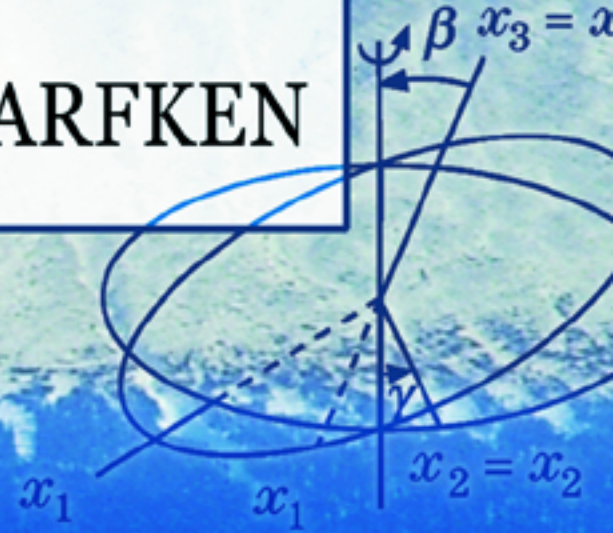
Essential

MATHEMATICAL Methods for Physicists

WEBER AND ARFKEN



Vector Identities

$$\mathbf{A} = A_x\hat{\mathbf{x}} + A_y\hat{\mathbf{y}} + A_z\hat{\mathbf{z}}, \quad A^2 = A_x^2 + A_y^2 + A_z^2, \quad \mathbf{A}\cdot\mathbf{B} = A_xB_x + A_yB_y + A_zB_z$$

$$\mathbf{A}\times\mathbf{B} = \begin{vmatrix} A_y & A_z \\ B_y & B_z \end{vmatrix}\hat{\mathbf{x}} - \begin{vmatrix} A_x & A_z \\ B_x & B_z \end{vmatrix}\hat{\mathbf{y}} + \begin{vmatrix} A_x & A_y \\ B_x & B_y \end{vmatrix}\hat{\mathbf{z}}$$

$$\mathbf{A}\cdot(\mathbf{B}\times\mathbf{C}) = \begin{vmatrix} A_x & A_y & A_z \\ B_x & B_y & B_z \\ C_x & C_y & C_z \end{vmatrix} = C_x\begin{vmatrix} A_y & A_z \\ B_y & B_z \end{vmatrix} - C_y\begin{vmatrix} A_x & A_z \\ B_x & B_z \end{vmatrix} + C_z\begin{vmatrix} A_x & A_y \\ B_x & B_y \end{vmatrix}$$

$$\mathbf{A}\times(\mathbf{B}\times\mathbf{C}) = \mathbf{B}\,\mathbf{A}\cdot\mathbf{C} - \mathbf{C}\,\mathbf{A}\cdot\mathbf{B}, \quad \sum_k \varepsilon_{ijk}\varepsilon_{pqk} = \delta_{ip}\delta_{jq} - \delta_{iq}\delta_{jp}$$

Vector Calculus

$$\mathbf{F} = -\nabla V(r) = -\frac{\mathbf{r}}{r}\frac{dV}{dr} = -\hat{\mathbf{r}}\frac{dV}{dr}, \quad \nabla\cdot(\mathbf{r}f(r)) = 3f(r) + r\frac{df}{dr},$$
$$\nabla\cdot(\mathbf{r}r^{n-1}) = (n+2)r^{n-1}$$

$$\nabla(\mathbf{A}\cdot\mathbf{B}) = (\mathbf{A}\cdot\nabla)\mathbf{B} + (\mathbf{B}\cdot\nabla)\mathbf{A} + \mathbf{A}\times(\nabla\times\mathbf{B}) + \mathbf{B}\times(\nabla\times\mathbf{A})$$

$$\nabla\cdot(S\mathbf{A}) = \nabla S\cdot\mathbf{A} + S\nabla\cdot\mathbf{A}, \quad \nabla\cdot(\mathbf{A}\times\mathbf{B}) = \mathbf{B}\cdot(\nabla\times\mathbf{A}) - \mathbf{A}\cdot(\nabla\times\mathbf{B})$$

$$\nabla\cdot(\nabla\times\mathbf{A}) = 0, \quad \nabla\times(S\mathbf{A}) = \nabla S\times\mathbf{A} + S\nabla\times\mathbf{A}, \quad \nabla\times(\mathbf{r}f(r)) = 0,$$
$$\nabla\times\mathbf{r} = 0$$

$$\nabla\times(\mathbf{A}\times\mathbf{B}) = \mathbf{A}\,\nabla\cdot\mathbf{B} - \mathbf{B}\,\nabla\cdot\mathbf{A} + (\mathbf{B}\cdot\nabla)\mathbf{A} - (\mathbf{A}\cdot\nabla)\mathbf{B},$$

$$\nabla\times(\nabla\times\mathbf{A}) = \nabla(\nabla\cdot\mathbf{A}) - \nabla^2\mathbf{A}$$

$$\int_V \nabla\cdot\mathbf{B}\,d^3r = \int_S \mathbf{B}\cdot d\mathbf{a}, \quad \text{(Gauss)}, \quad \int_S(\nabla\times\mathbf{A})\cdot d\mathbf{a} = \oint \mathbf{A}\cdot d\mathbf{l}, \quad \text{(Stokes)}$$

$$\int_V(\phi\nabla^2\psi - \psi\nabla^2\phi)d^3r = \int_S(\phi\nabla\psi - \psi\nabla\phi)\cdot d\mathbf{a}, \quad \text{(Green)}$$

$$\nabla^2\frac{1}{r} = -4\pi\delta(\mathbf{r}), \quad \delta(ax) = \frac{1}{|a|}\delta(x), \quad \delta(f(x)) = \sum_{i,f(x_i)=0,f'(x_i)\neq 0}\frac{\delta(x-x_i)}{|f'(x_i)|},$$

$$\delta(t-x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{i\omega(t-x)}d\omega, \quad \delta(\mathbf{r}) = \int\frac{d^3k}{(2\pi)^3}e^{-i\mathbf{k}\cdot\mathbf{r}},$$

$$\delta(x-t) = \sum_{n=0}^{\infty}\varphi_n^*(x)\varphi_n(t)$$

Curved Orthogonal Coordinates

Cylinder Coordinates

$$q_1 = \rho, \quad q_2 = \varphi, \quad q_3 = z; \quad h_1 = h_\rho = 1, \; h_2 = h_\varphi = \rho, \; h_3 = h_z = 1,$$

$$\mathbf{r} = \hat{\mathbf{x}}\rho\cos\varphi + \hat{\mathbf{y}}\rho\sin\varphi + z\hat{\mathbf{z}}$$

Spherical Polar Coordinates

$$q_1 = r, \; q_2 = \theta, \; q_3 = \varphi; h_1 = h_r = 1, \; h_2 = h_\theta = r, \; h_3 = h_\varphi = r\sin\theta,$$

$$\mathbf{r} = \hat{\mathbf{x}}r\sin\theta\cos\varphi + \hat{\mathbf{y}}r\sin\theta\sin\varphi + \hat{\mathbf{z}}r\cos\theta$$

$$d\mathbf{r} = \sum_i h_i dq_i \hat{\mathbf{q}}_i, \quad \mathbf{A} = \sum_i A_i \hat{\mathbf{q}}_i, \quad \mathbf{A}\cdot\mathbf{B} = \sum_i A_i B_i, \; \mathbf{A}\times\mathbf{B} = \begin{vmatrix} \hat{\mathbf{q}}_1 & \hat{\mathbf{q}}_2 & \hat{\mathbf{q}}_3 \\ A_1 & A_2 & A_3 \\ B_1 & B_2 & B_3 \end{vmatrix}$$

$$\int_V f\, d^3r = \int f(q_1, q_2, q_3) h_1 h_2 h_3\, dq_1\, dq_2\, dq_3 \qquad \int_L \mathbf{F}\cdot d\mathbf{r} = \sum_i \int F_i h_i\, dq_i$$

$$\int_S \mathbf{B}\cdot d\mathbf{a} = \int B_1 h_2 h_3\, dq_2\, dq_3 + \int B_2 h_1 h_3\, dq_1 dq_3 + \int B_3 h_1 h_2\, dq_1 dq_2,$$

$$\nabla V = \sum_i \hat{\mathbf{q}}_i \frac{1}{h_i}\frac{\partial V}{\partial q_i},$$

$$\nabla\cdot\mathbf{F} = \frac{1}{h_1 h_2 h_3}\left[\frac{\partial}{\partial q_1}(F_1 h_2 h_3) + \frac{\partial}{\partial q_2}(F_2 h_1 h_3) + \frac{\partial}{\partial q_3}(F_3 h_1 h_2)\right]$$

$$\nabla^2 V = \frac{1}{h_1 h_2 h_3}\left[\frac{\partial}{\partial q_1}\left(\frac{h_2 h_3}{h_1}\frac{\partial V}{\partial q_1}\right) + \frac{\partial}{\partial q_2}\left(\frac{h_1 h_3}{h_2}\frac{\partial V}{\partial q_2}\right) + \frac{\partial}{\partial q_3}\left(\frac{h_2 h_1}{h_3}\frac{\partial V}{\partial q_3}\right)\right]$$

$$\nabla\times\mathbf{F} = \frac{1}{h_1 h_2 h_3}\begin{vmatrix} h_1\hat{\mathbf{q}}_1 & h_2\hat{\mathbf{q}}_2 & h_3\hat{\mathbf{q}}_3 \\ \frac{\partial}{\partial q_1} & \frac{\partial}{\partial q_2} & \frac{\partial}{\partial q_3} \\ h_1 F_1 & h_2 F_2 & h_3 F_3 \end{vmatrix}$$

Mathematical Constants

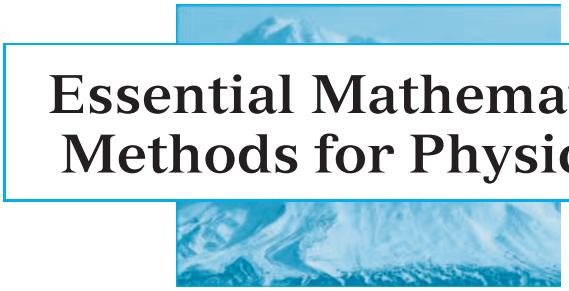
$$e = 2.718281828, \quad \pi = 3.14159265, \quad \ln 10 = 2.302585093,$$

$$1\text{ rad} = 57.29577951^\circ, \quad 1^\circ = 0.0174532925\text{ rad},$$

$$\gamma = \lim_{n\to\infty}\left[1 + \frac{1}{2} + \frac{1}{3} + \cdots + \frac{1}{n} - \ln(n+1)\right] = 0.577215661901532$$

(Euler-Mascheroni number)

$$B_1 = -\frac{1}{2}, \; B_2 = \frac{1}{6}, \; B_4 = B_8 = -\frac{1}{30}, \; B_6 = \frac{1}{42}, \ldots \text{ (Bernoulli numbers)}$$



Essential Mathematical Methods for Physicists

Essential Mathematical Methods for Physicists

Hans J. Weber
University of Virginia
Charlottesville, VA

George B. Arfken
Miami University
Oxford, Ohio

ACADEMIC PRESS
An imprint of Elsevier Science

Amsterdam Boston London New York Oxford Paris
San Diego San Francisco Singapore Sydney Tokyo

Sponsoring Editor Barbara Holland
Production Editor Angela Dooley
Editorial Assistant Karen Frost
Marketing Manager Marianne Rutter
Cover Design Richard Hannus
Printer and Binder Quebecor

This book is printed on acid-free paper. ♾

Academic Press
A Harcourt Science and Technology Company
525 B Street, Suite 1900, San Diego, CA 92101-4495, USA
http://www.academicpress.com

Academic Press
Harcourt Place, 32 Jamestown Road, London NW1 7BY, UK

Harcourt/Academic Press
200 Wheeler Road, Burlington, MA 01803
http://www.harcourt-ap.com

International Standard Book Number: 0-12-059877-9

PRINTED IN THE UNITED STATES OF AMERICA
03 04 05 06 07 Q 9 8 7 6 5 4 3 2 1

Contents

Preface

This text is designed for the usual introductory physics courses to prepare undergraduate students for the level of mathematics expected in more advanced undergraduate physics and engineering courses. One of its goals is to guide the student in learning the mathematical language physicists use by leading them through worked examples and then practicing problems. The pedagogy is that of introducing concepts, designing and refining methods, and practicing them repeatedly in physics examples and problems. Geometric and algebraic approaches and methods are included and are more or less emphasized in a variety of settings to accommodate different learning styles of students. Sometimes examples are solved in more than one way. Theorems are usually derived sketching the underlying ideas and describing the relevant mathematical relations so that one can recognize the assumptions they are based on and their limitations. These proofs are not rigorous in the sense of the professional mathematician, and no attempt was made to formulate theorems in their most general form or under the least restrictive assumptions.

An important objective of this text is to train the student to formulate physical phenomena in mathematical language, starting from intuitive and qualitative ideas. The examples in the text have been worked out so as to develop the mathematical treatment along with the physical intuition. A precise mathematical formulation of physical phenomena and problems is always the ultimate goal.

Text Overview

In Chapter 1 the basic concepts of vector algebra and vector analysis are introduced and applied to classical mechanics and electrodynamics. Chapter 2 deals with the extension of vector algebra and analysis to curved orthogonal coordinates, again with applications from classical mechanics and electrodynamics. These chapters lay the foundations for differential equations in Chapters 8, 9, and 16; variational calculus in Chapter 18; and nonlinear analysis in Chapter 19. Chapter 3 extends high school algebra of one or two linear

equations to determinants and matrix solutions of general systems of linear equations, eigenvalues and eigenvectors, and linear transformations in real and complex vector spaces. These chapters are extended to function spaces of solutions of differential equations in Chapter 9, thereby laying the mathematical foundations for and formulation of quantum mechanics. Chapter 4 on group theory is an introduction to the important concept of symmetry in modern physics. Chapter 5 gives a fairly extensive treatment of series that form the basis for the special functions discussed in Chapters 10–13 and also complex functions discussed in Chapters 6 and 7. Chapter 17 on probability and statistics is basic for the experimentally oriented physicist. Some of its content can be studied immediately after completion of Chapters 1 and 2, but later sections are based on Chapters 8 and 10. Chapter 19 on nonlinear methods can be studied immediately after completion of Chapter 8, and it complements and extends Chapter 8 in many directions. Chapters 10–13 on special functions contain many examples of physics problems requiring solutions of differential equations that can also be incorporated in Chapters 8 and 16. Chapters 14 and 15 on Fourier analysis are indispensible for a more advanced treatment of partial differential equations in Chapter 16.

Historical remarks are included that detail some physicists and mathematicians who introduced the ideas and methods that later generations perfected to the tools we now use routinely. We hope they provide motivation for students and generate some appreciation of the effort, devotion, and courage of past and present scientists.

Pathways through the Material

Because the text contains more than enough material for a two-semester undergraduate course, the instructor may select topics to suit the particular level of the class. Chapters 1–3 and 5–8 provide a basis for a one-semester course in mathematical physics. By omitting some topics, such as symmetries and group theory and tensors, it is possible in a one-semester course to also include parts of Chapters 10–13 on special functions, Chapters 14 and 15 on Fourier analysis, Chapter 17 on probability and statistics, Chapter 18 on variational calculus, or Chapter 19 on nonlinear methods.

A two-semester course can treat tensors and symmetries in Chapters 2 and 4 and special functions in Chapters 10–13 more extensively, as well as variational calculus in Chapter 18 in support of classical and quantum mechanics.

Problem-Solving Skills

Students should study the text until they are sure they understand the physical interpretation, can derive equations with the book closed, can make predictions in special cases, and can recognize the limits of applicability of the theories and equations of physics. However, physics and engineering courses routinely demand an even higher level of understanding involving active learning in which students can apply the material to solve problems because it is

common knowledge that we only learn the mathematical language that physicists use by repeatedly solving problems.

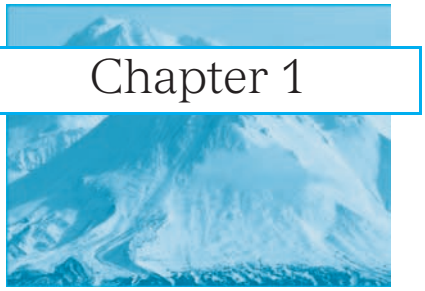
The problem sets at the end of sections and chapters are arranged in the order in which the material is covered in the text. A sufficient variety and level of difficulty of problems are provided to ensure that anyone who conscientiously solves them has mastered the material in the text beyond mere understanding of step-by-step derivations. More difficult problems that require some modification of routine methods are also included in various sets to engage the creative powers of the student, a skill that is expected of the professional physicist.

Computer Software

Problems in the text that can be solved analytically can also be solved by modern symbolic computer software, such as Macsyma, Mathcad, Maples, Mathematica, and Reduce, because these programs include the routine methods of mathematical physics texts. Once the student has developed an analytical result, these powerful programs are useful for checking and plotting the results. Finding an analytical solution by computer without understanding how it is derived is pointless. When computers are used too early for solving a problem, many instructors have found that students can be led astray by the computers. The available computer software is so diverse as to preclude any detailed discussion of it. Each instructor willing to make use of computers in the course will have to make a choice of a particular software and provide an introduction for the students. Many problems and examples in the text may then be adapted to it. However, their real utility and power lie in the graphics software they include and the ability to solve problems approximately and numerically that do not allow for an analytical solution. Special training is needed, and the text can be used to train students in approximation methods, such as series and asymptotic expansions, or integral representations that are suitable for further symbolic computer manipulations.

Acknowledgments

Many reviewers deserve special praise, particularly Prof. Frank Harris, although not all of their advice was always followed. We are particularly grateful to our untiring editor, Barbara Holland, for much help. We would like to thank Dr. Michael Beyer and Dr. Michael Bozoian for their invaluable help with the proofreading and Angela Dooley for expertly keeping the book on track in the production phase. Despite great care, we expect some misprints and errors to have survived the collective scrutiny of reviewers, proofreaders, editors, and authors. Although we are grateful for their efforts, we assume responsibility and welcome readers to point them out to us.



Chapter 1

Vector Analysis

1.1 Elementary Approach

In science and engineering we frequently encounter quantities that have only magnitude: mass, time, and temperature. This magnitude remains the same no matter how we orient the coordinate axes that we may use. These quantities we label scalar quantities. In contrast, many interesting physical quantities have magnitude or length and, in addition, an associated direction. Quantities with magnitude and direction are called vectors. Their length and the angle between any vectors remain unaffected by the orientation of coordinates we choose. To distinguish vectors from scalars, we identify vector quantities with boldface type (i.e., $\mathbf{V}$). Vectors are useful in solving systems of linear equations (Chapter 3). They are not only helpful in Euclidean geometry but also indispensable in classical mechanics and engineering because force, velocity, acceleration, and angular momentum are vectors. Electrodynamics is unthinkable without vector fields such as electric and magnetic fields.

Practical problems of mechanics and geometry, such as searching for the shortest distance between straight lines or parameterizing the orbit of a particle, will lead us to the differentiation of vectors and to vector analysis. Vector analysis is a powerful tool to formulate equations of motions of particles and then solve them in mechanics and engineering, or field equations of electrodynamics.

In this section, we learn to add and subtract vectors geometrically and algebraically in terms of their rectangular components.

A vector may be geometrically represented by an arrow with length proportional to the magnitude. The direction of the arrow indicates the direction of the vector, the positive sense of direction being indicated by the point. In

Figure 1.1

Triangle Law of Vector Addition

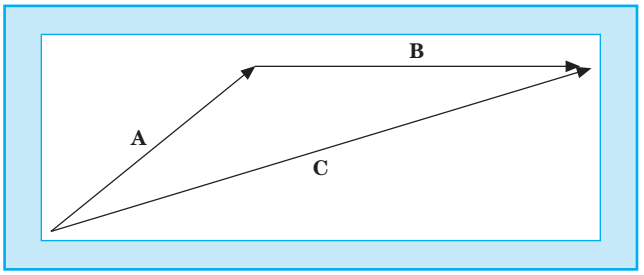
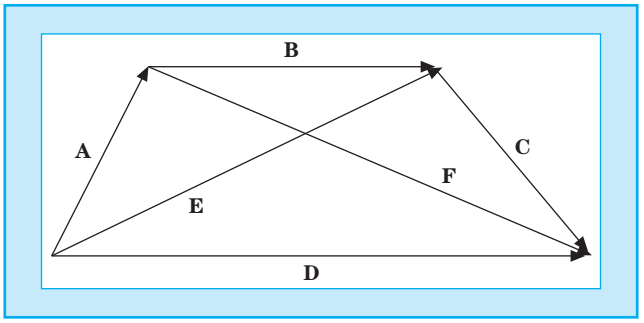


Figure 1.2

Vector Addition Is Associative



this representation, vector addition

$$\mathbf{C} = \mathbf{A} + \mathbf{B} \tag{1.1}$$

consists of placing the rear end of vector **B** at the point of vector **A** (head to tail rule). Vector **C** is then represented by an arrow drawn from the rear of **A** to the point of **B**. This procedure, the triangle law of addition, assigns meaning to Eq. (1.1) and is illustrated in Fig. 1.1. By completing the parallelogram (sketch it), we see that

$$\mathbf{C} = \mathbf{A} + \mathbf{B} = \mathbf{B} + \mathbf{A}. \tag{1.2}$$

In words, **vector addition is commutative**.

For the sum of three vectors

$$\mathbf{D} = \mathbf{A} + \mathbf{B} + \mathbf{C},$$

illustrated in Fig. 1.2, we first add **A** and **B**:

$$\mathbf{A} + \mathbf{B} = \mathbf{E}.$$

Then this sum is added to **C**:

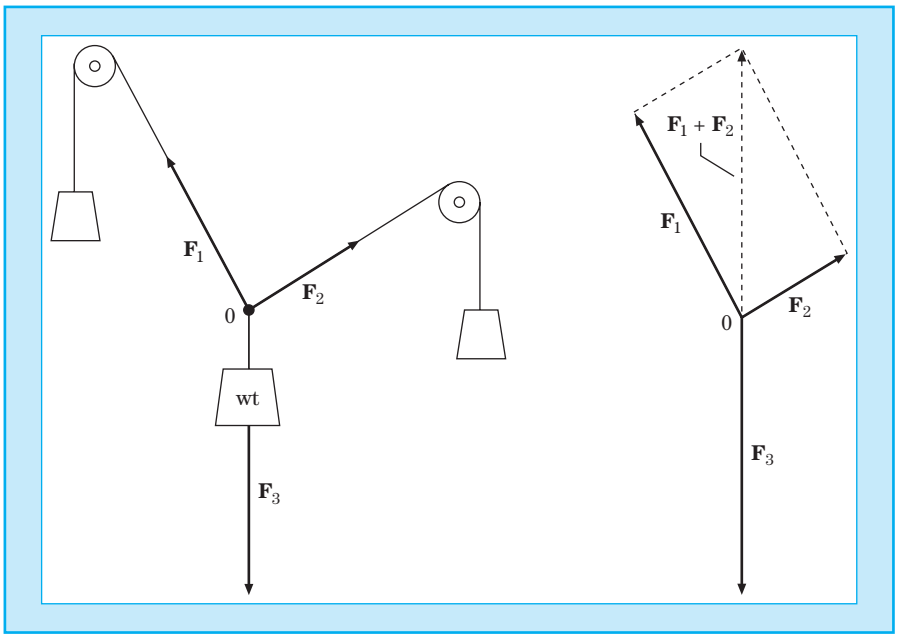
$$\mathbf{D} = \mathbf{E} + \mathbf{C}.$$

Alternatively, we may first add **B** and **C**:

$$\mathbf{B} + \mathbf{C} = \mathbf{F}.$$

Figure 1.3

Equilibrium of Forces: $\mathbf{F}_1 + \mathbf{F}_2 = -\mathbf{F}_3$



Then

$$\mathbf{D} = \mathbf{A} + \mathbf{F}.$$

In terms of the original expression,

$$(\mathbf{A} + \mathbf{B}) + \mathbf{C} = \mathbf{A} + (\mathbf{B} + \mathbf{C})$$

so that these alternative ways of summing three vectors lead to the same vector, or **vector addition is associative**.

A direct physical example of the parallelogram addition law is provided by a weight suspended by two cords in Fig. 1.3. If the junction point is in equilibrium, the vector sum of the two forces $\mathbf{F}_1$ and $\mathbf{F}_2$ must cancel the downward force of gravity, $\mathbf{F}_3$. Here, the parallelogram addition law is subject to immediate experimental verification.[1] Such a balance of forces is of immense importance for the stability of buildings, bridges, airplanes in flight, etc.

Subtraction is handled by defining the negative of a vector as a vector of the same magnitude but with reversed direction. Then

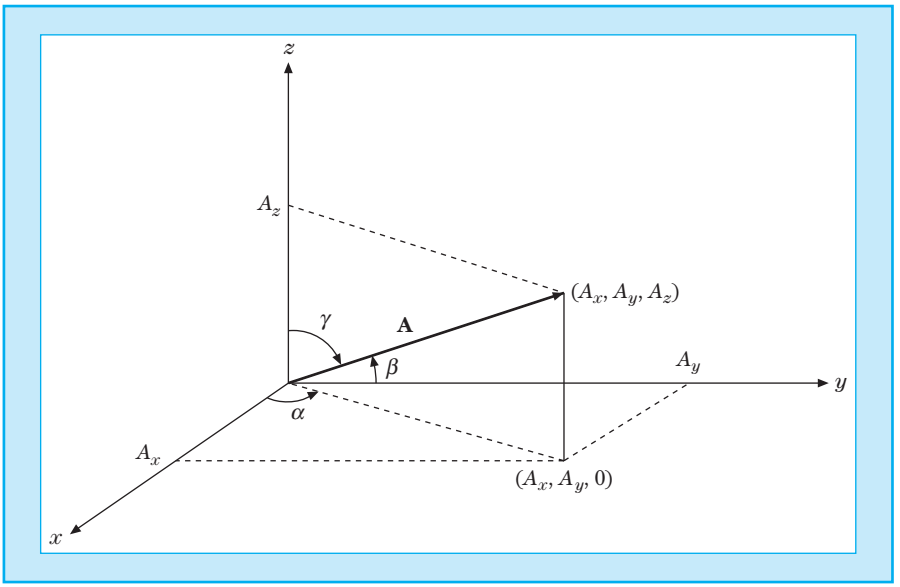
$$\mathbf{A} - \mathbf{B} = \mathbf{A} + (-\mathbf{B}).$$

The graphical representation of vector $\mathbf{A}$ by an arrow suggests using coordinates as a second possibility. Arrow $\mathbf{A}$ (Fig. 1.4), starting from the

[1]Strictly speaking, the parallelogram addition was introduced as a definition. Experiments show that forces are vector quantities that are combined by parallelogram addition, as required by the equilibrium condition of zero resultant force.

Figure 1.4

Components and Direction Cosines of A



origin,[2] terminates at the point (A_x, A_y, A_z). Thus, if we agree that the vector is to start at the origin, the positive end may be specified by giving the **rectangular** or **Cartesian** coordinates (A_x, A_y, A_z) of the arrow head.

Although **A** could have represented any vector quantity (momentum, electric field, etc.), one particularly important vector quantity, the distance from the origin to the point (x, y, z), is denoted by the special symbol **r**. We then have a choice of referring to the displacement as either the vector **r** or the collection (x, y, z), the coordinates of its end point:

$$\mathbf{r} \leftrightarrow (x, y, z). \tag{1.3}$$

Defining the magnitude r of vector **r** as its geometrical length, we find that Fig. 1.4 shows that the end point coordinates and the magnitude are related by

$$x = r\cos\alpha, \quad y = r\cos\beta, \quad z = r\cos\gamma. \tag{1.4}$$

$\cos\alpha$, $\cos\beta$, and $\cos\gamma$ are called the **direction cosines**, where α is the angle between the given vector and the positive x-axis, and so on. The (Cartesian) components A_x, A_y, and A_z can also be viewed as the **projections** of **A** on the respective axes.

Thus, any vector **A** may be resolved into its components (or projected onto the coordinate axes) to yield $A_x = A\cos\alpha$, etc., as in Eq. (1.4). We refer to the vector as a single quantity **A** or to its components (A_x, A_y, A_z). Note that the subscript x in A_x denotes the x component and not a dependence on the variable x. The choice between using **A** or its components (A_x, A_y, A_z) is

[2] We could start from any point; we choose the origin for simplicity. This freedom of shifting the origin of the coordinate system without affecting the geometry is called **translation invariance**.

essentially a choice between a **geometric or an algebraic representation**. The geometric "arrow in space" often aids in visualization. The algebraic set of components is usually more suitable for precise numerical or algebraic calculations. (This is illustrated in Examples 1.1.1–1.1.3 and also applies to Exercises 1.1.1, 1.1.3, 1.1.5, and 1.1.6.)

Vectors enter physics in two distinct forms:

- Vector $\mathbf{A}$ may represent a single force acting at a single point. The force of gravity acting at the center of gravity illustrates this form.
- Vector $\mathbf{A}$ may be defined over some extended region; that is, $\mathbf{A}$ and its components may be functions of position: $A_x = A_x(x, y, z)$, and so on.

Imagine a vector $\mathbf{A}$ attached to each point (x, y, z), whose length and direction change with position. Examples include the velocity of air around the wing of a plane in flight varying from point to point and electric and magnetic fields (made visible by iron filings). Thus, vectors defined at each point of a region are usually characterized as a **vector field**. The concept of the vector defined over a region and being a function of position will be extremely important in Section 1.2 and in later sections in which we differentiate and integrate vectors.

A **unit vector** has length 1 and may point in any direction. Coordinate unit vectors are implicit in the projection of $\mathbf{A}$ onto the coordinate axes to define its Cartesian components. Now, we define $\hat{\mathbf{x}}$ explicitly as a vector of unit magnitude pointing in the positive x-direction, $\hat{\mathbf{y}}$ as a vector of unit magnitude in the positive y-direction, and $\hat{\mathbf{z}}$ as a vector of unit magnitude in the positive z-direction. Then $\hat{\mathbf{x}}A_x$ is a vector with magnitude equal to A_x and in the positive x-direction; that is, the projection of $\mathbf{A}$ onto the x-direction, etc. By vector addition

$$\mathbf{A} = \hat{\mathbf{x}}A_x + \hat{\mathbf{y}}A_y + \hat{\mathbf{z}}A_z, \tag{1.5}$$

which states that a vector equals the vector sum of its components or projections. Note that if $\mathbf{A}$ vanishes, all of its components must vanish individually; that is, if

$$\mathbf{A} = 0, \quad \text{then } A_x = A_y = A_z = 0.$$

Finally, by the Pythagorean theorem, the length of vector $\mathbf{A}$ is

$$A = \left(A_x^2 + A_y^2 + A_z^2\right)^{1/2}. \tag{1.6}$$

This resolution of a vector into its components can be carried out in a variety of coordinate systems, as demonstrated in Chapter 2. Here, we restrict ourselves to Cartesian coordinates, where the unit vectors have the coordinates $\hat{\mathbf{x}} = (1, 0, 0)$, $\hat{\mathbf{y}} = (0, 1, 0)$, and $\hat{\mathbf{z}} = (0, 0, 1)$.

Equation (1.5) means that the three unit vectors $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$, and $\hat{\mathbf{z}}$ span the real three-dimensional space: Any constant vector may be written as a linear combination of $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$, and $\hat{\mathbf{z}}$. Since $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$, and $\hat{\mathbf{z}}$ are linearly independent (no one is a linear combination of the other two), they form a **basis** for the real three-dimensional space.

Complementary to the geometrical technique, algebraic addition and subtraction of vectors may now be carried out in terms of their components. For

$$\mathbf{A} = \hat{\mathbf{x}}A_x + \hat{\mathbf{y}}A_y + \hat{\mathbf{z}}A_z \quad \text{and} \quad \mathbf{B} = \hat{\mathbf{x}}B_x + \hat{\mathbf{y}}B_y + \hat{\mathbf{z}}B_z,$$

$$\mathbf{A} \pm \mathbf{B} = \hat{\mathbf{x}}(A_x \pm B_x) + \hat{\mathbf{y}}(A_y \pm B_y) + \hat{\mathbf{z}}(A_z \pm B_z). \tag{1.7}$$

Biographical Data

Descartes, René. Descartes, a French mathematician and philosopher, was born in La Haye, France, in 1596 and died in Stockholm, Sweden, in 1650. Cartesius is the latinized version of his name at a time when Latin was the language of sciences, although he mainly wrote in French. He discovered his love of mathematics in the army, when he had plenty of time for research. He introduced the concept of rectangular coordinates, thereby converting geometry to algebraic equations of the coordinates of points, now called analytic geometry. Thus, he paved the way for Newton's and Leibniz's calculus. He coined the phrase "Cogito, ergo sum," which translates to "I think, therefore I am."

EXAMPLE 1.1.1

Let

$$\mathbf{A} = 6\hat{\mathbf{x}} + 4\hat{\mathbf{y}} + 3\hat{\mathbf{z}}$$

$$\mathbf{B} = 2\hat{\mathbf{x}} - 3\hat{\mathbf{y}} - 3\hat{\mathbf{z}}.$$

Then by Eq. (1.7)

$$\mathbf{A} + \mathbf{B} = (6+2)\hat{\mathbf{x}} + (4-3)\hat{\mathbf{y}} + (3-3)\hat{\mathbf{z}} = 8\hat{\mathbf{x}} + \hat{\mathbf{y}},$$

$$\mathbf{A} - \mathbf{B} = (6-2)\hat{\mathbf{x}} + (4+3)\hat{\mathbf{y}} + (3+3)\hat{\mathbf{z}} = 4\hat{\mathbf{x}} + 7\hat{\mathbf{y}} + 6\hat{\mathbf{z}}. \quad \blacksquare$$

EXAMPLE 1.1.2

Parallelogram of Forces Find the sum of two forces $\mathbf{a}$ and $\mathbf{b}$. To practice the geometric meaning of vector addition and subtraction, consider two forces

$$\mathbf{a} = (3, 0, 1), \quad \mathbf{b} = (4, 1, 2)$$

(in units of newtons, $1\,\text{N} = 1\,\text{kgm/s}^2$, in the Standard International system of units) that span a parallelogram with the diagonals forming the sum

$$\mathbf{a} + \mathbf{b} = (3+4, 1, 1+2) = (7, 1, 3) = \mathbf{b} + \mathbf{a},$$

and the difference

$$\mathbf{b} - \mathbf{a} = (4-3, 1, 2-1) = (1, 1, 1),$$

as shown in Fig. 1.5. The midpoint $\mathbf{c}$ is half the sum,

$$\mathbf{c} = \frac{1}{2}(\mathbf{a} + \mathbf{b}) = \left(\frac{7}{2}, \frac{1}{2}, \frac{3}{2}\right).$$

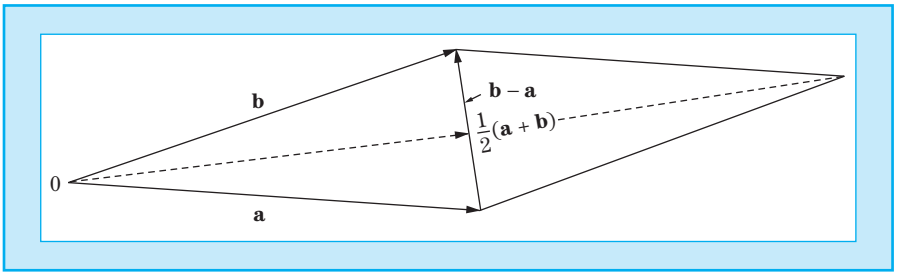


Figure 1.5
Parallelogram of Forces a and b

Alternately, to obtain the midpoint from **a**, add half of the second diagonal that points from **a** to **b**; that is,

$$\mathbf{a} + \frac{1}{2}(\mathbf{b} - \mathbf{a}) = \frac{1}{2}(\mathbf{a} + \mathbf{b}) = \mathbf{c} = \left(\frac{7}{2}, \frac{1}{2}, \frac{3}{2}\right). \quad \blacksquare$$

EXAMPLE 1.1.3

Center of Mass of Three Points at the Corners of a Triangle Consider each corner of a triangle to have a unit of mass and to be located $\mathbf{a}_i$ from the origin, where

$$\mathbf{a}_1 = (2, 0, 0), \mathbf{a}_2 = (4, 1, 1), \mathbf{a}_3 = (3, 3, 2).$$

Then, the center of mass of the triangle is

$$\frac{1}{3}(\mathbf{a}_1 + \mathbf{a}_2 + \mathbf{a}_3) = \mathbf{c} = \frac{1}{3}(2 + 4 + 3, 1 + 3, 1 + 2) = \left(3, \frac{4}{3}, 1\right).$$

THEOREM 1.1

If we draw a straight line from each corner to the midpoint of the opposite side of the triangle in Fig. 1.6, these lines meet in the center, which is at a distance of two-thirds of the line length to the corner.

The three midpoints are located at the point of the vectors

$$\frac{1}{2}(\mathbf{a}_1 + \mathbf{a}_2) = \frac{1}{2}(2 + 4, 1, 1) = \left(3, \frac{1}{2}, \frac{1}{2}\right)$$
$$\frac{1}{2}(\mathbf{a}_2 + \mathbf{a}_3) = \frac{1}{2}(4 + 3, 1 + 3, 1 + 2) = \left(\frac{7}{2}, 2, \frac{3}{2}\right)$$
$$\frac{1}{2}(\mathbf{a}_3 + \mathbf{a}_1) = \frac{1}{2}(3 + 2, 3, 2) = \left(\frac{5}{2}, \frac{3}{2}, 1\right).$$

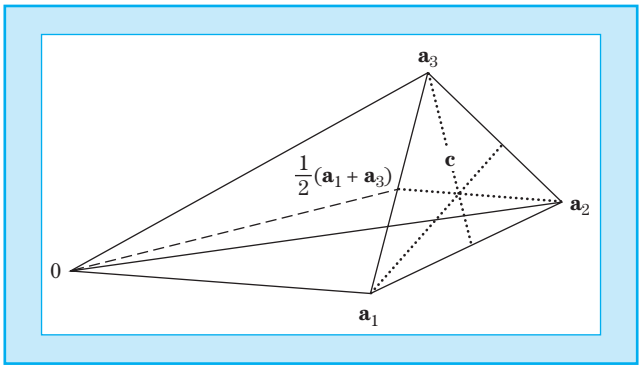


Figure 1.6

Center of a Triangle. The Dashed Line Goes from the Origin to the Midpoint of a Triangle Side, and the Dotted Lines Go from Each Corner to the Midpoint of the Opposite Triangle Side

To prove this theorem numerically or symbolically using general vectors, we start from each corner and end up in the center as follows:

$$(2,0,0)+\frac{2}{3}\left[\left(\frac{7}{2},2,\frac{3}{2}\right)-(2,0,0)\right]=\left(3,\frac{4}{3},1\right)$$

$$\mathbf{a}_1+\frac{2}{3}\left(\frac{1}{2}(\mathbf{a}_2+\mathbf{a}_3)-\mathbf{a}_1\right)=\frac{1}{3}(\mathbf{a}_1+\mathbf{a}_2+\mathbf{a}_3),$$

$$(4,1,1)+\frac{2}{3}\left[\left(\frac{5}{2},\frac{3}{2},1\right)-(4,1,1)\right]=\left(3,\frac{4}{3},1\right)$$

$$\mathbf{a}_2+\frac{2}{3}\left(\frac{1}{2}(\mathbf{a}_1+\mathbf{a}_3)-\mathbf{a}_2\right)=\frac{1}{3}(\mathbf{a}_1+\mathbf{a}_2+\mathbf{a}_3),$$

$$(3,3,2)+\frac{2}{3}\left[\left(3,\frac{1}{2},\frac{1}{2}\right)-(3,3,2)\right]=\left(3,\frac{4}{3},1\right)$$

$$\mathbf{a}_3+\frac{2}{3}\left(\frac{1}{2}(\mathbf{a}_1+\mathbf{a}_2)-\mathbf{a}_3\right)=\frac{1}{3}(\mathbf{a}_1+\mathbf{a}_2+\mathbf{a}_3).$$

This theorem is easy to establish using vector algebra, but it is much more tedious to prove working only with intersecting straight lines of Euclidean geometry. Thus, this example is not only useful practice but also lets us appreciate the power and versatility of the vector algebra. ■

EXAMPLE 1.1.4

Elastic Forces A movable point $\mathbf{a}$ is held elastically (denoted by springs in Fig. 1.7) by three fixed points $\mathbf{a}_i$, $i=1,2,3$; that is, the force $\mathbf{F}_i=k_i(\mathbf{a}_i-\mathbf{a})$ for each i that $\mathbf{a}$ experiences is pointed to $\mathbf{a}_i$ and proportional to the distance. Let us show that the elastic forces to three points can be replaced by an elastic force to a single point.

This holds because the total force is given by

$$\mathbf{F}=\sum_i \mathbf{F}_i=\sum_i k_i\mathbf{a}_i-\mathbf{a}\sum_i k_i=\left(\sum_i k_i\right)\left(\frac{\sum_i k_i\mathbf{a}_i}{\sum_i k_i}-\mathbf{a}\right)=k_0(\mathbf{a}_0-\mathbf{a}),$$

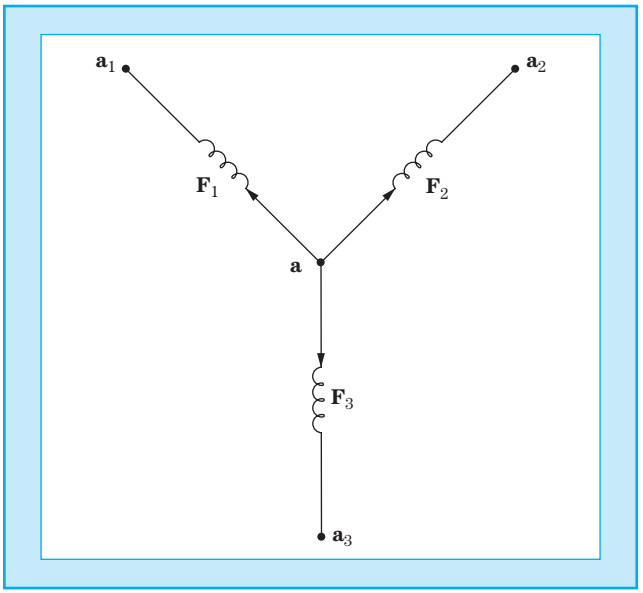


Figure 1.7

The Point a Is Held Elastically by Three Points $\mathbf{a}_i$

where $k_0 = \sum_i k_i$ and $\mathbf{a}_0 = \sum_i k_i \mathbf{a}_i / k_0$. This shows that the resulting force is equivalent to one with an effective spring constant k_0 acting from a point $\mathbf{a}_0$. Note that if all k_i's are the same, then $\mathbf{a}_0 = \frac{1}{3}(\mathbf{a}_1 + \mathbf{a}_2 + \mathbf{a}_3)$ is the center of mass.

Technical applications apply for bridges and buildings, for which the balance of forces is vital for stability. ■

Vectors and Vector Space Summary

An ordered triplet of real numbers (x_1, x_2, x_3) is labeled a **vector** $\mathbf{x}$. The number x_n is called the nth component of vector $\mathbf{x}$. The collection of all such vectors (obeying the properties that follow) forms a three-dimensional real **vector space**, or **linear space**. We ascribe five properties to our vectors: If $\mathbf{x} = (x_1, x_2, x_3)$ and $\mathbf{y} = (y_1, y_2, y_3)$,

1. Vector equality: $\mathbf{x} = \mathbf{y}$ means $x_i = y_i$, $i = 1, 2, 3$.
2. Vector addition: $\mathbf{x} + \mathbf{y} = \mathbf{z}$ means $x_i + y_i = z_i$, $i = 1, 2, 3$.
3. Scalar multiplication: $a\mathbf{x} = (ax_1, ax_2, ax_3)$.
4. Negative of a vector: $-\mathbf{x} = (-1)\mathbf{x} = (-x_1, -x_2, -x_3)$.
5. Null vector: There exists a null vector $\mathbf{0} = (0, 0, 0)$.

Since our vector components are numbers, the following properties also hold:

1. Addition of vectors is commutative: $\mathbf{x} + \mathbf{y} = \mathbf{y} + \mathbf{x}$.
2. Addition of vectors is associative: $(\mathbf{x} + \mathbf{y}) + \mathbf{z} = \mathbf{x} + (\mathbf{y} + \mathbf{z})$.

3. Scalar multiplication is distributive:

$$a(\mathbf{x}+\mathbf{y}) = a\mathbf{x} + a\mathbf{y}, \qquad \text{also} \quad (a+b)\mathbf{x} = a\mathbf{x} + b\mathbf{x}.$$

4. Scalar multiplication is associative: $(ab)\mathbf{x} = a(b\mathbf{x})$.

Furthermore, the null vector $\mathbf{0}$ is unique, as is the negative of a given vector $\mathbf{x}$.

With regard to the vectors, this approach merely formalizes the component discussion of Section 1.1. The importance lies in the extensions, which will be considered later. In Chapter 3, we show that vectors form a linear space, with the transformations in the linear space described by matrices. Finally, and perhaps most important, for advanced physics the concept of vectors presented here generalizes to (i) complex quantities,[3] (ii) functions, and (iii) an infinite number of components. This leads to infinite dimensional function spaces, the Hilbert spaces, which are important in quantum mechanics. A brief introduction to function expansions and Hilbert space is provided in Chapter 9.

SUMMARY

So far, we have defined the operations of addition and subtraction of vectors guided by the use of elastic and gravitational forces in classical mechanics, set up mechanical and geometrical problems such as finding the center of mass of a system of mass points, and solved these problems using the tools of vector algebra.

Next, we address three varieties of multiplication defined on the basis of their applicability in geometry and mechanics: a scalar or inner product in Section 1.2; a vector product peculiar to three-dimensional space in Section 1.3, for which the angular momentum in mechanics is a prime example; and a direct or outer product yielding a second-rank tensor in Section 2.7. Division by a vector cannot be consistently defined.

EXERCISES

1.1.1 A jet plane is flying eastward from Kennedy Airport at a constant speed of 500 mph. There is a crosswind from the south at 50 mph. What is the resultant speed of the plane relative to the ground? Draw the velocities (using graphical software, if available).

1.1.2 A boat travels straight across a river at a speed of 5 mph when there is no current. You want to go straight across the river in that boat when there is a constant current flowing at 1 mph. At what angle do you have to steer the boat? Plot the velocities.

1.1.3 A sphere of radius a is centered at a point $\mathbf{r}_1$.

(a) Write out the algebraic equation for the sphere. Explain in words why you chose a particular form. Name theorems from geometry you may have used.

[3] The n-dimensional vector space of real n-tuples is often labeled $\mathbf{R}^n$, and the n-dimensional vector space of complex n-tuples is labeled $\mathbf{C}^n$.

(b) Write out a **vector** equation for the sphere. Identify in words what you are doing.

ANS. (a) $(x - x_1)^2 + (y - y_1)^2 + (z - z_1)^2 = a^2$.
(b) $\mathbf{r} = \mathbf{r}_1 + \mathbf{a}$ ($\mathbf{a}$ takes on all directions but has a fixed magnitude, a).

1.1.4 Show that the medians of a triangle intersect at a point. Show that this point is two-thirds of the way from any corner of the triangle to the midpoint of the opposite side. Compare a geometrical proof with one using vectors. If you use a Cartesian coordinate system, place your triangle so as to simplify the analysis as much as possible. Explain in words why you are allowed to do so.

1.1.5 The velocity of sailboat A relative to sailboat B, $\mathbf{v}_{\text{rel}}$, is defined by the equation $\mathbf{v}_{\text{rel}} = \mathbf{v}_A - \mathbf{v}_B$, where $\mathbf{v}_A$ is the velocity of A and $\mathbf{v}_B$ is the velocity of B. Determine the velocity of A relative to B if

$$\mathbf{v}_A = 30 \text{ km/hr east}$$
$$\mathbf{v}_B = 40 \text{ km/hr north}.$$

Plot the velocities (using graphical software, if available).

ANS. $\mathbf{v}_{\text{rel}} = 50$ km/hr, 53.1° south of east.

1.1.6 A sailboat sails for 1 hr at 4 km/hr (relative to the water) on a steady compass heading of 40° east of north. The sailboat is simultaneously carried along by a current. At the end of the hour the boat is 6.12 km from its starting point. The line from its starting point to its location lies 60° east of north. Find the x (easterly) and y (northerly) components of the water's velocity. Plot all velocities.

ANS. $v_{\text{east}} = 2.73$ km/hr, $v_{\text{north}} \approx 0$ km/hr.

1.1.7 A triangle is defined by the vertices of three vectors, **A**, **B**, and **C**, that extend from the origin. In terms of **A**, **B**, and **C**, show that the **vector** sum of the successive sides of the triangle is zero. If software is available, plot a typical case.

1.1.8 Find the diagonal vectors of a unit cube with one corner at the origin and three adjacent sides lying along the three axes of a Cartesian coordinate system. Show that there are four diagonals with length $\sqrt{3}$. Representing these as vectors, what are their components? Show that the diagonals of the cube's surfaces have length $\sqrt{2}$. Determine their components.

1.1.9 Hubble's law: Hubble found that distant galaxies are receding with a velocity proportional to their distance (H_0 is the Hubble constant) from where we are on Earth. For the ith galaxy

$$\mathbf{v}_i = H_0 \mathbf{r}_i,$$

with our Milky Way galaxy at the origin. Show that this recession of the galaxies from us does **not** imply that we are at the center of the universe.

Specifically, take the galaxy at $\mathbf{r}_1$ as a new origin and show that Hubble's law is still obeyed.

1.2 Scalar or Dot Product

Having defined vectors, we now proceed to combine them in this section. The laws for combining vectors must be mathematically consistent. From the possibilities that are consistent we select two that are both mathematically and physically interesting. In this section, we start with the scalar product that is based on the geometric concept of projection that we used in Section 1.1 to define the Cartesian components of a vector. Also included here are some applications to particle orbits and analytic geometry that will prompt us to **differentiate vectors**, thus starting **vector analysis**.

The **projection of a vector A** onto a coordinate axis, which defines its Cartesian components in Eq. (1.5), **is a special case of the scalar product** of **A** and the coordinate unit vectors,

$$A_x = A\cos\alpha \equiv \mathbf{A}\cdot\hat{\mathbf{x}}, \quad A_y = A\cos\beta \equiv \mathbf{A}\cdot\hat{\mathbf{y}}, \quad A_z = A\cos\gamma \equiv \mathbf{A}\cdot\hat{\mathbf{z}} \tag{1.8}$$

and leads us to the general definition of the dot product. Just as the projection is linear in **A**, we want the scalar product of two vectors to be linear in **A** and **B**—that is, to obey the distributive and associative laws

$$\mathbf{A}\cdot(\mathbf{B}+\mathbf{C}) = \mathbf{A}\cdot\mathbf{B} + \mathbf{A}\cdot\mathbf{C} \tag{1.9}$$

$$\mathbf{A}\cdot(y\mathbf{B}) = (y\mathbf{A})\cdot\mathbf{B} = y\mathbf{A}\cdot\mathbf{B}, \tag{1.10}$$

where y is a real number. Now we can use the decomposition of **B** into its Cartesian components according to Eq. (1.5), $\mathbf{B} = B_x\hat{\mathbf{x}} + B_y\hat{\mathbf{y}} + B_z\hat{\mathbf{z}}$, to construct the general scalar or dot product of the vectors **A** and **B** from the special case as

$$\begin{aligned}
\mathbf{A}\cdot\mathbf{B} &= \mathbf{A}\cdot(B_x\hat{\mathbf{x}} + B_y\hat{\mathbf{y}} + B_z\hat{\mathbf{z}}),\\
&= B_x\mathbf{A}\cdot\hat{\mathbf{x}} + B_y\mathbf{A}\cdot\hat{\mathbf{y}} + B_z\mathbf{A}\cdot\hat{\mathbf{z}}, \qquad \text{applying Eqs. (1.9) and (1.10)}\\
&= B_xA_x + B_yA_y + B_zA_z, \qquad \text{upon substituting Eq. (1.8).}
\end{aligned}$$

Hence,

$$\mathbf{A}\cdot\mathbf{B} \equiv \sum_i A_iB_i = \sum_i B_iA_i = \mathbf{B}\cdot\mathbf{A} \tag{1.11}$$

because we are dealing with components.

If $\mathbf{A} = \mathbf{B}$ in Eq. (1.11), we recover the magnitude $A = (\sum_i A_i^2)^{1/2}$ of **A** in Eq. (1.6) from Eq. (1.11).

It is obvious from Eq. (1.11) that the scalar product treats **A** and **B** alike, is symmetric in **A** and **B**, or is commutative. Based on this observation, we can generalize Eq. (1.8) to the projection of **A** onto an arbitrary vector $\mathbf{B} \neq 0$

Figure 1.8

Scalar Product
$\mathbf{A} \cdot \mathbf{B} = AB\cos\theta$

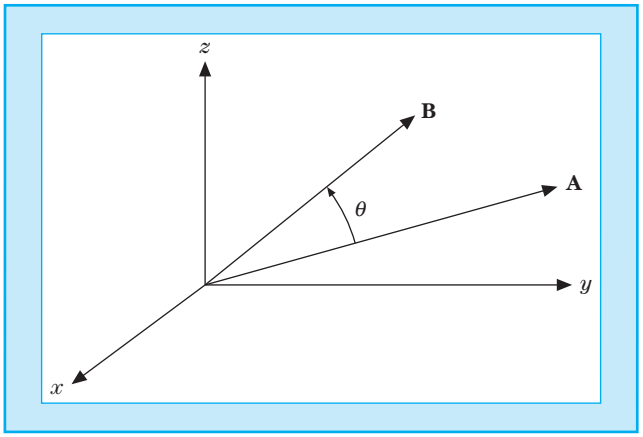
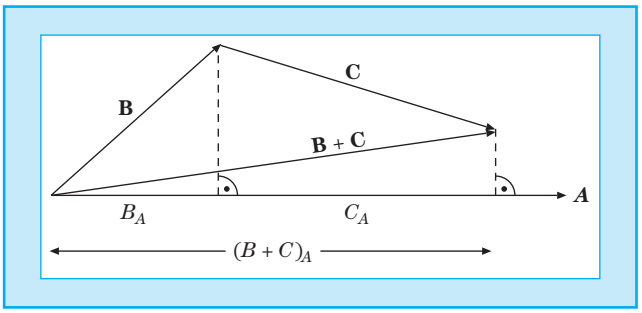


Figure 1.9

The Distributive Law
$\mathbf{A}\cdot(\mathbf{B}+\mathbf{C}) = AB_A + AC_A = A(\mathbf{B}+\mathbf{C})_A$
[Eq. (1.9)]



instead of the coordinate unit vectors. As a first step in this direction, we define A_B as $A_B = A\cos\theta \equiv \mathbf{A}\cdot\hat{\mathbf{B}}$, where $\hat{\mathbf{B}} = \mathbf{B}/B$ is the unit vector in the direction of $\mathbf{B}$ and θ is the angle between $\mathbf{A}$ and $\mathbf{B}$ as shown in Fig. 1.8. Similarly, we project $\mathbf{B}$ onto $\mathbf{A}$ as $B_A = B\cos\theta \equiv \mathbf{B}\cdot\hat{\mathbf{A}}$. These projections are not symmetric in $\mathbf{A}$ and $\mathbf{B}$. To make them symmetric in $\mathbf{A}$ and $\mathbf{B}$, we define

$$\mathbf{A}\cdot\mathbf{B} \equiv A_B B = AB_A = AB\cos\theta. \tag{1.12}$$

The distributive law in Eq. (1.9) is illustrated in Fig. 1.9, which states that the sum of the projections of $\mathbf{B}$ and $\mathbf{C}$ onto $\mathbf{A}$, $B_A + C_A$, is equal to the projection of $\mathbf{B}+\mathbf{C}$ onto $\mathbf{A}$, $(\mathbf{B}+\mathbf{C})_A$.

From Eqs. (1.8), (1.11), and (1.12), we infer that the coordinate unit vectors satisfy the relations

$$\hat{\mathbf{x}}\cdot\hat{\mathbf{x}} = \hat{\mathbf{y}}\cdot\hat{\mathbf{y}} = \hat{\mathbf{z}}\cdot\hat{\mathbf{z}} = 1, \tag{1.13}$$

whereas

$$\hat{\mathbf{x}}\cdot\hat{\mathbf{y}} = \hat{\mathbf{x}}\cdot\hat{\mathbf{z}} = \hat{\mathbf{y}}\cdot\hat{\mathbf{z}} = 0. \tag{1.14}$$

If the component definition of the dot product, Eq. (1.11), is labeled an algebraic definition, then Eq. (1.12) is a geometric definition. One of the most common applications of the scalar product in physics is in the definition of work = force · displacement · $\cos\theta$, where θ is the angle between the force and the displacement. This expression is interpreted as displacement times the projection of the force along the displacement direction—that is, the scalar product of force and displacement, $W = \mathbf{F} \cdot \mathbf{s}$.

If $\mathbf{A} \cdot \mathbf{B} = 0$ and we know that $\mathbf{A} \neq 0$ and $\mathbf{B} \neq 0$, then from Eq. (1.12) $\cos\theta = 0$ or $\theta = 90^\circ, 270^\circ$, and so on. The vectors **A** and **B** must be **perpendicular**. Alternately, we may say **A** and **B** are **orthogonal**. The unit vectors $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$, and $\hat{\mathbf{z}}$ are mutually orthogonal.

Free Motion and Other Orbits

EXAMPLE 1.2.1

Free Particle Motion To apply this notion of orthogonality in two dimensions, let us first deal with the motion of a particle free of forces along a straight line

$$\mathbf{r}(t) = (x(t), y(t)) = (-3t, 4t)$$

through the origin (dashed line in Fig. 1.10). The particle travels with the velocity $v_x = x/t = -3$ in the x-direction and $v_y = y/t = 4$ in the y-direction (in meters per second; e.g., 1 m/sec = 3.6 km/hr). The constant velocity $\mathbf{v} = (-3, 4)$ is characteristic of free motion according to Newton's equations.

Eliminating the time t, we find the homogeneous linear equation $4x + 3y = 0$, whose coefficient vector (4, 3) we normalize to unit length; that is, we write the linear equation as

$$\frac{4}{5}x + \frac{3}{5}y = 0 = \mathbf{n} \cdot \mathbf{r}.$$

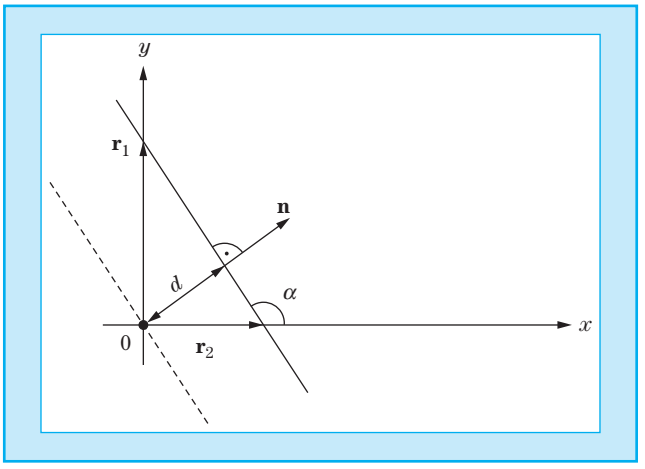


Figure 1.10

The Dashed Line Is $\mathbf{n} \cdot \mathbf{r} = 0$ and the Solid Line Is $\mathbf{n} \cdot \mathbf{r} = d$

where $\mathbf{n} = (4/5, 3/5)$ is a constant unit vector and $\mathbf{r}$ is the coordinate vector varying in the xy-plane; that is, $\mathbf{r} = \hat{\mathbf{x}}x + \hat{\mathbf{y}}y$. The scalar product

$$\mathbf{n} \cdot \mathbf{r} = 0 \tag{1.15}$$

means that the projection onto $\mathbf{n}$ of the vector $\mathbf{r}(t)$ pointing from the origin (a point on the line) to the general point on the line is zero so that **$\mathbf{n}$ is the normal of the straight line**. We verify that

$$(-3t, 4t) \cdot \left(\frac{4}{5}, \frac{3}{5}\right) = \frac{t}{5}(-3 \cdot 4 + 4 \cdot 3) = 0.$$

Because the particle's velocity is a tangent vector of the line, we can also write the scalar product as $\mathbf{v} \cdot \mathbf{n} = 0$, omitting the normalization factor $t/v = t/5$.

If we throw the particle from the origin in an arbitrary direction with some velocity v, it also will travel on a line through the origin. That is, upon varying the normal unit vector the linear Eq. (1.15) defines an arbitrary straight line through the origin in the xy-plane. Notice that in three dimensions Eq. (1.15) describes a plane through the origin, and a hyperplane ($(n-1)$-dimensional subspace) in n-dimensional space.

Now we shift the line by some constant distance d along the normal direction $\mathbf{n}$ so that it passes through the point $(3, 0)$ on the x-axis, for example. Because its tangent vector is $\mathbf{v}$, the line is parameterized as $x(t) = 3-3t,\ y(t) = 4t$. We can verify that it passes through the point $\mathbf{r}_2 = (3, 0)$ on the x-axis for $t = 0$ and $\mathbf{r}_1 = (0, 4)$ on the y-axis for $t = 1$. The particle has the same velocity and the path has the same normal. Eliminating the time as before, we find that the linear equation for the line becomes $4x + 3y = 12$, or

$$\mathbf{n} \cdot \mathbf{r} = d = \frac{12}{5}. \tag{1.16}$$

The line no longer goes through the origin (solid line in Fig. 1.10) but has the shortest distance $d = 12/5$ from the origin. If $\mathbf{r}_1 = (0, 4)$, $\mathbf{r}_2 = (3, 0)$ are our different points on that line, then $\mathbf{T} = \mathbf{r}_1 - \mathbf{r}_2 = (-3, 4) = \mathbf{v}$ is a tangent vector of the line and therefore orthogonal to the normal $\mathbf{n}$ because $\mathbf{n} \cdot \mathbf{T} = \mathbf{n} \cdot \mathbf{r}_1 - \mathbf{n} \cdot \mathbf{r}_2 = d - d = 0$ from Eq. (1.16). Then the general point on that line is parameterized by

$$\mathbf{r}(t) = \mathbf{r}_1 + t\mathbf{T} \tag{1.17}$$

because $\mathbf{n} \cdot \mathbf{r} = \mathbf{n} \cdot \mathbf{r}_1 + t\mathbf{n} \cdot \mathbf{T} = d + t \cdot 0 = d$.

Note that in general a straight line is defined by a linear relation, $\mathbf{n} \cdot \mathbf{r} = d$, and its points depend linearly on one variable t; that is, in two dimensions Eq. (1.17) represents $x = x_1 + tT_x$, $y = y_1 + tT_y$, with $\mathbf{T} = (T_x, T_y)$. The geometry of Fig. 1.10 shows that the projection of the vectors $\mathbf{r}_1$, $\mathbf{r}_2$, $\mathbf{r}$ on the normal $\mathbf{n}$ is always d—that is, the shortest distance of our line from the origin, consistent with the algebraic definition $\mathbf{n} \cdot \mathbf{r} = d$ of our line, from which we started.

Equations (1.16) and (1.17) are consistent with the conventional definition of a straight line by its constant slope (or angle α with the x-axis)

$$\tan\alpha = \frac{y - y_1}{x - x_1} \leftrightarrow (x - x_1)\sin\alpha - (y - y_1)\cos\alpha = 0, \tag{1.18}$$

where the normal $\mathbf{n} = (\sin\alpha, -\cos\alpha)$; upon comparing Eq. (1.18) with Eq. (1.16), $\mathbf{n}\cdot\mathbf{r} = d = x_1\sin\alpha - y_1\cos\alpha$.

Generalizing to three-dimensional analytic geometry, $\mathbf{n}\cdot\mathbf{r} = d$ is linear in the variables $(x, y, z) = \mathbf{r}$; that is, it represents a plane, and the unit vector $\mathbf{n} = (n_1, n_2, n_3)$ is perpendicular to the plane—it is the constant normal of the plane. If we divide the plane equation by d, the coefficients n_i/d of the coordinates x_i of the plane give the inverse lengths of the segments from the origin to the intersection of the Cartesian axes with the plane. For example, the point of the plane $6x + 3y + 2z = 6$ in Fig. 1.11 on the x-axis defined by $y = 0 = z$ is $(d/n_1 = 1, 0, 0)$ for $n_1 = 6/7$, $d = 6/7$, noting that $6^2+3^2+2^2 = 7^2$. The general point on the plane is parameterized as

$$\mathbf{r}(s, t) = \mathbf{r}_1 + s\mathbf{l}_1 + t\mathbf{l}_2,$$

where s and t are parameters, and it is constructed from three of its points $\mathbf{r}_i$, $i = 1, 2, 3$, that is, $\mathbf{r}_1 = (1, 0, 0)$, $\mathbf{r}_2 = (0, 2, 0)$, $\mathbf{r}_3 = (0, 0, 3)$ for the plane in Fig. 1.11, so that the tangent vectors $\mathbf{l}_1 = \mathbf{r}_2 - \mathbf{r}_1$, $\mathbf{l}_2 = \mathbf{r}_3 - \mathbf{r}_1$ of the plane are not parallel. All this generalizes to higher dimensions.

Geometry also tells us that two nonparallel planes $\mathbf{a}_1\cdot\mathbf{r} = d_1$, $\mathbf{a}_2\cdot\mathbf{r} = d_2$ in three-dimensional space have a line in common and three nonparallel planes a single point in general. Finding them amounts to solving linear equations, which is addressed in Section 3.1 using determinants.

Figure 1.11

The Plane $6x + 3y + 2z = 6$

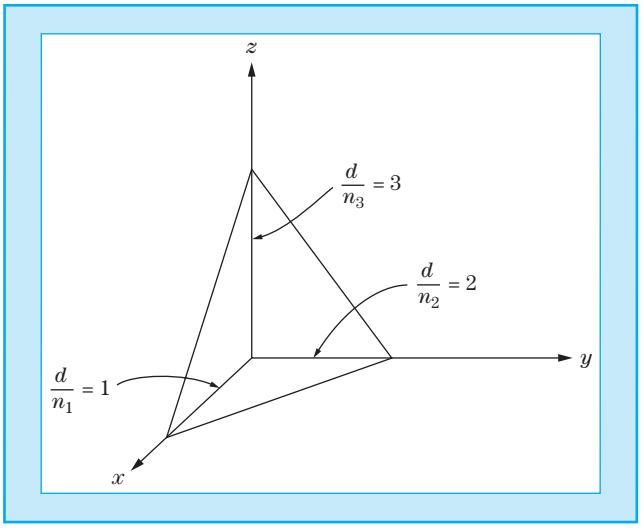
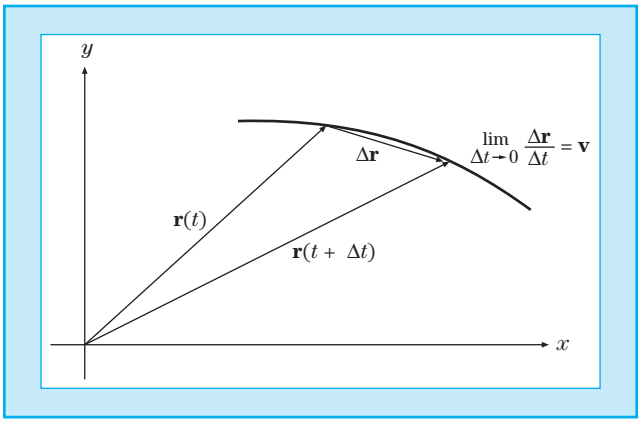


Figure 1.12

Differentiation of a Vector



More generally, the orbit of a particle or a curve in planar analytic geometry may be defined as $\mathbf{r}(t) = (x(t), y(t))$, where x and y are functions of the parameter t. In order to find the slope of a curve or the tangent to an orbit we need to differentiate vectors. Differentiating a vector function is a simple extension of differentiating scalar functions if we resolve $\mathbf{r}(t)$ into its Cartesian components. Then, for differentiation with respect to time, the linear velocity is given by

$$\frac{d\mathbf{r}(t)}{dt} = \lim_{\Delta t \to 0} \frac{\mathbf{r}(t + \Delta t) - \mathbf{r}(t)}{\Delta t} = \mathbf{v} = \left(\frac{dx}{dt}, \frac{dy}{dt}, \frac{dz}{dt}\right) \equiv (\dot{x}, \dot{y}, \dot{z})$$

because the Cartesian unit vectors are constant. Thus, differentiation of a vector always reduces directly to a vector sum of not more than three (for three-dimensional space) scalar derivatives. In other coordinate systems (see Chapter 2), the situation is more complicated because the unit vectors are no longer constant in direction. Differentiation with respect to the space coordinates is handled in the same way as differentiation with respect to time. Graphically, we have the slope of a curve, orbit, or trajectory, as shown in Fig. 1.12. ■

EXAMPLE 1.2.2

Shortest Distance of a Rocket from an Observer What is the shortest distance of a rocket traveling at a constant velocity $\mathbf{v} = (1, 2, 3)$ from an observer at $\mathbf{r}_0 = (2, 1, 3)$? The rocket is launched at **time** $t = 0$ at the point $\mathbf{r}_1 = (1, 1, 1)$.

The path of the rocket is the straight line

$$\mathbf{r} = \mathbf{r}_1 + t\mathbf{v}, \tag{1.19}$$

or, in Cartesian coordinates,

$$x(t) = 1 + t, \quad y(t) = 1 + 2t, \quad z(t) = 1 + 3t.$$

We now minimize the distance $|\mathbf{r}-\mathbf{r}_0|$ of the observer at the point $\mathbf{r}_0 = (2, 1, 3)$ from $\mathbf{r}(t)$, or equivalently $(\mathbf{r} - \mathbf{r}_0)^2 = \text{min}$. Differentiating Eq. (1.19) with respect to t yields $\dot{\mathbf{r}} = (\dot{x}, \dot{y}, \dot{z}) = \mathbf{v}$. Setting $\frac{d}{dt}(\mathbf{r} - \mathbf{r}_0)^2 = 0$, we obtain the condition

$$2(\mathbf{r} - \mathbf{r}_0) \cdot \dot{\mathbf{r}} = 2[\mathbf{r}_1 - \mathbf{r}_0 + t\mathbf{v}] \cdot \mathbf{v} = 0.$$

Because $\dot{\mathbf{r}} = \mathbf{v}$ is the tangent vector of the line, the geometric meaning of this condition is that the **shortest distance vector through $\mathbf{r}_0$ is perpendicular to the line.** Now solving for t yields the ratio of scalar products

$$t = -\frac{(\mathbf{r}_1 - \mathbf{r}_0) \cdot \mathbf{v}}{\mathbf{v}^2} = -\frac{(-1, 0, -2) \cdot (1, 2, 3)}{(1, 2, 3) \cdot (1, 2, 3)} = \frac{1 + 0 + 6}{1 + 4 + 9} = \frac{1}{2}.$$

Substituting this parameter value into Eq. (1.19) gives the point $\mathbf{r}_s = (3/2, 2, 5/2)$ on the line that is closest to $\mathbf{r}_0$. The shortest distance is $d = |\mathbf{r}_0 - \mathbf{r}_s| = |(-1/2, 1, -1/2)| = \sqrt{2/4 + 1} = \sqrt{3/2}$. ■

In two dimensions, $\mathbf{r}(t) = (x = a\cos t,\ y = b\sin t)$ describes an ellipse with half-axes a, b (so that $a = b$ gives a circle); for example, the orbit of a planet around the sun in a plane determined by the constant orbital angular momentum (the normal of the plane). If $\mathbf{r}_0 = (x(t_0), y(t_0)) = (x_0, y_0) = \mathbf{r}(t_0)$ is a point on our orbit, then the tangent at $\mathbf{r}_0$ has the slope $\dot{y}_0/\dot{x}_0$, where the dots denote the derivatives with respect to the time t as usual. Returning to the slope formula, imagine inverting $x = x(t)$ to find $t = t(x)$, which is substituted into $y = y(t) = y(t(x)) = f(x)$ to produce the standard form of a curve in analytic geometry. Using the **chain rule of differentiation**, the slope of $f(x)$ at x is

$$\frac{df}{dx} = f'(x) = \frac{dy(t(x))}{dx} = \frac{dy}{dt}\frac{dt}{dx} = \frac{\dot{y}}{\dot{x}}.$$

The tangent is a straight line and therefore depends linearly on one variable u,

$$\mathbf{r} = \mathbf{r}(t_0) + u\dot{\mathbf{r}}(t_0), \tag{1.20}$$

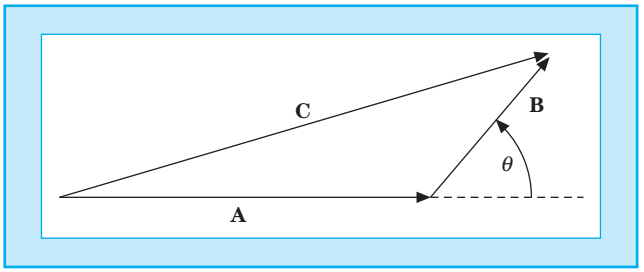
whereas the normal through the given point (x_0, y_0) obeys the linear equation

$$(x - x_0)\dot{x}_0 + (y - y_0)\dot{y}_0 = 0. \tag{1.21}$$

For the elliptical orbit mentioned previously, we check that the point $\mathbf{r}_0 = (0, b)$ for the parameter value $t = \pi/2$ lies on it. The slope at $t = \pi/2$ is zero, which we also know from geometry and because $\dot{y}_0 = b\cos t|_{t=\pi/2} = 0$, whereas $\dot{x}_0 = -a\sin t|_{\pi/2} = -a \neq 0$. The normal is the y-axis for which Eq. (1.21) yields $-ax = 0$.

A curve can also be defined implicitly by a functional relation, $F(x, y) = 0$, of the coordinates. This common case will be addressed in Section 1.5 because it involves partial derivatives.

Figure 1.13
The Law of Cosines



Law of Cosines In a similar geometrical approach, we take $\mathbf{C} = \mathbf{A} + \mathbf{B}$ and dot it into itself:

$$\mathbf{C} \cdot \mathbf{C} = (\mathbf{A} + \mathbf{B}) \cdot (\mathbf{A} + \mathbf{B}) = \mathbf{A} \cdot \mathbf{A} + \mathbf{B} \cdot \mathbf{B} + 2\mathbf{A} \cdot \mathbf{B}. \tag{1.22}$$

Since

$$\mathbf{C} \cdot \mathbf{C} = C^2, \tag{1.23}$$

the square of the magnitude of vector $\mathbf{C}$ is a scalar, we see that

$$\mathbf{A} \cdot \mathbf{B} = \frac{1}{2}(C^2 - A^2 - B^2) \tag{1.24}$$

is a scalar. Note that since the right-hand side of Eq. (1.24) is a scalar, the left-hand side $\mathbf{A} \cdot \mathbf{B}$ must also be a scalar, independent of the orientation of the coordinate system. We defer a proof that a scalar product is invariant under rotations to Section 2.6.

Equation (1.22) is another form of the **law of cosines**:

$$C^2 = A^2 + B^2 + 2AB\cos\theta. \tag{1.25}$$

Comparing Eqs. (1.22) and (1.25), we have another verification of Eq. (1.12) or, if preferred, a vector derivation of the law of cosines (Fig. 1.13). This law may also be derived from the triangle formed by the point of $\mathbf{C}$ and its line of shortest distance from the line along $\mathbf{A}$, which has the length $B\sin\theta$, whereas the projection of $\mathbf{B}$ onto $\mathbf{A}$ has length $B\cos\theta$. Applying the Pythagorean theorem to this triangle with a right angle formed by the point of $\mathbf{C}$, $\mathbf{A} + \mathbf{B} \cdot \hat{\mathbf{A}}$ and the shortest distance $B\sin\theta$ gives

$$C^2 = (A + \mathbf{B} \cdot \hat{\mathbf{A}})^2 + (B\sin\theta)^2 = A^2 + B^2(\cos^2\theta + \sin^2\theta) + 2AB\cos\theta.$$

SUMMARY

In this section, we defined the dot product as an algebraic generalization of the geometric concept of projection of vectors (their coordinates). We used it for geometrical purposes, such as finding the shortest distance of a point from a line or the cosine theorem for triangles. The geometrical meaning of the scalar product allowed us to go back and forth between the algebraic definition of a straight line as a linear equation and the parameterization of its general point $\mathbf{r}(t)$ as a linear function of time and similar steps for planes in three dimensions. We began differentiation of vectors as a tool for drawing tangents to orbits of particles, and this important step represents the start of vector analysis enlarging vector algebra.

The dot product, given by Eq. (1.11), may be generalized in two ways. The space need not be restricted to three dimensions. In n-dimensional space, Eq. (1.11) applies with the sum running from 1 to n; n may be infinity, with the sum then a convergent infinite series (see Section 5.2). The other generalization extends the concept of vector to embrace functions. The function analog of a dot or inner product is discussed in Section 9.4.

EXERCISES

1.2.1 A car is moving northward with a constant speed of 50 mph for 5 min, and then makes a 45° turn to the east and continues at 55 mph for 1 min. What is the average acceleration of the car?

1.2.2 A particle in an orbit is located at the point $\mathbf{r}$ (drawn from the origin) that terminates at and specifies the point in space (x, y, z). Find the surface swept out by the tip of $\mathbf{r}$ and draw it using graphical software if
(a) $(\mathbf{r} - \mathbf{a}) \cdot \mathbf{a} = 0$,
(b) $(\mathbf{r} - \mathbf{a}) \cdot \mathbf{r} = 0$.
The vector $\mathbf{a}$ is a constant (in magnitude and direction).

1.2.3 Develop a condition when two forces are parallel, with and without using their Cartesian coordinates.

1.2.4 The Newtonian equations of motion of two particles are

$$m_1\dot{\mathbf{v}}_1 = \mathbf{F}_1^i + \mathbf{F}_1^e, \quad m_2\dot{\mathbf{v}}_2 = \mathbf{F}_2^i + \mathbf{F}_2^e,$$

where m_i are their masses, $\mathbf{v}_i$ are their velocities, and the superscripts on the forces denote internal and external forces. What is the total force and the total external force? Write Newton's third law for the forces. Define the center of mass and derive its equation of motion. Define the relative coordinate vector of the particles and derive the relevant equation of motion. Plot a typical case at some time instant using graphical software.
Note. The resultant of all forces acting on particle 1, whose origin lies outside the system, is called external force $\mathbf{F}_1^e$; the force arising from the interaction of particle 2 with particle 1 is called the internal force $\mathbf{F}_1^i$ so that $\mathbf{F}_1^i = -\mathbf{F}_2^i$.

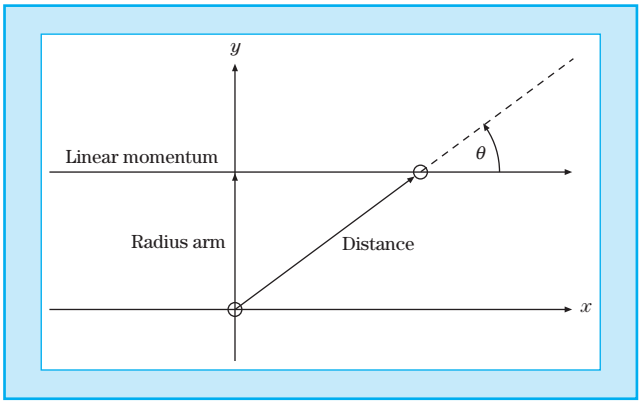
1.2.5 If $|\mathbf{A}|$, $|\mathbf{B}|$ are the magnitudes of the vectors $\mathbf{A}$, $\mathbf{B}$, show that $-|\mathbf{A}||\mathbf{B}| \leq \mathbf{A} \cdot \mathbf{B} \leq |\mathbf{A}||\mathbf{B}|$.

1.3 Vector or Cross Product

A second form of vector multiplication employs the sine of the included angle (denoted by θ) instead of the cosine and is called cross product. The cross product generates a vector from two vectors, in contrast with the dot product, which produces a scalar. Applications of the cross product in analytic geometry and mechanics are also discussed in this section. For instance, the orbital

Figure 1.14

Angular Momentum



angular momentum of a particle shown at the point of the distance vector in Fig. 1.14 is defined as

$$\begin{aligned}\text{Angular momentum} &= \text{radius arm} \cdot \text{ linear momentum} \\ &= \text{distance} \cdot \text{ linear momentum} \cdot \sin\theta. \end{aligned} \tag{1.26}$$

For convenience in treating problems relating to quantities such as angular momentum, torque, angular velocity, and area, we define the vector or cross product as

$$\mathbf{C} = \mathbf{A} \times \mathbf{B}, \tag{1.27}$$

with the magnitude (but not necessarily the dimensions of length)

$$C = AB\sin\theta. \tag{1.28}$$

Unlike the preceding case of the scalar product, $\mathbf{C}$ is now a vector, and we assign it a direction perpendicular to the plane of $\mathbf{A}$ and $\mathbf{B}$ such that $\mathbf{A}$, $\mathbf{B}$, and $\mathbf{C}$ form a right-handed system. If we curl the fingers of the right hand from the point of $\mathbf{A}$ to $\mathbf{B}$, then the extended thumb will point in the direction of $\mathbf{A} \times \mathbf{B}$, and these three vectors form a right-handed system. With this choice of direction, we have

$$\mathbf{A} \times \mathbf{B} = -\mathbf{B} \times \mathbf{A}, \qquad \text{anticommutation.} \tag{1.29}$$

In general, the cross product of two collinear vectors is zero so that

$$\hat{\mathbf{x}} \times \hat{\mathbf{x}} = \hat{\mathbf{y}} \times \hat{\mathbf{y}} = \hat{\mathbf{z}} \times \hat{\mathbf{z}} = 0, \tag{1.30}$$

whereas

$$\begin{aligned} &\hat{\mathbf{x}} \times \hat{\mathbf{y}} = \hat{\mathbf{z}}, \quad \hat{\mathbf{y}} \times \hat{\mathbf{z}} = \hat{\mathbf{x}}, \quad \hat{\mathbf{z}} \times \hat{\mathbf{x}} = \hat{\mathbf{y}}, \\ &\hat{\mathbf{y}} \times \hat{\mathbf{x}} = -\hat{\mathbf{z}}, \quad \hat{\mathbf{z}} \times \hat{\mathbf{y}} = -\hat{\mathbf{x}}, \quad \hat{\mathbf{x}} \times \hat{\mathbf{z}} = -\hat{\mathbf{y}}. \end{aligned} \tag{1.31}$$

Among the examples of the cross product in mathematical physics are the relation between linear momentum $\mathbf{p}$ and angular momentum $\mathbf{L}$ (defining angular momentum),

$$\mathbf{L} = \mathbf{r} \times \mathbf{p} \tag{1.32}$$

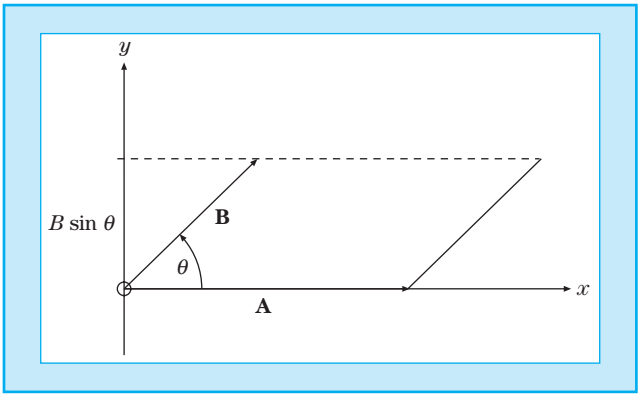


Figure 1.15

Parallelogram Representation of the Vector Product

and the relation between linear velocity $\mathbf{v}$ and angular velocity $\boldsymbol{\omega}$,

$$\mathbf{v} = \boldsymbol{\omega} \times \mathbf{r}. \tag{1.33}$$

Vectors $\mathbf{v}$ and $\mathbf{p}$ describe properties of the particle or physical system. However, the position vector $\mathbf{r}$ is determined by the choice of the origin of the coordinates. This means that $\boldsymbol{\omega}$ and $\mathbf{L}$ depend on the choice of the origin.

The familiar magnetic induction $\mathbf{B}$ occurs in the vector product force equation called Lorentz force

$$\mathbf{F}_M = q\mathbf{v} \times \mathbf{B} \qquad \text{(SI units)}, \tag{1.34}$$

where $\mathbf{v}$ is the velocity of the electric charge q, and $\mathbf{F}_M$ is the resulting magnetic force on the moving charge. The cross product has an important geometrical interpretation that we shall use in subsequent sections. In the parallelogram (Fig. 1.15) defined by $\mathbf{A}$ and $\mathbf{B}$, $B\sin\theta$ is the height if A is taken as the length of the base. Then $|\mathbf{A} \times \mathbf{B}| = AB\sin\theta$ is the **area of the parallelogram**. As a vector, $\mathbf{A} \times \mathbf{B}$ is the area of the parallelogram defined by $\mathbf{A}$ and $\mathbf{B}$, with the area vector normal to the plane of the parallelogram. This means that area (with its orientation in space) is treated as a vector.

An alternate definition of the vector product can be derived from the special case of the coordinate unit vectors in Eqs. (1.30) and (1.31) in conjunction with the linearity of the cross product in both vector arguments, in analogy with Eqs. (1.9) and (1.10) for the dot product,

$$\mathbf{A} \times (\mathbf{B} + \mathbf{C}) = \mathbf{A} \times \mathbf{B} + \mathbf{A} \times \mathbf{C}, \tag{1.35}$$

$$(\mathbf{A} + \mathbf{B}) \times \mathbf{C} = \mathbf{A} \times \mathbf{C} + \mathbf{B} \times \mathbf{C}, \tag{1.36}$$

$$\mathbf{A} \times (y\mathbf{B}) = y\mathbf{A} \times \mathbf{B} = (y\mathbf{A}) \times \mathbf{B}, \tag{1.37}$$

where y is a number, a scalar. Using the decomposition of $\mathbf{A}$ and $\mathbf{B}$ into their Cartesian components according to Eq. (1.5), we find

$$\begin{aligned}\mathbf{A}\times\mathbf{B}\equiv\mathbf{C}&=(C_x,C_y,C_z)=(A_x\hat{\mathbf{x}}+A_y\hat{\mathbf{y}}+A_z\hat{\mathbf{z}})\times(B_x\hat{\mathbf{x}}+B_y\hat{\mathbf{y}}+B_z\hat{\mathbf{z}})\\&=(A_xB_y-A_yB_x)\hat{\mathbf{x}}\times\hat{\mathbf{y}}+(A_xB_z-A_zB_x)\hat{\mathbf{x}}\times\hat{\mathbf{z}}\\&\quad+(A_yB_z-A_zB_y)\hat{\mathbf{y}}\times\hat{\mathbf{z}},\end{aligned}$$

upon applying Eqs. (1.35) and (1.37) and substituting Eqs. (1.30) and (1.31) so that the Cartesian components of $\mathbf{A}\times\mathbf{B}$ become

$$C_x=A_yB_z-A_zB_y,\quad C_y=A_zB_x-A_xB_z,\quad C_z=A_xB_y-A_yB_x,\tag{1.38}$$

or

$$C_i=A_jB_k-A_kB_j,\quad i,j,k\ \text{ all different},\tag{1.39}$$

and with cyclic permutation of the indices i, j, and k or $x\to y\to z\to x$ in Eq. (1.38). The vector product $\mathbf{C}$ may be represented by a determinant[4]

$$\mathbf{C}=\begin{vmatrix}\hat{\mathbf{x}}&\hat{\mathbf{y}}&\hat{\mathbf{z}}\\A_x&A_y&A_z\\B_x&B_y&B_z\end{vmatrix}\tag{1.40}$$

which, according to the expansion Eq. (3.11) of the determinant along the top row, is a shorthand form of the vector product

$$\mathbf{C}=\hat{\mathbf{x}}(A_yB_z-A_zB_y)+\hat{\mathbf{y}}(A_zB_x-A_xB_z)+\hat{\mathbf{z}}(A_xB_y-A_yB_x).$$

If Eqs. (1.27) and (1.28) are called a geometric definition of the vector product, then Eq. (1.38) is an algebraic definition.

To show the equivalence of Eqs. (1.27) and (1.28) and the component definition Eq. (1.38), let us form $\mathbf{A}\cdot\mathbf{C}$ and $\mathbf{B}\cdot\mathbf{C}$ using Eq. (1.38). We have

$$\begin{aligned}\mathbf{A}\cdot\mathbf{C}&=\mathbf{A}\cdot(\mathbf{A}\times\mathbf{B})\\&=A_x(A_yB_z-A_zB_y)+A_y(A_zB_x-A_xB_z)+A_z(A_xB_y-A_yB_x)\\&=0.\end{aligned}\tag{1.41}$$

Similarly,

$$\mathbf{B}\cdot\mathbf{C}=\mathbf{B}\cdot(\mathbf{A}\times\mathbf{B})=0.\tag{1.42}$$

Equations (1.41) and (1.42) show that $\mathbf{C}$ is perpendicular to both $\mathbf{A}$ and $\mathbf{B}$ and therefore perpendicular to the plane they determine. The positive direction is determined by considering special cases, such as the unit vectors $\hat{\mathbf{x}}\times\hat{\mathbf{y}}=\hat{\mathbf{z}}$.

[4]Determinants are discussed in detail in Section 3.1.

The magnitude is obtained from

$$\begin{aligned}(\mathbf{A}\times\mathbf{B})\cdot(\mathbf{A}\times\mathbf{B}) &= A^2B^2-(\mathbf{A}\cdot\mathbf{B})^2\\ &= A^2B^2-A^2B^2\cos^2\theta\\ &= A^2B^2\sin^2\theta,\end{aligned}\tag{1.43}$$

which implies Eq. (1.28). The first step in Eq. (1.43) may be verified by expanding out in component form using Eq. (1.38) for $\mathbf{A}\times\mathbf{B}$ and Eq. (1.11) for the dot product. From Eqs. (1.41)–(1.43), we see the equivalence of Eqs. (1.28) and (1.38), the two definitions of vector product.

EXAMPLE 1.3.1

Shortest Distance between Two Rockets in Free Flight Considering Example 1.2.2 as a similar but simpler case, we remember that the shortest distance between a point and a line is measured along the normal from the line through the point. Therefore, we expect that the shortest distance between two lines is normal to both tangent vectors of the straight lines. Establishing this fact will be our first and most important step. The second step involves the projection of a vector between two points, one on each line, onto that normal to both lines. However, we also need to locate the points where the normal starts and ends. This problem we address first.

Let us take the first line from Example 1.2.2, namely $\mathbf{r}=\mathbf{r}_1+t_1\mathbf{v}_1$ with time variable t_1 and tangent vector $\mathbf{v}_1=\mathbf{r}_2-\mathbf{r}_1=(1,2,3)$ that goes through the points $\mathbf{r}_1=(1,1,1)$ and $\mathbf{r}_2=(2,3,4)$ and is shown in Fig. 1.16, along with the second line $\mathbf{r}=\mathbf{r}_3+t_2\mathbf{v}_2$ with time variable t_2 that goes through the points $\mathbf{r}_3=(5,2,1)$ and $\mathbf{r}_4=(4,1,2)$, and so has the tangent vector $\mathbf{r}_4-\mathbf{r}_3=(-1,-1,1)=\mathbf{v}_2$ and the parameterization

$$x=5-t_2,\quad y=2-t_2,\quad z=1+t_2.$$

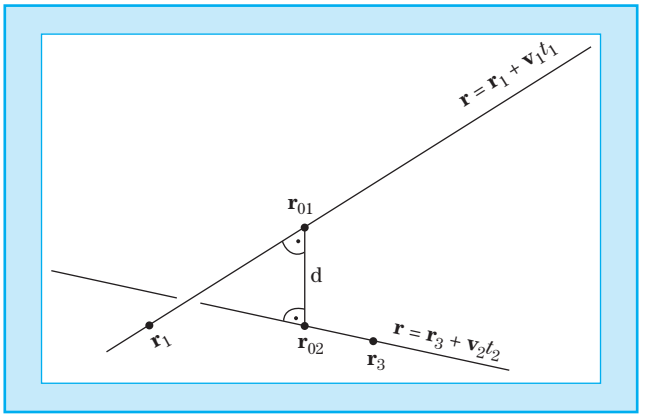


Figure 1.16

Shortest Distance Between Two Straight Lines That Do Not Intersect

In order to find the end points $\mathbf{r}_{0k}$ of this shortest distance we minimize the distances squared $(\mathbf{r}-\mathbf{r}_{0k})^2$ to obtain the conditions

$$0=\frac{d}{dt_1}(\mathbf{r}-\mathbf{r}_{02})^2=\frac{d}{dt_1}(\mathbf{r}_1-\mathbf{r}_{02}+t_1\mathbf{v}_1)^2=2\mathbf{v}_1\cdot(\mathbf{r}_1-\mathbf{r}_{02}+t_1\mathbf{v}_1),$$
$$0=\frac{d}{dt_2}(\mathbf{r}-\mathbf{r}_{01})^2=2\mathbf{v}_2\cdot(\mathbf{r}_3-\mathbf{r}_{01}+t_2\mathbf{v}_2). \tag{1.44}$$

We can solve for $t_1=-\mathbf{v}_1\cdot(\mathbf{r}_1-\mathbf{r}_{02})/\mathbf{v}_1^2$ and $t_2=-\mathbf{v}_2\cdot(\mathbf{r}_3-\mathbf{r}_{01})/\mathbf{v}_2^2$ and then plug these parameter values into the line coordinates to find the points $\mathbf{r}_{0k}$ and $d=|\mathbf{r}_{01}-\mathbf{r}_{02}|$. This is straightforward but tedious. Alternatively, we can exploit the geometric meaning of Eq. (1.44) that the distance vector $\mathbf{d}=\mathbf{r}_1+t_1\mathbf{v}_1-\mathbf{r}_{02}=-(\mathbf{r}_3+t_2\mathbf{v}_2-\mathbf{r}_{01})$ is perpendicular to both tangent vectors $\mathbf{v}_k$ as shown in Fig. 1.16. Thus, the distance vector $\mathbf{d}$ is along the normal unit vector

$$\mathbf{n}=\frac{\mathbf{v}_1\times\mathbf{v}_2}{|\mathbf{v}_1\times\mathbf{v}_2|}=\frac{1}{\sqrt{3}\sqrt{14}}\begin{vmatrix}\hat{\mathbf{x}}&\hat{\mathbf{y}}&\hat{\mathbf{z}}\\+1&+2&3\\-1&-1&1\end{vmatrix}=\frac{1}{\sqrt{42}}(5\hat{\mathbf{x}}-4\hat{\mathbf{y}}+\hat{\mathbf{z}})=\frac{1}{\sqrt{42}}(5,-4,1),$$

the **cross product** of both tangent vectors. We get the distance d by projecting the distance vector between two points $\mathbf{r}_1,\mathbf{r}_3$, one on each line, onto that normal $\mathbf{n}$—that is, $d=(\mathbf{r}_3-\mathbf{r}_1)\cdot\mathbf{n}=\frac{1}{\sqrt{42}}(4,1,0)\cdot(5,-4,1)=\frac{20-4+0}{\sqrt{42}}=\frac{16}{\sqrt{42}}$.

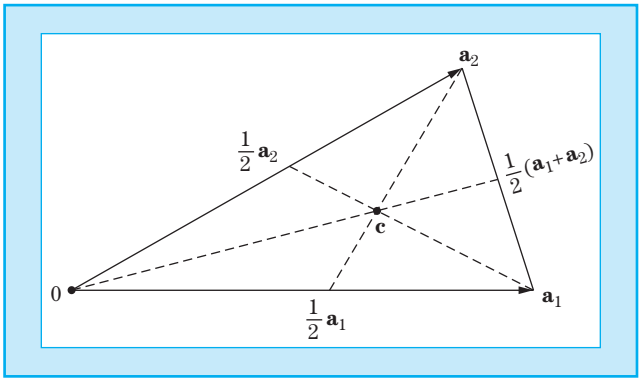
This example generalizes to the shortest distance between two orbits by examining the shortest distance beween their tangent lines. In this form, there are many applications in mechanics, space travel, and satellite orbits. ■

EXAMPLE 1.3.2

Medians of a Triangle Meet in the Center Let us consider Example 1.1.3 and Fig. 1.6 again, but now without using the 2:1 ratio of the segments from the center to the end points of each median. We put the origin of the coordinate system in one corner of the triangle, as shown in Fig. 1.17, so that the median from the origin will be given by the vector $\mathbf{m}_3=(\mathbf{a}_1+\mathbf{a}_2)/2$. The medians

Figure 1.17

Medians of a Triangle Meet in the Center



from the triangle corners $\mathbf{a}_1$ and $\mathbf{a}_2$ intersect at a point we call the center that is given by the vector $\mathbf{c}$ from the origin. We want to show that $\mathbf{m}_3$ and $\mathbf{c}$ are parallel (and therefore collinear), indicating that the center will also lie on the median from the origin.

From Fig. 1.17, we see that the vector $\mathbf{c}-\mathbf{a}_1$ from the corner $\mathbf{a}_1$ to the center will be parallel to $\frac{1}{2}\mathbf{a}_2-\mathbf{a}_1$; similarly, $\mathbf{c}-\mathbf{a}_2$ will be collinear with $\frac{1}{2}\mathbf{a}_1-\mathbf{a}_2$. We write these conditions as follows:

$$(\mathbf{c}-\mathbf{a}_1)\times\left(\frac{1}{2}\mathbf{a}_2-\mathbf{a}_1\right)=0,\quad (\mathbf{c}-\mathbf{a}_2)\times\left(\frac{1}{2}\mathbf{a}_1-\mathbf{a}_2\right)=0.$$

Expanding, and using the fact that $\mathbf{a}_1\times\mathbf{a}_1=0=\mathbf{a}_2\times\mathbf{a}_2$, we find

$$\mathbf{c}\times\frac{1}{2}\mathbf{a}_2-\mathbf{c}\times\mathbf{a}_1-\frac{1}{2}(\mathbf{a}_1\times\mathbf{a}_2)=0,\quad \mathbf{c}\times\frac{1}{2}\mathbf{a}_1-\mathbf{c}\times\mathbf{a}_2-\frac{1}{2}(\mathbf{a}_2\times\mathbf{a}_1)=0.$$

Adding these equations, the last terms on the left-hand sides cancel, and the other terms combine to yield

$$-\frac{1}{2}\mathbf{c}\times(\mathbf{a}_1+\mathbf{a}_2)=0,$$

proving that $\mathbf{c}$ and $\mathbf{m}_3$ are parallel.

The center of mass (see Example 1.1.3) will be at the point $\frac{1}{3}(\mathbf{a}_1+\mathbf{a}_2)$ and is therefore on the median from the origin. By symmetry it must be on the other medians as well, confirming both that they meet at a point and that the distance from the triangle corner to the intersection is two-thirds of the total length of the median. ■

SUMMARY

If we define a vector as an ordered triplet of numbers (or functions) as in Section 1.2, then there is no problem identifying the cross product as a vector. The cross product operation maps the two triples **A** and **B** into a third triple **C**, which by definition is a vector. In Section 2.6, we shall see that the cross product also transforms like a vector.

The cross product combines two vectors antisymmetrically and involves the sine of the angle between the vectors, in contrast to their symmetric combination in the scalar product involving the cosine of their angle, and it unifies the angular momentum and velocity of mechanics with the area concept of geometry. The vector nature of the cross product is peculiar to three-dimensional space, but it can naturally be generalized to higher dimensions. The cross product occurs in many applications such as conditions for parallel forces or other vectors and the shortest distance between lines or curves more generally.

We now have two ways of multiplying vectors; a third form is discussed in Chapter 2. However, what about division by a vector? The ratio $\mathbf{B}/\mathbf{A}$ is not uniquely specified (see Exercise 3.2.21) unless **A** and **B** are also required to be parallel. Hence, division of one vector by another is meaningless.

EXERCISES

1.3.1 Prove the law of cosines starting from $\mathbf{A}^2 = (\mathbf{B} - \mathbf{C})^2$, where $\mathbf{A}$, $\mathbf{B}$, and $\mathbf{C}$ are the vectors collinear with the sides of a triangle. Plot the triangle and describe the theorem in words. State the analog of the law of cosines on the unit sphere (Fig. 1.18), if $\mathbf{A}$, $\mathbf{B}$, and $\mathbf{C}$ go from the origin to the corners of the triangle.

1.3.2 A coin with a mass of 2 g rolls on a horizontal plane at a constant velocity of 5 cm/sec. What is its kinetic energy?
Hint. Show that the radius of the coin drops out.

1.3.3 Starting with $\mathbf{C} = \mathbf{A} + \mathbf{B}$, show that $\mathbf{C} \times \mathbf{C} = 0$ leads to

$$\mathbf{A} \times \mathbf{B} = -\mathbf{B} \times \mathbf{A}.$$

1.3.4 Show that
(a) $(\mathbf{A} - \mathbf{B}) \cdot (\mathbf{A} + \mathbf{B}) = A^2 - B^2$,
(b) $(\mathbf{A} - \mathbf{B}) \times (\mathbf{A} + \mathbf{B}) = 2\mathbf{A} \times \mathbf{B}$.
The distributive laws needed here,

$$\mathbf{A} \cdot (\mathbf{B} + \mathbf{C}) = \mathbf{A} \cdot \mathbf{B} + \mathbf{A} \cdot \mathbf{C}$$

and

$$\mathbf{A} \times (\mathbf{B} + \mathbf{C}) = \mathbf{A} \times \mathbf{B} + \mathbf{A} \times \mathbf{C},$$

may be verified by expansion in Cartesian components.

1.3.5 If $\mathbf{P} = \hat{\mathbf{x}}P_x + \hat{\mathbf{y}}P_y$ and $\mathbf{Q} = \hat{\mathbf{x}}Q_x + \hat{\mathbf{y}}Q_y$ are any two nonparallel (also non-antiparallel) vectors in the xy-plane, show that $\mathbf{P} \times \mathbf{Q}$ is in the z-direction.

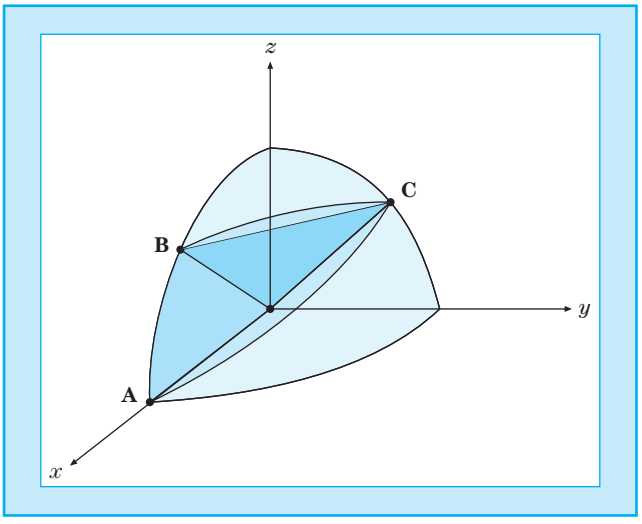
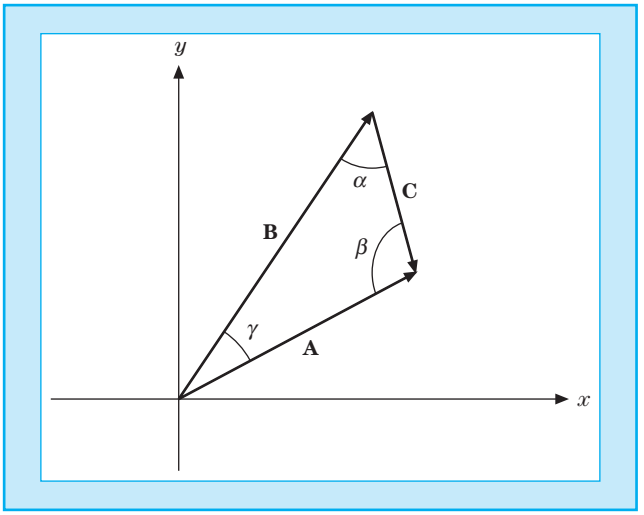


Figure 1.18
Spherical Triangle

Figure 1.19

Law of Sines



1.3.6 Prove that $(\mathbf{A} \times \mathbf{B}) \cdot (\mathbf{A} \times \mathbf{B}) = \mathbf{A}^2\mathbf{B}^2 - (\mathbf{A} \cdot \mathbf{B})^2$. Write the identity appropriately and describe it in geometric language. Make a plot for a typical case using graphical software.

1.3.7 Using the vectors

$$\mathbf{P} = \hat{\mathbf{x}}\cos\theta + \hat{\mathbf{y}}\sin\theta,$$

$$\mathbf{Q} = \hat{\mathbf{x}}\cos\varphi - \hat{\mathbf{y}}\sin\varphi,$$

$$\mathbf{R} = \hat{\mathbf{x}}\cos\varphi + \hat{\mathbf{y}}\sin\varphi,$$

prove the familiar trigonometric identities

$$\sin(\theta + \varphi) = \sin\theta\cos\varphi + \cos\theta\sin\varphi,$$

$$\cos(\theta + \varphi) = \cos\theta\cos\varphi - \sin\theta\sin\varphi.$$

1.3.8 If four vectors **a**, **b**, **c**, and **d** all lie in the same plane, show that

$$(\mathbf{a} \times \mathbf{b}) \times (\mathbf{c} \times \mathbf{d}) = 0.$$

If graphical software is available, plot all vectors for a specific numerical case.
Hint. Consider the directions of the cross product vectors.

1.3.9 Derive the law of sines (Fig. 1.19):

$$\frac{\sin\alpha}{|\mathbf{A}|} = \frac{\sin\beta}{|\mathbf{B}|} = \frac{\sin\gamma}{|\mathbf{C}|}.$$

1.3.10 A proton of mass m, charge $+e$, and (asymptotic) momentum $p = mv$ is incident on a nucleus of charge $+Ze$ at an impact parameter b. Determine its distance of closest approach.

Hint. Consider only the Coulomb repulsion and classical mechanics, not the strong interaction and quantum mechanics.

1.3.11 Expand a vector $\mathbf{x}$ in components parallel to three linearly independent vectors $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$.

ANS. $(\mathbf{a}\times\mathbf{b}\cdot\mathbf{c})\mathbf{x}=(\mathbf{x}\times\mathbf{b}\cdot\mathbf{c})\mathbf{a}+(\mathbf{a}\times\mathbf{x}\cdot\mathbf{c})\mathbf{b}+(\mathbf{a}\times\mathbf{b}\cdot\mathbf{x})\mathbf{c}$.

1.3.12 Let $\mathbf{F}$ be a force vector drawn from the coordinate vector $\mathbf{r}$. If $\mathbf{r}'$ goes from the origin to another point on the line through the point of $\mathbf{r}$ with tangent vector given by the force, show that the torque $\mathbf{r}'\times\mathbf{F}=\mathbf{r}\times\mathbf{F}$—that is, the torque about the origin due to the force stays the same.

1.3.13 A car drives in a horizontal circular track of radius R (to its center of mass). Find the speed at which it will overturn, if h is the height of its center of mass and d the distance between its left and right wheels.
Hint. Find the speed at which there is no vertical force on the inner wheels. (The mass of the car drops out.)

1.3.14 A force $\mathbf{F}=(3,2,4)$ acts at the point $(1,4,2)$. Find the torque about the origin. Plot the vectors using graphical software.

1.3.15 Generalize the cross product to n-dimensional space ($n=2,4,5,\ldots$) and give a geometrical interpretation of your construction. Give realistic examples in four- and higher dimensional spaces.

1.3.16 A jet plane flies due south over the north pole with a constant speed of 500 mph. Determine the angle between a plumb line hanging freely in the plane and the radius vector from the center of the earth to the plane above the north pole.
Hint. Assume that the earth's angular velocity is 2π radians in 24 hr, which is a good approximation. Why?

1.4 Triple Scalar Product and Triple Vector Product

Triple Scalar Product

Sections 1.2 and 1.3 discussed the two types of vector multiplication. However, there are combinations of three vectors, $\mathbf{A}\cdot(\mathbf{B}\times\mathbf{C})$ and $\mathbf{A}\times(\mathbf{B}\times\mathbf{C})$, that occur with sufficient frequency in mechanics, electrodynamics, and analytic geometry to deserve further attention. The combination

$$\mathbf{A}\cdot(\mathbf{B}\times\mathbf{C}) \tag{1.45}$$

is known as the **triple scalar product**. $\mathbf{B}\times\mathbf{C}$ yields a vector that, dotted into $\mathbf{A}$, gives a scalar. We note that $(\mathbf{A}\cdot\mathbf{B})\times\mathbf{C}$ represents a scalar crossed into a vector, an operation that is not defined. Hence, if we agree to exclude this undefined interpretation, the parentheses may be omitted and the triple scalar product written as $\mathbf{A}\cdot\mathbf{B}\times\mathbf{C}$.

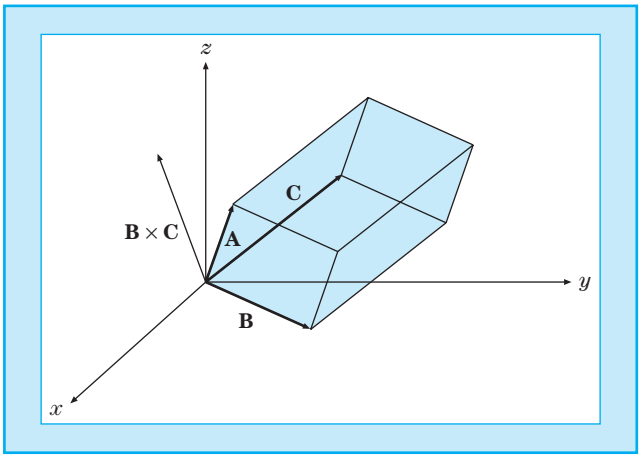


Figure 1.20

Parallelepiped Representation of Triple Scalar Product

Using Eq. (1.38) for the cross product and Eq. (1.11) for the dot product, we obtain

$$\begin{aligned}\mathbf{A}\cdot\mathbf{B}\times\mathbf{C} &= A_x(B_yC_z - B_zC_y) + A_y(B_zC_x - B_xC_z) + A_z(B_xC_y - B_yC_x)\\ &= \mathbf{B}\cdot\mathbf{C}\times\mathbf{A} = \mathbf{C}\cdot\mathbf{A}\times\mathbf{B} = -\mathbf{A}\cdot\mathbf{C}\times\mathbf{B}\\ &= -\mathbf{C}\cdot\mathbf{B}\times\mathbf{A} = -\mathbf{B}\cdot\mathbf{A}\times\mathbf{C}. \qquad (1.46)\end{aligned}$$

The high degree of symmetry present in the component expansion should be noted. Every term contains the factors A_i, B_j, and C_k. If i, j, and k are in cyclic order (x, y, z), the sign is positive. If the order is anticyclic, the sign is negative. Furthermore, the dot and the cross may be interchanged:

$$\mathbf{A}\cdot\mathbf{B}\times\mathbf{C} = \mathbf{A}\times\mathbf{B}\cdot\mathbf{C}. \qquad (1.47)$$

A convenient representation of the component expansion of Eq. (1.46) is provided by the determinant

$$\mathbf{A}\cdot\mathbf{B}\times\mathbf{C} = \begin{vmatrix} A_x & A_y & A_z \\ B_x & B_y & B_z \\ C_x & C_y & C_z \end{vmatrix}, \qquad (1.48)$$

which follows from Eq. (1.38) by dotting $\mathbf{B}\times\mathbf{C}$ into $\mathbf{A}$. The rules for interchanging rows and columns of a determinant[5] provide an immediate verification of the permutations listed in Eq. (1.46), whereas the symmetry of $\mathbf{A}$, $\mathbf{B}$, and $\mathbf{C}$ in the determinant form suggests the relation given in Eq. (1.46). The triple products discussed in Section 1.3, which showed that $\mathbf{A}\times\mathbf{B}$ was perpendicular to both $\mathbf{A}$ and $\mathbf{B}$, were special cases of the general result [Eq. (1.46)].

The triple scalar product has a direct **geometrical interpretation** in which the three vectors $\mathbf{A}$, $\mathbf{B}$, and $\mathbf{C}$ are interpreted as defining a **parallelepiped** (Fig. 1.20):

$$|\mathbf{B}\times\mathbf{C}| = BC\sin\theta = \text{ area of parallelogram base.} \qquad (1.49)$$

[5]See Section 3.1 for a detailed discussion of the properties of determinants.

The direction, of course, is normal to the base. Dotting $\mathbf{A}$ into this means multiplying the base area by the projection of $\mathbf{A}$ onto the normal, or base times height. Therefore,

$$\mathbf{A} \cdot \mathbf{B} \times \mathbf{C} = \text{ volume of parallelepiped defined by } \mathbf{A}, \mathbf{B}, \text{ and } \mathbf{C}. \tag{1.50}$$

Note that $\mathbf{A} \cdot \mathbf{B} \times \mathbf{C}$ may sometimes be negative. This is not a problem, and its proper interpretation is provided in Chapter 2.

EXAMPLE 1.4.1 **A Parallelepiped** For

$$\mathbf{A} = \hat{\mathbf{x}} + 2\hat{\mathbf{y}} - \hat{\mathbf{z}}, \quad \mathbf{B} = \hat{\mathbf{y}} + \hat{\mathbf{z}}, \quad \mathbf{C} = \hat{\mathbf{x}} - \hat{\mathbf{y}},$$

$$\mathbf{A} \cdot \mathbf{B} \times \mathbf{C} = \begin{vmatrix} 1 & 2 & -1 \\ 0 & 1 & 1 \\ 1 & -1 & 0 \end{vmatrix} = 4.$$

This is the volume of the parallelepiped defined by $\mathbf{A}$, $\mathbf{B}$, and $\mathbf{C}$. ■

Recall that we already encountered a triple scalar product, namely the distance $d \sim (\mathbf{r}_3 - \mathbf{r}_1) \cdot (\mathbf{v}_1 \times \mathbf{v}_2)$ between two straight lines in Example 1.3.1.

Triple Vector Product

The second triple product of interest is $\mathbf{A} \times (\mathbf{B} \times \mathbf{C})$, which is a vector. Here, the parentheses must be retained, as is seen from a special case $(\hat{\mathbf{x}} \times \hat{\mathbf{x}}) \times \hat{\mathbf{y}} = 0$, whereas $\hat{\mathbf{x}} \times (\hat{\mathbf{x}} \times \hat{\mathbf{y}}) = \hat{\mathbf{x}} \times \hat{\mathbf{z}} = -\hat{\mathbf{y}}$. Let us start with an example that illustrates a key property of the triple product.

EXAMPLE 1.4.2 **A Triple Vector Product** By using the three vectors given in Example 1.4.1, we obtain

$$\mathbf{B} \times \mathbf{C} = \begin{vmatrix} \hat{\mathbf{x}} & \hat{\mathbf{y}} & \hat{\mathbf{z}} \\ 0 & 1 & 1 \\ 1 & -1 & 0 \end{vmatrix} = \hat{\mathbf{x}} + \hat{\mathbf{y}} - \hat{\mathbf{z}}$$

and

$$\mathbf{A} \times (\mathbf{B} \times \mathbf{C}) = \begin{vmatrix} \hat{\mathbf{x}} & \hat{\mathbf{y}} & \hat{\mathbf{z}} \\ 1 & 2 & -1 \\ 1 & 1 & -1 \end{vmatrix} = -\hat{\mathbf{x}} - \hat{\mathbf{z}} = -(\hat{\mathbf{y}} + \hat{\mathbf{z}}) - (\hat{\mathbf{x}} - \hat{\mathbf{y}}).$$ ■

By rewriting the result in the last line as a linear combination of $\mathbf{B}$ and $\mathbf{C}$, we notice that, taking a geometric approach, the triple product vector is perpendicular to $\mathbf{A}$ and to $\mathbf{B} \times \mathbf{C}$. The plane spanned by $\mathbf{B}$ and $\mathbf{C}$ is perpendicular to $\mathbf{B} \times \mathbf{C}$, so the triple product lies in this plane (Fig. 1.21):

$$\mathbf{A} \times (\mathbf{B} \times \mathbf{C}) = u\mathbf{B} + v\mathbf{C}, \tag{1.51}$$

where u and v are numbers. Multiplying Eq. (1.51) by $\mathbf{A}$ gives zero for the left-hand side so that $u\mathbf{A} \cdot \mathbf{B} + v\mathbf{A} \cdot \mathbf{C} = 0$. Hence, $u = w\mathbf{A} \cdot \mathbf{C}$ and $v = -w\mathbf{A} \cdot \mathbf{B}$ for

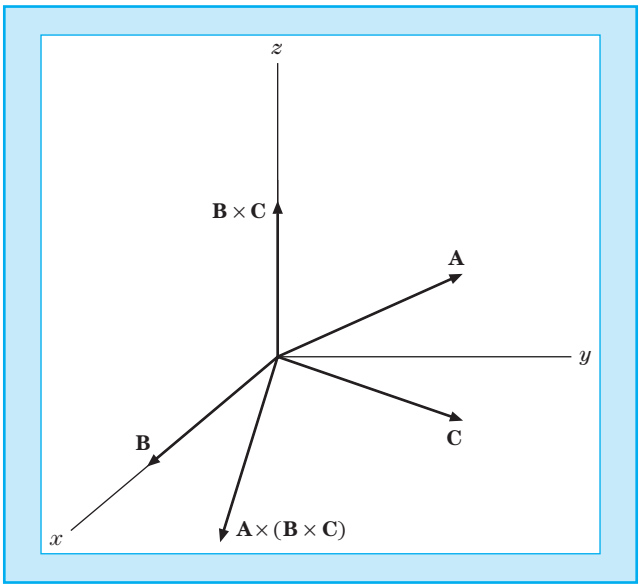


Figure 1.21

B and C Are in the *xy*-Plane. B × C Is Perpendicular to the *xy*-Plane and Is Shown Here Along the *z*-Axis. Then A × (B × C) Is Perpendicular to the *z*-Axis and Therefore Is Back in the *xy*-Plane

a suitable number w. Substituting these values into Eq. (1.50) gives

$$\mathbf{A} \times (\mathbf{B} \times \mathbf{C}) = w[\mathbf{B}(\mathbf{A} \cdot \mathbf{C}) - \mathbf{C}(\mathbf{A} \cdot \mathbf{B})]. \tag{1.52}$$

Equation (1.51), with $w = 1$, which we now prove, is known as the ***BAC–CAB* rule**. Since Eq. (1.52) is linear in A, B, and C, w is independent of these magnitudes. That is, we only need to show that $w = 1$ for unit vectors $\hat{\mathbf{A}}$, $\hat{\mathbf{B}}$, $\hat{\mathbf{C}}$. Let us denote $\hat{\mathbf{B}} \cdot \hat{\mathbf{C}} = \cos\alpha$, $\hat{\mathbf{C}} \cdot \hat{\mathbf{A}} = \cos\beta$, $\hat{\mathbf{A}} \cdot \hat{\mathbf{B}} = \cos\gamma$, and square Eq. (1.52) to obtain

$$\begin{aligned}
[\hat{\mathbf{A}} \times (\hat{\mathbf{B}} \times \hat{\mathbf{C}})]^2 &= \hat{\mathbf{A}}^2(\hat{\mathbf{B}} \times \hat{\mathbf{C}})^2 - [\hat{\mathbf{A}} \cdot (\hat{\mathbf{B}} \times \hat{\mathbf{C}})]^2 \\
&= 1 - \cos^2\alpha - [\hat{\mathbf{A}} \cdot (\hat{\mathbf{B}} \times \hat{\mathbf{C}})]^2 \\
&= w^2[(\hat{\mathbf{A}} \cdot \hat{\mathbf{C}})^2 + (\hat{\mathbf{A}} \cdot \hat{\mathbf{B}})^2 - 2\hat{\mathbf{A}} \cdot \hat{\mathbf{B}}\,\hat{\mathbf{A}} \cdot \hat{\mathbf{C}}\,\hat{\mathbf{B}} \cdot \hat{\mathbf{C}}] \\
&= w^2(\cos^2\beta + \cos^2\gamma - 2\cos\alpha\cos\beta\cos\gamma),
\end{aligned} \tag{1.53}$$

using $(\hat{\mathbf{A}} \times \hat{\mathbf{B}})^2 = \hat{\mathbf{A}}^2\hat{\mathbf{B}}^2 - (\hat{\mathbf{A}} \cdot \hat{\mathbf{B}})^2$ repeatedly. Consequently, the (squared) volume spanned by $\hat{\mathbf{A}}$, $\hat{\mathbf{B}}$, $\hat{\mathbf{C}}$ that occurs in Eq. (1.53) can be written as

$$[\hat{\mathbf{A}} \cdot (\hat{\mathbf{B}} \times \hat{\mathbf{C}})]^2 = 1 - \cos^2\alpha - w^2(\cos^2\beta + \cos^2\gamma - 2\cos\alpha\cos\beta\cos\gamma).$$

Here, we must have $w^2 = 1$ because this volume is symmetric in α, β, γ. That is, $w = \pm 1$ and is independent of $\hat{\mathbf{A}}$, $\hat{\mathbf{B}}$, $\hat{\mathbf{C}}$. Again using the special case $\hat{\mathbf{x}} \times (\hat{\mathbf{x}} \times \hat{\mathbf{y}}) = -\hat{\mathbf{y}}$ in Eq. (1.51) finally gives $w = 1$.

An alternate and easier algebraic derivation using the Levi-Civita ε_{ijk} of Chapter 2 is the topic of Exercise 2.9.8.

Note that because vectors are independent of the coordinates, a vector equation is independent of the particular coordinate system. The coordinate system only determines the components. If the vector equation can be established in Cartesian coordinates, it is established and valid in any of the coordinate systems, as will be shown in Chapter 2. Thus, Eq. (1.52) may be verified by a direct though not very elegant method of expanding into Cartesian components (see Exercise 1.4.1).

Other, more complicated, products may be simplified by using these forms of the triple scalar and triple vector products.

SUMMARY

We have developed the geometric meaning of the triple scalar product as a volume spanned by three vectors and exhibited its component form that is directly related to a determinant whose entries are the Cartesian components of the vectors.

The main property of the triple vector product is its decomposition expressed in the *BAC–CAB* rule. It plays a role in electrodynamics, a vector field theory in which cross products abound.

EXERCISES

1.4.1 Verify the expansion of the triple vector product

$$\mathbf{A} \times (\mathbf{B} \times \mathbf{C}) = \mathbf{B}(\mathbf{A} \cdot \mathbf{C}) - \mathbf{C}(\mathbf{A} \cdot \mathbf{B})$$

by direct expansion in Cartesian coordinates.

1.4.2 Show that the first step in Eq. (1.43),

$$(\mathbf{A} \times \mathbf{B}) \cdot (\mathbf{A} \times \mathbf{B}) = A^2B^2 - (\mathbf{A} \cdot \mathbf{B})^2,$$

is consistent with the $BAC–CAB$ rule for a triple vector product.

1.4.3 The orbital angular momentum $\mathbf{L}$ of a particle is given by $\mathbf{L} = \mathbf{r} \times \mathbf{p} = m\mathbf{r} \times \mathbf{v}$, where $\mathbf{p}$ is the linear momentum. With linear and angular velocity related by $\mathbf{v} = \boldsymbol{\omega} \times \mathbf{r}$, show that

$$\mathbf{L} = mr^2[\boldsymbol{\omega} - \hat{\mathbf{r}}(\hat{\mathbf{r}} \cdot \boldsymbol{\omega})],$$

where $\hat{\mathbf{r}}$ is a unit vector in the $\mathbf{r}$ direction. For $\mathbf{r} \cdot \boldsymbol{\omega} = 0$, this reduces to $\mathbf{L} = I\boldsymbol{\omega}$, with the moment of inertia I given by mr^2.

1.4.4 The kinetic energy of a single particle is given by $T = \frac{1}{2}mv^2$. For rotational motion this becomes $\frac{1}{2}m(\boldsymbol{\omega} \times \mathbf{r})^2$. Show that

$$T = \frac{1}{2}m[r^2\omega^2 - (\mathbf{r} \cdot \boldsymbol{\omega})^2].$$

For $\mathbf{r} \cdot \boldsymbol{\omega} = 0$, this reduces to $T = \frac{1}{2}I\omega^2$, with the moment of inertia I given by mr^2.

1.4.5 Show that

$$\mathbf{a} \times (\mathbf{b} \times \mathbf{c}) + \mathbf{b} \times (\mathbf{c} \times \mathbf{a}) + \mathbf{c} \times (\mathbf{a} \times \mathbf{b}) = 0.^{6}$$

1.4.6 A vector $\mathbf{A}$ is decomposed into a radial vector $\mathbf{A}_r$ and a tangential vector $\mathbf{A}_t$. If $\hat{\mathbf{r}}$ is a unit vector in the radial direction, show that
(a) $\mathbf{A}_r = \hat{\mathbf{r}}(\mathbf{A} \cdot \hat{\mathbf{r}})$ and
(b) $\mathbf{A}_t = -\hat{\mathbf{r}} \times (\hat{\mathbf{r}} \times \mathbf{A})$.

1.4.7 Prove that a necessary and sufficient condition for the three (nonvanishing) vectors $\mathbf{A}$, $\mathbf{B}$, and $\mathbf{C}$ to be coplanar is the vanishing of the triple scalar product

$$\mathbf{A} \cdot \mathbf{B} \times \mathbf{C} = 0.$$

1.4.8 Vector $\mathbf{D}$ is a linear combination of three noncoplanar (and nonorthogonal) vectors:

$$\mathbf{D} = a\mathbf{A} + b\mathbf{B} + c\mathbf{C}.$$

Show that the coefficients are given by a ratio of triple scalar products,

$$a = \frac{\mathbf{D} \cdot \mathbf{B} \times \mathbf{C}}{\mathbf{A} \cdot \mathbf{B} \times \mathbf{C}}, \quad \text{and so on.}$$

If symbolic software is available, evaluate numerically the triple scalar products and coefficients for a typical case.

1.4.9 Show that

$$(\mathbf{A} \times \mathbf{B}) \cdot (\mathbf{C} \times \mathbf{D}) = (\mathbf{A} \cdot \mathbf{C})(\mathbf{B} \cdot \mathbf{D}) - (\mathbf{A} \cdot \mathbf{D})(\mathbf{B} \cdot \mathbf{C}).$$

1.4.10 Show that

$$(\mathbf{A} \times \mathbf{B}) \times (\mathbf{C} \times \mathbf{D}) = (\mathbf{A} \cdot \mathbf{B} \times \mathbf{D})\mathbf{C} - (\mathbf{A} \cdot \mathbf{B} \times \mathbf{C})\mathbf{D}.$$

1.4.11 Given

$$\mathbf{a}' = \frac{\mathbf{b} \times \mathbf{c}}{\mathbf{a} \cdot \mathbf{b} \times \mathbf{c}}, \quad \mathbf{b}' = \frac{\mathbf{c} \times \mathbf{a}}{\mathbf{a} \cdot \mathbf{b} \times \mathbf{c}}, \quad \mathbf{c}' = \frac{\mathbf{a} \times \mathbf{b}}{\mathbf{a} \cdot \mathbf{b} \times \mathbf{c}},$$

and $\mathbf{a} \cdot \mathbf{b} \times \mathbf{c} \neq 0$, show that
(a) $\mathbf{x}' \cdot \mathbf{y}' = 0$ (if $\mathbf{x} \neq \mathbf{y}$) and $\mathbf{x}' \cdot \mathbf{y}' = 1$ (if $\mathbf{x} = \mathbf{y}$), for ($\mathbf{x}$, $\mathbf{y} = \mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$),
(b) $\mathbf{a}' \cdot \mathbf{b}' \times \mathbf{c}' = (\mathbf{a} \cdot \mathbf{b} \times \mathbf{c})^{-1}$,
(c) $\mathbf{a} = \frac{\mathbf{b}' \times \mathbf{c}'}{\mathbf{a}' \cdot \mathbf{b}' \times \mathbf{c}'}$.

1.4.12 If $\mathbf{x}' \cdot \mathbf{y}' = 0$ if $\mathbf{x} \neq \mathbf{y}$ and $\mathbf{x}' \cdot \mathbf{y}' = 1$ if $\mathbf{x} = \mathbf{y}$, for ($\mathbf{x}$, $\mathbf{y} = \mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$), prove that

$$\mathbf{a}' = \frac{\mathbf{b} \times \mathbf{c}}{\mathbf{a} \cdot \mathbf{b} \times \mathbf{c}}.$$

(This is the converse of Problem 1.4.11.)

[6] This is Jacobi's identity for vector products.

1.4.13 Show that any vector $\mathbf{V}$ may be expressed in terms of the reciprocal vectors $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$ (of Problem 1.4.11) by

$$\mathbf{V} = (\mathbf{V}\cdot\mathbf{a})\,\mathbf{a}' + (\mathbf{V}\cdot\mathbf{b})\,\mathbf{b}' + (\mathbf{V}\cdot\mathbf{c})\,\mathbf{c}'.$$

1.4.14 An electric charge q_1 moving with velocity $\mathbf{v}_1$ produces a magnetic induction $\mathbf{B}$ given by

$$\mathbf{B} = \frac{\mu_0}{4\pi} q_1 \frac{\mathbf{v}_1 \times \hat{\mathbf{r}}}{r^2} \quad \text{(SI units)},$$

where $\hat{\mathbf{r}}$ points from q_1 to the point at which $\mathbf{B}$ is measured (Biot and Savart's law).

(a) Show that the magnetic force on a second charge q_2, velocity $\mathbf{v}_2$, is given by the triple vector product

$$\mathbf{F}_2 = \frac{\mu_0}{4\pi}\frac{q_1 q_2}{r^2}\mathbf{v}_2 \times (\mathbf{v}_1 \times \hat{\mathbf{r}}).$$

(b) Write out the corresponding magnetic force $\mathbf{F}_1$ that q_2 exerts on q_1. Define your unit radial vector. How do $\mathbf{F}_1$ and $\mathbf{F}_2$ compare?

(c) Calculate $\mathbf{F}_1$ and $\mathbf{F}_2$ for the case of q_1 and q_2 moving along parallel trajectories side by side.

ANS.

(b) $\mathbf{F}_1 = -\dfrac{\mu_0}{4\pi}\dfrac{q_1 q_2}{r^2}\mathbf{v}_1 \times (\mathbf{v}_2 \times \hat{\mathbf{r}})$.

(c) $\mathbf{F}_1 = \dfrac{\mu_0}{4\pi}\dfrac{q_1 q_2}{r^2} v^2 \hat{\mathbf{r}} = -\mathbf{F}_2$.

1.5 Gradient, ∇

Partial Derivatives

In this section, we deal with derivatives of functions of several variables that will lead us to the concept of directional derivative or gradient operator, which is of central importance in mechanics, electrodynamics, and engineering.

We can view a function $z = \varphi(x, y)$ of two variables geometrically as a surface over the xy-plane in three-dimensional Euclidean space because for each point (x, y) we find the z value from φ. For a fixed value y then, $z = \varphi(x, y) \equiv f(x)$ is a function of x only, viz. a curve on the intersection of the surface with the xz-plane going through y. The slope of this curve,

$$\frac{df}{dx} \equiv \frac{\partial\varphi(x, y)}{\partial x} = \lim_{h\to 0}\frac{\varphi(x+h, y) - \varphi(x, y)}{h}, \tag{1.54}$$

is the **partial derivative** of φ with respect to x defined with the understanding that the other variable y is held fixed. It is useful for drawing tangents and locating a maximum or minimum on the curve where the slope is zero. The partial derivative $\partial\varphi/\partial y$ is similarly defined holding x fixed (i.e., it is the slope of the surface in the y-direction), and so on for the higher partial derivatives.

EXAMPLE 1.5.1

Error Estimate Error estimates usually involve many partial derivatives. Let us calculate the moment of inertia of a rectangular slab of metal of length $a = 10 \pm 1$ cm, width $b = 15 \pm 2$ cm, and height $c = 5 \pm 1$ cm about an axis through its center of gravity and perpendicular to the area ab and estimate the error. The uniform density is $\rho = 5 \pm 0.1$ g/cm^3. The moment of inertia is given by

$$\begin{aligned} I &= \rho \int (x^2 + y^2)\, d\tau = \rho c \left(\int_{-a/2}^{a/2} x^2\, dx \int_{-b/2}^{b/2} dy + \int_{-a/2}^{a/2} dx \int_{-b/2}^{b/2} y^2\, dy \right) \\ &= \frac{\rho c}{3} 2 \left(b \left(\frac{a}{2} \right)^3 + a \left(\frac{b}{2} \right)^3 \right) = \frac{\rho abc}{12} (a^2 + b^2) \qquad (1.55) \\ &= \frac{1}{2} 5^6 (4 + 9)\ \text{g cm}^2 = 10.15625 \times 10^{-3}\ \text{kg m}^2, \end{aligned}$$

where $d\tau = cdxdy$ has been used.

The corresponding error in I derives from the errors in all variables, each being weighted by the corresponding partial derivative,

$$(\Delta I)^2 = \left(\frac{\partial I}{\partial \rho} \right)^2 (\Delta \rho)^2 + \left(\frac{\partial I}{\partial a} \right)^2 (\Delta a)^2 + \left(\frac{\partial I}{\partial b} \right)^2 (\Delta b)^2 + \left(\frac{\partial I}{\partial c} \right)^2 (\Delta c)^2,$$

where Δx is the error in the variable x, that is, $\Delta a = 1$ cm, etc. The partial derivatives

$$\begin{aligned} \frac{\partial I}{\partial \rho} &= \frac{abc}{12}(a^2 + b^2), & \frac{\partial I}{\partial a} &= \frac{\rho bc}{12}(3a^2 + b^2), \\ \frac{\partial I}{\partial b} &= \frac{\rho ac}{12}(a^2 + 3b^2), & \frac{\partial I}{\partial c} &= \frac{\rho ab}{12}(a^2 + b^2) \qquad (1.56) \end{aligned}$$

are obtained from Eq. (1.55). Substituting the numerical values of all parameters, we get

$$\begin{aligned} \frac{\partial I}{\partial \rho} \Delta\rho &= 0.203125 \times 10^{-3}\ \text{kg m}^2, & \frac{\partial I}{\partial a} \Delta a &= 1.640625 \times 10^{-3}\ \text{kg m}^2, \\ \frac{\partial I}{\partial b} \Delta b &= 3.2291667 \times 10^{-3}\ \text{kg m}^2, & \frac{\partial I}{\partial c} \Delta c &= 2.03125 \times 10^{-3}\ \text{kg m}^2. \end{aligned}$$

Squaring and summing up, we find $\Delta I = 4.1577 \times 10^{-3}$ kg m^2. This error of more than 40% of the value I is much higher than the largest error $\Delta c \sim 20\%$ of the variables on which I depends and shows how errors in several variables can add up. Thus, all decimals except the first one can be dropped safely. ■

EXAMPLE 1.5.2

Partials of a Plane Let us now take a plane $F(\mathbf{r}) = \mathbf{n} \cdot \mathbf{r} - d = 0$ that cuts the coordinate axes at $x = 1$, $y = 2$, $z = 3$ so that $n_x = d$, $2n_y = d$, $3n_z = d$. Because the normal $\mathbf{n}^2 = 1$, we have the constraint $d^2(1 + \frac{1}{4} + \frac{1}{9}) = 1$ so that

$d = 6/7$. Hence, the partial derivatives

$$\frac{\partial F}{\partial x} = n_x = 6/7, \quad \frac{\partial F}{\partial y} = n_y = 3/7, \quad \frac{\partial F}{\partial z} = n_z = 2/7$$

are the components of a vector **n** (the normal) for our plane $6x + 3y + 2z = 6$. This suggests the partial derivatives of any function F are a vector. ■

To provide more motivation for the vector nature of the partial derivatives, we now introduce the **total variation of a function** $F(x, y)$,

$$dF = \frac{\partial F}{\partial x}dx + \frac{\partial F}{\partial y}dy. \tag{1.57}$$

It consists of independent variations in the x- and y-directions. We write dF as a sum of two increments, one purely in the x- and the other in the y-direction,

$$\begin{aligned} dF(x, y) \equiv F(x + dx, y + dy) - F(x, y) &= [F(x + dx, y + dy) - F(x, y + dy)] \\ &+ [F(x, y + dy) - F(x, y)] = \frac{\partial F}{\partial x}dx + \frac{\partial F}{\partial y}dy, \end{aligned}$$

by adding and subtracting $F(x, y + dy)$. The mean value theorem (i.e., continuity of F) tells us that here $\partial F/\partial x$, $\partial F/\partial y$ are evaluated at some point ξ, η between x and $x + dx$, y and $y + dy$, respectively. As $dx \to 0$ and $dy \to 0$, $\xi \to x$ and $\eta \to y$. This result generalizes to three and higher dimensions. For example, for a function φ of three variables,

$$\begin{aligned} d\varphi(x, y, z) \equiv\ & [\varphi(x + dx, y + dy, z + dz) - \varphi(x, y + dy, z + dz)] \\ &+ [\varphi(x, y + dy, z + dz) - \varphi(x, y, z + dz)] \\ &+ [\varphi(x, y, z + dz) - \varphi(x, y, z)] \\ =\ & \frac{\partial \varphi}{\partial x}dx + \frac{\partial \varphi}{\partial y}dy + \frac{\partial \varphi}{\partial z}dz. \end{aligned} \tag{1.58}$$

Note that if F is a scalar function, dF is also a scalar and the form of Eq. (1.57) suggests an interpretation as a scalar product of the coordinate displacement vector $d\mathbf{r} = (dx, dy)$ with the partial derivatives of F; the same holds for $d\varphi$ in three dimensions. These observations pave the way for the gradient in the next section.

As an application of the total variation, we consider the slope of an implicitly defined curve $F(x, y) = 0$, a general theorem that we postponed in Section 1.3. Because also $dF = 0$ on the curve, we find the slope of the curve

$$\frac{dy}{dx} = -\frac{\frac{\partial F}{\partial x}}{\frac{\partial F}{\partial y}} \tag{1.59}$$

from Eq. (1.57). Compare this result with $\dot{y}/\dot{x}$ for the slope of a curve defined in terms of two functions $x(t)$, $y(t)$ of time t in Section 1.2.

Often, we are confronted with more difficult problems of finding a slope given some constraint. A case in point is the next example.

EXAMPLE 1.5.3

Extremum under a Constraint Find the points of shortest (or longest) distance from the origin on the curve $G(x, y) \equiv x^2 + xy + y^2 - 1 = 0$.

From analytic geometry we know that the points on such a quadratic form with center at the origin (there are no terms linear in x or y that would shift the center) represent a conic section. But which kind? To answer this question, note that $(x + y)^2 = x^2 + 2xy + y^2 \geq 0$ implies that $xy \geq -(x^2 + y^2)/2$ so that the quadratic form is positive definite, that is, $G(x, y) + 1 \geq 0$, and G must therefore be an ellipse (Fig. 1.22). Hence, our problem is equivalent to finding the orientation of its principal axes (see Section 3.5 for the alternative matrix diagonalization method). The square of the distance from the origin is defined by the function $F(x, y) = x^2 + y^2$, subject to the constraint that the point (x, y) lie on the ellipse defined by G. The constraint G defines $y = y(x)$. Therefore, we look for the solutions of

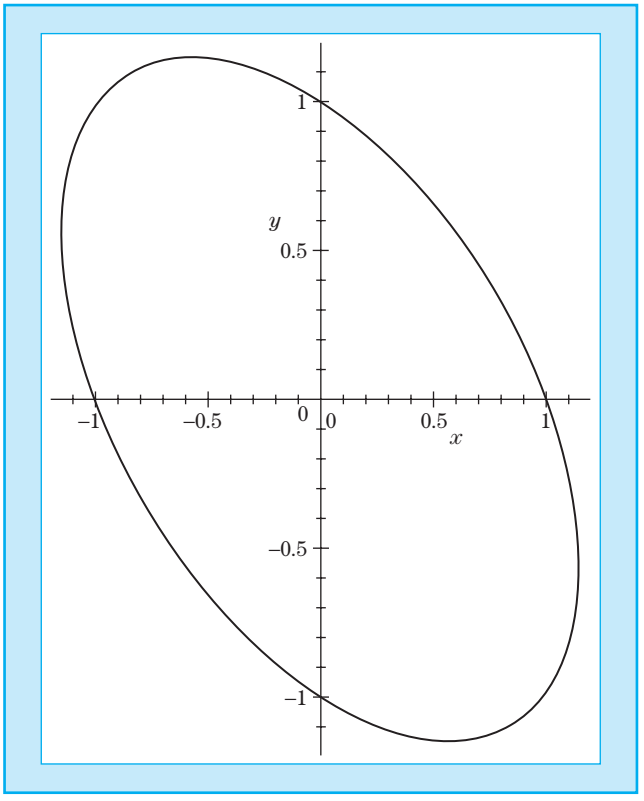
$$0 = \frac{dF(x, y(x))}{dx} = 2x + 2y\frac{dy}{dx}.$$

Differentiating G, we find

$$y' = -\frac{2x + y}{2y + x} \text{ from } 2x + y + xy' + 2yy' = 0,$$

Figure 1.22

The Ellipse $x^2 + xy + y^2 = 1$



which we substitute into our min/max condition $dF/dx = 0$. This yields

$$x(2y + x) = y(2x + y), \quad \text{or} \quad y = \pm x.$$

Substituting $x = y$ into G gives the solutions $x = \pm 1/\sqrt{3}$, while $x = -y$ yields the points $x = \pm 1$ on the ellipse. Substituting $x = 1$ into G gives $y = 0$ and $y = -1$, while $x = -1$ yields $y = 0$ and $y = 1$. Although the points $(x, y) = (1, 0), (-1, 0)$ lie on the ellipse, their distance $(= 1)$ from the origin is neither shortest nor longest. However, the points $(1, -1), (-1, 1)$ have the longest distance $(= \sqrt{2})$ and define the line $x + y = 0$ through the origin (at $135°$) as a principal axis. The points $(1/\sqrt{3}, 1/\sqrt{3}), (-1/\sqrt{3}, -1/\sqrt{3})$ define the line at $45°$ through the origin as the second principal axis that is orthogonal to the first axis.

It is also instructive to apply the slope formula (1.59) at the intersection points of the principal axes and the ellipse, that is, $(\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}), (1, -1)$. The partial derivatives there are given by $G_x \equiv \frac{\partial G}{\partial x} = 2x + y = \frac{3}{\sqrt{3}} = \sqrt{3}$ and $2 - 1 = 1$, respectively, $G_y \equiv \frac{\partial G}{\partial y} = 2y + x = \frac{3}{\sqrt{3}} = \sqrt{3}$ and $-2 + 1 = -1$, so that the slopes become $-G_x/G_y = -\frac{\sqrt{3}}{\sqrt{3}} = -1$ equal to that of the principal axis $x + y = 0$, and $-1/(-1) = 1$ equal to that of the other principal axis $x - y = 0$. ■

Although this problem was straightforward to solve, there is the more elegant **Lagrange multiplier method** for finding a maximum or minimum of a function $F(x, y)$ subject to a constraint $G(x, y) = 0$.

Introducing a Lagrange multiplier λ helps us avoid the direct (and often messy algebraic) solution for x and y as follows. Because we look for the solution of

$$dF = \frac{\partial F}{\partial x}dx + \frac{\partial F}{\partial y}dy = 0, \qquad dG = \frac{\partial G}{\partial x}dx + \frac{\partial G}{\partial y}dy = 0, \tag{1.60}$$

we can solve for the slope dy/dx from one equation and substitute that solution into the other one. Equivalently, we use the function $F + \lambda G$ of three variables x, y, λ, and solve

$$d(F + \lambda G) = \left(\frac{\partial F}{\partial x} + \lambda\frac{\partial G}{\partial x}\right)dx + \left(\frac{\partial F}{\partial y} + \lambda\frac{\partial G}{\partial y}\right)dy + \frac{\partial(F + \lambda G)}{\partial \lambda}d\lambda = 0$$

by choosing λ to satisfy $\frac{\partial F}{\partial y} + \lambda\frac{\partial G}{\partial y} = 0$, for example, and then eliminating the last term by the constraint $G = 0$ (note that F does not depend on λ) so that $\frac{\partial F}{\partial x} + \lambda\frac{\partial G}{\partial x} = 0$ follows. Including the constraint, we now have three equations for three unknowns x, y, λ, where the slope λ is not usually needed.

EXAMPLE 1.5.4

Lagrange Multiplier Method Let us illustrate the method by solving Example 1.5.3 again, this time using the Lagrange multiplier method. The x

and y partial derivative equations of the Lagrange multiplier method are given by

$$\frac{\partial F}{\partial x} + \lambda \frac{\partial G}{\partial x} \equiv 2x + \lambda(2x + y) = 0,$$
$$\frac{\partial F}{\partial y} + \lambda \frac{\partial G}{\partial y} \equiv 2y + \lambda(2y + x) = 0.$$

We find for the ratio $\xi \equiv y/x = -2(\lambda + 1)/\lambda$ and $\xi = -\lambda/2(1 + \lambda)$, that is, $\xi = 1/\xi$, or $\xi = \pm 1$, so that the principal axes are along the lines $x + y = 0$ and $x - y = 0$ through the origin. Substituting these solutions into the conic section G yields $x = 1/\sqrt{3} = y$ and $x = 1 = -y$, respectively. Contrast this simple, yet sophisticated approach with our previous lengthy solution. ■

Biographical Data

Lagrange, Joseph Louis comte de. Lagrange, a French mathematician and physicist, was born in Torino to a wealthy French-Italian family in 1736 and died in Paris in 1813. While in school, an essay on calculus by the English astronomer Halley sparked his enthusiasm for mathematics. In 1755, he became a professor in Torino. In 1766, he succeeded L. Euler (who moved to St. Petersburg to serve Catherine the Great) as director of the mathematics–physics section of the Prussian Academy of Sciences in Berlin. In 1786, he left Berlin for Paris after the death of king Frederick the Great. He was the founder of analytical mechanics. His famous book, *Mécanique Analytique*, contains not a single geometric figure.

Gradient as a Vector Operator

The **total variation** $dF(x, y)$ in Eq. (1.57) looks like a scalar product of the incremental length vector $d\mathbf{r} = (dx, dy)$ with a vector $(\frac{\partial F}{\partial x}, \frac{\partial F}{\partial y})$ of partial derivatives in two dimensions, that is, the change of F depends on the direction in which we go. For example, F could be a wave function in quantum mechanics or describe a temperature distribution in space. When we are at the peak value, the height will fall off at different rates in different directions, just like a ski slope: One side might be for beginners, whereas another has only expert runs. When we generalize this to a function $\varphi(x, y, z)$ of three variables, we obtain Eq. (1.58),

$$d\varphi = \frac{\partial \varphi}{\partial x}\, dx + \frac{\partial \varphi}{\partial y}\, dy + \frac{\partial \varphi}{\partial z}\, dz, \tag{1.61}$$

for the total change in the scalar function φ consisting of additive contributions of each coordinate change corresponding to a change in position

$$d\mathbf{r} = \hat{\mathbf{x}}\, dx + \hat{\mathbf{y}}\, dy + \hat{\mathbf{z}}\, dz, \tag{1.62}$$

the increment of length $d\mathbf{r}$. Algebraically, $d\varphi$ in Eq. (1.58) is a scalar product of the change in position $d\mathbf{r}$ and the **directional** change of φ. Now we are ready to recognize the three-dimensional partial derivative as a vector, which leads

us to the concept of gradient. A convenient notation is

$$\nabla \equiv \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}\right) = \hat{\mathbf{x}}\frac{\partial}{\partial x} + \hat{\mathbf{y}}\frac{\partial}{\partial y} + \hat{\mathbf{z}}\frac{\partial}{\partial z}, \tag{1.63}$$

$$\nabla\varphi = \hat{\mathbf{x}}\frac{\partial\varphi}{\partial x} + \hat{\mathbf{y}}\frac{\partial\varphi}{\partial y} + \hat{\mathbf{z}}\frac{\partial\varphi}{\partial z}, \tag{1.64}$$

so that ∇ (del) is a vector that differentiates (scalar) functions. As such, it is a **vector operator**. All the relations for ∇ can be derived from the hybrid nature of del in terms of both the partial derivatives and its vector nature.

The gradient of a scalar is extremely important in physics and engineering in expressing the relation between a force field and a potential field

$$\text{force } \mathbf{F} = -\nabla(\text{ potential } V), \tag{1.65}$$

which holds for both gravitational and electrostatic fields, among others. Note that the minus sign in Eq. (1.65) results in water flowing downhill rather than uphill. If a force can be described as in Eq. (1.65) by a single function $V(\mathbf{r})$ everywhere, we call the scalar function V its **potential**. Because the force is the directional derivative of the potential, we can find the potential, if it exists, by integrating the force along a suitable path. Because the total variation $dV = \nabla V \cdot d\mathbf{r} = -\mathbf{F} \cdot d\mathbf{r}$ is the work done against the force along the path $d\mathbf{r}$, we recognize the physical meaning of the potential (difference) as work and energy. Moreover, in a sum of path increments the intermediate points cancel,

$$\begin{aligned}&[V(\mathbf{r} + d\mathbf{r}_1 + d\mathbf{r}_2) - V(\mathbf{r} + d\mathbf{r}_1)] + [V(\mathbf{r} + d\mathbf{r}_1) - V(\mathbf{r})]\\ &\quad = V(\mathbf{r} + d\mathbf{r}_2 + d\mathbf{r}_1) - V(\mathbf{r}),\end{aligned}$$

so that the integrated work along some path from an initial point $\mathbf{r}_i$ to a final point $\mathbf{r}$ is given by the potential difference $V(\mathbf{r}) - V(\mathbf{r}_i)$ at the end points of the path. Therefore, such forces are especially simple and well behaved: They are called **conservative**. When there is loss of energy due to friction along the path or some other dissipation, the work will depend on the path and such forces cannot be conservative: No potential exists. We discuss conservative forces in more detail in Section 1.12.

EXAMPLE 1.5.5

The Gradient of a Function of r Because we often deal with **central forces** in physics and engineering, we start with the gradient of the radial distance $r = \sqrt{x^2 + y^2 + z^2}$. From r as a function of x, y, z,

$$\frac{\partial r}{\partial x} = \frac{\partial(x^2 + y^2 + z^2)^{1/2}}{\partial x} = \frac{x}{(x^2 + y^2 + z^2)^{1/2}} = \frac{x}{r},$$

etc. Now we can calculate the more general gradient of a spherically symmetric potential $f(r)$ of a central force law so that

$$\nabla f(r) = \hat{\mathbf{x}}\frac{\partial f(r)}{\partial x} + \hat{\mathbf{y}}\frac{\partial f(r)}{\partial y} + \hat{\mathbf{z}}\frac{\partial f(r)}{\partial z}, \tag{1.66}$$

where $f(r)$ depends on x through the dependence of r on x. Therefore[7],

$$\frac{\partial f(r)}{\partial x} = \frac{df(r)}{dr} \cdot \frac{\partial r}{\partial x}.$$

Therefore,

$$\frac{\partial f(r)}{\partial x} = \frac{df(r)}{dr} \cdot \frac{x}{r}. \tag{1.67}$$

Permuting coordinates ($x \to y$, $y \to z$, $z \to x$) to obtain the y and z derivatives, we get

$$\nabla f(r) = (\hat{\mathbf{x}}x + \hat{\mathbf{y}}y + \hat{\mathbf{z}}z)\frac{1}{r}\frac{df}{dr} = \frac{\mathbf{r}}{r}\frac{df}{dr} = \hat{\mathbf{r}}\frac{df}{dr}, \tag{1.68}$$

where $\hat{\mathbf{r}}$ is a unit vector ($\mathbf{r}/r$) in the **positive** radial direction. The gradient of a function of r is a vector in the (positive or negative) radial direction. ■

A Geometrical Interpretation

Example 1.5.2 illustrates the geometric meaning of the gradient of a plane: It is its normal vector. This is a special case of the general geometric meaning of the gradient of an implicitly defined surface $\varphi(\mathbf{r}) = \text{const}$. Consider P and Q to be two points on a surface $\varphi(x, y, z) = C$, a constant. If φ is a potential, the surface is an **equipotential surface**. These points are chosen so that Q is a distance $d\mathbf{r}$ from P. Then, moving from P to Q, the change in $\varphi(x, y, z)$, given by Eq. (1.58) that is now written in vector notation, must be

$$d\varphi = (\nabla\varphi) \cdot d\mathbf{r} = 0 \tag{1.69}$$

since we stay on the surface $\varphi(x, y, z) = C$. This shows that $\nabla\varphi$ is perpendicular to $d\mathbf{r}$. Since $d\mathbf{r}$ may have any direction from P **as long as it stays in the surface** $\varphi = \text{const.}$, the point Q being restricted to the surface but having arbitrary direction, $\nabla\varphi$ is seen as **normal to the surface** $\varphi = \text{const.}$ (Fig. 1.23).

If we now permit $d\mathbf{r}$ to take us from one surface $\varphi = C_1$ to an adjacent surface $\varphi = C_2$ (Fig. 1.24),

$$d\varphi = C_1 - C_2 = \Delta C = (\nabla\varphi) \cdot d\mathbf{r}. \tag{1.70}$$

For a given $d\varphi$, $|d\mathbf{r}|$ is a minimum when it is chosen parallel to $\nabla\varphi$ ($\cos\theta = 1$); for a given $|d\mathbf{r}|$, the change in the scalar function φ is maximized by choosing $d\mathbf{r}$ parallel to $\nabla\varphi$. **This identifies $\nabla\varphi$ as a vector having the direction of the maximum space rate of change of** φ, an identification that will be useful in Chapter 2 when we consider non-Cartesian coordinate systems.

[7] This is a special case of the **chain rule** generalized to partial derivatives:

$$\frac{\partial f(r, \theta, \varphi)}{\partial x} = \frac{\partial f}{\partial r}\frac{\partial r}{\partial x} + \frac{\partial f}{\partial \theta}\frac{\partial \theta}{\partial x} + \frac{\partial f}{\partial \varphi}\frac{\partial \varphi}{\partial x},$$

where $\partial f/\partial\theta = \partial f/\partial\varphi = 0$, $\partial f/\partial r \to df/dr$.

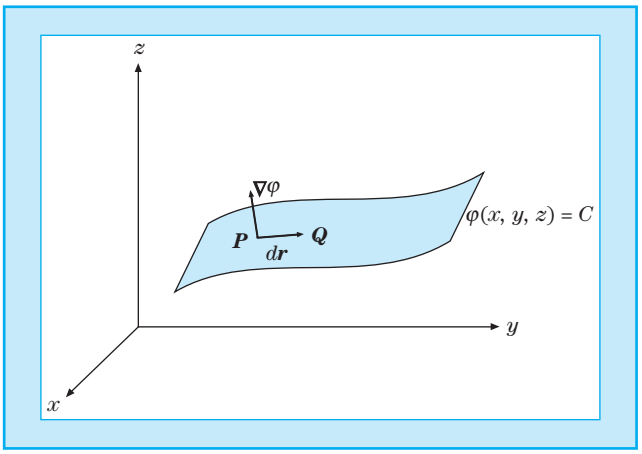


Figure 1.23

The Length Increment *dr* is Required to Stay on the Surface $\varphi = C$

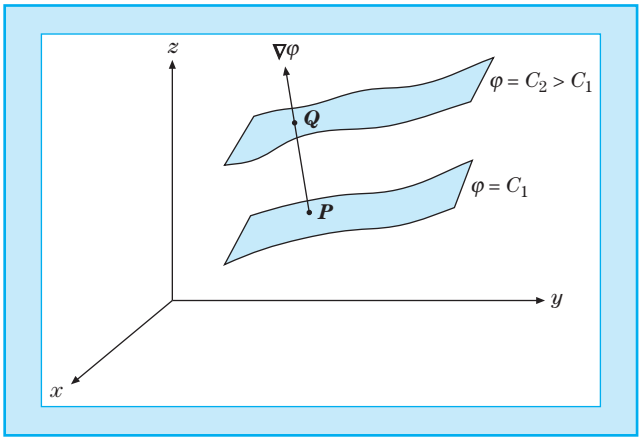


Figure 1.24

Gradient

SUMMARY

We have constructed the gradient operator as a vector of derivatives. The total variation of a function is the dot product of its gradient with the coordinate displacement vector. A conservative force is the (negative) gradient of a scalar called its potential.

EXERCISES

1.5.1 The dependence of the free fall acceleration g on geographical latitude ϕ at sea level is given by $g = g_0(1+0.0053\sin^2\phi)$. What is the southward displacement near $\phi = 30^\circ$ that changes g by 1 part in 10^8?

1.5.2 Given a vector $\mathbf{r}_{12} = \hat{\mathbf{x}}(x_1 - x_2) + \hat{\mathbf{y}}(y_1 - y_2) + \hat{\mathbf{z}}(z_1 - z_2)$, show that $\nabla_1 r_{12}$ (gradient with respect to x_1, y_1, and z_1, of the magnitude r_{12}) is a unit vector in the direction of r_{12}. Note that a central force and a potential may depend on r_{12}.

1.5.3 If a vector function $\mathbf{F}$ depends on both space coordinates (x, y, z) and time t, show that

$$d\mathbf{F} = (d\mathbf{r} \cdot \nabla)\mathbf{F} + \frac{\partial \mathbf{F}}{\partial t}\, dt.$$

1.5.4 Show that $\nabla(uv) = v\nabla u + u\nabla v$, where u and v are differentiable scalar functions of x, y, and z (product rule).

(a) Show that a necessary and sufficient condition that $u(x, y, z)$ and $v(x, y, z)$ are related by some function $f(u, v) = 0$ is that $(\nabla u) \times (\nabla v) = 0$. Describe this geometrically. If graphical software is available, plot a typical case.

(b) If $u = u(x, y)$ and $v = v(x, y)$, show that the condition $(\nabla u) \times (\nabla v) = 0$ leads to the two-dimensional Jacobian

$$J\left(\frac{u, v}{x, y}\right) = \begin{vmatrix} \frac{\partial u}{\partial x} & \frac{\partial u}{\partial y} \\ \frac{\partial v}{\partial x} & \frac{\partial v}{\partial y} \end{vmatrix} = \frac{\partial u}{\partial x}\frac{\partial v}{\partial y} - \frac{\partial u}{\partial y}\frac{\partial v}{\partial x} = 0.$$

The functions u and v are assumed differentiable.

1.6 Divergence, ∇

In Section 1.5, ∇ was defined as a vector operator. Now, paying careful attention to both its vector and its differential properties, we let it operate on a vector. First, as a vector we dot it into a second vector to obtain

$$\nabla \cdot \mathbf{V} = \frac{\partial V_x}{\partial x} + \frac{\partial V_y}{\partial y} + \frac{\partial V_z}{\partial z}, \tag{1.71}$$

known as the divergence of $\mathbf{V}$, which we expect to be a scalar.

EXAMPLE 1.6.1

Divergence of a Central Force Field From Eq. (1.71) we obtain for the coordinate vector with radial outward flow

$$\nabla \cdot \mathbf{r} = \frac{\partial x}{\partial x} + \frac{\partial y}{\partial y} + \frac{\partial z}{\partial z} = 3. \tag{1.72}$$

Because the gravitational (or electric) force of a mass (or charge) at the origin is proportional to $\mathbf{r}$ with a radial $1/r^3$ dependence, we also consider the more general and important case of the divergence of a central force field

$$\begin{aligned} \nabla \cdot \mathbf{r} f(r) &= \frac{\partial}{\partial x}[x f(r)] + \frac{\partial}{\partial y}[y f(r)] + \frac{\partial}{\partial z}[z f(r)] \\ &= f(r)\nabla \cdot \mathbf{r} + x\frac{\partial f}{\partial x} + y\frac{\partial f}{\partial y} + z\frac{\partial f}{\partial z} = 3f(r) + \frac{df}{dr}\mathbf{r} \cdot \nabla r \\ &= 3f(r) + \frac{x^2}{r}\frac{df}{dr} + \frac{y^2}{r}\frac{df}{dr} + \frac{z^2}{r}\frac{df}{dr} = 3f(r) + r\frac{df}{dr}, \end{aligned} \tag{1.73}$$

using the product and chain rules of differentiation in conjunction with Example 1.5.5 and Eq. (1.71). In particular, if $f(r) = r^{n-1}$,

$$\nabla \cdot \mathbf{r} r^{n-1} = \nabla \cdot (\hat{\mathbf{r}} r^n) = 3r^{n-1} + (n-1)r^{n-1} = (n+2)r^{n-1}. \tag{1.74}$$

This divergence vanishes for $n = -2$, except at $r = 0$ (where $\hat{\mathbf{r}}/r^2$ is singular). This is relevant for the Coulomb potential

$$V(r) = A_0 = -\frac{q}{4\pi\epsilon_0 r}$$

with the electric field

$$\mathbf{E} = -\nabla V = \frac{q\hat{\mathbf{r}}}{4\pi\epsilon_0 r^2}.$$

Using Eq. (1.74) we obtain the divergence $\nabla \cdot \mathbf{E} = 0$ (except at $r = 0$, where the derivatives are undefined). ■

A Physical Interpretation

To develop an understanding of the physical significance of the divergence, consider $\nabla \cdot (\rho \mathbf{v})$, with $\mathbf{v}(x, y, z)$, the velocity of a compressible fluid, and $\rho(x, y, z)$, its density at point (x, y, z). If we consider a small volume $dx\,dy\,dz$ (Fig. 1.25), the fluid flowing into this volume per unit time (positive x-direction) through the face $EFGH$ is (rate of flow in)$_{EFGH} = \rho v_x|_{x=0}\,dy\,dz$. The components of the flow ρv_y and ρv_z tangential to this face contribute nothing to the flow through this face. The rate of flow out (still positive x-direction) through face $ABCD$ is $\rho v_x|_{x=dx}\,dy\,dz$. To compare these flows and to find the net flow out, we add the change of ρv_x in the x-direction for an increment dx that

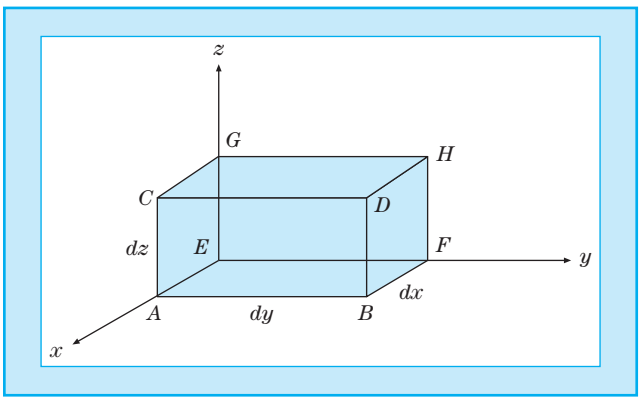


Figure 1.25

Differential Rectangular Parallelepiped (in the First or Positive Octant)

is given by its partial derivative (i.e., expand this last result in a Maclaurin series).[8] This yields

$$\begin{aligned}(\text{rate of flow out})_{ABCD} &= \rho v_x|_{x=dx}\, dy\,dz \\ &= \left[\rho v_x + \frac{\partial}{\partial x}(\rho v_x)\,dx\right]_{x=0} dy\,dz.\end{aligned}$$

Here, the derivative term is a first correction term allowing for the possibility of nonuniform density or velocity or both.[9] The zero-order term $\rho v_x|_{x=0}$ (corresponding to uniform flow) cancels out:

$$\text{Net rate of flow out}|_x = \frac{\partial}{\partial x}(\rho v_x)\,dx\,dy\,dz.$$

Equivalently, we can arrive at this result by

$$\lim_{\Delta x\to 0}\frac{\rho v_x(\Delta x, 0, 0) - \rho v_x(0, 0, 0)}{\Delta x} \equiv \left.\frac{\partial\left[\rho v_x(x, y, z)\right]}{\partial x}\right|_{(0,0,0)}.$$

Now the x-axis is not entitled to any preferred treatment. The preceding result for the two faces perpendicular to the x-axis must hold for the two faces perpendicular to the y-axis, with x replaced by y and the corresponding changes for y and z: $y \to z$, $z \to x$. This is a cyclic permutation of the coordinates. A further cyclic permutation yields the result for the remaining two faces of our parallelepiped. Adding the net rate of flow out for all three pairs of surfaces of our volume element, we have

$$\begin{aligned}\text{Net flow out (per unit time)} &= \left[\frac{\partial}{\partial x}(\rho v_x) + \frac{\partial}{\partial y}(\rho v_y) + \frac{\partial}{\partial z}(\rho v_z)\right] dx\,dy\,dz \\ &= \nabla\cdot(\rho\mathbf{v})\,dx\,dy\,dz. \qquad (1.75)\end{aligned}$$

Therefore, the net flow of our compressible fluid out of the volume element $dx\,dy\,dz$ per unit volume per unit time is $\nabla\cdot(\rho\mathbf{v})$. Hence the name **divergence**. A direct application is in the **continuity equation**

$$\frac{\partial\rho}{\partial t} + \nabla\cdot(\rho\mathbf{v}) = 0, \qquad (1.76)$$

which states that a net flow out of the volume results in a decreased density inside the volume. Note that in Eq. (1.76), ρ is considered to be a possible function of time as well as of space: $\rho(x, y, z, t)$. The divergence appears in a wide variety of physical problems, ranging from a probability current density in quantum mechanics to neutron leakage in a nuclear reactor.

[8] A Maclaurin expansion for a single variable is given by Eq. (5.75) in Section 5.6. Here, we have the increment x of Eq. (5.75) replaced by dx. We show a partial derivative with respect to x because ρv_x may also depend on y and z.

[9] Strictly speaking, ρv_x is averaged over face *EFGH* and the expression $\rho v_x + (\partial/\partial x)(\rho v_x)\,dx$ is similarly averaged over face *ABCD*. Using an arbitrarily small differential volume, we find that the averages reduce to the values employed here.

The combination $\nabla\cdot(f\mathbf{V})$, in which f is a scalar function and $\mathbf{V}$ a vector function, may be written as

$$\begin{aligned}\nabla\cdot(f\mathbf{V}) &= \frac{\partial}{\partial x}(fV_x)+\frac{\partial}{\partial y}(fV_y)+\frac{\partial}{\partial z}(fV_z)\\ &= \frac{\partial f}{\partial x}V_x+f\frac{\partial V_x}{\partial x}+\frac{\partial f}{\partial y}V_y+f\frac{\partial V_y}{\partial y}+\frac{\partial f}{\partial z}V_z+f\frac{\partial V_z}{\partial z}\\ &= (\nabla f)\cdot\mathbf{V}+f\nabla\cdot\mathbf{V}, \qquad (1.77)\end{aligned}$$

which is what we would expect for the derivative of a product. Notice that ∇ as a differential operator differentiates both f and $\mathbf{V}$; as a vector it is dotted into $\mathbf{V}$ (in each term).

SUMMARY

The divergence of a vector field is constructed as the dot product of the gradient with the vector field, and it locally measures its spatial outflow. In this sense, the continuity equation captures the essence of the divergence: the temporal change of the density balances the spatial outflow of the current density.

EXERCISES

1.6.1 For a particle moving in a circular orbit $\mathbf{r}=\hat{\mathbf{x}}r\cos\omega t+\hat{\mathbf{y}}r\sin\omega t$,

(a) evaluate $\mathbf{r}\times\dot{\mathbf{r}}$.

(b) Show that $\ddot{\mathbf{r}}+\omega^2\mathbf{r}=0$.

The radius r and the angular velocity ω are constant.

ANS. (a) $\hat{\mathbf{z}}\omega r^2$. *Note:* $\dot{\mathbf{r}}=d\mathbf{r}/dt$, $\ddot{\mathbf{r}}=d^2\mathbf{r}/dt^2$.

1.6.2 Show, by differentiating components, that

(a) $\frac{d}{dt}(\mathbf{A}\cdot\mathbf{B})=\frac{d\mathbf{A}}{dt}\cdot\mathbf{B}+\mathbf{A}\cdot\frac{d\mathbf{B}}{dt}$,

(b) $\frac{d}{dt}(\mathbf{A}\times\mathbf{B})=\frac{d\mathbf{A}}{dt}\times\mathbf{B}+\mathbf{A}\times\frac{d\mathbf{B}}{dt}$,

in the same way as the derivative of the product of two scalar functions.

1.7 Curl, $\nabla\times$

Another possible application of the vector ∇ is to cross it into a vector field called its curl, which we discuss in this section along with its physical interpretation and applications. We obtain

$$\begin{aligned}\nabla\times\mathbf{V} &= \hat{\mathbf{x}}\left(\frac{\partial}{\partial y}V_z-\frac{\partial}{\partial z}V_y\right)+\hat{\mathbf{y}}\left(\frac{\partial}{\partial z}V_x-\frac{\partial}{\partial x}V_z\right)+\hat{\mathbf{z}}\left(\frac{\partial}{\partial x}V_y-\frac{\partial}{\partial y}V_x\right)\\ &= \begin{vmatrix}\hat{\mathbf{x}} & \hat{\mathbf{y}} & \hat{\mathbf{z}}\\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z}\\ V_x & V_y & V_z\end{vmatrix}, \qquad (1.78)\end{aligned}$$

which is called the **curl** of $\mathbf{V}$. In expanding this determinant we must consider the derivative nature of ∇. Specifically, $\mathbf{V} \times \nabla$ is meaningless unless it acts on a function or a vector. Then it is certainly not equal, in general, to $-\nabla \times \mathbf{V}$.[10] In the case of Eq. (1.78), the determinant must be expanded **from the top down** so that we get the derivatives as shown in the middle of Eq. (1.78). If ∇ is crossed into the product of a scalar and a vector, we can show

$$\begin{aligned}\nabla \times (f\mathbf{V})|_x &= \left[\frac{\partial}{\partial y}(fV_z) - \frac{\partial}{\partial z}(fV_y)\right] \\ &= \left(f\frac{\partial V_z}{\partial y} + \frac{\partial f}{\partial y}V_z - f\frac{\partial V_y}{\partial z} - \frac{\partial f}{\partial z}V_y\right) \\ &= f\nabla \times \mathbf{V}|_x + (\nabla f) \times \mathbf{V}|_x . \end{aligned} \tag{1.79}$$

If we permute the coordinates $x \to y, y \to z, z \to x$ to pick up the y-component and then permute them a second time to pick up the z-component,

$$\nabla \times (f\mathbf{V}) = f\nabla \times \mathbf{V} + (\nabla f) \times \mathbf{V}, \tag{1.80}$$

which is the vector product analog of Eq. (1.77). Again, as a differential operator, ∇ differentiates both f and $\mathbf{V}$. As a vector, it is crossed into $\mathbf{V}$ (in each term).

EXAMPLE 1.7.1

Vector Potential of a Constant B Field From electrodynamics we know that $\nabla \cdot \mathbf{B} = 0$, which has the general solution $\mathbf{B} = \nabla \times \mathbf{A}$, where $\mathbf{A}(\mathbf{r})$ is called the vector potential (of the magnetic induction) because $\nabla \cdot (\nabla \times \mathbf{A}) = (\nabla \times \nabla) \cdot \mathbf{A} \equiv 0$ as a triple scalar product with two identical vectors. This last identity will not change if we add the gradient of some scalar function to the vector potential, which is therefore not unique.

In our case, we want to show that a vector potential is $\mathbf{A} = \frac{1}{2}(\mathbf{B} \times \mathbf{r})$.

Using the *BAC–CAB* rule in conjunction with Eq. (1.72), we find that

$$2\nabla \times \mathbf{A} = \nabla \times (\mathbf{B} \times \mathbf{r}) = (\nabla \cdot \mathbf{r})\mathbf{B} - (\mathbf{B} \cdot \nabla)\mathbf{r} = 3\mathbf{B} - \mathbf{B} = 2\mathbf{B},$$

where we indicate by the ordering of the scalar product of the second term that the gradient still acts on the coordinate vector. ■

EXAMPLE 1.7.2

Curl of a Central Force As in Example 1.6.1, let us start with the curl of the coordinate vector

$$\nabla \times \mathbf{r} = \begin{vmatrix} \hat{\mathbf{x}} & \hat{\mathbf{y}} & \hat{\mathbf{z}} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ x & y & z \end{vmatrix} = 0. \tag{1.81}$$

[10] Note that for the quantum mechanical angular momentum **operator**, $\mathbf{L} = -i(\mathbf{r} \times \nabla)$, we find that $\mathbf{L} \times \mathbf{L} = i\mathbf{L}$. See Sections 4.3 and 4.4 for more details.

Algebraically, this comes about because each Cartesian coordinate is independent of the other two.

Now we are ready to calculate the curl of a central force $\nabla \times \mathbf{r} f(r)$, where we expect zero for the same reason. By Eq. (1.80),

$$\nabla \times \mathbf{r} f(r) = f(r)\nabla \times \mathbf{r} + [\nabla f(r)] \times \mathbf{r}. \tag{1.82}$$

Second, using $\nabla f(r) = \hat{\mathbf{r}}(df/dr)$ (Example 1.5.5), we obtain

$$\nabla \times \mathbf{r} f\,(r) = \frac{df}{dr}\hat{\mathbf{r}} \times \mathbf{r} = 0. \tag{1.83}$$

This vector product vanishes because $\mathbf{r} = \hat{\mathbf{r}}r$ and $\hat{\mathbf{r}} \times \hat{\mathbf{r}} = 0$.

This central force case is important in potential theory of classical mechanics and engineering (see Section 1.12). ■

To develop a better understanding of the physical significance of the curl, we consider the circulation of fluid around a differential loop in the xy-plane (Fig. 1.26).

Although the circulation is technically given by a vector line integral $\int \mathbf{V} \cdot d\boldsymbol{\lambda}$, we can set up the equivalent scalar integrals here. Let us take the circulation to be

$$\begin{aligned}\text{Circulation}_{1234} = &\int_1 V_x(x, y)\, d\lambda_x + \int_2 V_y(x, y)\, d\lambda_y \\ &+ \int_3 V_x(x, y)\, d\lambda_x + \int_4 V_y(x, y)\, d\lambda_y.\end{aligned} \tag{1.84}$$

The numbers 1–4 refer to the numbered line segments in Fig. 1.26. In the first integral $d\lambda_x = +dx$ but in the third integral $d\lambda_x = -dx$ because the third line segment is traversed in the negative x-direction. Similarly, $d\lambda_y = +dy$ for the

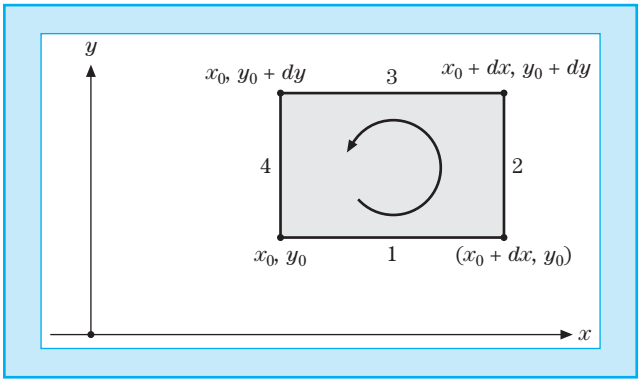


Figure 1.26

Circulation Around a Differential Loop

second integral and $-dy$ for the fourth. Next, the integrands are referred to the point (x_0, y_0) with a Taylor expansion,[11] taking into account the displacement of line segment 3 from 1 and 2 from 4. For our differential line segments, this leads to

$$\begin{aligned}\text{Circulation}_{1234} &= V_x(x_0, y_0)\,dx + \left[V_y(x_0, y_0) + \frac{\partial V_y}{\partial x}\,dx\right]dy \\ &\quad + \left[V_x(x_0, y_0) + \frac{\partial V_x}{\partial y}\,dy\right](-dx) + V_y(x_0, y_0)\,(-dy) \\ &= \left(\frac{\partial V_y}{\partial x} - \frac{\partial V_x}{\partial y}\right)dx\,dy. \end{aligned} \tag{1.85}$$

Dividing by $dx\,dy$, we have

$$\text{Circulation per unit area} = \nabla \times \mathbf{V}|_z\,. \tag{1.86}$$

This is an infinitesimal case of Stokes's theorem in Section 1.11. The circulation[12] about our differential area in the xy-plane is given by the z-component of $\nabla \times \mathbf{V}$. In principle, the curl $\nabla \times \mathbf{V}$ at (x_0, y_0) could be determined by inserting a (differential) paddle wheel into the moving fluid at point (x_0, y_0). The rotation of the little paddle wheel would be a measure of the curl and its axis along the direction of $\nabla \times \mathbf{V}$, which is perpendicular to the plane of circulation.

In light of this connection of the curl with the concept of circulation, we now understand intuitively the vanishing curl of a central force in Example 1.7.2 because $\mathbf{r}$ flows radially outward from the origin with no rotation, and any scalar $f(r)$ will not affect this situation. When

$$\nabla \times \mathbf{V} = 0, \tag{1.87}$$

$\mathbf{V}$ is labeled **irrotational**. The most important physical examples of irrotational vectors are the gravitational and electrostatic forces. In each case,

$$\mathbf{V} = C\frac{\hat{\mathbf{r}}}{r^2} = C\frac{\mathbf{r}}{r^3}, \tag{1.88}$$

where C is a constant and $\hat{\mathbf{r}}$ is the unit vector in the outward radial direction. For the gravitational case, we have $C = -Gm_1m_2$, given by Newton's law of universal gravitation. If $C = q_1q_2/(4\pi\varepsilon_0)$, we have Coulomb's law of electrostatics (SI units). The force $\mathbf{V}$ given in Eq. (1.88) may be shown to be irrotational by direct expansion into Cartesian components as we did in Example 1.7.2 [Eq. (1.83)].

In Section 1.15 of Arfken and Weber's *Mathematical Methods for Physicists* (5th ed.), it is shown that a vector field may be resolved into an irrotational part and a solenoidal part (subject to conditions at infinity).

[11] $V_y(x_0 + dx, y_0) = V_y(x_0, y_0) + (\frac{\partial V_y}{\partial x})_{x_0y_0}dx + \cdots$. The higher order terms will drop out in the limit as $dx \to 0$.

[12] In fluid dynamics, $\nabla \times \mathbf{V}$ is called the vorticity.

For waves in an elastic medium, if the displacement $\mathbf{u}$ is irrotational, $\nabla \times \mathbf{u} = 0$, plane waves (or spherical waves at large distances) become longitudinal. If $\mathbf{u}$ is solenoidal, $\nabla \cdot \mathbf{u} = 0$, then the waves become transverse. A seismic disturbance will produce a displacement that may be resolved into a solenoidal part and an irrotational part. The irrotational part yields the longitudinal P (primary) earthquake waves. The solenoidal part gives rise to the slower transverse S (secondary) waves.

Using the gradient, divergence, curl, and the *BAC–CAB* rule, we may construct or verify a large number of useful vector identities. For verification, complete expansion into Cartesian components is always a possibility. Sometimes if we use insight instead of routine shuffling of Cartesian components, the verification process can be shortened drastically.

Remember that ∇ is a vector operator, a hybrid object satisfying two sets of rules: vector rules and partial differentiation rules, including differentiation of a product.

EXAMPLE 1.7.3

Gradient of a Dot Product Verify that

$$\nabla(\mathbf{A}\cdot\mathbf{B}) = (\mathbf{B}\cdot\nabla)\mathbf{A} + (\mathbf{A}\cdot\nabla)\mathbf{B} + \mathbf{B}\times(\nabla\times\mathbf{A}) + \mathbf{A}\times(\nabla\times\mathbf{B}). \tag{1.89}$$

This particular example hinges on the recognition that $\nabla(\mathbf{A}\cdot\mathbf{B})$ is the type of term that appears in the *BAC–CAB* expansion of a triple vector product [Eq. (1.52)]. For instance,

$$\mathbf{A}\times(\nabla\times\mathbf{B}) = \nabla(\mathbf{A}\cdot\mathbf{B}) - (\mathbf{A}\cdot\nabla)\mathbf{B},$$

with the ∇ differentiating only $\mathbf{B}$, not $\mathbf{A}$. From the commutativity of factors in a scalar product we may interchange $\mathbf{A}$ and $\mathbf{B}$ and write

$$\mathbf{B}\times(\nabla\times\mathbf{A}) = \nabla(\mathbf{A}\cdot\mathbf{B}) - (\mathbf{B}\cdot\nabla)\mathbf{A},$$

now with ∇ differentiating only $\mathbf{A}$, not $\mathbf{B}$. Adding these two equations, we obtain ∇ differentiating the product $\mathbf{A}\cdot\mathbf{B}$ and the identity [Eq. (1.89)]. This identity is used frequently in electromagnetic theory. Exercise 1.7.9 is an illustration. ■

SUMMARY

The curl is constructed as the cross product of the gradient and a vector field, and it measures the local rotational flow or circulation of the vector field. When the curl of a force field is zero, then the force is labeled conservative and derives from the gradient of a scalar, its potential. In Chapter 6, we shall see that an analytic function of a complex variable describes a two-dimensional irrotational fluid flow.

EXERCISES

1.7.1 Show that $\mathbf{u}\times\mathbf{v}$ is solenoidal if $\mathbf{u}$ and $\mathbf{v}$ are each irrotational. Start by formulating the problem in terms of mathematical equations.

1.7.2 If $\mathbf{A}$ is irrotational, show that $\mathbf{A}\times\mathbf{r}$ is solenoidal.

1.7.3 A rigid body is rotating with constant angular velocity $\boldsymbol{\omega}$. Show that the linear velocity $\mathbf{v}$ is solenoidal.

1.7.4 If a vector function $\mathbf{f}(x, y, z)$ is not irrotational but the product of f and a scalar function $g(x, y, z)$ is irrotational, show that

$$\mathbf{f} \cdot \nabla \times \mathbf{f} = 0.$$

1.7.5 Verify the vector identity

$$\nabla \times (\mathbf{A} \times \mathbf{B}) = (\mathbf{B} \cdot \nabla)\mathbf{A} - (\mathbf{A} \cdot \nabla)\mathbf{B} - \mathbf{B}(\nabla \cdot \mathbf{A}) + \mathbf{A}(\nabla \cdot \mathbf{B}).$$

Describe in words what causes the last two terms to appear in the identity beyond the *BAC–CAB* rule. If symbolic software is available, test the Cartesian components for a typical case, such as $\mathbf{A} = \mathbf{L}$, $\mathbf{B} = \mathbf{r}/r^3$.

1.7.6 As an alternative to the vector identity of Example 1.7.5, show that

$$\nabla(\mathbf{A} \cdot \mathbf{B}) = (\mathbf{A} \times \nabla) \times \mathbf{B} + (\mathbf{B} \times \nabla) \times \mathbf{A} + \mathbf{A}(\nabla \cdot \mathbf{B}) + \mathbf{B}(\nabla \cdot \mathbf{A}).$$

1.7.7 Verify the identity

$$\mathbf{A} \times (\nabla \times \mathbf{A}) = \frac{1}{2}\nabla(A^2) - (\mathbf{A} \cdot \nabla)\mathbf{A}.$$

Test this identity for a typical vector field, such as $\mathbf{A} \sim \mathbf{r}$ or $\mathbf{r}/r^3$.

1.7.8 If $\mathbf{A}$ and $\mathbf{B}$ are constant vectors, show that

$$\nabla(\mathbf{A} \cdot \mathbf{B} \times \mathbf{r}) = \mathbf{A} \times \mathbf{B}.$$

1.7.9 A distribution of electric currents creates a constant magnetic moment $\mathbf{m}$. The force on $\mathbf{m}$ in an external magnetic induction $\mathbf{B}$ is given by

$$\mathbf{F} = \nabla \times (\mathbf{B} \times \mathbf{m}).$$

Show that

$$\mathbf{F} = \nabla(\mathbf{m} \cdot \mathbf{B}).$$

Note. Assuming no time dependence of the fields, Maxwell's equations yield $\nabla \times \mathbf{B} = 0$. Also, $\nabla \cdot \mathbf{B} = 0$.

1.7.10 An electric dipole of moment $\mathbf{p}$ is located at the origin. The dipole creates an electric potential at $\mathbf{r}$ given by

$$\psi(\mathbf{r}) = \frac{\mathbf{p} \cdot \mathbf{r}}{4\pi\varepsilon_0 r^3}.$$

Find the electric field $\mathbf{E} = -\nabla\psi$ at $\mathbf{r}$.

1.7.11 The vector potential $\mathbf{A}$ of a magnetic dipole, dipole moment $\mathbf{m}$, is given by $\mathbf{A}(\mathbf{r}) = (\mu_0/4\pi)(\mathbf{m} \times \mathbf{r}/r^3)$. Show that the magnetic induction $\mathbf{B} = \nabla \times \mathbf{A}$ is given by

$$\mathbf{B} = \frac{\mu_0}{4\pi}\frac{3\hat{\mathbf{r}}(\hat{\mathbf{r}} \cdot \mathbf{m}) - \mathbf{m}}{r^3}.$$

1.7.12 Classically, orbital angular momentum is given by $\mathbf{L} = \mathbf{r} \times \mathbf{p}$, where $\mathbf{p}$ is the linear momentum. To go from classical mechanics to quantum mechanics, replace $\mathbf{p}$ by the operator $-i\nabla$ (Section 14.6). Show that the quantum mechanical angular momentum operator has Cartesian components

$$L_x = -i\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)$$
$$L_y = -i\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)$$
$$L_z = -i\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)$$

(in units of $\hbar$).

1.7.13 Using the angular momentum operators previously given, show that they satisfy commutation relations of the form

$$[L_x, L_y] \equiv L_xL_y - L_yL_x = iL_z$$

and, hence,

$$\mathbf{L} \times \mathbf{L} = i\mathbf{L}.$$

These commutation relations will be taken later as the defining relations of an angular momentum operator—see Exercise 3.2.15 and the following one and Chapter 4.

1.7.14 With the commutator bracket notation $[L_x, L_y] = L_xL_y - L_yL_x$, the angular momentum vector $\mathbf{L}$ satisfies $[L_x, L_y] = iL_z$, etc., or $\mathbf{L} \times \mathbf{L} = i\mathbf{L}$. If two other vectors $\mathbf{a}$ and $\mathbf{b}$ commute with each other and with $\mathbf{L}$, that is, $[\mathbf{a}, \mathbf{b}] = [\mathbf{a}, \mathbf{L}] = [\mathbf{b}, \mathbf{L}] = 0$, show that

$$[\mathbf{a} \cdot \mathbf{L}, \mathbf{b} \cdot \mathbf{L}] = i(\mathbf{a} \times \mathbf{b}) \cdot \mathbf{L}.$$

This vector version of the angular momentum commutation relations is an alternative to that given in Exercise 1.7.13.

1.7.15 Prove $\nabla \cdot (\mathbf{a} \times \mathbf{b}) = \mathbf{b} \cdot (\nabla \times \mathbf{a}) - \mathbf{a} \cdot (\nabla \times \mathbf{b})$. Explain in words why the identity is valid.
Hint. Treat as a triple scalar product.

1.8 Successive Applications of ∇

We have now defined gradient, divergence, and curl to obtain vector, scalar, and vector quantities, respectively. Letting ∇ operate on each of these quantities, we obtain

(a) $\nabla \cdot \nabla\varphi$ (b) $\nabla \times \nabla\varphi$ (c) $\nabla\nabla \cdot \mathbf{V}$
(d) $\nabla \cdot \nabla \times \mathbf{V}$ (e) $\nabla \times (\nabla \times \mathbf{V})$.

All five expressions involve second derivatives and all five appear in the second-order differential equations of mathematical physics, particularly in electromagnetic theory.

The first expression, $\nabla \cdot \nabla\varphi$, the divergence of the gradient, is called the Laplacian of φ. We have

$$\nabla \cdot \nabla\varphi = \left(\hat{\mathbf{x}}\frac{\partial}{\partial x} + \hat{\mathbf{y}}\frac{\partial}{\partial y} + \hat{\mathbf{z}}\frac{\partial}{\partial z}\right) \cdot \left(\hat{\mathbf{x}}\frac{\partial\varphi}{\partial x} + \hat{\mathbf{y}}\frac{\partial\varphi}{\partial y} + \hat{\mathbf{z}}\frac{\partial\varphi}{\partial z}\right)$$
$$= \frac{\partial^2\varphi}{\partial x^2} + \frac{\partial^2\varphi}{\partial y^2} + \frac{\partial^2\varphi}{\partial z^2}. \tag{1.90}$$

When φ is the electrostatic potential, in a charge-free region we have

$$\nabla \cdot \nabla\varphi = 0, \tag{1.91}$$

which is Laplace's equation of electrostatics. Often, the combination $\nabla \cdot \nabla$ is written ∇^2, or Δ in the European literature.

Biographical Data

Laplace, Pierre Simon. Laplace, a French mathematician, physicist, and astronomer, was born in Beaumont-en-Auge in 1749 and died in Paris in 1827. He developed perturbation theory for the solar system, published a monumental treatise *Celestial Mechanics*, and applied mathematics to artillery. He made contributions of fundamental importance to hydrodynamics, differential equations and probability, the propagation of sound, and surface tension in liquids. To Napoleon's remark missing "God" in his treatise, he replied "I had no need for that hypothesis." He generally disliked giving credit to others.

EXAMPLE 1.8.1

Laplacian of a Radial Function Calculate $\nabla \cdot \nabla g(r)$. Referring to Examples 1.5.5 and 1.6.1,

$$\nabla \cdot \nabla g(r) = \nabla \cdot \hat{\mathbf{r}}\frac{dg}{dr} = \frac{2}{r}\frac{dg}{dr} + \frac{d^2g}{dr^2},$$

replacing $f(r)$ in Example 1.6.1 by $1/r \cdot dg/dr$. If $g(r) = r^n$, this reduces to

$$\nabla \cdot \nabla r^n = n(n+1)r^{n-2}.$$

This vanishes for $n = 0$ [$g(r) =$ constant] and for $n = -1$; that is, $g(r) = 1/r$ is a solution of Laplace's equation, $\nabla^2 g(r) = 0$. This is for $r \neq 0$. At the origin there is a singularity. ■

Expression (b) may be written as

$$\nabla \times \nabla\varphi = \begin{vmatrix} \hat{\mathbf{x}} & \hat{\mathbf{y}} & \hat{\mathbf{z}} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ \frac{\partial\varphi}{\partial x} & \frac{\partial\varphi}{\partial y} & \frac{\partial\varphi}{\partial z} \end{vmatrix}.$$

By expanding the determinant, we obtain

$$\nabla \times \nabla\varphi = \hat{\mathbf{x}}\left(\frac{\partial^2\varphi}{\partial y\,\partial z} - \frac{\partial^2\varphi}{\partial z\,\partial y}\right) + \hat{\mathbf{y}}\left(\frac{\partial^2\varphi}{\partial z\,\partial x} - \frac{\partial^2\varphi}{\partial x\,\partial z}\right) + \hat{\mathbf{z}}\left(\frac{\partial^2\varphi}{\partial x\,\partial y} - \frac{\partial^2\varphi}{\partial y\,\partial x}\right) = 0, \tag{1.92}$$

assuming that the order of partial differentiation may be interchanged. This is true as long as these second partial derivatives of φ are continuous functions. Then, from Eq. (1.92), the curl of a gradient is identically zero. All gradients, therefore, are irrotational. Note that the zero in Eq. (1.92) comes as a mathematical identity, independent of any physics. The zero in Eq. (1.91) is a consequence of physics.

Expression (d) is a triple scalar product that may be written as

$$\nabla \cdot \nabla \times \mathbf{V} = \begin{vmatrix} \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ V_x & V_y & V_z \end{vmatrix}. \tag{1.93}$$

Again, assuming continuity so that the order of differentiation is immaterial, we obtain

$$\nabla \cdot \nabla \times \mathbf{V} = 0. \tag{1.94}$$

The divergence of a curl vanishes or all curls are solenoidal.

One of the most important cases of a vanishing divergence of a vector is

$$\nabla \cdot \mathbf{B} = 0, \tag{1.95}$$

where $\mathbf{B}$ is the magnetic induction, and Eq. (1.95) appears as one of Maxwell's equations. When a vector is solenoidal, it may be written as the curl of another vector known as its vector potential, $\mathbf{B} = \nabla \times \mathbf{A}$. This form solves one of the four vector equations that make up Maxwell's field equations of electrodynamics. Because a vector field may be determined from its curl and divergence (Helmholtz's theorem), solving Maxwell's (often called Oersted's) equation involving the curl of $\mathbf{B}$ determines $\mathbf{A}$ and thereby $\mathbf{B}$. Similar considerations apply to the other pair of Maxwell's equations involving the divergence and curl of $\mathbf{E}$ and make plausible the fact that there are precisely four vector equations as part of Maxwell's equations.

The two remaining expressions satisfy a relation

$$\nabla \times (\nabla \times \mathbf{V}) = \nabla(\nabla \cdot \mathbf{V}) - (\nabla \cdot \nabla)\mathbf{V}. \tag{1.96}$$

This decomposition of the Laplacian $\nabla \cdot \nabla$ into a longitudinal part (the gradient) and a transverse part (the curl term) follows from Eq. (1.52), the *BAC–CAB* rule, which we rewrite so that $\mathbf{C}$ appears at the extreme right of each term. The term $(\nabla \cdot \nabla)\mathbf{V}$ was not included in our list, but it appears in the Navier–Stokes's equation and may be **defined** by Eq. (1.96). In words, this is the Laplacian (a scalar operator) acting on a vector, so it is a vector with three components in three-dimensional space. ■

EXAMPLE 1.8.2

Electromagnetic Wave Equations One important application of this vector relation [Eq. (1.96)] is in the derivation of the electromagnetic wave equation. In vacuum Maxwell's equations become

$$\nabla \cdot \mathbf{B} = 0, \tag{1.97a}$$

$$\nabla \cdot \mathbf{E} = 0, \tag{1.97b}$$

$$\nabla \times \mathbf{B} = \varepsilon_0 \mu_0 \frac{\partial \mathbf{E}}{\partial t} = \frac{1}{c^2} \frac{\partial \mathbf{E}}{\partial t}, \tag{1.97c}$$

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}, \tag{1.97d}$$

where $\mathbf{E}$ is the electric field, $\mathbf{B}$ the magnetic induction, ε_0 the electric permittivity, and μ_0 the magnetic permeability (SI units), so that $\varepsilon_0 \mu_0 = 1/c^2$, where c is the velocity of light. This relation has important consequences. Because ε_0, μ_0 can be measured in any frame, the velocity of light is the same in any frame.

Suppose we eliminate $\mathbf{B}$ from Eqs. (1.97c) and (1.97d). We may do this by taking the curl of both sides of Eq. (1.97d) and the time derivative of both sides of Eq. (1.97c). Since the space and time derivatives commute,

$$\frac{\partial}{\partial t} \nabla \times \mathbf{B} = \nabla \times \frac{\partial \mathbf{B}}{\partial t},$$

and we obtain

$$\nabla \times (\nabla \times \mathbf{E}) = -\frac{1}{c^2} \frac{\partial^2 \mathbf{E}}{\partial t^2}.$$

Application of Eqs. (1.96) and (1.97b) yields

$$(\nabla \cdot \nabla)\mathbf{E} = \frac{1}{c^2} \frac{\partial^2 \mathbf{E}}{\partial t^2}, \tag{1.98}$$

the electromagnetic vector wave equation. Again, if $\mathbf{E}$ is expressed in Cartesian coordinates, Eq. (1.98) separates into three scalar wave equations, each involving a scalar Laplacian.

When external electric charge and current densities are kept as driving terms in Maxwell's equations, similar wave equations are valid for the electric potential and the vector potential. To show this, we solve Eq. (1.97a) by writing $\mathbf{B} = \nabla \times \mathbf{A}$ as a curl of the vector potential. This expression is substituted into Faraday's induction law in differential form [Eq. (1.97d)] to yield $\nabla \times (\mathbf{E} + \frac{\partial \mathbf{A}}{\partial t}) = 0$. The vanishing curl implies that $\mathbf{E} + \frac{\partial \mathbf{A}}{\partial t}$ is a gradient and therefore can be written as $-\nabla \varphi$, where $\varphi(\mathbf{r}, t)$ is defined as the (nonstatic) electric potential. These results

$$\mathbf{B} = \nabla \times \mathbf{A}, \qquad \mathbf{E} = -\nabla \varphi - \frac{\partial \mathbf{A}}{\partial t} \tag{1.99}$$

for the $\mathbf{B}$ and $\mathbf{E}$ fields solve the homogeneous Maxwell's equations.

We now show that the inhomogeneous Maxwell's equations,

$$\text{Gauss's law: } \nabla \cdot \mathbf{E} = \rho/\varepsilon_0;$$
$$\text{Oersted's law: } \nabla \times \mathbf{B} - \frac{1}{c^2}\frac{\partial \mathbf{E}}{\partial t} = \mu_0 \mathbf{J} \tag{1.100}$$

in differential form lead to wave equations for the potentials φ and $\mathbf{A}$, provided that $\nabla \cdot \mathbf{A}$ is determined by the constraint $\frac{1}{c^2}\frac{\partial \varphi}{\partial t} + \nabla \cdot \mathbf{A} = 0$. This choice of fixing the divergence of the vector potential is called the **Lorentz gauge** and serves to uncouple the partial differential equations of both potentials. This gauge constraint is not a restriction; it has no physical effect.

Substituting our electric field solution into Gauss's law yields

$$\frac{\rho}{\varepsilon_0} = \nabla \cdot \mathbf{E} = -\nabla^2 \varphi - \frac{\partial}{\partial t}\nabla \cdot \mathbf{A} = -\nabla^2 \varphi + \frac{1}{c^2}\frac{\partial^2 \varphi}{\partial t^2},$$

the wave equation for the electric potential. In the last step, we used the Lorentz gauge to replace the divergence of the vector potential by the time derivative of the electric potential and thus decouple φ from $\mathbf{A}$.

Finally, we substitute $\mathbf{B} = \nabla \times \mathbf{A}$ into Oersted's law and use Eq. (1.96), which expands ∇^2 in terms of a longitudinal (the gradient term) and a transverse component (the curl term). This yields

$$\mu_0 \mathbf{J} + \frac{1}{c^2}\frac{\partial \mathbf{E}}{\partial t} = \nabla \times (\nabla \times \mathbf{A}) = \nabla(\nabla \cdot \mathbf{A}) - \nabla^2 \mathbf{A} = \mu_0 \mathbf{J} - \frac{1}{c^2}\left(\nabla \frac{\partial \varphi}{\partial t} + \frac{\partial^2 \mathbf{A}}{\partial t^2}\right),$$

where we have used the electric field solution [Eq. (1.99)] in the last step. Now we see that the Lorentz gauge condition eliminates the gradient terms so that the wave equation

$$\frac{1}{c^2}\frac{\partial^2 \mathbf{A}}{\partial t^2} - \nabla^2 \mathbf{A} = \mu_0 \mathbf{J}$$

for the vector potential remains.

Finally, looking back at Oersted's law, taking the divergence of Eq. (1.100), dropping $\nabla \cdot (\nabla \times \mathbf{B}) = 0$ and substituting Gauss's law for $\nabla \cdot \mathbf{E} = \rho/\epsilon_0$, we find $\mu_0 \nabla \cdot \mathbf{J} = -\frac{1}{\epsilon_0 c^2}\frac{\partial \rho}{\partial t}$, where $\epsilon_0 \mu_0 = 1/c^2$, that is, the continuity equation for the current density. This step justifies the inclusion of Maxwell's displacement current in the generalization of Oersted's law to nonstationary situations. ■

EXERCISES

1.8.1 Verify Eq. (1.96)

$$\nabla \times (\nabla \times \mathbf{V}) = \nabla(\nabla \cdot \mathbf{V}) - (\nabla \cdot \nabla)\mathbf{V}$$

by direct expansion in Cartesian coordinates. If symbolic software is available, check the identity for typical fields, such as $\mathbf{V} = \mathbf{r}, \mathbf{r}/r^3$, $\mathbf{a} \cdot \mathbf{rb}$, $\mathbf{a} \times \mathbf{r}$.

1.8.2 Show that the identity

$$\nabla \times (\nabla \times \mathbf{V}) = \nabla(\nabla \cdot \mathbf{V}) - (\nabla \cdot \nabla)\mathbf{V}$$

follows from the *BAC–CAB* rule for a triple vector product. Justify any alteration of the order of factors in the *BAC* and *CAB* terms.

1.8.3 Prove that $\nabla \times (\varphi \nabla \varphi) = 0$.

1.8.4 Prove that $(\nabla u) \times (\nabla v)$ is solenoidal, where u and v are differentiable scalar functions. Start by formulating the problem as a mathematical equation.

1.8.5 φ is a scalar satisfying Laplace's equation, $\nabla^2 \varphi = 0$. Show that $\nabla \varphi$ is **both** solenoidal and irrotational.

1.8.6 With ψ a scalar function, show that

$$(\mathbf{r} \times \nabla) \cdot (\mathbf{r} \times \nabla)\psi = r^2 \nabla^2 \psi - r^2 \frac{\partial^2 \psi}{\partial r^2} - 2r \frac{\partial \psi}{\partial r}.$$

(This can actually be shown more easily in spherical polar coordinates; see Section 2.5.)

1.8.7 In the Pauli theory of the electron one encounters the expression

$$(\mathbf{p} - e\mathbf{A}) \times (\mathbf{p} - e\mathbf{A})\psi,$$

where ψ is a scalar function. $\mathbf{A}$ is the magnetic vector potential related to the magnetic induction $\mathbf{B}$ by $\mathbf{B} = \nabla \times \mathbf{A}$. Given that $\mathbf{p} = -i\nabla$, show that this expression reduces to $ie\mathbf{B}\psi$. Show that this leads to the orbital g-factor $g_L = 1$ upon writing the magnetic moment as $\boldsymbol{\mu} = g_L \mathbf{L}$ in units of Bohr magnetons. See also Example 1.7.1.

1.8.8 Show that any solution of the equation

$$\nabla \times \nabla \times \mathbf{A} - k^2 \mathbf{A} = 0$$

automatically satisfies the vector Helmholtz equation

$$\nabla^2 \mathbf{A} + k^2 \mathbf{A} = 0$$

and the solenoidal condition

$$\nabla \cdot \mathbf{A} = 0.$$

Hint. Let $\nabla \cdot$ operate on the first equation.

1.9 Vector Integration

The next step after differentiating vectors is to integrate them. Let us start with line integrals and then proceed to surface and volume integrals. In each case, the method of attack will be to reduce the vector integral to one-dimensional integrals over a coordinate interval.

Line Integrals

Using an increment of length $d\mathbf{r} = \hat{\mathbf{x}}\,dx + \hat{\mathbf{y}}\,dy + \hat{\mathbf{z}}\,dz$, we often encounter the line integral

$$\int_C \mathbf{V} \cdot d\mathbf{r}, \tag{1.101}$$

in which the integral is over some contour C that may be open (with starting point and ending point separated) or closed (forming a loop) instead of an interval of the x-axis. The Riemann integral is defined by subdividing the curve into ever smaller segments whose number grows indefinitely. The form [Eq. (1.101)] is exactly the same as that encountered when we calculate the work done by a force that varies along the path

$$W = \int \mathbf{F} \cdot d\mathbf{r} = \int F_x(x, y, z)\,dx + \int F_y(x, y, z)\,dy + \int F_z(x, y, z)\,dz, \tag{1.102}$$

that is, a sum of conventional integrals over intervals of one variable each. In this expression, $\mathbf{F}$ is the force exerted on a particle. In general, such integrals depend on the path except for conservative forces, whose treatment we postpone to Section 1.12.

EXAMPLE 1.9.1

Path-Dependent Work The force exerted on a body is $\mathbf{F} = -\hat{\mathbf{x}}y + \hat{\mathbf{y}}x$. The problem is to calculate the work done going from the origin to the point (1, 1),

$$W = \int_{0,0}^{1,1} \mathbf{F} \cdot d\mathbf{r} = \int_{0,0}^{1,1} (-y\,dx + x\,dy). \tag{1.103}$$

Separating the two integrals, we obtain

$$W = -\int_0^1 y\,dx + \int_0^1 x\,dy. \tag{1.104}$$

The first integral cannot be evaluated until we specify the values of y as x ranges from 0 to 1. Likewise, the second integral requires x as a function of y. Consider first the path shown in Fig. 1.27. Then

$$W = -\int_0^1 0\,dx + \int_0^1 1\,dy = 1 \tag{1.105}$$

because $y = 0$ along the first segment of the path and $x = 1$ along the second. If we select the path $[x = 0, 0 \le y \le 1]$ and $[0 \le x \le 1, y = 1]$, then Eq. (1.103) gives $W = -1$. For this force, the work done depends on the choice of path. ■

EXAMPLE 1.9.2

Line Integral for Work Find the work done going around a unit circle clockwise from 0 to $-\pi$ shown in Fig. 1.28 in the xy-plane doing work against a force field given by

$$\mathbf{F} = \frac{-\hat{\mathbf{x}}y}{x^2 + y^2} + \frac{\hat{\mathbf{y}}x}{x^2 + y^2}.$$

Figure 1.27

A Path of Integration

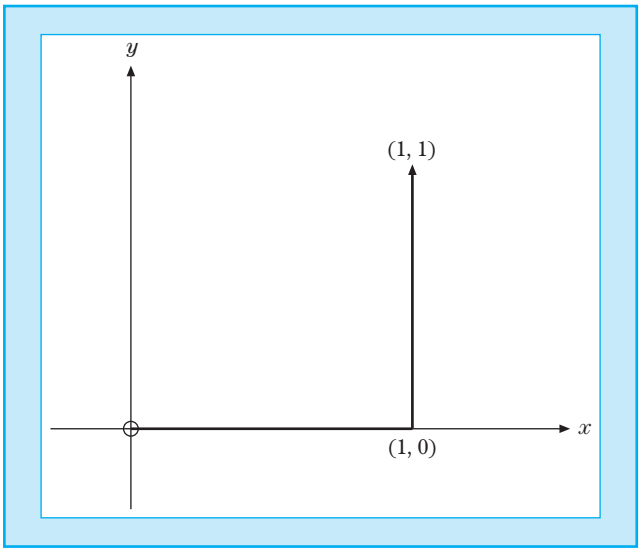
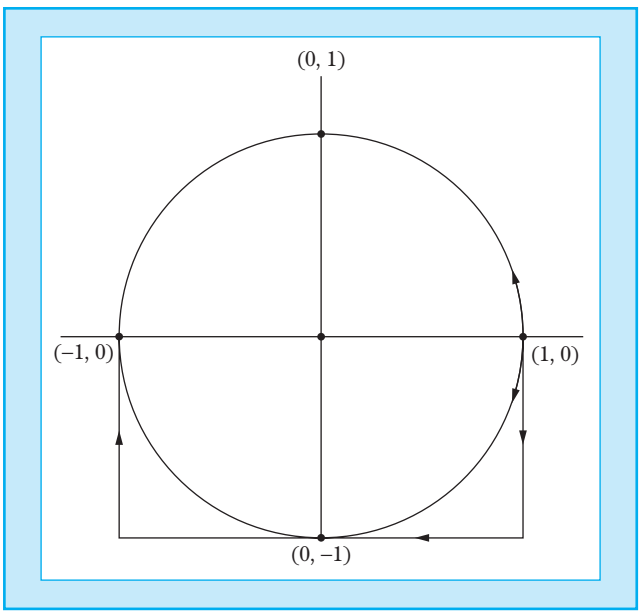


Figure 1.28

Circular and Square Integration Paths



Let us parameterize the circle C as $x = \cos\varphi$, $y = \sin\varphi$ with the polar angle φ so that $dx = -\sin\varphi d\varphi$, $dy = \cos\varphi d\varphi$. Then the force can be written as $\mathbf{F} = -\hat{\mathbf{x}}\sin\varphi + \hat{\mathbf{y}}\cos\varphi$. The work becomes

$$-\int_C \frac{xdy - ydx}{x^2 + y^2} = \int_0^{-\pi} (-\sin^2\varphi - \cos^2\varphi)\, d\varphi = \pi.$$

Here we spend energy. If we integrate anticlockwise from $\varphi = 0$ to π we find the value $-\pi$ because we are riding with the force. The work is path dependent, which is consistent with the physical interpretation that $\mathbf{F} \cdot d\mathbf{r} \sim x dy - y dx = L_z$ is proportional to the z-component of orbital angular momentum (involving circulation, as discussed in Section 1.7).

If we integrate along the square through the points $(\pm 1, 0)$, $(0, -1)$ surrounding the circle, we find for the clockwise lower half square path of Fig. 1.28

$$\begin{aligned} -\int \mathbf{F} \cdot d\mathbf{r} &= -\int_0^{-1} F_y\, dy|_{x=1} - \int_1^{-1} F_x\, dx|_{y=-1} - \int_{-1}^{0} F_y\, dy|_{x=-1} \\ &= \int_0^1 \frac{dy}{1+y^2} + \int_{-1}^{1} \frac{dx}{x^2+(-1)^2} + \int_{-1}^{0} \frac{dy}{(-1)^2+y^2} \\ &= \arctan(1) + \arctan(1) - \arctan(-1) - \arctan(-1) \\ &= 4 \cdot \frac{\pi}{4} = \pi, \end{aligned}$$

which is consistent with the circular path.

For the circular paths we used the $x = \cos\varphi$, $y = \sin\varphi$ parameterization, whereas for the square shape we used the standard definitions $y = f(x)$ or $x = g(y)$ of a curve, that is, $y = -1 = \text{const.}$ and $x = \pm 1 = \text{const.}$ We could have used the implicit definition $F(x, y) \equiv x^2 + y^2 - 1 = 0$ of the circle. Then the total variation

$$dF = \frac{\partial F}{\partial x} dx + \frac{\partial F}{\partial y} dy = 2x\, dx + 2y\, dy \equiv 0$$

so that

$$dy = -x\, dx/y \text{ with } y = -\sqrt{1-x^2}$$

on our half circle. The work becomes

$$\begin{aligned} -\int_C \frac{x\, dy - y\, dx}{x^2+y^2} &= \int \left(\frac{x^2}{y} + y\right) dx = \int \frac{dx}{y} = \int_1^{-1} \frac{dx}{-\sqrt{1-x^2}} \\ &= \arcsin 1 - \arcsin(-1) = 2 \cdot \frac{\pi}{2} = \pi, \end{aligned}$$

in agreement with our previous results. ■

EXAMPLE 1.9.3

Gravitational Potential If a force can be described by a scalar function V_G as $\mathbf{F} = -\nabla V_G(\mathbf{r})$ [Eq. (1.65)], everywhere we call V_G its potential in mechanics and engineering. Because the total variation $dV_G = \nabla V_G \cdot d\mathbf{r} = -\mathbf{F}_G \cdot d\mathbf{r}$ is the work done against the force along the path $d\mathbf{r}$, the integrated work along any path from the initial point $\mathbf{r}_0$ to the final point $\mathbf{r}$ is given by a line integral $\int_{\mathbf{r}_0}^{\mathbf{r}} dV_G = V_G(\mathbf{r}) - V_G(\mathbf{r}_0)$, the potential difference between the end points of

the path. Thus, to find the scalar potential for the gravitational force on a unit mass m_1,

$$\mathbf{F}_G = -\frac{Gm_1m_2\hat{\mathbf{r}}}{r^2} = -\frac{k\hat{\mathbf{r}}}{r^2}, \qquad \text{radially } \textbf{inward} \tag{1.106}$$

we integrate from infinity, where V_G is zero into position $\mathbf{r}$. We obtain

$$V_G(r) - V_G(\infty) = -\int_{\infty}^{\mathbf{r}} \mathbf{F}_G \cdot d\mathbf{r} = +\int_{\mathbf{r}}^{\infty} \mathbf{F}_G \cdot d\mathbf{r}. \tag{1.107}$$

By use of $\mathbf{F}_G = -\mathbf{F}_{\text{applied}}$, the potential is the work done in bringing the unit mass in from infinity. (We can define only the potential difference. Here, we arbitrarily assign infinity to be a zero of potential.) Since $\mathbf{F}_G$ is radial, we obtain a contribution to V_G only when $d\mathbf{r}$ is radial or

$$V_G(r) = -\int_r^{\infty} \frac{k\,dr}{r^2} = -\frac{k}{r} = -\frac{Gm_1m_2}{r}. \tag{1.108}$$

The negative sign reflects the attractive nature of gravity. ■

Surface Integrals

Surface integrals appear in the same forms as line integrals, the element of area also being a vector, $d\boldsymbol{\sigma}$.[13] Often this area element is written $\mathbf{n}\,dA$, where $\mathbf{n}$ is a unit (normal) vector to indicate the positive direction.[14] There are two conventions for choosing the positive direction. First, if the surface is a closed surface, we agree to take the outward normal as positive. Second, if the surface is an open surface, the positive normal depends on the direction in which the perimeter of the open surface is traversed. If the right-hand fingers are curled in the direction of travel around the perimeter, the positive normal is indicated by the thumb of the right hand. As an illustration, a circle in the xy-plane (Fig. 1.29) mapped out from x to y to $-x$ to $-y$ and back to x will have its positive normal parallel to the positive z-axis (for the right-handed coordinate system).

Analogous to the line integrals, Eq. (1.101), surface integrals may appear in the form

$$\int \mathbf{V} \cdot d\boldsymbol{\sigma}. \tag{1.109}$$

This surface integral $\int \mathbf{V} \cdot d\boldsymbol{\sigma}$ may be interpreted as a flow or flux through the given surface. This is really what we did in Section 1.6 to understand the significance of the concept of divergence. Note that both physically and from the dot product the tangential components of the velocity contribute nothing to the flow through the surface.

[13] Recall that in Section 1.3 the area (of a parallelogram) is represented by a cross product **vector**.
[14] Although $\mathbf{n}$ always has unit length, its direction may well be a function of position.

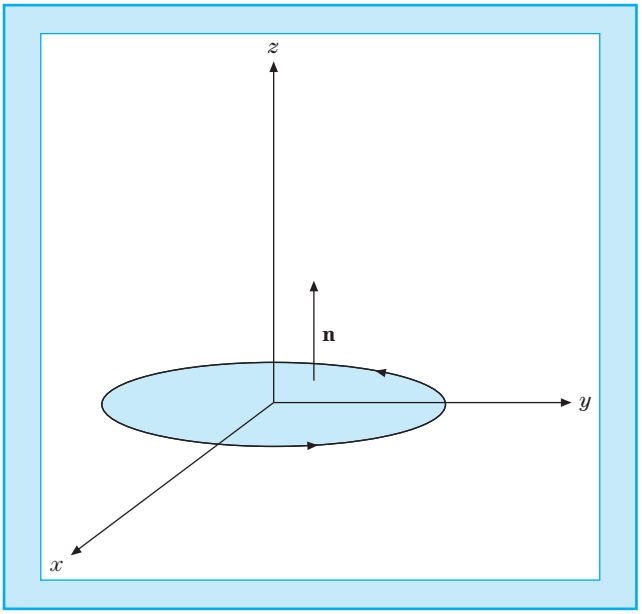


Figure 1.29

Right-Hand Rule for the Positive Normal

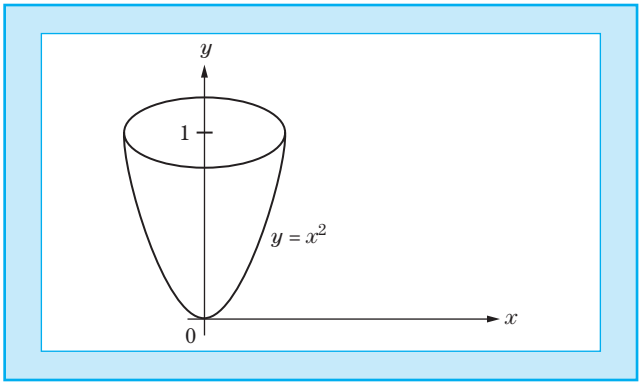


Figure 1.30

The Parabola $y = x^2$ for $0 \le y \le 1$ Rotated About the y-Axis

EXAMPLE 1.9.4

Moment of Inertia Let us determine the moment of inertia I_y of a segment of the parabola $y = x^2$ cut off by the line $y = 1$ and rotated about the y-axis (Fig. 1.30). We find

$$I_y = 2\mu \int_{x=0}^{1} \int_{y=x^2}^{1} x^2 \, dx \, dy = 2\mu \int_0^1 (1 - x^2) x^2 dx = 2\mu \left(\frac{x^3}{3} - \frac{x^5}{5} \right) \Big|_0^1 = \frac{4\mu}{15}.$$

The factor of 2 originates in the reflection symmetry of $x \to -x$, and μ is the constant mass density. ■

A surface in three-dimensional space may be explicitly given as $z = f(x, y)$ or by the coordinate functions of its points

$$x = x(u, v), \quad y = y(u, v), \quad z = z(u, v)$$

in terms of two parameters u, v or in implicit form $F(x, y, z) = 0$. The explicit form is a special case

$$F(x, y, z) \equiv z - f(x, y)$$

of the general implicit definition of a surface. We find the area $dA = dx\,dy/n_z$ over the projection $dx\,dy$ of the surface onto the xy-plane for the latter case. Here, $n_z = \cos\gamma$ is the z-component of the normal unit vector $\mathbf{n}$ at $\mathbf{r}$ on the surface so that γ is the angle of $d\mathbf{A}$ with the xy-plane. Thus, when we project $d\mathbf{A}$ to the xy-plane, we get $dA\cos\gamma = dx\,dy$, which proves this useful formula for measuring the **area of a curved surface**. From the gradient properties we also know that $\mathbf{n} = \nabla f/\sqrt{\nabla f^2}$.

EXAMPLE 1.9.5

A Surface Integral Here we apply the general formula for surface integrals to find the area on $z = xy = f(x, y)$ cut out by the unit circle in the xy-plane shown in Fig. 1.31. We start from

$$\frac{\partial f}{\partial x} = \frac{\partial z}{\partial x} = y, \quad \frac{\partial f}{\partial y} = \frac{\partial z}{\partial y} = x, \quad \frac{\partial f}{\partial z} = \frac{\partial z}{\partial z} = 1,$$

which we substitute into

$$n_z = 1/\sqrt{1 + \left(\frac{\partial z}{\partial x}\right)^2 + \left(\frac{\partial z}{\partial y}\right)^2}$$

for the normal to yield the area

$$A = \int_{x=-1}^{x=1} \int_{y=-\sqrt{1-x^2}}^{y=\sqrt{1-x^2}} \sqrt{1 + x^2 + y^2}\,dx\,dy.$$

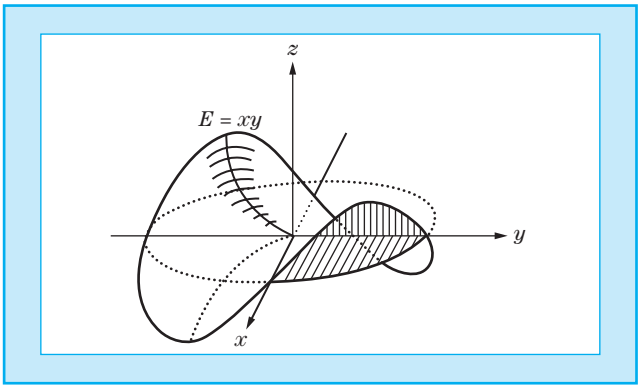


Figure 1.31

The Surface $z = xy$ Above and Below the Unit Circle $x^2 + y^2 = 1$

For the circular geometry plane polar coordinates r, φ are more appropriate, where the radial integral is evaluated by substituting $u = 1 + r^2$ in

$$A = \int_0^1 \sqrt{1+r^2}\, r\, dr \int_0^{2\pi} d\varphi = \pi \int \sqrt{u}\, du = \frac{2\pi}{3} \left|(1+r^2)^{3/2}\right|_0^1 = \frac{2\pi}{3}(2\sqrt{2}-1).$$

More examples of line and surface integrals are provided in Chapter 2.

Volume Integrals

Volume integrals are simpler because the volume element $d\tau$ is a scalar quantity.[15] We have

$$\int_v \mathbf{V}\, d\tau = \hat{\mathbf{x}} \int_v V_x\, d\tau + \hat{\mathbf{y}} \int_v V_y\, d\tau + \hat{\mathbf{z}} \int_v V_z\, d\tau, \tag{1.110}$$

again reducing the vector integral to a vector sum of scalar integrals.

If the vector

$$\mathbf{V} = V_\rho(\rho, \varphi, z)\hat{\boldsymbol{\rho}} + V_\varphi(\rho, \varphi, z)\hat{\boldsymbol{\varphi}} + V_z(\rho, \varphi, z)\hat{\mathbf{z}}$$

and its components are given in cylindrical coordinates $x = \rho\cos\varphi$, $y = \rho\sin\varphi$ with volume element $d\tau = \rho\, d\rho\, d\varphi\, dz$, the volume integral

$$\int_v \mathbf{V}\, d\tau = \hat{\mathbf{z}} \int_v V_z\, d\tau + \iiint (V_\rho \hat{\boldsymbol{\rho}} + V_\varphi \hat{\boldsymbol{\varphi}})\rho\, d\rho\, d\varphi\, dz$$

involves integrals over the varying unit vectors of the polar coordinates. To reduce them to scalar integrals, we need to expand the polar coordinate unit vectors in Cartesian unit vectors as follows. Dividing the plane coordinates by ρ, we find

$$\hat{\boldsymbol{\rho}} = \frac{1}{\rho}(x, y) = (\cos\varphi, \sin\varphi) = \hat{\mathbf{x}}\cos\varphi + \hat{\mathbf{y}}\sin\varphi.$$

Differentiating $\hat{\boldsymbol{\rho}}^2 = 1$, we see from $0 = \frac{d\hat{\rho}^2}{d\varphi} = 2\hat{\boldsymbol{\rho}} \cdot \frac{d\hat{\boldsymbol{\rho}}}{d\varphi}$ that

$$\frac{d\hat{\boldsymbol{\rho}}}{d\varphi} = -\hat{\mathbf{x}}\sin\varphi + \hat{\mathbf{y}}\cos\varphi = \hat{\boldsymbol{\varphi}}$$

is perpendicular to $\hat{\boldsymbol{\rho}}$ and a unit vector; therefore, it is equal to $\hat{\boldsymbol{\varphi}}$. Substituting these expressions into the second integral yields the final result

$$\begin{aligned}\int_v \mathbf{V}\, d\tau = \hat{\mathbf{z}} \int_v V_z\, d\tau + \hat{\mathbf{x}} \iiint [V_\rho \cos\varphi - V_\varphi \sin\varphi]\rho\, d\rho\, d\varphi\, dz \\ + \hat{\mathbf{y}} \iiint [V_\rho \sin\varphi + V_\varphi \cos\varphi]\rho\, d\rho\, d\varphi\, dz.\end{aligned} \tag{1.111}$$

The terms in brackets are the Cartesian components V_x, V_y expressed in plane polar coordinates.

[15] Frequently, the symbols d^3r and d^3x are used to denote a volume element in coordinate (xyz or $x_1x_2x_3$) space.

In spherical polar coordinates, all of the unit vectors depend on the coordinates, none can be pulled out of the integrals, and all have to be expanded in Cartesian unit vectors. This task of rewriting Eq. (1.110) is left as an exercise.

EXAMPLE 1.9.6

Volume of Rotated Gaussian Rotate the Gaussian $y = \exp(-x^2)$ about the z-axis leading to $z = \exp(-x^2 - y^2)$. Then the volume in the polar (cylindrical) coordinates appropriate for the geometry is given by

$$V = \int_{r=0}^{\infty}\int_{\varphi=0}^{2\pi}\int_{z=0}^{e^{-r^2}} r\,dr\,d\varphi\,dz = 2\pi\int_0^{\infty} re^{-r^2}dr = \pi\int_0^{\infty} e^{-u}du = \pi,$$

upon substituting $\exp(-x^2 - y^2) = \exp(-r^2)$, $dx\,dy = r\,dr\,d\varphi$, $u = r^2$, and $du = 2rdr$. ■

Integral Definitions of Gradient, Divergence, and Curl

One interesting and significant application of our surface and volume integrals is their use in developing alternate definitions of our differential relations. We find

$$\nabla\varphi = \lim_{\int d\tau\to 0}\frac{\int \varphi\,d\boldsymbol{\sigma}}{\int d\tau}, \tag{1.112}$$

$$\nabla\cdot\mathbf{V} = \lim_{\int d\tau\to 0}\frac{\int \mathbf{V}\cdot d\boldsymbol{\sigma}}{\int d\tau}, \tag{1.113}$$

$$\nabla\times\mathbf{V} = \lim_{\int d\tau\to 0}\frac{\int d\boldsymbol{\sigma}\times\mathbf{V}}{\int d\tau}. \tag{1.114}$$

In these three equations, $\int d\tau$ is the volume of a small region of space and $d\boldsymbol{\sigma}$ is the vector area element of this volume. The identification of Eq. (1.113) as the divergence of $\mathbf{V}$ was carried out in Section 1.6. Here, we show that Eq. (1.112) is consistent with our earlier definition of $\nabla\varphi$ [Eq. (1.64)]. For simplicity, we choose $d\tau$ to be the differential volume $dx\,dy\,dz$ (Fig. 1.32). This

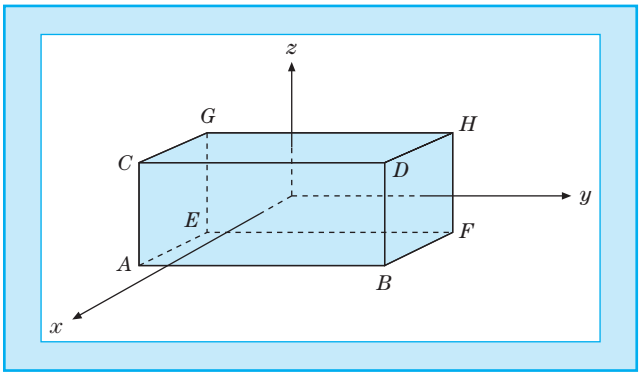


Figure 1.32

Differential Rectangular Parallelepiped (Origin at Center)

time, we place the origin at the geometric center of our volume element. The area integral leads to six integrals, one for each of the six faces. Remembering that $d\boldsymbol{\sigma}$ is outward, $d\boldsymbol{\sigma}\cdot\hat{\mathbf{x}} = -|d\boldsymbol{\sigma}|$ for surface *EFHG*, and $+|d\boldsymbol{\sigma}|$ for surface *ABDC*, we have

$$\begin{aligned}\int \varphi\, d\boldsymbol{\sigma} = &-\hat{\mathbf{x}}\int_{EFHG}\left(\varphi - \frac{\partial\varphi}{\partial x}\frac{dx}{2}\right)dy\,dz + \hat{\mathbf{x}}\int_{ABDC}\left(\varphi + \frac{\partial\varphi}{\partial x}\frac{dx}{2}\right)dy\,dz\\ &-\hat{\mathbf{y}}\int_{AEGC}\left(\varphi - \frac{\partial\varphi}{\partial y}\frac{dy}{2}\right)dx\,dz + \hat{\mathbf{y}}\int_{BFHD}\left(\varphi + \frac{\partial\varphi}{\partial y}\frac{dy}{2}\right)dx\,dz\\ &-\hat{\mathbf{z}}\int_{ABFE}\left(\varphi - \frac{\partial\varphi}{\partial z}\frac{dz}{2}\right)dx\,dy + \hat{\mathbf{z}}\int_{CDHG}\left(\varphi + \frac{\partial\varphi}{\partial z}\frac{dz}{2}\right)dx\,dy.\end{aligned}$$

Using the first two terms of a Maclaurin expansion, we evaluate each integrand at the origin with a correction included to correct for the displacement ($\pm dx/2$, etc.) of the center of the face from the origin. Having chosen the total volume to be of differential size ($\int d\tau = dx\,dy\,dz$), we drop the integral signs on the right and obtain

$$\int \varphi\, d\boldsymbol{\sigma} = \left(\hat{\mathbf{x}}\frac{\partial\varphi}{\partial x} + \hat{\mathbf{y}}\frac{\partial\varphi}{\partial y} + \hat{\mathbf{z}}\frac{\partial\varphi}{\partial z}\right)dx\,dy\,dz. \tag{1.115}$$

Dividing by

$$\int d\tau = dx\,dy\,dz,$$

we verify Eq. (1.112).

This verification has been oversimplified in ignoring other correction terms beyond the first derivatives. These additional terms, which are introduced in Section 5.6 when the Taylor expansion is developed, vanish in the limit

$$\int d\tau \to 0\,(dx \to 0, dy \to 0, dz \to 0).$$

This, of course, is the reason for specifying in Eqs. (1.112)–(1.114) that this limit be taken. Verification of Eq. (1.114) follows these same lines, using a differential volume $d\tau = dx\,dy\,dz$.

EXERCISES

1.9.1 Find the potential for the electric field generated by a charge q at the origin. Normalize the potential to zero at spatial infinity.

1.9.2 Determine the gravitational field of the earth taken to be spherical and of uniform mass density. Punch out a concentric spherical cavity and show that the field is zero inside it. Show that the field is constant if the cavity is not concentric.

1.9.3 Evaluate

$$\frac{1}{3}\int_s \mathbf{r}\cdot d\boldsymbol{\sigma}$$

over the unit cube defined by the point (0, 0, 0) and the unit intercepts on the positive x-, y-, and z-axes. Note that (a) $\mathbf{r}\cdot d\boldsymbol{\sigma}$ is zero for three of the surfaces, and (b) each of the three remaining surfaces contributes the same amount to the integral.

1.9.4 Show by expansion of the surface integral that

$$\lim_{\int d\tau\to 0}\frac{\int_s d\boldsymbol{\sigma}\times\mathbf{V}}{\int d\tau} = \boldsymbol{\nabla}\times\mathbf{V}.$$

Hint. Choose the volume to be a differential volume, $dx\,dy\,dz$.

1.10 Gauss's Theorem

Here, we derive a useful relation between a surface integral of a vector and the volume integral of the divergence of that vector. Let us assume that the vector $\mathbf{V}$ and its first derivatives are continuous over the simply connected region (without holes) of interest. Then, **Gauss's theorem** states that

$$\int_S \mathbf{V}\cdot d\boldsymbol{\sigma} = \int_V \boldsymbol{\nabla}\cdot\mathbf{V}\,d\tau. \tag{1.116a}$$

In words, the surface integral of a vector over a closed surface equals the volume integral of the divergence of that vector integrated over the volume enclosed by the surface.

Imagine that volume V is subdivided into an arbitrarily large number of tiny (differential) parallelepipeds. For each parallelepiped,

$$\sum_{\text{six surfaces}} \mathbf{V}\cdot d\boldsymbol{\sigma} = \boldsymbol{\nabla}\cdot\mathbf{V}\,d\tau \tag{1.116b}$$

from the analysis of Section 1.6, Eq. (1.75), with $\rho\mathbf{v}$ replaced by $\mathbf{V}$. The summation is over the six faces of the parallelepiped. Summing over all parallelepipeds, we find that the $\mathbf{V}\cdot d\boldsymbol{\sigma}$ terms cancel (pairwise) for all **interior** faces; only the contributions of the **exterior** surfaces survive (Fig. 1.33). Analogous to the definition of a Riemann integral as the limit of a sum, we take the limit as the number of parallelepipeds approaches infinity ($\to\infty$) and the dimensions of each approach zero ($\to 0$):

$$\sum_{\text{exterior surfaces}} \mathbf{V}\cdot_{\downarrow} d\boldsymbol{\sigma} = \sum_{\text{volumes}} \boldsymbol{\nabla}\cdot_{\downarrow}\mathbf{V}\,d\tau$$

$$\int_S \mathbf{V}\cdot d\boldsymbol{\sigma} = \int_V \boldsymbol{\nabla}\cdot\mathbf{V}\,d\tau.$$

The result is Eq. (1.116a), Gauss's theorem.

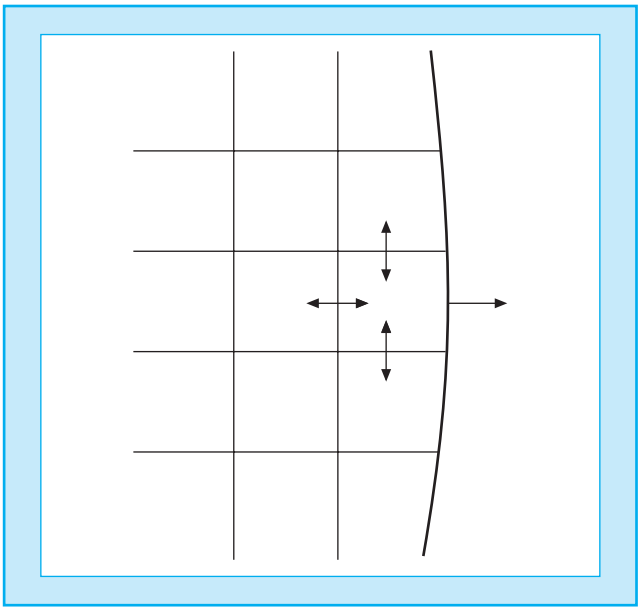


Figure 1.33

Exact Cancellation of $\mathbf{V} \cdot d\boldsymbol{\sigma}$'s on Interior Surfaces. No Cancellation on the Exterior Surface

From a physical standpoint, Eq. (1.75) has established $\nabla \cdot \mathbf{V}$ as the net outflow of field per unit volume. The volume integral then gives the total net outflow. However, the surface integral $\int \mathbf{V} \cdot d\boldsymbol{\sigma}$ is just another way of expressing this same quantity, which is the equality, Gauss's theorem.

Biographical Data

Gauss, Carl Friedrich. Gauss, a German mathematician, physicist, and astronomer, was born in Brunswick in 1777 and died in Göttingen in 1855. He was an infant prodigy in mathematics whose education was directed and financed by the Duke of Brunswick. As a teenager, he proved that regular n-polygons can be constructed in Euclidean geometry provided n is a Fermat prime number such as 3, 5, 17, and 257, a major advance in geometry since antiquity. This feat convinced him to stay in mathematics and give up the study of foreign languages. For his Ph.D., he proved the fundamental theorem of algebra, avoiding the then controversial complex numbers he had used to discover it. In his famous treatise *Disquisitiones Arithmetica* on number theory, he first proved the quadratic reciprocity theorem and originated the terse style and rigor of mathematical proofs as a series of logical steps, discarding any trace of the original heuristic ideas used in the discovery and checks of examples. Not surprisingly, he hated teaching. He is considered by many as the greatest mathematician of all times and was the last to provide major contributions to all then existing branches of mathematics. As the founder of differential geometry, he developed the intrinsic properties of surfaces, such as curvature, which later motivated B. Riemann to develop the geometry of metric spaces, the mathematical foundation

of Einstein's General Relativity. In astronomy (for the orbit of the asteroid Ceres), he developed the method of least squares for fitting curves to data. In physics, he developed potential theory, and the unit of the magnetic induction is named after him in honor of his measurements and development of units in physics.

Green's Theorem

A frequently useful corollary of Gauss's theorem is a relation known as Green's theorem. If u and v are two scalar functions, we have the identities

$$\nabla \cdot (u\nabla v) = u\nabla \cdot \nabla v + (\nabla u) \cdot (\nabla v), \tag{1.117}$$

$$\nabla \cdot (v\nabla u) = v\nabla \cdot \nabla u + (\nabla v) \cdot (\nabla u), \tag{1.118}$$

which follow from the product rule of differentiation. Subtracting Eq. (1.118) from Eq. (1.117), integrating over a volume (u, v, and their derivatives, assumed continuous), and applying Eq. (1.116a) (Gauss's theorem), we obtain

$$\int_V (u\nabla \cdot \nabla v - v\nabla \cdot \nabla u)\, d\tau = \int_S (u\nabla v - v\nabla u) \cdot d\boldsymbol{\sigma}. \tag{1.119}$$

This is **Green's theorem**, which states that the antisymmetric Laplacian of a pair of functions integrated over a simply connected volume (no holes) is equivalent to the antisymmetric gradient of the pair integrated over the bounding surface. An alternate form of Green's theorem derived from Eq. (1.117) alone is

$$\int_S u\nabla v \cdot d\boldsymbol{\sigma} = \int_V u\nabla \cdot \nabla v\, d\tau + \int_V \nabla u \cdot \nabla v\, d\tau. \tag{1.120}$$

Finally, Gauss's theorem may also be extended to tensors (see Section 2.11).

Biographical Data

Green, George. Green, an English mathematician, was born in Nottingham in 1793 and died near Nottingham in 1841. He studied Laplace's papers in Cambridge and developed potential theory in electrodynamics.

EXERCISES

1.10.1 If $\mathbf{B} = \nabla \times \mathbf{A}$, show that

$$\int_S \mathbf{B} \cdot d\boldsymbol{\sigma} = 0$$

for any closed surface S. State this in words. If symbolic software is available, check this for a typical vector potential and specific surfaces, such as a sphere or cube.

1.10.2 Over some volume V, let ψ be a solution of Laplace's equation (with the derivatives appearing there continuous). Prove that the integral over

any closed surface in V of the normal derivative of ψ ($\partial\psi/\partial n$, or $\nabla\psi\cdot\mathbf{n}$) will be zero.

1.10.3 In analogy to the integral definition of gradient, divergence, and curl of Section 1.10, show that

$$\nabla^2\varphi = \lim_{\int d\tau\to 0} \frac{\int \nabla\varphi\cdot d\boldsymbol{\sigma}}{\int d\tau}.$$

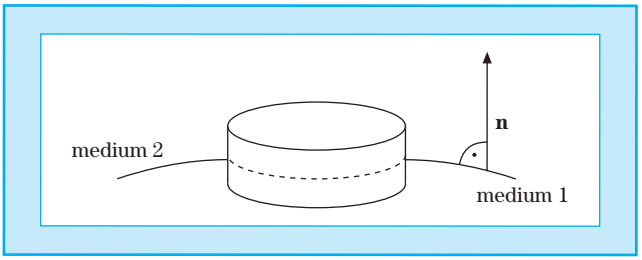
1.10.4 The electric displacement vector $\mathbf{D}$ satisfies the Maxwell equation $\nabla\cdot\mathbf{D} = \rho$, where ρ is the charge density (per unit volume). At the boundary between two media there is a surface charge density σ (per unit area). Show that a boundary condition for $\mathbf{D}$ is

$$(\mathbf{D}_2 - \mathbf{D}_1)\cdot\mathbf{n} = \sigma,$$

where $\mathbf{n}$ is a unit vector normal to the surface and out of medium 1.
Hint. Consider a thin pillbox as shown in Fig. 1.34.

Figure 1.34

Pillbox



1.10.5 From Eq. (1.77) and Example 1.6.1, with $\mathbf{V}$ the electric field $\mathbf{E}$ and f the electrostatic potential φ, show that

$$\int \rho\varphi\, d\tau = \varepsilon_0 \int E^2\, d\tau.$$

This corresponds to a three-dimensional integration by parts.
Hint. $\mathbf{E} = -\nabla\varphi$, $\nabla\cdot\mathbf{E} = \rho/\varepsilon_0$. You may assume that φ vanishes at large r at least as fast as r^{-1}.

1.10.6 The creation of a **localized** system of steady electric currents (current density $\mathbf{J}$) and magnetic fields may be shown to require an amount of work

$$W = \frac{1}{2}\int \mathbf{H}\cdot\mathbf{B}\, d\tau.$$

Transform this into

$$W = \frac{1}{2}\int \mathbf{J}\cdot\mathbf{A}\, d\tau,$$

where $\mathbf{A}$ is the magnetic vector potential, $\nabla\times\mathbf{A} = \mathbf{B}$.

Hint. In Maxwell's equations, take the displacement current term $\partial \mathbf{D}/\partial t = 0$ and explain why using Ohm's law. If the fields and currents are localized, a bounding surface may be taken far enough out so that the integrals of the fields and currents over the surface yield zero.

1.11 Stokes's Theorem

Gauss's theorem relates the volume integral of a derivative of a function to an integral of the function over the closed surface bounding the volume. Here, we consider an analogous relation between the surface integral of a derivative of a function and the line integral of the function, the path of integration being the perimeter bounding the surface.

Let us take the surface and subdivide it into a network of arbitrarily small rectangles. In Section 1.7, we showed that the circulation about such a differential rectangle (in the xy-plane) is $\nabla \times \mathbf{V}|_z \, dx\, dy$. From Eq. (1.85) applied to **one** differential rectangle,

$$\sum_{\text{four sides}} \mathbf{V} \cdot d\boldsymbol{\lambda} = \nabla \times \mathbf{V} \cdot d\boldsymbol{\sigma}. \tag{1.121}$$

We sum over all the little rectangles as in the definition of a Riemann integral. The surface contributions [right-hand side of Eq. (1.121)] are added together. The line integrals [left-hand side of Eq. (1.121)] of all **interior** line segments cancel identically. Only the line integral around the perimeter survives (Fig. 1.35). Taking the usual limit as the number of rectangles approaches

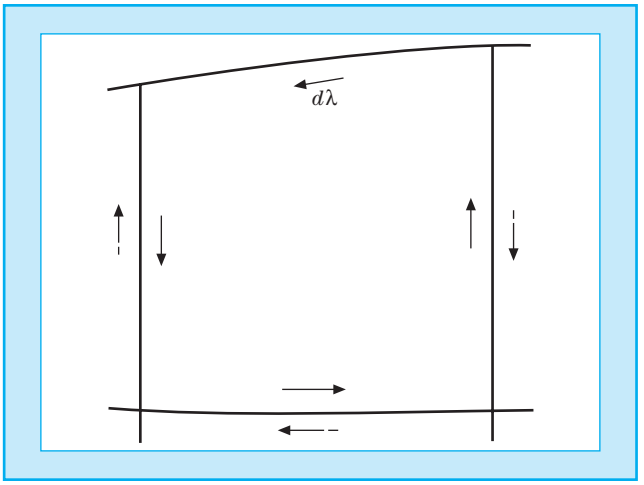


Figure 1.35

Exact Cancellation on Interior Paths; No Cancellation on the Exterior Path

infinity while $dx \to 0$, $dy \to 0$, we have

$$\sum_{\substack{\text{exterior line}\\ \text{segments}}} \mathbf{V}\cdot d\boldsymbol{\lambda} = \sum_{\text{rectangles}} \boldsymbol{\nabla}\times\mathbf{V}\cdot d\boldsymbol{\sigma}$$

$$\downarrow \qquad\qquad \downarrow$$

$$\oint \mathbf{V}\cdot d\boldsymbol{\lambda} = \int_S \boldsymbol{\nabla}\times\mathbf{V}\cdot d\boldsymbol{\sigma}. \tag{1.122}$$

This is Stokes's theorem. The surface integral on the right is over the surface bounded by the perimeter or contour for the line integral on the left. The direction of the vector representing the area is out of the paper plane toward the reader if the direction of traversal around the contour for the line integral is in the positive mathematical sense as shown in Fig. 1.35.

This demonstration of Stokes's theorem is limited by the fact that we used a Maclaurin expansion of $\mathbf{V}(x, y, z)$ in establishing Eq. (1.85) in Section 1.7. Actually, we need only demand that the curl of $\mathbf{V}(x, y, z)$ exists and that it be integrable over the surface. Stokes's theorem obviously applies to an open, simply connected surface. It is possible to consider a closed surface as a limiting case of an open surface with the opening (and therefore the perimeter) shrinking to zero. This is the point of Exercise 1.11.4.

As a special case of Stokes's theorem, consider the curl of a two-dimensional vector field $\mathbf{V} = (V_1(x, y), V_2(x, y), 0)$. The curl $\boldsymbol{\nabla}\times\mathbf{V} = (0, 0, \frac{\partial V_2}{\partial x} - \frac{\partial V_1}{\partial y})$ so

$$\int_S \boldsymbol{\nabla}\times\mathbf{V}\cdot\hat{\mathbf{z}}\,dx\,dy = \int_S \left(\frac{\partial V_2}{\partial x} - \frac{\partial V_1}{\partial y}\right) dx\,dy = \int_C \mathbf{V}\cdot d\mathbf{r} = \int_C (V_1 dx + V_2 dy),$$

where the curve C is the boundary of the simply connected surface S that is integrated in the positive mathematical sense (anticlockwise). This relation is sometimes also called Green's theorem. In Chapter 6, we shall use it to prove Cauchy's theorem for analytic functions.

EXAMPLE 1.11.1

Area as a Line Integral For the two-dimensional Stokes's theorem, we first choose $\mathbf{V} = x\hat{\mathbf{y}}$, which gives the area $S = \int_S dx\,dy = \int_C x\,dy$, and for $\mathbf{V} = (y\hat{\mathbf{x}})$ we get similarly $S = \int_S dx\,dy = -\int_C y\,dx$. Adding both results gives the area

$$S = \frac{1}{2}\int_C (x\,dy - y\,dx). \quad \blacksquare$$

We can use Stokes's theorem to derive Oersted's and Faraday's laws from two of Maxwell's equations and vice versa, thus recognizing that the former are an integrated form of the latter.

EXAMPLE 1.11.2

Oersted's and Faraday's Laws Consider the magnetic field generated by a long wire that carries a stationary current I (Fig. 1.36). Starting from Maxwell's differential law $\boldsymbol{\nabla}\times\mathbf{H} = \mathbf{J}$ [Eq. (1.97c); with Maxwell's displacement current $\partial\mathbf{D}/\partial t = 0$ for a stationary current case by Ohm's law], we integrate over a closed area S perpendicular to and surrounding the wire and apply Stokes's

Figure 1.36

Oersted's Law for a Long Wire Carrying a Current

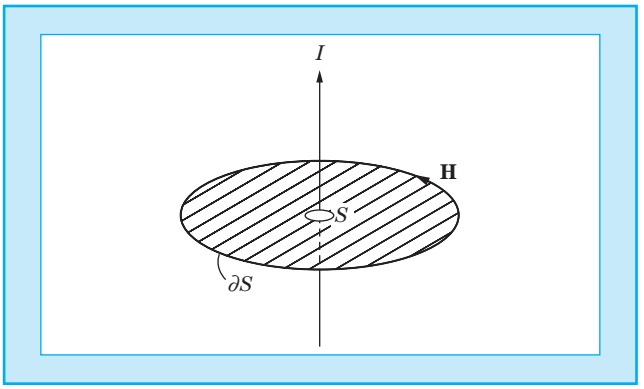
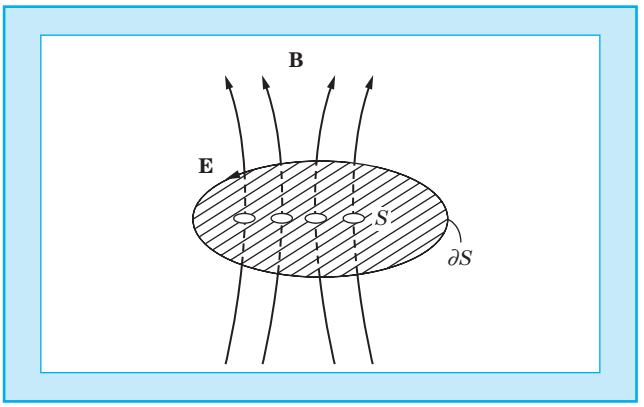


Figure 1.37

Faraday's Induction Law Across a Magnetic Induction Field



theorem to get

$$I = \int_S \mathbf{J} \cdot d\boldsymbol{\sigma} = \int_S (\boldsymbol{\nabla} \times \mathbf{H}) \cdot d\boldsymbol{\sigma} = \oint_{\partial S} \mathbf{H} \cdot d\mathbf{r},$$

which is Oersted's law. Here, the line integral is along ∂S, the closed curve surrounding the cross section area S.

Similarly, we can integrate Maxwell's equation for $\boldsymbol{\nabla} \times \mathbf{E}$ [Eq. (1.97d)] to yield Faraday's induction law. Imagine moving a closed loop (∂S) of wire (of area S) across a magnetic induction field $\mathbf{B}$ (Fig. 1.37). At a fixed moment of time we integrate Maxwell's equation and use Stokes's theorem, yielding

$$\int_{\partial S} \mathbf{E} \cdot d\mathbf{r} = \int_S (\boldsymbol{\nabla} \times \mathbf{E}) \cdot d\boldsymbol{\sigma} = -\frac{d}{dt} \int_S \mathbf{B} \cdot d\boldsymbol{\sigma} = -\frac{d\Phi}{dt},$$

which is Faraday's law. The line integral on the left-hand side represents the voltage induced in the wire loop, whereas the right-hand side is the change with time of the magnetic flux Φ through the moving surface S of the wire. ■

SUMMARY

Both Stokes's and Gauss's theorems are of tremendous importance in a wide variety of problems involving vector calculus in electrodynamics, where they

allow us to derive the local form of Maxwell's differential equations from the global (integral) form of the experimental laws. An indication of their power and versatility may be obtained from the exercises in Sections 1.10 and 1.11 and the development of potential theory in Section 1.12.

Biographical Data

Stokes, Sir George Gabriel. Stokes, a British mathematician and physicist, was born in Skreen, Ireland, in 1819 and died in Cambridge in 1903. Son of a clergyman, his talent for mathematics was already evident in school. In 1849, he became Lucasian professor at Cambridge, the chair Isaac Newton once held and currently held by S. Hawking. In 1885, he became president of the Royal Society. He is known for the theory of viscous fluids, with practical applications to the motion of ships in water. He demonstrated his vision by hailing Joule's work early on and recognizing X-rays as electromagnetic radiation. He received the Rumford and Copley medals of the Royal Society and served as a member of Parliament for Cambridge University in 1887–1892.

EXERCISES

1.11.1 The calculation of the magnetic moment of a current loop leads to the line integral

$$\oint \mathbf{r} \times d\mathbf{r}.$$

(a) Integrate around the perimeter of a current loop (in the xy-plane) and show that the scalar magnitude of this line integral is twice the area of the enclosed surface.

(b) The perimeter of an ellipse is described by $\mathbf{r} = \hat{\mathbf{x}}a\cos\theta + \hat{\mathbf{y}}b\sin\theta$. From part (a), show that the area of the ellipse is πab.

1.11.2 In steady state, the magnetic field $\mathbf{H}$ satisfies the Maxwell equation $\nabla \times \mathbf{H} = \mathbf{J}$, where $\mathbf{J}$ is the current density (per square meter). At the boundary between two media there is a surface current density $\mathbf{K}$ (perimeter). Show that a boundary condition on $\mathbf{H}$ is

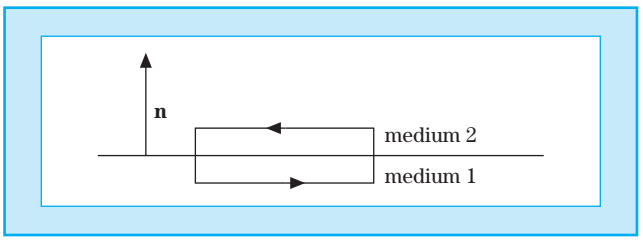
$$\mathbf{n} \times (\mathbf{H}_2 - \mathbf{H}_1) = \mathbf{K},$$

where $\mathbf{n}$ is a unit vector normal to the surface and out of medium 1.

Hint. Consider a narrow loop perpendicular to the interface as shown in Fig. 1.38.

Figure 1.38

Loop Contour



1.11.3 A magnetic induction **B** is generated by electric current in a ring of radius R. Show that the **magnitude** of the vector potential **A** ($\mathbf{B} = \nabla \times \mathbf{A}$) at the ring is

$$|\mathbf{A}| = \frac{\Phi}{2\pi R},$$

where Φ is the total magnetic flux passing through the ring.
Note. **A** is tangential to the ring.

1.11.4 Prove that

$$\int_S \nabla \times \mathbf{V} \cdot d\boldsymbol{\sigma} = 0$$

if S is a closed surface.

1.11.5 Prove that

$$\oint u \nabla v \cdot d\boldsymbol{\lambda} = -\oint v \nabla u \cdot d\boldsymbol{\lambda}.$$

1.11.6 Prove that

$$\oint u \nabla v \cdot d\boldsymbol{\lambda} = \int_S (\nabla u) \times (\nabla v) \cdot d\boldsymbol{\sigma}.$$

1.12 Potential Theory

Scalar Potential

This section formulates the conditions under which a force field **F** is conservative. From a mathematical standpoint, it is a practice session of typical applications of Gauss's and Stokes's theorems in physics.

If a force in a given **simply connected region** of space V (i.e., no holes in it) can be expressed as the negative gradient of a scalar function φ,

$$\mathbf{F} = -\nabla\varphi, \tag{1.123}$$

we call φ a scalar potential that describes the force by one function instead of three, which is a significant simplification. A scalar potential is only determined up to an additive constant, which can be used to adjust its value at infinity (usually zero) or at some other point. The force **F** appearing as the negative gradient of a single-valued scalar potential is labeled a **conservative** force. We want to know when a scalar potential function exists. To answer this question, we establish two other relations as equivalent to Eq. (1.123):

$$\nabla \times \mathbf{F} = 0 \tag{1.124}$$

and

$$\oint \mathbf{F} \cdot d\mathbf{r} = 0, \tag{1.125}$$

for every closed path in our simply connected region V. We proceed to show that each of these three equations implies the other two. Let us start with

$$\mathbf{F} = -\nabla\varphi. \tag{1.126}$$

Then

$$\nabla \times \mathbf{F} = -\nabla \times \nabla\varphi = 0 \tag{1.127}$$

by Eq. (1.92), or Eq. (1.123) implies Eq. (1.124). Turning to the line integral, we have

$$\oint \mathbf{F} \cdot d\mathbf{r} = -\oint \nabla\varphi \cdot d\mathbf{r} = -\oint d\varphi \tag{1.128}$$

using Eq. (1.58). Now $d\varphi$ integrates to give φ. Because we have specified a closed loop, the end points coincide and we get zero for every closed path in our region S for which Eq. (1.123) holds. It is important to note the restriction that the potential be single-valued and that Eq. (1.123) hold for **all** points in S. This derivation may also apply to a scalar magnetic potential as long as no net current is encircled. As soon as we choose a path in space that encircles a net current, the scalar magnetic potential ceases to be single-valued and our analysis no longer applies because V is no longer simply connected.

Continuing this demonstration of equivalence, let us assume that Eq. (1.125) holds. If $\oint \mathbf{F} \cdot d\mathbf{r} = 0$ for all paths in S, the value of the integral joining two distinct points A and B is independent of the path (Fig. 1.39). Our premise is that

$$\oint_{ACBDA} \mathbf{F} \cdot d\mathbf{r} = 0. \tag{1.129}$$

Therefore,

$$\oint_{ACB} \mathbf{F} \cdot d\mathbf{r} = -\int_{BDA} \mathbf{F} \cdot d\mathbf{r} = \int_{ADB} \mathbf{F} \cdot d\mathbf{r}, \tag{1.130}$$

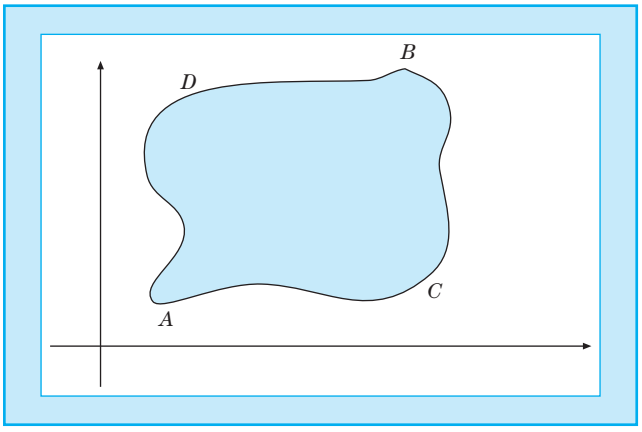


Figure 1.39

Possible Paths for Doing Work

reversing the sign by reversing the direction of integration. Physically, this means that the work done in going from A to B is independent of the path and that the work done in going around a closed path is zero. This is the reason for labeling such a force conservative: Energy is conserved.

With the result shown in Eq. (1.130), we have the work done dependent only on the end points A and B. That is,

$$\text{Work done by force} = \int_A^B \mathbf{F} \cdot d\mathbf{r} = \varphi(A) - \varphi(B). \tag{1.131}$$

Equation (1.131) defines a scalar potential (strictly speaking, the difference in potential between points A and B) and provides a means of calculating the potential. If point B is taken as a variable such as (x, y, z), then differentiation with respect to x, y, and z will recover Eq. (1.123).

The choice of sign on the right-hand side is arbitrary. The choice here is made to achieve agreement with Eq. (1.123) and to ensure that water will run downhill rather than uphill. For points A and B separated by a length $d\mathbf{r}$, Eq. (1.131) becomes

$$\mathbf{F} \cdot d\mathbf{r} = -d\varphi = -\nabla\varphi \cdot d\mathbf{r}. \tag{1.132}$$

This may be rewritten

$$(\mathbf{F} + \nabla\varphi) \cdot d\mathbf{r} = 0, \tag{1.133}$$

and since $d\mathbf{r} \neq 0$ is arbitrary, Eq. (1.126) must follow. If

$$\oint \mathbf{F} \cdot d\mathbf{r} = 0, \tag{1.134}$$

we may obtain Eq. (1.123) by using Stokes's theorem [Eq. (1.122)]:

$$\oint \mathbf{F} \cdot d\mathbf{r} = \int \nabla \times \mathbf{F} \cdot d\boldsymbol{\sigma}. \tag{1.135}$$

If we take the path of integration to be the perimeter of an arbitrary differential area $d\boldsymbol{\sigma}$, the integrand in the surface integral must vanish. Hence, Eq. (1.125) implies Eq. (1.123).

Finally, if $\nabla \times \mathbf{F} = 0$, we need only reverse our statement of Stokes's theorem [Eq. (1.135)] to derive Eq. (1.125). Then, by Eqs. (1.131)–(1.133) the initial statement $\mathbf{F} = -\nabla\varphi$ is derived. The triple equivalence is illustrated in Fig. 1.40.

SUMMARY

A single-valued scalar potential function φ exists if and only if $\mathbf{F}$ is irrotational so that the work done around every closed loop is zero. The gravitational and electrostatic force fields given by Eq. (1.88) are irrotational and therefore conservative. Gravitational and electrostatic scalar potentials exist. Now, by calculating the work done [Eq. (1.131)], we proceed to determine three potentials (Fig. 1.41).

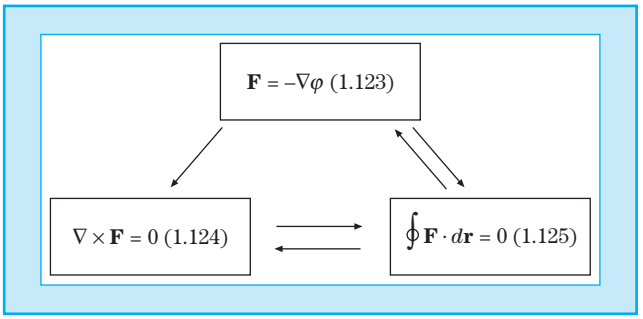


Figure 1.40

Equivalent Formulations of a Conservative Force

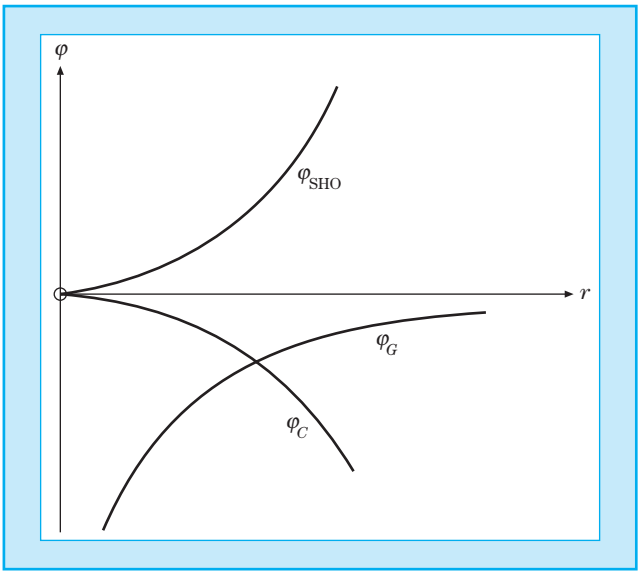


Figure 1.41

Potential Energy Versus Distance (Gravitational, Centrifugal, and Simple Harmonic Oscillator)

EXAMPLE 1.12.1

Centrifugal Potential Calculate the scalar potential for the **centrifugal** force per unit mass, $\mathbf{F}_C = \omega^2\mathbf{r}$, radially **outward**. Physically, the centrifugal force is what you feel when on a merry-go-round. Proceeding as in Example 1.9.3, but integrating from the origin outward and taking $\varphi_C(0) = 0$, we have

$$\varphi_C(r) = -\int_0^r \mathbf{F}_C \cdot d\mathbf{r} = -\frac{\omega^2 r^2}{2}.$$

If we reverse signs, taking $\mathbf{F}_{\text{SHO}} = -k\mathbf{r}$, we obtain $\varphi_{\text{SHO}} = \frac{1}{2}kr^2$, the simple harmonic oscillator potential.

The gravitational, centrifugal, and simple harmonic oscillator potentials are shown in Fig. 1.41. Clearly, the simple harmonic oscillator yields stability and describes a restoring force. The centrifugal potential describes an unstable situation. ■

SUMMARY

When a vector **B** is solenoidal, a vector potential **A** exists such that $\mathbf{B} = \nabla \times \mathbf{A}$. **A** is undetermined to within an additive gradient of a scalar function. This is similar to the arbitrary zero of a potential, due to an additive constant of the scalar potential.

In many problems, the magnetic vector potential **A** will be obtained from the current distribution that produces the magnetic induction **B**. This means solving Poisson's (vector) equation (see Exercise 1.13.4).

EXERCISES

1.12.1 The usual problem in classical mechanics is to calculate the motion of a particle given the potential. For a uniform density (ρ_0), nonrotating massive sphere, Gauss's law (Section 1.10) leads to a gravitational force on a unit mass m_0 at a point r_0 produced by the attraction of the mass at $r \le r_0$. The mass at $r > r_0$ contributes nothing to the force.

(a) Show that $\mathbf{F}/m_0 = -(4\pi G\rho_0/3)\mathbf{r}$, $0 \le r \le a$, where a is the radius of the sphere.

(b) Find the corresponding gravitational potential, $0 \le r \le a$.

(c) Imagine a vertical hole running completely through the center of the earth and out to the far side. Neglecting the rotation of the earth and assuming a uniform density $\rho_0 = 5.5\,\text{g/cm}^3$, calculate the nature of the motion of a particle dropped into the hole. What is its period? *Note.* $\mathbf{F} \propto \mathbf{r}$ is actually a very poor approximation. Because of varying density, the approximation $\mathbf{F} =$ constant, along the outer half of a radial line, and $\mathbf{F} \propto \mathbf{r}$, along the inner half, is much closer.

1.12.2 The origin of the Cartesian coordinates is at the earth's center. The moon is on the z-axis, a fixed distance R away (center-to-center distance). The tidal force exerted by the moon on a particle at the earth's surface (point x, y, z) is given by

$$F_x = -GMm\frac{x}{R^3}, \quad F_y = -GMm\frac{y}{R^3}, \quad F_z = +2GMm\frac{z}{R^3}.$$

Find the potential that yields this tidal force.

ANS. $$-\frac{GMm}{R^3}\left(z^2 - \frac{1}{2}x^2 - \frac{1}{2}y^2\right)$$

In terms of the Legendre polynomials of Chapter 11, this becomes

$$-\frac{GMm}{R^3}r^2 P_2(\cos\theta).$$

1.12.3 Vector **B** is formed by the product of two gradients

$$\mathbf{B} = (\nabla u) \times (\nabla v),$$

where u and v are scalar functions.

(a) Show that $\mathbf{B}$ is solenoidal.
(b) Show that

$$\mathbf{A} = \frac{1}{2}(u\,\nabla v - v\,\nabla u)$$

is a vector potential for $\mathbf{B}$ in that

$$\mathbf{B} = \nabla \times \mathbf{A}.$$

1.12.4 The magnetic induction $\mathbf{B}$ is related to the magnetic vector potential $\mathbf{A}$ by $\mathbf{B} = \nabla \times \mathbf{A}$. By Stokes's theorem,

$$\int \mathbf{B} \cdot d\boldsymbol{\sigma} = \oint \mathbf{A} \cdot d\mathbf{r}.$$

Show that each side of this equation is invariant under the **gauge transformation**, $\mathbf{A} \to \mathbf{A} + \nabla\Lambda$, where Λ is an arbitrary scalar function.
Note. Take the function Λ to be single-valued.

1.12.5 With $\mathbf{E}$ as the electric field and $\mathbf{A}$ as the magnetic vector potential, show that $[\mathbf{E} + \partial\mathbf{A}/\partial t]$ is irrotational and that we may therefore write

$$\mathbf{E} = -\nabla\varphi - \frac{\partial \mathbf{A}}{\partial t}.$$

1.12.6 The total force on a charge q moving with velocity $\mathbf{v}$ is

$$\mathbf{F} = q(\mathbf{E} + \mathbf{v} \times \mathbf{B}).$$

Using the scalar and vector potentials, show that

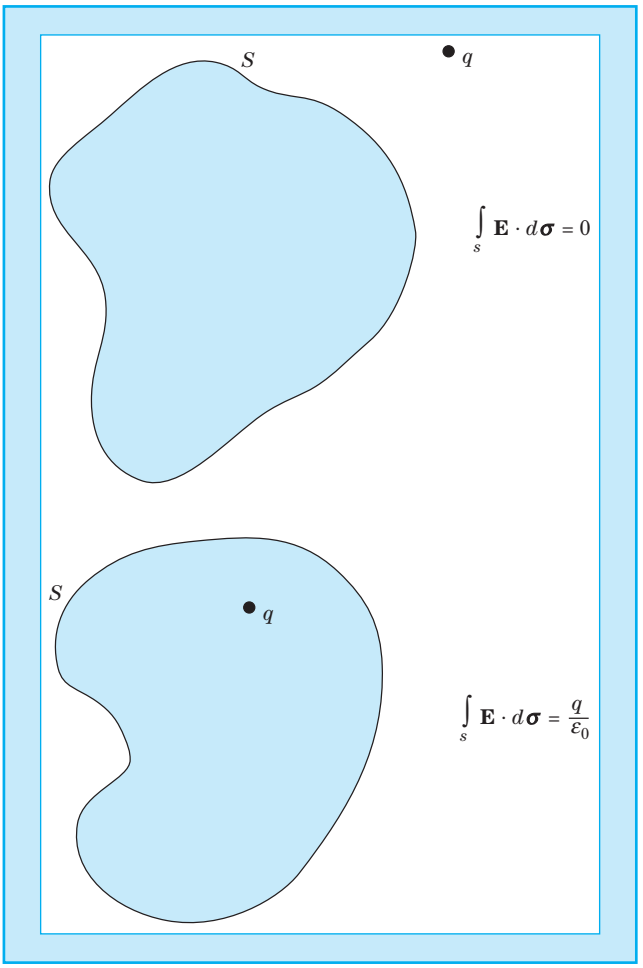
$$\mathbf{F} = q\left[-\nabla\varphi - \frac{d\mathbf{A}}{dt} + \nabla(\mathbf{A} \cdot \mathbf{v})\right].$$

Note that we now have a total time derivative of $\mathbf{A}$ in place of the partial derivative of Exercise 1.12.5.

1.12.7 A planet of mass m moves on a circular orbit of radius r around a star in an attractive gravitational potential $V = kr^n$. Find the conditions on the exponent n for the orbit to be stable.
Note. You can set $k = -GmM$, where M is the mass of the star, and use classical mechanics. Einstein's General Relativity gives $n = -1$, whereas in Newton's gravitation the Kepler laws are needed in addition to determining that $n = -1$.

Figure 1.42

Gauss's Law



1.13 Gauss's Law and Poisson's Equation

Gauss's Law

Consider a point electric charge q at the origin of our coordinate system. This produces an electric field $\mathbf{E}$[16] given by

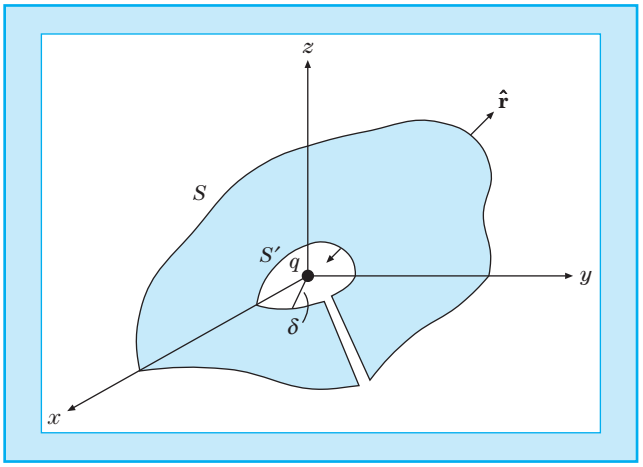
$$\mathbf{E} = \frac{q\hat{\mathbf{r}}}{4\pi\varepsilon_0 r^2}. \tag{1.136}$$

We now derive Gauss's law, which states that the surface integral in Fig. 1.42 is q/ε_0 if the closed surface S includes the origin (where q is located) and zero

[16]The electric field $\mathbf{E}$ is defined as the force per unit charge on a small stationary test charge q_t: $\mathbf{E} = \mathbf{F}/q_t$. From Coulomb's law, the force on q_t due to q is $\mathbf{F} = (qq_t/4\pi\varepsilon_0)(\hat{\mathbf{r}}/r^2)$. When we divide by q_t, Eq. (1.136) follows.

Figure 1.43

Exclusion of the Origin



if the surface does not include the origin. The surface S is any closed surface; it need not be spherical.

Using Gauss's theorem [Eq. (1.116a)] (and neglecting the scale factor $q/4\pi\varepsilon_0$), we obtain

$$\int_S \frac{\hat{\mathbf{r}}\cdot d\boldsymbol{\sigma}}{r^2} = \int_V \boldsymbol{\nabla}\cdot\left(\frac{\hat{\mathbf{r}}}{r^2}\right) d\tau = 0 \tag{1.137}$$

by Example 1.6.1, provided the surface S does not include the origin, where the integrands are not defined. This proves the second part of Gauss's law.

The first part, in which the surface S must include the origin, may be handled by surrounding the origin with a small sphere S' of radius δ (Fig. 1.43). So that there will be no question as to what is inside and what is outside, imagine the volume outside the outer surface S and the volume inside surface $S'(r < \delta)$ connected by a small hole. This joins surfaces S and S', combining them into one **single, simply connected closed surface**. Because the radius of the imaginary hole may be made vanishingly small, there is no additional contribution to the surface integral. The inner surface is deliberately chosen to be spherical so that we will be able to integrate over it. Gauss's theorem now applies to the volume between S and S' without any difficulty. We have

$$\int_S \frac{\hat{\mathbf{r}}\cdot d\boldsymbol{\sigma}}{r^2} + \int_{S'} \frac{\hat{\mathbf{r}}\cdot d\boldsymbol{\sigma}'}{\delta^2} = 0. \tag{1.138}$$

We may evaluate the second integral for $d\boldsymbol{\sigma}' = -\hat{\mathbf{r}}\delta^2\, d\Omega$, in which $d\Omega$ is an element of solid angle. The minus sign appears because we agreed in Section 1.9 to have the positive normal $\hat{\mathbf{r}}'$ **outward** from the volume. In this case, the outward $\hat{\mathbf{r}}'$ is in the negative radial direction, $\hat{\mathbf{r}}' = -\hat{\mathbf{r}}$. By integrating over all angles, we have

$$\int_{S'} \frac{\hat{\mathbf{r}}\cdot d\boldsymbol{\sigma}'}{\delta^2} = -\int_{S'} \frac{\hat{\mathbf{r}}\cdot\hat{\mathbf{r}}\delta^2 d\Omega}{\delta^2} = -4\pi, \tag{1.139}$$

independent of the radius δ. With the constants from Eq. (1.136), this results in

$$\int_S \mathbf{E}\cdot d\boldsymbol{\sigma} = \frac{q}{4\pi\varepsilon_0}4\pi = \frac{q}{\varepsilon_0}, \tag{1.140}$$

completing the proof of Gauss's law. Notice that although the surface S may be spherical, it **need not** be spherical.

Going a bit further, we consider a distributed charge so that

$$q = \int_V \rho\, d\tau. \tag{1.141}$$

Equation (1.140) still applies, with q now interpreted as the total distributed charge enclosed by surface S:

$$\int_S \mathbf{E}\cdot d\boldsymbol{\sigma} = \int_V \frac{\rho}{\varepsilon_0}\, d\tau. \tag{1.142}$$

Using Gauss's theorem, we have

$$\int_V \boldsymbol{\nabla}\cdot\mathbf{E}\, d\tau = \int_V \frac{\rho}{\varepsilon_0}\, d\tau. \tag{1.143}$$

Since our volume is completely arbitrary, the integrands must be equal or

$$\boldsymbol{\nabla}\cdot\mathbf{E} = \frac{\rho}{\varepsilon_0}, \tag{1.144}$$

one of Maxwell's equations. If we reverse the argument, Gauss's law follows immediately from Maxwell's equation by integration.

Poisson's Equation

Replacing $\mathbf{E}$ by $-\boldsymbol{\nabla}\varphi$, Eq. (1.144) becomes

$$\boldsymbol{\nabla}\cdot\boldsymbol{\nabla}\varphi = -\frac{\rho}{\varepsilon_0}, \tag{1.145}$$

which is Poisson's equation. We know a solution,

$$\varphi(\mathbf{r}) = \frac{1}{4\pi\epsilon_0}\int \frac{\rho(\mathbf{r}')d\tau'}{|\mathbf{r}-\mathbf{r}'|},$$

from generalizing a sum of Coulomb potentials for discrete charges in electrostatics to a continuous charge distribution.

For the condition $\rho = 0$ this reduces to an even more famous equation, the **Laplace equation**.

$$\boldsymbol{\nabla}\cdot\boldsymbol{\nabla}\varphi = 0. \tag{1.146}$$

We encounter Laplace's equation frequently in discussing various curved coordinate systems (Chapter 2) and the special functions of mathematical physics that appear as its solutions in Chapter 11.

From direct comparison of the Coulomb electrostatic force law and Newton's law of universal gravitation,

$$\mathbf{F}_E = \frac{1}{4\pi\varepsilon_0}\frac{q_1q_2}{r^2}\hat{\mathbf{r}}, \qquad \mathbf{F}_G = -G\frac{m_1m_2}{r^2}\hat{\mathbf{r}}.$$

All of the potential theory of this section therefore applies equally well to gravitational potentials. For example, the gravitational Poisson equation is

$$\nabla \cdot \nabla\varphi = +4\pi G\rho, \tag{1.147}$$

with ρ now a mass density.

Biographical Data

Poisson, Siméon Denis. Poisson, a French mathematician, was born in Pithiviers, France in 1781 and died in Paris in 1840. He studied mathematics at the Ecole Polytechnique under Laplace and Lagrange, whom he so impressed with his talent that he became professor there in 1802. He contributed to their celestial mechanics, Fourier's heat theory, and probability theory, among others.

EXERCISES

1.13.1 Develop Gauss's law for the two-dimensional case in which

$$\varphi = -q\frac{\ln\rho}{2\pi\varepsilon_0}, \quad \mathbf{E} = -\nabla\varphi = q\frac{\hat{\boldsymbol{\rho}}}{2\pi\varepsilon_0\rho},$$

where q is the charge at the origin or the line charge per unit length if the two-dimensional system is a unit thickness slice of a three-dimensional (circular cylindrical) system. The variable ρ is measured radially outward from the line charge. $\hat{\boldsymbol{\rho}}$ is the corresponding unit vector (see Section 2.2). If graphical software is available, draw the potential and field for the $q/2\pi\varepsilon_0 = 1$ case.

1.13.2 (a) Show that Gauss's law follows from Maxwell's equation

$$\nabla \cdot \mathbf{E} = \frac{\rho}{\varepsilon_0}$$

by integrating over a closed surface. Here, ρ is the charge density.

(b) Assuming that the electric field of a point charge q is spherically symmetric, show that Gauss's law implies the Coulomb inverse square expression

$$\mathbf{E} = \frac{q\hat{\mathbf{r}}}{4\pi\varepsilon_0 r^2}.$$

1.13.3 Show that the value of the electrostatic potential φ at any point P is equal to the average of the potential over any spherical surface centered on P. There are no electric charges on or within the sphere.
Hint. Use Green's theorem [Eq. (1.119)], with $u^{-1} = r$, the distance from P, and $v = \varphi$.

1.13.4 Using Maxwell's equations, show that for a system (steady current) the magnetic vector potential $\mathbf{A}$ satisfies a vector Poisson equation

$$\nabla^2\mathbf{A} = -\mu\mathbf{J},$$

provided we require $\nabla \cdot \mathbf{A} = 0$ in Coulomb gauge.

1.14 Dirac Delta Function

From Example 1.6.1 and the development of Gauss's law in Section 1.13,

$$\int \nabla\cdot\nabla\left(\frac{1}{r}\right)d\tau = -\int \nabla\cdot\left(\frac{\hat{\mathbf{r}}}{r^2}\right)d\tau = \begin{cases} -4\pi \\ 0 \end{cases}, \tag{1.148}$$

depending on whether the integration includes the origin $\mathbf{r} = 0$ or not. This result may be conveniently expressed by introducing the Dirac delta function,

$$\nabla^2\left(\frac{1}{r}\right) = -4\pi\,\delta(\mathbf{r}) = -4\pi\,\delta(x)\delta(y)\delta(z). \tag{1.149}$$

This Dirac delta function is **defined** by its assigned properties

$$\delta(x) = 0, \qquad x \neq 0 \tag{1.150}$$

$$f(0) = \int_{-\infty}^{\infty} f(x)\,\delta(x)\,dx, \tag{1.151}$$

where $f(x)$ is any well-behaved function and the integration includes the origin. As a special case of Eq. (1.151),

$$\int_{-\infty}^{\infty} \delta(x)\,dx = 1. \tag{1.152}$$

From Eq. (1.151), $\delta(x)$ must be an infinitely high, infinitely thin spike at $x = 0$, as in the description of an impulsive force or the charge density for a point charge.[17] The problem is that **no such function exists** in the usual sense of function. However, the crucial property in Eq. (1.151) can be developed rigorously as the limit of a **sequence** of functions, a distribution. For example, the delta function may be approximated by the sequences of functions in n for $n \to \infty$ [Eqs. (1.153)–(1.156) and Figs. 1.44–1.47]:

$$\delta_n(x) = \begin{cases} 0, & x < -\frac{1}{2n} \\ n, & -\frac{1}{2n} < x < \frac{1}{2n} \\ 0, & x > \frac{1}{2n} \end{cases} \tag{1.153}$$

$$\delta_n(x) = \frac{n}{\sqrt{\pi}}\exp(-n^2x^2) \tag{1.154}$$

$$\delta_n(x) = \frac{n}{\pi}\cdot\frac{1}{1+n^2x^2} \tag{1.155}$$

$$\delta_n(x) = \frac{\sin nx}{\pi x} = \frac{1}{2\pi}\int_{-n}^{n} e^{ixt}\,dt. \tag{1.156}$$

[17] The delta function is frequently invoked to describe very short-range forces such as nuclear forces. It also appears in the normalization of continuum wave functions of quantum mechanics.

Figure 1.44

δ Sequence Function Eq. (1.153)

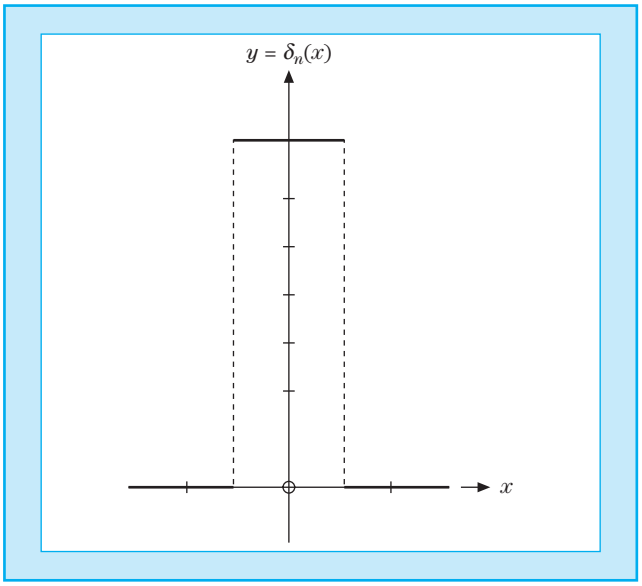
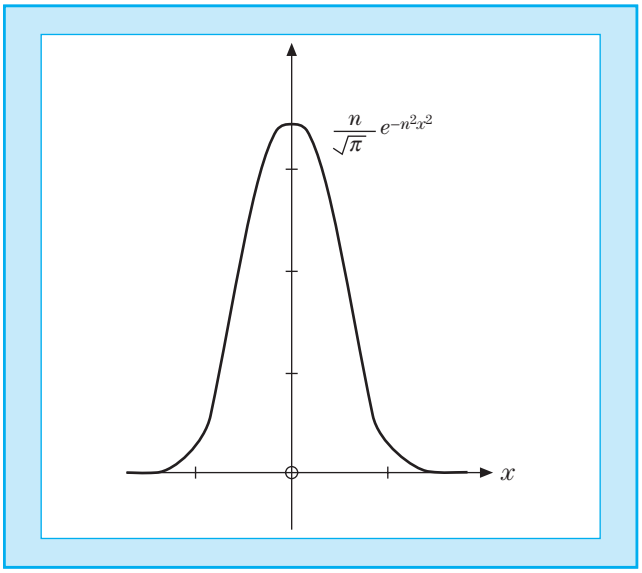


Figure 1.45

δ Sequence Function Eq. (1.154)



EXAMPLE 1.14.1

Let us evaluate $\int_{-\pi}^{\pi} \cos x \delta(x) dx = \cos 0 = 1$ using the sequence of Eq. (1.153). We find

$$\int_{-1/2n}^{1/2n} n \cos x \, dx = n \sin x \Big|_{-1/2n}^{1/2n} = n\left(\sin\left(\frac{1}{2n}\right) - \sin\left(-\frac{1}{2n}\right)\right)$$

$$= 2n \sin \frac{1}{2n} = 2n\left(\frac{1}{2n} + O(1/n^3)\right) \to 1 \quad \text{for } n \to \infty.$$

Figure 1.46

δ Sequence Function Eq. (1.155)

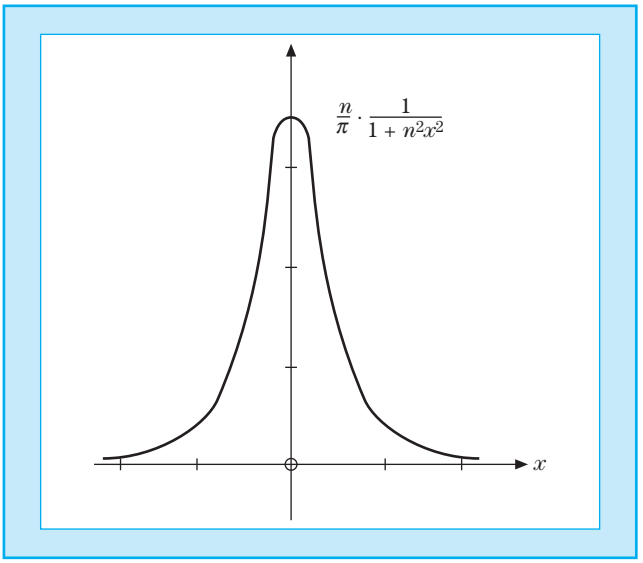
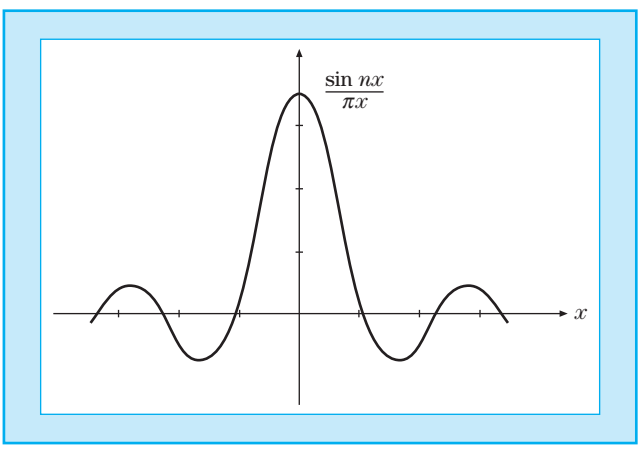


Figure 1.47

δ Sequence Function Eq. (1.156)



Notice how the integration limits change in the first step. Similarly, $\int_{-\pi}^{\pi} \sin x\delta(x) \cdot dx = \sin 0 = 0$. We could have used Eq. (1.155) instead,

$$\begin{aligned}\frac{n}{\pi}\int_{-\pi}^{\pi}\frac{\cos x\,dx}{1+n^2x^2} &= \frac{n}{\pi}\int_{-\pi}^{\pi}\frac{1-x^2/2+\cdots}{1+n^2x^2}dx = \frac{n}{\pi}\int_{-\pi}^{\pi}\frac{dx}{1+n^2x^2}\\ &= \frac{1}{\pi}\int_{-n\pi}^{n\pi}\frac{dy}{1+y^2} = \frac{1}{\pi}[\arctan(n\pi)-\arctan(-n\pi)]\\ &= \frac{2}{\pi}\arctan(n\pi) \to \frac{2}{\pi}\frac{\pi}{2} = 1, \quad \text{for } n \to \infty,\end{aligned}$$

by keeping just the first term of the power expansion of $\cos x$. Again, we could have changed the integration limits to $\pm\pi/n$ in the first step for all terms with positive powers of x because the denominator is so large, except close to $x = 0$ for large n. This explains why the higher order terms of the $\cos x$ power series do not contribute. ■

These approximations have varying degrees of usefulness. Equation (1.153) is useful in providing a simple derivation of the integral property [Eq. (1.151)]. Equation (1.154) is convenient to differentiate. Its derivatives lead to the Hermite polynomials. Equation (1.156) is particularly useful in Fourier analysis and in its applications to quantum mechanics. In the theory of Fourier series, Eq. (1.156) often appears (modified) as the Dirichlet kernel:

$$\delta_n(x) = \frac{1}{2\pi}\frac{\sin[(n+\frac{1}{2})x]}{\sin(\frac{1}{2}x)}. \tag{1.157}$$

In using these approximations in Eq. (1.151) and later, we assume that $f(x)$ is integrable—it offers no problems at large x.

For most physical purposes such approximations are quite adequate. From a mathematical standpoint, the situation is still unsatisfactory: The limits

$$\lim_{n\to\infty} \delta_n(x)$$

do not exist.

A way out of this difficulty is provided by the theory of distributions. Recognizing that Eq. (1.151) is the fundamental property, we focus our attention on it rather than on $\delta(x)$. Equations (1.153)–(1.156), with $n = 1, 2, 3, \ldots$, may be interpreted as **sequences** of normalized functions:

$$\int_{-\infty}^{\infty} \delta_n(x)\,dx = 1. \tag{1.158}$$

The sequence of integrals has the limit

$$\lim_{n\to\infty} \int_{-\infty}^{\infty} \delta_n(x) f(x)\,dx = f(0). \tag{1.159}$$

Note that Eq. (1.158) is the limit of a sequence of integrals. Again, the limit of $\delta_n(x)$, $n \to \infty$, does not exist. [The limits for all four forms of $\delta_n(x)$ diverge at $x = 0$.]

We may treat $\delta(x)$ consistently in the form

$$\int_{-\infty}^{\infty} \delta(x) f(x)\,dx = \lim_{n\to\infty} \int_{-\infty}^{\infty} \delta_n(x) f(x)\,dx. \tag{1.160}$$

$\delta(x)$ is labeled a distribution (not a function) defined by the sequences $\delta_n(x)$ as indicated in Eq. (1.158). We might emphasize that the integral on the left-hand side of Eq. (1.160) is not a Riemann integral.[18] It is a limit.

[18] It can be treated as a Stieltjes integral if desired. $\delta(x)\,dx$ is replaced by $du(x)$, where $u(x)$ is the Heaviside step function.

This distribution $\delta(x)$ is only one of an infinity of possible distributions, but it is the one we are interested in because of Eq. (1.151).

From these sequences of functions, we see that Dirac's delta function must be even in x, $\delta(-x) = \delta(x)$.

Let us now consider a detailed application of the Dirac delta function to a single charge and illustrate the singularity of the electric field at the origin.

EXAMPLE 1.14.2

Total Charge inside a Sphere Consider the total electric flux $\oint \mathbf{E} \cdot d\boldsymbol{\sigma}$ out of a sphere of radius R around the origin surrounding n charges e_j located at the points $\mathbf{r}_j$ with $r_j < R$ (i.e., inside the sphere). The electric field strength $\mathbf{E} = -\nabla\varphi(\mathbf{r})$, where the potential

$$\varphi = \sum_{j=1}^{n} \frac{e_j}{|\mathbf{r} - \mathbf{r}_j|} = \int \frac{\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d^3r'$$

is the sum of the Coulomb potentials generated by each charge and the total charge density is $\rho(\mathbf{r}) = \sum_j e_j \delta(\mathbf{r} - \mathbf{r}_j)$. The delta function is used here as an abbreviation of a pointlike density. Now we use Gauss's theorem for

$$\oint \mathbf{E} \cdot d\boldsymbol{\sigma} = -\oint \nabla\varphi \cdot d\boldsymbol{\sigma} = -\int \nabla^2\varphi d\tau = \int \frac{\rho(\mathbf{r})}{\varepsilon_0} d\tau = \frac{\sum_j e_j}{\varepsilon_0}$$

in conjunction with the differential form of Gauss's law $\nabla \cdot \mathbf{E} = -\rho/\varepsilon_0$ and $\sum_j e_j \int \delta(\mathbf{r} - \mathbf{r}_j) d\tau = \sum_j e_j$. ■

The integral property [Eq. (1.151)] is useful in cases in which the argument of the delta function is a function $g(x)$ with **simple zeros** on the real axis, which leads to the rules

$$\delta(ax) = \frac{1}{a}\delta(x), \quad a > 0, \tag{1.161}$$

$$\delta(g(x)) = \sum_{\substack{a,\\ g(a)=0,\\ g'(a)\neq 0}} \frac{\delta(x-a)}{|g'(a)|}. \tag{1.162}$$

To obtain Eq. (1.161) we change the integration variable in

$$\int_{-\infty}^{\infty} f(x)\delta(ax)dx = \frac{1}{a}\int_{-\infty}^{\infty} f\left(\frac{y}{a}\right)\delta(y)dy = \frac{1}{a}f(0)$$

and apply Eq. (1.151). To prove Eq. (1.162), we decompose the integral

$$\int_{-\infty}^{\infty} f(x)\delta(g(x))dx = \sum_a \int_{a-\varepsilon}^{a+\varepsilon} f(x)\delta((x-a)g'(a))dx \tag{1.163}$$

into a sum of integrals over small intervals containing the first-order zeros of $g(x)$. In these intervals, $g(x) \approx g(a) + (x-a)g'(a) = (x-a)g'(a)$. Using Eq. (1.161) on the right-hand side of Eq. (1.163), we obtain the integral of Eq. (1.162).

EXAMPLE 1.14.3

Evaluate $I \equiv \int_{-\infty}^{\infty} f(x)\delta(x^2-2)dx$ Because the zeros of the argument of the delta function, $x^2 = 2$, are $x = \pm\sqrt{2}$, we can write the integral as a sum of two contributions:

$$\begin{aligned} I &= \int_{\sqrt{2}-\epsilon}^{\sqrt{2}+\epsilon} \delta(x-\sqrt{2}) \frac{f(x)dx}{\frac{d(x^2-2)}{dx}|_{x=\sqrt{2}}} dx + \int_{-\sqrt{2}-\epsilon}^{-\sqrt{2}+\epsilon} \delta(x+\sqrt{2}) \frac{f(x)dx}{\frac{d(x^2-2)}{dx}|_{x=-\sqrt{2}}} \\ &= \int_{\sqrt{2}-\epsilon}^{\sqrt{2}+\epsilon} \delta(x-\sqrt{2}) \frac{f(x)dx}{2\sqrt{2}} + \int_{-\sqrt{2}-\epsilon}^{-\sqrt{2}+\epsilon} \delta(x+\sqrt{2}) \frac{f(x)dx}{2\sqrt{2}} \\ &= \frac{f(\sqrt{2}) + f(-\sqrt{2})}{2\sqrt{2}}. \end{aligned}$$ ■

This example is good training for the following one.

EXAMPLE 1.14.4

Phase Space In the scattering theory of relativistic particles using Feynman diagrams, we encounter the following integral over energy of the scattered particle (we set the velocity of light $c = 1$):

$$\begin{aligned} \int d^4p\delta(p^2-m^2)f(p) &\equiv \int d^3p \int dp_0 \delta\left(p_0^2 - \mathbf{p}^2 - m^2\right) f(p) \\ &= \int_{E>0} \frac{d^3p f(E,\mathbf{p})}{2\sqrt{m^2+\mathbf{p}^2}} - \int_{E<0} \frac{d^3p f(E,\mathbf{p})}{2\sqrt{m^2+\mathbf{p}^2}}, \end{aligned}$$

where we have used Eq. (1.162) at the zeros $E = \pm\sqrt{m^2+\mathbf{p}^2}$ of the argument of the delta function. The physical meaning of $\delta(p^2-m^2)$ is that the particle of mass m and four-momentum $p^\mu = (p_0, \mathbf{p})$ is on its mass shell because $p^2 = m^2$ is equivalent to $E = \pm\sqrt{m^2+\mathbf{p}^2}$. Thus, the on-mass-shell volume element in momentum space is the Lorentz invariant $\frac{d^3p}{2E}$, in contrast to the nonrelativistic d^3p of momentum space. The fact that a negative energy occurs is a peculiarity of relativistic kinematics that is related to the antiparticle. ■

Using integration by parts we can also **define the derivative** $\delta'(x)$ of the Dirac delta function by the relation

$$\int_{-\infty}^{\infty} f(x)\delta'(x-x')\,dx = -\int_{-\infty}^{\infty} f'(x)\delta(x-x')\,dx = -f'(x'). \tag{1.164}$$

It should be understood that our Dirac delta function has significance only as part of an integrand. Thus, the Dirac delta function is often regarded as a linear operator: $\delta(x-x_0)$ operates on $f(x)$ and yields $f(x_0)$:

$$\mathcal{L}(x_0)f(x) \equiv \int_{-\infty}^{\infty} \delta(x-x_0)f(x)\,dx = f(x_0). \tag{1.165}$$

It may also be classified as a linear mapping or simply as a generalized function. Shifting our singularity to the point $x = x'$, we write the Dirac delta function as $\delta(x - x')$. Equation (1.151) becomes

$$\int_{-\infty}^{\infty} f(x)\delta(x - x')\,dx = f(x'). \tag{1.166}$$

As a description of a singularity at $x = x'$, the Dirac delta function may be written as $\delta(x - x')$ or as $\delta(x' - x)$. Expanding to three dimensions and using spherical polar coordinates, we obtain

$$\begin{aligned} f(0) &= \int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} f(\mathbf{r})\delta(\mathbf{r})\,r^2\,dr\sin\theta\,d\theta\,d\varphi \\ &= \iiint_{-\infty}^{\infty} f(x, y, z)\delta(x)\,\delta(y)\,\delta(z)\,dx\,dy\,dz, \\ &\int_0^{\infty}\frac{\delta(r)}{r^2}r^2dr\int_{-1}^{1}\delta(\cos\theta)\,d\cos\theta\int_0^{2\pi}\delta(\varphi)\,d\varphi = 1, \end{aligned} \tag{1.167}$$

where each one-dimensional integral is equal to unity. This corresponds to a singularity (or source) at the origin. Again, if our source is at $\mathbf{r} = \mathbf{r}_1$, Eq. (1.167) generalizes to

$$\iiint f(\mathbf{r}_2)\delta(\mathbf{r}_2 - \mathbf{r}_1)\,r_2^2dr_2\sin\theta_2\,d\theta_2\,d\varphi_2 = f(\mathbf{r}_1), \tag{1.168}$$

where

$$\int_0^{\infty}\frac{\delta(r_2 - r_1)}{r_2^2}r_2^2dr_2\int_{-1}^{1}\delta(\cos\theta_2 - \cos\theta_1)d\cos\theta_2\int_0^{2\pi}\delta(\varphi_2 - \varphi_1)d\varphi_2 = 1.$$

SUMMARY

We use $\delta(x)$ frequently and call it the Dirac delta function—for historical reasons.[19] Remember that it is not really a function. It is essentially a shorthand notation, defined implicitly as the limit of integrals in a sequence, $\delta_n(x)$, according to Eq. (1.160).

Biographical Data

Dirac, Paul Adrien Maurice. Dirac, an English physicist, was born in Bristol in 1902 and died in Bristol in 1984. He obtained a degree in electrical engineering at Bristol and obtained his Ph.D. in mathematical physics in 1926 at Cambridge. By 1932, he was Lucasian professor, like Stokes, the chair Newton once held. In the 1920s, he advanced quantum mechanics, became one of the founders of quantum field theory, and, in 1928, discovered his relativistic equation for the electron that predicted antiparticles for which he was awarded the Nobel prize in 1933.

[19] Dirac introduced the delta function to quantum mechanics. Actually, the delta function can be traced back to Kirchhoff, 1882. For further details, see M. Jammer (1966). *The Conceptual Development of Quantum Mechanics*, p. 301. McGraw-Hill, New York.

EXERCISES

1.14.1 Let

$$\delta_n(x) = \begin{cases} 0, & x < -\frac{1}{2n} \\ n, & -\frac{1}{2n} < x < \frac{1}{2n}, \\ 0, & \frac{1}{2n} < x. \end{cases}$$

Show that

$$\lim_{n\to\infty} \int_{-\infty}^{\infty} f(x)\delta_n(x)\,dx = f(0),$$

assuming that $f(x)$ is continuous at $x = 0$.

1.14.2 Verify that the sequence $\delta_n(x)$, based on the function

$$\delta_n(x) = \begin{cases} 0, & x < 0, \\ ne^{-nx} & x > 0, \end{cases}$$

is a delta sequence [satisfying Eq. (1.159)]. Note that the singularity is at $+0$, the positive side of the origin.
Hint. Replace the upper limit (∞) by c/n, where c is large but finite, and use the mean value theorem of integral calculus.

1.14.3 For

$$\delta_n(x) = \frac{n}{\pi} \cdot \frac{1}{1 + n^2x^2},$$

[Eq. (1.155)], show that

$$\int_{-\infty}^{\infty} \delta_n(x)\,dx = 1.$$

1.14.4 Demonstrate that $\delta_n = \sin nx/\pi x$ is a delta distribution by showing that

$$\lim_{n\to\infty} \int_{-\infty}^{\infty} f(x)\frac{\sin nx}{\pi x}\,dx = f(0).$$

Assume that $f(x)$ is continuous at $x = 0$ and vanishes as $x \to \pm\infty$.
Hint. Replace x by y/n and take $\lim n \to \infty$ **before** integrating.

1.14.5 Fejer's method of summing series is associated with the function

$$\delta_n(t) = \frac{1}{2\pi n}\left[\frac{\sin(nt/2)}{\sin(t/2)}\right]^2.$$

Show that $\delta_n(t)$ is a delta distribution in the sense that

$$\lim_{n\to\infty} \frac{1}{2\pi n} \int_{-\infty}^{\infty} f(t)\left[\frac{\sin(nt/2)}{\sin(t/2)}\right]^2 dt = f(0).$$

1.14.6 Using the Gaussian delta sequence (δ_n), Eq. (1.154), show that

$$x\frac{d}{dx}\delta(x) = -\delta(x),$$

treating $\delta(x)$ and its derivative as in Eq. (1.151).

1.14.7 Show that

$$\int_{-\infty}^{\infty} \delta'(x) f(x)\, dx = -f'(0).$$

Assume that $f'(x)$ is continuous at $x = 0$.

1.14.8 Prove that

$$\delta(f(x)) = \left|\frac{df(x)}{dx}\right|^{-1} \delta(x - x_0),$$

where x_0 is chosen so that $f(x_0) = 0$ with $df/dx \neq 0$; that is, $f(x)$ has a simple zero at x_0.
Hint. Use $\delta(f)\, df = \delta(x)\, dx$ after explaining why this holds.

1.14.9 Show that in spherical polar coordinates $(r, \cos\theta, \varphi)$ the delta function $\delta(\mathbf{r}_1 - \mathbf{r}_2)$ becomes

$$\frac{1}{r_1^2}\delta(r_1 - r_2)\delta(\cos\theta_1 - \cos\theta_2)\delta(\varphi_1 - \varphi_2).$$

1.14.10 For the finite interval $(-\pi, \pi)$ expand the Dirac delta function $\delta(x-t)$ in a series of sines and cosines: $\sin nx$, $\cos nx$, $n = 0, 1, 2, \ldots$. Note that although these functions are orthogonal, they are not normalized to unity.

1.14.11 In the interval $(-\pi, \pi)$, $\delta_n(x) = \frac{n}{\sqrt{\pi}} \exp(-n^2x^2)$.

(a) Expand $\delta_n(x)$ as a Fourier cosine series.
(b) Show that your Fourier series agrees with a Fourier expansion of $\delta(x)$ in the limit as $n \to \infty$.
(c) Confirm the delta function nature of your Fourier series by showing that for any $f(x)$ that is finite in the interval $[-\pi, \pi]$ and continuous at $x = 0$,

$$\int_{-\pi}^{\pi} f(x)[\text{Fourier expansion of } \delta_\infty(x)]\, dx = f(0).$$

1.14.12 (a) Expand $\delta_n(x) = \frac{n}{\sqrt{\pi}} \exp(-n^2x^2)$ in the interval $(-\infty, \infty)$ as a Fourier integral.
(b) Expand $\delta_n(x) = n\exp(-nx)$ as a Laplace transform.

1.14.13 We may define a sequence

$$\delta_n(x) = \begin{cases} n, & |x| < 1/2n, \\ 0, & |x| > 1/2n. \end{cases}$$

[Eq. (1.153)]. Express $\delta_n(x)$ as a Fourier integral (via the Fourier integral theorem, inverse transform, etc.). Finally, show that we may write

$$\delta(x) = \lim_{n\to\infty} \delta_n(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-ikx}\, dk.$$

1.14.14 Using the sequence

$$\delta_n(x) = \frac{n}{\sqrt{\pi}} \exp(-n^2x^2),$$

show that

$$\delta(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-ikx}\, dk.$$

Note. Remember that $\delta(x)$ is defined in terms of its behavior as part of an integrand, especially Eq. (1.159).

1.14.15 Derive sine and cosine representations of $\delta(t - x)$.

ANS. $\dfrac{2}{\pi} \displaystyle\int_0^{\infty} \sin \omega t \sin \omega x\, d\omega$, $\dfrac{2}{\pi} \displaystyle\int_0^{\infty} \cos \omega t \cos \omega x\, d\omega$.

Additional Reading

Borisenko, A. I., and Taropov, I. E. (1968). *Vector and Tensor Analysis with Applications*. Prentice-Hall, Englewood Cliffs, NJ. Reprinted, Dover, New York (1980).

Davis, H. F., and Snider, A. D. (1995). *Introduction to Vector Analysis*, 7th ed. Allyn & Bacon, Boston.

Kellogg, O. D. (1953). *Foundations of Potential Theory*. Dover, New York. Originally published 1929. The classic text on potential theory.

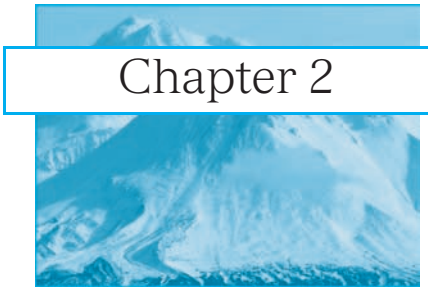
Lewis, P. E., and Ward, J. P. (1989). *Vector Analysis for Engineers and Scientists*. Addison-Wesley, Reading, MA.

Marion, J. B. (1965). *Principles of Vector Analysis*. Academic Press, New York. A moderately advanced presentation of vector analysis oriented toward tensor analysis. Rotations and other transformations are described with the appropriate matrices.

Spiegel, M. R. (1989). *Vector Analysis*. McGraw-Hill, New York.

Tai, C.-T. (1996). *Generalized Vector and Dyadic Analysis*. Oxford Univ. Press, Oxford.

Wrede, R. C. (1963). *Introduction to Vector and Tensor Analysis*. Wiley, New York. Reprinted, Dover, New York (1972). Fine historical introduction; excellent discussion of differentiation of vectors and applications to mechanics.



Chapter 2

Vector Analysis in Curved Coordinates and Tensors

In Chapter 1 we restricted ourselves almost completely to rectangular or Cartesian coordinate systems. A Cartesian coordinate system offers the unique advantage that all three unit vectors, $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$, and $\hat{\mathbf{z}}$ are constant in direction as well as in magnitude. We did introduce the radial distance r, but even this was treated as a function of x, y, and z, as $r = \sqrt{x^2 + y^2 + z^2}$. Unfortunately, not all physical problems are well adapted to solution in Cartesian coordinates. For instance, if we have a central force problem, $\mathbf{F} = \hat{\mathbf{r}} F(r)$, such as gravitational or electrostatic force, Cartesian coordinates may be unusually inappropriate. Such a problem requires the use of a coordinate system in which the radial distance is taken to be one of the coordinates, that is, spherical polar coordinates.

The point is that the coordinate system should be chosen to fit the problem to exploit any constraint or symmetry present in it. For example, rectangular (spherical) boundary conditions call for Cartesian (polar) coordinates, or a rectangular (cylindrical) shape of the system demands Cartesian (cylindrical) coordinates. With such a choice, it is hoped that the problem will be more readily soluble than if we had forced it into an inappropriate framework.

Naturally, there is a price that must be paid for the use of a non-Cartesian coordinate system. In Chapter 1 we developed the gradient, divergence, and curl in Cartesian coordinates, but we have not yet written expressions for gradient, divergence, or curl in any of the non-Cartesian coordinate systems. Such expressions are developed first for cylindrical coordinates in Section 2.2 and then developed in a general form in Section 2.3. This system of curvilinear coordinates is then specialized to spherical polar coordinates in Section 2.5. There are other useful coordinates, 11 of which can be found in the second edition of *Mathematical Methods* and some in Margenau and Murphy (1956).

2.1 Special Coordinate Systems

As mentioned previously, there are 11 coordinate systems in which the three-dimensional Helmholtz partial differential equation can be separated into three ordinary differential equations. Some of these coordinate systems have achieved prominence in the historical development of quantum mechanics. Other systems, such as bipolar coordinates, satisfy special needs. Partly because the needs are rather infrequent, but mostly because the development of computers and efficient programming techniques reduce the need for these coordinate systems, the discussion in this chapter is limited to (i) a brief summary of Cartesian coordinates dealt with extensively in Chapter 1, (ii) circular cylindrical coordinates, and (iii) spherical polar coordinates. Specifications and details of the other coordinate systems can be found in the first two editions of this work and in Morse and Feshbach (1953) and Margenau and Murphy (1956).

Rectangular Cartesian Coordinates

In Cartesian coordinates we deal with three mutually perpendicular families of planes: $x =$ constant, $y =$ constant, and $z =$ constant. These are the Cartesian coordinates on which Chapter 1 is based. In this simplest of all systems, the coordinate vector and a vector $\mathbf{V}$ are written as

$$\mathbf{r} = \hat{\mathbf{x}}x + \hat{\mathbf{y}}y + \hat{\mathbf{z}}z, \quad \mathbf{V} = \hat{\mathbf{x}}V_x + \hat{\mathbf{y}}V_y + \hat{\mathbf{z}}V_z. \tag{2.1}$$

The coordinate unit vectors $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$, $\hat{\mathbf{z}}$ are constant in direction and length, and they are mutually orthogonal, making Cartesian coordinates the simplest for developing vector analysis.

Now we turn our attention to line, area, and volume elements in order to perform multiple integrals and differentiations. From the Pythagorean theorem in Cartesian coordinates, the square of the distance between two infinitesimally close points is

$$ds^2 = dx^2 + dy^2 + dz^2, \tag{2.2}$$

where the sum of squares means that these coordinates are called orthogonal. That is, no bilinear terms $dx\,dy$, $dy\,dz$, $dx\,dz$ occur.

From Eqs. (1.63), (1.71), and (1.78) we reproduce the main results of vector analysis in Chapter 1:

$$\nabla\psi = \hat{\mathbf{x}}\frac{\partial\psi}{\partial x} + \hat{\mathbf{y}}\frac{\partial\psi}{\partial y} + \hat{\mathbf{z}}\frac{\partial\psi}{\partial z}, \tag{2.3}$$

$$\nabla\cdot\mathbf{V} = \frac{\partial V_x}{\partial x} + \frac{\partial V_y}{\partial y} + \frac{\partial V_z}{\partial z}, \tag{2.4}$$

$$\nabla \cdot \nabla \psi = \frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2}, \tag{2.5}$$

$$\nabla \times \mathbf{V} = \begin{vmatrix} \hat{\mathbf{x}} & \hat{\mathbf{y}} & \hat{\mathbf{z}} \\ \dfrac{\partial}{\partial x} & \dfrac{\partial}{\partial y} & \dfrac{\partial}{\partial z} \\ V_x & V_y & V_z \end{vmatrix}. \tag{2.6}$$

Integrals in Cartesian Coordinates

The simplest integrals are one-dimensional scalars such as the length of a space curve

$$s = \int_{t_1}^{t_2} \sqrt{\dot{x}^2 + \dot{y}^2 + \dot{z}^2}\, dt,$$

if the curve is parameterized as $\mathbf{r}(t) = (x(t), y(t), z(t))$.

The most common line integrals are of the form (see Examples 1.9.1 and 1.9.2)

$$\int \mathbf{A} \cdot d\mathbf{r} = \int (A_x dx + A_y dy + A_z dz) = \int (A_x \dot{x} + A_y \dot{y} + A_z \dot{z}) dt,$$

thus reducing them to a sum of ordinary integrals in Cartesian coordinates.

From the general formula discussed before Example 1.9.5 and employed in it, the area A of a surface $z = z(x, y)$ is given by

$$A = \int \frac{dx\, dy}{n_z}, \quad \frac{1}{n_z} = \sqrt{1 + \left(\frac{\partial z}{\partial x}\right)^2 + \left(\frac{\partial z}{\partial y}\right)^2}.$$

Here the integration ranges over the projection of the surface onto the xy-plane.

The volume bounded by a surface $z = z(x, y)$ is given by $V = \iint z(x, y)\, dx\, dy$, which is the three-dimensional generalization of the two-dimensional area $A = \int f(x) dx$ under a curve $y = f(x)$.

For examples of line, surface, and volume integrals in rectangular coordinates, refer to Chapter 1.

2.2 Circular Cylinder Coordinates

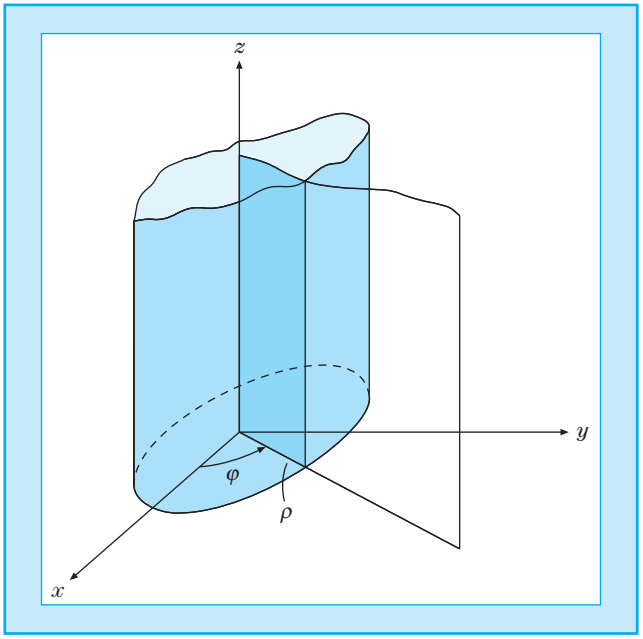
In the circular cylindrical coordinate system the three curvilinear coordinates are (ρ, φ, z). The limits on ρ, φ and z are

$$0 \le \rho < \infty, \qquad 0 \le \varphi < 2\pi, \qquad \text{and} \qquad -\infty < z < \infty,$$

and φ is not well defined for $\rho = 0$. Note that we are using ρ for the perpendicular distance from the z-axis and saving r for the distance from the origin. The z-coordinate remains unchanged. This is essentially a two-dimensional

Figure 2.1

Circular Cylinder Coordinates



curvilinear system with a Cartesian z-axis added on to form a three-dimensional system. The coordinate surfaces, shown in Fig. 2.1, are

1. Right circular cylinders having the z-axis as a common axis,

$$\rho = (x^2 + y^2)^{1/2} = \text{constant}.$$

2. Half planes through the z-axis,

$$\varphi = \tan^{-1}\left(\frac{y}{x}\right) = \text{constant}.$$

3. Planes parallel to the xy-plane, as in the Cartesian system,

$$z = \text{constant}.$$

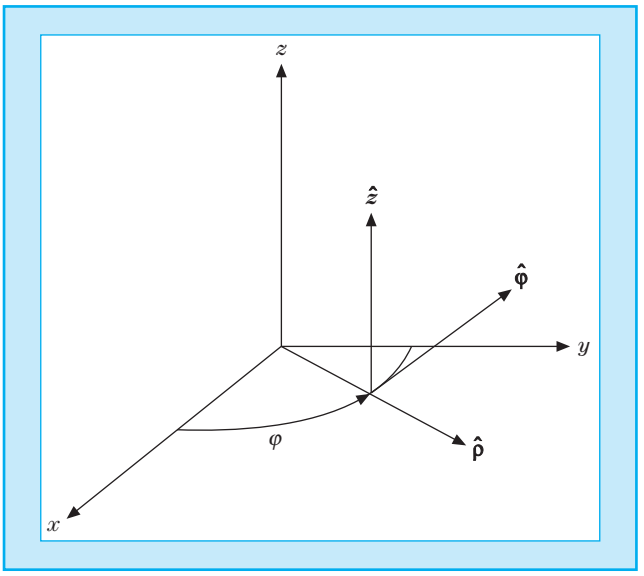
Inverting the preceding equations for ρ and φ (or going directly to Fig. 2.2), we obtain the transformation relations

$$x = \rho\cos\varphi, \quad y = \rho\sin\varphi, \quad z = z. \tag{2.7}$$

The coordinate unit vectors are $\hat{\boldsymbol{\rho}}$, $\hat{\boldsymbol{\varphi}}$, $\hat{\mathbf{z}}$ (Fig. 2.2). Note that $\hat{\boldsymbol{\varphi}}$ is not well defined at $\rho = 0$. The unit vector $\hat{\boldsymbol{\rho}}$ is normal to the cylindrical surface pointing in the direction of increasing radius ρ. The unit vector $\hat{\boldsymbol{\varphi}}$ is tangential to the cylindrical surface, perpendicular to the half plane $\varphi =$ constant, and pointing in the direction of increasing azimuth angle φ. The third unit vector, $\hat{\mathbf{z}}$, is the

Figure 2.2

Circular Cylindrical Coordinate Unit Vectors



usual Cartesian unit vector. They are mutually orthogonal, that is,

$$\hat{\boldsymbol{\rho}} \cdot \hat{\boldsymbol{\varphi}} = \hat{\boldsymbol{\varphi}} \cdot \hat{\mathbf{z}} = \hat{\mathbf{z}} \cdot \hat{\boldsymbol{\rho}} = 0.$$

For example, in circular cylindrical coordinates we have

$$\mathbf{r} = \hat{\boldsymbol{\rho}}\rho + \hat{\mathbf{z}}z, \quad \mathbf{V} = \hat{\boldsymbol{\rho}}V_\rho + \hat{\boldsymbol{\varphi}}V_\varphi + \hat{\mathbf{z}}V_z. \tag{2.8}$$

EXAMPLE 2.2.1

Distance in Cylindrical Coordinates We now derive the distance ds^2 in circular cylindrical coordinates ρ, φ, z with $x = \rho\cos\varphi$, $y = \rho\sin\varphi$ of plane polar coordinates. Differentiating we obtain

$$dx = \cos\varphi d\rho - \rho\sin\varphi d\varphi, \quad dz = dz,$$

using

$$\frac{\partial x}{\partial \rho} = \frac{\partial(\rho\cos\varphi)}{\partial\rho} = \cos\varphi, \quad \frac{\partial x}{\partial\varphi} = -\rho\sin\varphi, \quad \frac{\partial x}{\partial z} = 0.$$

Similarly, we find

$$dy = \sin\varphi d\rho + \rho\cos\varphi d\varphi$$

using

$$\frac{\partial y}{\partial\rho} = \frac{\partial(\rho\sin\varphi)}{\partial\rho} = \sin\varphi, \quad \frac{\partial y}{\partial\varphi} = \rho\cos\varphi$$

and, upon squaring and adding,

$$ds^2 = dx^2 + dy^2 = d\rho^2 + \rho^2 d\varphi^2 + dz^2 \tag{2.9}$$

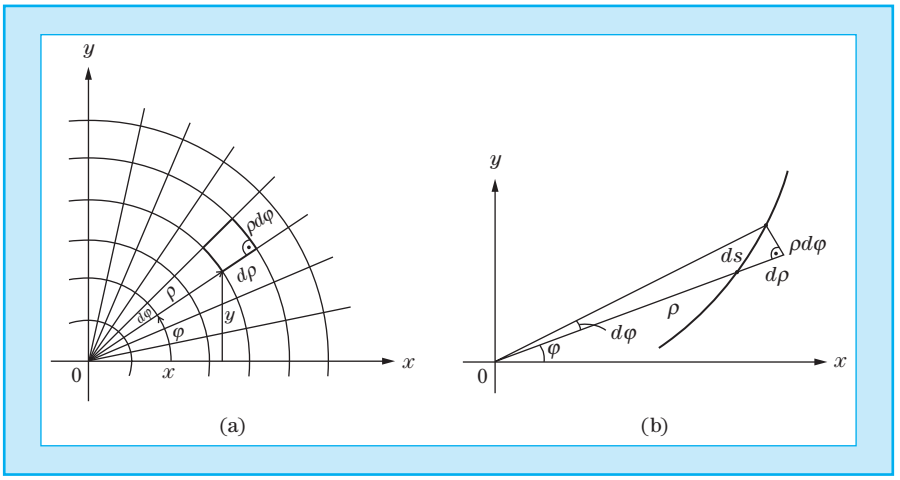


Figure 2.3

(a) Line Elements of Polar Coordinates. (b) Infinitesimal Triangle on a Space Curve

becomes a sum of squares, again showing that these coordinates are orthogonal. That is, the terms $d\rho d\varphi$, $d\rho dz$, $d\varphi dz$ drop out, and the straight lines through the origin with $z = 0$, $\varphi = \text{const.}$, are perpendicular to the circles $z = 0$, $\rho = \text{const.}$, wherever they intersect; they are orthogonal to the z-axis as well. The geometry is illustrated in Fig. 2.3. ■

Integrals in Cylindrical Coordinates

To develop the length of a space curve, we start from the line element $ds^2 = d\rho^2 + \rho^2 d\varphi^2 + dz^2$ from Example 2.2.1 and divide it by dt^2 to obtain $\dot{s}^2 = \dot{\rho}^2 + \rho^2\dot{\varphi}^2 + \dot{z}^2$, in case the curve is parameterized as $\mathbf{r}(t) = (\rho(t),\ \varphi(t),\ z(t))$. Using the chain rule, the length of a space curve becomes

$$s = \int_{t_1}^{t_2} \sqrt{\dot{\rho}^2 + \rho^2\dot{\varphi}^2 + \dot{z}^2}\, dt \tag{2.10}$$

and is a scalar integral. For example, for a sector of a circle of radius R in Fig. 2.4, the line element reduces to $\rho|_{\rho=R} d\varphi = R d\varphi$ because $d\rho = 0 = dz$. Therefore, we have $R\int_{\varphi_1}^{\varphi_2} d\varphi = R(\varphi_2 - \varphi_1)$ for the length of arc.

The line integral is a sum of ordinary integrals if we expand the dot product as

$$\begin{aligned}\int \mathbf{A}\cdot d\mathbf{r} &= \int (A_\rho d\rho + \rho A_\varphi d\varphi + A_z dz)\\ &= \int (A_\rho\dot{\rho} + \rho A_\varphi\dot{\varphi} + A_z\dot{z})\, dt\end{aligned} \tag{2.11}$$

using the chain rule.

When $\mathbf{A}$ is the vector potential of the magnetic field $\mathbf{B} = \nabla \times \mathbf{A}$, then Stokes's theorem relates the **line** integral

$$\oint \mathbf{A}\cdot d\mathbf{r} = \int_S (\nabla\times\mathbf{A})\cdot d\boldsymbol{\sigma} = \int \mathbf{B}\cdot d\boldsymbol{\sigma}$$

Figure 2.4

Length of Arc

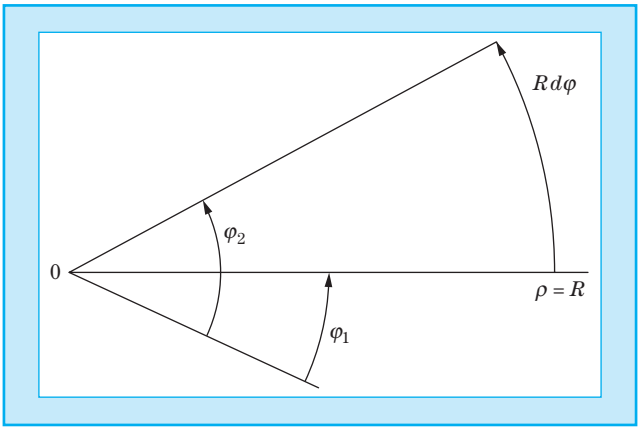
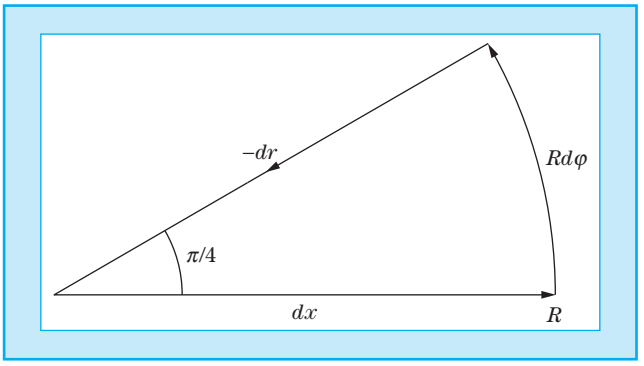


Figure 2.5

Sector Integration Path



to the magnetic flux through the surface S bounded by the closed curve, that is, a **surface** integral.

EXAMPLE 2.2.2

Magnetic Flux For a constant magnetic field $\mathbf{B} = B\hat{\mathbf{z}}$ in the z-direction, the flux through a circle of radius R around the origin of the xy-plane is obviously given by $B\pi R^2$. Let us see what $\oint \mathbf{A} \cdot d\mathbf{r}$ gives. From Example 1.7.1, we take $\mathbf{A} = \frac{1}{2}(\mathbf{B} \times \mathbf{r})$, with $\mathbf{r} = R\hat{\mathbf{r}}$ but $d\mathbf{r} = \rho|_{\rho=R} d\varphi\hat{\boldsymbol{\varphi}} = Rd\varphi\hat{\boldsymbol{\varphi}}$, the same as for the arc section in Fig. 2.4 because $d\rho = 0 = dz$. Hence,

$$\mathbf{B} \times \mathbf{r}|_{\rho=R} = \begin{vmatrix} \hat{\boldsymbol{\rho}} & \hat{\boldsymbol{\varphi}} & \hat{\mathbf{z}} \\ 0 & 0 & B \\ \rho & 0 & 0 \end{vmatrix}_{\rho=R} = BR\hat{\boldsymbol{\varphi}},$$

so that, with $\rho = R$,

$$\frac{1}{2}\oint_{\rho=R} (\mathbf{B} \times \mathbf{r}) \cdot d\mathbf{r} = \frac{1}{2}BR^2 \int_0^{2\pi} d\varphi = B\pi R^2. \quad \blacksquare$$

EXAMPLE 2.2.3

Work Integral As an illustration of a line integral, we want to find the work done by the angular momentum type force of Example 1.9.2: $\mathbf{F} = -\hat{\mathbf{x}}\sin\varphi + \hat{\mathbf{y}}\cos\varphi$ around a pielike sector shown in Fig. 2.5 from the origin to $x = R$, then at constant radial distance R from azimuthal angle $\varphi = 0$ to $\pi/4$ and finally back radially to the origin.

The geometry of the path tells us to use plane polar coordinates ($x = \rho\cos\varphi$, $y = \rho\sin\varphi$). In vector notation, we have

$$\boldsymbol{\rho} = \rho\hat{\boldsymbol{\rho}} = (x, y), \quad \hat{\boldsymbol{\rho}} = \hat{\mathbf{x}}\cos\varphi + \hat{\mathbf{y}}\sin\varphi.$$

However, the work in these coordinates is $\int \mathbf{F}\cdot d\boldsymbol{\rho}$, where $\mathbf{F}$ still needs to be expressed as a linear combination of $\hat{\boldsymbol{\rho}}$ and $\hat{\boldsymbol{\varphi}}$ like the path element

$$d\boldsymbol{\rho} = d\rho\hat{\boldsymbol{\rho}} + \rho d\varphi\frac{d\hat{\boldsymbol{\rho}}}{d\varphi}$$

with

$$\frac{d\hat{\boldsymbol{\rho}}}{d\varphi} = -\hat{\mathbf{x}}\sin\varphi + \hat{\mathbf{y}}\cos\varphi,$$

that follows from differentiating $\hat{\boldsymbol{\rho}} = \hat{\mathbf{x}}\cos\varphi + \hat{\mathbf{y}}\sin\varphi$ with respect to φ. Next, let us express $\hat{\boldsymbol{\varphi}}$ in Cartesian unit vectors.

Differentiating $1 = \hat{\boldsymbol{\rho}}^2$ we obtain $0 = 2\hat{\boldsymbol{\rho}}\cdot\frac{d\hat{\rho}}{d\varphi}$. The vanishing dot product means that $\frac{d\hat{\rho}}{d\varphi}$ is perpendicular to $\hat{\boldsymbol{\rho}}$, just like $\hat{\boldsymbol{\varphi}}$. Because $-\hat{\mathbf{x}}\sin\varphi + \hat{\mathbf{y}}\cos\varphi$ is already a unit vector, it must be equal to $\pm\hat{\boldsymbol{\varphi}}$. Geometry tells us that the $+$ sign is correct.

Applying this to the force, we notice $\mathbf{F} = \hat{\boldsymbol{\varphi}}$ so that the radial integrals do not contribute to the work, only the arc does. Therefore, dropping the radial paths from $d\boldsymbol{\rho}$, we only keep

$$W = \int_0^{\pi/4} \hat{\boldsymbol{\varphi}}\cdot\hat{\boldsymbol{\varphi}}\rho d\varphi|_{\rho=R} = R\int_0^{\pi/4} d\varphi = R\frac{\pi}{4}. \quad \blacksquare$$

EXAMPLE 2.2.4

Magnetic Flux and Stokes's Theorem When a stationary current I flows in a long circular coil of wire (Fig. 2.6), Oersted's law $\oint \mathbf{H}\cdot d\mathbf{r} = I$ and the geometry tell us that the magnetic induction $\mathbf{B} = B_z\hat{\mathbf{z}}$ is along the z-direction (i.e., the coil axis). Moreover, cylindrical coordinates are appropriate to formulate Stokes's theorem

$$\Phi \equiv \int \mathbf{B}\cdot d\boldsymbol{\sigma} = \int (\nabla\times\mathbf{A})\cdot d\boldsymbol{\sigma} = \oint \mathbf{A}\cdot d\mathbf{r}.$$

The latter links the magnetic flux through **one wire loop of the coil** shown in Fig. 2.7 to the integral of the vector potential along the wire and $\mathbf{A} = A_\phi\hat{\boldsymbol{\varphi}}$ is nonvanishing only in the azimuthal direction. With

$$d\boldsymbol{\sigma} = \hat{\mathbf{z}}\rho\, d\rho\, d\varphi, \quad d\mathbf{r}|_{\rho=R} = \rho d\varphi\hat{\boldsymbol{\varphi}}|_{\rho=R} = Rd\varphi\hat{\boldsymbol{\varphi}}$$

Figure 2.6

Magnetic Flux Through a Long Coil

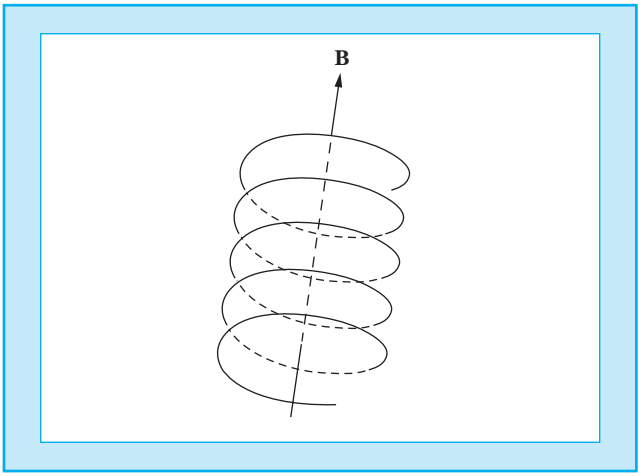
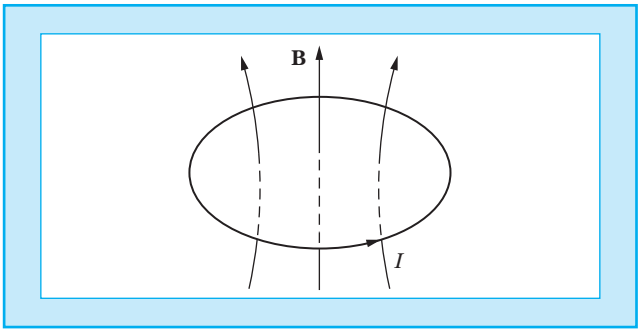


Figure 2.7

Magnetic Flux Through Wire Loop with Current *I*



we obtain the magnetic flux through the cross section of the coil as

$$\Phi = \int_{\rho=0}^{R}\int_{\varphi=0}^{2\pi} B_z \rho \, d\rho \, d\varphi = \int_{\varphi=0}^{2\pi} A_\phi \rho d\varphi|_{\rho=R} = 2\pi R A_\phi,$$

so that $A_\phi = \frac{\Phi}{2\pi R}$. From Oersted's law, we infer $B_z = \frac{\mu_0 I}{2\pi R} = \text{const.}$ ■

EXAMPLE 2.2.5

Area Law for Planetary Motion First, we derive Kepler's law in cylindrical coordinates, which states that the radius vector sweeps out equal areas in equal time from angular momentum conservation.

We consider the sun at the origin as a source of the **central** gravitational force $\mathbf{F} = f(\mathbf{r})\hat{\mathbf{r}}$. Then the orbital angular momentum $\mathbf{L} = m\mathbf{r} \times \mathbf{v}$ of a planet of mass m and velocity $\mathbf{v}$ is conserved because the torque

$$\frac{d\mathbf{L}}{dt} = m\frac{d\mathbf{r}}{dt} \times \frac{d\mathbf{r}}{dt} + \mathbf{r} \times \frac{d\mathbf{p}}{dt} = \mathbf{r} \times \mathbf{F} = \frac{f(\mathbf{r})}{r}\mathbf{r} \times \mathbf{r} = 0.$$

Hence, $\mathbf{L} = \text{const}$. Now we can choose the z-axis to lie along the direction of the orbital angular momentum vector, $\mathbf{L} = L\hat{\mathbf{z}}$, and work in cylindrical coordinates $\mathbf{r} = (\rho, \varphi, z) = \rho\hat{\boldsymbol{\rho}}$ with $z = 0$ [compare with Eq. (2.8)]. The planet moves in the xy-plane because $\mathbf{r}$ and $\mathbf{v}$ are perpendicular to $\mathbf{L}$. Thus, we expand its velocity as follows:

$$\mathbf{v} = \frac{d\mathbf{r}}{dt} = \dot{\rho}\hat{\boldsymbol{\rho}} + \rho\frac{d\hat{\boldsymbol{\rho}}}{dt} = \dot{\rho}\hat{\boldsymbol{\rho}} + \rho\dot{\varphi}\hat{\boldsymbol{\varphi}},$$

and with

$$\hat{\boldsymbol{\rho}} = (\cos\varphi, \sin\varphi), \quad \frac{\partial\hat{\boldsymbol{\rho}}}{d\varphi} = (-\sin\varphi, \cos\varphi) = \hat{\boldsymbol{\varphi}},$$

find that $\frac{d\hat{\rho}}{dt} = \frac{d\hat{\rho}}{d\varphi}\frac{d\varphi}{dt} = \dot{\varphi}\hat{\boldsymbol{\varphi}}$ using the chain rule. As a result,

$$\mathbf{L} = m\boldsymbol{\rho} \times \mathbf{v} = m\rho(\rho\dot{\varphi})(\hat{\boldsymbol{\rho}} \times \hat{\boldsymbol{\varphi}}) = m\rho^2\dot{\varphi}\hat{\mathbf{z}} = \text{ constant}$$

when we substitute the expansions of $\hat{\boldsymbol{\rho}}$ and $\mathbf{v}$ in polar coordinates.

The triangular area swept by the radius vector $\boldsymbol{\rho}$ in the time dt (**area law**) is then given by

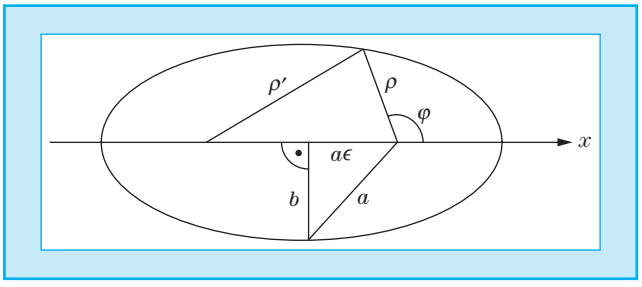
$$A = \frac{1}{2}\int \rho(\rho d\varphi) = \frac{1}{2}\int \rho^2\dot{\varphi}dt = \frac{L}{2m}\int dt = \frac{L\tau}{2m}, \tag{2.12}$$

if we substitute $m\rho^2\dot{\varphi} = L = \text{const}$. Here, τ is the period, that is, the time for one revolution of the planet in its orbit.

Kepler's first law states that the orbit is an ellipse. Now we derive the orbit equation $\rho(\varphi)$ of the ellipse in polar coordinates, where in Fig. 2.8 the sun is at one focus, which is the origin of our cylindrical coordinates. From the geometrical construction of the ellipse we know that $\rho' + \rho = 2a$, where a is the major half-axis; we shall show that this is equivalent to the conventional form of the ellipse equation. The distance between both foci is $0 < 2a\epsilon < 2a$, where $0 < \epsilon < 1$ is the eccentricity of the ellipse. For a circle, $\epsilon = 0$ because both foci coincide with the center. At the angle $\varphi = 3\pi/2$, the distances $\rho' = \rho = a$ are equal in Fig. 2.8, and the Pythagorean theorem applied to this rectangular triangle gives $b^2 + a^2\epsilon^2 = a^2$. As a result, $\sqrt{1-\epsilon^2} = b/a$ is given by the ratio of the minor (b) to the major half-axis a.

Figure 2.8

Ellipse in Polar Coordinates



Now we use the cosine theorem for the right angle triangle with the sides labeled by ρ', ρ, $2a\epsilon$ in Fig. 2.8 and angle $\pi - \varphi$. Then, squaring the vector $\boldsymbol{\rho}' = \boldsymbol{\rho} - 2\epsilon a\hat{\mathbf{x}}$ gives

$$\rho'^2 = \rho^2 + 4a^2\epsilon^2 + 4\rho a\epsilon\cos\varphi,$$

and substituting $\rho' = 2a - \rho$, canceling ρ^2 on both sides, and dividing by $4a$, yields

$$\rho(1 + \epsilon\cos\varphi) = a(1 - \epsilon^2) \equiv p, \tag{2.13}$$

the **Kepler orbit equation** in polar coordinates.

Alternatively, we revert to Cartesian coordinates to find from Eq. (2.13) with $x = \rho\cos\varphi$ that

$$\rho^2 = x^2 + y^2 = (p - x\epsilon)^2 = p^2 + x^2\epsilon^2 - 2px\epsilon,$$

so that the familiar ellipse equation in Cartesian coordinates

$$(1 - \epsilon^2)\left(x + \frac{p\epsilon}{1 - \epsilon^2}\right)^2 + y^2 = p^2 + \frac{p^2\epsilon^2}{1 - \epsilon^2} = \frac{p^2}{1 - \epsilon^2}$$

obtains. If we compare this result with the standard form

$$\frac{(x - x_0)^2}{a^2} + \frac{y^2}{b^2} = 1$$

of the ellipse, we confirm that

$$b = \frac{p}{\sqrt{1 - \epsilon^2}} = a\sqrt{1 - \epsilon^2}, \quad a = \frac{p}{1 - \epsilon^2},$$

and that the distance x_0 between the center and focus is $a\epsilon$, as shown in Fig. 2.8.

In Example 1.11.1, we derived the formula $2A = \int_C (x\,dy - y\,dx)$ for the area A of a simply connected region R enclosed by the simple curve C from Green's theorem taking $P = -y$, $Q = x$ in

$$\int_C (P\,dx + Q\,dy) = \int_R \left(\frac{\partial Q}{\partial x} - \frac{\partial P}{\partial y}\right) dx\,dy.$$

Applying this formula to the Kepler ellipse in the form $x = a\cos\varphi$, $y = b\sin\varphi$ yields

$$2A = ab\int (\cos^2\varphi + \sin^2\varphi)\,d\varphi = 2\pi ab$$

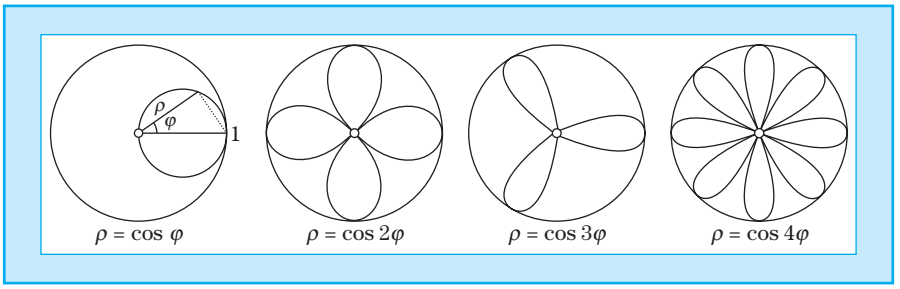
for its area A. This concludes our Kepler orbit example.

A closely related case is the area of the rosetta curve $\rho = \cos n\varphi$ shown in Fig. 2.9 for the cases $n = 1, 2, 3, 4$. As for the area law, we have

$$A = \frac{1}{2}\int_0^{2\pi} \cos^2 n\varphi\,d\varphi = \frac{1}{2n}\int_0^{2n\pi} \cos^2 u\,du = \frac{1}{4n}\int_0^{2n\pi} du = \frac{\pi}{2},$$

independent of n.

Figure 2.9
Rosetta Curves



Another interesting family of curves is given by $\rho = 1 + \epsilon \cos\varphi$. Compare this with the form of the Kepler orbit equation. For $\epsilon = 0$ we have a unit circle and for $\epsilon = 1$ a cardioid (plot it). ■

Gradient

The starting point for developing the gradient operator in curvilinear coordinates is the geometric interpretation of the gradient as the vector having the magnitude and direction of the maximum rate of spacial change of a function ψ (compare Section 1.5). From this interpretation the component of $\nabla\psi(\rho, \varphi, z)$ in the direction normal to the family of surfaces $\rho =$ constant is given by

$$\hat{\boldsymbol{\rho}} \cdot \nabla\psi = \frac{\partial\psi}{\partial\rho} \tag{2.14}$$

because this is the rate of change of ψ for varying ρ, holding φ and z fixed. The φ-component of the gradient in circular cylindrical coordinates has the form

$$\hat{\boldsymbol{\varphi}} \cdot \nabla\psi = \nabla\psi|_{\varphi} = \frac{1}{\rho}\frac{\partial\psi}{\partial\varphi} \tag{2.15}$$

because $ds_{\varphi} = \rho d\varphi$ is the angular line element [Eq. (2.9) and Fig. 2.3]. By repeating this for z and adding vectorially, we see that the gradient becomes

$$\nabla\psi(\rho, \varphi, z) = \hat{\boldsymbol{\rho}}\frac{\partial\psi}{\partial\rho} + \hat{\boldsymbol{\varphi}}\frac{1}{\rho}\frac{\partial\psi}{\partial\varphi} + \hat{\mathbf{z}}\frac{\partial\psi}{\partial z}. \tag{2.16}$$

EXAMPLE 2.2.6

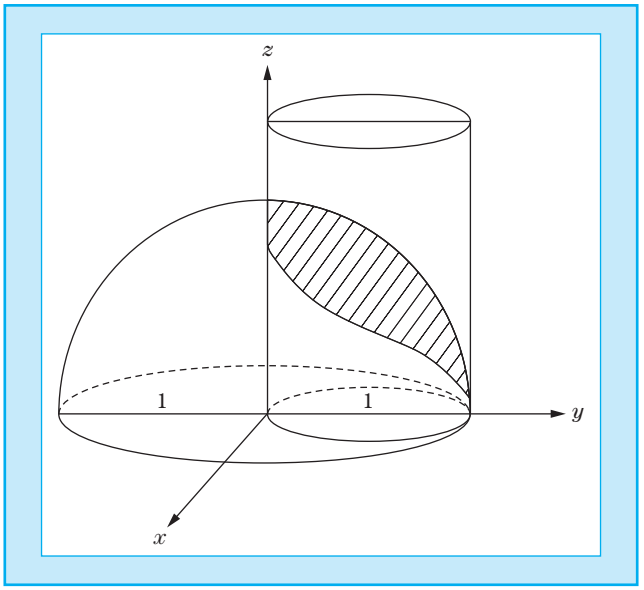
Area Cut from Sphere by Cylinder Consider the unit sphere $\Phi = \rho^2 + z^2 - 1 = 0$ cut by the cylinder $\rho = \sin\varphi$, which has radius $1/2$ and is parallel to the z-axis with center at $y = 1/2$ (Fig. 2.10). Let us calculate the area cut out by the cylinder. We want to apply the area formula of Example 1.9.5, which in cylindrical coordinates has the form

$$A = \int \frac{|\nabla\Phi|}{\frac{\partial\Phi}{\partial z}} \rho\, d\rho\, d\varphi$$

if the surface is given as $\Phi(\rho, \varphi, z) = 0$. If the surface is defined by $z = f(\rho, \varphi)$, then $\nabla\Phi = (-\frac{\partial f}{\partial\rho}, -\frac{1}{\rho}\frac{\partial f}{\partial\varphi}, 1)$ and $|\nabla\Phi|^2 = 1 + (\frac{\partial f}{\partial\rho})^2 + (\frac{1}{\rho}\frac{\partial f}{\partial\varphi})^2$.

Figure 2.10

Area Cut from Unit Sphere by a Cylinder



In the xy-plane the cylinder is given by the circle $x^2 + (y - 1/2)^2 = 1/4$, or $\rho^2 = y$, that is, $\rho = \sin\varphi$ as stated above. Also, $\nabla\Phi = (2\rho, 0, 2z)$, $\frac{\partial\Phi}{\partial z} = 2z$ so that $|\nabla\Phi|^2 = 4(\rho^2 + z^2) = 4$ and

$$\frac{|\nabla\Phi|}{\frac{\partial\Phi}{\partial z}} = \frac{1}{z}.$$

Hence, the surface area cut out on the sphere becomes

$$\begin{aligned} 2\int_0^{\pi/2}\int_0^{\sin\varphi} \frac{\rho\, d\rho\, d\varphi}{\sqrt{1-\rho^2}} &= -2\int_0^{\pi/2} \sqrt{1-\rho^2}\Big|_{\rho=0}^{\sin\varphi} d\varphi \\ &= 2\int_0^{\pi/2} \left(1 - \sqrt{1-\sin^2\varphi}\right) d\varphi = 2\int_0^{\pi/2} (1-\cos\varphi)\, d\varphi \\ &= 2(\varphi - \sin\varphi)\Big|_0^{\pi/2} = 2\left(\frac{\pi}{2} - 1\right) = \pi - 2 \end{aligned}$$

upon integrating over the semicircle in the first quadrant and multiplying by 2 because of symmetry. If we cut out two such cylindrical windows, the remaining spherical surface is $2\pi - 2(\pi - 2) = 4$, independent of π. ■

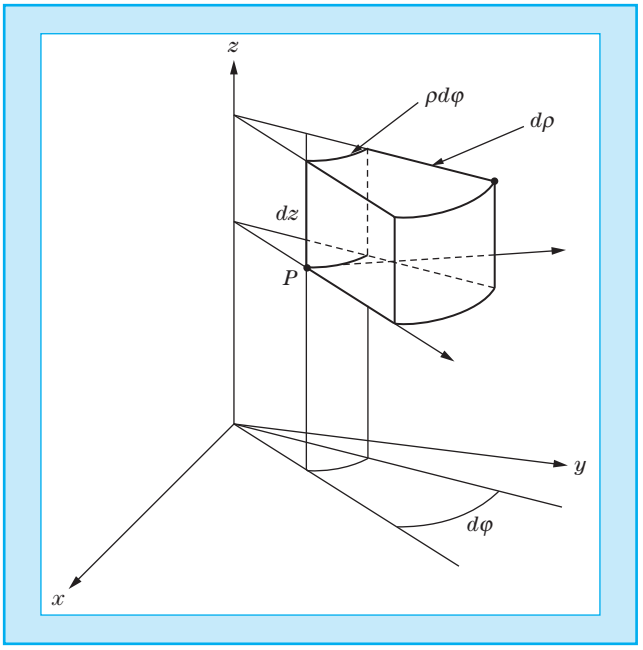
Divergence

The divergence operator may be obtained from the second definition [Eq. (1.113)] of Chapter 1 or equivalently from Gauss's theorem (Section 1.11). Let us use Eq. (1.113),

$$\nabla \cdot \mathbf{V}(\rho, \varphi, z) = \lim_{\int d\tau \to 0} \frac{\int \mathbf{V} \cdot d\boldsymbol{\sigma}}{\int d\tau}, \tag{2.17}$$

Figure 2.11

Volume Element in Cylindrical Coordinates



with a differential volume $d\tau = \rho\, d\rho\, d\varphi\, dz$ (Fig. 2.11). Note that the positive directions have been chosen so that (ρ, φ, z) or $(\hat{\boldsymbol{\rho}}, \hat{\boldsymbol{\varphi}}, \hat{\mathbf{z}})$ form a right-handed set, $\hat{\boldsymbol{\rho}} \times \hat{\boldsymbol{\varphi}} = \hat{\mathbf{z}}$.

The area integral for the two faces $\rho =$ constant in Fig. 2.11 is given by

$$\left[V_\rho \rho + \frac{\partial}{\partial \rho}(V_\rho \rho) d\rho\right] dz\, d\varphi - V_\rho \rho\, d\varphi\, dz = \frac{\partial}{\partial \rho}(V_\rho \rho) d\rho\, d\varphi\, dz, \tag{2.18}$$

exactly as in Sections 1.6 and 1.9.[1] Here, V_ρ is the component of $\mathbf{V}$ in the $\hat{\boldsymbol{\rho}}$-direction, etc., increasing ρ; that is, $V_\rho = \hat{\boldsymbol{\rho}} \cdot \mathbf{V}$ is the projection of $\mathbf{V}$ onto the $\hat{\boldsymbol{\rho}}$-direction. Adding in the similar results for the other two pairs of surfaces, we obtain (for the differential volume $d\tau = \rho d\rho\, d\varphi\, dz$)

$$\int \mathbf{V}(\rho, \varphi, z) \cdot d\boldsymbol{\sigma} = \left[\frac{\partial}{\partial \rho}(V_\rho \rho) + \frac{\partial}{\partial \varphi} V_\varphi + \frac{\partial}{\partial z}(V_z \rho)\right] d\rho\, d\varphi\, dz. \tag{2.19}$$

Division by our differential volume $d\tau$ yields

$$\boldsymbol{\nabla} \cdot \mathbf{V}(\rho, \varphi, z) = \frac{1}{\rho}\left[\frac{\partial}{\partial \rho}(V_\rho \rho) + \frac{\partial}{\partial \varphi} V_\varphi + \frac{\partial}{\partial z}(V_z \rho)\right]. \tag{2.20}$$

We may obtain the Laplacian by combining Eqs. (2.16) and (2.20) using $\mathbf{V} = \boldsymbol{\nabla}\psi(\rho, \varphi, z)$. This leads to

$$\boldsymbol{\nabla} \cdot \boldsymbol{\nabla}\psi(\rho, \varphi, z) = \frac{1}{\rho}\left[\frac{\partial}{\partial \rho}\left(\rho \frac{\partial \psi}{\partial \rho}\right) + \frac{\partial}{\partial \varphi}\left(\frac{1}{\rho}\frac{\partial \psi}{\partial \varphi}\right) + \frac{\partial}{\partial z}\left(\rho \frac{\partial \psi}{\partial z}\right)\right]. \tag{2.21}$$

[1] Since we take the limit $d\rho, d\varphi, dz \to 0$, the second- and higher order derivatives will drop out.

Curl

Finally, to develop $\nabla \times \mathbf{V}$, let us apply Stokes's theorem (Section 1.11) and, as with the divergence, take the limit as the surface area becomes vanishingly small. Working on one component at a time, we consider a differential surface element in the curvilinear surface $\rho =$ constant. For such a small surface the mean value theorem of integral calculus tells us that an integral is given by the surface times the function at a mean value on the small surface. Thus, from

$$\int_s \nabla \times \mathbf{V}|_\rho \cdot d\boldsymbol{\sigma}_\rho = \hat{\boldsymbol{\rho}} \cdot (\nabla \times \mathbf{V}) \rho \, d\varphi \, dz \tag{2.22}$$

Stokes's theorem yields

$$\hat{\boldsymbol{\rho}} \cdot (\nabla \times \mathbf{V}) \rho \, d\varphi \, dz = \oint \mathbf{V} \cdot d\mathbf{r}, \tag{2.23}$$

with the line integral lying in the surface $\rho =$ constant. Following the loop (1, 2, 3, 4) of Fig. 2.12,

$$\begin{aligned} \oint \mathbf{V}(\rho, \varphi, z) \cdot d\mathbf{r} &= V_\varphi \rho \, d\varphi + \left[V_z + \frac{\partial}{\partial \varphi}(V_z) \, d\varphi \right] dz \\ &\quad - \left[V_\varphi \rho + \frac{\partial}{\partial z}(V_\varphi \rho) dz \right] d\varphi - V_z \, dz \\ &= \left[\frac{\partial}{\partial \varphi} V_z - \frac{\partial}{\partial z}(\rho V_\varphi) \right] d\varphi \, dz. \end{aligned} \tag{2.24}$$

We pick up a positive sign when going in the positive direction on parts 1 and 2, and a negative sign on parts 3 and 4, because here we are going in the negative direction. Higher order terms have been omitted. They will vanish in the limit as the surface becomes vanishingly small ($d\varphi \to 0$, $dz \to 0$).

Combining Eqs. (2.23) and (2.24) we obtain

$$\nabla \times \mathbf{V}|_\rho = \frac{1}{\rho} \left[\frac{\partial}{\partial \varphi} V_z - \frac{\partial}{\partial z}(\rho V_\varphi) \right]. \tag{2.25}$$

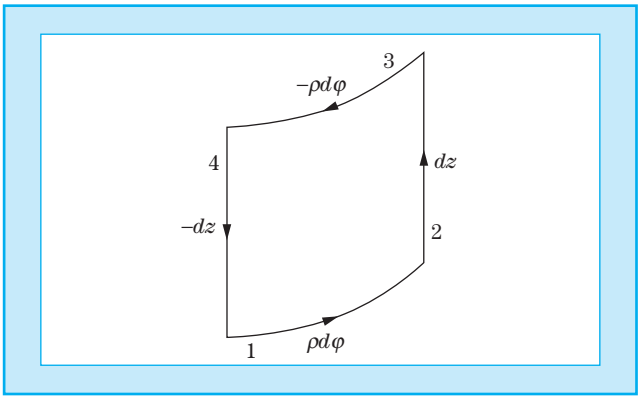


Figure 2.12

Surface Element with $\rho =$ Constant in Cylindrical Coordinates

The remaining two components of $\nabla \times \mathbf{V}$ may be picked up by cyclic permutation of the indices. As in Chapter 1, it is often convenient to write the curl in determinant form:

$$\nabla \times \mathbf{V} = \frac{1}{\rho}\begin{vmatrix} \hat{\boldsymbol{\rho}} & \rho\hat{\boldsymbol{\varphi}} & \hat{\mathbf{z}} \\ \dfrac{\partial}{\partial \rho} & \dfrac{\partial}{\partial \varphi} & \dfrac{\partial}{\partial z} \\ V_\rho & \rho V_\varphi & V_z \end{vmatrix}. \tag{2.26}$$

Remember that because of the presence of the differential operators, this determinant must be expanded from the top down (Eq. 3.11). Note that this equation is **not** identical with the form for the cross product of two vectors. ∇ is not an ordinary vector; it is a vector **operator**.

Our geometric interpretation of the gradient and the use of Gauss's and Stokes's theorems (or integral definitions of divergence and curl) have enabled us to obtain these quantities **without having to differentiate the unit vectors** $\hat{\rho}$, $\hat{\varphi}$.

EXAMPLE 2.2.7

Magnetic Induction of a Long Wire This problem involves the magnetic induction $\mathbf{B}$ and vector potential $\mathbf{A}$ generated by a long wire in the z-direction carrying a stationary current I shown in Fig. 2.13. Oersted's law $\oint \mathbf{H} \cdot d\mathbf{r} = I$ and the geometry tell us that $\mathbf{B}$ has only an azimuthal component, and the vector potential has only a z-component from the Biot–Savart law. With $d\mathbf{r} = \rho d\varphi \hat{\boldsymbol{\varphi}}$ and $\mathbf{B} = \mu_0 \mathbf{H}$ we obtain $\mathbf{B} = \frac{\mu_0 I}{2\pi\rho}\hat{\boldsymbol{\varphi}}$. Using $\mathbf{B} = \nabla \times \mathbf{A}$ we verify that $\mathbf{A} = -\hat{\mathbf{z}}\frac{\mu_0 I}{2\pi} \ln \rho$ because Eq. (2.26) gives

$$\nabla \times (\ln \rho \hat{\mathbf{z}}) = \frac{1}{\rho}\begin{vmatrix} \hat{\boldsymbol{\rho}} & \rho\hat{\boldsymbol{\varphi}} & \hat{\mathbf{z}} \\ \dfrac{\partial}{\partial \rho} & \dfrac{\partial}{\partial \varphi} & \dfrac{\partial}{\partial z} \\ 0 & 0 & \ln \rho \end{vmatrix} = -\hat{\boldsymbol{\varphi}}\frac{d \ln \rho}{d\rho} = -\frac{\hat{\boldsymbol{\varphi}}}{\rho}.$$

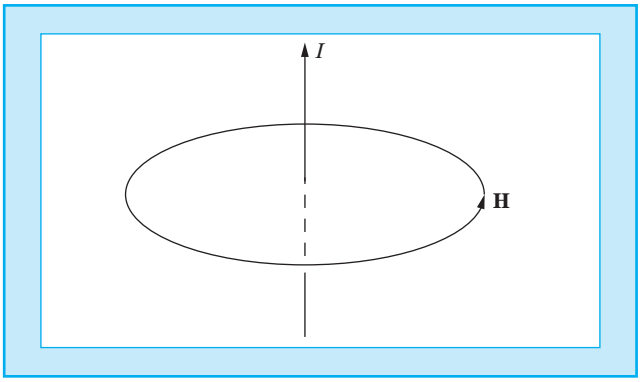


Figure 2.13

Magnetic Field of a Long Wire with Current *I*

An example of a line integral of the form $\int \mathbf{A} \times d\mathbf{r}$ is a loop of wire C carrying a current I that is placed in a constant magnetic field $\mathbf{B}$; then the force element is given by $d\mathbf{F} = Id\mathbf{r} \times \mathbf{B}$ so that the force is $\mathbf{F} = I \int_C d\mathbf{r} \times \mathbf{B}$. ■

EXERCISES

2.2.1 Resolve the circular cylindrical unit vectors into their Cartesian components (Fig. 2.2).

ANS. $\hat{\boldsymbol{\rho}} = \hat{\mathbf{x}} \cos\varphi + \hat{\mathbf{y}} \sin\varphi,$
$\hat{\boldsymbol{\varphi}} = -\hat{\mathbf{x}} \sin\varphi + \hat{\mathbf{y}} \cos\varphi,$
$\hat{\mathbf{z}} = \hat{\mathbf{z}}.$

2.2.2 Resolve the Cartesian unit vectors into their circular cylindrical components (Fig. 2.2).

ANS. $\hat{\mathbf{x}} = \hat{\boldsymbol{\rho}} \cos\varphi - \hat{\boldsymbol{\varphi}} \sin\varphi,$
$\hat{\mathbf{y}} = \hat{\boldsymbol{\rho}} \sin\varphi + \hat{\boldsymbol{\varphi}} \cos\varphi,$
$\hat{\mathbf{z}} = \hat{\mathbf{z}}.$

2.2.3 From the results of Exercise 2.2.1, show that

$$\frac{\partial \hat{\boldsymbol{\rho}}}{\partial \varphi} = \hat{\boldsymbol{\varphi}}, \qquad \frac{\partial \hat{\boldsymbol{\varphi}}}{\partial \varphi} = -\hat{\boldsymbol{\rho}}$$

and that all other first derivatives of the circular cylindrical unit vectors with respect to the circular cylindrical coordinates vanish.

2.2.4 Compare $\nabla \cdot \mathbf{V}$ [Eq. (2.20)] with the gradient operator

$$\nabla = \hat{\boldsymbol{\rho}} \frac{\partial}{\partial \rho} + \hat{\boldsymbol{\varphi}} \frac{1}{\rho} \frac{\partial}{\partial \varphi} + \hat{\mathbf{z}} \frac{\partial}{\partial z}$$

[Eq. (2.16)] dotted into $\mathbf{V}$. Explain why they differ.

2.2.5 A rigid body is rotating about a fixed axis with a constant angular velocity ω. Take ω to lie along the z-axis. Express $\mathbf{r}$ in circular cylindrical coordinates and, using circular cylindrical coordinates, calculate
(a) $\mathbf{v} = \boldsymbol{\omega} \times \mathbf{r}$, (b) $\nabla \times \mathbf{v}$.

ANS. (a) $\mathbf{v} = \varphi \omega \rho$ (b) $\nabla \times \mathbf{v} = 2\omega$.

2.2.6 Halley's comet has a period of about 76 years, and its closest distance from the sun is 9×10^7 km. What is its greatest distance from the sun?

2.2.7 A planet is in a circular orbit about a star that explodes, shedding 2% of its mass in an expanding spherical shell. Find the eccentricity of the new orbit of the planet, which otherwise is not affected by the shell.

2.2.8 Find the circular cylindrical components of the velocity and acceleration of a moving particle,

$$v_\rho = \dot{\rho}, \qquad a_\rho = \ddot{\rho} - \rho\dot{\varphi}^2,$$
$$v_\varphi = \rho\dot{\varphi}, \qquad a_\varphi = \rho\ddot{\varphi} + 2\dot{\rho}\dot{\varphi},$$
$$v_z = \dot{z}, \qquad a_z = \ddot{z}.$$

Hint.

$$\begin{aligned}\mathbf{r}(t) &= \hat{\boldsymbol{\rho}}(t)\rho(t) + \hat{\mathbf{z}}z(t)\\ &= [\hat{\mathbf{x}}\cos\varphi(t) + \hat{\mathbf{y}}\sin\varphi(t)]\rho(t) + \hat{\mathbf{z}}z(t).\end{aligned}$$

Note. $\dot{\rho} = d\rho/dt$, $\ddot{\rho} = d^2\rho/dt^2$, and so on.

2.2.9 In right circular cylindrical coordinates a particular vector function is given by

$$\mathbf{V}(\rho, \varphi) = \hat{\boldsymbol{\rho}}V_\rho(\rho, \varphi) + \hat{\boldsymbol{\varphi}}V_\varphi(\rho, \varphi).$$

Show that $\nabla \times \mathbf{V}$ has only a z-component.

2.2.10 The linear velocity of particles in a rigid body rotating with angular velocity ω is given by

$$\mathbf{v} = \hat{\boldsymbol{\varphi}}\rho\omega.$$

Integrate $\oint \mathbf{v}\cdot d\boldsymbol{\lambda}$ around a circle in the xy-plane and verify that

$$\frac{\oint \mathbf{v}\cdot d\boldsymbol{\lambda}}{\text{area}} = \nabla \times \mathbf{v}|_z.$$

2.2.11 Two protons are moving toward each other. Describe their orbits if they approach (a) head-on and (b) on parallel lines a distance b (impact parameter) apart.
Hint. Ignore the strong interaction but keep the Coulomb repulsion.

2.2.12 A stationary current I flows in the wire loop A anticlockwise. If the loop A moves toward a parallel loop B of the same size and shape, in which direction will the induced current flow in loop B?

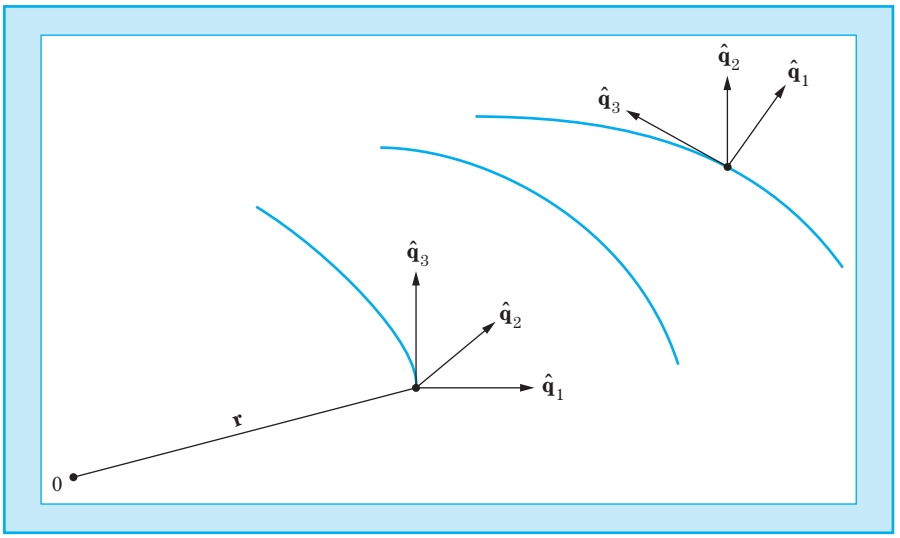
2.2.13 A particle of mass m and charge e moves in a circular orbit in a magnetic field $\mathbf{B}$ perpendicular to the orbit. Show that the time the particle takes for one orbit does not depend on its velocity. Is this still true if you change the direction of the magnetic field?

2.3 Orthogonal Coordinates

In Cartesian coordinates we deal with three mutually perpendicular families of planes: $x =$ constant, $y =$ constant, and $z =$ constant. Imagine that we superimpose on this system three other families of surfaces $q_i(x, y, z)$, $i = 1, 2, 3$. The surfaces of any one family need not be parallel to each other and they need not be planes. If this is difficult to visualize, see Fig. 2.14, or the figure of a specific coordinate system such as Fig. 2.1 may be helpful. The three new families of surfaces need not be mutually perpendicular, but for simplicity we impose such a condition below [Eq. (2.33)]. This orthogonality has many advantages: Locally perpendicular coordinates are almost like Cartesian coordinates, where areas and volumes are products of coordinate differentials, and two-dimensional motion may be separated into analogs of one-dimensional

Figure 2.14

Curved Coordinates q_i with Varying Directions $\hat{\mathbf{q}}_i$



radial and angular components. A relevant example is the motion of a planet around a central star in plane polar coordinates (Example 2.2.5). In other words, we can again break vectors into components efficiently: $(x, y) \to (\rho, \varphi)$, a powerful concept of physics and engineering. In this section, we develop the general formalism of orthogonal coordinates, **derive from the geometry of orthogonal coordinates the coordinate differentials, and use them for line, area, and volume elements in multiple integrals.**

We may describe any point (x, y, z) as the intersection of three planes in Cartesian coordinates or as the intersection of the three surfaces that form our new, curvilinear coordinates as sketched in Fig. 2.14. Describing the curvilinear coordinate surfaces by $q_1 = \text{constant}$, $q_2 = \text{constant}$, $q_3 = \text{constant}$, we may identify our point by (q_1, q_2, q_3) as well as by (x, y, z). This means that in principle we may write

General curvilinear coordinates	Circular cylindrical coordinates
q_1, q_2, q_3	ρ, φ, z
$x = x(q_1, q_2, q_3)$	$-\infty < x = \rho\cos\varphi < \infty$
$y = y(q_1, q_2, q_3)$	$-\infty < y = \rho\sin\varphi < \infty$
$z = z(q_1, q_2, q_3)$	$-\infty < z = z < \infty$

(2.27)

specifying x, y, z in terms of the q's and the inverse relations,

$$\begin{aligned} q_1 &= q_1(x, y, z) & 0 \le \rho &= (x^2 + y^2)^{1/2} < \infty \\ q_2 &= q_2(x, y, z) & 0 \le \varphi &= \arctan(y/x) < 2\pi \\ q_3 &= q_3(x, y, z) & -\infty < z &= z < \infty. \end{aligned} \tag{2.28}$$

As a specific illustration of the general, abstract q_1, q_2, q_3, the transformation equations for circular cylindrical coordinates (Section 2.2) are included in Eqs. (2.27) and (2.28). With each family of surfaces q_i = constant, we can associate a unit vector $\hat{\mathbf{q}}_i$ normal to the surface q_i = constant and in the direction of increasing q_i. Because the normal to the q_i = constant surfaces can point in different directions depending on the position in space (remember that these surfaces are not planes), **the unit vectors $\hat{\mathbf{q}}_i$ can depend on the position in space**, just like $\hat{\boldsymbol{\varphi}}$ in cylindrical coordinates. Then the coordinate vector and a vector $\mathbf{V}$ may be written as

$$\mathbf{r} = \hat{\mathbf{q}}_1 q_1 + \hat{\mathbf{q}}_2 q_2 + \hat{\mathbf{q}}_3 q_3, \qquad \mathbf{V} = \hat{\mathbf{q}}_1 V_1 + \hat{\mathbf{q}}_2 V_2 + \hat{\mathbf{q}}_3 V_3. \tag{2.29}$$

The $\hat{\mathbf{q}}_i$ are normalized to $\hat{\mathbf{q}}_i^2 = 1$ and form a right-handed coordinate system with volume $\hat{\mathbf{q}}_1 \cdot (\hat{\mathbf{q}}_2 \times \hat{\mathbf{q}}_3) = 1$.

This example tells us that we need to differentiate $x(q_1, q_2, q_3)$ in Eq. (2.27), and this leads to (see total differential in Section 1.5)

$$dx = \frac{\partial x}{\partial q_1} dq_1 + \frac{\partial x}{\partial q_2} dq_2 + \frac{\partial x}{\partial q_3} dq_3, \tag{2.30}$$

and similarly for differentiation of y and z, that is, $d\mathbf{r} = \sum_i \frac{\partial \mathbf{r}}{\partial q_i} dq_i$.

In curvilinear coordinate space the most general expression for the square of the distance element can be written as a quadratic form:

$$\begin{aligned} ds^2 &= g_{11}\, dq_1^2 + g_{12}\, dq_1\, dq_2 + g_{13}\, dq_1\, dq_3 \\ &\quad + g_{21}\, dq_2\, dq_1 + g_{22}\, dq_2^2 + g_{23}\, dq_2\, dq_3 \\ &\quad + g_{31}\, dq_3\, dq_1 + g_{32}\, dq_3\, dq_2 + g_{33}\, dq_3^2 \\ &= \sum_{ij} g_{ij}\, dq_i\, dq_j, \end{aligned} \tag{2.31}$$

where the mixed terms $dq_i dq_j$ with $i \neq j$, signal that these coordinates are not orthogonal. Spaces for which Eq. (2.31) is the definition of distance are called metric and Riemannian. Substituting Eq. (2.30) (squared) and the corresponding results for dy^2 and dz^2 into Eq. (2.2) and equating coefficients of $dq_i\, dq_j$,[2] we find

$$g_{ij} = \frac{\partial x}{\partial q_i}\frac{\partial x}{\partial q_j} + \frac{\partial y}{\partial q_i}\frac{\partial y}{\partial q_j} + \frac{\partial z}{\partial q_i}\frac{\partial z}{\partial q_j} = \sum_l \frac{\partial x_l}{\partial q_i}\frac{\partial x_l}{\partial q_j}. \tag{2.32}$$

These coefficients g_{ij}, which we now proceed to investigate, may be viewed as specifying the nature of the coordinate system (q_1, q_2, q_3). Collectively, these coefficients are referred to as the **metric**.[3] In general relativity the metric components are determined by the properties of matter, that is, the g_{ij} are solutions of Einstein's nonlinear field equations that are driven by the energy-momentum tensor of matter: Geometry is merged with physics.

[2]The dq are arbitrary. For instance, setting $dq_2 = dq_3 = 0$ isolates g_{11}. Note that Eq. (2.32) can be derived from Eq. (2.30) more elegantly with the matrix notation of Chapter 3.

[3]The tensor nature of the set of g_{ij} follows from the quotient rule (Section 2.8). Then the tensor transformation law yields Eq. (2.32).

From this point on, we limit ourselves to **orthogonal** coordinate systems (defined by mutually **perpendicular** surfaces or, equivalently, sums of squares in ds^2),[4] which means (Exercise 2.3.1)

$$g_{ij} = 0, \qquad i \neq j, \quad \text{or} \quad \hat{\mathbf{q}}_i \cdot \hat{\mathbf{q}}_j = \delta_{ij}. \tag{2.33}$$

Now, to simplify the notation, we write $g_{ii} = h_i^2$ so that

$$ds^2 = (h_1\, dq_1)^2 + (h_2\, dq_2)^2 + (h_3\, dq_3)^2 = \sum_i (h_i\, dq_i)^2. \tag{2.34}$$

The specific orthogonal coordinate systems in Sections 2.2 and 2.5 are described by specifying **scale factors** h_1, h_2, and h_3. Conversely, the scale factors may be conveniently identified by the relation

$$ds_i = h_i\, dq_i \tag{2.35}$$

for any given dq_i, holding the other q's constant. Note that the three curvilinear coordinates q_1, q_2, q_3 need not be lengths. The scale factors h_i may depend on the q's and they may have dimensions. The **product** $h_i\, dq_i$ must have dimensions of length and be positive. Because Eq. (2.32) can also be written as a scalar product of the **tangent vectors**

$$g_{ij} = \frac{\partial \mathbf{r}}{\partial q_i} \cdot \frac{\partial \mathbf{r}}{\partial q_j}, \tag{2.36}$$

the orthogonality condition in Eq. (2.33) in conjunction with the sum of squares in Eq. (2.34) tell us that for each displacement along a coordinate axis (see Fig. 2.14)

$$\frac{\partial \mathbf{r}}{\partial q_i} = h_i \hat{\mathbf{q}}_i, \tag{2.37}$$

they are the coordinate tangent vectors so that the differential distance vector $d\mathbf{r}$ becomes

$$d\mathbf{r} = \sum_i h_i\, dq_i\, \hat{\mathbf{q}}_i = \sum_i h_i d\mathbf{q}_i. \tag{2.38}$$

Using the curvilinear component form we find that a **line integral** becomes

$$\int \mathbf{V} \cdot d\mathbf{r} = \sum_i \int V_i h_i\, dq_i. \tag{2.39}$$

The work $dW = \mathbf{F} \cdot d\mathbf{r}$ done by a force $\mathbf{F}$ along a line element $d\mathbf{r}$ is the most prominent example in physics for a line integral. In this context, we often use the **chain rule** in the form

$$\int_{\mathbf{r}(t_1)}^{\mathbf{r}(t_2)} \mathbf{A}(\mathbf{r}(\mathbf{t})) \cdot d\mathbf{r} = \int_{t_1}^{t_2} \mathbf{A}(\mathbf{r}(\mathbf{t})) \cdot \frac{d\mathbf{r}}{dt} dt. \tag{2.40}$$

[4] In relativistic cosmology the nondiagonal elements of the metric g_{ij} are usually set equal to zero as a consequence of physical assumptions such as no rotation.

EXAMPLE 2.3.1

Energy Conservation for Conservative Force Using Eq. (2.40) for a force $\mathbf{F} = m\frac{d\mathbf{v}}{dt}$ in conjunction with Newton's equation of motion for a particle of mass m allows us to integrate analytically the work

$$\int_{\mathbf{r}(t_1)}^{\mathbf{r}(t_2)} \mathbf{F}\cdot d\mathbf{r} = \int_{t_1}^{t_2} \mathbf{F}\cdot\frac{d\mathbf{r}(t)}{dt}dt = m\int \frac{d\mathbf{v}}{dt}\cdot\mathbf{v}dt = \frac{m}{2}\int\frac{d\mathbf{v}^2}{dt}dt = \frac{m}{2}\mathbf{v}^2|_{t_1}^{t_2}$$
$$= \frac{m}{2}[\mathbf{v}^2(t_2) - \mathbf{v}^2(t_1)]$$

as the difference of kinetic energies. If the force derives from a potential as $\mathbf{F} = -\boldsymbol{\nabla}V$, then we can **integrate that line integral explicitly because it contains the gradient**

$$\int_{\mathbf{r}(t_1)}^{\mathbf{r}(t_2)} \mathbf{F}\cdot d\mathbf{r} = -\int_{\mathbf{r}(t_1)}^{\mathbf{r}(t_2)} \boldsymbol{\nabla}V(\mathbf{r})\cdot d\mathbf{r} = -V|_{\mathbf{r}(t_1)}^{\mathbf{r}(t_2)} = -[V(\mathbf{r}(t_2)) - V(\mathbf{r}(t_1))]$$

and identify the work as minus the potential difference. Comparing both expressions, we have **energy conservation**

$$\frac{m}{2}\mathbf{v}^2(t_2) + V(\mathbf{r}(t_2)) = \frac{m}{2}\mathbf{v}^2(t_1) + V(\mathbf{r}(t_1))$$

for a conservative force. The path independence of the work is discussed in detail in Section 1.12. Thus, in this case only the end points of the path $\mathbf{r}(t)$ matter. ■

In Cartesian coordinates the **length of a space curve** is given by $\int ds$, with $ds^2 = dx^2 + dy^2 + dz^2$. If a space curve in curved coordinates is parameterized as $(q_1(t),\ q_2(t),\ q_3(t))$, we find its length by integrating the length element of Eq. (2.34) so that

$$L = \int_{t_1}^{t_2} \sqrt{h_1^2\left(\frac{dq_1}{dt}\right)^2 + h_2^2\left(\frac{dq_2}{dt}\right)^2 + h_3^2\left(\frac{dq_3}{dt}\right)^2}\,dt \tag{2.41}$$

using the chain rule [Eq. (2.40)]. From Eq. (2.35) we immediately develop the **area and volume elements**

$$d\sigma_{ij} = ds_i\,ds_j = h_i h_j\,dq_i\,dq_j \tag{2.42}$$

and

$$d\tau = ds_1\,ds_2\,ds_3 = h_1h_2h_3\,dq_1\,dq_2\,dq_3. \tag{2.43}$$

From Eq. (2.42) an area element may be expanded:

$$d\boldsymbol{\sigma} = ds_2\,ds_3\,\hat{\mathbf{q}}_1 + ds_3\,ds_1\,\hat{\mathbf{q}}_2 + ds_1\,ds_2\,\hat{\mathbf{q}}_3$$
$$= h_2h_3\,dq_2\,dq_3\,\hat{\mathbf{q}}_1 + h_3h_1\,dq_3\,dq_1\,\hat{\mathbf{q}}_2$$
$$+ h_1h_2\,dq_1\,dq_2\,\hat{\mathbf{q}}_3. \tag{2.44}$$

Thus, a **surface integral** becomes

$$\int \mathbf{V}\cdot d\boldsymbol{\sigma} = \int V_1 h_2 h_3\, dq_2\, dq_3 + \int V_2 h_3 h_1\, dq_3\, dq_1 + \int V_3 h_1 h_2\, dq_1\, dq_2. \tag{2.45}$$

More examples of such line and surface integrals in cylindrical and spherical polar coordinates appear in Sections 2.2 and 2.5.

In anticipation of the new forms of equations for vector **calculus** that appear in the next section, we emphasize that vector **algebra** is the same in orthogonal curvilinear coordinates as in Cartesian coordinates. Specifically, for the dot product

$$\mathbf{A}\cdot\mathbf{B} = \sum_{i,k} A_i \hat{\mathbf{q}}_i \cdot \hat{\mathbf{q}}_k B_k = \sum_{i,k} A_i B_k \delta_{ik} = \sum_i A_i B_i, \tag{2.46}$$

where the subscripts indicate curvilinear components. For the cross product

$$\mathbf{A}\times\mathbf{B} = \sum_{i,k} A_i \hat{\mathbf{q}}_i \times \hat{\mathbf{q}}_k B_k = \begin{vmatrix} \hat{\mathbf{q}}_1 & \hat{\mathbf{q}}_2 & \hat{\mathbf{q}}_3 \\ A_1 & A_2 & A_3 \\ B_1 & B_2 & B_3 \end{vmatrix}, \tag{2.47}$$

as in Eq. (1.40).

EXAMPLE 2.3.2 **Orbital Angular Momentum in Cylindrical Coordinates** In circular cylindrical coordinates the orbital angular momentum takes the form [see Eq. (2.8)] for the coordinate vector $\mathbf{r} = \boldsymbol{\rho} + \mathbf{z}$ and Example 2.2.5 for the velocity $\mathbf{v} = \dot{\rho}\hat{\boldsymbol{\rho}} + \rho\dot{\varphi}\hat{\boldsymbol{\varphi}} + \dot{z}\hat{\mathbf{z}}$

$$\mathbf{L} = \mathbf{r}\times\mathbf{p} = m\begin{vmatrix} \hat{\boldsymbol{\rho}} & \hat{\boldsymbol{\varphi}} & \hat{\mathbf{z}} \\ \rho & 0 & z \\ \dot{\rho} & \rho\dot{\varphi} & \dot{z} \end{vmatrix}. \tag{2.48}$$

Now let us take the mass to be 3 kg, the lever arm as 1 m in the radial direction of the xy-plane, and the velocity as 2 m/s in the z-direction. Then we expect $\mathbf{L}$ to be in the $\hat{\boldsymbol{\varphi}}$ direction and quantitatively

$$\mathbf{L} = 3\begin{vmatrix} \hat{\boldsymbol{\rho}} & \hat{\boldsymbol{\varphi}} & \hat{\mathbf{z}} \\ 1 & 0 & 0 \\ 0 & 0 & 2 \end{vmatrix} = 3\hat{\boldsymbol{\rho}}\begin{vmatrix} 0 & 0 \\ 0 & 2 \end{vmatrix} - 3\hat{\boldsymbol{\varphi}}\begin{vmatrix} 1 & 0 \\ 0 & 2 \end{vmatrix} + 3\hat{\mathbf{z}}\begin{vmatrix} 1 & 0 \\ 0 & 0 \end{vmatrix} = -6\hat{\boldsymbol{\varphi}}\ \text{mkg/s}. \tag{2.49}$$

■

Previously, we specialized to locally rectangular coordinates that are adapted to special symmetries. Let us now briefly examine the more general case in which the coordinates are not necessarily orthogonal. Surface and volume elements are part of multiple integrals, which are common in physical applications such as center of mass determinations and moments of inertia. Typically, we choose coordinates according to the symmetry of the particular problem. In Chapter 1 we used Gauss's theorem to transform a volume integral into a

surface integral and Stokes's theorem to transform a surface integral into a line integral. For orthogonal coordinates, the surface and volume elements are simply products of the line elements $h_i dq_i$ [see Eqs. (2.42) and (2.43)]. For the general case, we use the geometric meaning of $\partial\mathbf{r}/\partial q_i$ in Eq. (2.37) as tangent vectors. We start with the Cartesian surface element $dx\,dy$, which becomes an infinitesimal rectangle in the new coordinates q_1, q_2 formed by the two incremental vectors

$$d\mathbf{r}_1 = \mathbf{r}(q_1 + dq_1, q_2) - \mathbf{r}(q_1, q_2) = \frac{\partial \mathbf{r}}{\partial q_1} dq_1,$$
$$d\mathbf{r}_2 = \mathbf{r}(q_1, q_2 + dq_2) - \mathbf{r}(q_1, q_2) = \frac{\partial \mathbf{r}}{\partial q_2} dq_2, \tag{2.50}$$

whose area is the z-component of their cross product, or

$$dx\,dy = d\mathbf{r}_1 \times d\mathbf{r}_2\big|_z = \left[\frac{\partial x}{\partial q_1}\frac{\partial y}{\partial q_2} - \frac{\partial x}{\partial q_2}\frac{\partial y}{\partial q_1}\right] dq_1\,dq_2$$
$$= \begin{vmatrix} \frac{\partial x}{\partial q_1} & \frac{\partial x}{\partial q_2} \\ \frac{\partial y}{\partial q_1} & \frac{\partial y}{\partial q_2} \end{vmatrix} dq_1\,dq_2. \tag{2.51}$$

The transformation coefficient in determinant form is called the **Jacobian**.

Similarly, the volume element $dx\,dy\,dz$ becomes the triple scalar product of the three infinitesimal displacement vectors $d\mathbf{r}_i = dq_i \frac{\partial \mathbf{r}}{\partial q_i}$ along the q_i directions $\hat{\mathbf{q}}_i$, which according to Section 1.4 takes on the form

$$dx\,dy\,dz = \begin{vmatrix} \frac{\partial x}{\partial q_1} & \frac{\partial x}{\partial q_2} & \frac{\partial x}{\partial q_3} \\ \frac{\partial y}{\partial q_1} & \frac{\partial y}{\partial q_2} & \frac{\partial y}{\partial q_3} \\ \frac{\partial z}{\partial q_1} & \frac{\partial z}{\partial q_2} & \frac{\partial z}{\partial q_3} \end{vmatrix} dq_1\,dq_2\,dq_3. \tag{2.52}$$

Here, the coefficient is also called the Jacobian, and so on in higher dimensions.

For orthogonal coordinates the Jacobians simplify to products of the orthogonal vectors in Eq. (2.38). It follows that they are products of h_i; for example, the volume Jacobian in Eq. (2.52) becomes

$$h_1 h_2 h_3 (\hat{\mathbf{q}}_1 \times \hat{\mathbf{q}}_2) \cdot \hat{\mathbf{q}}_3 = h_1 h_2 h_3.$$

EXAMPLE 2.3.3

Jacobians for Polar Coordinates Let us illustrate the transformation of the Cartesian two-dimensional volume element $dx\,dy$ to polar coordinates ρ, φ, with $x = \rho\cos\varphi$, $y = \rho\sin\varphi$. (See also Section 2.2.) Here,

$$dx\,dy = \begin{vmatrix} \frac{\partial x}{\partial \rho} & \frac{\partial x}{\partial \varphi} \\ \frac{\partial y}{\partial \rho} & \frac{\partial y}{\partial \varphi} \end{vmatrix} d\rho\,d\varphi = \begin{vmatrix} \cos\varphi & -\rho\sin\varphi \\ \sin\varphi & \rho\cos\varphi \end{vmatrix} d\rho\,d\varphi = \rho\,d\rho\,d\varphi. \tag{2.53}$$

Similarly, in spherical coordinates (see Section 2.5), we get from $x = r\sin\theta\cos\varphi$, $y = r\sin\theta\sin\varphi$, $z = r\cos\theta$ the Jacobian

$$J = \begin{vmatrix} \frac{\partial x}{\partial r} & \frac{\partial x}{\partial \theta} & \frac{\partial x}{\partial \varphi} \\ \frac{\partial y}{\partial r} & \frac{\partial y}{\partial \theta} & \frac{\partial y}{\partial \varphi} \\ \frac{\partial z}{\partial r} & \frac{\partial z}{\partial \theta} & \frac{\partial z}{\partial \varphi} \end{vmatrix} = \begin{vmatrix} \sin\theta\cos\varphi & r\cos\theta\cos\varphi & -r\sin\theta\sin\varphi \\ \sin\theta\sin\varphi & r\cos\theta\sin\varphi & r\sin\theta\cos\varphi \\ \cos\theta & -r\sin\theta & 0 \end{vmatrix}$$

$$= \cos\theta \begin{vmatrix} r\cos\theta\cos\varphi & -r\sin\theta\sin\varphi \\ r\cos\theta\sin\varphi & r\sin\theta\cos\varphi \end{vmatrix} + r\sin\theta \begin{vmatrix} \sin\theta\cos\varphi & -r\sin\theta\sin\varphi \\ \sin\theta\sin\varphi & r\sin\theta\cos\varphi \end{vmatrix}$$

$$= r^2(\cos^2\theta\sin\theta + \sin^3\theta) = r^2\sin\theta \tag{2.54}$$

by expanding the determinant along the third line. Hence, the volume element becomes $dx\,dy\,dz = r^2 dr\sin\theta d\theta d\varphi$. The volume integral can be written as

$$\int f(x, y, z)dx\,dy\,dz = \int f(x(r,\theta,\varphi), y(r,\theta,\varphi), z(r,\theta,\varphi))r^2 dr\sin\theta d\theta d\varphi. \quad \blacksquare$$

SUMMARY

We have developed the general formalism for vector analysis in curvilinear coordinates. For most applications, locally orthogonal coordinates can be chosen, for which surface and volume elements in multiple integrals are products of line elements. For the general nonorthogonal case, Jacobian determinants apply.

Biographical Data

Jacobi, Carl Gustav Jacob. Jacobi, a German mathematician, was born in Potsdam, Prussia, in 1804 and died in Berlin in 1851. He obtained his Ph.D. in Berlin in 1824. Praised by Legendre for his work on elliptical functions, he became a professor at the University of Königsberg in 1827 (East Prussia, which is now Russia). He also developed determinants and partial differential equations, among other contributions.

EXERCISES

2.3.1 Show that limiting our attention to orthogonal coordinate systems implies that $g_{ij} = 0$ for $i \neq j$ [Eq. (2.33)].
Hint. Construct a triangle with sides ds_1, ds_2, and ds_3. Equation (2.42) must hold regardless of whether $g_{ij} = 0$. Then compare ds^2 from Eq. (2.34) with a calculation using the law of cosines. Show that $\cos\theta_{12} = g_{12}/\sqrt{g_{11}g_{22}}$.

2.3.2 In the spherical polar coordinate system $q_1 = r$, $q_2 = \theta$, $q_3 = \varphi$. The transformation equations corresponding to Eq. (2.27) are

$$x = r\sin\theta\cos\varphi, \quad y = r\sin\theta\sin\varphi, \quad z = r\cos\theta.$$

(a) Calculate the spherical polar coordinate scale factors: h_r, h_θ, and h_φ.
(b) Check your calculated scale factors by the relation $ds_i = h_i\,dq_i$.

2.3.3 The u-, v-, z-coordinate system frequently used in electrostatics and in hydrodynamics is defined by

$$xy = u, \quad x^2 - y^2 = v, \quad z = z.$$

This u-, v-, z-system is orthogonal.

(a) In words, describe briefly the nature of each of the three families of coordinate surfaces.

(b) Sketch the system in the xy-plane showing the intersections of surfaces of constant u and surfaces of constant v with the xy-plane (using graphical software if available).

(c) Indicate the directions of the unit vector $\hat{\mathbf{u}}$ and $\hat{\mathbf{v}}$ in all four quadrants.

(d) Is this u-, v-, z-system right-handed ($\hat{\mathbf{u}} \times \hat{\mathbf{v}} = +\hat{\mathbf{z}}$) or left-handed ($\hat{\mathbf{u}} \times \hat{\mathbf{v}} = -\hat{\mathbf{z}}$)?

2.3.4 The elliptic cylindrical coordinate system consists of three families of surfaces:

$$\frac{x^2}{a^2 \cosh^2 u} + \frac{y^2}{a^2 \sinh^2 u} = 1, \qquad \frac{x^2}{a^2 \cos^2 v} - \frac{y^2}{a^2 \sin^2 v} = 1, \qquad z = z.$$

Sketch the coordinate surfaces $u =$ constant and $v =$ constant as they intersect the first quadrant of the xy-plane (using graphical software if available). Show the unit vectors $\hat{\mathbf{u}}$ and $\hat{\mathbf{v}}$. The range of u is $0 \le u < \infty$, and the range of v is $0 \le v \le 2\pi$.

Hint. It is easier to work with the square of each side of this equation.

2.3.5 Determine the volume of an n-dimensional sphere of radius r.

Hint. Use generalized polar coordinates.

2.3.6 Minkowski space is defined as $x_1 = x$, $x_2 = y$, $x_3 = z$, and $x_0 = ct$. This is done so that the space–time interval $ds^2 = dx_0^2 - dx_1^2 - dx_2^2 - dx_3^2$ ($c =$ velocity of light). Show that the metric in Minkowski space is

$$(g_{ij}) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}.$$

We use Minkowski space in Section 4.4 for describing Lorentz transformations.

2.4 Differential Vector Operators

Gradient

The starting point for developing the gradient, divergence, and curl operators in curvilinear coordinates is the geometric interpretation of the gradient as the vector having the magnitude and direction of the maximum space rate of change of a function ψ (compare Section 1.5). From this interpretation the

component of $\nabla\psi(q_1, q_2, q_3)$ in the direction normal to the family of surfaces $q_1 =$ constant is given by[5]

$$\hat{\mathbf{q}}_1 \cdot \nabla\psi = \nabla\psi|_1 = \frac{\partial\psi}{\partial s_1} = \frac{1}{h_1}\frac{\partial\psi}{\partial q_1} \tag{2.55}$$

since this is the rate of change of ψ for varying q_1, holding q_2 and q_3 fixed. For example, from Example 2.2.1 [and $h_\rho = 1,\ h_\varphi = \rho,\ h_z = 1$ from Eq. (2.9)] the φ-component of the gradient in circular cylindrical coordinates has the form given by Eq. (2.15). The quantity ds_1 is a differential length in the direction of increasing q_1 [compare Eq. (2.35)]. In Section 2.3, we introduced a unit vector $\hat{\mathbf{q}}_1$ to indicate this direction. By repeating Eq. (2.55) for q_2 and again for q_3 and adding vectorially, the gradient becomes

$$\begin{aligned}\nabla\psi(q_1, q_2, q_3) &= \hat{\mathbf{q}}_1\frac{\partial\psi}{\partial s_1} + \hat{\mathbf{q}}_2\frac{\partial\psi}{\partial s_2} + \hat{\mathbf{q}}_3\frac{\partial\psi}{\partial s_3}\\ &= \hat{\mathbf{q}}_1\frac{1}{h_1}\frac{\partial\psi}{\partial q_1} + \hat{\mathbf{q}}_2\frac{1}{h_2}\frac{\partial\psi}{\partial q_2} + \hat{\mathbf{q}}_3\frac{1}{h_3}\frac{\partial\psi}{\partial q_3}\\ &= \sum_i \hat{\mathbf{q}}_i\frac{1}{h_i}\frac{\partial\psi}{\partial q_i}.\end{aligned} \tag{2.56}$$

Exercise 2.2.4 offers a mathematical alternative independent of this physical interpretation of the gradient. Examples are given for cylindrical coordinates in Section 2.2 and spherical polar coordinates in Section 2.5.

Divergence

The divergence operator may be obtained from the second definition [Eq. (1.113)] of Chapter 1 or equivalently from Gauss's theorem (Section 1.11). Let us use Eq. (1.113),

$$\nabla \cdot \mathbf{V}(q_1, q_2, q_3) = \lim_{\int d\tau \to 0} \frac{\int \mathbf{V} \cdot d\boldsymbol{\sigma}}{\int d\tau}, \tag{2.57}$$

with a differential volume $d\tau = h_1h_2h_3\, dq_1\, dq_2\, dq_3$ (Fig. 2.15). Note that the positive directions have been chosen so that (q_1, q_2, q_3) or $(\hat{\mathbf{q}}_1, \hat{\mathbf{q}}_2, \hat{\mathbf{q}}_3)$ form a right-handed set, $\hat{\mathbf{q}}_1 \times \hat{\mathbf{q}}_2 = \hat{\mathbf{q}}_3$.

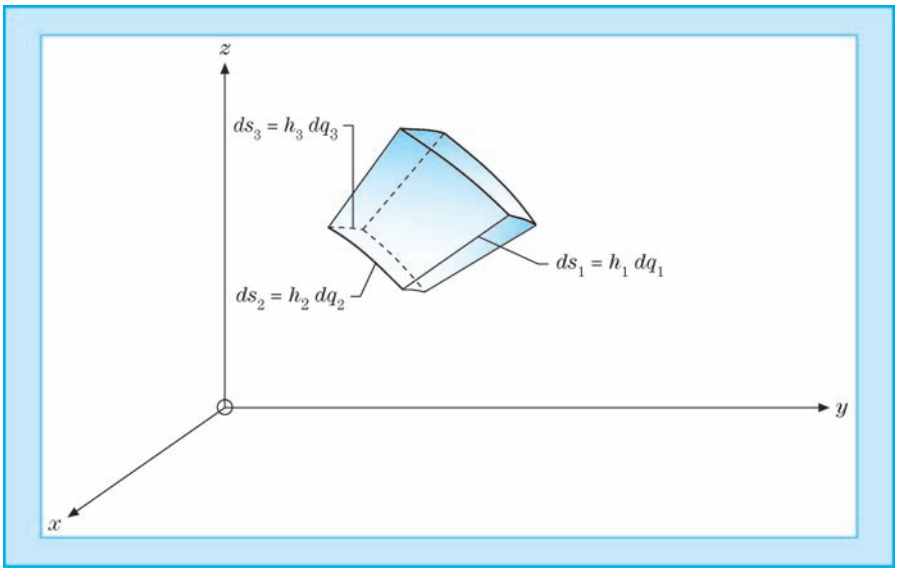
The area integral for the two faces $q_1 =$ constant in Fig. 2.15 is given by

$$\begin{aligned}&\left[V_1h_2h_3 + \frac{\partial}{\partial q_1}(V_1h_2h_3)dq_1\right]dq_2\, dq_3 - V_1h_2h_3\, dq_2\, dq_3\\ &\quad = \frac{\partial}{\partial q_1}(V_1h_2h_3)dq_1\, dq_2\, dq_3,\end{aligned} \tag{2.58}$$

[5]Here, the use of φ to label a function is avoided because it is conventional to use this symbol to denote an azimuthal coordinate.

Figure 2.15

Curvilinear Volume Element



as in Sections 1.6 and 1.9.[6] Here, V_i is the component of $\mathbf{V}$ in the $\hat{\mathbf{q}}_i$-direction, increasing q_i; that is, $V_i = \hat{\mathbf{q}}_i \cdot \mathbf{V}$ is the projection of $\mathbf{V}$ onto the $\hat{\mathbf{q}}_i$-direction. Adding in the similar results for the other two pairs of surfaces, we obtain

$$\int \mathbf{V}(q_1, q_2, q_3) \cdot d\boldsymbol{\sigma} = \left[\frac{\partial}{\partial q_1}(V_1 h_1 h_3) + \frac{\partial}{\partial q_2}(V_2 h_3 h_1) + \frac{\partial}{\partial q_3}(V_3 h_1 h_2) \right] dq_1\, dq_2\, dq_3. \tag{2.59}$$

Division by our differential volume [see $d\tau$ after Eq. (2.57)] yields

$$\nabla \cdot \mathbf{V}(q_1, q_2, q_3) = \frac{1}{h_1 h_2 h_3} \left[\frac{\partial}{\partial q_1}(V_1 h_2 h_3) + \frac{\partial}{\partial q_2}(V_2 h_3 h_1) + \frac{\partial}{\partial q_3}(V_3 h_1 h_2) \right]. \tag{2.60}$$

Applications and examples of this general result will be given in the following section for a special coordinate system. We may obtain the Laplacian by combining Eqs. (2.56) and (2.60), using $\mathbf{V} = \nabla\psi(q_1, q_2, q_3)$. This leads to

$$\nabla \cdot \nabla\psi(q_1, q_2, q_3) = \frac{1}{h_1 h_2 h_3} \left[\frac{\partial}{\partial q_1} \left(\frac{h_2 h_3}{h_1} \frac{\partial \psi}{\partial q_1} \right) + \frac{\partial}{\partial q_2} \left(\frac{h_3 h_1}{h_2} \frac{\partial \psi}{\partial q_2} \right) + \frac{\partial}{\partial q_3} \left(\frac{h_1 h_2}{h_3} \frac{\partial \psi}{\partial q_3} \right) \right]. \tag{2.61}$$

Examples and numerical applications of the central Eqs. (2.56), (2.60), (2.61), and (2.66) are shown for cylindrical coordinates in Section 2.2 and for spherical polar coordinates in Section 2.5.

[6] Since we take the limit $dq_1, dq_2, dq_3 \to 0$, the second- and higher order derivatives will drop out.

Curl

Finally, to develop $\nabla \times \mathbf{V}$, let us apply Stokes's theorem (Section 1.11) and, as with divergence, take the limit as the surface area becomes vanishingly small. Working on one component at a time, we consider a differential surface element in the curvilinear surface $q_1 =$ constant. For such a small surface the mean value theorem of integral calculus states that an integral is given by the surface times the function at a mean value on the small surface. Thus, from

$$\int_s \nabla \times \mathbf{V}|_1 \cdot d\boldsymbol{\sigma}_1 = \hat{\mathbf{q}}_1 \cdot (\nabla \times \mathbf{V}) h_2 h_3 \, dq_2 \, dq_3, \tag{2.62}$$

Stokes's theorem yields

$$\hat{\mathbf{q}}_1 \cdot (\nabla \times \mathbf{V}) h_2 h_3 \, dq_2 \, dq_3 = \oint \mathbf{V} \cdot d\mathbf{r}, \tag{2.63}$$

with the line integral lying in the surface $q_1 =$ constant. Following the loop (1, 2, 3, 4) of Fig. 2.16,

$$\begin{aligned} \oint \mathbf{V}(q_1, q_2, q_3) \cdot d\mathbf{r} &= V_2 h_2 \, dq_2 + \left[V_3 h_3 + \frac{\partial}{\partial q_2}(V_3 h_3) \, dq_2 \right] dq_3 \\ &\quad - \left[V_2 h_2 + \frac{\partial}{\partial q_3}(V_2 h_2) dq_3 \right] dq_2 - V_3 h_3 \, dq_3 \\ &= \left[\frac{\partial}{\partial q_2}(h_3 V_3) - \frac{\partial}{\partial q_3}(h_2 V_2) \right] dq_2 \, dq_3. \end{aligned} \tag{2.64}$$

We pick up a positive sign when going in the positive direction on parts 1 and 2 and a negative sign on parts 3 and 4 because here we are going in the negative direction. Higher order terms have been omitted. They will vanish in the limit as the surface becomes vanishingly small ($dq_2 \to 0$, $dq_3 \to 0$).

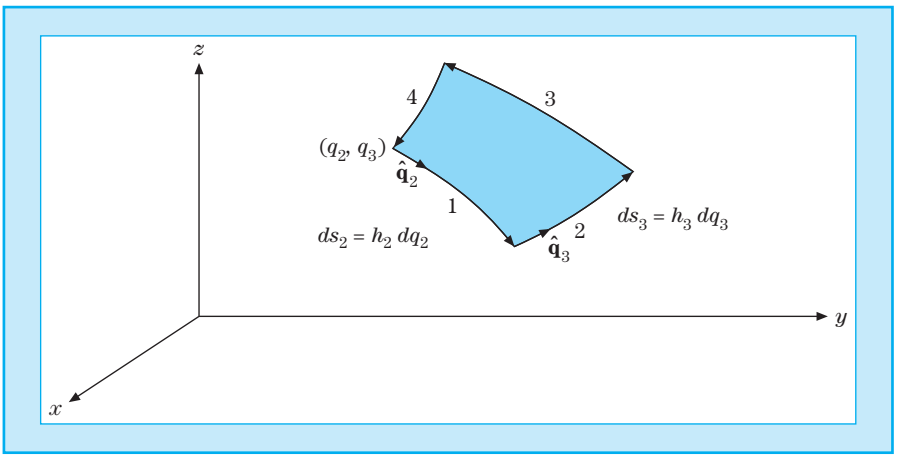


Figure 2.16

Curvilinear Surface Element with $q_1 =$ Constant

Combining Eqs. (2.63) and (2.64), we obtain

$$\nabla \times \mathbf{V}|_1 = \frac{1}{h_2 h_3}\left[\frac{\partial}{\partial q_2}(h_3 V_3) - \frac{\partial}{\partial q_3}(h_2 V_2)\right]. \tag{2.65}$$

The remaining two components of $\nabla \times \mathbf{V}$ may be picked up by cyclic permutation of the indices. As in Chapter 1, it is often convenient to write the curl in determinant form:

$$\nabla \times \mathbf{V} = \frac{1}{h_1 h_2 h_3}\begin{vmatrix} \hat{\mathbf{q}}_1 h_1 & \hat{\mathbf{q}}_2 h_2 & \hat{\mathbf{q}}_3 h_3 \\ \dfrac{\partial}{\partial q_1} & \dfrac{\partial}{\partial q_2} & \dfrac{\partial}{\partial q_3} \\ h_1 V_1 & h_2 V_2 & h_3 V_3 \end{vmatrix}. \tag{2.66}$$

Remember that because of the presence of the differential operators, this determinant must be expanded from the top down. Note that this equation is **not** identical to the form for the cross product of two vectors [Eq. (1.40)]. ∇ is not an ordinary vector; it is a vector **operator**.

Our geometric interpretation of the gradient and the use of Gauss's and Stokes's theorems (or integral definitions of divergence and curl) have enabled us to obtain these general formulas **without having to differentiate the unit vectors** $\hat{\mathbf{q}}_i$. There exist alternate ways to determine grad, div, and curl based on direct differentiation of the $\hat{\mathbf{q}}_i$. One approach resolves the $\hat{\mathbf{q}}_i$ of a specific coordinate system into its Cartesian components (Exercises 2.2.1 and 2.5.1) and differentiates this Cartesian form (Exercises 2.4.3 and 2.5.2). The point is that the derivatives of the Cartesian $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$, and $\hat{\mathbf{z}}$ vanish since $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$, and $\hat{\mathbf{z}}$ are constant in direction as well as in magnitude. A second approach [L. J. Kijewski, *Am. J. Phys.* **33**, 816 (1965)] starts from the equality of $\partial^2\mathbf{r}/\partial q_i\,\partial q_j$ and $\partial^2\mathbf{r}/\partial q_j\,\partial q_i$ and develops the derivatives of $\hat{\mathbf{q}}_i$ in a general curvilinear form. Exercises 2.3.3 and 2.3.4 are based on this method.

EXERCISES

2.4.1 Develop arguments to show that ordinary dot and cross products (not involving ∇) in orthogonal curvilinear coordinates proceed as in Cartesian coordinates **with no involvement of scale factors**.

2.4.2 With $\hat{\mathbf{q}}_1$ a unit vector in the direction of increasing q_1, show that

(a) $\nabla \cdot \hat{\mathbf{q}}_1 = \dfrac{1}{h_1 h_2 h_3}\dfrac{\partial(h_2 h_3)}{\partial q_1}$

(b) $\nabla \times \hat{\mathbf{q}}_1 = \dfrac{1}{h_1}\left[\hat{\mathbf{q}}_2 \dfrac{1}{h_3}\dfrac{\partial h_1}{\partial q_3} - \hat{\mathbf{q}}_3 \dfrac{1}{h_2}\dfrac{\partial h_1}{\partial q_2}\right]$.

Note that even though $\hat{\mathbf{q}}_1$ is a unit vector, its divergence and curl **do not necessarily vanish** (because it varies with position).

2.4.3 Start from Eq. (2.37) and show (i) that $\hat{\mathbf{q}}_i \cdot \hat{\mathbf{q}}_i = 1$ leads to an expression for h_i in agreement with Eq. (2.32) and (ii) derive

$$\frac{\partial \hat{\mathbf{q}}_i}{\partial q_j} = \hat{\mathbf{q}}_j \frac{1}{h_i}\frac{\partial h_j}{\partial q_i}, \qquad i \neq j$$

and

$$\frac{\partial \hat{\mathbf{q}}_i}{\partial q_i} = -\sum_{j \neq i} \hat{\mathbf{q}}_j \frac{1}{h_j}\frac{\partial h_i}{\partial q_j}.$$

2.4.4 Derive

$$\nabla\psi = \hat{\mathbf{q}}_1 \frac{1}{h_1}\frac{\partial \psi}{\partial q_1} + \hat{\mathbf{q}}_2 \frac{1}{h_2}\frac{\partial \psi}{\partial q_2} + \hat{\mathbf{q}}_3 \frac{1}{h_3}\frac{\partial \psi}{\partial q_3}$$

by direct application of Eq. (1.112),

$$\nabla\psi = \lim_{\int d\tau} \frac{\int \psi \, d\boldsymbol{\sigma}}{\int d\tau}.$$

Hint. Evaluation of the surface integral will lead to terms such as $(h_1h_2h_3)^{-1}\,(\partial/\partial q_1)(\hat{\mathbf{q}}_1 h_2 h_3)$. The results listed in Exercise 2.4.3 will be helpful. Cancellation of unwanted terms occurs when the contributions of all three pairs of surfaces are added together.

2.5 Spherical Polar Coordinates

Relabeling (q_1, q_2, q_3) as (r, θ, φ), we see that the spherical polar coordinate system consists of the following:

1. Concentric spheres centered at the origin,

$$r = (x^2 + y^2 + z^2)^{1/2} = \text{const.}$$

2. Right circular cones centered on the z-(polar) axis, vertices at the origin,

$$\theta = \arccos \frac{z}{(x^2 + y^2 + z^2)^{1/2}} = \text{const.}$$

3. Half planes through the z-(polar) axis,

$$\varphi = \arctan \frac{y}{x} = \text{const.}$$

By our arbitrary choice of definitions of θ (the polar angle) and φ (the azimuth angle), the z-axis is singled out for special treatment. The transformation equations corresponding to Eq. (2.27) are

$$x = r\sin\theta\cos\varphi, \quad y = r\sin\theta\sin\varphi, \quad z = r\cos\theta, \tag{2.67}$$

measuring θ from the positive z-axis and φ in the xy-plane from the positive x-axis. The ranges of values are $0 \le r < \infty$, $0 \le \theta < \pi$, and $0 \le \varphi \le 2\pi$. At $r = 0$, θ and φ are undefined. The coordinate vector measured from the origin

is $\mathbf{r} = r\hat{\mathbf{r}}$. From Eqs. (2.32) and (2.35),

$$\begin{aligned} h_1 &= h_r = 1, \\ h_2 &= h_\theta = r, \\ h_3 &= h_\varphi = r\sin\theta. \end{aligned} \tag{2.68}$$

This gives a (vectorial) line element

$$d\mathbf{r} = \hat{\mathbf{r}}\,dr + \hat{\boldsymbol{\theta}} r\,d\theta + \hat{\boldsymbol{\varphi}} r\sin\theta\,d\varphi$$

so that

$$ds^2 = d\mathbf{r}\cdot d\mathbf{r} = dr^2 + r^2 d\theta^2 + r^2\sin^2\theta d\varphi^2$$

because the unit vectors are mutually orthogonal.

In this spherical coordinate system, the area element [for r = constant; compare Eqs. (2.42) and (2.44)] is

$$dA = d\sigma_{\theta\varphi} = r^2\sin\theta\,d\theta\,d\varphi, \tag{2.69}$$

the light, unshaded area in Fig. 2.17. Integrating over the azimuth φ, the area element becomes a ring of width $d\theta$,

$$dA = 2\pi r^2\sin\theta\,d\theta. \tag{2.70}$$

This form will appear repeatedly in problems in spherical polar coordinates with azimuthal symmetry, such as the scattering of an unpolarized beam of particles. By definition of solid radians or steradians, an element of solid angle $d\Omega$ is given by

$$d\Omega = \frac{dA}{r^2} = \sin\theta\,d\theta\,d\varphi = |d(\cos\theta)d\varphi|. \tag{2.71}$$

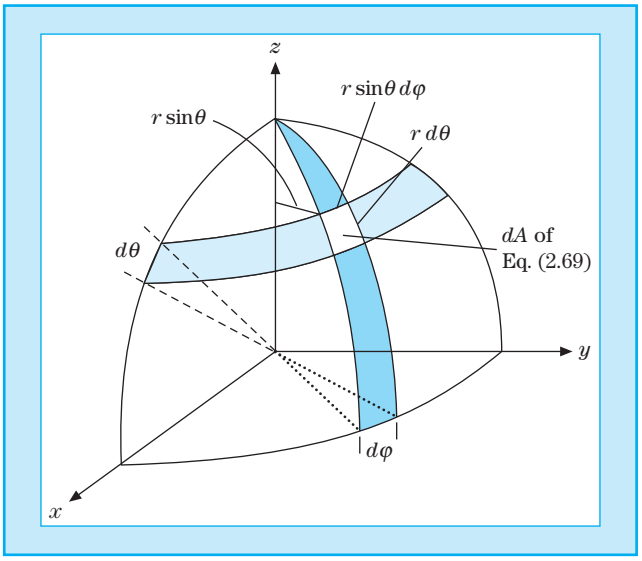
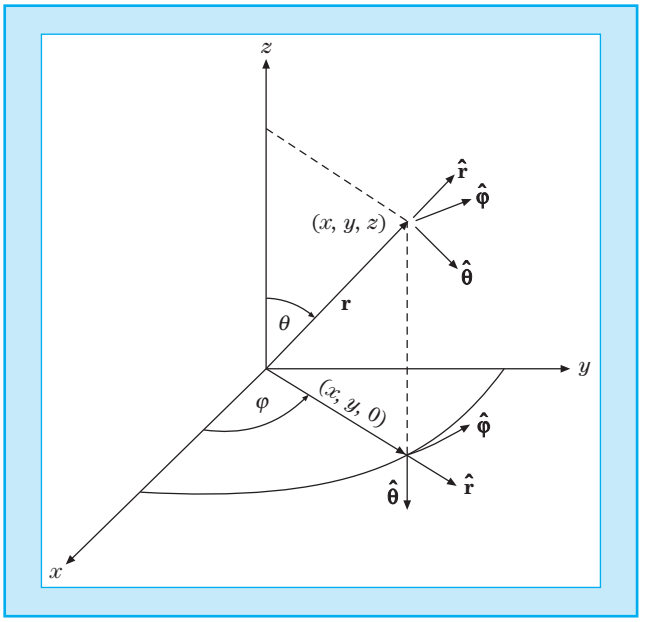


Figure 2.17

Spherical Polar Coordinate Area Elements

Figure 2.18

Spherical Polar Coordinates



Integrating over the entire spherical surface, we obtain

$$\int d\Omega = 4\pi.$$

From Eq. (2.43) the volume element is

$$d\tau = r^2\, dr \sin\theta\, d\theta\, d\varphi = r^2\, dr\, d\Omega. \tag{2.72}$$

The spherical polar coordinate unit vectors are shown in Fig. 2.18.

It must be emphasized that **the unit vectors $\hat{\mathbf{r}}$, $\hat{\boldsymbol{\theta}}$, and $\hat{\boldsymbol{\varphi}}$ vary in direction as the angles θ and φ vary**. Specifically, the θ and φ derivatives of these spherical polar coordinate unit vectors do not vanish (Exercise 2.5.2). When differentiating vectors in spherical polar (or in any non-Cartesian system) this variation of the unit vectors with position must not be neglected. In terms of the fixed-direction Cartesian unit vectors $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$ and $\hat{\mathbf{z}}$,

$$\begin{aligned}
\hat{\mathbf{r}} &= \hat{\mathbf{x}}\sin\theta\cos\varphi + \hat{\mathbf{y}}\sin\theta\sin\varphi + \hat{\mathbf{z}}\cos\theta,\\
\hat{\boldsymbol{\theta}} &= \hat{\mathbf{x}}\cos\theta\cos\varphi + \hat{\mathbf{y}}\cos\theta\sin\varphi - \hat{\mathbf{z}}\sin\theta,\\
\hat{\boldsymbol{\varphi}} &= -\hat{\mathbf{x}}\sin\varphi + \hat{\mathbf{y}}\cos\varphi.
\end{aligned} \tag{2.73}$$

Note that Exercise 2.5.4 gives the inverse transformation.

A given vector can now be expressed in a number of different (but equivalent) ways. For instance, the position vector $\mathbf{r}$ may be written

$$\begin{aligned}
\mathbf{r} &= \hat{\mathbf{r}}r = \hat{\mathbf{r}}(x^2 + y^2 + z^2)^{1/2}\\
&= \hat{\mathbf{x}}x + \hat{\mathbf{y}}y + \hat{\mathbf{z}}z\\
&= \hat{\mathbf{x}}r\sin\theta\cos\varphi + \hat{\mathbf{y}}r\sin\theta\sin\varphi + \hat{\mathbf{z}}r\cos\theta.
\end{aligned} \tag{2.74}$$

Select the form that is most useful for your particular problem, that is, r for spherical polar coordinates, the second form for Cartesian coordinates, and the third when converting from Cartesian to spherical polar coordinates.

From Section 2.4, relabeling the curvilinear coordinate unit vectors $\hat{\mathbf{q}}_1$, $\hat{\mathbf{q}}_2$, and $\hat{\mathbf{q}}_3$ as $\hat{\mathbf{r}}$, $\hat{\boldsymbol{\theta}}$, and $\hat{\boldsymbol{\varphi}}$ gives

$$\nabla\psi = \hat{\mathbf{r}}\frac{\partial\psi}{\partial r} + \hat{\boldsymbol{\theta}}\frac{1}{r}\frac{\partial\psi}{\partial\theta} + \hat{\boldsymbol{\varphi}}\frac{1}{r\sin\theta}\frac{\partial\psi}{\partial\varphi}, \tag{2.75}$$

$$\nabla\cdot\mathbf{V} = \frac{1}{r^2\sin\theta}\left[\sin\theta\frac{\partial}{\partial r}(r^2V_r) + r\frac{\partial}{\partial\theta}(\sin\theta V_\theta) + r\frac{\partial V_\varphi}{\partial\varphi}\right], \tag{2.76}$$

$$\nabla\cdot\nabla\psi = \frac{1}{r^2\sin\theta}\left[\sin\theta\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{\sin\theta}\frac{\partial^2\psi}{\partial\varphi^2}\right], \tag{2.77}$$

$$\nabla\times\mathbf{V} = \frac{1}{r^2\sin\theta}\begin{vmatrix} \hat{\mathbf{r}} & r\hat{\boldsymbol{\theta}} & r\sin\theta\hat{\boldsymbol{\varphi}} \\ \dfrac{\partial}{\partial r} & \dfrac{\partial}{\partial\theta} & \dfrac{\partial}{\partial\varphi} \\ V_r & rV_\theta & r\sin\theta V_\varphi \end{vmatrix}. \tag{2.78}$$

EXAMPLE 2.5.1

∇, $\nabla\cdot$, $\nabla\times$ for Central Force Using Eqs. (2.75)–(2.78), we can reproduce by inspection some of the results derived in Chapter 1 by laborious application of Cartesian coordinates.

From Eq. (2.75)

$$\begin{aligned} \nabla f(r) &= \hat{\mathbf{r}}\frac{df}{dr}, \\ \nabla r^n &= \hat{\mathbf{r}}nr^{n-1}. \end{aligned} \tag{2.79}$$

For example, for the Coulomb potential $V = Ze^2/r$, the electric field is $\mathbf{E} = -\nabla V/e = -Ze\nabla\frac{1}{r} = \frac{Ze}{r^2}\hat{\mathbf{r}}$.

From Eq. (2.76)

$$\begin{aligned} \nabla\cdot\hat{\mathbf{r}}f(r) &= \frac{2}{r}f(r) + \frac{df}{dr}, \\ \nabla\cdot\hat{\mathbf{r}}r^n &= (n+2)r^{n-1}. \end{aligned} \tag{2.80}$$

For example, for $r > 0$ the charge density of the electric field of the Coulomb potential is $\rho = \nabla\cdot\mathbf{E} = Ze\nabla\cdot\frac{\hat{\mathbf{r}}}{r^2} = 0$.

From Eq. (2.77)

$$\nabla^2 f(r) = \frac{2}{r}\frac{df}{dr} + \frac{d^2f}{dr^2}, \tag{2.81}$$

$$\nabla^2 r^n = n(n+1)r^{n-2}, \tag{2.82}$$

in contrast to the ordinary radial second derivative of r^n involving $n-1$ instead of $n+1$.

Finally, from Eq. (2.78)

$$\nabla \times \hat{\mathbf{r}} f(r) = 0. \tag{2.83}$$

■

Integrals in Spherical Polar Coordinates

The length of a space curve

$$s = \int_{t_1}^{t_2} \sqrt{\dot{r}^2 + r^2\dot{\theta}^2 + r^2 \sin^2\theta\,\dot{\varphi}^2}\,dt$$

is a scalar integral, in case the curve is parameterized as $\mathbf{r}(t) = (r(t),\ \theta(t),\ \varphi(t))$.

The line integral is a sum of ordinary integrals if we expand the dot product as

$$\begin{aligned}\int \mathbf{A}\cdot d\mathbf{r} &= \int (A_r dr + rA_\theta d\theta + r\sin\theta A_\varphi d\varphi)\\ &= \int (A_r\dot{r} + rA_\theta\dot{\theta} + r\sin\theta A_\varphi\dot{\varphi})\,dt.\end{aligned}$$

See Example 1.9.2 for a line integral in plane polar coordinates, or for an ellipse $x = a\cos\omega t,\ \ y = b\sin\omega t$ see Example 2.2.5 and the rosetta curves.

EXAMPLE 2.5.2 **Surface of Hemisphere** We can write the area formula as

$$\begin{aligned}\int h_\theta h_\varphi d\theta d\varphi &= \int_0^{2\pi}\int_0^{\pi/2} r^2\sin\theta d\theta d\varphi = 2\pi r^2\int_0^{\pi/2}\sin\theta d\theta\\ &= -2\pi r^2\cos\theta|_0^{\pi/2} = 2\pi r^2,\end{aligned}$$

as expected. ■

EXAMPLE 2.5.3 **Area Cut from Sphere by Cylinder** We take up the unit sphere cut by a cylinder from Example 2.2.6 and Fig. 2.10 again, but now we use the **spherical** area element $\sin\theta d\theta d\varphi$. The cylinder is described (in the xy-plane) by $r = \cos\varphi$, which is the $n = 1$ case of the rosetta curves in Fig. 2.9 of Example 2.2.5, and $z = \cos\theta$ holds on the sphere. Inserting $x^2+y^2 = \cos^2\varphi$ and $z = \cos\theta$ into $x^2 + y^2 + z^2 = 1$, we get $\cos\varphi = \sin\theta$, implying $\varphi = \pm(\frac{\pi}{2} - \theta)$ as integration limits for θ. Hence, the area cut from the sphere is given by

$$\begin{aligned}A &= \int_{\theta=0}^{\pi/2}\int_{\varphi=\theta-\pi/2}^{\pi/2-\theta}\sin\theta d\theta d\varphi = 2\int_0^{\pi/2}\left(\frac{\pi}{2}-\theta\right)\sin\theta d\theta\\ &= \pi - 2\int_0^{\pi/2}\theta\sin\theta d\theta = \pi - 2[-\theta\cos\theta + \sin\theta]|_0^{\pi/2} = \pi - 2,\end{aligned}$$

upon integrating the second term by parts. This agrees with our previous result, although the intermediate steps are quite different. ■

The volume bounded by a surface $z = z(x, y)$ is given by $V = \iint z(x, y)dx\,dy$, the three-dimensional generalization of the two-dimensional area $A = \int f(x)dx$ under a curve $y = f(x)$, which we apply in the next example.

EXAMPLE 2.5.4

Volume of Ellipsoid The ellipsoid equation with half axes a, b, c is given by

$$\frac{x^2}{a^2} + \frac{y^2}{b^2} + \frac{z^2}{c^2} = 1, \quad \text{so that } z(x, y) = c\sqrt{1 - \frac{x^2}{a^2} - \frac{y^2}{b^2}}.$$

The complicated square-root form of z demonstrates that Cartesian coordinates are inappropriate to calculate the volume of an ellipsoid. It is easier to parameterize the ellipsoid in spherical polar coordinates as

$$x = a\sin\theta\cos\varphi, \quad y = b\sin\theta\sin\varphi, \quad z = c\cos\theta.$$

We check that the ellipsoid equation is satisfied by squaring the coordinates and adding them up. Next, we transform the volume integral to polar coordinates using the Jacobian

$$dx\,dy = \begin{vmatrix} \frac{\partial x}{\partial\theta} & \frac{\partial x}{\partial\varphi} \\ \frac{\partial y}{\partial\theta} & \frac{\partial y}{\partial\varphi} \end{vmatrix} d\theta d\varphi = \begin{vmatrix} a\cos\theta\cos\varphi & -a\sin\theta\sin\varphi \\ b\cos\theta\sin\varphi & b\sin\theta\cos\varphi \end{vmatrix} d\theta d\varphi$$
$$= abd\theta d\varphi\sin\theta\cos\theta,$$

with the volume in the positive octant given by

$$V = \int z(x, y)dx\,dy = \int_{\varphi=0}^{\pi/2}\int_{\theta=0}^{\pi/2} c\cos\theta ab\sin\theta\cos\theta d\theta d\varphi$$
$$= \frac{\pi}{2}abc\int_0^1 \cos^2\theta d\cos\theta = \frac{\pi}{6}abc\cos^3\theta|_{\cos\theta=0}^1 = \frac{\pi}{6}abc.$$

Multiplying by 8, we find the ellipsoid volume $\frac{4}{3}\pi abc$, which reduces to that of a sphere for $a = b = c = R$. ■

EXAMPLE 2.5.5

Surface of Rotation Ellipsoid The ellipsoid surface is a much more complicated function of its half axes. For simplicity, we specialize to a rotation ellipsoid with $a = b$, for which we use the general area formula employed in Example 1.9.5:

$$A = \int \frac{dx\,dy}{n_z}, \quad \frac{1}{n_z} = \sqrt{1 + \left(\frac{\partial z}{\partial x}\right)^2 + \left(\frac{\partial z}{\partial y}\right)^2}. \tag{2.84}$$

The partial derivatives

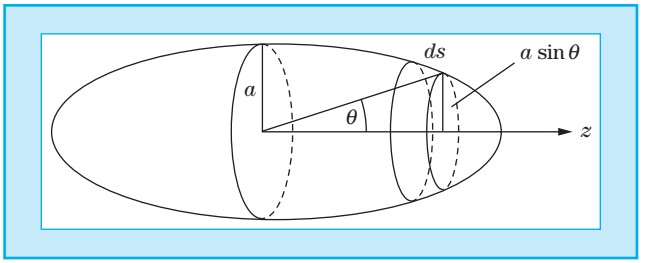
$$\frac{\partial z(x, y)}{\partial x} = -\frac{c^2 x}{a^2 z} = -\frac{c\sin\theta\cos\varphi}{a\cos\theta}, \quad \frac{\partial z(x, y)}{\partial y} = -\frac{c^2 y}{b^2 z} = -\frac{c\sin\theta\sin\varphi}{b\cos\theta}$$

enter the area formula via

$$\frac{1}{n_z} = \sqrt{1 + \frac{c^4}{z^2}\left(\frac{x^2}{a^4} + \frac{y^2}{b^4}\right)} = \sqrt{1 + \frac{c^2}{a^2}\tan^2\theta},$$

Figure 2.19

Rotation Ellipsoid



where the φ-dependence drops out for $a = b$ (only) so that the ellipsoidal area is given by

$$A = a^2 \int_{\varphi=0}^{2\pi} \int_{\theta=0}^{\pi} \sin\theta \cos\theta \sqrt{1 + \frac{c^2}{a^2} \tan^2\theta} d\theta$$
$$= \int_{\theta=0}^{\pi} 2\pi a \sin\theta \sqrt{a^2 \cos^2\theta + c^2 \sin^2\theta} d\theta. \tag{2.85}$$

The last expression has a direct geometric interpretation shown in Fig. 2.19 as the surface area of a rotation ellipsoid $A = \int 2\pi y ds$, with radius $y = a \sin\theta$ and arc length

$$ds = \sqrt{(dx)^2 + (dz)^2} = \sqrt{\left(\frac{dx}{d\theta}\right)^2 + \left(\frac{dz}{d\theta}\right)^2} d\theta = \sqrt{a^2 \cos^2\theta + c^2 \sin^2\theta}\, d\theta$$

with $z = c\cos\theta$, a result that we could have used from the start, of course. Instead, we have shown as a by-product that the general area formula Eq. (2.84) is consistent with that generated by rotating the ellipse $x = a\sin\theta$, $z = c\cos\theta$ about the z-axis. The area integral [Eq. (2.85)] can be evaluated for $c > a$ by substituting $t = \epsilon\cos\theta$, $dt = -\epsilon \sin\theta d\theta$ in conjunction with the eccentricity $\epsilon = \sqrt{(c^2 - a^2)/c^2}$ to yield

$$A = 4\pi ac \int_0^1 \sqrt{1 - \frac{c^2 - a^2}{c^2} \cos^2\theta}\, d\cos\theta = 2\pi \frac{ac}{\epsilon} \int_0^{\epsilon} \sqrt{1 - t^2} dt$$
$$= 2\pi \frac{ac}{\epsilon} \left[t\sqrt{1 - t^2} + \arcsin t\right]_0^{\epsilon} = 2\pi ac \left[\sqrt{1 - \epsilon^2} + \frac{1}{\epsilon} \arcsin\epsilon\right].$$

This result goes over into the area $4\pi R^2$ of a sphere in the limit $a = c = R$ and $\epsilon \to 0$, where the term in brackets goes to 2 using l'Hôpital's rule for $\arcsin\epsilon/\epsilon$.

The substitution used for the area integral in the case $c > a$ amounted to solving

$$A = 2\pi \int_{-c}^{c} x \sqrt{1 + \left(\frac{dx}{dz}\right)^2} dz = 2\pi a \int_{-c}^{c} \sqrt{1 - \frac{\epsilon^2 z^2}{c^2}} dz$$

for the rotating ellipse $\frac{x^2}{a^2}+\frac{z^2}{c^2}$. We now handle the case $a > c$ using the same formula but involving $\epsilon^2 = (a^2-c^2)/c^2$ defined with the **opposite sign**. Thus,

$$A = 2\pi\int_{-c}^{c} x\sqrt{1+\left(\frac{dx}{dz}\right)^2}\,dz = 2\pi\int_{-c}^{c}\sqrt{x^2+\left(x\frac{dx}{dz}\right)^2}\,dz$$

$$= 2\pi\int_{-c}^{c}\sqrt{a^2\left(1-\frac{z^2}{c^2}\right)+\frac{z^2a^4}{c^4}}dz = 4\pi a\int_0^c\sqrt{1+\frac{z^2\epsilon^2}{c^2}}dz,$$

where the ellipse equation implied $x\frac{dx}{dz} = -\frac{za^2}{c^2}$. We solve the integral by substituting $t = z\epsilon/c$, which yields

$$A = 4\pi\frac{ac}{\epsilon}\int_0^{\epsilon}\sqrt{1+t^2}dt = 2\pi\frac{ac}{\epsilon}[t\sqrt{1+t^2}+\ln(t+\sqrt{1+t^2})]|_0^{\epsilon}$$

$$= 2\pi ac\left[\sqrt{1+\epsilon^2}+\frac{1}{\epsilon}\ln(\epsilon+\sqrt{1+\epsilon^2})\right].$$

In the limit $a = c = R$, $\epsilon \to 0$ we obtain $4\pi R^2$ again.

The general formula for the area of an ellipsoid with $a \neq b \neq c \neq a$ is even more complicated, which shows that solutions to elementary problems are sometimes surprisingly tricky. ■

EXERCISES

2.5.1 Resolve the spherical polar unit vectors into their Cartesian components.

ANS.
$$\hat{\mathbf{r}} = \hat{\mathbf{x}}\sin\theta\cos\varphi + \hat{\mathbf{y}}\sin\theta\sin\varphi + \hat{\mathbf{z}}\cos\theta,$$
$$\hat{\boldsymbol{\theta}} = \hat{\mathbf{x}}\cos\theta\cos\varphi + \hat{\mathbf{y}}\cos\theta\sin\varphi - \hat{\mathbf{z}}\sin\theta,$$
$$\hat{\boldsymbol{\varphi}} = -\hat{\mathbf{x}}\sin\varphi + \hat{\mathbf{y}}\cos\varphi.$$

2.5.2 (a) From the results of Exercise 2.5.1, calculate the partial derivatives of $\hat{\mathbf{r}}$, $\hat{\boldsymbol{\theta}}$, and $\hat{\boldsymbol{\varphi}}$ with respect to r, θ, and φ.

(b) With ∇ given by

$$\hat{\mathbf{r}}\frac{\partial}{\partial r}+\hat{\boldsymbol{\theta}}\frac{1}{r}\frac{\partial}{\partial\theta}+\hat{\boldsymbol{\varphi}}\frac{1}{r\sin\theta}\frac{\partial}{\partial\varphi}$$

(greatest space rate of change), use the results of part (a) to calculate $\nabla\cdot\nabla\psi$. This is an alternate derivation of the Laplacian.

Note. The derivatives of the left-hand ∇ operate on the unit vectors of the right-hand ∇ **before** the unit vectors are dotted together.

2.5.3 A rigid body is rotating about a fixed axis with a constant angular velocity ω. Take ω to be along the z-axis. Using spherical polar coordinates,

(a) Calculate

$$\mathbf{v} = \boldsymbol{\omega} \times \mathbf{r}.$$

(b) Calculate

$$\nabla \times \mathbf{v}.$$

ANS. (a) $\mathbf{v} = \hat{\boldsymbol{\varphi}}\omega r \sin\theta$
(b) $\nabla \times \mathbf{v} = 2\boldsymbol{\omega}$.

2.5.4 Resolve the Cartesian unit vectors into their spherical polar components.

$$\hat{\mathbf{x}} = \hat{\mathbf{r}}\sin\theta\cos\varphi + \hat{\boldsymbol{\theta}}\cos\theta\cos\varphi - \hat{\boldsymbol{\varphi}}\sin\varphi,$$
$$\hat{\mathbf{y}} = \hat{\mathbf{r}}\sin\theta\sin\varphi + \hat{\boldsymbol{\theta}}\cos\theta\sin\varphi + \hat{\boldsymbol{\varphi}}\cos\varphi,$$
$$\hat{\mathbf{z}} = \hat{\mathbf{r}}\cos\theta - \hat{\boldsymbol{\theta}}\sin\theta.$$

2.5.5 With $\mathbf{A}$ any vector

$$\mathbf{A} \cdot \nabla\mathbf{r} = \mathbf{A}.$$

(a) Verify this result in Cartesian coordinates.
(b) Verify this result using spherical polar coordinates [Equation (2.75) provides ∇].

2.5.6 Find the spherical coordinate components of the velocity and acceleration of a moving particle:

$$v_r = \dot{r},$$
$$v_\theta = r\dot{\theta},$$
$$v_\varphi = r\sin\theta\dot{\varphi},$$
$$a_r = \ddot{r} - r\dot{\theta}^2 - r\sin^2\theta\dot{\varphi}^2,$$
$$a_\theta = r\ddot{\theta} + 2\dot{r}\dot{\theta} - r\sin\theta\cos\theta\dot{\varphi}^2,$$
$$a_\varphi = r\sin\theta\ddot{\varphi} + 2\dot{r}\sin\theta\dot{\varphi} + 2r\cos\theta\dot{\theta}\dot{\varphi}.$$

Hint.

$$\mathbf{r}(t) = \hat{\mathbf{r}}(t)r(t)$$
$$= [\hat{\mathbf{x}}\sin\theta(t)\cos\varphi(t) + \hat{\mathbf{y}}\sin\theta(t)\sin\varphi(t) + \hat{\mathbf{z}}\cos\theta(t)]r(t).$$

Note. The dot in $\dot{r}$ means time derivative, $\dot{r} = dr/dt$. The notation was originated by Newton. There are no $\hat{\boldsymbol{\theta}}$ or $\hat{\boldsymbol{\varphi}}$ components for $\mathbf{r}$.

2.5.7 A particle m moves in response to a central force according to Newton's second law

$$m\ddot{\mathbf{r}} = \hat{\mathbf{r}}f(\mathbf{r}).$$

Show that $\mathbf{r} \times \dot{\mathbf{r}} = \mathbf{c}$, a constant and that the geometric interpretation of this (angular momentum conservation) leads to Kepler's second law, the area law. Also explain why the particle moves in a plane.

2.5.8 Express $\partial/\partial x$, $\partial/\partial y$, $\partial/\partial z$ in spherical polar coordinates.

ANS.
$$\frac{\partial}{\partial x} = \sin\theta\cos\varphi\frac{\partial}{\partial r} + \cos\theta\cos\varphi\frac{1}{r}\frac{\partial}{\partial\theta} - \frac{\sin\varphi}{r\sin\theta}\frac{\partial}{\partial\varphi},$$
$$\frac{\partial}{\partial y} = \sin\theta\sin\varphi\frac{\partial}{\partial r} + \cos\theta\sin\varphi\frac{1}{r}\frac{\partial}{\partial\theta} + \frac{\cos\varphi}{r\sin\theta}\frac{\partial}{\partial\varphi},$$
$$\frac{\partial}{\partial z} = \cos\theta\frac{\partial}{\partial r} - \sin\theta\frac{1}{r}\frac{\partial}{\partial\theta}.$$

Hint. Equate ∇_{xyz} and $\nabla_{r\theta\varphi}$.

2.5.9 From Exercise 2.5.8, show that
$$-i\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) = -i\frac{\partial}{\partial\varphi}.$$
This is the quantum mechanical operator corresponding to the z-component of orbital angular momentum.

2.5.10 With the quantum mechanical orbital angular momentum operator defined as $\mathbf{L} = -i(\mathbf{r}\times\nabla)$, show that

(a) $L_x + iL_y = e^{i\varphi}\left(\dfrac{\partial}{\partial\theta} + i\cot\theta\dfrac{\partial}{\partial\varphi}\right)$,

(b) $L_x - iL_y = -e^{-i\varphi}\left(\dfrac{\partial}{\partial\theta} - i\cot\theta\dfrac{\partial}{\partial\varphi}\right)$.

These are the raising and lowering operators of Section 4.3.

2.5.11 Verify that $\mathbf{L}\times\mathbf{L} = i\mathbf{L}$ in spherical polar coordinates. $\mathbf{L} = -i(\mathbf{r}\times\nabla)$, the quantum mechanical orbital angular momentum operator.
Hint. Use spherical polar coordinates for $\mathbf{L}$ but Cartesian components for the cross product.

2.5.12 (a) From Eq. (2.75), show that
$$\mathbf{L} = -i(\mathbf{r}\times\nabla) = i\left(\hat{\boldsymbol{\theta}}\frac{1}{\sin\theta}\frac{\partial}{\partial\varphi} - \hat{\boldsymbol{\varphi}}\frac{\partial}{\partial\theta}\right).$$

(b) Resolving $\hat{\boldsymbol{\theta}}$ and $\hat{\boldsymbol{\varphi}}$ into Cartesian components, determine L_x, L_y, and L_z in terms of θ, φ, and their derivatives.

(c) From $L^2 = L_x^2 + L_y^2 + L_z^2$, show that
$$\mathbf{L}^2 = -\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) - \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}$$
$$= -r^2\nabla^2 + \frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right).$$
This latter identity is useful in relating orbital angular momentum and Legendre's differential equation (Exercise 8.9.2).

2.5.13 With $\mathbf{L} = -i\mathbf{r}\times\nabla$, verify the operator identities

(a) $\nabla = \hat{\mathbf{r}}\dfrac{\partial}{\partial r} - i\dfrac{\mathbf{r}\times\mathbf{L}}{r^2}$,

(b) $\mathbf{r}\nabla^2 - \nabla\left(1 + r\dfrac{\partial}{\partial r}\right) = i\nabla \times \mathbf{L}$.

2.5.14 Show that the following three forms (spherical coordinates) of $\nabla^2\psi(r)$ are equivalent:

$$\text{(a)}\ \frac{1}{r^2}\frac{d}{dr}\left[r^2\frac{d\psi(r)}{dr}\right], \quad \text{(b)}\ \frac{1}{r}\frac{d^2}{dr^2}[r\psi(r)], \quad \text{(c)}\ \frac{d^2\psi(r)}{dr^2} + \frac{2}{r}\frac{d\psi(r)}{dr}.$$

The second form is particularly convenient in establishing a correspondence between spherical polar and Cartesian descriptions of a problem. A generalization of this appears in Exercise 8.6.11.

2.5.15 (a) Explain why ∇^2 in plane polar coordinates follows from ∇^2 in circular cylindrical coordinates with $z =$ constant.

(b) Explain why taking ∇^2 in spherical polar coordinates and restricting θ to $\pi/2$ does **not** lead to the plane polar form of ∇.

Note.

$$\nabla^2(\rho, \varphi) = \frac{\partial^2}{\partial\rho^2} + \frac{1}{\rho}\frac{\partial}{\partial\rho} + \frac{1}{\rho^2}\frac{\partial^2}{\partial\varphi^2}.$$

2.6 Tensor Analysis

In Chapter 1, vectors were defined or represented in two equivalent ways: (i) geometrically by specifying magnitude and direction, as an arrow, and (ii) algebraically by specifying the components relative to Cartesian (orthogonal) coordinate axes. The second definition has been adequate for vector analysis so far. However, the definition of a vector as a quantity with magnitude and direction is not unique and therefore incomplete. We encounter quantities, such as elastic constants and index of refraction in anisotropic crystals, that have magnitude and depend on direction but that are not vectors. We seek a new definition of a vector using the coordinate vector $\mathbf{r}$ as a prototype. In this section, two more refined, sophisticated, and powerful definitions are presented that are central to the concept of a tensor generally.

Tensors are important in many areas of physics, including general relativity and electrodynamics. Scalars and vectors (Sections 1.1–1.5) are special cases of tensors. A scalar is specified by one real number and is called a **tensor of rank zero**. In three-dimensional space, a vector is specified by $3 = 3^1$ real numbers (e.g., its Cartesian components) and is called a **tensor of rank one**. We shall see that a **tensor of rank** n has 3^n components that transform in a definite manner.[7]

We start by defining a vector in three-dimensional Euclidean space in terms of the behavior of its three components under rotations of the coordinate axes. This **transformation theory** philosophy is of central importance for tensor analysis and groups of transformations (discussed in Chapter 4 as well) and conforms with the mathematician's concepts of vector and vector (or linear)

[7] In N-dimensional space a tensor of rank n has N^n components.

space and the physicist's notion that observables must not depend on the choice of coordinate frames. There is an important physical basis for such a philosophy: We describe our physical world by mathematics, but any physical predictions we make must be **independent** of our mathematical conventions such as a coordinate system with its arbitrary origin and directions of its axes.

Rotation of Coordinate Axes

When we assume that space is isotropic—that is, there is no preferred direction or all directions are equivalent—then the physical system being analyzed or the relevant physical law cannot and must not depend on our choice or **orientation** of the coordinate axes. Thus, a quantity S that does not change under rotations of the coordinate system in three-dimensional space, $S' = S$, is a rotational invariant; it is labeled a scalar. Examples are the mass of a particle, the scalar product of two vectors whose invariance $\mathbf{A}' \cdot \mathbf{B}' = \mathbf{A} \cdot \mathbf{B}$ under rotations we show in the next subsection, and the volume spanned by three vectors. Similarly, a quantity whose components transform under rotations like those of the coordinates of a point is called a vector. The transformation of the components of the vector under a rotation of the coordinates preserves the vector as a geometric entity (such as an arrow in space), independent of the orientation of the reference frame. Now we return to the concept of vector $\mathbf{r}$ as a geometric object independent of the coordinate system. Let us examine $\mathbf{r}$ in two different systems, one rotated in relation to the other. For simplicity, we consider first the two-dimensional case. If the x-, y-coordinates are rotated counterclockwise through an angle φ, **keeping r fixed** (i.e., the physical system is held fixed), we read off Fig. 2.20 the following relations between the

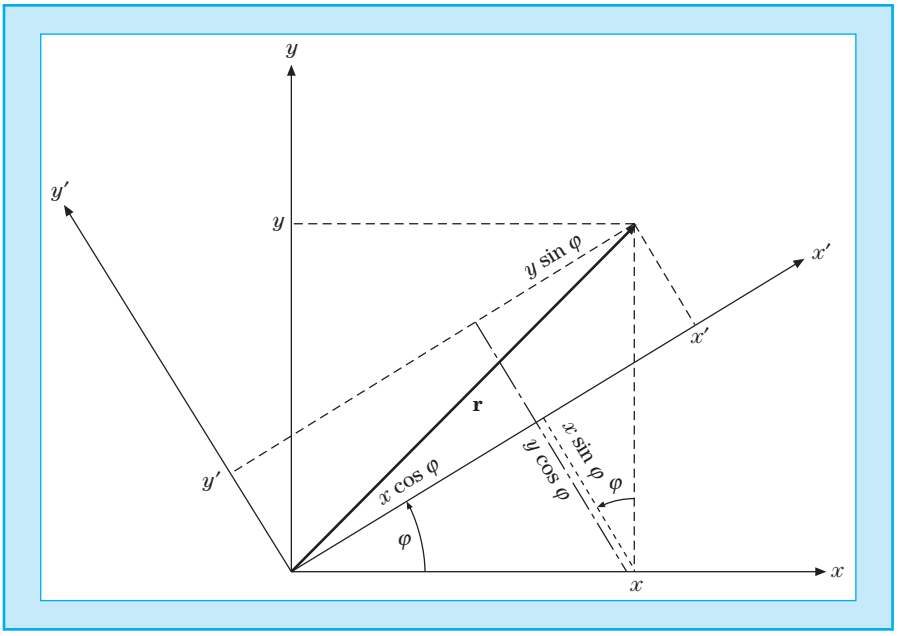


Figure 2.20

Rotation of Cartesian Coordinate Axes About the z-Axis

components resolved in the original system (unprimed) and those resolved in the new rotated system (primed):

$$\begin{aligned} x' &= x\cos\varphi + y\sin\varphi, \\ y' &= -x\sin\varphi + y\cos\varphi. \end{aligned} \tag{2.86}$$

We saw in Section 1.1 that a vector could be represented by the Cartesian coordinates of a point; that is, the coordinates were proportional to the vector components. Hence, the components of a vector must transform under rotation as coordinates of a point (such as $\mathbf{r}$). Therefore, whenever any pair of quantities A_x and A_y in the xy-coordinate system is transformed in (A'_x, A'_y) by this rotation of the coordinate system with

$$\begin{aligned} A'_x &= A_x\cos\varphi + A_y\sin\varphi \\ A'_y &= -A_x\sin\varphi + A_y\cos\varphi, \end{aligned} \tag{2.87}$$

we **define**[8] A_x and A_y as the components of a vector $\mathbf{A}$. Our vector is now defined in terms of the transformation of its components under rotation of the coordinate system. From a comparison of Eqs. (2.86) and (2.87), we can conclude that A_x and A_y transform in the same way as x and y, the components of the two-dimensional coordinate vector $\mathbf{r}$. In other words, the vector $\mathbf{A}$ varies as $\mathbf{r}$ does under rotations; that is, it "covaries." If a pair of numbers A_x and A_y do not show this **form invariance (or covariance)** when the coordinates are rotated, they are not the components of a vector. In this sense, the coordinates of a vector belong together. In contrast, from Fig. 2.20 we see that any single component, such as A_x, of the vector $\mathbf{A}$ is not invariant under rotations, that is, changes its length in a rotated coordinate system.

The vector components A_x and A_y satisfying the defining equations [Eq. (2.87)] associate a magnitude A and a direction with each point in space. The magnitude is a scalar quantity, invariant to the rotation of the coordinate system. The direction (relative to the unprimed system) is likewise invariant to the rotation of the coordinate system (see Exercise 2.6.1). The result is that the components of a vector may vary according to the rotation of the primed coordinate system. This is what Eq. (2.87) states. However, the variation with the angle is such that the components in the rotated coordinate system A'_x and A'_y define a vector with the same magnitude and the same direction as the vector defined by the components A_x and A_y relative to the x-, y-coordinate axes (compare Exercise 2.6.1). The components of $\mathbf{A}$ in a particular coordinate system constitute the representation of $\mathbf{A}$ in that coordinate system. Equation (2.87), the transformation relation, is a guarantee that the entity $\mathbf{A}$ is independent of the rotation of the coordinate system.

[8]The corresponding definition of a scalar quantity is $S' = S$, that is, invariant under rotation of the coordinates like the scalar product of two vectors $\mathbf{x}'_1 \cdot \mathbf{x}'_2 = \mathbf{x}_1 \cdot \mathbf{x}_2$.

To go on to three, four, and higher dimensions, we use a more compact notation. Let

$$\begin{aligned} x &\to x_1 \\ y &\to x_2 \end{aligned} \tag{2.88}$$

$$\begin{aligned} a_{11} &= \cos\varphi, \qquad a_{12} = \sin\varphi, \\ a_{21} &= -\sin\varphi, \qquad a_{22} = \cos\varphi, \end{aligned} \tag{2.89}$$

and $z \to x_3$, etc. in higher dimensions. Then Eq. (2.86) becomes

$$\begin{aligned} x_1' &= a_{11}x_1 + a_{12}x_2, \\ x_2' &= a_{21}x_1 + a_{22}x_2. \end{aligned} \tag{2.90}$$

The coefficient a_{ij} is a direction cosine, the cosine of the angle $\varphi_{i'j}$ between x_i' and x_j; that is,

$$\begin{aligned} a_{12} &= \cos\varphi_{1'2} = \sin\varphi, \\ a_{21} &= \cos\varphi_{2'1} = \cos\left(\varphi + \frac{\pi}{2}\right) = -\sin\varphi. \end{aligned} \tag{2.91}$$

The advantage of the new notation[9] is that it permits us to use the summation symbol $\sum$ and to rewrite Eq. (2.90) as

$$x_i' = \sum_{j=1}^{2} a_{ij}x_j, \qquad i = 1, 2. \tag{2.92}$$

Note that i remains as a parameter that gives rise to one equation when it is set equal to 1 and to a second equation when it is set equal to 2. The index j, of course, is a summation index, a dummy index. As with a variable of integration, j may be replaced by any other convenient symbol.

The generalization to three, four, or N dimensions is now very simple. The set of N quantities, V_j, is said to be the components of an N–dimensional vector, $\mathbf{V}$, if and only if their values relative to the rotated coordinate axes are given by

$$V_i' = \sum_{j=1}^{N} a_{ij}V_j, \qquad i = 1, 2, \ldots, N. \tag{2.93}$$

As before, a_{ij} is the cosine of the angle between the x_i' and x_j directions. When the number of dimensions that our space has is clear, the upper limit N and the corresponding range of i will often not be indicated.

[9] If you wonder about the replacement of one parameter φ by four parameters a_{ij}, clearly the a_{ij} do not constitute a minimum set of parameters. For two dimensions, the four a_{ij} are subject to the three constraints given in Eq. (2.97). The justification for the redundant set of direction cosines is the convenience it provides. It is hoped that this convenience will become more apparent in the following discussion. For three-dimensional rotations (nine a_{ij}, of which only three are independent) alternate descriptions are provided by (i) the Euler angles discussed in Section 3.3, (ii) quaternions, and (iii) the Cayley–Klein parameters. These alternatives have their respective advantages and disadvantages.

From the definition of a_{ij} as the cosine of the angle between the positive x_i' direction and the positive x_j direction, we may write (Cartesian coordinates)[10]

$$a_{ij} = \frac{\partial x_i'}{\partial x_j}. \tag{2.94}$$

Using the inverse rotation ($\varphi \to -\varphi$) yields

$$x_j = \sum_{i=1}^{2} a_{ij} x_i', \quad \text{or} \quad \frac{\partial x_j}{\partial x_i'} = a_{ij}. \tag{2.95}$$

Notice that $\frac{\partial x_i'}{\partial x_j} = \frac{\partial x_j}{\partial x_i'}$; this is only true for Cartesian coordinates.

By use of Eqs. (2.94) and (2.95), Eq. (2.93) becomes

$$V_i' = \sum_{j=1}^{N} \frac{\partial x_i'}{\partial x_j} V_j = \sum_{j=1}^{N} \frac{\partial x_j}{\partial x_i'} V_j. \tag{2.96}$$

The direction cosines a_{ij} satisfy an **orthogonality condition**

$$\sum_i a_{ij} a_{ik} = \delta_{jk} \tag{2.97}$$

or, equivalently,

$$\sum_i a_{ji} a_{ki} = \delta_{jk}. \tag{2.98}$$

The symbol δ_{jk} in Eqs. (2.97) and (2.98) is the Kronecker delta, defined by

$$\begin{aligned} \delta_{jk} &= 1 \quad \text{for} \quad j = k, \\ \delta_{jk} &= 0 \quad \text{for} \quad j \neq k. \end{aligned} \tag{2.99}$$

Equations (2.97) and (2.98) can be verified in the two-dimensional case by substituting the specific a_{ij} from Eq. (2.89). The result is the well-known identity $\sin^2\varphi + \cos^2\varphi = 1$. To verify Eq. (2.98) in general form, we use the partial derivative forms of Eqs. (2.94) and (2.95) to obtain

$$\sum_i \frac{\partial x_j}{\partial x_i'} \frac{\partial x_k}{\partial x_i'} = \sum_i \frac{\partial x_j}{\partial x_i'} \frac{\partial x_i'}{\partial x_k} = \frac{\partial x_j}{\partial x_k}. \tag{2.100}$$

The last step follows by the standard rules for partial differentiation, assuming that x_j is a function of x_1', x_2', x_3', and so on. The final result, $\partial x_j/\partial x_k$, is equal to δ_{jk} since x_j and x_k as coordinate lines ($j \neq k$) are assumed to be perpendicular (two or three dimensions) or orthogonal (for any number of dimensions). Equivalently, x_j and x_k ($j \neq k$) are totally independent variables. If $j = k$, the partial derivative is clearly equal to 1.

In redefining a vector in terms of the way its components transform under a rotation of the coordinate system, we should emphasize two points:

- This more precise definition is not only useful but necessary in describing our physical world. When all vectors in a vector equation transform covariantly (i.e., transform just like the coordinate vector), the vector equation is

[10] Differentiate x_i' with respect to x_j. See the discussion at the start of Section 1.6 for the definition of partial derivatives. Section 3.3 provides an alternate approach.

in essence independent of any particular coordinate system. (The coordinate system need not even be Cartesian.) A vector equation can always be expressed in some coordinate system. This **independence of reference frame** (implied by **covariance**) is needed to formulate universal laws of physics involving vectors or tensors more generally.

- This definition is subject to a generalization that will form the basis of the branch of mathematics known as tensor analysis.

On this basis, the behavior of the vector components under rotation of the coordinates is used next to prove that an inner product is a scalar, and then to prove that an outer product is a vector, and finally to show that the gradient of a scalar, $\nabla\psi$, is a vector.

Biographical Data

Kronecker, Leopold. Kronecker, a German mathematician, was born in Liegnitz, Germany (now Poland), in 1823 and died in Berlin in 1891. Son of a Jewish merchant, he ran the family business and was well off, so he could afford to retire at age 30. He obtained his Ph.D. in 1845 in Berlin, and by 1883 he was a professor. He developed number theory and algebra but was obsessed with integers to the point of dismissing Cantor's transfinite numbers and Weierstrass's analysis, coining the phrase "God made the integers, all else is the work of man."

Invariance of the Scalar Product under Rotations

We have not formally shown that the word scalar is justified or that the scalar product is indeed a scalar quantity—that is, stays invariant under rotations of the coordinates. To show this, we investigate the behavior of $\mathbf{A}\cdot\mathbf{B}$ under a rotation of the coordinate system. By use of Eq. (2.93),

$$\mathbf{A}'\cdot\mathbf{B}' = \sum_i A_i'B_i' = \sum_i a_{1i}A_i \sum_j a_{1j}B_j + \sum_i a_{2i}A_i \sum_j a_{2j}B_j + \sum_i a_{3i}A_i \sum_j a_{3j}B_j. \tag{2.101}$$

Using the indices k and l to sum over 1, 2, and 3 indices, we obtain

$$\sum_k A_k'B_k' = \sum_l \sum_i \sum_j a_{li}\, A_i\, a_{lj}B_j, \tag{2.102}$$

and, by rearranging the terms on the right-hand side, we have

$$\sum_k A_k'B_k' = \sum_l \sum_i \sum_j (a_{li}\, a_{lj})A_iB_j = \sum_i \sum_j \delta_{ij}A_iB_j = \sum_j A_jB_j. \tag{2.103}$$

The last two steps follow by using Eq. (2.98), the orthogonality condition of the direction cosines, and Eq. (2.99), which defines the Kronecker delta. The effect of the Kronecker delta is to cancel all terms in a summation over either

index except the term for which the indices are equal. In Eq. (2.103), its effect is to set $j = i$ and to eliminate the summation over j. Of course, we could equally well set $i = j$ and eliminate the summation over i. Equation (2.103) gives us

$$\sum_k A'_k B'_k = \sum_i A_i B_i, \tag{2.104}$$

which is our definition of a scalar quantity—one that remains invariant under the rotation of the coordinate system.

Covariance of Cross Product

For the cross product there remains the problem of verifying that $\mathbf{C} = \mathbf{A} \times \mathbf{B}$ is indeed a vector; that is, it obeys Eq. (2.93), the vector transformation law. That is, we want to show that the cross product transforms like the coordinate vector, which is the meaning of covariance here. Starting in a rotated (primed) system

$$\begin{aligned} C'_i &= A'_j B'_k - A'_k B'_j, \quad i, j, \text{ and } k \text{ in cyclic order,} \\ &= \sum_l a_{jl} A_l \sum_m a_{km} B_m - \sum_l a_{kl} A_l \sum_m a_{jm} B_m \\ &= \sum_{l,m} (a_{jl} a_{km} - a_{kl} a_{jm}) A_l B_m. \end{aligned} \tag{2.105}$$

The combination of direction cosines in parentheses vanishes for $m = l$. We therefore have j and k taking on fixed values, dependent on the choice of i, and six combinations of l and m. If $i = 3$, then $j = 1$, $k = 2$ (cyclic order), and we have the following direction cosine combinations:[11]

$$\begin{aligned} a_{11}a_{22} - a_{21}a_{12} &= a_{33}, \\ a_{13}a_{21} - a_{23}a_{11} &= a_{32}, \\ a_{12}a_{23} - a_{22}a_{13} &= a_{31}. \end{aligned} \tag{2.106}$$

Equations (2.106) are identities satisfied by the direction cosines. They can be verified with the use of determinants and matrices (see Exercise 3.3.3). Substituting back into Eq. (2.105),

$$\begin{aligned} C'_3 &= a_{33}(A_1 B_2 - A_2 B_1) + a_{32}(A_3 B_1 - A_1 B_3) + a_{31}(A_2 B_3 - A_3 B_2) \\ &= a_{31} C_1 + a_{32} C_2 + a_{33} C_3 = \sum_n a_{3n} C_n. \end{aligned} \tag{2.107}$$

By permuting indices to pick up C'_1 and C'_2, we see that Eq. (2.93) is satisfied and $\mathbf{C}$ is indeed a vector. It should be mentioned here that this **vector nature** of the **cross product** is an accident associated with the **three-dimensional**

[11] Equations (2.106) hold for rotations because they preserve volumes. For a more general orthogonal transformation the r.h.s. of Eq. (2.106) is multiplied by the determinant of the transformation matrix (see Chapter 3 for matrices and determinants). As a consequence, the cross product is a pseudovector rather than a vector.

nature of ordinary space.[12] We shall also see that the cross product of two vectors may be treated as a second-rank antisymmetric tensor.

Covariance of Gradient

There is one more ambiguity in the transformation law of a vector, Eq. (2.93), in which a_{ij} is the cosine of the angle between the x_i'-axis and the x_j-axis. If we start with a differential distance vector $d\mathbf{r}$, and taking dx_i' to be a function of the unprimed variables

$$dx_i' = \sum_j \frac{\partial x_i'}{\partial x_j}\, dx_j \tag{2.108}$$

by partial differentiation (see Section 1.5 for the total differential), then Eqs. (2.108) and (2.92) are consistent. Any set of quantities V_j transforming according to Eq. (2.96) is defined as a **contravariant** vector.

However, we have already encountered a slightly different type of vector transformation. The gradient $\nabla\varphi$ defined by Eq. (1.64) (using x_1, x_2, x_3 for x, y, z) transforms as

$$\frac{\partial\varphi'}{\partial x_i'} = \sum_j \frac{\partial\varphi}{\partial x_j}\frac{\partial x_j}{\partial x_i'} = \sum_j \frac{\partial x_j}{\partial x_i'}\frac{\partial\varphi}{\partial x_j} \tag{2.109}$$

using the chain rule and $\varphi = \varphi(x, y, z) = \varphi(x', y', z') = \varphi'$ with φ defined as a scalar quantity. Notice that this differs from Eqs. (2.93) and (2.94) in that we have $\partial x_j/\partial x_i'$ instead of $\partial x_i'/\partial x_j$. Equation (2.109) is taken as the definition of a **covariant** vector with the gradient as the prototype.

In Cartesian coordinates only,

$$\frac{\partial x_j}{\partial x_i'} = \frac{\partial x_i'}{\partial x_j} = a_{ij}, \tag{2.110}$$

and there is no difference between contravariant and covariant transformations.

In other systems, Eq. (2.110) in general does not apply, and the distinction between contravariant and covariant is real and must be observed. This is of prime importance in the curved Riemannian space of general relativity. Let us illustrate the difference between covariant and contravariant vectors in Minkowski space of special relativity.

In the remainder of this section, the components of a **contravariant** vector are denoted by a **superscript**, A^i, whereas a **subscript** is used for the components of a **covariant** vector A_i.[13]

[12] Specifically, Eq. (2.106) holds only for three-dimensional space. For a far-reaching generalization of the cross product, see D. Hestenes and G. Sobczyk, *Clifford Algebra to Geometric Calculus*. Reidel, Dordrecht (1984).

[13] This means that the coordinates (x, y, z) should be written (x^1, x^2, x^3) since $\mathbf{r}$ transforms as a contravariant vector. Because we restrict our attention to Cartesian tensors (where the distinction between contravariance and covariance disappears), we continue to use subscripts on the coordinates. This avoids the ambiguity of x^2 representing both x squared and y.

EXAMPLE 2.6.1

Gradient in Minkowski Space The distance $x^2 = c^2t^2 - \mathbf{r}^2$ of the coordinate four-vector $x^\mu = (ct, \mathbf{r})$ defines the (indefinite) metric of Minkowski space, the four-dimensional space–time of special relativity. The scalar product $a\cdot b = a_0b_0 - \mathbf{a}\cdot\mathbf{b}$ has the same relative minus sign. Four-vectors transforming like x^μ are called contravariant and those like $x_\mu = (ct, -\mathbf{r})$ that contain the minus sign of the metric are called covariant so that the distance becomes $x^2 = \sum_\mu x^\mu x_\mu$ and the scalar product simply $a \cdot b = \sum_\mu a^\mu b_\mu$. Covariant and contravariant four-vectors clearly differ. The relative minus sign between them is important, as the gradient $\partial^\mu \equiv (\frac{1}{c}\frac{\partial}{\partial t}, -\boldsymbol{\nabla})$ and the continuity equation of the current $J^\mu = (c\rho, \mathbf{J})$,

$$\sum_\mu \partial^\mu J_\mu = \frac{\partial \rho}{\partial t} - (-\boldsymbol{\nabla}\cdot\mathbf{J}) = \partial \cdot J,$$

show. The reason for the minus sign in the definition of the gradient is that $\partial^\mu = \frac{\partial}{\partial x_\mu}$. This can be checked by the derivative of the metric

$$\frac{\partial x^2}{\partial x_\mu} = \frac{\partial \sum_\nu x^\nu x_\nu}{\partial x_\mu} = 2x^\mu,$$

which transforms (contravariantly) like the coordinate vector x^μ, and $\frac{\partial}{\partial x_\mu} = (\frac{1}{c}\frac{\partial}{\partial t}, -\boldsymbol{\nabla})$. ■

Definition of Tensors of Rank Two

To derive the principal moments of inertia, we rotate the inertia ellipsoid to its principal axes. Thus, we need to obtain the principal moments from the original moments. That is, we have to generalize the transformation theory of vectors to tensors as well. Now we proceed to define **contravariant, mixed, and covariant tensors of rank 2** by the following equations for their components under coordinate transformations (which are separate vector transformations for each index of a tensor):

$$\begin{aligned} A'^{ij} &= \sum_{kl} \frac{\partial x'_i}{\partial x_k}\frac{\partial x'_j}{\partial x_l} A^{kl}, \\ B'^i_j &= \sum_{kl} \frac{\partial x'_i}{\partial x_k}\frac{\partial x_l}{\partial x'_j} B^k_l, \\ C'_{ij} &= \sum_{kl} \frac{\partial x_k}{\partial x'_i}\frac{\partial x_l}{\partial x'_j} C_{kl}. \end{aligned} \tag{2.111}$$

Clearly, the rank goes as the number of indices and, therefore, partial derivatives (or direction cosines) in the definition: zero for a scalar, one for a vector, two for a second-rank tensor, and so on. Each index (subscript or superscript) ranges over the number of dimensions of the space. The number of indices (rank of tensor) is independent of the dimensions of the space. A^{kl} is contravariant with respect to both indices, C_{kl} is covariant with respect to both indices, and B^k_l transforms contravariantly with respect to the first index k but covariantly with respect to the second index l. Again, if we are using Cartesian

coordinates, all three forms of the tensors of second rank—contravariant, mixed, and covariant—are the same.

As with the components of a vector, the transformation laws for the components of a tensor [Eq. (2.111)] yield entities (and properties) that are independent of the choice of reference frame. This is what makes tensor analysis important in physics. The independence of reference frame (covariance) is ideal for expressing and investigating universal physical laws.

The second-rank tensor $\mathbf{A}$ (components A^{kl}) may be conveniently represented by writing out its components in a square array (3×3 if we are in three-dimensional space),

$$\mathbf{A} = \begin{pmatrix} A^{11} & A^{12} & A^{13} \\ A^{21} & A^{22} & A^{23} \\ A^{31} & A^{32} & A^{33} \end{pmatrix}. \tag{2.112}$$

This does not mean that any square array of numbers or functions forms a tensor. The essential condition is that the components transform according to Eq. (2.111).

Examples of tensors abound in physics and engineering: The inertia tensor [see Eqs. (3.126)–(3.128)], the Kronecker δ, multipole moments of electrostatics and gravity, the antisymmetric Levi–Civita symbol [see Eq. (2.133)] of rank three in three-dimensional Euclidean space, the metric, Ricci and energy-momentum tensors of general relativity, and the electromagnetic field tensor (see Example 2.6.2) are all second-rank tensors, and the Riemann curvature tensor is of rank four.

In the context of matrix analysis, the preceding transformation equations become (for Cartesian coordinates) an orthogonal similarity transformation (Section 3.3). A geometrical interpretation of a second-rank tensor (the inertia tensor) is developed in Section 3.5.

Addition and Subtraction of Tensors

The addition and subtraction of tensors is defined in terms of the individual elements just as for vectors. If

$$\mathbf{A} + \mathbf{B} = \mathbf{C}, \tag{2.113}$$

then

$$A^{ij} + B^{ij} = C^{ij}.$$

Of course, $\mathbf{A}$ and $\mathbf{B}$ must be tensors of the same rank and both expressed in a space of the same number of dimensions.

Summation Convention

In tensor analysis it is customary to adopt a summation convention to put Eq. (2.111) and subsequent tensor equations in a more compact form. As long as we are distinguishing between contravariance and covariance, let us agree that when an index appears on one side of an equation, once as a superscript and

once as a subscript (except for the coordinates, where both are subscripts), we automatically sum over that index. Then we may write the second expression in Eq. (2.111) as

$$B'^{i}_{j} = \frac{\partial x'_i}{\partial x_k}\frac{\partial x_l}{\partial x'_j}B^k_l, \tag{2.114}$$

with the summation of the right-hand side over k and i implied. This is **Einstein's summation convention**.[14]

To illustrate the use of the summation convention and some of the techniques of tensor analysis, let us show that the now familiar Kronecker delta, δ_{kl}, is really a mixed tensor of rank two, δ^k_l.[15] Does δ^k_l transform according to Eq. (2.111)? This is our criterion for calling it a tensor. Using the summation convention, δ^k_l transforms into

$$\delta^k_l\frac{\partial x'_i}{\partial x_k}\frac{\partial x_l}{\partial x'_j} = \frac{\partial x'_i}{\partial x_k}\frac{\partial x_k}{\partial x'_j}, \tag{2.115}$$

the last step by definition of the Kronecker delta. Now

$$\frac{\partial x'_i}{\partial x_k}\frac{\partial x_k}{\partial x'_j} = \frac{\partial x'_i}{\partial x'_j} \tag{2.116}$$

by direct partial differentiation of the right-hand side (chain rule). However, x'_i and x'_j are independent coordinates, and therefore the variation of one with respect to the other must be zero if they are different and unity if they coincide; that is,

$$\frac{\partial x'_i}{\partial x'_j} = \delta'^{i}_{j}. \tag{2.117}$$

Hence,

$$\delta'^{i}_{j} = \frac{\partial x'_i}{\partial x_k}\frac{\partial x_l}{\partial x'_j}\delta^k_l,$$

showing that the δ^k_l are indeed the components of a mixed second-rank tensor. Notice that this result is independent of the number of dimensions of our space.

Because the Kronecker delta has the same components in all of our rotated coordinate systems, it is called **isotropic**. In Section 2.9, we discuss a third-rank isotropic tensor and three fourth-rank isotropic tensors. No isotropic first-rank tensor (vector) exists.

Symmetry–Antisymmetry

The order in which the indices appear in our description of a tensor is important. In general, A^{mn} is independent of A^{nm}, but there are some cases of special interest. If, for all m and n,

$$A^{mn} = A^{nm}, \tag{2.118}$$

[14] In this context, $\partial x'_i/\partial x_k$ might better be written as a^i_k and $\partial x_l/\partial x'_j$ as b^l_j.

[15] It is common practice to refer to a tensor $\mathbf{A}$ by specifying a typical component, A_{ij}. As long as one refrains from writing nonsense such as $\mathbf{A} = A_{ij}$, no harm is done.

we call the tensor **symmetric**. If, on the other hand,

$$A^{mn} = -A^{nm}, \tag{2.119}$$

the tensor is **antisymmetric**. Clearly, every (second-rank) tensor can be resolved into symmetric and antisymmetric parts by the identity

$$A^{mn} = \frac{1}{2}(A^{mn} + A^{nm}) + \frac{1}{2}(A^{mn} - A^{nm}), \tag{2.120}$$

the first term on the right being a symmetric tensor and the second term an antisymmetric tensor. A similar resolution of functions into symmetric and antisymmetric parts is of extreme importance in quantum mechanics.

EXAMPLE 2.6.2

Inertia, Quadrupole, and Electromagnetic Field Tensors The off-diagonal moments of inertia, such as $I_{xy} = -\sum_{i,j} m_{ij}x_i y_j = I_{yx}$, show that the inertia tensor is symmetric. Similarly, the electric quadrupole moments $Q_{ij} = \int (3x_i x_j - r^2\delta_{ij})\rho(\mathbf{r})d^3r = Q_{ji}$ form a manifestly symmetric tensor. In contrast, the electromagnetic field tensor $F^{\mu\nu} = \partial^\mu A^\nu - \partial^\nu A^\mu$ with the four-vector gradient $\partial^\mu \equiv (\frac{1}{c}\frac{\partial}{\partial t}, -\boldsymbol{\nabla})$ is manifestly antisymmetric. ■

Spinors

It was once thought that the system of scalars, vectors, tensors (second rank), and so on formed a complete mathematical system—one that is adequate for describing a physics independent of the choice of reference frame. However, the universe and mathematical physics are not this simple. In the realm of elementary particles, for example, spin zero particles[16] (π mesons and α particles) may be described with scalars, spin 1 particles (deuterons) by vectors, and spin 2 particles (gravitons) by tensors. This listing omits the most common particles: electrons, protons, neutrinos, and neutrons, all with spin $\frac{1}{2}$. These particles are properly described by **spinors**, which are two-component wave functions—one for spin up and the other for the spin down state. A spinor is not a scalar, vector, or tensor. A brief introduction to spinors in the context of group theory appears in Section 4.3.

SUMMARY

Tensors are systems of components organized by one, two, or more indices that transform according to specific rules under a set (group) of transformations. The number of indices is called the rank of the tensor. If the transformations are rotations in three-dimensional space, then tensor analysis amounts to what we did in the sections on curvilinear coordinates and in Cartesian coordinates in Chapter 1. In four dimensions of Minkowski space–time, the transformations are Lorentz transformations. Here, tensors of rank 1 are the four-vectors of Chapter 4.

[16] The particle spin is intrinsic angular momentum (in units of $\hbar$). It is distinct from classical, orbital angular momentum due to motion.

EXERCISES

2.6.1 (a) Show that the magnitude of a vector **A**, $A = (A_x^2 + A_y^2)^{1/2}$, is independent of the orientation of the rotated coordinate system

$$\left(A_x^2 + A_y^2\right)^{1/2} = \left(A_x'^2 + A_y'^2\right)^{1/2}$$

independent of the rotation angle φ.
This independence of angle is expressed by saying that A is **invariant** under rotations.

(b) At a given point (x, y), **A** defines an angle α relative to the positive x-axis and α' relative to the positive x'-axis. The angle from x to x' is φ. Show that $\mathbf{A} = \mathbf{A}'$ defines the **same** direction in space when expressed in terms of its primed components and in terms of its unprimed components; that is,

$$\alpha' = \alpha - \varphi.$$

2.6.2 Show that if all components of a tensor of any rank vanish in one particular coordinate system, they vanish in all coordinate systems.
Note. This point takes on special importance in the four-dimensional curved space of general relativity. If a quantity, expressed as a tensor, is defined in one coordinate system, it exists in all coordinate systems and is not just a consequence of a **choice** of a coordinate system (as are centrifugal and Coriolis forces in Newtonian mechanics).

2.6.3 The components of tensor **A** are equal to the corresponding components of tensor **B** in one particular coordinate system; that is,

$$A_{ij}^0 = B_{ij}^0.$$

Show that tensor **A** is equal to tensor **B**, $A_{ij} = B_{ij}$, in all coordinate systems.

2.6.4 The first three components of a four-dimensional vector vanish in each of two reference frames. If the second reference frame is not merely a rotation of the first about the x_4 axis—that is, if at least one of the coefficients a_{i4} $(i = 1, 2, 3) \neq 0$—show that the fourth component vanishes in all reference frames. Translated into relativistic mechanics this means that if momentum is conserved in two Lorentz frames, then energy is conserved in all Lorentz frames.

2.6.5 From an analysis of the behavior of a general second-rank tensor under 90° and 180° rotations about the coordinate axes, show that an isotropic second-rank tensor in three-dimensional space must be a multiple of δ_{ij}.

2.6.6 T_{iklm} is antisymmetric with respect to all pairs of indices. How many independent components has it (in three-dimensional space)?

2.7 Contraction and Direct Product

Contraction

When dealing with vectors, we formed a scalar product (Section 1.2) by summing products of corresponding components:

$$\mathbf{A}\cdot\mathbf{B} = A_iB_i \qquad (\textbf{summation convention}). \tag{2.121}$$

The generalization of this expression in tensor analysis is a process known as contraction. Two indices, one covariant and the other contravariant, are set equal to each other and then (as implied by the summation convention) we sum over this repeated index. For example, let us contract the second-rank mixed tensor $B_j'^i$:

$$B_j'^i \to B_i'^i = \frac{\partial x_i'}{\partial x_k}\frac{\partial x_l}{\partial x_i'}B_l^k = \frac{\partial x_l}{\partial x_k}B_l^k \tag{2.122}$$

by Eq. (2.98), and then by Eq. (2.99),

$$B_i'^i = \delta_k^l B_l^k = B_k^k. \tag{2.123}$$

Remember that i and k are both summed. Our contracted second-rank mixed tensor is invariant and therefore a scalar.[17] This is exactly what we obtained in Eq. (2.102) for the dot product of two vectors and in Section 1.6 for the divergence of a vector.

SUMMARY In general, the operation of contraction reduces the rank of a tensor by two. Examples of the use of contraction abound in physics and engineering: The scalar product of two vectors, the triple scalar product for the volume spanned by three vectors, determinants as contractions of the antisymmetric Levi–Civita tensor with n vectors in n-dimensional Euclidean space are discussed in Chapter 3.

Direct Product

The components of a covariant vector (first-rank tensor) a_i and those of a contravariant vector (first-rank tensor) b^j may be multiplied component by component to give the general term a_ib^j. By Eq. (2.111), this is actually a mixed second-rank tensor for

$$a_i'b'^j = \frac{\partial x_k}{\partial x_i'}a_k\frac{\partial x_j'}{\partial x_l}b^l = \frac{\partial x_k}{\partial x_i'}\frac{\partial x_j'}{\partial x_l}(a_kb^l). \tag{2.124}$$

Note that the tensors a_ib^j, b_ia^j, a_ib_j, a^ib^j are all different. Contracting, we obtain

$$a_i'b'^i = a_kb^k, \tag{2.125}$$

as in Eq. (2.104) to give the regular scalar product.

[17] In matrix analysis, this scalar is the **trace** of the matrix (Section 3.2).

The operation of adjoining two vectors a_i and b^j as in the last paragraph is known as forming the **direct product**. For the case of two vectors, the direct product is a tensor of second rank. In this sense, we may attach meaning to $\nabla\mathbf{E}$, which was not defined within the framework of vector analysis. In general, the direct product of two tensors is a tensor of rank equal to the sum of the two initial ranks; that is,

$$A_j^i B^{kl} = C_j^{ikl}, \tag{2.126a}$$

where C_j^{ikl} is a tensor of fourth rank. From Eqs. (2.111),

$$C'^{ikl}_j = \frac{\partial x_i'}{\partial x_m}\frac{\partial x_n}{\partial x_j'}\frac{\partial x_k'}{\partial x_p}\frac{\partial x_l'}{\partial x_q} C_n^{mpq}. \tag{2.126b}$$

EXAMPLE 2.7.1

Direct Product of Vectors Let us consider two-particle spin states in quantum mechanics that are constructed as direct products of single-particle states. The spin-$\frac{1}{2}$ states $|\uparrow\rangle$, $|\downarrow\rangle$ combine to spin 0 and spin 1. We may also describe them by unit vectors

$$|\uparrow\rangle = \begin{pmatrix}1\\0\end{pmatrix}, \quad |\downarrow\rangle = \begin{pmatrix}0\\1\end{pmatrix},$$

and direct product states, such as $|\uparrow\uparrow\rangle = |\uparrow\rangle|\uparrow\rangle$, are examples of $a_i b_j$ for $i = 1,\ j = 1$ in Eq. (2.124), etc. The triplet spin states can be described as

$$|\uparrow\uparrow\rangle = \begin{pmatrix}1 & 0\\0 & 0\end{pmatrix}, \quad \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) = \frac{1}{\sqrt{2}}\begin{pmatrix}0 & 1\\1 & 0\end{pmatrix} = \frac{1}{\sqrt{2}}\sigma_1,$$

$$|\downarrow\downarrow\rangle = \begin{pmatrix}0 & 0\\0 & 1\end{pmatrix}.$$

The spin 0 singlet state $\frac{1}{\sqrt{2}}(|\uparrow\rangle|\downarrow\rangle - |\downarrow\rangle|\uparrow\rangle)$ as a direct product can then be represented by the matrix

$$\begin{pmatrix}0 & 1\\-1 & 0\end{pmatrix} = i\sigma_2,$$

one of the Pauli spin matrices. ■

The direct product is a technique for creating higher rank tensors. Exercise 2.7.1 is a form of the direct product in which the first factor is ∇. Other applications appear in Section 4.6.

When $\mathbf{T}$ is an nth rank Cartesian tensor, $(\partial/\partial x_i)T_{jkl}\ldots$, an element of $\nabla\mathbf{T}$, is a **Cartesian** tensor of rank $n+1$ (Exercise 2.7.1). However, $(\partial/\partial x_i)T_{jkl}\ldots$ is not a tensor under more general transformations. In non-Cartesian systems $\partial/\partial x_i'$ will act on the partial derivatives $\partial x_p/\partial x_q'$ and destroy the simple tensor transformation relation.

So far, the distinction between a covariant transformation and a contravariant transformation has been maintained because it does exist in non-Cartesian space and because it is of great importance in general relativity. Now, however, because of the simplification achieved, we restrict ourselves to Cartesian tensors. As noted in Section 2.6, the distinction between contravariance

and covariance disappears and all indices from now on are shown as subscripts. We restate the summation convention and the operation of contraction.

SUMMARY

The operations of tensor algebra include contracting two indices, which generalizes the trace of a matrix and the scalar or dot product of two vectors to arbitrary tensors. The direct product of tensors is converse to contraction by forming products of all individual tensor components and enlarging the set of indices to comprise those of all tensors involved.

EXERCISES

2.7.1 If $T_{i\ldots}$ is a tensor of rank n, show that $\partial T_{\ldots i}/\partial x_j$ is a tensor of rank $n+1$ (Cartesian coordinates).
Note. In non-Cartesian coordinate systems the coefficients a_{ij} are, in general, functions of the coordinates, and the simple derivative of a tensor of rank n is not a tensor except in the special case of $n = 0$. In this case, the derivative does yield a covariant vector (tensor of rank 1) by Eq. (2.109).

2.7.2 If $T_{ijk\ldots}$ is a tensor of rank n, show that $\sum_j \partial T_{ijk\ldots}/\partial x_j$ is a tensor of rank $n-1$ (Cartesian coordinates).

2.7.3 Show that the operator

$$\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \nabla^2$$

is a **scalar** operator in Minkowski space–time.

2.8 Quotient Rule

If A_i and B_j are vectors, as defined in Section 2.6, then the direct product A_iB_j is a second-rank tensor. Here, we are concerned with recognizing tensors that are implicitly defined in some relation. For example, consider such equations as

$$K^iA_i = B \tag{2.127a}$$

$$K^i_jA^j = B^i \tag{2.127b}$$

$$K^i_jA^j_k = B^i_k \tag{2.127c}$$

$$K^{ijkl}A_{ij} = B^{kl} \tag{2.127d}$$

$$K_{ij}A_k = B_{ijk}, \tag{2.127e}$$

where in each of these relations **A** and **B** are known to be tensors of a rank indicated by the number of indices. In each case, K is an unknown quantity. We wish to establish the transformation properties of K. Let us demonstrate the **quotient rule** for Eq. (2.127b), which asserts that if the equation of interest

holds in all (rotated) Cartesian coordinate systems, then K is a tensor of the indicated rank. The proof for the other equations is similar and left as an exercise. The importance in physical theory is that the quotient rule can establish the tensor nature of quantities that are defined in relations. Exercise 2.8.1 is a simple illustration of this. The quotient rule shows that **the inertia matrix** appearing in the angular momentum equation $\mathbf{L} = I\boldsymbol{\omega}$ (Section 3.5) **is a tensor of rank 2**.

In proving the quotient rule, we consider Eq. (2.127b) as a typical case. In our primed coordinate system

$$K'^{i}_{j} A'^{j} = B'^{i} = a^{i}_{k} B^{k}, \tag{2.128}$$

using the vector transformation properties of $\mathbf{B}$. Since the equation holds in all rotated Cartesian coordinate systems,

$$a^{i}_{k} B^{k} = a^{i}_{k} \left(K^{k}_{l} A^{l}\right). \tag{2.129}$$

Now, transforming $\mathbf{A}$ back into the primed coordinate system[18] [compare Eq. (2.96)], we have

$$K'^{i}_{j} A'^{j} = a^{i}_{k} K^{k}_{l} a^{l}_{j} A'^{j}. \tag{2.130}$$

Rearranging, we obtain

$$\left(K'^{i}_{j} - a^{i}_{k} a^{l}_{j} K^{k}_{l}\right) A'^{j} = 0. \tag{2.131}$$

This must hold for each value of the index i and for every primed coordinate system. Since the A'^{j} is arbitrary,[19] we conclude

$$K'^{i}_{j} = a^{i}_{k} a^{l}_{j} K^{k}_{l}, \tag{2.132}$$

which is our definition of a mixed second-rank tensor.

The other equations may be treated similarly, giving rise to other forms of the quotient rule. One minor pitfall should be noted: The quotient rule does not necessarily apply if B is zero. The transformation properties of zero are indeterminate.

EXAMPLE 2.8.1

Equations of Motion and Field Equations In classical mechanics, Newton's equations of motion $m\dot{\mathbf{v}} = \mathbf{F}$ indicate, on the basis of the quotient rule, that if the mass is a scalar and the force a vector, then the acceleration $\mathbf{a} \equiv \dot{\mathbf{v}}$ is a vector. In other words, the vector character of the force as the driving term imposes its vector character on the acceleration provided the scale factor m is scalar.

---

[18] Note the order of the indices of the a^{j}_{l} in this **inverse** transformation. We have

$$A^{l} = \sum_{j} \frac{\partial x_l}{\partial x'_j} A'^{j} = \sum_{j} a^{l}_{j} A'^{j}.$$

[19] We might, for instance, take $A'^{1} = 1$ and $A'^{m} = 0$ for $m \neq 1$. Then the equation $K'^{i}_{1} = a^{i}_{k} a^{l}_{1} K^{k}_{l}$ follows immediately. The rest of Eq. (2.132) derives from other special choices of the arbitrary A'^{j}.

The wave equation of electrodynamics $\partial^2 A^\mu = J^\mu$ involves the Lorentz scalar four-dimensional version of the Laplacian $\partial^2 = \frac{\partial^2}{c^2 \partial t^2} - \nabla^2$ and the external four-vector current J^μ as its driving term. From the quotient rule, we infer that the vector potential A^μ is a four-vector as well. If the driving current is a four-vector, the vector potential must be of rank one by the quotient rule. ■

SUMMARY The quotient rule is a substitute for the illegal division of tensors.

EXERCISES

2.8.1 The double summation $K^{ij} A_i B_j$ is invariant for any two vectors A_i and B_j. Prove that K^{ij} is a second-rank tensor.

2.8.2 The equation $K^{ij} A_{jk} = B^i_k$ holds for all orientations of the coordinate system. If **A** and **B** are second-rank tensors, show that **K** is also a second-rank tensor.

2.8.3 The exponential in a plane wave is $\exp[i(\mathbf{k} \cdot \mathbf{r} - \omega t)]$. We recognize $x^\mu = (ct, x_1, x_2, x_3)$ as a prototype vector in Minkowski space. If $\mathbf{k} \cdot \mathbf{r} - \omega t$ is a scalar under Lorentz transformations (Chapter 4), show that $k^\mu = (\omega/c, k_1, k_2, k_3)$ is a four-vector in Minkowski space.
Note. Multiplication by $\hbar$ yields $(E/c, \mathbf{p})$ as a four-vector momentum in Minkowski space.

2.9 Dual Tensors

Levi–Civita Symbol

For future use, it is convenient to introduce the three-dimensional Levi–Civita symbol ε_{ijk} defined by

$$\begin{aligned} \varepsilon_{123} = \varepsilon_{231} = \varepsilon_{312} &= 1, \\ \varepsilon_{132} = \varepsilon_{213} = \varepsilon_{321} &= -1, \\ \text{all other } \varepsilon_{ijk} &= 0 \end{aligned} \tag{2.133}$$

in three-dimensional Cartesian space (where we do not have to distinguish between upper and lower indices). Note that ε_{ijk} is antisymmetric with respect to all pairs of indices. Suppose now that we have a third-rank tensor δ_{ijk}, which in one particular coordinate system is equal to ε_{ijk}. Then we can show that

$$\delta'_{ijk} = \det(a) a_{ip} a_{jq} a_{kr} \varepsilon_{pqr}, \tag{2.134}$$

where $\det(a)$ is the determinant (or volume; see Chapter 1) of the coordinate rotation. Recall that this determinant factor already occurred in the transformation law of the cross product in Section 2.6. A tensor transforming according to Eq. (2.134) is called a **pseudotensor** to distinguish it from tensors whose

transformation laws do not contain $\det(a)$. For a rotation of the coordinates $\det(a) = 1$, but if an axis is inverted or reflected, $x \to -x$, $\det(a) = -1$. Now,

$$a_{1p}a_{2q}a_{3r}\varepsilon_{pqr} = \det(a) \tag{2.135}$$

by direct expansion of the determinant, showing that $\delta'_{123} = \det(a)^2 = 1 = \varepsilon_{123}$. Considering the other possibilities, we find

$$\delta'_{ijk} = \varepsilon_{ijk} \tag{2.136}$$

for rotations and reflections. Hence, ε_{ijk} is a pseudotensor.[20,21] Furthermore, it is an isotropic pseudotensor with the same components in all rotated Cartesian coordinate systems.

Dual Tensors

With any **antisymmetric** second-rank tensor $\mathbf{C}$ (in three-dimensional space) we may associate a dual pseudovector C_i defined by

$$C_i = \frac{1}{2}\varepsilon_{ijk}C_{jk}. \tag{2.137}$$

Here, the antisymmetric $\mathbf{C}$ may be written as a 3×3 square array:

$$\mathbf{C} = \begin{pmatrix} C_{11} & C_{12} & C_{13} \\ C_{21} & C_{22} & C_{23} \\ C_{31} & C_{32} & C_{33} \end{pmatrix} = \begin{pmatrix} 0 & C_{12} & -C_{31} \\ -C_{12} & 0 & C_{23} \\ C_{31} & -C_{23} & 0 \end{pmatrix}. \tag{2.138}$$

We know that C_i must transform as a vector under rotations from the double contraction of the fifth-rank (pseudo) tensor $\varepsilon_{ijk}C_{mn}$, but it is really a pseudovector because of the pseudo nature of ε_{ijk}. Specifically, the components of $\mathbf{C}$ are given by

$$(C_1, C_2, C_3) = (C_{23}, C_{31}, C_{12}). \tag{2.139}$$

Notice the cyclic order of the indices that derives from the cyclic order of the components of ε_{ijk}. This duality, given by Eq. (2.139), means that our three-dimensional vector product may be taken to be either a pseudovector or an antisymmetric second-rank tensor, depending on how we choose to write it out.

If we take three (polar) vectors $\mathbf{A}$, $\mathbf{B}$, and $\mathbf{C}$, we may define the direct product

$$V_{ijk} = A_iB_jC_k. \tag{2.140}$$

[20]The usefulness of ε_{ijk} extends far beyond this section. For instance, the matrices M_k of Exercise 3.2.11 are derived from $(\mathsf{M}_k)_{ij} = -i\varepsilon_{ijk}$. Much of elementary vector analysis can be written in a very compact form by using ε_{ijk} and the identity of Exercise 2.9.4. See A. A. Evett, Permutation symbol approach to elementary vector analysis. *Am. J. Phys.* **34**, 503 (1966).

[21]The numerical value of ε_{ijk} is given by the triple scalar product of coordinate unit vectors:

$$\hat{\mathbf{q}}_i \cdot \hat{\mathbf{q}}_j \times \hat{\mathbf{q}}_k.$$

From this standpoint, each element of ε_{ijk} is a pseudoscalar, but the ε_{ijk} collectively form a third-rank pseudotensor.

By an extension of the analysis of Section 2.6, V_{ijk} is a tensor of third rank. The dual quantity is

$$V = \frac{1}{3!}\varepsilon_{ijk}V_{ijk}, \tag{2.141}$$

clearly a pseudoscalar. By expansion, it is seen that

$$V = \begin{vmatrix} A_1 & B_1 & C_1 \\ A_2 & B_2 & C_2 \\ A_3 & B_3 & C_3 \end{vmatrix} \tag{2.142}$$

is our familiar triple scalar product.

For use in writing Maxwell's equations in covariant form, we want to extend this dual vector analysis to four-dimensional Minkowski space and, in particular, to indicate that the four-dimensional volume element, $dx_0\,dx_1\,dx_2\,dx_3$, is a pseudoscalar.

We introduce the Levi–Civita symbol ε_{ijkl}, the four-dimensional analog of ε_{ijk}. This quantity ε_{ijkl} is defined as totally antisymmetric in all four indices, which run from 0 to 3. If $(ijkl)$ is an even permutation[22] of (0, 1, 2, 3), then ε_{ijkl} is defined as $+1$; if it is an odd permutation, then ε_{ijkl} is -1; and it is defined as 0 if any two indices are equal. The Levi–Civita ε_{ijkl} may be proved to be a pseudotensor of rank 4 by analysis similar to that used for establishing the tensor nature of ε_{ijk}. Introducing the direct product of four vectors as fourth-rank tensor with components

$$H^{ijkl} = A^iB^jC^kD^l, \tag{2.143}$$

built from the four-vectors **A**, **B**, **C**, and **D**, we may define the dual quantity

$$H = \frac{1}{4!}\varepsilon_{ijkl}H^{ijkl}. \tag{2.144}$$

We actually have a quadruple contraction that reduces the rank to zero. From the pseudo nature of ε_{ijkl}, H is a pseudoscalar. Now we let **A**, **B**, **C**, and **D** be infinitesimal displacements along the four coordinate axes (Minkowski space),

$$\begin{aligned} \mathbf{A} &= (dx_0, 0, 0, 0) \\ \mathbf{B} &= (0, dx_1, 0, 0), \qquad \text{and so on,} \end{aligned} \tag{2.145}$$

and

$$H = dx_0\,dx_1\,dx_2\,dx_3. \tag{2.146}$$

The four-dimensional volume element is now identified as a pseudoscalar. This result could have been expected from the results of the special theory of relativity. The Lorentz–Fitzgerald contraction of $dx_1\,dx_2\,dx_3$ balances the time dilation of dx_0.

We slipped into this four-dimensional space as a simple mathematical extension of the three-dimensional space and, indeed, we could just as easily

[22] A permutation is odd if it involves an odd number of interchanges of adjacent indices, such as (0 1 2 3)→ (0 2 1 3). Even permutations arise from an even number of transpositions of adjacent indices. (Actually the word "adjacent" is not necessary.) $\varepsilon_{0123} = +1$.

have discussed 5-, 6-, or N-dimensional space, where the Levi–Civita symbol is defined similarly. This is typical of the power of the component analysis. Physically, this four-dimensional space may be taken as Minkowski space,

$$(x_0, x_1, x_2, x_3) = (ct, x, y, z), \tag{2.147}$$

where t is time. This is the merger of space and time achieved in special relativity. The transformations of four-dimensional space are the Lorentz transformations of special relativity. We encounter these Lorentz transformations in Section 4.4.

SUMMARY

Contraction of the antisymmetric Levi-Civita tensor with another antisymmetric tensor or the direct product of vectors leads to their dual tensors. Determinants are pseudoscalar examples, and the cross product of two vectors is their dual, another well-known example.

EXERCISES

2.9.1 An antisymmetric square array is given by

$$\begin{pmatrix} 0 & C_3 & -C_2 \\ -C_3 & 0 & C_1 \\ C_2 & -C_1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & C_{12} & C_{13} \\ -C_{12} & 0 & C_{23} \\ -C_{13} & -C_{23} & 0 \end{pmatrix},$$

where (C_1, C_2, C_3) form a pseudovector. Assuming that the relation

$$C_i = \frac{1}{2!}\varepsilon_{ijk}C_{jk}$$

holds in all coordinate systems, prove that C_{jk} is a tensor. (This is another form of the quotient theorem.)

2.9.2 Show that the vector product is unique to three-dimensional space; that is, only in three dimensions can we establish a one-to-one correspondence between the components of an antisymmetric tensor (second-rank) and the components of a vector.

2.9.3 Show that

(a) $\delta_{ii} = 3$, (b) $\delta_{ij}\varepsilon_{ijk} = 0$, (c) $\varepsilon_{ipq}\varepsilon_{jpq} = 2\delta_{ij}$, (d) $\varepsilon_{ijk}\varepsilon_{ijk} = 6$.

2.9.4 Show that

$$\varepsilon_{ijk}\varepsilon_{pqk} = \delta_{ip}\delta_{jq} - \delta_{iq}\delta_{jp}.$$

2.9.5 (a) Express the components of a cross product vector $\mathbf{C}$, $\mathbf{C} = \mathbf{A} \times \mathbf{B}$, in terms of ε_{ijk} and the components of $\mathbf{A}$ and $\mathbf{B}$.

(b) Use the antisymmetry of ε_{ijk} to show that $\mathbf{A} \cdot \mathbf{A} \times \mathbf{B} = 0$.

ANS. (a) $C_i = \varepsilon_{ijk}A_jB_k$.

2.9.6 (a) Show that the inertia tensor (Section 3.5) may be written as

$$I_{ij} = m(x_n x_n \delta_{ij} - x_i x_j)$$

for a particle of mass m at (x_1, x_2, x_3). Here, $x_n x_n = \mathbf{r}^2$.

(b) Show that

$$I_{ij} = -M_{il}M_{lj} = -m\varepsilon_{ilk}x_k\varepsilon_{ljm}x_m,$$

where $M_{il} = m^{1/2}\varepsilon_{ilk}x_k$. This is the contraction of two second-rank tensors and is identical with the matrix product of Section 3.2.

2.9.7 Write $\nabla \cdot \nabla \times \mathbf{A}$ and $\nabla \times \nabla\varphi$ in ε_{ijk} notation so that it becomes obvious that each expression vanishes.

ANS. $$\nabla \cdot \nabla \times \mathbf{A} = \varepsilon_{ijk}\frac{\partial}{\partial x_i}\frac{\partial}{\partial x_j}A_k$$

$$(\nabla \times \nabla\varphi)_i = \varepsilon_{ijk}\frac{\partial}{\partial x_j}\frac{\partial}{\partial x_k}\varphi.$$

2.9.8 Expressing cross products in terms of Levi–Civita symbols (ε_{ijk}), derive the *BAC–CAB* rule [Eq. (1.52)].
Hint. The relation of Exercise 2.9.4 is helpful.

2.9.9 Verify that each of the following fourth-rank tensors is isotropic; that is, it has the same form independent of any rotation of the coordinate systems:
(a) $A_{ijkl} = \delta_{ij}\delta_{kl}$,
(b) $B_{ijkl} = \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}$,
(c) $C_{ijkl} = \delta_{ik}\delta_{jl} - \delta_{il}\delta_{jk}$.

2.9.10 Show that the two-index Levi–Civita symbol ε_{ij} is a second-rank pseudotensor (in two-dimensional space). Does this contradict the uniqueness of δ_{ij} (Exercise 2.6.5)?

2.9.11 (1) Given $A_k = \frac{1}{2}\varepsilon_{ijk}B_{ij}$ with $B_{ij} = -B_{ji}$, antisymmetric, show that

$$B_{mn} = \varepsilon_{mnk}A_k.$$

(2) Show that the vector identity

$$(\mathbf{A} \times \mathbf{B}) \cdot (\mathbf{C} \times \mathbf{D}) = (\mathbf{A} \cdot \mathbf{C})(\mathbf{B} \cdot \mathbf{D}) - (\mathbf{A} \cdot \mathbf{D})(\mathbf{B} \cdot \mathbf{C})$$

(Exercise 1.4.9) follows directly from the description of a cross product with ε_{ijk} and the identity of Exercise 2.9.4.

Additional Reading

Jeffreys, H. (1952). *Cartesian Tensors*. Cambridge Univ. Press, Cambridge. This is an excellent discussion of Cartesian tensors and their application to a wide variety of fields of classical physics.

Lawden, D. F. (1982). *An Introduction to Tensor Calculus, Relativity and Cosmology*, 3rd ed. Wiley, New York.

Margenau, H., and Murphy, G. M. (1956). *The Mathematics of Physics and Chemistry*, 2nd ed. Van Nostrand, Princeton, NJ. Chapter 5 covers curvilinear coordinates and 13 specific coordinate systems.

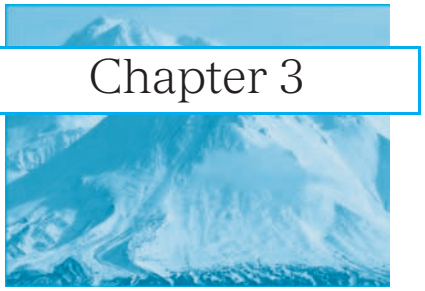
Morse, P. M., and Feshbach, H. (1953). *Methods of Theoretical Physics*. McGraw-Hill, New York. Chapter 5 includes a description of several

different coordinate systems. Note that Morse and Feshbach are not above using left-handed coordinate systems even for Cartesian coordinates. Elsewhere in this excellent (and difficult) book there are many examples of the use of the various coordinate systems in solving physical problems. Eleven additional fascinating but seldom encountered orthogonal coordinate systems are discussed in the second edition of *Mathematical Methods for Physicists* (1970).

Ohanian, H. C., and Ruffini, R. (1994). *Gravitation and Spacetime*, 2nd ed. Norton, New York. A well-written introduction to Riemannian geometry.

Sokolnikoff, I. S. (1964). *Tensor Analysis—Theory and Applications*, 2nd ed. Wiley, New York. Particularly useful for its extension of tensor analysis to non-Euclidean geometries.

Young, E. C. (1993). *Vector and Tensor Analysis*, 2nd ed. Dekker, New York.



Chapter 3

Determinants and Matrices

3.1 Determinants

We begin the study of matrices by solving linear equations, which will lead us to determinants and matrices. The concept of determinant and the notation were introduced by the renowned German mathematician, physicist, and philosopher G. W. von Leibniz and developed further by the German mathematician C. Jacobi. One of the major applications of determinants is in the establishment of conditions for the existence of nontrivial solutions for a set of linear equations. Matrices serve to write linear equations more compactly and also represent coordinate transformations such as rotations in Section 3.3 on orthogonal matrices and unitary matrices as their complex analogs in Section 3.4. Eigenvector–eigenvalue problems of symmetric matrices (Hermitian matrices for complex numbers) in Section 3.5 are of central importance in geometry, physics, engineering, and astronomy.

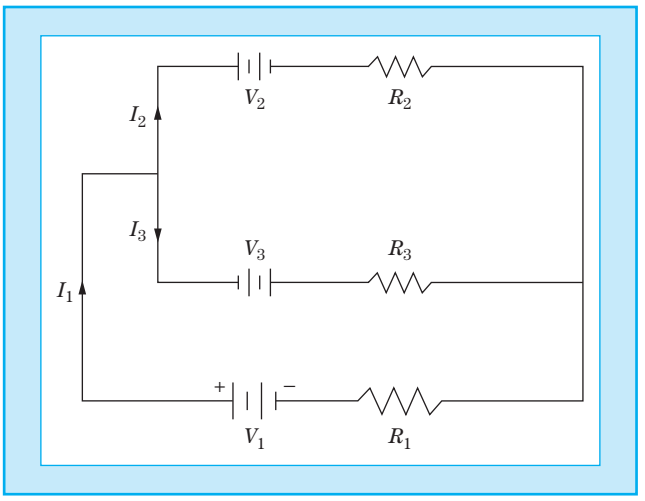
Linear Equations: Examples

Electrical circuits typically lead one to sets of linear equations. When a battery supplies a DC voltage V across a resistance R, the current I flowing is related to the voltage by Ohm's law $V = RI$. (At this stage, we do not include a capacitance or an inductance with AC voltage because they would lead us to complex numbers.) More complicated circuitry involves **Kirchhoff's law**, which stipulates that at a junction the sum of all incoming currents equals that of all outflowing currents. The sum of potential drops around a loop is equal to the input voltage. Let us illustrate a case.

EXAMPLE 3.1.1 **Battery-Powered Circuit** The circuit shown in Fig. 3.1 contains two loops: one involving the voltage V_1 and V_3 reinforcing each other and one involving

Figure 3.1

Battery-Powered Circuit



V_1 and V_2 in opposite directions. Using the lower loop with currents I_1, I_3 we set up the linear equations

$$R_1 I_1 + R_3 I_3 = V_1 + V_3, \quad I_1 = I_2 + I_3.$$

The upper loop with currents I_1, I_2 sets up the second set of linear equations

$$R_1 I_1 + R_2 I_2 = V_1 - V_2, \quad I_3 = I_1 - I_2,$$

where I_j are unknown. For $R_1 = 4$ ohm, $R_2 = 3$ ohm, $R_3 = 2$ ohm and $V_1 = 1$ V, $V_2 = 2$ V, $V_3 = 3$ V, we have to solve

$$4I_1 + 3I_2 = 1 - 2 = -1, \quad 4I_1 + 2I_3 = 1 + 3 = 4, \quad I_3 = I_1 - I_2$$

for I_1, I_2, I_3. Upon substituting $I_3 = I_1 - I_2$ we find the linear equations

$$4I_1 + 3I_2 = -1, \quad 3I_1 - I_2 = 2.$$

Multiplying the second equation by 3 and adding it to the first eliminates I_2 so that $I_1 = \frac{5}{13}$ A results. The second equation yields $I_2 = -2 + 3I_1 = \frac{15-26}{13} = -\frac{11}{13}$ A and finally $I_3 = I_1 - I_2 = \frac{5-(-11)}{13} = \frac{16}{13}$ A. Given the large resistance R_1 and small voltage V_1, it is reasonable that I_1 is the smallest current and I_3 the biggest because the resistance R_3 is the smallest and the driving voltage V_3 is the highest. ■

Homogeneous Linear Equations

We start with homogeneous equations, where no terms independent of the unknown x_i occur. Determinants give a condition when homogeneous algebraic equations have nontrivial solutions. Suppose we have three unknowns

x_1, x_2, x_3

$$\begin{aligned} a_1x_1 + a_2x_2 + a_3x_3 &= 0, \\ b_1x_1 + b_2x_2 + b_3x_3 &= 0, \\ c_1x_1 + c_2x_2 + c_3x_3 &= 0. \end{aligned} \tag{3.1}$$

The problem is to determine under what conditions there is any solution, apart from the trivial one $x_1 = 0, x_2 = 0, x_3 = 0$. If we use vector notation $\mathbf{x} = (x_1, x_2, x_3)$ for the solution and three rows $\mathbf{a} = (a_1, a_2, a_3)$, $\mathbf{b} = (b_1, b_2, b_3)$, $\mathbf{c} = (c_1, c_2, c_3)$ of coefficients, then the three equations of Eq. (3.1) become

$$\mathbf{a} \cdot \mathbf{x} = 0, \quad \mathbf{b} \cdot \mathbf{x} = 0, \quad \mathbf{c} \cdot \mathbf{x} = 0. \tag{3.2}$$

These three vector equations have the **geometrical** interpretation that $\mathbf{x}$ is orthogonal to $\mathbf{a}$, $\mathbf{b}$, and $\mathbf{c}$ or lies in the intersection of the planes through the origin that are orthogonal to $\mathbf{a}$, $\mathbf{b}$, and $\mathbf{c}$, respectively, because each homogeneous linear equation represents a plane through the origin. If the volume spanned by $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ given by the triple scalar product [see Eq. (1.49) of Section 1.4] or the determinant

$$D_3 = (\mathbf{a} \times \mathbf{b}) \cdot \mathbf{c} \equiv \det(\mathbf{a}, \mathbf{b}, \mathbf{c}) = \begin{vmatrix} a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \\ c_1 & c_2 & c_3 \end{vmatrix} \tag{3.3}$$

is not zero, then there is only the trivial solution $\mathbf{x} = 0$ because $\mathbf{x}$ cannot be perpendicular to all $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ unless $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ are not all independent. Conversely, if the previous triple scalar product or determinant of coefficients vanishes, then one of the row vectors is a linear combination of the other two. Let us assume that $\mathbf{c}$ lies in the plane spanned by $\mathbf{a}$ and $\mathbf{b}$, that is, the third equation Eq. (3.2) is a linear combination of the first two and not independent. Then $\mathbf{x}$ is orthogonal to $\mathbf{a}$ and $\mathbf{b}$ so that $\mathbf{x} \sim \mathbf{a} \times \mathbf{b}$. To get rid of the unknown proportionality constant we form ratios of the unknown x_i. Since homogeneous equations can be multiplied by arbitrary numbers, only ratios of the x_i are relevant, for which we then obtain ratios of the components of the cross product, or 2×2 determinants,

$$\begin{aligned} x_1/x_3 &= (a_2b_3 - a_3b_2)/(a_1b_2 - a_2b_1) \\ x_2/x_3 &= -(a_1b_3 - a_3b_1)/(a_1b_2 - a_2b_1) \end{aligned} \tag{3.4}$$

from the components of the cross product $\mathbf{a} \times \mathbf{b}$ provided $x_3 \sim a_1b_2 - a_2b_1 \neq 0$. If $x_3 = 0$ but $x_2 \neq 0$, we can similarly find the ratio x_1/x_2. That is, x_3 does not play a special role.

Inhomogeneous Linear Equations

The simplest case of two equations with two unknowns

$$a_1x_1 + a_2x_2 = a_3, \qquad b_1x_1 + b_2x_2 = b_3 \tag{3.5}$$

has the geometrical meaning of the solution as the intersection of two lines. This problem can be reduced to the previous homogeneous case by imbedding it in three-dimensional space with a solution vector $\mathbf{x} = (x_1, x_2, -1)$ and row vectors $\mathbf{a} = (a_1, a_2, a_3)$, $\mathbf{b} = (b_1, b_2, b_3)$. Note that -1 is the third component of $\mathbf{x}$ in order to account for the inhomogeneous constants a_3, b_3 in Eq. (3.5). As before, Eq. (3.5) in vector notation, $\mathbf{a} \cdot \mathbf{x} = 0$ and $\mathbf{b} \cdot \mathbf{x} = 0$, implies that $\mathbf{x} \sim \mathbf{a} \times \mathbf{b}$ so that the analog of Eq. (3.4) holds. For this to apply, though, the third component of $\mathbf{a} \times \mathbf{b}$ must not be zero (i.e., $a_1 b_2 - a_2 b_1 \neq 0$) because the third component of $\mathbf{x}$ is -1 and not zero. This yields the x_i as

$$x_1 = (a_3 b_2 - b_3 a_2)/(a_1 b_2 - a_2 b_1) = \begin{vmatrix} a_3 & a_2 \\ b_3 & b_2 \end{vmatrix} \Big/ \begin{vmatrix} a_1 & a_2 \\ b_1 & b_2 \end{vmatrix}, \tag{3.6a}$$

$$x_2 = (a_1 b_3 - a_3 b_1)/(a_1 b_2 - a_2 b_1) = \begin{vmatrix} a_1 & a_3 \\ b_1 & b_3 \end{vmatrix} \Big/ \begin{vmatrix} a_1 & a_2 \\ b_1 & b_2 \end{vmatrix}. \tag{3.6b}$$

This is **Cramer's rule** for two inhomogeneous linear equations with two unknowns x_1, x_2: The determinant $D_1(D_2)$ in the numerator of $x_1(x_2)$ is obtained from the determinant of the coefficients $D = \left|\begin{smallmatrix} a_1 & a_2 \\ b_2 & b_2 \end{smallmatrix}\right|$ in the denominator by replacing the first (second) column vector by the vector $\left(\begin{smallmatrix} a_3 \\ b_3 \end{smallmatrix}\right)$ of the inhomogeneous side of Eq. (3.5). Cramer's rule generalizes to $x_i = D_i/D$ for n inhomogeneous linear equations with n unknowns, $n = 2, 3, \ldots$, where D_i and D are the corresponding $n \times n$ determinants.

Biographical Data

Cramer, Gabriel. Cramer, a Swiss mathematician, was born in 1704 and died in 1752. His main contributions are in algebra and geometry. Cramer's rule was known to Leibniz already but was first published posthumously by Mclaurin in his *Treatise on Algebra* in 1748. Cramer's form of the rule appeared in his well-written book in French (1750) on algebraic curves, which became a standard reference so that he is often given credit for the rule.

EXAMPLE 3.1.2

Battery-Powered Circuit In order to apply this solution to Example 3.1.1, let us write the current equations as

$$R_1 I_1 + R_2 I_2 = V_1 - V_2, \quad R_1 I_1 + R_3 (I_1 - I_2) = (R_1 + R_3) I_1 - R_3 I_2 = V_1 + V_3$$

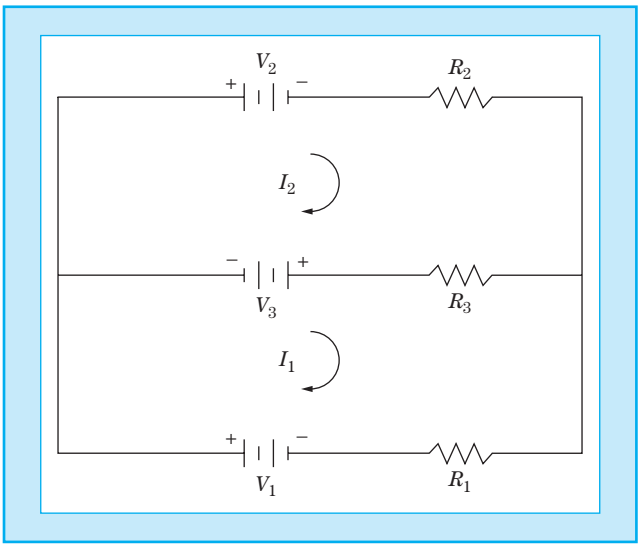
so that $a_3 = V_1 - V_2$, $b_3 = V_1 + V_3$, and the determinants are

$$D = \begin{vmatrix} R_1 & R_2 \\ R_1 + R_3 & -R_3 \end{vmatrix}, \quad D_1 = \begin{vmatrix} V_1 - V_2 & R_2 \\ V_1 + V_3 & -R_3 \end{vmatrix}, \quad D_2 = \begin{vmatrix} R_1 & V_1 - V_2 \\ R_1 + R_3 & V_1 + V_3 \end{vmatrix}.$$

If we plot Fig. 3.1 in the simpler form of Fig. 3.2, then the last equation can be read off the lower loop involving the current I_1. According to Cramer's rule

Figure 3.2

Battery-Powered Circuit



the general solution becomes

$$I_1 = \frac{D_1}{D} = \frac{(V_1 - V_2)(-R_3) - (V_1 + V_3)R_2}{R_1(-R_3) - R_2(R_1 + R_3)},$$

$$I_2 = \frac{D_2}{D} = -\frac{R_1(V_1 + V_3) - (V_1 - V_2)(R_1 + R_3)}{R_1R_3 + R_2(R_1 + R_3)}.$$

Plugging in the numbers we get (in amps)

$$I_1 = \frac{2 - 4 \cdot 3}{-4 \cdot 2 - 3 \cdot 6} = \frac{5}{13}, \qquad I_2 = -\frac{4 \cdot 4 + 6}{26} = -\frac{11}{13},$$

confirming our previous results. ■

These solutions in terms of ratios of determinants can be generalized to n dimensions. The $n \times n$ determinant is a number that is represented by a square array

$$D_n = \begin{vmatrix} a_1 & a_2 & \cdots & a_n \\ b_1 & b_2 & \cdots & b_n \\ c_1 & c_2 & \cdots & c_n \\ . & . & \cdots & . \end{vmatrix} \tag{3.7}$$

of numbers (or functions), the coefficients of n linear equations in our case. The number n of columns (and of rows) in the array is sometimes called the **order** of the determinant. The generalization of the expansion in Eq. (1.46) of the triple scalar product (of row vectors of three linear equations) leads to the

following value of the determinant D_n in n dimensions:

$$D_n = \sum_{i,j,k\cdots=1}^{n} \varepsilon_{ijk\cdots} a_i b_j c_k \cdots, \tag{3.8}$$

where $\varepsilon_{ijk\cdots}$, the Levi–Civita symbol introduced in Section 2.9, is $+1$ for even permutations[1] $(ijk\cdots)$ of $(123\cdots n)$, -1 for odd permutations, and zero if any index is repeated.

Specifically, for the third-order determinant D_3 of Eq. (3.3), Eq. (3.7) leads to

$$D_3 = +a_1b_2c_3 - a_1b_3c_2 - a_2b_1c_3 + a_2b_3c_1 + a_3b_1c_2 - a_3b_2c_1. \tag{3.9}$$

Several useful properties of the nth-order determinants follow from Eq. (3.8). Again, to be specific, Eq. (3.9) for third-order determinants is used to illustrate these properties.

Laplacian Development by Minors

Equation (3.9) may be written as follows:

$$\begin{aligned} D_3 &= a_1(b_2c_3 - b_3c_2) - a_2(b_1c_3 - b_3c_1) + a_3(b_1c_2 - b_2c_1) \\ &= a_1\begin{vmatrix} b_2 & b_3 \\ c_2 & c_3 \end{vmatrix} - a_2\begin{vmatrix} b_1 & b_3 \\ c_1 & c_3 \end{vmatrix} + a_3\begin{vmatrix} b_1 & b_2 \\ c_1 & c_2 \end{vmatrix}. \end{aligned} \tag{3.10}$$

The number of terms in the sum [Eq. (3.8)] is 24 for a fourth-order determinant and $n!$ for an nth-order determinant. Because of the appearance of the negative signs in Eq. (3.9) (and possibly in the individual elements as well), there may be considerable cancellation. It is quite possible that a determinant of large elements will have a very small value.

EXAMPLE 3.1.3 **Numerical Evaluation of a Hilbert Determinant** To illustrate this point, let us calculate the 3×3 Hilbert determinant expanding it according to Eq. (3.10) along the top row

$$\begin{aligned} \begin{vmatrix} 1 & 1/2 & 1/3 \\ 1/2 & 1/3 & 1/4 \\ 1/3 & 1/4 & 1/5 \end{vmatrix} &= \begin{vmatrix} 1/3 & 1/4 \\ 1/4 & 1/5 \end{vmatrix} - \frac{1}{2}\begin{vmatrix} 1/2 & 1/4 \\ 1/3 & 1/5 \end{vmatrix} + \frac{1}{3}\begin{vmatrix} 1/2 & 1/3 \\ 1/3 & 1/4 \end{vmatrix} \\ &= \left(\frac{1}{15} - \frac{1}{16}\right) - \frac{1}{2}\left(\frac{1}{10} - \frac{1}{12}\right) + \frac{1}{3}\left(\frac{1}{8} - \frac{1}{9}\right) \\ &= \frac{1}{15\cdot 16} - \frac{1}{10\cdot 12} + \frac{1}{3\cdot 8\cdot 9} = \frac{1}{2^4\cdot 3^3\cdot 5}. \end{aligned}$$

[1] In a linear sequence $abcd\cdots$, any single, simple transposition of adjacent elements yields an **odd** permutation of the original sequence: $abcd \to bacd$. Two such transpositions yield an even permutation. In general, an odd number of such interchanges of adjacent elements results in an odd permutation; an even number of such transpositions yields an even permutation.

Its value is rather small compared to any of its entries because of significant cancellations that are typical of Hilbert determinants. ■

In general, the nth-order determinant may be expanded as a linear combination of the products of the elements of any row (or any column) and the $(n-1)$-order determinants formed by striking out the row and column of the original determinant in which the element appears. This reduced array (2×2 in this example) is called a minor. If the element is in the ith row and jth column, the sign associated with the product is $(-1)^{i+j}$. The minor with this sign is called the cofactor. If M_{ij} is used to designate the minor formed by omitting the ith row and the jth column and C_{ij} is the corresponding cofactor, Eq. (3.10) becomes

$$D_3 = \sum_{j=1}^{3} (-1)^{1+j} a_j M_{1j} = \sum_{j=1}^{3} a_j C_{1j}. \tag{3.11}$$

In this case, expanding along the first row, we have $i = 1$ and the summation over j, the columns.

This Laplace expansion may be used to advantage in the evaluation of high-order determinants in which many of the elements are zero.

EXAMPLE 3.1.4 **Expansion across the Top Row** To find the value of the determinant

$$D = \begin{vmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{vmatrix}, \tag{3.12}$$

we expand across the top row to obtain (upon striking the first line and second column)

$$D = (-1)^{1+2} \cdot (1) \begin{vmatrix} -1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{vmatrix}. \tag{3.13}$$

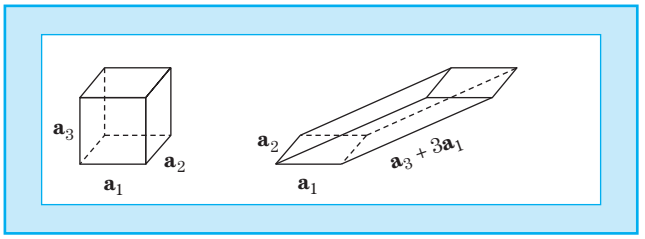
Again, expanding across the top row, we get (upon striking the first line and first column)

$$D = (-1) \cdot (-1)^{1+1} \cdot (-1) \begin{vmatrix} 0 & 1 \\ -1 & 0 \end{vmatrix} = \begin{vmatrix} 0 & 1 \\ -1 & 0 \end{vmatrix} = 1. \tag{3.14}$$

It is straightforward to check that we obtain the same result expanding any other row or column. ■

Figure 3.3

Shifting the Top Parallel to the Bottom Leaves Volume Unchanged



Antisymmetry

The determinant changes sign if any two rows are interchanged or if any two columns are interchanged. This follows from the even–odd character of the Levi–Civita ε in Eq. (3.8).[2]

This property was used in Section 2.9 to develop a totally antisymmetric linear combination (a third rank tensor from three vectors). It is also frequently used in quantum mechanics in the construction of a many particle wave function that, in accordance with the (Pauli) exclusion principle, will be antisymmetric under the interchange of any two identical spin $\frac{1}{2}$ particles (electrons, protons, neutrons, quarks, etc.). To summarize:

- As a special case of antisymmetry, any determinant with two rows equal or two columns equal equals zero.
- If each element in a row or each element in a column is zero, the determinant is equal to zero (seen by expanding across this row or column).
- If each element in a row or each element in a column is multiplied by a constant, the determinant is multiplied by that constant (scaling up the volume with one of its sides).
- The value of a determinant is unchanged if a multiple of one row is added (column by column) to another row or if a multiple of one column is added (row by row) to another column.[3]
- As a special case, a determinant is equal to zero if any two rows are proportional or any two columns are proportional.

EXAMPLE 3.1.5

Rules on Determinants To illustrate the next to last point, which derives from the linearity and additivity of determinants, $D(\mathbf{a}_1+k\mathbf{a}_1', \ldots) = D(\mathbf{a}_1, \ldots) + kD(\mathbf{a}_1', \ldots)$ in terms of their column (or row) vectors, we show that

$$\begin{vmatrix} a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \\ c_1 & c_2 & c_3 \end{vmatrix} = \begin{vmatrix} a_1 + ka_2 & a_2 & a_3 \\ b_1 + kb_2 & b_2 & b_3 \\ c_1 + kc_2 & c_2 & c_3 \end{vmatrix}. \tag{3.15}$$

[2]The sign reversal for the interchange of two adjacent rows (or columns) is an odd permutation. The interchange of **any** two rows is also an odd permutation.

[3]This derives from the geometric meaning of the determinant as the volume of the parallelepiped $(\mathbf{a}_1 \times \mathbf{a}_2) \cdot \mathbf{a}_3$ spanned by its column vectors. Pulling it to the side along the direction of $\mathbf{a}_1$ (i.e., replacing $\mathbf{a}_3 \to \mathbf{a}_3 + k\mathbf{a}_1$), without changing its height, leaves the volume unchanged, etc. This is illustrated in Fig. 3.3.

Using the Laplace development on the right-hand side, we obtain

$$\begin{vmatrix} a_1 + ka_2 & a_2 & a_3 \\ b_1 + kb_2 & b_2 & b_3 \\ c_1 + kc_2 & c_2 & c_3 \end{vmatrix} = \begin{vmatrix} a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \\ c_1 & c_2 & c_3 \end{vmatrix} + k \begin{vmatrix} a_2 & a_2 & a_3 \\ b_2 & b_2 & b_3 \\ c_2 & c_2 & c_3 \end{vmatrix}. \tag{3.16}$$

Then, by the property of antisymmetry, the second determinant on the right-hand side of Eq. (3.16) vanishes because two columns are identical, verifying Eq. (3.15).

Using these rules, let us evaluate the following determinant by subtracting twice the third column from the second and three times the third from the first column in order to create zeros in the first line:

$$\begin{vmatrix} 3 & 2 & 1 \\ 2 & 3 & 1 \\ 1 & 1 & 4 \end{vmatrix} = \begin{vmatrix} 3-3\cdot 1 & 2-2\cdot 1 & 1 \\ 2-3\cdot 1 & 3-2\cdot 1 & 1 \\ 1-3\cdot 4 & 1-2\cdot 4 & 4 \end{vmatrix} = \begin{vmatrix} 0 & 0 & 1 \\ -1 & 1 & 1 \\ -11 & -7 & 4 \end{vmatrix}$$

$$= \begin{vmatrix} -1 & 1 \\ -11 & -7 \end{vmatrix} = 7 + 11 = 18. \quad \blacksquare$$

Some useful relations involving determinants or matrices appear in Exercises of Sections 3.2 and 3.4.

EXAMPLE 3.1.6

Solving Linear Equations Returning to the homogeneous Eq. (3.1) and multiplying the determinant of the coefficients by x_1, then adding x_2 times the second column and x_3 times the third column to the first column, we can directly establish the condition for the presence of a nontrivial solution for Eq. (3.1):

$$x_1 \begin{vmatrix} a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \\ c_1 & c_2 & c_3 \end{vmatrix} = \begin{vmatrix} a_1x_1 & a_2 & a_3 \\ b_1x_1 & b_2 & b_3 \\ c_1x_1 & c_2 & c_3 \end{vmatrix} = \begin{vmatrix} a_1x_1 + a_2x_2 + a_3x_3 & a_2 & a_3 \\ b_1x_1 + b_2x_2 + b_3x_3 & b_2 & b_3 \\ c_1x_1 + c_2x_2 + c_3x_3 & c_2 & c_3 \end{vmatrix} \tag{3.17}$$

$$= \begin{vmatrix} 0 & a_2 & a_3 \\ 0 & b_2 & b_3 \\ 0 & c_2 & c_3 \end{vmatrix} = 0.$$

Similar reasoning applies for x_2 and x_3. Therefore, x_1, x_2, and x_3 must all be zero **unless the determinant of the coefficients vanishes**. Conversely [see text following Eq. (3.3)], we can show that if the determinant of the coefficients vanishes, a nontrivial solution does indeed exist.

If our linear equations are **inhomogeneous**—that is, as in Eq. (3.5) if the zeros on the right-hand side of Eq. (3.1) are replaced by a_4, b_4, and c_4, respectively—then from Eq. (3.17) we obtain, instead,

$$x_1 = \begin{vmatrix} a_4 & a_2 & a_3 \\ b_4 & b_2 & b_3 \\ c_4 & c_2 & c_3 \end{vmatrix} \Big/ \begin{vmatrix} a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \\ c_1 & c_2 & c_3 \end{vmatrix}, \tag{3.18}$$

which generalizes Eq. (3.6a) to $n = 3$ dimensions, etc. This is **Cramer's rule** generalized to three dimensions, and it can be shown to hold in n dimensions for any positive integer n. If the determinant of the coefficients vanishes, the inhomogeneous set of equations has no solution, unless the numerators also vanish. In this case solutions may exist, but they are not unique (see Exercise 3.1.3 for a specific example). ■

For numerical work, the determinant solution of Eq. (3.18) is exceedingly unwieldy. The determinant may involve large numbers with alternate signs, and in the subtraction of two large numbers the relative error may soar to a point that makes the result worthless. Also, although the determinant method is illustrated here with 3 equations and 3 unknowns, we might easily have 200 equations with 200 unknowns, which, involving up to 200! terms in each determinant, pose a challenge even to high-speed electronic computers. There must be a better way.

In fact, there are better ways. One of the best is a straightforward process often called Gauss elimination. To illustrate this technique, consider the following set of linear equations:

EXAMPLE 3.1.7 **Gauss Elimination** Solve

$$\begin{aligned} 3x + 2y + z &= 11 \\ 2x + 3y + z &= 13 \\ x + y + 4z &= 12. \end{aligned} \tag{3.19}$$

The determinant of the inhomogeneous linear equations [Eq. (3.19)] is obtained as 18 by subtracting twice the third column from the second and three times the third from the first column (see Example 3.1.5):

$$\begin{vmatrix} 3 & 2 & 1 \\ 2 & 3 & 1 \\ 1 & 1 & 4 \end{vmatrix} = \begin{vmatrix} 0 & 0 & 1 \\ -1 & 1 & 1 \\ -11 & -7 & 0 \end{vmatrix} = \begin{vmatrix} -1 & 1 \\ -11 & -7 \end{vmatrix} = 7 + 11 = 18,$$

so that a solution exists.

For convenience and for the optimum numerical accuracy, the equations are rearranged so that the largest coefficients run along the main diagonal (upper left to lower right). This has already been done in Eq. (3.19).

In the Gauss technique, the first equation is used to eliminate the first unknown, x, from the remaining equations. Then the (new) second equation is used to eliminate y from the last equation. In general, we work down through the set of equations; then, with one unknown determined, we work back up to solve for each of the other unknowns in succession.

Dividing each row by its initial coefficient, we see that Eqs. (3.19) become

$$\begin{aligned} x + \frac{2}{3}y + \frac{1}{3}z &= \frac{11}{3} \\ x + \frac{3}{2}y + \frac{1}{2}z &= \frac{13}{2} \\ x + y + 4z &= 12. \end{aligned} \tag{3.20}$$

Now, subtracting the first equation, we eliminate x from the second and third:

$$\begin{aligned} x + \frac{2}{3}y + \frac{1}{3}z &= \frac{11}{3} \\ \frac{5}{6}y + \frac{1}{6}z &= \frac{17}{6} \\ \frac{1}{3}y + \frac{11}{3}z &= \frac{25}{3} \end{aligned} \tag{3.21}$$

and then normalize the y-coefficients to 1 again:

$$\begin{aligned} x + \frac{2}{3}y + \frac{1}{3}z &= \frac{11}{3} \\ y + \frac{1}{5}z &= \frac{17}{5} \\ y + 11z &= 25. \end{aligned} \tag{3.22}$$

Repeating the technique, we use the new second equation to eliminate y from the third equation:

$$\begin{aligned} x + \frac{2}{3}y + \frac{1}{3}z &= \frac{11}{3} \\ y + \frac{1}{5}z &= \frac{17}{5} \\ 54z &= 108, \end{aligned} \tag{3.23}$$

or

$$z = 2.$$

Finally, working back up, we get

$$y + \frac{1}{5} \times 2 = \frac{17}{5},$$

or

$$y = 3.$$

Then with z and y determined,

$$x + \frac{2}{3} \times 3 + \frac{1}{3} \times 2 = \frac{11}{3}$$

and

$$x = 1.$$

The technique may not seem as elegant as Eq. (3.18), but it is well adapted to computers and is far faster than using determinants.

This Gauss technique is used to convert a determinant into **triangular** form:

$$D = \begin{vmatrix} \alpha_1 & \beta_1 & \gamma_1 \\ 0 & \beta_2 & \gamma_2 \\ 0 & 0 & \gamma_3 \end{vmatrix} \tag{3.24}$$

for a third-order determinant. In this form $D = \alpha_1\beta_2\gamma_3$. For an nth-order determinant the evaluation of the triangular form requires only $n-1$ multiplications compared with the $n!$ terms required for the general case.

A variation of this progressive elimination is known as Gauss–Jordan elimination. We start as with the preceding Gauss elimination, but each new equation considered is used to eliminate a variable from **all** the other equations, not just those below it. If we had used this Gauss–Jordan elimination, Eq. (3.23) would become

$$\begin{aligned} x + \frac{1}{5}z &= \frac{7}{5} \\ y + \frac{1}{5}z &= \frac{17}{5} \\ z &= 2, \end{aligned} \tag{3.25}$$

using the second equation of Eq. (3.22) to eliminate y from both the first and third equations. Then the third equation of Eq. (3.23) is used to eliminate z from the first and second, giving

$$\begin{aligned} x &= 1 \\ y &= 3 \\ z &= 2. \end{aligned} \tag{3.26}$$

Let us compare the Gauss method with Cramer's rule, where we have to evaluate the determinants

$$D = \begin{vmatrix} 3 & 2 & 1 \\ 2 & 3 & 1 \\ 1 & 1 & 4 \end{vmatrix} = 18$$

from above, then D_1 with the inhomogeneous column vector replacing the first column of D,

$$D_1 = \begin{vmatrix} 11 & 2 & 1 \\ 13 & 3 & 1 \\ 12 & 1 & 4 \end{vmatrix} = \begin{vmatrix} 11 & 2 & 1 \\ 2 & 1 & 0 \\ 12 & 1 & 4 \end{vmatrix} = \begin{vmatrix} 2 & 1 \\ 12 & 1 \end{vmatrix} + 4 \begin{vmatrix} 11 & 2 \\ 2 & 1 \end{vmatrix}$$
$$= (2 - 12) + 4(11 - 4) = 18,$$

where we subtract the first from the second row and then expand the determinant along the last column. Hence, from Cramer's rule, $x = D_1/D = 1$.

Next, proceeding with D_2 the same way, we obtain

$$D_2 = \begin{vmatrix} 3 & 11 & 1 \\ 2 & 13 & 1 \\ 1 & 12 & 4 \end{vmatrix} = \begin{vmatrix} 3 & 11 & 1 \\ -1 & 2 & 0 \\ 1 & 12 & 4 \end{vmatrix} = \begin{vmatrix} -1 & 2 \\ 1 & 12 \end{vmatrix} + 4 \begin{vmatrix} 3 & 11 \\ -1 & 2 \end{vmatrix}$$
$$= (-12 - 2) + 4(6 + 11) = 54$$

so that $y = D_2/D = 54/18 = 3$. Finally,

$$D_3 = \begin{vmatrix} 3 & 2 & 11 \\ 2 & 3 & 13 \\ 1 & 1 & 12 \end{vmatrix} = \begin{vmatrix} 3 & -1 & 11 \\ 2 & 1 & 13 \\ 1 & 0 & 12 \end{vmatrix} = \begin{vmatrix} -1 & 11 \\ 1 & 13 \end{vmatrix} + 12 \begin{vmatrix} 3 & -1 \\ 2 & 1 \end{vmatrix}$$
$$= (-13 - 11) + 12(3 + 2) = 36,$$

where we subtract the first from the second row and expand D_3 along the last line so that $z = D_3/D = 36/18 = 2$. ■

We return to the Gauss–Jordan technique in Section 3.2 on inverting matrices. Another technique suitable for computer use is the Gauss–Seidel iteration technique. Each technique has advantages and disadvantages. The Gauss and Gauss–Jordan methods may have accuracy problems for large determinants. This is also a problem for matrix inversion (Section 3.2). The Gauss–Seidel method, as an iterative method, may have convergence problems. The Gauss–Seidel iterative method and the Gauss and Gauss–Jordan elimination methods are discussed in considerable detail by Ralston and Wilf and also by Pennington.[4] Computer codes in FORTRAN and other programming languages and extensive literature on the Gauss–Jordan elimination and others are also given by Press *et al.*[5] Symbolic mathematical manipulation computer software, such as Mathematica, Maple, Reduce, Matlab, and Mathcad, include matrix diagonalization and inversion programs.

[4]Ralston, A., and Wilf, H. (Eds.) (1960). *Mathematical Methods for Digital Computers*. Wiley, New York; Pennington, R. H. (1970). *Introductory Computer Methods and Numerical Analysis*. Macmillan, New York.

[5]Press, W. H., Flannery, B. P., Teukolsky, S. A., and Vetterling, W. T. (1992). *Numerical Recipes*, 2nd ed., Chapter 2. Cambridge Univ. Press, Cambridge, UK.

SUMMARY

Linear equations are formally solved by ratios of determinants, that is, Cramer's rule. However, a systematic elimination of variables leads to a solution much more efficiently, and computer codes are based on this Gauss method.

Biographical Data

Leibniz, Gottfried Wilhelm von. Leibniz, a German mathematician, philosopher, and physicist, was born in Leipzig, Saxony (now Germany) in 1646 and died in Hannover in 1716. Son of a professor of philosophy, he was a child prodigy whose universal talents remained at the genius level throughout his life. He is thought by many to have been the last person knowledgeable in all fields of human scholarship. He taught himself Latin at age 8, Greek at age 14, and obtained a law degree in 1665. He studied mathematics and physics with the Dutch physicist C. Huygens. In 1667, he started a logical symbolism that was a precursor of Boolean logics. In 1671, he devised a calculating machine superior to that of the French mathematician Blaise Pascal. When he visited the English physicist Boyle in London in 1673, he was promptly elected a member of the Royal Society. In 1684, he published his version of differential and integral calculus, which eventually drew him into a nasty priority fight with Newton, each all but accusing the other of plagiarism (which from Leibniz's superior notations and approach and Newton's famous applications to gravity was practically ruled out). In 1693, he recognized the conservation law of mechanical energy. Using variational techniques in philosophy, he tried to prove that "ours is the best of all possible worlds," for which he was satirized by the French rationalist Voltaire. Determinants are one of his minor achievements. In 1714, the Duke of Hannover became King George I of England but left Leibniz there to die neglected and forgotten: Like Newton, he had never married and had no family.

EXERCISES

3.1.1 Find the currents of the circuits in Fig. 3.4.

3.1.2 Test the set of linear homogeneous equations

$$x + 3y + 3z = 0, \qquad x - y + z = 0, \qquad 2x + y + 3z = 0$$

to see if it possesses a nontrivial solution and find one.

3.1.3 Given the pair of equations

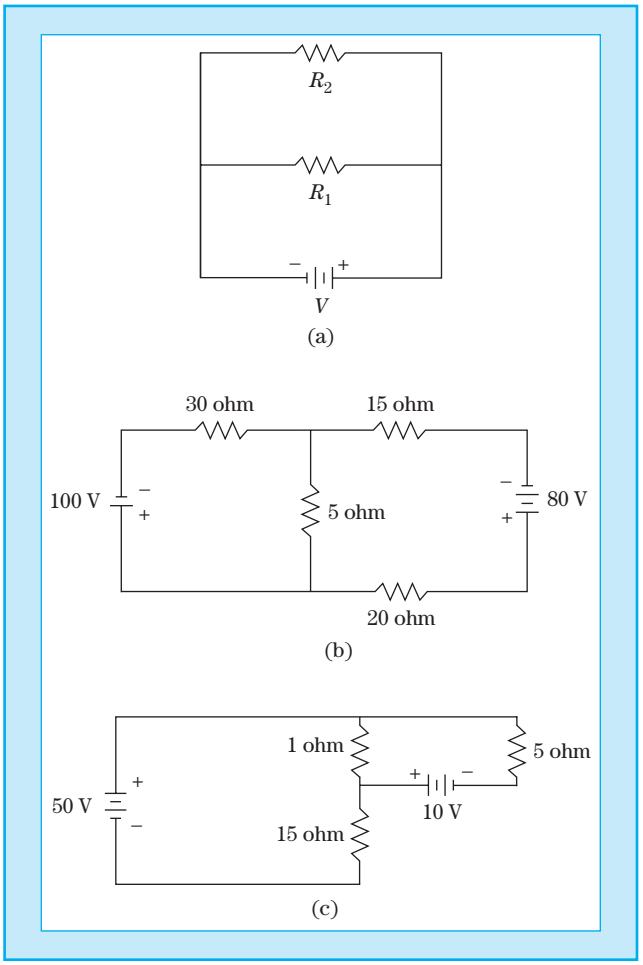
$$x + 2y = 3, \qquad 2x + 4y = 6,$$

(a) show that the determinant of the coefficients vanishes;
(b) show that the numerator determinants [Eq. (3.6)] also vanish;
(c) find at least two solutions.

3.1.4 Express the **components** of $\mathbf{A} \times \mathbf{B}$ as 2×2 determinants. Then show that the dot product $\mathbf{A} \cdot (\mathbf{A} \times \mathbf{B})$ yields a Laplacian expansion of a 3×3

Figure 3.4

Electric Circuits (a), (b), (c)



determinant. Finally, note that two rows of the 3×3 determinant are identical and hence $\mathbf{A} \cdot (\mathbf{A} \times \mathbf{B}) = 0$.

3.1.5 If C_{ij} is the cofactor of element a_{ij} [formed by striking out the ith row and jth column and including a sign $(-1)^{i+j}$], show that

(a) $\sum_i a_{ij}C_{ij} = \sum_i a_{ji}C_{ji} = \det(A)$, where $\det(A)$ is the determinant with the elements a_{ij},

(b) $\sum_i a_{ij}C_{ik} = \sum_i a_{ji}C_{ki} = 0$, $j \neq k$.

3.1.6 A determinant with all elements of order unity may be surprisingly small. The Hilbert determinant $H_{ij} = (i + j - 1)^{-1}$, $i, j = 1, 2, \ldots, n$ is notorious for its small values.

(a) Calculate the value of the Hilbert determinants of order n for $n = 1, 2,$ and 4. See Example 3.1.3 for the case $n = 3$.

(b) Find the Hilbert determinants of order n for $n = 5$ and 6.

ANS.

n	$\text{Det}(H_n)$
1	1
2	8.33333×10^{-2}
3	4.62963×10^{-4}
4	1.65344×10^{-7}
5	3.74930×10^{-12}
6	5.36730×10^{-18}

3.1.7 Solve the following set of linear simultaneous equations. Give the results to five decimal places or as rational numbers and check the solution using symbolic software (if available):

$$\begin{aligned}
1.0x_1 + 0.9x_2 + 0.8x_3 + 0.4x_4 + 0.1x_5 &= 1.0\\
0.9x_1 + 1.0x_2 + 0.8x_3 + 0.5x_4 + 0.2x_5 + 0.1x_6 &= 0.9\\
0.8x_1 + 0.8x_2 + 1.0x_3 + 0.7x_4 + 0.4x_5 + 0.2x_6 &= 0.8\\
0.4x_1 + 0.5x_2 + 0.7x_3 + 1.0x_4 + 0.6x_5 + 0.3x_6 &= 0.7\\
0.1x_1 + 0.2x_2 + 0.4x_3 + 0.6x_4 + 1.0x_5 + 0.5x_6 &= 0.6\\
0.1x_2 + 0.2x_3 + 0.3x_4 + 0.5x_5 + 1.0x_6 &= 0.5.
\end{aligned}$$

3.2 Matrices

We can write the linear Eqs. (3.1), (3.5), and (3.19), more elegantly and compactly by collecting the coefficients in a 3×3 square array of numbers called a **matrix**:

$$\mathsf{A} = \begin{pmatrix} a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \\ c_1 & c_2 & c_3 \end{pmatrix} \tag{3.27}$$

so that

$$\mathsf{A} = \begin{pmatrix} 3 & 2 & 1 \\ 2 & 3 & 1 \\ 1 & 1 & 4 \end{pmatrix} \tag{3.28}$$

for the inhomogeneous Eqs. (3.19). This concept will be useful if we define appropriate ways of dealing with these arrays of numbers. Note that a matrix does not have a numerical value like a determinant. The entries, or individual matrix elements, need not be numbers; they can also be functions.

Basic Definitions, Equality, and Rank

A matrix is defined as a square or rectangular array of numbers that obeys certain laws. This is a perfectly logical extension of familiar mathematical concepts. In arithmetic, we deal with single numbers. In the theory of complex

variables (Chapter 6), we deal with ordered pairs of numbers as $(1, 2) = 1+2i$, called complex numbers, in which the ordering is important. We now consider numbers (or functions) ordered in a square or rectangular array. For convenience in later work the entry numbers, or matrix elements, are distinguished by two subscripts, the first indicating the row (horizontal) and the second indicating the column (vertical) in which the number appears. For instance, a_{13} is the matrix element in the first row, third column. Hence, if A is a matrix with m rows and n columns, that is, an $m \times n$ array,

$$\mathsf{A} = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \cdots & & \cdots & \cdot \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{pmatrix}. \tag{3.29}$$

Perhaps the most important fact is that the elements a_{ij} are not combined with one another. A matrix is not a determinant. It is an ordered array of numbers, not a single number. For a $n \times n$ matrix, n is its **order**.

The matrix A, so far just an array of numbers, has the properties we assign to it. Literally, this means constructing a new form of mathematics. We postulate that matrices A, B, and C, with elements a_{ij}, b_{ij}, and c_{ij}, respectively, combine according to the following rules.

Two **matrices** $\mathsf{A} = \mathsf{B}$ **are defined to be equal** if and only if $a_{ij} = b_{ij}$ for **all** values of i and j. This, of course, requires that A and B each be m by n (or $m \times n$) arrays (m rows, n columns).

Looking back at the homogeneous linear Eq. (3.1), we note that the matrix of coefficients, A, is made up of three row vectors that each represent one linear equation of the set. If their triple scalar product is not zero, they span a nonzero volume, are linearly independent, and the homogeneous linear equations have only the trivial solution. In this case, the matrix is said to have **rank** 3. In n dimensions the volume represented by the triple scalar product becomes the determinant, det(A), for a square matrix. If $\det(\mathsf{A}) \neq 0$, the $n \times n$ matrix A has **rank** n. The case of Eq. (3.1), where the vector **c** lies in the plane spanned by **a** and **b**, corresponds to rank 2 of the matrix of coefficients because only two of its row vectors (**a**, **b** corresponding to two equations) are independent. In general, the **rank** m **of a matrix is the maximal number of linearly independent row vectors** it has; with $0 \leq m \leq n$.

Matrix Multiplication, Inner Product

We now write linear equations in terms of matrices because their coefficients represent an array of numbers that we just defined as a matrix, and the column vector of unknown x_i we recognize as a 3×1 matrix consisting of three rows and one column. In terms of matrices, the homogeneous linear equations take the form

$$\begin{pmatrix} a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \\ c_1 & c_2 & c_3 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} \equiv \begin{pmatrix} a_1x_1 + a_2x_2 + a_3x_3 \\ b_1x_1 + b_2x_2 + b_3x_3 \\ c_1x_1 + c_2x_2 + c_3x_3 \end{pmatrix} = 0, \tag{3.30}$$

which is a 3×3 matrix A multiplied by a single column vector $\mathbf{x}$, by forming scalar products of the row vectors of the matrix with the column vector of the unknown x_i. The inhomogeneous Eqs. (3.19) can be written similarly

$$\begin{pmatrix} 3 & 2 & 1 \\ 2 & 3 & 1 \\ 1 & 1 & 4 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} \equiv \begin{pmatrix} 3x_1 + 2x_2 + x_3 \\ 2x_1 + 3x_2 + x_3 \\ x_1 + x_2 + 4x_3 \end{pmatrix} = \begin{pmatrix} 11 \\ 13 \\ 12 \end{pmatrix}, \tag{3.31}$$

and Eq. (3.5) can be formulated as

$$\begin{pmatrix} a_1 & a_2 \\ b_1 & b_2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \equiv \begin{pmatrix} a_1 x_1 + a_2 x_2 \\ b_1 x_1 + b_2 x_2 \end{pmatrix} = \begin{pmatrix} a_3 \\ b_3 \end{pmatrix}, \tag{3.32}$$

where we label the array of coefficients a 2×2 matrix A consisting of two rows and two columns and consider the vector x as a 2×1 matrix.

We take **the summation of products in Eq. (3.30) as a definition of matrix multiplication involving the scalar product of each row vector of** A **with the column vector** $\mathbf{x}$. Thus, in matrix notation Eq. (3.30) becomes

$$\mathbf{x}' = \mathsf{A}\mathbf{x}. \tag{3.33}$$

Matrix analysis belongs to linear algebra because matrices may be used as linear operators or maps such as rotations. Suppose we rotate the Cartesian coordinates of a two-dimensional space as in Section 2.6 so that, in vector notation,

$$\begin{pmatrix} x_1' \\ x_2' \end{pmatrix} = \begin{pmatrix} x_1 \cos\varphi + x_2 \sin\varphi \\ -x_1 \sin\varphi + x_2 \cos\varphi \end{pmatrix} \equiv \begin{pmatrix} \cos\varphi & \sin\varphi \\ -\sin\varphi & \cos\varphi \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} \sum_j a_{ij} x_j \end{pmatrix}, \tag{3.34}$$

where we label the array of elements a_{ij} a 2×2 matrix A consisting of two rows and two columns and consider the vectors $\mathbf{x}$, $\mathbf{x}'$ as 2×1 matrices.

To extend this definition of multiplication of a matrix times a column vector to the product of two 2×2 matrices, let the coordinate rotation be followed by a second rotation given by matrix B such that

$$\mathbf{x}'' = \mathsf{B}\mathbf{x}'. \tag{3.35}$$

Therefore, symbolically

$$\mathbf{x}'' = \mathsf{B}\mathsf{A}\mathbf{x}. \tag{3.36}$$

In component form,

$$x_i'' = \sum_j b_{ij} x_j' = \sum_j b_{ij} \sum_k a_{jk} x_k = \sum_k \left(\sum_j b_{ij} a_{jk} \right) x_k. \tag{3.37}$$

Thus, the summation over j is matrix multiplication defining a matrix $\mathsf{C} = \mathsf{BA}$ such that

$$x_i'' = \sum_{k=1}^{2} c_{ik}\, x_k, \tag{3.38}$$

or $x'' = \mathsf{C}x$ in matrix notation, where the elements of C are given by

$$c_{ik} = \sum_j b_{ij} a_{jk}.$$

Again, this definition involves the scalar products of row vectors of B with column vectors of A. This definition of matrix multiplication generalizes to rectangular $m \times n$ matrices but makes sense only when **the number m of columns of A equals the number of rows of B**. This definition is useful and indeed **this usefulness is the justification for its existence**.

The geometrical interpretation is that the matrix product of the two matrices, BA, is the rotation that carries the unprimed system directly into the double-primed coordinate system. (Before discussing formal definitions, the reader should note that a matrix A as an operator is described by its effect on the coordinates or basis vectors. The matrix elements a_{ij} constitute a **representation** of the operator that depends on the choice of coordinates or a basis.)

From these examples we extract the **general multiplication rule**:

$$\mathsf{AB} = \mathsf{C} \quad \text{if and only if } c_{ij} = \sum_k a_{ik} b_{kj}. \tag{3.39}$$

The ij element of C is formed as a scalar product of the ith row of A with the jth column of B [which demands that A have the same number of columns (n) as B has rows]. The dummy index k takes on all values $1, 2, \ldots, n$ in succession, that is,

$$c_{ij} = a_{i1}b_{1j} + a_{i2}b_{2j} + a_{i3}b_{3j} \tag{3.40}$$

for $n = 3$. Obviously, the dummy index k may be replaced by any other symbol that is not already in use without altering Eq. (3.39). Perhaps the situation may be clarified by stating that Eq. (3.39) defines the method of combining certain matrices. This method of combination is called **matrix multiplication** because, as emphasized earlier, Eq. (3.39) is useful.

EXAMPLE 3.2.1

Matrix Multiplication To illustrate, consider two (so-called Pauli) matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \text{and} \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

The $_{11}$ element of the product, $(\sigma_1\sigma_3)_{11}$, is given by the sum of the products of elements of the first **row** of σ_1 with the corresponding elements of the first **column** of σ_3:

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \rightarrow 0 \cdot 1 + 1 \cdot 0 = 0;$$

that is, writing σ_1 in terms of two row vectors $\mathbf{a}_1$, $\mathbf{a}_2$ and σ_3 in terms of two column vectors $\mathbf{b}_1$, $\mathbf{b}_2$, we have

$$\sigma_1\sigma_3 = \begin{pmatrix} \mathbf{a}_1 \\ \mathbf{a}_2 \end{pmatrix} (\mathbf{b}_1\ \mathbf{b}_2) = \begin{pmatrix} \mathbf{a}_1\cdot\mathbf{b}_1 & \mathbf{a}_1\cdot\mathbf{b}_2 \\ \mathbf{a}_2\cdot\mathbf{b}_1 & \mathbf{a}_2\cdot\mathbf{b}_2 \end{pmatrix}$$
$$= \begin{pmatrix} 0\cdot 1+1\cdot 0 & 0\cdot 0+1\cdot(-1) \\ 1\cdot 1+0\cdot 0 & 1\cdot 0+0\cdot(-1) \end{pmatrix} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}.$$

Here,

$$(\sigma_1\sigma_3)_{ij} = (\sigma_1)_{i1}(\sigma_3)_{1j} + (\sigma_1)_{i2}(\sigma_3)_{2j}.$$

Thus, direct application of the definition of matrix multiplication shows that

$$\sigma_3\sigma_1 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

and therefore

$$\sigma_3\sigma_1 = -\sigma_1\sigma_3. \quad \blacksquare$$

Dirac Bra-ket, Transposition

The vector of unknown x_i in linear equations represents a special case of a matrix with one column and n rows. A shorthand notation, Dirac's ket[6] $|x\rangle$, is common for such a column vector with components x_i, $i = 1, 2, \ldots, n$. If A is an $n \times n$ matrix and $|x\rangle$ an n-component column vector, $A|x\rangle$ is defined as in Eqs. (3.30) and (3.32). Similarly, if a matrix has one row and n columns, it is called a **row vector**, $\langle x|$, with components x_i, $i = 1, 2, \ldots, n$. Clearly, $\langle x|$ and $|x\rangle$ are related by interchanging rows and columns, a **matrix operation** called **transposition**, and for any matrix A, $\tilde{\mathsf{A}}$ is called A transpose,[7] with matrix elements $(\tilde{\mathsf{A}})_{ik} = A_{ki}$. For example,

$$\begin{pmatrix} 3 & 5 & 0 \\ 2 & 3 & 1 \\ 1 & 1 & 4 \end{pmatrix}^T = \begin{pmatrix} 3 & 2 & 1 \\ 5 & 3 & 1 \\ 0 & 1 & 4 \end{pmatrix}.$$

Transposing a product of matrices AB reverses the order and gives $\tilde{\mathsf{B}}\tilde{\mathsf{A}}$; similarly, $\mathsf{A}|x\rangle$ transpose is $\langle x|\tilde{\mathsf{A}}$. The scalar product of vectors takes the form $\langle x|y\rangle = \sum_i x_i y_i$.

(For the determinant $|\mathsf{A}|$ of an orthogonal matrix A, we have $|\mathsf{A}| = |\tilde{\mathsf{A}}|$ because of the symmetric role that rows and columns play for determinants.)

Multiplication (by a Scalar)

We can multiply each linear Eq. (3.30) by a number, α, which means that each coefficient is multiplied by α. This suggests that we complement the multiplication by the following rule: The **multiplication of a matrix** A **by**

[6] The Dirac's bra $\langle x|$ and ket $|x\rangle$ are abstract vectors. Only when we choose a basis of coordinates $x_1, x_2, \ldots, x_n$, as we have here, are the components $x_i = \langle i|x\rangle$. In a complex space, $x_i^* = \langle x|i\rangle$.

[7] Some texts denote A transpose by A^T.

the scalar quantity α is defined as

$$\alpha \mathsf{A} = (\alpha a_{ij}), \tag{3.41}$$

in which the elements of $\alpha\mathsf{A}$ are αa_{ij}; that is, each element of matrix A is multiplied by the scalar factor. This rule is in striking contrast to the behavior of determinants, in which the factor α multiplies only one column or one row and not every element of the entire determinant. A consequence of this scalar multiplication is that

$$\alpha \mathsf{A} = \mathsf{A}\alpha, \quad \text{commutation.}$$

If A is a square matrix, we can evaluate its determinant det(A) and compare α det(A) with

$$\det(\alpha \mathsf{A}) = \alpha^n \det(\mathsf{A}),$$

where we extract a factor α from each row (or column) of αA.

Addition

We also need to add and subtract matrices according to rules that, again, are suggested by and consistent with adding and subtracting linear equations. When we deal with two sets of linear equations in the same unknowns that we can add or subtract, then we add or subtract individual coefficients keeping the unknowns the same. This leads us to the definition

$$\mathsf{A} + \mathsf{B} = \mathsf{C} \text{ if and only if } a_{ij} + b_{ij} = c_{ij} \text{ for all values of } i \text{ and } j, \tag{3.42}$$

with the elements combining according to the laws of ordinary algebra (or arithmetic if they are simple numbers). This means that

$$\mathsf{A} + \mathsf{B} = \mathsf{B} + \mathsf{A}, \quad \text{commutation.} \tag{3.43}$$

EXAMPLE 3.2.2

Matrix Addition To illustrate matrix addition, let us add the Pauli matrices σ_1 and σ_3 of Example 3.2.1:

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} 0+1 & 1+0 \\ 1+0 & 0-1 \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}. \quad \blacksquare$$

Also, an associative addition law is satisfied:

$$(\mathsf{A} + \mathsf{B}) + \mathsf{C} = \mathsf{A} + (\mathsf{B} + \mathsf{C}). \tag{3.44}$$

If all elements are zero, the matrix is called the **null matrix** and is denoted by O. For all A,

$$\mathsf{A} + \mathsf{O} = \mathsf{O} + \mathsf{A} = \mathsf{A}, \tag{3.45}$$

with

$$\mathsf{O} = \begin{pmatrix} 0 & 0 & 0 & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix}. \tag{3.46}$$

Such $m \times n$ matrices form a linear space with respect to addition and subtraction.

Except in special cases, **matrix multiplication is not commutative.**[8]

$$\mathsf{AB} \neq \mathsf{BA}.$$

However, from the definition of matrix multiplication[9] we can show that an **associative law**

$$(\mathsf{AB})\mathsf{C} = \mathsf{A}(\mathsf{BC})$$

holds. There is also a **distributive law:**

$$\mathsf{A}(\mathsf{B} + \mathsf{C}) = \mathsf{AB} + \mathsf{AC}.$$

The **unit matrix** 1 has elements δ_{ij}, Kronecker delta, and the property that $1\mathsf{A} = \mathsf{A}1 = \mathsf{A}$ for all A,

$$1 = \begin{pmatrix} 1 & 0 & 0 & 0 & \cdot & \cdot & \cdot \\ 0 & 1 & 0 & 0 & \cdot & \cdot & \cdot \\ 0 & 0 & 1 & 0 & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix}. \tag{3.47}$$

It should be noted that it is possible for the product of two matrices to be the null matrix without either one being the null matrix. For example, if

$$\mathsf{A} = \begin{pmatrix} 1 & 1 \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad \mathsf{B} = \begin{pmatrix} 1 & 0 \\ -1 & 0 \end{pmatrix},$$

$\mathsf{AB} = \mathsf{O}$. This differs from the multiplication of real or complex numbers, which form a **field**, whereas the additive and multiplicative structure of matrices is called a **ring** by mathematicians.

Product Theorem

An important theorem links the determinant of a product of square matrices to the product of their determinants. Specifically, the **product theorem** states that **the determinant of the product**, $\det(\mathsf{AB})$, of two $n \times n$ matrices A and B **is equal to the product of the determinants**, $\det(\mathsf{A})\det(\mathsf{B})$.

To prove the product theorem, consider the n column vectors

$$\mathbf{c}_k = \left(\sum_j a_{ij} b_{jk}, \, i = 1, 2, \ldots, n \right)$$

[8] Commutation or the lack of it is conveniently described by the **commutator** bracket symbol, $[\mathsf{A}, \mathsf{B}] \equiv \mathsf{AB} - \mathsf{BA}$. $\mathsf{AB} \neq \mathsf{BA}$ becomes $[\mathsf{A}, \mathsf{B}] \neq 0$.

[9] Note that the basic definitions of equality, addition, and multiplication are given in terms of the matrix elements, the a_{ij}. All our matrix operations can be carried out in terms of the matrix elements. However, we can also treat a matrix as an algebraic operator, as in Eq. (3.33). Matrix elements and single operators each have their advantages, as will be seen in the following section. We shall use both approaches.

of the product matrix $\mathsf{C} = \mathsf{AB}$ for $k = 1, 2, \ldots, n$. Each transpose column vector can be displayed as a row vector

$$\tilde{\mathbf{c}}_k = \left(\sum_j a_{1j} b_{jk}, \sum_j a_{2j} b_{jk}, \ldots \sum_j a_{nj} b_{jk} \right) = \sum_{j_k} b_{j_k k} \tilde{\mathbf{a}}_{j_k}.$$

Thus, each column vector

$$\mathbf{c}_k = \sum_{j_k} b_{j_k k} \mathbf{a}_{j_k}$$

is a sum of n column vectors $\mathbf{a}_{j_k} = (a_{i j_k}, i = 1, 2, \ldots, n)$. Note that we are now using a different product summation index j_k for each column vector $\mathbf{c}_k$. Since any determinant

$$D(b_1 \mathbf{a}_1 + b_2 \mathbf{a}_2) = b_1 D(\mathbf{a}_1) + b_2 D(\mathbf{a}_2)$$

is linear in its column vectors, we can pull out the summation sign in front of the determinant from each column vector in C together with the common column factor $b_{j_k k}$ so that

$$\det(\mathsf{C}) = \sum_{j_k} b_{j_1 1} b_{j_2 2} \cdots b_{j_n n} \det(\mathbf{a}_{j_1} \mathbf{a}_{j_2}, \ldots, \mathbf{a}_{j_n}). \tag{3.48}$$

If we rearrange the column vectors $\mathbf{a}_{j_k}$ of the determinant factor in Eq. (3.48) in the proper order $1, 2, \ldots n$, then we can pull the common factor $\det(\mathbf{a}_1, \mathbf{a}_2, \ldots, \mathbf{a}_n) = |\mathsf{A}|$ in front of the n summation signs in Eq. (3.48). These column permutations generate just the right sign $\varepsilon_{j_1 j_2 \cdots j_n}$ to produce in Eq. (3.48) the expression in Eq. (3.8) for $\det(\mathsf{B})$ so that

$$\det(\mathsf{AB}) = \det(\mathsf{C}) = \det(\mathsf{A}) \sum_{j_k} \varepsilon_{j_1 j_2 \cdots j_n} b_{j_1 1} b_{j_2 2} \cdots b_{j_n n} = \det(\mathsf{A}) \det(\mathsf{B}). \tag{3.49}$$

EXAMPLE 3.2.3 **Determinant of Matrix Product** Consider

$$\mathsf{A} = \begin{pmatrix} -1/2 & -\sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{pmatrix}, \quad \mathsf{B} = \begin{pmatrix} -1 & \sqrt{3} \\ -\sqrt{3} & -1 \end{pmatrix}.$$

Then $\det(\mathsf{A}) = 1/4 + 3/4 = 1$ and $\det(\mathsf{B}) = 1 + 3 = 4$, whereas the matrix product is

$$\begin{aligned} \mathsf{AB} &= \begin{pmatrix} -1/2 & -\sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{pmatrix} \begin{pmatrix} -1 & \sqrt{3} \\ -\sqrt{3} & -1 \end{pmatrix} \\ &= \begin{pmatrix} 1/2 + 3/2 & -\sqrt{3}/2 + \sqrt{3}/2 \\ -\sqrt{3}/2 + \sqrt{3}/2 & 3/2 + 1/2 \end{pmatrix} = 2 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \end{aligned}$$

The determinant of the unit matrix is 1, of course. The product theorem gives

$$\det(\mathsf{AB}) = \det(\mathsf{A})\det(\mathsf{B}) = 2^2 \begin{vmatrix} 1 & 0 \\ 0 & 1 \end{vmatrix} = 4. \quad \blacksquare$$

Direct Product

A second procedure for multiplying matrices is known as the **direct** tensor or Kronecker **product**. If A is an $m \times m$ matrix and B an $n \times n$ matrix, then the direct product is

$$\mathsf{A} \otimes \mathsf{B} = \mathsf{C}. \tag{3.50}$$

C is an $mn \times mn$ matrix with elements

$$C_{\alpha\beta} = A_{ij}B_{kl}, \tag{3.51}$$

with

$$\alpha = n(i-1)+k, \quad \beta = n(j-1)+l.$$

EXAMPLE 3.2.4 **A Direct Product** If $\mathsf{A} = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}$ and $\mathsf{B} = \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix}$ are both 2×2 matrices,

$$\mathsf{A} \otimes \mathsf{B} = \begin{pmatrix} a_{11}\mathsf{B} & a_{12}\mathsf{B} \\ a_{21}\mathsf{B} & a_{22}\mathsf{B} \end{pmatrix} = \begin{pmatrix} a_{11}b_{11} & a_{11}b_{12} & a_{12}b_{11} & a_{12}b_{12} \\ a_{11}b_{21} & a_{11}b_{22} & a_{12}b_{21} & a_{12}b_{22} \\ a_{21}b_{11} & a_{21}b_{12} & a_{22}b_{11} & a_{22}b_{12} \\ a_{21}b_{21} & a_{21}b_{22} & a_{22}b_{21} & a_{22}b_{22} \end{pmatrix}. \tag{3.52}$$

$\blacksquare$

The direct product is associative but not commutative. Examples appear in the construction of groups (see Chapter 4) and in vector or Hilbert space in quantum theory.

Direct Sum of Vector Spaces If the vector space V_1 is made up of all linear combinations of the vectors $\mathbf{a}_1, \mathbf{a}_1, \ldots, \mathbf{a}_m$ and V_2 of $\mathbf{b}_1, \mathbf{b}_1, \ldots, \mathbf{b}_n$, then their direct sum $V_1 + V_2$ consists of all linear combinations of the $\mathbf{a}_\mathrm{i}$ and $\mathbf{b}_\mathrm{j}$.

Diagonal Matrices

An important special type of matrix is the square matrix in which all the non-diagonal elements are zero; it is called diagonal. Specifically, if a 3×3 matrix A is diagonal,

$$\mathsf{A} = \begin{pmatrix} a_{11} & 0 & 0 \\ 0 & a_{22} & 0 \\ 0 & 0 & a_{33} \end{pmatrix}.$$

Obvious examples are the unit and zero matrices. A physical interpretation of such diagonal matrices and the method of reducing matrices to this diagonal form are considered in Section 3.5. Here, we simply note a significant property of diagonal matrices: Multiplication of diagonal matrices is commutative,

$$\mathsf{AB} = \mathsf{BA}, \quad \text{if A and B are each diagonal.}$$

Multiplication by a diagonal matrix $[d_1, d_2, \ldots, d_n]$ that has only nonzero elements in the diagonal is particularly simple,

$$\begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix} \begin{pmatrix} 1 & 2 \\ 3 & 4 \end{pmatrix} = \begin{pmatrix} 1 & 2 \\ 2 \cdot 3 & 2 \cdot 4 \end{pmatrix},$$

whereas the opposite order gives

$$\begin{pmatrix} 1 & 2 \\ 3 & 4 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix} = \begin{pmatrix} 1 & 2 \cdot 2 \\ 3 & 2 \cdot 4 \end{pmatrix}.$$

Thus, **a diagonal matrix does not commute with another matrix unless both are diagonal, or the diagonal matrix is proportional to the unit matrix.** This is borne out by the more general form

$$\begin{aligned} [d_1, d_2, \ldots, d_n]\mathsf{A} &= \begin{pmatrix} d_1 & 0 & \cdots & 0 \\ 0 & d_2 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdot \\ 0 & 0 & \cdots & d_n \end{pmatrix} \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \cdots & \cdots & \cdots & \cdot \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{pmatrix} \\ &= \begin{pmatrix} d_1 a_{11} & d_1 a_{12} & \cdots & d_1 a_{1n} \\ d_2 a_{21} & d_2 a_{22} & \cdots & d_2 a_{2n} \\ \cdots & \cdots & \cdots & \cdot \\ d_n a_{n1} & d_n a_{n2} & \cdots & d_n a_{nn} \end{pmatrix}, \end{aligned}$$

whereas

$$\begin{aligned} \mathsf{A}[d_1, d_2, \ldots, d_n] &= \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \cdots & \cdots & \cdots & \cdot \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{pmatrix} \begin{pmatrix} d_1 & 0 & \cdots & 0 \\ 0 & d_2 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdot \\ 0 & 0 & \cdots & d_n \end{pmatrix} \\ &= \begin{pmatrix} d_1 a_{11} & d_2 a_{12} & \cdots & d_n a_{1n} \\ d_1 a_{21} & d_2 a_{22} & \cdots & d_n a_{2n} \\ \cdots & \cdots & \cdots & \cdot \\ d_1 a_{n1} & d_2 a_{n2} & \cdots & d_n a_{nn} \end{pmatrix}. \end{aligned}$$

In the special case of multiplying two diagonal matrices, we simply multiply the corresponding diagonal matrix elements, which obviously is commutative.

Trace

In any square matrix the **sum of the diagonal elements is called the trace.** For example,

$$\text{trace}\begin{pmatrix}1 & 2\\ 3 & 4\end{pmatrix} = 1 + 4 = 5.$$

Clearly, the trace is a linear operation:

$$\text{trace}(\mathsf{A} - \mathsf{B}) = \text{trace}(\mathsf{A}) - \text{trace}(\mathsf{B}).$$

One of its interesting and useful properties is that the trace of a product of two matrices A and B is independent of the order of multiplication:

$$\begin{aligned}\text{trace}(\mathsf{AB}) &= \sum_i (\mathsf{AB})_{ii} = \sum_i \sum_j a_{ij} b_{ji}\\ &= \sum_j \sum_i b_{ji} a_{ij} = \sum_j (\mathsf{BA})_{jj}\\ &= \text{trace}(\mathsf{BA}).\end{aligned} \tag{3.53}$$

This holds even though $\mathsf{AB} \neq \mathsf{BA}$. [Equation (3.53) means that the trace of any commutator, $[\mathsf{A}, \mathsf{B}] = \mathsf{AB} - \mathsf{BA}$, is zero.] From Eq. (3.53) we obtain

$$\text{trace}(\mathsf{ABC}) = \text{trace}(\mathsf{BCA}) = \text{trace}(\mathsf{CAB}),$$

which shows that **the trace is invariant under cyclic permutation of the matrices in a product**.

Matrix Inversion

We cannot define division of matrices, but for a square matrix A with nonzero determinant we can find a matrix A^{-1}, called the inverse of A, so that[10]

$$\mathsf{A}^{-1}\mathsf{A} = \mathsf{A}\mathsf{A}^{-1} = 1. \tag{3.54}$$

This concept has immediate applications: If the matrix A represents a linear transformation, such as a rotation of the coordinate axes, we would expect the inverse transformation that restores the original coordinate axes to be given by A^{-1}. If the matrix A describes a linear coordinate transformation, the inverse matrix A^{-1} allows us to formally write

$$|x\rangle = \mathsf{A}^{-1}|x'\rangle. \tag{3.55}$$

That is, A^{-1} describes the reverse of the transformation given by A and returns the coordinate system to its original position.

[10]Here and throughout this chapter, our matrices have finite rank. If A is an infinite rank matrix ($n \times n$ with $n \to \infty$), then life is more difficult. For A^{-1} to be the inverse we must demand that both

$$\mathsf{A}\mathsf{A}^{-1} = 1 \quad \text{and} \quad \mathsf{A}^{-1}\mathsf{A} = 1.$$

One relation no longer implies the other.

If A is the matrix of coefficients of a system of inhomogeneous linear equations $\mathsf{A}|x\rangle = |b\rangle$, then the inverse matrix allows us to write the formal solution as $|x\rangle = \mathsf{A}^{-1}|b\rangle$. These examples indicate that the concept of inverse matrix is useful.

EXAMPLE 3.2.5

Inverse 2×2 Matrix The general 2×2 matrix

$$\mathsf{A} = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}$$

has the inverse

$$\mathsf{A}^{-1} = \frac{1}{\det(\mathsf{A})} \begin{pmatrix} a_{22} & -a_{12} \\ -a_{21} & a_{11} \end{pmatrix}$$

if and only if $\det(\mathsf{A}) = a_{11}a_{22} - a_{12}a_{21} \neq 0$. To verify this, we check that

$$\begin{aligned} \mathsf{A}\mathsf{A}^{-1} &= \frac{1}{\det(\mathsf{A})} \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \begin{pmatrix} a_{22} & -a_{12} \\ -a_{21} & a_{11} \end{pmatrix} \\ &= \frac{1}{\det(\mathsf{A})} \begin{pmatrix} a_{11}a_{22} - a_{12}a_{21} & -a_{11}a_{12} + a_{12}a_{11} \\ a_{21}a_{22} - a_{22}a_{21} & -a_{21}a_{12} + a_{22}a_{11} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \end{aligned}$$

■

Inverse of Diagonal Matrix The **inverse of a diagonal matrix is also diagonal with inverse matrix elements along the diagonal**:

$$[d_1, d_2, \ldots, d_n]\left[\frac{1}{d_1}, \frac{1}{d_2}, \cdots, \frac{1}{d_n}\right] = \begin{pmatrix} d_1 & 0 & \cdots & 0 \\ 0 & d_2 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdot \\ 0 & 0 & \cdots & d_n \end{pmatrix} \begin{pmatrix} \frac{1}{d_1} & 0 & \cdots & 0 \\ 0 & \frac{1}{d_2} & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdot \\ 0 & 0 & \cdots & \frac{1}{d_n} \end{pmatrix}$$

$$= \begin{pmatrix} \frac{d_1}{d_1} & 0 & \cdots & 0 \\ 0 & \frac{d_2}{d_2} & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdot \\ 0 & 0 & \cdots & \frac{d_n}{d_n} \end{pmatrix} = \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdot \\ 0 & 0 & \cdots & 1 \end{pmatrix}.$$

Inverse of Product AB If A is an $n \times n$ matrix with determinant $\det(\mathsf{A}) \neq 0$, then it has a unique inverse A^{-1} so that $\mathsf{A}\mathsf{A}^{-1} = \mathsf{A}^{-1}\mathsf{A} = 1$. If B is also an $n \times n$ matrix with inverse B^{-1}, then the product AB has the inverse

$$(\mathsf{A}\mathsf{B})^{-1} = \mathsf{B}^{-1}\mathsf{A}^{-1} \tag{3.56}$$

because $\mathsf{A}\mathsf{B}\mathsf{B}^{-1}\mathsf{A}^{-1} = 1 = \mathsf{B}^{-1}\mathsf{A}^{-1}\mathsf{A}\mathsf{B}$.

Derivative of a Matrix and Its Inverse When the matrix elements $a_{jk}(t)$ of A are functions of the variable t, we define the derivative of A as $\frac{d\mathsf{A}}{dt} = \left(\frac{da_{jk}(t)}{dt}\right)$. To define the derivative of the inverse matrix, we differentiate $\mathsf{A}\mathsf{A}^{-1} = 1$, obtaining

$$0 = \frac{d(\mathsf{A}\mathsf{A}^{-1})}{dt} = \frac{d\mathsf{A}}{dt}\mathsf{A}^{-1} + \mathsf{A}\frac{d\mathsf{A}^{-1}}{dt}.$$

Multiplying this relation by A^{-1} on the left yields the formula

$$\frac{d\mathsf{A}^{-1}}{dt} = -\mathsf{A}^{-1}\frac{d\mathsf{A}}{dt}\mathsf{A}^{-1}.$$

The generalization of the inverse of a 2×2 matrix in Example 3.2.5 is given in Exercise 3.2.24, with the inverse matrix having matrix elements $(\mathsf{A}^{-1})_{ij}$,

$$(\mathsf{A}^{-1})_{ij} = \frac{C_{ji}}{|\mathsf{A}|}, \tag{3.57}$$

with the assumption that the determinant of A, $|\mathsf{A}| \neq 0$. If it is zero, we label A singular. No inverse exists. However, as explained at the end of Section 3.1, this determinant form is **totally unsuited for numerical work** with large matrices.

In Example 3.2.5, $C_{11} = a_{22}$, $C_{12} = -a_{21}$, $C_{21} = -a_{12}$, $C_{22} = a_{11}$ so that $(\mathsf{A}^{-1})_{12} = C_{21}/|A| = -a_{12}/|A|$, etc., as noted in the example.

There is a wide variety of alternative techniques. One of the best and most commonly used is the Gauss–Jordan matrix inversion technique (demonstrated in Example 3.2.6), which shows how to find matrices M_L such that the product $\mathsf{M}_L\mathsf{A}$ will be A but with

- one row multiplied by a constant, or
- one row replaced by the original row minus a multiple of another row, or
- rows interchanged.

Other matrices M_R operating on the right ($\mathsf{A}\mathsf{M}_R$) can carry out the same operations on the **columns** of A.

This means that the matrix rows and columns may be altered (by matrix multiplication) as though we were dealing with determinants, so we can apply the Gauss–Jordan elimination techniques of Section 3.1 to the matrix elements. Hence, there exists a matrix M_L (or M_R) such that[11]

$$\mathsf{M}_L\mathsf{A} = 1. \tag{3.58}$$

Then $\mathsf{M}_L = \mathsf{A}^{-1}$. We determine M_L by carrying out the identical elimination operations on the unit matrix. Then

$$\mathsf{M}_L 1 = \mathsf{M}_L. \tag{3.59}$$

To illustrate this, we consider a specific example.

EXAMPLE 3.2.6

Gauss–Jordan Matrix Inversion We want to invert the matrix

$$\mathsf{A} = \begin{pmatrix} 3 & 2 & 1 \\ 2 & 3 & 1 \\ 1 & 1 & 4 \end{pmatrix} \tag{3.60}$$

[11] Remember that $\det(\mathsf{A}) \neq 0$.

corresponding to the simultaneous linear equations of Example 3.1.7. For convenience we write A and 1 side by side and carry out the identical operations on each:

$$\begin{pmatrix} 3 & 2 & 1 \\ 2 & 3 & 1 \\ 1 & 1 & 4 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{3.61}$$

To be systematic, we multiply the first row by 1/3 and the second row by 1/2 to get $a_{k1} = 1$:

$$\begin{pmatrix} 1 & \frac{2}{3} & \frac{1}{3} \\ 1 & \frac{3}{2} & \frac{1}{2} \\ 1 & 1 & 4 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} \frac{1}{3} & 0 & 0 \\ 0 & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{3.62}$$

Subtracting the first row from the second and third, we obtain

$$\begin{pmatrix} 1 & \frac{2}{3} & \frac{1}{3} \\ 0 & \frac{5}{6} & \frac{1}{6} \\ 0 & \frac{1}{3} & \frac{11}{3} \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} \frac{1}{3} & 0 & 0 \\ -\frac{1}{3} & \frac{1}{2} & 0 \\ -\frac{1}{3} & 0 & 1 \end{pmatrix}. \tag{3.63}$$

Then we divide the second row (of **both** matrices) by $\frac{5}{6}$ and subtract $\frac{2}{3}$ times it from the first row and $\frac{1}{3}$ times it from the third row. The results for both matrices are

$$\begin{pmatrix} 1 & 0 & \frac{1}{5} \\ 0 & 1 & \frac{1}{5} \\ 0 & 0 & \frac{18}{5} \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} \frac{3}{5} & -\frac{2}{5} & 0 \\ -\frac{2}{5} & \frac{3}{5} & 0 \\ -\frac{1}{5} & -\frac{1}{5} & 1 \end{pmatrix}. \tag{3.64}$$

We divide the third row (of **both** matrices) by $\frac{18}{5}$. Then, as the last step, $\frac{1}{5}$ times the third row is subtracted from each of the first two rows (of both matrices). Our final pair is

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \text{and} \quad \mathsf{A}^{-1} = \begin{pmatrix} \frac{11}{18} & -\frac{7}{18} & -\frac{1}{18} \\ -\frac{7}{18} & \frac{11}{18} & -\frac{1}{18} \\ -\frac{1}{18} & -\frac{1}{18} & \frac{5}{18} \end{pmatrix}. \tag{3.65}$$

The check is to multiply the original A by the calculated A^{-1} to see if we really do get the unit matrix 1. Instead, we check that the column vector of solution x_i

$$\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \mathsf{A}^{-1} \begin{pmatrix} 11 \\ 13 \\ 12 \end{pmatrix} = \begin{pmatrix} \frac{11\cdot 11 - 7\cdot 13 - 12}{18} \\ \frac{-7\cdot 11 + 11\cdot 13 - 12}{18} \\ \frac{-11 - 13 + 5\cdot 12}{18} \end{pmatrix} = \begin{pmatrix} \frac{18}{18} \\ \frac{54}{18} \\ \frac{36}{18} \end{pmatrix} = \begin{pmatrix} 1 \\ 3 \\ 2 \end{pmatrix}$$

coincides with that of Example 3.1.7. ■

As with the Gauss–Jordan solution of simultaneous linear algebraic equations, this technique is well adapted to computers. Indeed, this Gauss–Jordan matrix inversion technique will be available in the program library as a FORTRAN code or in other programming languages as well as in Mathematica, Maple, and other symbolic computer manipulation software (see Sections 2.3 and 2.4 of Press *et al.*, 1992).

For **matrices of special form the inverse matrix can be given in closed form**; for example, for

$$\mathsf{A} = \begin{pmatrix} a & b & c \\ b & d & b \\ c & b & e \end{pmatrix} \tag{3.66}$$

the inverse matrix has a similar but slightly more general form

$$\mathsf{A}^{-1} = \begin{pmatrix} \alpha & \beta_1 & \gamma \\ \beta_1 & \delta & \beta_2 \\ \gamma & \beta_2 & \epsilon \end{pmatrix}, \tag{3.67}$$

with matrix elements given by

$$D\alpha = ed - b^2, \quad D\gamma = -(cd - b^2), \quad D\beta_1 = (c - e)b, \quad D\beta_2 = (c - a)b,$$
$$D\delta = ae - c^2, \quad D\epsilon = ad - b^2, \quad D = b^2(2c - a - e) + d(ae - c^2),$$

where $D = \det(\mathsf{A})$ is the determinant of the matrix A. If $e = a$ in A, then the inverse matrix A^{-1} also simplifies to

$$\beta_1 = \beta_2, \quad \epsilon = \alpha, \quad D = (a^2 - c^2)d + 2(c - a)b^2.$$

As a check, let us work out the $_{11}$ matrix element of the product $\mathsf{A}\mathsf{A}^{-1} = 1$. We find

$$\begin{aligned} a\alpha + b\beta_1 + c\gamma &= \frac{1}{D}[a(ed - b^2) + b^2(c - e) - c(cd - b^2)] \\ &= \frac{1}{D}(-ab^2 + aed + 2b^2c - b^2e - c^2d) = \frac{D}{D} = 1. \end{aligned}$$

Similarly, we check that the $_{12}$ matrix element vanishes,

$$a\beta_1 + b\delta + c\beta_2 = \frac{1}{D}[ab(c - e) + b(ae - c^2) + cb(c - a)] = 0,$$

etc.

Note that we cannot always find an inverse of A^{-1} by solving for the matrix elements $a, b, \cdots$ of A because not every inverse matrix A^{-1} of the form in Eq. (3.67) has a corresponding A of the special form in Eq. 3.66, as Example 3.2.6 clearly shows.

SUMMARY

Matrices are square or rectangular arrays of numbers that define linear transformations like rotations of a coordinate system. As such, they are linear operators. Square matrices may be inverted when their determinant is nonzero. When a matrix defines a system of linear equations, the inverse matrix solves it. Matrices with the same number of rows and columns may be added and

subtracted. They form what mathematicians call a ring, with a unit and a zero matrix. Matrices are also useful for representing group operations and operators in Hilbert spaces.

EXERCISES

3.2.1 Show that matrix multiplication is associative: $(AB)C = A(BC)$.

3.2.2 Show that

$$(A + B)(A - B) = A^2 - B^2$$

if and only if A and B commute,

$$AB - BA \equiv [A, B] = 0.$$

3.2.3 Show that matrix A is a **linear operator** by showing that

$$A(c_1\mathbf{r}_1 + c_2\mathbf{r}_2) = c_1A\mathbf{r}_1 + c_2A\mathbf{r}_2,$$

where c_j are arbitrary constants and $\mathbf{r}_j$ are vectors. It can be shown that an $n \times n$ matrix is the **most general** linear operator in an n-dimensional vector space. This means that every linear operator in this n-dimensional vector space is equivalent to a matrix.

3.2.4 If A is an $n \times n$ matrix, show that

$$\det(-A) = (-1)^n \det A.$$

3.2.5 (a) The matrix equation $A^2 = 0$ does not imply $A = 0$. Show that the most general 2×2 matrix whose square is zero may be written as

$$\begin{pmatrix} ab & b^2 \\ -a^2 & -ab \end{pmatrix},$$

where a and b are real or complex numbers.

(b) If $C = A + B$, in general

$$\det C \neq \det A + \det B.$$

Construct a specific numerical example to illustrate this inequality.

3.2.6 Verify the **Jacobi identity**

$$[A, [B, C]] = [B, [A, C]] - [C, [A, B]].$$

This is useful in quantum mechanics and for generators of Lie groups (see Chapter 4). As a mnemonic aid, the reader might note that the Jacobi identity has the same form as the *BAC–CAB* rule of Section 1.5.

3.2.7 Show that the matrices

$$A = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad B = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}, \quad C = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

satisfy the commutation relations

$$[\mathsf{A}, \mathsf{B}] = \mathsf{C}, \quad [\mathsf{A}, \mathsf{C}] = 0, \quad \text{and} \quad [\mathsf{B}, \mathsf{C}] = 0.$$

These matrices can be interpreted as raising operators for angular momentum 1.

3.2.8 A matrix with elements $a_{ij} = 0$ for $j < i$ may be called upper right triangular. The elements in the lower left (below and to the left of the main diagonal) vanish.

Show that the product of two upper right triangular matrices is an upper right triangular matrix. The same applies to lower left triangular matrices.

3.2.9 The three Pauli spin matrices are

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \text{and} \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Show that

(a) $\sigma_i^2 = 1$,

(b) $\sigma_i \sigma_j = i\sigma_k$, $(i, j, k) = (1, 2, 3), (2, 3, 1), (3, 1, 2)$ (cyclic permutation), and

(c) $\sigma_i \sigma_j + \sigma_j \sigma_i = 2\delta_{ij} 1_2$, where 1_2 is the identity 2×2 matrix.

These matrices were used by Pauli in the nonrelativistic theory of electron spin.

3.2.10 Using the Pauli σ of Exercise 3.2.9, show that

$$(\boldsymbol{\sigma} \cdot \mathbf{a})(\boldsymbol{\sigma} \cdot \mathbf{b}) = \mathbf{a} \cdot \mathbf{b}\, 1_2 + i\boldsymbol{\sigma} \cdot (\mathbf{a} \times \mathbf{b}).$$

Here

$$\boldsymbol{\sigma} \equiv \hat{\mathbf{x}}\sigma_1 + \hat{\mathbf{y}}\sigma_2 + \hat{\mathbf{z}}\sigma_3$$

and $\mathbf{a}$ and $\mathbf{b}$ are ordinary vectors and 1_2 is the 2×2 unit matrix.

3.2.11 One description of spin 1 particles uses the matrices

$$\mathsf{M}_x = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad \mathsf{M}_y = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix},$$

and

$$\mathsf{M}_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

Show that

(a) $[M_x, M_y] = iM_z$, and so on[12] (cyclic permutation of indices). Using the Levi–Civita symbol of Sections 2.9 and 3.4, we may write

$$[M_i, M_j] = i\varepsilon_{ijk}M_k,$$

which are the commutation relations of angular momentum.

(b) $M^2 \equiv M_x^2 + M_y^2 + M_z^2 = 2\,1_3$,
where 1_3 is the 3×3 unit matrix.

(c) $[M^2, M_i] = 0$,
$[M_z, L^+] = L^+$,
$[L^+, L^-] = 2M_z$,
where
$L^+ \equiv M_x + iM_y$,
$L^- \equiv M_x - iM_y$.

3.2.12 Repeat Exercise 3.2.11 using an alternate representation,

$$M_x = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad M_y = \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix},$$

and

$$M_z = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

In Chapter 4 these matrices appear as the **generators** of the rotation group.

3.2.13 Repeat Exercise 3.2.11 using the matrices for a spin of $3/2$,

$$M_x = \frac{1}{2}\begin{pmatrix} 0 & \sqrt{3} & 0 & 0 \\ \sqrt{3} & 0 & 2 & 0 \\ 0 & 2 & 0 & \sqrt{3} \\ 0 & 0 & \sqrt{3} & 0 \end{pmatrix}, \quad M_y = \frac{i}{2}\begin{pmatrix} 0 & -\sqrt{3} & 0 & 0 \\ \sqrt{3} & 0 & -2 & 0 \\ 0 & 2 & 0 & -\sqrt{3} \\ 0 & 0 & \sqrt{3} & 0 \end{pmatrix},$$

and

$$M_z = \frac{1}{2}\begin{pmatrix} 3 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -3 \end{pmatrix}.$$

3.2.14 An operator P commutes with J_x and J_y, the x and y components of an angular momentum operator. Show that P commutes with the third component of angular momentum; that is,

$$[P, J_z] = 0.$$

Hint. The angular momentum components must satisfy the commutation relation of Exercise 3.2.11(a).

[12] $[A, B] = AB - BA$.

3.2.15 The L^+ and L^- matrices of Exercise 3.2.11 are ladder operators (see Chapter 4): L^+ operating on a system of spin projection m will raise the spin projection to $m+1$ if m is below its maximum. L^+ operating on $m_{\max}$ yields zero. L^- reduces the spin projection in unit steps in a similar fashion. Dividing by $\sqrt{2}$, we have

$$\mathsf{L}^+ = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}, \quad \mathsf{L}^- = \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}.$$

Show that

$$\mathsf{L}^+|-1\rangle = |0\rangle, \mathsf{L}^-|-1\rangle = \text{null column vector},$$

$$\mathsf{L}^+|0\rangle = |1\rangle, \mathsf{L}^-|0\rangle = |-1\rangle,$$

$$\mathsf{L}^+|1\rangle = \text{null column vector}, \mathsf{L}^-|1\rangle = |0\rangle,$$

where

$$|-1\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \quad |0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad \text{and} \quad |1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$

represent states of spin projection -1, 0, and 1, respectively.
Note. Differential operator analogs of these ladder operators appear in Exercise 11.6.7.

3.2.16 Vectors **A** and **B** are related by the tensor T:

$$\mathbf{B} = \mathsf{T}\mathbf{A}.$$

Given **A** and **B** show that there is **no unique solution** for the components of T. This is why **vector division B/A is undefined** (apart from the special case of **A** and **B** parallel and T then a scalar).

3.2.17 We might ask for a vector $\mathbf{A}^{-1}$, an inverse of a given vector **A** in the sense that

$$\mathbf{A} \cdot \mathbf{A}^{-1} = \mathbf{A}^{-1} \cdot \mathbf{A} = 1.$$

Show that this relation does not suffice to define $\mathbf{A}^{-1}$ uniquely. **A** has literally an infinite number of inverses.

3.2.18 If A is a diagonal matrix, with all diagonal elements different, and A and B commute, show that B is diagonal.

3.2.19 If A and B are diagonal matrices, show that A and B commute.

3.2.20 Angular momentum matrices satisfy commutation relations

$$[\mathsf{M}_i, \mathsf{M}_j] = i\mathsf{M}_k, \quad i, j, k \text{ cyclic}.$$

Show that the trace of each angular momentum matrix vanishes. Explain why.

3.2.21 (a) The operator tr replaces a matrix A by its trace; that is,

$$\mathrm{tr}(\mathsf{A}) = \mathrm{trace}(\mathsf{A}) = \sum_i a_{ii}.$$

Show that tr is a **linear** operator.

(b) The operator det replaces a matrix A by its determinant; that is,

$$\det(\mathsf{A}) = \text{determinant of A}.$$

Show that det is **not** a linear operator.

3.2.22 A and B anticommute. Also, $\mathsf{A}^2 = 1$, $\mathsf{B}^2 = 1$. Show that $\mathrm{trace}(\mathsf{A}) = \mathrm{trace}(\mathsf{B}) = 0$.
Note. The Pauli (Section 3.4) matrices are specific examples.

3.2.23 If a matrix has an inverse, show that the inverse is unique.

3.2.24 If A^{-1} has elements

$$(\mathsf{A}^{-1})_{ij} = \frac{C_{ji}}{|\mathsf{A}|},$$

where C_{ji} is the jith cofactor of $|\mathsf{A}|$, show that

$$\mathsf{A}^{-1}\mathsf{A} = 1.$$

Hence, A^{-1} is the inverse of A (if $|\mathsf{A}| \neq 0$).
Note. In numerical work it sometimes happens that $|\mathsf{A}|$ is almost equal to zero. Then there is trouble.

3.2.25 Show that $\det \mathsf{A}^{-1} = (\det \mathsf{A})^{-1}$.
Hint. Apply the product theorem of Section 3.2.
Note. If $\det \mathsf{A}$ is zero, then A has no inverse. A is singular.

3.2.26 Find the inverse of

$$\mathsf{A} = \begin{pmatrix} 3 & 2 & 1 \\ 2 & 2 & 1 \\ 1 & 1 & 4 \end{pmatrix}.$$

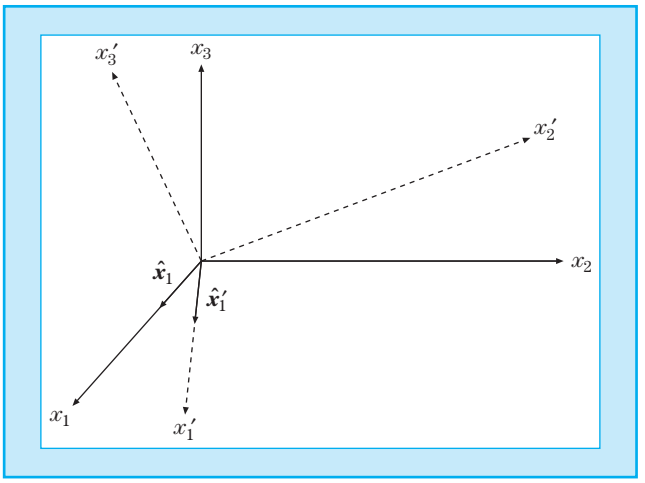
3.2.27 Explain why the inverse process starting from a matrix A^{-1} of the form in Eq. (3.67) and solving for the matrix elements $a, b, \cdots$ of A does not always work.

3.3 Orthogonal Matrices

Ordinary three-dimensional space may be described with the Cartesian coordinates (x_1, x_2, x_3). We consider a second set of Cartesian coordinates (x_1', x_2', x_3'), whose origin and handedness coincide with those of the first set but whose orientation is different (Fig. 3.5). We can say that the primed coordinate **axes** have been **rotated** relative to the initial, unprimed coordinate axes. Since this rotation is a **linear** operation, we expect a matrix equation relating the primed coordinates to the unprimed coordinates.

Figure 3.5

Rotation of Cartesian Coordinate Systems



This section repeats portions of Chapter 2 in a slightly different context and with a different emphasis. Previously, attention was focused on a vector or tensor. Transformation properties were strongly stressed and were critical. Here, emphasis is on the description of the coordinate rotation—the matrix. Transformation properties, the behavior of the matrix when the coordinate system is changed, appear at the end of this section. Sections 3.4 and 3.5 continue with transformation properties of complex vector spaces.

Direction Cosines

A unit vector along the x_1'-axis ($\hat{\mathbf{x}}_1'$) may be resolved into components along the x_1-, x_2-, and x_3-axes by the usual projection technique:

$$\hat{\mathbf{x}}_1' = \hat{\mathbf{x}}_1 \cos(x_1', x_1) + \hat{\mathbf{x}}_2 \cos(x_1', x_2) + \hat{\mathbf{x}}_3 \cos(x_1', x_3). \tag{3.68}$$

Equation (3.68) is a specific example of the linear relations discussed at the beginning of Section 3.2. In two dimensions, this decomposition of a vector in rotated coordinates is illustrated in Fig. 2.18 in conjunction with Fig. 3.5.

For convenience, these cosines, which are the direction cosines, are labeled

$$\begin{aligned} \cos(x_1', x_1) &= \hat{\mathbf{x}}_1' \cdot \hat{\mathbf{x}}_1 = a_{11}, \\ \cos(x_1', x_2) &= \hat{\mathbf{x}}_1' \cdot \hat{\mathbf{x}}_2 = a_{12}, \\ \cos(x_1', x_3) &= \hat{\mathbf{x}}_1' \cdot \hat{\mathbf{x}}_3 = a_{13}. \end{aligned} \tag{3.69}$$

Continuing, we have

$$\begin{aligned} \cos(x_2', x_1) &= \hat{\mathbf{x}}_2' \cdot \hat{\mathbf{x}}_1 = a_{21}, \\ \cos(x_2', x_2) &= \hat{\mathbf{x}}_2' \cdot \hat{\mathbf{x}}_2 = a_{22}, \end{aligned} \tag{3.70}$$

and so on, where $a_{21} \neq a_{12}$ in general. Now Eq. (3.68) may be rewritten as

$$\hat{\mathbf{x}}_1' = \hat{\mathbf{x}}_1 a_{11} + \hat{\mathbf{x}}_2 a_{12} + \hat{\mathbf{x}}_3 a_{13}$$

and also

$$\begin{aligned} \hat{\mathbf{x}}_2' &= \hat{\mathbf{x}}_1 a_{21} + \hat{\mathbf{x}}_2 a_{22} + \hat{\mathbf{x}}_3 a_{23}, \\ \hat{\mathbf{x}}_3' &= \hat{\mathbf{x}}_1 a_{31} + \hat{\mathbf{x}}_2 a_{32} + \hat{\mathbf{x}}_3 a_{33}. \end{aligned} \tag{3.71}$$

We may also go the other way by resolving $\hat{\mathbf{x}}_1$, $\hat{\mathbf{x}}_2$, and $\hat{\mathbf{x}}_3$ into components in the primed system. Then

$$\begin{aligned} \hat{\mathbf{x}}_1 &= \hat{\mathbf{x}}_1' a_{11} + \hat{\mathbf{x}}_2' a_{21} + \hat{\mathbf{x}}_3' a_{31}, \\ \hat{\mathbf{x}}_2 &= \hat{\mathbf{x}}_1' a_{12} + \hat{\mathbf{x}}_2' a_{22} + \hat{\mathbf{x}}_3' a_{32}, \\ \hat{\mathbf{x}}_3 &= \hat{\mathbf{x}}_1' a_{13} + \hat{\mathbf{x}}_2' a_{23} + \hat{\mathbf{x}}_3' a_{33}. \end{aligned} \tag{3.72}$$

Associating $\hat{\mathbf{x}}_1$ and $\hat{\mathbf{x}}_1'$ with the subscript 1, $\hat{\mathbf{x}}_2$ and $\hat{\mathbf{x}}_2'$ with the subscript 2, $\hat{\mathbf{x}}_3$ and $\hat{\mathbf{x}}_3'$ with the subscript 3, we see that in each case the first subscript of a_{ij} refers to the primed unit vector ($\hat{\mathbf{x}}_1'$, $\hat{\mathbf{x}}_2'$, $\hat{\mathbf{x}}_3'$), whereas the second subscript refers to the unprimed unit vector ($\hat{\mathbf{x}}_1$, $\hat{\mathbf{x}}_2$, $\hat{\mathbf{x}}_3$).

Applications to Vectors

If we consider a vector whose components are functions of the position in space, then

$$\begin{aligned} \mathbf{V}(x_1, x_2, x_3) &= \hat{\mathbf{x}}_1 V_1 + \hat{\mathbf{x}}_2 V_2 + \hat{\mathbf{x}}_3 V_3, \\ \mathbf{V}(x_1', x_2', x_3') &= \hat{\mathbf{x}}_1' V_1' + \hat{\mathbf{x}}_2' V_2' + \hat{\mathbf{x}}_3' V_3' \end{aligned} \tag{3.73}$$

since the point may be given by both the coordinates (x_1, x_2, x_3) and the coordinates (x_1', x_2', x_3'). Note that $\mathbf{V}$ and $\mathbf{V}'$ are geometrically the same vector (but with different components). The coordinate axes are being rotated; the vector stays fixed. Using Eq. (3.72) to eliminate $\hat{\mathbf{x}}_1$, $\hat{\mathbf{x}}_2$, and $\hat{\mathbf{x}}_3$, we may separate Eq. (3.73) into three scalar equations:

$$\begin{aligned} V_1' &= a_{11} V_1 + a_{12} V_2 + a_{13} V_3, \\ V_2' &= a_{21} V_1 + a_{22} V_2 + a_{23} V_3, \\ V_3' &= a_{31} V_1 + a_{32} V_2 + a_{33} V_3. \end{aligned} \tag{3.74}$$

In particular, these relations will hold for the coordinates of a point (x_1, x_2, x_3) and (x_1', x_2', x_3'), giving

$$\begin{aligned} x_1' &= a_{11} x_1 + a_{12} x_2 + a_{13} x_3, \\ x_2' &= a_{21} x_1 + a_{22} x_2 + a_{23} x_3, \\ x_3' &= a_{31} x_1 + a_{32} x_2 + a_{33} x_3, \end{aligned} \tag{3.75}$$

and similarly for the primed coordinates. In this notation, the set of three equations may be written as

$$x_i' = \sum_{j=1}^{3} a_{ij} x_j, \tag{3.76}$$

where i takes on the values 1, 2, and 3 and the result is three **separate** equations, or it is just one matrix equation

$$|x'\rangle = \mathsf{A}|x\rangle$$

involving the matrix A, the column vector $|x\rangle$, and matrix multiplication.

Now let us set aside these results and try a different approach to the same problem. We consider two coordinate systems (x_1, x_2, x_3) and (x_1', x_2', x_3') with a common origin and one point (x_1, x_2, x_3) in the unprimed system, (x_1', x_2', x_3') in the primed system. Note the usual ambiguity. The same symbol x denotes both the coordinate axis and a particular distance along that axis. Since our system is linear, x_i' must be a linear combination of x_i. Let

$$x_i' = \sum_{j=1}^{3} a_{ij} x_j. \tag{3.77}$$

The a_{ij} may be identified as our old friends, the direction cosines. This identification is carried out for the two-dimensional case later.

If we have two sets of quantities (V_1, V_2, V_3) in the unprimed system and (V_1', V_2', V_3') in the primed system, related in the same way as the coordinates of a point in the two different systems [Eq. (3.77)],

$$V_i' = \sum_{j=1}^{3} a_{ij} V_j, \tag{3.78}$$

then, as in Section 2.6, the quantities (V_1, V_2, V_3) are defined as the components of a vector that stay fixed while the coordinates rotate; that is, a vector is defined in terms of transformation properties of its components under a rotation of the coordinate axes. In a sense, the coordinates of a point have been taken as a prototype vector. The power and usefulness of this definition became apparent in Chapter 2, in which it was extended to define pseudovectors and tensors.

From Eq. (3.76) we can derive interesting information about a_{ij} that describe the orientation of coordinate system (x_1', x_2', x_3') relative to the system (x_1, x_2, x_3). The length from the origin to the point is the same in both systems. Squaring,[13]

$$\sum_i x_i^2 = \sum_i x_i'^2 = \sum_i \left(\sum_j a_{ij} x_j \right) \left(\sum_k a_{ik} x_k \right) = \sum_{j,k} x_j x_k \sum_i a_{ij} a_{ik}. \tag{3.79}$$

This can be true for all points if and only if

$$\sum_i a_{ij} a_{ik} = \delta_{jk}, \quad j, k = 1, 2, 3. \tag{3.80}$$

[13]Note that **two** independent indices j and k are used.

Note that Eq. (3.80), the orthogonality condition, does not conform to our definition of matrix multiplication, but it can be put in the required form by using the transpose matrix $\tilde{\mathsf{A}}$ such that

$$\tilde{a}_{ji} = a_{ij}. \tag{3.81}$$

Then Eq. (3.80) becomes

$$\tilde{\mathsf{A}}\mathsf{A} = 1. \tag{3.82}$$

This is a restatement of the orthogonality condition and may be taken as a definition of orthogonality. Multiplying Eq. (3.82) by A^{-1} from the right and using Eq. (3.55), we have

$$\tilde{\mathsf{A}} = \mathsf{A}^{-1}. \tag{3.83}$$

This important matrix result that the **inverse equals the transpose** holds only **for orthogonal matrices** and indeed may be taken as a further restatement of the orthogonality condition.

Multiplying Eq. (3.83) by A from the left, we obtain

$$\mathsf{A}\tilde{\mathsf{A}} = 1 \tag{3.84}$$

or

$$\sum_i a_{ji}a_{ki} = \delta_{jk}, \tag{3.85}$$

which is still another form of the orthogonality condition.

Summarizing, the orthogonality condition may be stated in several equivalent ways:

$$\sum_i a_{ij}a_{ik} = \delta_{jk} \tag{3.86}$$

$$\sum_i a_{ji}a_{ki} = \delta_{jk} \tag{3.87}$$

$$\tilde{\mathsf{A}}\mathsf{A} = \mathsf{A}\tilde{\mathsf{A}} = 1 \tag{3.88}$$

$$\tilde{\mathsf{A}} = \mathsf{A}^{-1}. \tag{3.89}$$

Any one of these relations is a necessary and a sufficient condition for A to be orthogonal.

Taking determinants of Eq. (3.84) implies (recall $|\tilde{\mathsf{A}}| = |\mathsf{A}|$)

$$|\mathsf{A}||\tilde{\mathsf{A}}| = |\mathsf{A}|^2 = 1, \quad \text{so that } |\mathsf{A}| = \pm 1.$$

Moreover, we may describe Eq. (3.79) as stating that rotations leave lengths invariant. Verification of Eq. (3.80), if needed, may be obtained by returning to Eq. (3.79) and setting

$$\mathbf{r} = (x_1, x_2, x_3) = (1, 0, 0), (0, 1, 0), (0, 0, 1), (1, 1, 0),$$

and so on to evaluate the nine relations given by Eq. (3.80). This process is valid since Eq. (3.79) must hold for all **r** for a given set of a_{ij}. Equation (3.80), a consequence of requiring that the **length remain constant (invariant) under rotation of the coordinate system**, is called the **orthogonality condition**. The a_{ij}, written as a matrix A, **define an orthogonal matrix**. Finally, in matrix notation Eq. (3.76) becomes

$$|x'\rangle = \mathsf{A}|x\rangle. \tag{3.90}$$

Orthogonality Conditions: Two-Dimensional Case

A better understanding of a_{ij} and the orthogonality condition may be gained by considering rotation in two dimensions in detail. (This can be thought of as a three-dimensional system with the x_1-, x_2-axes rotated about x_3.) From Fig. 3.6,

$$\begin{aligned} x_1' &= x_1 \cos\varphi + x_2 \sin\varphi, \\ x_2' &= -x_1 \sin\varphi + x_2 \cos\varphi. \end{aligned} \tag{3.91}$$

Therefore, by Eq. (3.81),

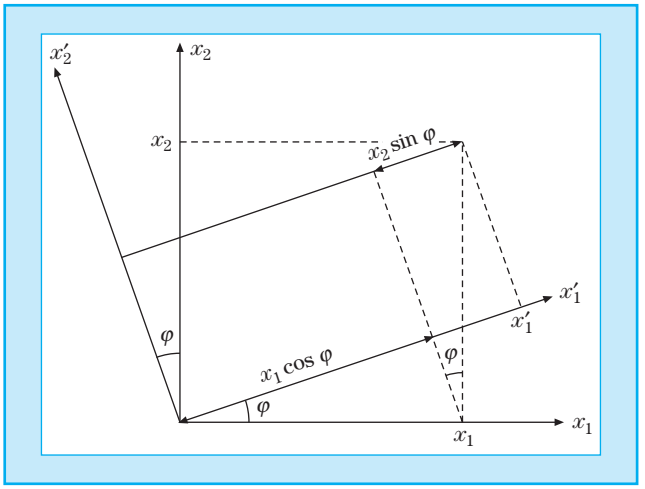
$$\mathsf{A} = \begin{pmatrix} \cos\varphi & \sin\varphi \\ -\sin\varphi & \cos\varphi \end{pmatrix}. \tag{3.92}$$

Notice that A reduces to the unit matrix for $\varphi = 0$. Zero angle rotation means nothing has changed. It is clear from Fig. 3.6 that

$$\begin{aligned} a_{11} &= \cos\varphi = \cos(x_1', x_1), \\ a_{12} &= \sin\varphi = \cos\left(\frac{\pi}{2} - \varphi\right) = \cos(x_1', x_2), \end{aligned} \tag{3.93}$$

Figure 3.6

Rotation



and so on, thus identifying the matrix elements a_{ij} as the direction cosines. Equation (3.80), the orthogonality condition, becomes

$$\begin{aligned} \sin^2\varphi + \cos^2\varphi &= 1, \\ \sin\varphi\cos\varphi - \sin\varphi\cos\varphi &= 0. \end{aligned} \tag{3.94}$$

The extension to three dimensions (rotation of the coordinates through an angle φ counterclockwise about x_3) is simply

$$\mathsf{A} = \begin{pmatrix} \cos\varphi & \sin\varphi & 0 \\ -\sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{3.95}$$

The matrix element a_{33} being equal to 1 expresses the fact that $x_3' = x_3$ since the rotation is about the x_3-axis. The zeros guarantee that x_1' and x_2' do not depend on x_3 and that x_3' does not depend on x_1 and x_2.

It is now possible to see and understand why the term **orthogonal** is appropriate for these matrices. We have the general form

$$\mathsf{A} = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix},$$

a matrix of direction cosines in which a_{ij} is the cosine of the angle between x_i' and x_j. Therefore, a_{11}, a_{12}, a_{13} are the direction cosines of x_1' relative to x_1, x_2, x_3. These three elements of A **define** a unit length along x_1', that is, a unit vector $\hat{\mathbf{x}}_1'$:

$$\hat{\mathbf{x}}_1' = \hat{\mathbf{x}}_1 a_{11} + \hat{\mathbf{x}}_2 a_{12} + \hat{\mathbf{x}}_3 a_{13}.$$

The orthogonality relations [Eqs. (3.86–3.89)] are simply a statement that the **unit vectors $\hat{\mathbf{x}}_1'$, $\hat{\mathbf{x}}_2'$, and $\hat{\mathbf{x}}_3'$ are mutually perpendicular or orthogonal**. Our orthogonal transformation matrix A transforms one orthogonal coordinate system into a second orthogonal coordinate system by rotation [and reflection if $\det(\mathsf{A}) = -1$].

As an example of the use of matrices, the unit vectors in spherical polar coordinates may be written as

$$\begin{pmatrix} \hat{\mathbf{r}} \\ \hat{\boldsymbol{\theta}} \\ \hat{\boldsymbol{\varphi}} \end{pmatrix} = \mathsf{C} \begin{pmatrix} \hat{\mathbf{x}} \\ \hat{\mathbf{y}} \\ \hat{\mathbf{z}} \end{pmatrix}, \tag{3.96}$$

where C is given in Exercise 2.5.1. This is equivalent to Eq. (3.68) with $\mathbf{x}_1'$, $\mathbf{x}_2'$, and $\mathbf{x}_3'$ replaced by $\hat{\mathbf{r}}$, $\hat{\boldsymbol{\theta}}$, and $\hat{\boldsymbol{\varphi}}$. From the preceding analysis, C is orthogonal. Therefore, the inverse relation becomes

$$\begin{pmatrix} \hat{\mathbf{x}} \\ \hat{\mathbf{y}} \\ \hat{\mathbf{z}} \end{pmatrix} = \mathsf{C}^{-1} \begin{pmatrix} \hat{\mathbf{r}} \\ \hat{\boldsymbol{\theta}} \\ \hat{\boldsymbol{\varphi}} \end{pmatrix} = \tilde{\mathsf{C}} \begin{pmatrix} \hat{\mathbf{r}} \\ \hat{\boldsymbol{\theta}} \\ \hat{\boldsymbol{\varphi}} \end{pmatrix}, \tag{3.97}$$

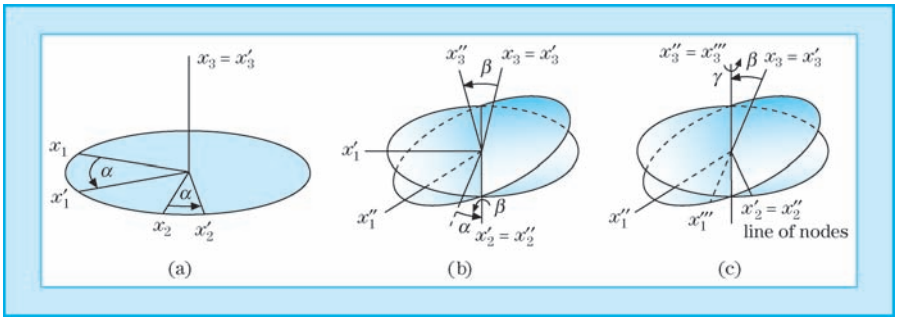


Figure 3.7

(a) Rotation About x_3 Through Angle α, (b) Rotation About x_2' Through Angle β, and (c) Rotation About x_3'' Through Angle γ

and Exercise 2.5.5 is solved by inspection. Similar applications of matrix inverses appear in connection with the transformation of a power series into a series of orthogonal functions (Gram–Schmidt orthogonalization in Section 9.3).

Euler Angles

Our transformation matrix A contains nine direction cosines. Clearly, only three of these are independent; Eq. (3.80) provides six constraints. Equivalently, we may say that two parameters (θ and φ in spherical polar coordinates) are required to fix the axis of rotation. Then one additional parameter describes the amount of rotation about the specified axis. In the Lagrangian formulation of mechanics (Section 17.3) it is necessary to describe A by using some set of three independent parameters rather than the redundant direction cosines. The usual choice of parameters is the Euler angles.[14]

The goal is to describe the orientation of a final rotated system (x_1''', x_2''', x_3''') relative to some initial coordinate system (x_1, x_2, x_3). The final system is developed in three steps, with each step involving one rotation described by one Euler angle (Fig. 3.7):

1. The coordinates are rotated about the x_3-axis through an angle α counterclockwise relative to x_1, x_2, x_3 into new axes denoted by x_1', x_2', x_3'. (The x_3- and x_3'-axes coincide.)
2. The coordinates are rotated about the x_2'-axis[15] through an angle β counterclockwise relative to x_1', x_2', x_3' into new axes denoted by x_1'', x_2'', x_3''. (The x_2'- and the x_2''-axes coincide.)
3. The third and final rotation is through an angle γ counterclockwise about the x_3''- axis, yielding the x_1''', x_2''', x_3''' system. (The x_3''- and x_3'''-axes coincide.)

[14]There are almost as many definitions of the Euler angles as there are authors. Here, we follow the choice generally made by workers in the area of group theory and the quantum theory of angular momentum (compare Sections 4.3 and 4.4).

[15]Some authors choose this second rotation to be about the x_1'-axis.

The three matrices describing these rotations are

$$R_z(\alpha) = \begin{pmatrix} \cos\alpha & \sin\alpha & 0 \\ -\sin\alpha & \cos\alpha & 0 \\ 0 & 0 & 1 \end{pmatrix}, \tag{3.98}$$

exactly like Eq. (3.92), but different sign for β in

$$R_y(\beta) = \begin{pmatrix} \cos\beta & 0 & -\sin\beta \\ 0 & 1 & 0 \\ \sin\beta & 0 & \cos\beta \end{pmatrix} \tag{3.99}$$

and

$$R_z(\gamma) = \begin{pmatrix} \cos\gamma & \sin\gamma & 0 \\ -\sin\gamma & \cos\gamma & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{3.100}$$

The total rotation is described by the triple matrix product:

$$A(\alpha, \beta, \gamma) = R_z(\gamma)R_y(\beta)R_z(\alpha). \tag{3.101}$$

Note the order: $R_z(\alpha)$ operates first, then $R_y(\beta)$, and finally $R_z(\gamma)$. Direct multiplication gives

$$A(\alpha, \beta, \gamma) = \begin{pmatrix} \cos\gamma\cos\beta\cos\alpha - \sin\gamma\sin\alpha & \cos\gamma\cos\beta\sin\alpha + \sin\gamma\cos\alpha & -\cos\gamma\sin\beta \\ -\sin\gamma\cos\beta\cos\alpha - \cos\gamma\sin\alpha & -\sin\gamma\cos\beta\sin\alpha + \cos\gamma\cos\alpha & \sin\gamma\sin\beta \\ \sin\beta\cos\alpha & \sin\beta\sin\alpha & \cos\beta \end{pmatrix}. \tag{3.102}$$

Equating $A(a_{ij})$ with $A(\alpha, \beta, \gamma)$, element by element, yields the direction cosines in terms of the three Euler angles. We could use this Euler angle identification to verify the direction cosine identities [Eq. (2.106) of Section 2.6], but the approach of Exercise 3.3.3 is much more elegant.

Biographical Data

Euler, Leonhard. Euler, a Swiss mathematician, was born in Basel in 1707 and died in St. Petersburg, Russia, in 1783. He studied with the Bernoulli brothers and eventually became the most prolific mathematician of all time, contributing to all then-existing branches of mathematics, and he founded new ones such as graph theory. There are many Euler identities, equations, and formulas, for example, for the exponential function of pure imaginary argument, another relating Bernoulli numbers to the Riemann zeta function at even integer argument, or in the calculus of variations. In 1733, he became professor at the St. Petersburg Academy of Catherine I, widow of Peter the Great. He left Russia during the terror reign of Ivan IV for Frederic the Great's

court of Prussia but returned to Russia when Catherine the Great invited him back. He lost both eyes, one due to solar observations and the other in 1766 due to intense work on mathematics, but continued his productive work to his death.

Symmetry Properties and Similarity Transformations

Our matrix formalism leads to the Euler angle description of rotations (which forms a basis for developing the rotation group in Chapter 4). The power and flexibility of matrices pushed quaternions into obscurity early in the century.[16]

It will be noted that matrices have been handled in two ways in the foregoing discussion: by their components and as single entities. Each technique has its own advantages and both are useful.

The transpose matrix is useful in a discussion of symmetry properties. If

$$\mathsf{A} = \tilde{\mathsf{A}}, \quad a_{ij} = a_{ji}, \tag{3.103}$$

the matrix is called **symmetric**, whereas if

$$\mathsf{A} = -\tilde{\mathsf{A}}, \quad a_{ij} = -a_{ji}, \tag{3.104}$$

it is called antisymmetric or skewsymmetric. The diagonal elements of an antisymmetric matrix vanish. It is easy to show that any square matrix may be written as the sum of a symmetric matrix and an antisymmetric matrix. Consider the identity

$$\mathsf{A} = \frac{1}{2}[\mathsf{A} + \tilde{\mathsf{A}}] + \frac{1}{2}[\mathsf{A} - \tilde{\mathsf{A}}]. \tag{3.105}$$

$[\mathsf{A} + \tilde{\mathsf{A}}]$ is clearly symmetric, whereas $[\mathsf{A} - \tilde{\mathsf{A}}]$ is clearly antisymmetric. This is the matrix analog of Eq. (2.120) for tensors. Similarly, a function may be broken up into its even and odd parts.

So far, we have interpreted the orthogonal matrix as rotating the coordinate system. This changes the components of a fixed vector (not rotating with the coordinates) (see Fig. 3.6). However, an orthogonal matrix A may be interpreted equally well as a rotation of the **vector** in the **opposite** direction (Fig. 3.8). These are the two possibilities: active transformation—rotating the vector keeping the coordinates fixed; and passive transformation—rotating the coordinates (in the opposite sense) keeping the vector fixed.

Suppose we interpret matrix A as a linear transformation of a **vector r** into the position shown by $\mathbf{r}_1$; that is, in a particular coordinate system we have a relation

$$\mathbf{r}_1 = \mathsf{A}\mathbf{r}. \tag{3.106}$$

[16]Stephenson, R. J. (1966). Development of vector analysis from quaternions. *Am. J. Phys.* **34**, 194.

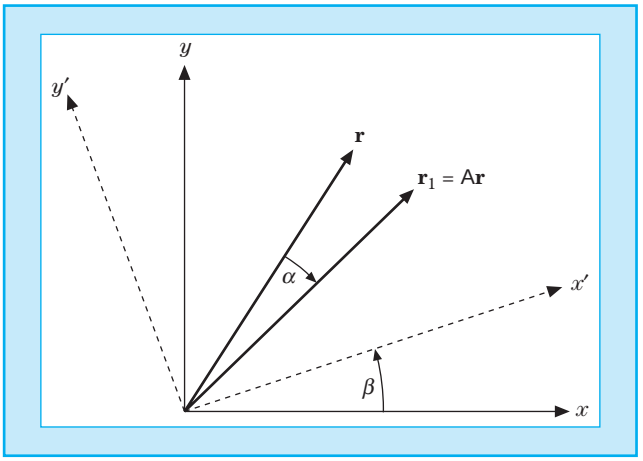


Figure 3.8

Fixed Coordinates-rotated Vector

Now let us transform the **coordinates** linearly by applying matrix B, which transforms (x, y, z) into (x', y', z'):

$$\begin{aligned}\mathbf{r}_1' &= \mathsf{B}\mathbf{r}_1 = \mathsf{BA}\mathbf{r} = \mathsf{BA}(\mathsf{B}^{-1}\mathsf{B})\mathbf{r} \\ &= (\mathsf{BAB}^{-1})\mathsf{B}\mathbf{r} = (\mathsf{BAB}^{-1})\mathbf{r}'. \end{aligned} \tag{3.107}$$

$\mathsf{B}\mathbf{r}_1$ is just $\mathbf{r}_1'$ in the new coordinate system with a similar interpretation holding for $\mathsf{B}\mathbf{r}$. Hence, **in this new system** $(\mathsf{B}\mathbf{r})$ is transformed into position $(\mathsf{B}\mathbf{r}_1)$ by the matrix BAB^{-1}:

$$\begin{array}{ccccc} \mathsf{B}\mathbf{r}_1 & = & (\mathsf{BAB}^{-1}) & & \mathsf{B}\mathbf{r} \\ \downarrow & & \downarrow & & \downarrow \\ \mathbf{r}_1' & = & \mathsf{A}' & & \mathbf{r}'. \end{array}$$

In the new system the coordinates have been transformed by matrix B, and A has the form A′, in which

$$\mathsf{A}' = \mathsf{BAB}^{-1}. \tag{3.108}$$

A′ operates in the x', y', z' space as A operates in the x, y, z space.

For the determinant $|\mathsf{A}'|$ the product theorem gives

$$|\mathsf{A}'| = |\mathsf{B}||\mathsf{A}||\mathsf{B}^{-1}| = |\mathsf{A}|. \tag{3.109a}$$

For the trace we find

$$\text{trace}(\mathsf{BAB}^{-1}) = \text{trace}(\mathsf{B}^{-1}\mathsf{BA}) = \text{trace}(\mathsf{A}) \tag{3.109b}$$

so that both the trace and the determinant of a square matrix stay invariant under a coordinate transformation, and rotations in particular.

The coordinate transformation defined by Eq. (3.108) with B any matrix, not necessarily orthogonal, is known as a **similarity transformation**. In component form, Eq. (3.108) becomes

$$a'_{ij} = \sum_{k,l} b_{ik} a_{kl} (\mathsf{B}^{-1})_{lj}. \tag{3.110}$$

Now if B is orthogonal,

$$(\mathsf{B}^{-1})_{lj} = (\tilde{\mathsf{B}})_{lj} = b_{jl}, \tag{3.111}$$

and we have

$$a'_{ij} = \sum_{k,l} b_{ik} a_{kl} b_{jl}. \tag{3.112}$$

It may be helpful to think of A again as an operator, possibly as rotating coordinate axes, relating angular momentum and angular velocity of a rotating solid (Section 3.5). Matrix A is the representation in a given coordinate system. However, there are directions associated with A-crystal axes, symmetry axes in the rotating solid, and so on so that the representation A depends on the coordinates. The similarity transformation shows how the representation changes with a change of coordinates.

Relation to Tensors

Comparing Eq. (3.112) with the equations of Section 2.6, we see that it defines a tensor of second rank. Hence, a matrix that transforms by an **orthogonal** similarity transformation is, by definition, a tensor. Clearly, then, any matrix A, interpreted as linearly transforming a vector [Eq. (3.106)], may be called a tensor. If, however, we consider an **orthogonal** matrix as a collection of fixed direction cosines, giving the new orientation of a coordinate system, there is no tensor transformation involved.

The symmetry and antisymmetry properties defined earlier are preserved under **orthogonal** similarity transformations. Let A be a symmetric matrix, $\mathsf{A} = \tilde{\mathsf{A}}$, and

$$\mathsf{A}' = \mathsf{B}\mathsf{A}\mathsf{B}^{-1}. \tag{3.113}$$

Now

$$\tilde{\mathsf{A}}' = \tilde{\mathsf{B}}^{-1}\tilde{\mathsf{A}}\tilde{\mathsf{B}} = \mathsf{B}\tilde{\mathsf{A}}\mathsf{B}^{-1} \tag{3.114}$$

since B is orthogonal. However, $\mathsf{A} = \tilde{\mathsf{A}}$. Therefore,

$$\tilde{\mathsf{A}}' = \mathsf{B}\mathsf{A}\mathsf{B}^{-1} = \mathsf{A}', \tag{3.115}$$

showing that the property of symmetry is invariant under an orthogonal similarity transformation. In general, symmetry is **not** preserved under a nonorthogonal similarity transformation.

SUMMARY

Matrices that define rotations are composed of mutually orthogonal row and column vectors. Their inverse is the transposed matrix.

EXERCISES

Note. Assume all matrix elements are real.

3.3.1 Show that the product of two orthogonal matrices is orthogonal. Show that the inverse of an orthogonal matrix is orthogonal.
Note. These are key steps in showing that all $n \times n$ orthogonal matrices form a group (Section 4.1).

3.3.2 If A is orthogonal, show that its determinant $|\mathsf{A}| = \pm 1$.

3.3.3 If A is orthogonal and $\det \mathsf{A} = +1$, show that $(\det \mathsf{A})a_{ij} = C_{ij}$, where C_{ij} is the **cofactor** of a_{ij}. This yields the identities of Eq. (2.106) used in Section 2.6 to show that a cross product of vectors (in three-space) is itself a vector.
Hint. Note Exercise 3.2.24.

3.3.4 Another set of Euler rotations in common use is
(1) a rotation about the x_3-axis through an angle φ, counterclockwise,
(2) a rotation about the x_1'-axis through an angle θ, counterclockwise,
(3) a rotation about the x_3''-axis through an angle ψ, counterclockwise.
If

$$\begin{aligned} \alpha &= \varphi - \pi/2 \quad & \varphi &= \alpha + \pi/2 \\ \beta &= \theta & \theta &= \beta \\ \gamma &= \psi + \pi/2 & \psi &= \gamma - \pi/2, \end{aligned}$$

show that the final systems are identical.

3.3.5 Suppose the earth is moved (rotated) so that the north pole goes to 30° north, 20° west (original latitude and longitude system) and the 10° west meridian points due south.
(a) What are the Euler angles describing this rotation?
(b) Find the corresponding direction cosines.

$$\textit{ANS.}\ (b)\ \mathsf{A} = \begin{pmatrix} 0.9551 & -0.2552 & -0.1504 \\ 0.0052 & 0.5221 & -0.8529 \\ 0.2962 & 0.8138 & 0.5000 \end{pmatrix}.$$

3.3.6 Verify that the Euler angle rotation matrix, Eq. (3.102), is invariant under the transformation

$$\alpha \to \alpha + \pi, \quad \beta \to -\beta, \quad \gamma \to \gamma - \pi.$$

3.3.7 Show that the Euler angle rotation matrix $\mathsf{A}(\alpha, \beta, \gamma)$ satisfies the following relations:
(a) $\mathsf{A}^{-1}(\alpha, \beta, \gamma) = \tilde{\mathsf{A}}(\alpha, \beta, \gamma)$
(b) $\mathsf{A}^{-1}(\alpha, \beta, \gamma) = \mathsf{A}(-\gamma, -\beta, -\alpha)$.

3.3.8 Show that the trace of the product of a symmetric and an antisymmetric matrix is zero.

3.3.9 Show that the trace of a matrix remains invariant under similarity transformations.

3.3.10 Show that the determinant of a matrix remains invariant under similarity transformations.
Note. These Exercises 3.3.9 and 3.3.10 show that the trace and the determinant are independent of the coordinates. They are characteristics of the matrix (operator).

3.3.11 Show that the property of antisymmetry is invariant under orthogonal similarity transformations.

3.3.12 A is 2×2 and orthogonal. Find its most general form. Compare with two-dimensional rotation.

3.3.13 $|\mathbf{x}\rangle$ and $|\mathbf{y}\rangle$ are column vectors. Under an orthogonal transformation S, $|\mathbf{x}'\rangle = \mathsf{S}|\mathbf{x}\rangle$, $|\mathbf{y}'\rangle = \mathsf{S}|\mathbf{y}\rangle$. Show that the scalar product $\langle\mathbf{x}|\mathbf{y}\rangle$ is invariant under this orthogonal transformation.
Note. This is equivalent to the invariance of the dot product of two vectors (Section 2.6).

3.3.14 Show that the sum of the squares of the elements of a matrix remains invariant under orthogonal similarity transformations.

3.3.15 A rotation $\varphi_1 + \varphi_2$ about the z-axis is carried out as two successive rotations φ_1 and φ_2, each about the z-axis. Use the matrix representation of the rotations to derive the trigonometric identities:

$$\cos(\varphi_1 + \varphi_2) = \cos\varphi_1 \cos\varphi_2 - \sin\varphi_1 \sin\varphi_2$$
$$\sin(\varphi_1 + \varphi_2) = \sin\varphi_1 \cos\varphi_2 + \cos\varphi_1 \sin\varphi_2.$$

3.3.16 A column vector $\mathbf{V}$ has components V_1 and V_2 in an initial (unprimed) system. Calculate V_1' and V_2' for a
(a) rotation of the coordinates through an angle of θ **counterclockwise**,
(b) rotation of the vector through an angle of θ **clockwise**.
The results for parts (a) and (b) should be identical.

3.4 Hermitian Matrices and Unitary Matrices

Definitions

Thus far, it has generally been assumed that our linear vector space is a real space and that the matrix elements (the representations of the linear operators) are real. For many calculations in classical physics, real matrix elements will suffice. However, in quantum mechanics complex variables are unavoidable because of the form of the basic commutation relations (or the form of the time-dependent Schrödinger equation). With this in mind, we generalize to the case of complex matrix elements. To handle these elements, let us define, or label, some new properties:

1. Complex conjugate, $\mathsf{A}^* = (a_{ik}^*)$, formed by taking the complex conjugate $(i \to -i)$ of each element a_{ik} of A, where $i = \sqrt{-1}$.
2. Adjoint, $\mathsf{A}^\dagger$, formed by transposing A^*,
$$\mathsf{A}^\dagger = (a_{ik})^\dagger = \widetilde{\mathsf{A}^*} = \tilde{\mathsf{A}}^* = (a_{ki}^*). \tag{3.116}$$
3. Hermitian matrix: The matrix A is labeled **Hermitian** (or **self-adjoint**) if
$$\mathsf{A} = \mathsf{A}^\dagger. \tag{3.117}$$
If A is real, then $\mathsf{A}^\dagger = \tilde{\mathsf{A}}$ and real Hermitian matrices are real symmetric matrices. In quantum mechanics (or matrix mechanics) matrices are usually constructed to be Hermitian.
4. Unitary matrix: Matrix U is labeled **unitary** if
$$\mathsf{U}^\dagger = \mathsf{U}^{-1}. \tag{3.118}$$
If U is real, then $\mathsf{U}^{-1} = \tilde{\mathsf{U}}$ so that **real unitary matrices are orthogonal matrices**. This represents a generalization of the concept of orthogonal matrix [compare Eq. (3.83)].
5. $(\mathsf{AB})^* = \mathsf{A}^*\mathsf{B}^*$, $(\mathsf{AB})^\dagger = \mathsf{B}^\dagger\mathsf{A}^\dagger$.

If the matrix elements are complex, the physicist is almost always concerned with Hermitian and unitary matrices. **Unitary matrices** are especially important in quantum mechanics because they **leave the length of a (complex) vector unchanged**—analogous to the operation of an orthogonal matrix on a real vector. It is for this reason that the S matrix of scattering theory is a unitary matrix. The transformation of an operator A^S in the Schrödinger representation of quantum mechanics to the Heisenberg representation $\mathsf{A}^\mathsf{H} = \mathsf{U}^\dagger\mathsf{A}^\mathsf{S}\mathsf{U}$ with the unitary evolution operator $e^{-i\mathsf{H}t/\hbar}$ is another example.

In a complex n-dimensional linear space the square of the **length of a vector** $\tilde{\mathbf{x}} = (x_1, x_2, \ldots, x_n)$, or the square of its distance from the origin 0, is defined as

$$\mathbf{x}^\dagger\mathbf{x} = \sum_{i=1}^{n} x_i^* x_i = \sum_{i=1}^{n} |x_i|^2.$$

If a coordinate transformation $\mathbf{y} = \mathsf{U}\mathbf{x}$ leaves the distance unchanged, then

$$\mathbf{x}^\dagger\mathbf{x} = \mathbf{y}^\dagger\mathbf{y} = (\mathsf{U}\mathbf{x})^\dagger\mathsf{U}\mathbf{x} = \mathbf{x}^\dagger\mathsf{U}^\dagger\mathsf{U}\mathbf{x}.$$

Since $\mathbf{x}$ is arbitrary it follows that $\mathsf{U}^\dagger\mathsf{U} = 1_n$; that is, U is a unitary $n \times n$ matrix.

If $\mathbf{x}' = \mathsf{A}\mathbf{x}$ is a linear map, then its matrix in the new coordinates becomes the unitary (complex analog of a similarity) transformation

$$\mathsf{A}' = \mathsf{U}\mathsf{A}\mathsf{U}^\dagger \tag{3.119}$$

because

$$\mathsf{U}\mathbf{x}' = \mathbf{y}' = \mathsf{U}\mathsf{A}\mathbf{x} = \mathsf{U}\mathsf{A}\mathsf{U}^{-1}\mathbf{y} = \mathsf{U}\mathsf{A}\mathsf{U}^\dagger\mathbf{y}.$$

Once we have the notion of length in a complex vector space, we can proceed to **define a scalar or inner product of vectors** as

$$\sum_i y_i^* x_i = \mathbf{y}^\dagger \cdot \mathbf{x} \equiv \langle y|x\rangle.$$

Two vectors are orthogonal if their scalar product is zero, $\langle y|x\rangle = 0$. The Pauli spin matrices introduced next are also unitary.

Pauli Matrices

The set of three 2×2 Pauli matrices $\boldsymbol{\sigma}$,

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{3.120}$$

were introduced by W. Pauli to describe a particle of spin $1/2$ in nonrelativistic quantum mechanics. It can readily be shown that (compare Exercises 3.2.9 and 3.2.10) the Pauli $\boldsymbol{\sigma}$ satisfy

$$\sigma_i\sigma_j + \sigma_j\sigma_j = 2\delta_{ij}1_2, \quad \text{anticommutation} \tag{3.121}$$

$$\sigma_i\sigma_j = i\sigma_k, \quad \text{cyclic permutation of indices} \tag{3.122}$$

$$(\sigma_i)^2 = 1_2, \tag{3.123}$$

where 1_2 is the 2×2 unit matrix. Thus, the vector $\boldsymbol{\sigma}/2$ satisfies the same commutation relations

$$[\sigma_i, \sigma_j] \equiv \sigma_i\sigma_j - \sigma_j\sigma_i = 2i\varepsilon_{ijk}\sigma_k \tag{3.124}$$

as the orbital angular momentum $\mathbf{L}$ ($\mathbf{L} \times \mathbf{L} = i\mathbf{L}$; see Exercise 2.5.11).

The three Pauli matrices $\boldsymbol{\sigma}$ and the unit matrix form a complete set of 2×2 matrices so that any 2×2 matrix M may be expanded as

$$\mathsf{M} = m_0 1 + m_1\sigma_1 + m_2\sigma_2 + m_3\sigma_3 = m_0 + \mathbf{m} \cdot \boldsymbol{\sigma}, \tag{3.125}$$

where the m_i form a constant vector $\mathbf{m} = (m_1, m_2, m_3)$. Using $\sigma_i^2 = 1$ and $\text{trace}(\sigma_i) = 0$, we obtain from Eq. (3.125) the expansion coefficients m_i by forming traces,

$$2m_0 = \text{trace}(\mathsf{M}), \quad 2m_i = \text{trace}(\mathsf{M}\sigma_i), \quad i = 1, 2, 3. \tag{3.126}$$

Adding and multiplying such 2×2 matrices, we generate the Pauli algebra.[17] Note that $\text{trace}(\sigma_i) = 0$ for $i = 1, 2, 3$.

The spin algebra generated by the Pauli matrices is a matrix representation of the four-dimensional Clifford algebra, whereas Hestenes and coworkers have developed in their **geometric calculus** a representation-free (i.e., coordinate-free) algebra that contains complex numbers, vectors, the quaternion subalgebra, and generalized cross products as directed areas (called bivectors). This algebraic–geometric framework is tailored to nonrelativistic

[17] For its geometrical significance, see Baylis, W. E., Huschilt, J., and Jiansu Wei (1992). *Am. J. Phys.* **60**, 788.

quantum mechanics where spinors acquire geometric aspects and the Gauss's and Stokes's theorems appear as components of a unified theorem.

The discussion of orthogonal matrices in Section 3.3 and unitary matrices in this section is only a beginning. Further extensions are of vital concern in modern particle physics. With the Pauli matrices, we can develop **spinor** wave functions for electrons, protons, and other spin $\frac{1}{2}$ particles.

SUMMARY

Unitary matrices for a complex vector space play the role that orthogonal matrices perform in a real vector space: they represent coordinate transformations. Therefore, unitary matrices are composed of mutually orthogonal unit vectors. Hermitian matrices define quadratic forms in complex spaces and are complex analogs of real symmetric matrices. Both have numerous applications in quantum mechanics.

Biographical Data

Pauli, Wolfgang. Pauli, an Austrian American theoretical physicist, was born in Vienna, Austria, in 1900 and died in Zürich, Switzerland, in 1958. He was a prodigy, publishing in his teens a lucid review of relativity while still a student in Sommerfeld's group in Munich, Germany, where he obtained his Ph.D. in 1921. In 1925, he found the exclusion principle named after him, for which he was eventually honored with the Nobel prize in 1945. He was a scathing critic of numerous physicists of his times ("conscience of physics"). With Heisenberg, and independently of Dirac, he founded quantum field theory and QED. In 1931, he proposed the neutrino (thus named by Fermi) to conserve energy and quantum numbers in the weak interaction in a letter to colleagues at a conference but never published this suggestion for fear of ridicule or making a mistake. The elusive neutrino was finally tracked down experimentally in 1956 and F. Reines received the Nobel prize in 1995.

EXERCISES

3.4.1 Show that

$$\det(\mathsf{A}^*) = (\det \mathsf{A})^* = \det(\mathsf{A}^\dagger).$$

3.4.2 Three angular momentum matrices satisfy the basic commutation relation

$$[\mathsf{J}_x, \mathsf{J}_y] = i\mathsf{J}_z$$

(and cyclic permutation of indices). If two of the matrices have real elements, show that the elements of the third must be pure imaginary.

3.4.3 Show that $(\mathsf{AB})^\dagger = \mathsf{B}^\dagger\mathsf{A}^\dagger$.

3.4.4 A matrix $\mathsf{C} = \mathsf{S}^\dagger\mathsf{S}$. Show that the trace is positive definite unless S is the null matrix, in which case $\text{trace}(\mathsf{C}) = 0$.

3.4.5 If A and B are Hermitian matrices, show that $(\mathsf{AB} + \mathsf{BA})$ and $i(\mathsf{AB} - \mathsf{BA})$ are also Hermitian.

3.4.6 The matrix C is **not** Hermitian. Show that $\mathsf{C} + \mathsf{C}^\dagger$ and $i(\mathsf{C} - \mathsf{C}^\dagger)$ are Hermitian. This means that a non-Hermitian matrix may be resolved into two Hermitian parts:

$$\mathsf{C} = \frac{1}{2}(\mathsf{C} + \mathsf{C}^\dagger) + \frac{1}{2i} i(\mathsf{C} - \mathsf{C}^\dagger).$$

This decomposition of a matrix into two Hermitian matrix parts parallels the decomposition of a complex number z into $x + iy$, where $x = (z + z^*)/2$ and $y = (z - z^*)/2i$.

3.4.7 A and B are two noncommuting Hermitian matrices:

$$\mathsf{AB} - \mathsf{BA} = i\mathsf{C}.$$

Prove that C is Hermitian.

3.4.8 Show that a Hermitian matrix remains Hermitian under unitary similarity transformations.

3.4.9 Two matrices A and B are each Hermitian. Find a necessary and sufficient condition for their product AB to be Hermitian.

ANS. $[\mathsf{A}, \mathsf{B}] = 0$.

3.4.10 Show that the reciprocal (i.e., inverse) of a unitary matrix is unitary. Show that the product of two unitary matrices is unitary.
Hint. These are key steps in proving that unitary matrices form a group.

3.4.11 A particular similarity transformation yields

$$\mathsf{A}' = \mathsf{UAU}^{-1}$$
$$\mathsf{A}'^\dagger = \mathsf{UA}^\dagger\mathsf{U}^{-1}.$$

If the adjoint relationship is preserved ($\mathsf{A}^{\dagger\prime} = \mathsf{A}'^\dagger$) and $\det \mathsf{U} = 1$, show that U must be unitary.

3.4.12 Two matrices U and H are related by

$$\mathsf{U} = e^{ia\mathsf{H}}$$

with a real. (The exponential function is defined by a Maclaurin expansion. This will be done in Section 5.11.)
(a) If H is Hermitian, show that U is unitary.
(b) If U is unitary, show that H is Hermitian. (H is independent of a.)
Note. With H the Hamiltonian,

$$\psi(x, t) = \mathsf{U}(x, t)\psi(x, 0) = \exp(-it\mathsf{H}/\hbar)\psi(x, 0)$$

is a solution of the time-dependent Schrödinger equation. $\mathsf{U}(x, t) = \exp(-it\mathsf{H}/\hbar)$ is the evolution operator.

3.4.13 An operator $T(t + \varepsilon, t)$ describes the change in the wave function from t to $t + \varepsilon$. For ε real and small enough so that ε^2 may be neglected

$$T(t + \varepsilon, t) = 1 - \frac{i}{\hbar}\varepsilon\mathsf{H}(t).$$

(a) If T is unitary, show that H is Hermitian.
(b) If H is Hermitian, show that T is unitary.
Note. When $\mathsf{H}(t)$ is independent of time, this relation may be put in exponential form (Exercise 3.4.12).

3.4.14 (a) Given $\mathbf{r}' = \mathsf{U}\mathbf{r}$, with U a unitary matrix and $\mathbf{r}$ a (column) vector with complex elements, show that the norm (magnitude) of $\mathbf{r}$ is invariant under this operation.
(b) The matrix U transforms any column vector $\mathbf{r}$ with complex elements into $\mathbf{r}'$ leaving the magnitude invariant: $\mathbf{r}^\dagger\mathbf{r} = \mathbf{r}'^\dagger\mathbf{r}'$. Show that U is unitary.

3.5 Diagonalization of Matrices

Moment of Inertia Matrix

In Example 1.5.3, we analyzed a quadratic form G that can be defined by symmetric 2×2 matrix A as

$$x^2 + xy + y^2 = (x, y)\begin{pmatrix} 1 & 1/2 \\ 1/2 & 1 \end{pmatrix}\begin{pmatrix} x \\ y \end{pmatrix} \equiv \langle \mathbf{x}|\mathsf{A}|\mathbf{x}\rangle,$$

where $\langle \mathbf{x}| = (x, y)$ is the two-dimensional (transpose) coordinate vector. We found that $G(x, y) = 1$ is an ellipse with rotated axes. In the rotated coordinate system along the major and minor axes $x \pm y$ of the ellipse G becomes the familiar sum of squares $3(x + y)^2 + (x - y)^2 = 4$. This situation suggests that using a suitable rotation of coordinates, we can transform a general quadratic form into a sum of squares, that is, diagonalize the associated (real) symmetric matrix.

In many physical problems involving real symmetric or complex Hermitian matrices it is desirable to carry out a (real) orthogonal similarity transformation or a unitary transformation (corresponding to a rotation of the coordinate system) to reduce the matrix to a diagonal form, with nondiagonal elements all equal to zero. One particularly direct example is the moment of inertia matrix I of a rigid body. From the definition of angular momentum $\mathbf{L}$ we have

$$\mathbf{L} = \mathsf{I}\boldsymbol{\omega}, \tag{3.127}$$

where $\boldsymbol{\omega}$ is the angular velocity.[18] The inertia matrix I is found to have diagonal components

$$I_{11} = \sum_i m_i(r_i^2 - x_i^2), \quad \text{and so on,} \tag{3.128}$$

[18]The moment of inertia matrix may also be developed from the kinetic energy of a rotating body, $T = 1/2\langle\boldsymbol{\omega}|\mathsf{I}|\boldsymbol{\omega}\rangle$ defined as in Eq. (3.130) with the three-dimensional vector $|\boldsymbol{\omega}\rangle$ replacing $\hat{\mathbf{n}}$.

where the subscript i refers to mass m_i located at $\mathbf{r}_i = (x_i, y_i, z_i)$. For the nondiagonal components we have

$$I_{12} = -\sum_i m_i x_i y_i = I_{21}. \tag{3.129}$$

By inspection, matrix I is symmetric. Also, since I appears in a physical equation of the form (3.127), which holds for all orientations of the coordinate system, it may be considered to be a tensor (quotient rule; Section 2.8). Note that $\mathbf{L}$ and $\boldsymbol{\omega}$ are not necessarily parallel, except when $\boldsymbol{\omega}$ is along special directions (the principal axes that we want to find).

The key now is to orient the coordinate axes (along a body-fixed frame) so that the I_{12} and the other nondiagonal elements will vanish. As a consequence of this orientation and an indication of it, if the angular velocity is along one such realigned **principal axis**, the angular velocity and the angular momentum will be parallel. As an illustration, the stability of rotation is used by football players when they throw the ball spinning about its long principal axis.

Eigenvectors and Eigenvalues

It is instructive to consider a geometrical picture of this principal axes problem. If the inertia matrix I is multiplied from each side by a unit vector of variable direction, $\hat{\mathbf{n}} = (n_1, n_2, n_3)$, then in the Dirac bracket notation of Section 3.2 as for the quadratic form $G = \langle \mathbf{x}|\mathsf{A}|\mathbf{x}\rangle$,

$$\langle \hat{\mathbf{n}}|\mathsf{I}|\hat{\mathbf{n}}\rangle = (n_1, n_2, n_3)\begin{pmatrix} I_{11} & I_{12} & I_{13} \\ I_{21} & I_{22} & I_{23} \\ I_{31} & I_{32} & I_{33} \end{pmatrix}\begin{pmatrix} n_1 \\ n_2 \\ n_3 \end{pmatrix} = I, \tag{3.130}$$

where I is the moment of inertia about the direction $\hat{\mathbf{n}}$. Carrying out the multiplications, we obtain

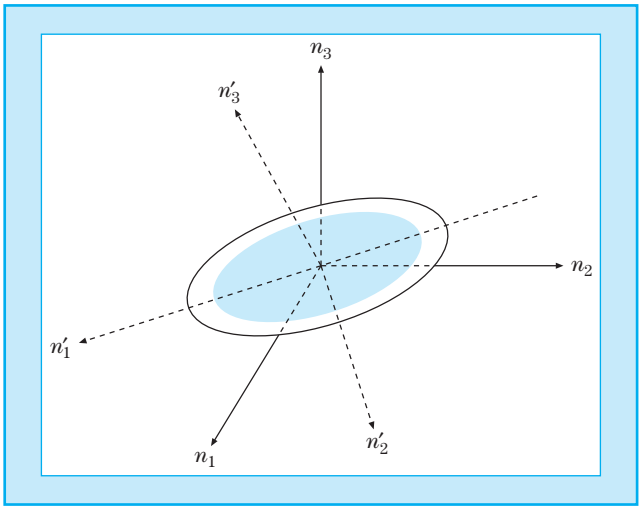
$$I = I_{11}n_1^2 + I_{22}n_2^2 + I_{33}n_3^2 + 2I_{12}n_1n_2 + 2I_{13}n_1n_3 + 2I_{23}n_2n_3, \tag{3.131}$$

a positive definite quadratic form that must be an ellipsoid (Fig. 3.9) because the moment of inertia about any axis is a positive observable. From analytic geometry and Example 1.5.3 we know that the coordinate axes can be rotated to coincide with the axes of our ellipsoid. In many elementary cases, especially when symmetry is present, these new axes, called the principal axes, can be found by inspection. This ellipsoid is a three-dimensional generalization of Example 1.5.3. Thus, we can find the axes by locating the local extrema of the ellipsoid in terms of the variable components of $\hat{\mathbf{n}}$, subject to the constraint $\hat{\mathbf{n}}^2 = 1$. To deal with the constraint, we introduce a Lagrange multiplier λ, just as we did in Example 1.5.4. Differentiating $\langle \hat{\mathbf{n}}|\mathsf{I}|\hat{\mathbf{n}}\rangle - \lambda\langle \hat{\mathbf{n}}|\hat{\mathbf{n}}\rangle$,

$$\frac{\partial}{\partial n_j}(\langle \hat{n}|\mathsf{I}|\hat{n}\rangle - \lambda\langle \hat{n}|\hat{n}\rangle) = 2\sum_k I_{jk}n_k - 2\lambda n_j = 0, \quad j = 1, 2, 3 \tag{3.132}$$

Figure 3.9

Moment of Inertia Ellipsoid



yields the eigenvalue equation

$$\mathsf{I}|\hat{\mathbf{n}}\rangle = \lambda|\hat{\mathbf{n}}\rangle. \tag{3.133}$$

The same result can be found by purely geometric methods. We now proceed to develop the geometric method of finding the diagonal elements and the principal axes.

If $\mathsf{R}^{-1} = \tilde{\mathsf{R}}$ is the real orthogonal matrix such that $\hat{\mathbf{n}}' = \mathsf{R}\hat{\mathbf{n}}$, or $|\hat{\mathbf{n}}'\rangle = \mathsf{R}|\hat{\mathbf{n}}\rangle$ in Dirac notation, are the coordinates along the principal axes, then we obtain using $\langle\hat{\mathbf{n}}'|\mathsf{R} = \langle\hat{\mathbf{n}}|$ in Eq. (3.130),

$$\langle\hat{\mathbf{n}}|\mathsf{I}|\hat{\mathbf{n}}\rangle = \langle\hat{\mathbf{n}}'|\mathsf{R}\mathsf{I}\tilde{\mathsf{R}}|\hat{\mathbf{n}}'\rangle = I_1' n_1'^2 + I_2' n_2'^2 + I_3' n_3'^2, \tag{3.134}$$

where $I_i' > 0$ are the principal moments of inertia. The inertia matrix I' in Eq. (3.134) is diagonal in the new coordinates,

$$\mathsf{I}' = \mathsf{R}\mathsf{I}\tilde{\mathsf{R}} = \begin{pmatrix} I_1' & 0 & 0 \\ 0 & I_2' & 0 \\ 0 & 0 & I_3' \end{pmatrix}. \tag{3.135}$$

If we rewrite Eq. (3.135) using $\mathsf{R}^{-1} = \tilde{\mathsf{R}}$ in the form

$$\tilde{\mathsf{R}}\mathsf{I}' = \mathsf{I}\tilde{\mathsf{R}}, \tag{3.136}$$

and take $\tilde{\mathsf{R}} = (\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3)$ to consist of three column vectors, then Eq. (3.136) splits into three eigenvalue equations

$$\mathsf{I}\mathbf{v}_i = I_i'\mathbf{v}_i, \quad i = 1, 2, 3 \tag{3.137}$$

with **eigenvalues** I_i' and **eigenvectors** $\mathbf{v}_i$. The names were introduced from the early German literature on quantum mechanics. Because these equations are linear and homogeneous (for fixed i), by Section 3.1 their determinants

have to vanish (for a nontrivial solution to exist):

$$\begin{vmatrix} I_{11} - I_i' & I_{12} & I_{13} \\ I_{12} & I_{22} - I_i' & I_{23} \\ I_{13} & I_{23} & I_{33} - I_i' \end{vmatrix} = 0. \tag{3.138}$$

Replacing the eigenvalue I_i' by a variable λ times the unit matrix 1, we may rewrite Eq. (3.137) as

$$(\mathsf{I} - \lambda 1)|\mathbf{v}\rangle = 0, \tag{3.139}$$

whose determinant

$$|\mathsf{I} - \lambda 1| = 0, \tag{3.140}$$

is a cubic polynomial in λ; its three roots, of course, are the I_i'. Substituting one root at a time back into Eq. (3.137) [or Eq. (3.139)], we can find the corresponding eigenvectors from Eq. (3.135).

Because of its applications in astronomical theories, Eq. (3.138) [or Eq. (3.140)] is known as the **secular equation**.[19] This method is also used in quantum mechanics to find the eigenvalues and eigenvectors of observables such as the Hamiltonian or angular momentum. The same treatment applies to any real symmetric matrix I, except that its eigenvalues need not all be positive, but they are real, of course. Because Eq. (3.137) is homogeneous, eigenvectors can always be normalized to unity, remaining eigenvectors. Also, the orthogonality condition in Eqs. (3.86)–(3.89) for R states that, in geometric terms, the eigenvectors v_i are mutually orthogonal unit vectors. (It is possible for two eigenvectors to have the same eigenvalue, which then are called degenerate eigenvalues.) Indeed, they form the new coordinate system. The fact that any two eigenvectors $\mathbf{v}_i$, $\mathbf{v}_j$ are orthogonal if $I_i' \neq I_j'$ follows from Eq. (3.137) in conjunction with the symmetry of $\mathbf{I}$ by multiplying with $\mathbf{v}_i$ and $\mathbf{v}_j$, respectively,

$$\langle \mathbf{v}_j|\mathsf{I}|\mathbf{v}_i\rangle = I_i'\mathbf{v}_j \cdot \mathbf{v}_i = \langle \mathbf{v}_i|\mathsf{I}|\mathbf{v}_j\rangle = I_j'\mathbf{v}_i \cdot \mathbf{v}_j. \tag{3.141}$$

Since $I_i' \neq I_j'$ and Eq. (3.137) implies that $(I_j' - I_i')\mathbf{v}_i \cdot \mathbf{v}_j = 0$, $\mathbf{v}_i \cdot \mathbf{v}_j = 0$.

Hermitian Matrices

For complex vector spaces Hermitian and unitary matrices play the same role as symmetric and orthogonal matrices for real vector spaces, respectively. First, let us generalize the important theorem about the diagonal elements and the principal axes for the eigenvalue equation

$$\mathsf{A}|\mathbf{r}\rangle = \lambda|\mathbf{r}\rangle. \tag{3.142}$$

We now show that if A is a Hermitian matrix,[20] its eigenvalues are real and its eigenvectors orthogonal.

[19] Equation (3.127) will take on this form when ω is along one of the principal axes. Then $\mathbf{L} = \lambda\boldsymbol{\omega}$ and $\mathsf{I}\boldsymbol{\omega} = \lambda\boldsymbol{\omega}$. In the mathematics literature λ is usually called a **characteristic value** and $\boldsymbol{\omega}$ a **characteristic vector**.

[20] If A is real, the Hermitian requirement is replaced by a requirement of symmetry.

Let λ_i and λ_j be two eigenvalues and $|\mathbf{r}_i\rangle$ and $|\mathbf{r}_j\rangle$ the corresponding eigenvectors of A, a Hermitian matrix. Then

$$\mathsf{A}|\mathbf{r}_i\rangle = \lambda_i|\mathbf{r}_i\rangle, \tag{3.143}$$

$$\mathsf{A}|\mathbf{r}_j\rangle = \lambda_j|\mathbf{r}_j\rangle. \tag{3.144}$$

Equation (3.143) is multiplied by $\langle\mathbf{r}_j|$:

$$\langle\mathbf{r}_j|\mathsf{A}|\mathbf{r}_i\rangle = \lambda_i\langle\mathbf{r}_j|\mathbf{r}_i\rangle. \tag{3.145}$$

Equation (3.144) is multiplied by $\langle\mathbf{r}_i|$ to give

$$\langle\mathbf{r}_i|\mathsf{A}|\mathbf{r}_j\rangle = \lambda_j\langle\mathbf{r}_i|\mathbf{r}_j\rangle. \tag{3.146}$$

Taking the adjoint[21] of this equation, we have

$$\langle\mathbf{r}_j|\mathsf{A}^\dagger|\mathbf{r}_i\rangle = \lambda_j^*\langle\mathbf{r}_j|\mathbf{r}_i\rangle \tag{3.147}$$

or

$$\langle\mathbf{r}_j|\mathsf{A}|\mathbf{r}_i\rangle = \lambda_j^*\langle\mathbf{r}_j|\mathbf{r}_i\rangle \tag{3.148}$$

as A is Hermitian. Subtracting Eq. (3.148) from Eq. (3.147), we obtain

$$(\lambda_i - \lambda_j^*)\langle\mathbf{r}_j|\mathbf{r}_i\rangle = 0. \tag{3.149}$$

This is a general result for all possible combinations of i and j. First, let $j = i$. Then Eq. (3.149) becomes

$$(\lambda_i - \lambda_i^*)\langle\mathbf{r}_i|\mathbf{r}_i\rangle = 0. \tag{3.150}$$

Because $\langle\mathbf{r}_i|\mathbf{r}_i\rangle = 0$ would be a trivial solution [$\langle\mathbf{r}_i| = (0, 0, 0)$] of Eq. (3.143), we conclude that

$$\lambda_i = \lambda_i^*, \tag{3.151}$$

or λ_i is real, for all i.

Second, for $i \neq j$, and $\lambda_i \neq \lambda_j$,

$$(\lambda_i - \lambda_j)\langle\mathbf{r}_j|\mathbf{r}_i\rangle = 0, \tag{3.152}$$

or

$$\langle\mathbf{r}_j|\mathbf{r}_i\rangle = 0, \tag{3.153}$$

which means that the eigenvectors of **distinct** eigenvalues are orthogonal, Eq. (3.153) being our generalization of orthogonality in this complex space.[22]

[21] Note $\langle\mathbf{r}_j| = |\mathbf{r}_j\rangle^\dagger$ for complex vectors, and $\langle\mathbf{r}|(\mathsf{A} - \lambda\cdot 1) = 0$ because $(\mathsf{A} - \lambda\cdot 1)^\dagger = \mathsf{A} - \lambda^*\cdot 1$.

[22] The corresponding theory for differential operators (Sturm–Liouville theory) appears in Section 9.2.

If $\lambda_i = \lambda_j$ (degenerate case), $|\mathbf{r}_i\rangle$ is not automatically orthogonal to $|\mathbf{r}_j\rangle$, but it may be **made** orthogonal.[23] Consider the physical problem of the moment of inertia matrix again. If x_1 is an axis of rotational symmetry, then we will find that $\lambda_2 = \lambda_3$. Eigenvectors $|\mathbf{r}_2\rangle$ and $|\mathbf{r}_3\rangle$ are each perpendicular to the symmetry axis, $|\mathbf{r}_1\rangle$, but they lie anywhere in the plane perpendicular to $|\mathbf{r}_1\rangle$; that is, any linear combination of $|\mathbf{r}_2\rangle$ and $|\mathbf{r}_3\rangle$ is also an eigenvector. Consider $(a_2|\mathbf{r}_2\rangle + a_3|\mathbf{r}_3\rangle)$ with a_2 and a_3 constants. Then

$$\begin{aligned} \mathsf{A}(a_2|\mathbf{r}_2\rangle + a_3|\mathbf{r}_3\rangle) &= a_2\lambda_2|\mathbf{r}_2\rangle + a_3\lambda_3|\mathbf{r}_3\rangle \\ &= \lambda_2(a_2|\mathbf{r}_2\rangle + a_3|\mathbf{r}_3\rangle), \end{aligned} \tag{3.154}$$

as is to be expected because x_1 is an axis of rotational symmetry. Therefore, if $|\mathbf{r}_1\rangle$ and $|\mathbf{r}_2\rangle$ are fixed, $|\mathbf{r}_3\rangle$ may simply be chosen to lie in the plane perpendicular to $|\mathbf{r}_1\rangle$ and also perpendicular to $|\mathbf{r}_2\rangle$. A general method of orthogonalizing solutions, the Gram–Schmidt process, is applied to functions in Section 9.3 but works for vectors similarly.

The set of n-orthogonal eigenvectors of our $n \times n$ Hermitian matrix forms a **complete** set, spanning the n-dimensional (complex) space. Eigenvalues and eigenvectors are not limited to Hermitian matrices. All matrices have at least one eigenvalue and eigenvector. However, only Hermitian matrices have a complete set of orthogonal eigenvectors **and** all eigenvalues real.

Anti-Hermitian Matrices

Occasionally, in quantum theory we encounter anti-Hermitian matrices:

$$\mathsf{A}^\dagger = -\mathsf{A}.$$

Following the analysis of the first portion of this section, we can show that

(a) The eigenvalues are pure imaginary (or zero).
(b) The eigenvectors corresponding to distinct eigenvalues are orthogonal.

The matrix R formed from the normalized eigenvectors is unitary. This anti-Hermitian property is preserved under unitary transformations.

EXAMPLE 3.5.1 **Eigenvalues and Eigenvectors of a Real Symmetric Matrix** Find the eigenvalues and eigenvectors of

$$\mathsf{A} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \tag{3.155}$$

[23] We are assuming here that the eigenvectors of the n-fold degenerate λ_i span the corresponding n-dimensional space. This may be shown by including a parameter ε in the original matrix to remove the degeneracy and then letting ε approach zero. This is analogous to breaking a degeneracy in atomic spectroscopy by applying an external magnetic field (Zeeman effect).

The secular equation is

$$\begin{vmatrix} -\lambda & 1 & 0 \\ 1 & -\lambda & 0 \\ 0 & 0 & -\lambda \end{vmatrix} = 0, \tag{3.156}$$

or

$$-\lambda(\lambda^2 - 1) = 0, \tag{3.157}$$

expanding by minors. The roots are $\lambda = -1, 0, 1$. To find the eigenvector corresponding to $\lambda = -1$, we substitute this value back into the eigenvalue equation [Eq. (3.142)],

$$\begin{pmatrix} -\lambda & 1 & 0 \\ 1 & -\lambda & 0 \\ 0 & 0 & -\lambda \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}. \tag{3.158}$$

With $\lambda = -1$, this yields

$$x + y = 0, \quad z = 0. \tag{3.159}$$

Within an arbitrary scale factor, and an arbitrary sign (or phase factor), $\langle \mathbf{r}_1| = (1, -1, 0)$. Note that (for real $|\mathbf{r}\rangle$ in ordinary space) the eigenvector singles out a line in space. The positive or negative sense is not determined. This indeterminacy could be expected if we noted that Eq. (3.158) is homogeneous in $|\mathbf{r}\rangle$ so that $|\mathbf{r}_1\rangle$ remains an eigenvector if multiplied by a nonzero constant. For convenience, we will require that the eigenvectors be normalized to unity, $\langle \mathbf{r}_1|\mathbf{r}_1\rangle = 1$. With this choice of sign,

$$\langle \mathbf{r}_1| = \left(\frac{1}{\sqrt{2}}, \frac{-1}{\sqrt{2}}, 0 \right) \tag{3.160}$$

is fixed. For $\lambda = 0$, Eq. (3.158) yields

$$y = 0, \quad x = 0. \tag{3.161}$$

$\langle \mathbf{r}_2| = (0, 0, 1)$ is a suitable eigenvector. Finally, for $\lambda = 1$, we get

$$-x + y = 0, \quad z = 0, \tag{3.162}$$

or

$$\langle \mathbf{r}_3| = \left(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0 \right). \tag{3.163}$$

The orthogonality of $\mathbf{r}_1$, $\mathbf{r}_2$, and $\mathbf{r}_3$, corresponding to three distinct eigenvalues, may be easily verified. ■

EXAMPLE 3.5.2 **Degenerate Eigenvalues** Consider

$$\mathsf{A} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}. \tag{3.164}$$

The secular equation is

$$\begin{vmatrix} 1-\lambda & 0 & 0 \\ 0 & -\lambda & 1 \\ 0 & 1 & -\lambda \end{vmatrix} = 0 \tag{3.165}$$

or

$$(1-\lambda)(\lambda^2-1)=0, \quad \lambda=-1,\,1,\,1, \tag{3.166}$$

a degenerate case. If $\lambda=-1$, the eigenvalue equation (3.142) yields

$$2x=0, \quad y+z=0. \tag{3.167}$$

A suitable normalized eigenvector is

$$\langle \mathbf{r}_1| = \left(0, \frac{1}{\sqrt{2}}, \frac{-1}{\sqrt{2}}\right). \tag{3.168}$$

For $\lambda=1$, we get

$$-y+z=0. \tag{3.169}$$

Any eigenvector satisfying Eq. (3.169) is perpendicular to $\mathbf{r}_1$. We have an infinite number of choices. Suppose, as one possible choice, $\mathbf{r}_2$ is taken as

$$\langle \mathbf{r}_2| = \left(0, \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right), \tag{3.170}$$

which clearly satisfies Eq. (3.169). Then $\mathbf{r}_3$ must be perpendicular to $\mathbf{r}_1$ and may be made perpendicular to $\mathbf{r}_2$ by[24]

$$\mathbf{r}_3 = \mathbf{r}_1 \times \mathbf{r}_2 = (1, 0, 0). \tag{3.171}$$

■

Normal Modes of Vibration

We consider the vibrations of a classical model of the CO_2 molecule. It is an illustration of the application of matrix techniques to a problem that does not start as a matrix problem. It also provides an example of the eigenvalues and eigenvectors of an asymmetric real matrix.

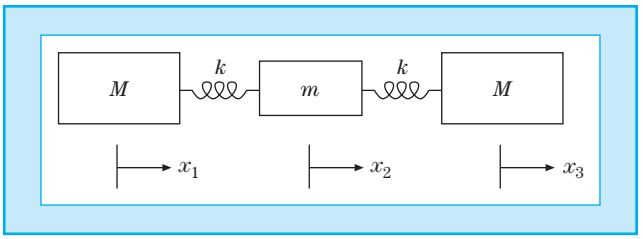
EXAMPLE 3.5.3

Normal Modes Consider three masses on the x-axis joined by springs as shown in Fig. 3.10. The spring forces are assumed to be linear (small displacements; Hooke's law) and the mass is constrained to stay on the x-axis.

[24]The use of the cross product is limited to three-dimensional space (see Section 1.3).

Figure 3.10

Double Oscillator



Using a different coordinate for each mass, Newton's second law yields the set of equations

$$\begin{aligned}\ddot{x}_1 &= -\frac{k}{M}(x_1 - x_2)\\ \ddot{x}_2 &= -\frac{k}{m}(x_2 - x_1) - \frac{k}{m}(x_2 - x_3)\\ \ddot{x}_3 &= -\frac{k}{M}(x_3 - x_2).\end{aligned} \tag{3.172}$$

The system of masses is vibrating. We seek the common frequencies, ω, such that all masses vibrate at this same frequency. These are the **normal** modes. Let

$$x_i = x_{i0}e^{i\omega t}, \quad i = 1, 2, 3.$$

Substituting this set into Eq. (3.172), we may rewrite it as

$$\begin{pmatrix} \frac{k}{M} & -\frac{k}{M} & 0 \\ -\frac{k}{m} & \frac{2k}{m} & -\frac{k}{m} \\ 0 & -\frac{k}{M} & \frac{k}{M} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = +\omega^2 \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}, \tag{3.173}$$

with the common factor $e^{i\omega t}$ divided out. We have an eigenvalue problem whose matrix is not symmetric. Therefore, the eigenvectors will not be mutually orthogonal. The secular equation is

$$\begin{vmatrix} \frac{k}{M} - \omega^2 & -\frac{k}{M} & 0 \\ -\frac{k}{m} & \frac{2k}{m} - \omega^2 & -\frac{k}{m} \\ 0 & -\frac{k}{M} & \frac{k}{M} - \omega^2 \end{vmatrix} = 0. \tag{3.174}$$

This leads to

$$\omega^2\left(\frac{k}{M} - \omega^2\right)\left(\omega^2 - \frac{2k}{m} - \frac{k}{M}\right) = 0.$$

The eigenvalues are

$$\omega^2 = 0, \quad \frac{k}{M}, \quad \frac{k}{M} + \frac{2k}{m},$$

all real.

The corresponding eigenvectors are determined by substituting the eigenvalues back into Eq. (3.173), one at a time. For $\omega^2 = 0$, this yields

$$x_1 - x_2 = 0, \qquad -x_1 + 2x_2 - x_3 = 0, \qquad -x_2 + x_3 = 0.$$

Then, we get

$$x_1 = x_2 = x_3.$$

This describes pure translation with no relative motion of the masses and no vibration.

For $\omega^2 = k/M$, Eq. (3.173) yields

$$x_1 = -x_3, \quad x_2 = 0.$$

The two outer masses are moving in opposite direction. The center mass is stationary.

For $\omega^2 = k/M + 2k/m$ the eigenvector components are

$$x_1 = x_3, \quad x_2 = -\frac{2M}{m}x_1.$$

The two outer masses are moving together. The center mass is moving opposite to the two outer ones. The net momentum is zero.

Any displacement of the three masses along the x-axis can be described as a linear combination of these three types of motion: translation plus two forms of vibration. ■

Ill-Conditioned Systems

A system of simultaneous linear equations may be written as

$$\mathsf{A}|\mathbf{x}\rangle = |\mathbf{y}\rangle \quad \text{or} \quad \mathsf{A}^{-1}|\mathbf{y}\rangle = |\mathbf{x}\rangle, \tag{3.175}$$

with A and $|\mathbf{y}\rangle$ known and $|\mathbf{x}\rangle$ unknown. The reader may encounter examples in which a small error in $|\mathbf{y}\rangle$ results in a larger error in $|\mathbf{x}\rangle$. In this case, the matrix A is called ill-conditioned. With $|\delta\mathbf{x}\rangle$ an error in $|\mathbf{x}\rangle$ and $|\delta\mathbf{y}\rangle$ an error in $|\mathbf{y}\rangle$, the relative errors may be written as

$$\left[\frac{\langle\delta\mathbf{x}|\delta\mathbf{x}\rangle}{\langle\mathbf{x}|\mathbf{x}\rangle}\right]^{1/2} \le K(\mathsf{A})\left[\frac{\langle\delta\mathbf{y}|\delta\mathbf{y}\rangle}{\langle\mathbf{y}|\mathbf{y}\rangle}\right]^{1/2}, \tag{3.176}$$

where $K(\mathsf{A})$, a property of matrix A, is the **condition number**. For A Hermitian one form of the condition number is given by[25]

$$K(\mathsf{A}) = \frac{|\lambda|_{\max}}{|\lambda|_{\min}}. \tag{3.177}$$

[25]Forsythe, G. E., and Moler, C. B. (1967). *Computer Solution of Linear Algebraic Systems*. Prentice Hall, Englewood Cliffs, NJ.

An approximate form due to Turing[26] is

$$K(\mathsf{A}) = n[A_{ij}]_{\max}\left[A_{ij}^{-1}\right]_{\max}, \tag{3.178}$$

in which n is the order of the matrix and $[A_{ij}]_{\max}$ is the maximum element in A.

EXAMPLE 3.5.4

An Ill-Conditioned Matrix A common example of an ill-conditioned matrix is the Hilbert matrix, $H_{ij} = (i + j - 1)^{-1}$. The Hilbert matrix of order 4, H_4, is encountered in a least-squares fit of data to a third-degree polynomial. We have

$$\mathsf{H}_4 = \begin{pmatrix} 1 & \frac{1}{2} & \frac{1}{3} & \frac{1}{4} \\ \frac{1}{2} & \frac{1}{3} & \frac{1}{4} & \frac{1}{5} \\ \frac{1}{3} & \frac{1}{4} & \frac{1}{5} & \frac{1}{6} \\ \frac{1}{4} & \frac{1}{5} & \frac{1}{6} & \frac{1}{7} \end{pmatrix}. \tag{3.179}$$

The elements of the inverse matrix (order n) are given by

$$\left(\mathsf{H}_n^{-1}\right)_{ij} = \frac{(-1)^{i+j}}{i+j-1} \cdot \frac{(n+i-1)!(n+j-1)!}{[(i-1)!(j-1)!]^2(n-i)!(n-j)!}. \tag{3.180}$$

For $n = 4$

$$\mathsf{H}_4^{-1} = \begin{pmatrix} 16 & -120 & 240 & -140 \\ -120 & 1200 & -2700 & 1680 \\ 240 & -2700 & 6480 & -4200 \\ -140 & 1680 & -4200 & 2800 \end{pmatrix}. \tag{3.181}$$

From Eqs. (3.179), (3.181), the Turing estimate of the condition number for H_4 becomes

$$K_{\text{Turing}} = 4 \times 1 \times 6480 = 2.59 \times 10^4. \quad \blacksquare$$

This is a warning that an input error may be multiplied by 26,000 in the calculation of the output result. It is a statement that H_4 is ill-conditioned. If you encounter a highly ill-conditioned system, you have two alternatives (besides abandoning the problem):

(a) Try a different mathematical attack.
(b) Arrange to carry more significant figures and push through by brute force.

As previously seen, matrix eigenvector–eigenvalue techniques are not limited to the solution of strictly matrix problems.

Functions of Matrices

Polynomials with one or more matrix arguments are well defined and occur often. Power series of a matrix may also be defined provided the series

[26] Compare Todd, J., *The Condition of the Finite Segments of the Hilbert Matrix*, Applied Mathematics Series No. 313. National Bureau of Standards, Washington, DC.

converge (see Chapter 5) for each matrix element. For example, if A is any $n \times n$ matrix, then the power series

$$\exp(\mathsf{A}) = \sum_{i=0}^{\infty} \frac{1}{i!}\mathsf{A}^i, \tag{3.182a}$$

$$\sin(\mathsf{A}) = \sum_{i=0}^{\infty} \frac{(-1)^i}{(2i+1)!}\mathsf{A}^{2i+1}, \tag{3.182b}$$

$$\cos(\mathsf{A}) = \sum_{i=0}^{\infty} \frac{(-1)^i}{(2i)!}\mathsf{A}^{2i} \tag{3.182c}$$

are well-defined $n \times n$ matrices. For the Pauli matrices σ_k the **Euler identity** for real θ and $k = 1, 2,$ or 3

$$\exp(i\sigma_k\theta) = 1_2 \cos\theta + i\sigma_k \sin\theta, \tag{3.183}$$

follows from the Mclaurin series for the exponential collecting all even and odd powers of θ in an even and odd power series using $\sigma_k^2 = 1$:

$$\begin{aligned} e^{i\sigma_k\theta} = \sum_{n=0}^{\infty} \frac{1}{n!}(i\sigma_k\theta)^n &= \sum_{m=0}^{\infty} \frac{i^{2m}}{(2m)!}(\sigma_k)^{2m}\theta^{2m} \\ &\quad + \sum_{m=0}^{\infty} \frac{i^{2m+1}}{(2m+1)!}(\sigma_k)^{2m+1}\theta^{2m+1} \\ &= \sum_{m=0}^{\infty} \frac{(-1)^m}{(2m)!}\theta^{2m} + i\sigma_k \sum_{m=0}^{\infty} \frac{(-1)^m}{(2m+1)!}\theta^{2m+1}. \end{aligned}$$

EXAMPLE 3.5.5

Exponential of a Diagonal Matrix If the matrix A is diagonal, such as $\sigma_3 = \left(\begin{smallmatrix} 1 & 0 \\ 0 & -1 \end{smallmatrix}\right)$, then its nth power is also diagonal, with its diagonal matrix elements raised to the nth power: $(\sigma_3)^n = \left(\begin{smallmatrix} 1 & 0 \\ 0 & (-1)^n \end{smallmatrix}\right)$. Then summing the exponential series element for element yields

$$e^{\sigma_3} = \begin{pmatrix} \sum_{n=0}^{\infty} \frac{1}{n!} & 0 \\ 0 & \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \end{pmatrix} = \begin{pmatrix} e & 0 \\ 0 & \frac{1}{e} \end{pmatrix}.$$

If we write the general diagonal matrix as $\mathsf{A} = [a_1, a_2, \cdots, a_n]$ with diagonal elements a_j, then $\mathsf{A}^m = [a_1^m, a_2^m, \cdots, a_n^m]$, and summing the exponentials elementwise again we obtain $e^{\mathsf{A}} = [e^{a_1}, e^{a_2}, \ldots, e^{a_n}]$. ■

For a Hermitian matrix A there is a unitary matrix U that diagonalizes it; that is, $\mathsf{UAU}^\dagger = [a_1, a_2, \ldots, a_n]$. Then the **trace formula**

$$\det(\exp(\mathsf{A})) = \exp(\text{trace}\,(\mathsf{A})) \tag{3.184}$$

is obtained (see Exercises 3.5.2 and 3.5.9) from

$$\begin{aligned}\det(\exp(\mathsf{A})) &= \det(\mathsf{U}\exp(\mathsf{A})\mathsf{U}^\dagger) = \det(\exp(\mathsf{U}\mathsf{A}\mathsf{U}^\dagger))\\ &= \det(\exp[a_1, a_2, \ldots, a_n] = \det[e^{a_1}, e^{a_2}, \ldots, e^{a_n}]\\ &= \prod e^{a_i} = \exp\left(\sum a_i\right) = \exp(\text{trace}(\mathsf{A})),\end{aligned}$$

using $\mathsf{U}\mathsf{A}^i\mathsf{U}^\dagger = (\mathsf{U}\mathsf{A}\mathsf{U}^\dagger)^i$ in the power series Eq. (3.182a) for $\exp(\mathsf{U}\mathsf{A}\mathsf{U}^\dagger)$ and the product theorem for determinants in Section 3.2.

Another important relation is the **Baker–Hausdorff formula**

$$\exp(i\mathsf{G})\mathsf{H}\exp(-i\mathsf{G}) = \mathsf{H} + [i\mathsf{G}, \mathsf{H}] + \frac{1}{2}[i\mathsf{G}, [i\mathsf{G}, \mathsf{H}]] + \cdots, \tag{3.185}$$

which follows from multiplying the power series for $\exp(iG)$ and collecting the terms with the same powers of iG. Here we define

$$[\mathsf{G}, \mathsf{H}] = \mathsf{G}\mathsf{H} - \mathsf{H}\mathsf{G}$$

as the **commutator** of G and H.

The preceding analysis has the advantage of exhibiting and clarifying conceptual relationships in the diagonalization of matrices. However, for matrices larger than 3×3, or perhaps 4×4, the process rapidly becomes so cumbersome that we turn gratefully to computers and iterative techniques.[27] One such technique is the Jacobi method for determining eigenvalues and eigenvectors of real symmetric matrices. This Jacobi technique and the Gauss–Seidel method of solving systems of simultaneous linear equations are examples of relaxation methods. They are iterative techniques in which the errors will, it is hoped, decrease or relax as the iterations continue. Relaxation methods are used extensively for the solution of partial differential equations.

SUMMARY

The diagonalization of a real symmetric matrix rotates the quadratic form that it defines to its principal axes. A unitary matrix achieves the same for a Hermitian matrix in a complex space. The eigenvectors define the principal axes and the eigenvalues the principal moments. Eigenvalue problems occur in classical mechanics in the search for the normal modes of oscillators and in quantum mechanics as solutions of the Schrödinger equation.

EXERCISES

3.5.1 (a) Starting with the orbital angular momentum of the ith element of mass,

$$\mathbf{L}_i = \mathbf{r}_i \times \mathbf{p}_i = m_i\mathbf{r}_i \times (\boldsymbol{\omega} \times \mathbf{r}_i),$$

derive the inertia matrix such that $\mathbf{L} = \mathsf{I}\boldsymbol{\omega}$, $|\mathbf{L}\rangle = \mathsf{I}|\boldsymbol{\omega}\rangle$.

[27] In higher dimensional systems the secular equation may be strongly ill-conditioned with respect to the determination of its roots (the eigenvalues). Direct solution by computer may be very inaccurate. Iterative techniques for diagonalizing the original matrix are usually preferred. See Sections 2.7 and 2.9 of Press *et al.*, loc. cit.

(b) Repeat the derivation starting with kinetic energy

$$T_i = \frac{1}{2} m_i (\boldsymbol{\omega} \times \mathbf{r}_i)^2 \quad \left(T = \frac{1}{2} \langle \omega | \mathsf{I} | \omega \rangle \right).$$

3.5.2 Show that the eigenvalues of a matrix are unaltered if the matrix is transformed by a similarity transformation. This property is not limited to symmetric or Hermitian matrices. It holds for any matrix satisfying the eigenvalue equation [Eq. (3.139)]. If our matrix can be brought into diagonal form by a similarity transformation, then two immediate consequences are

(1) The trace (sum of eigenvalues) is invariant under a similarity transformation.

(2) The determinant (product of eigenvalues) is invariant under a similarity transformation.

Note. Prove this **separately** (for matrices that cannot be diagonalized). The invariance of the trace and determinant are often demonstrated by using the Cayley–Hamilton theorem: A matrix satisfies its own characteristic (secular) equation.

3.5.3 As a converse of the theorem that Hermitian matrices have real eigenvalues and that eigenvectors corresponding to distinct eigenvalues are orthogonal, show that if

(a) the eigenvalues of a matrix are real and

(b) the eigenvectors satisfy $\mathbf{r}_i^\dagger \mathbf{r}_j = \delta_{ij} = \langle \mathbf{r}_i | \mathbf{r}_j \rangle$,

then the matrix is Hermitian.

3.5.4 Show that a real matrix that is not symmetric cannot be diagonalized by an orthogonal similarity transformation.

Hint. Assume that the nonsymmetric real matrix can be diagonalized and develop a contradiction.

3.5.5 The matrices representing the angular momentum components J_x, J_y, and J_z are all Hermitian. Show that the eigenvalues of $\mathbf{J}^2$, where $\mathbf{J}^2 = J_x^2 + J_y^2 + J_z^2$, are real and nonnegative.

3.5.6 A has eigenvalues λ_i and corresponding eigenvectors $|\mathbf{x}_i\rangle$. Show that A^{-1} has the same eigenvectors but with eigenvalues λ_i^{-1}.

3.5.7 A square matrix with zero determinant is labeled **singular**.

(a) If A is singular, show that there is at least one nonzero column vector $\mathbf{v}$ such that

$$\mathsf{A}|\mathbf{v}\rangle = 0.$$

(b) If there is a nonzero vector $|\mathbf{v}\rangle$ such that

$$\mathsf{A}|\mathbf{v}\rangle = 0,$$

show that A is a singular matrix. This means that if a matrix (or operator) has zero as an eigenvalue, the matrix (or operator) has no inverse and its determinant is zero.

3.5.8 The same similarity transformation diagonalizes each of two matrices. Show that the original matrices must commute. [This is particularly important in the matrix (Heisenberg) formulation of quantum mechanics.]

3.5.9 Two Hermitian matrices A and B have the same eigenvalues. Show that A and B are related by a unitary similarity transformation.

3.5.10 Show that the inertia matrix for a single particle of mass m at (x, y, z) has a zero determinant. Explain this result in terms of the invariance of the determinant of a matrix under similarity transformations (Exercise 3.3.10) and a possible rotation of the coordinate system.

3.5.11 Unit masses are at the eight corners of a cube $(\pm 1, \pm 1, \pm 1)$. Find the moment of inertia matrix and show that there is a triple degeneracy. This means that as far as moments of inertia are concerned, the cubic structure exhibits spherical symmetry.

3.5.12 Find the eigenvalues and corresponding orthonormal eigenvectors of the following matrices (as a numerical check, note that the sum of the eigenvalues equals the sum of the diagonal elements of the original matrix; Exercise 3.3.9). Note also the correspondence between $\det \mathsf{A} = 0$ and the existence of $\lambda = 0$, as required by Exercises 3.5.2 and 3.5.7:

$$\mathsf{A} = \begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix}. \qquad \textit{ANS.}\ \ \lambda = 0, 1, 2.$$

3.5.13

$$\mathsf{A} = \begin{pmatrix} 5 & 0 & \sqrt{3} \\ 0 & 3 & 0 \\ \sqrt{3} & 0 & 3 \end{pmatrix}. \qquad \textit{ANS.}\ \ \lambda = 2, 3, 6.$$

3.5.14

$$\mathsf{A} = \begin{pmatrix} 1 & \sqrt{2} & 0 \\ \sqrt{2} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \qquad \textit{ANS.}\ \ \lambda = -1, 0, 2.$$

3.5.15

$$\mathsf{A} = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix}. \qquad \textit{ANS.}\ \ \lambda = 0, 0, 3.$$

3.5.16 Write $x^2 + 2xy + 2yz + z^2$ as a sum of squares $x'^2 - y'^2 + 2z'^2$ in a rotated coordinate system.

3.5.17 Describe the geometric properties of the surface

$$x^2 + 2xy + 2y^2 + 2xz + z^2 = 1.$$

How is it oriented in three-space? Is it a conic section? If so, which kind?

3.5.18 Show that every 2×2 matrix has two eigenvectors and corresponding eigenvalues. The eigenvectors are not necessarily orthogonal or different. The eigenvalues are not necessarily real.

3.5.19 As an illustration of Exercise 3.5.18, find the eigenvalues and corresponding eigenvectors for

$$\begin{pmatrix} 2 & 4 \\ 1 & 2 \end{pmatrix}.$$

Note that the eigenvectors are **not** orthogonal.

ANS. $\lambda_1 = 0$, $\langle \mathbf{r}_1| = (2, -1)$;
$\lambda_2 = 4$, $\langle \mathbf{r}_2| = (2, \ 1)$.

3.5.20 If A is a 2×2 matrix, show that its eigenvalues λ satisfy the equation

$$\lambda^2 - \lambda \ \text{trace}(\mathsf{A}) + \det \mathsf{A} = 0.$$

3.5.21 Assuming a unitary matrix U to satisfy an eigenvalue equation $\mathsf{U}\mathbf{r} = \lambda\mathbf{r}$, show that the eigenvalues of the unitary matrix have unit magnitude. This same result holds for real orthogonal matrices.

3.5.22 Since an orthogonal matrix describing a rotation in real three-dimensional space is a special case of a unitary matrix, such an orthogonal matrix can be diagonalized by a unitary transformation.

(a) Show that the sum of the three eigenvalues is $1 + 2\cos\varphi$, where φ is the net angle of rotation about a single fixed axis.

(b) Given that one eigenvalue is 1, show that the other two eigenvalues must be $e^{i\varphi}$ and $e^{-i\varphi}$.

Our orthogonal rotation matrix (real elements) has complex eigenvalues.

3.5.23 A is an nth-order Hermitian matrix with orthonormal eigenvectors $|\mathbf{x}_i\rangle$ and real eigenvalues $\lambda_1 \le \lambda_2 \le \lambda_3 \le \cdots \le \lambda_n$. Show that for a unit magnitude vector $|\mathbf{y}\rangle$,

$$\lambda_1 \le \langle \mathbf{y}|\mathsf{A}|\mathbf{y}\rangle \le \lambda_n.$$

3.5.24 A particular matrix is both Hermitian and unitary. Show that its eigenvalues are all ± 1.

Note. The Pauli matrices are specific examples.

3.5.25 A has eigenvalues 1 and -1 and corresponding eigenvectors $\binom{1}{0}$ and $\binom{0}{1}$. Construct A.

ANS. $\mathsf{A} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$.

3.5.26 A non-Hermitian matrix A has eigenvalues λ_i and corresponding eigenvectors $|\mathbf{u}_i\rangle$. The adjoint matrix $\mathsf{A}^\dagger$ has the same set of eigenvalues but **different** corresponding eigenvectors, $|\mathbf{v}_i\rangle$. Show that the eigenvectors form a **biorthogonal** set in the sense that

$$\langle \mathbf{v}_i | \mathbf{u}_j \rangle = 0 \quad \text{for} \quad \lambda_i^* \neq \lambda_j.$$

3.5.27 An $n \times n$ matrix A has n eigenvalues A_i. If $\mathsf{B} = e^{\mathsf{A}}$ show that B has the same eigenvectors as A, with the corresponding eigenvalues B_i given by $B_i = \exp(A_i)$.
Note. e^{A} is defined by the Maclaurin expansion of the exponential:

$$e^{\mathsf{A}} = 1 + \mathsf{A} + \frac{\mathsf{A}^2}{2!} + \frac{\mathsf{A}^3}{3!} + \cdots.$$

3.5.28 A matrix P is a projection operator satisfying the condition

$$\mathsf{P}^2 = \mathsf{P}.$$

Show that the corresponding eigenvalues $(\rho^2)_\lambda$ and ρ_λ satisfy the relation

$$(\rho^2)_\lambda = (\rho_\lambda)^2 = \rho_\lambda.$$

This means that the eigenvalues of P are 0 and 1.

3.5.29 In the **matrix** eigenvector–eigenvalue equation

$$\mathsf{A}|\mathbf{r}_i\rangle = \lambda_i |\mathbf{r}_i\rangle,$$

A is an $n \times n$ Hermitian matrix. For simplicity, assume that its n real eigenvalues are distinct, λ_1 being the largest. If $|\mathbf{r}\rangle$ is an approximation to $|\mathbf{r}_1\rangle$,

$$|\mathbf{r}\rangle = |\mathbf{r}_1\rangle + \sum_{i=2}^{n} \delta_i |\mathbf{r}_i\rangle,$$

show that

$$\frac{\langle \mathbf{r}|\mathsf{A}|\mathbf{r}\rangle}{\langle \mathbf{r}|\mathbf{r}\rangle} \leq \lambda_1$$

and that the error in λ_1 is of the order $|\delta_i|^2$. Take $|\delta_i| \ll 1$.
Hint. The n $|\mathbf{r}_i\rangle$ form a **complete** orthogonal set spanning the n-dimensional (complex) space.

3.5.30 Two equal masses are connected to each other and to walls by springs as shown in Fig. 3.11. The masses are constrained to stay on a horizontal line.

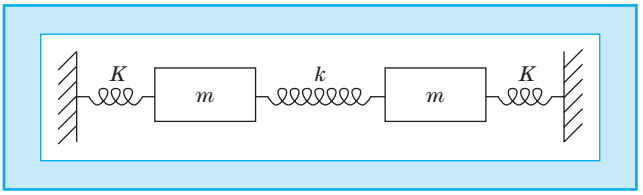


Figure 3.11
Coupled Harmonic Oscillators

(a) Set up the Newtonian acceleration equation for each mass.
(b) Solve the secular equation for the eigenvectors.
(c) Determine the eigenvectors and thus the normal modes of motion.

Additional Reading

Aitken A. C. (1956). *Determinants and Matrices*. Interscience, New York. Reprinted, Greenwood (1983). A readable introduction to determinants and matrices.

Barnett, S. (1990). *Matrices: Methods and Applications*. Clarendon, Oxford.

Bickley, W. G., and Thompson, R. S. H. G. (1964). *Matrices—Their Meaning and Manipulation*. Van Nostrand, Princeton, NJ. A comprehensive account of the occurrence of matrices in physical problems, their analytic properties, and numerical techniques.

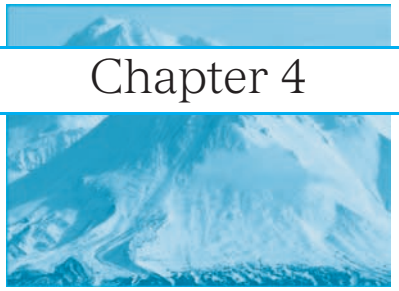
Brown, W. C. (1991). *Matrices and Vector Spaces*. Dekker, New York.

Gilbert, J., and Gilbert, L. (1995). *Linear Algebra and Matrix Theory*. Academic Press, San Diego.

Heading, J. (1958). *Matrix Theory for Physicists*. Longmans, Green, London. A readable introduction to determinants and matrices with applications to mechanics, electromagnetism, special relativity, and quantum mechanics.

Vein, R., and Dale, P. (1998). *Determinants and Their Applications in Mathematical Physics*. Springer, Berlin.

Watkins, D. S. (1991). *Fundamentals of Matrix Computations*. Wiley, New York.



Chapter 4

Group Theory

Disciplined judgment, about what is neat and symmetrical and elegant, has time and time again proved an excellent guide to how nature works.

—Murray Gell-Mann

4.1 Introduction to Group Theory

In classical mechanics the **symmetry** of a physical system leads to **conservation laws**. Conservation of angular momentum ($\mathbf{L}$) is a direct consequence of rotational symmetry, which means **invariance** of some physical observables (such as $\mathbf{L}^2$) or geometrical quantities (such as length of a vector or distance between points) under spatial rotations. In the first third of this century, Wigner and others realized that invariance was a key concept in understanding the new quantum phenomena and in developing appropriate theories. For example, Noether's theorem establishes a conserved current from an invariance of the Lagrangian of a field theory. Thus, in quantum mechanics the concept of angular momentum and spin has become even more central. Its generalizations, **isospin** in nuclear physics and the **flavor symmetry** in particle physics, are indispensable tools in building and solving theories. Generalizations of the concept of **gauge invariance** of classical electrodynamics to the isospin symmetry lead to the electroweak gauge theory.

In each case the set of these symmetry operations forms a group, a mathematical concept we shall soon define. Group theory is the mathematical tool to treat invariants and symmetries. It brings unification and formalization of

principles such as spatial reflections, or parity, angular momentum, and geometry that are widely used by physicists.

In geometry the fundamental role of group theory was recognized more than a century ago by mathematicians (e.g., Felix Klein's Erlanger Programm). In Euclidean geometry the distance between two points, the scalar product of two vectors or metric, does not change under rotations or translations. These symmetries are characteristic of this geometry. In special relativity the metric, or scalar product of four-vectors, differs from that of Euclidean geometry in that it is no longer positive definite and is invariant under Lorentz transformations.

For a crystal, the symmetry group contains only a finite number of rotations at discrete values of angles or reflections. The theory of such **discrete** or **finite** groups, developed originally as a branch of pure mathematics, is now a useful tool for the development of crystallography and condensed matter physics. When the rotations depend on continuously varying angles (e.g., the Euler angles of Section 3.3) the rotation groups have an infinite number of elements. Such continuous (or **Lie**)[1] **groups** are the topic of this chapter.

Definition of Group

A group G may be defined as a set of objects or, in physics usually, symmetry operations (such as rotations or Lorentz transformations), called the elements g of G, that may be combined or "multiplied" to form a well-defined product in G that satisfies the following conditions:

1. If a and b are any two elements of G, then the product ab is also an element of G. In terms of symmetry operations, b is applied to the physical system before a in the product, and the product ab is equivalent to a single symmetry operation in G. Multiplication associates (or maps) an element ab of G with the pair (a, b) of elements of G; this property is known as **closure** under multiplication.
2. This multiplication is **associative**, $(ab)c = a(bc)$.
3. There is a **unit or identity** element[2] 1 in G such that $1a = a1 = a$ for every element a in G.
4. G must contain an **inverse or reciprocal** of every element a of G, labeled a^{-1} such that $aa^{-1} = a^{-1}a = 1$.

Note that the unit is unique, as is the inverse. The inverse of 1 is 1 because $1a = a1 = a$ for $a = 1$ yields $1 \cdot 1 = 1$. If a second unit $1'$ existed we would have $11' = 1'1 = 1'$ and $1'1 = 11' = 1$. Comparing we see that $1' = 1$. Similarly, if a second inverse a'^{-1} existed we would have $a^{-1}a = aa^{-1} = 1 = aa'^{-1}$. Multiplying by a^{-1}, we get $a^{-1} = a'^{-1}$.

[1] After the Norwegian mathematician Sophus Lie.

[2] Following E. Wigner, the unit element of a group is often labeled E, from the German **Einheit** (i.e., unit) or just 1 or I for identity.

EXAMPLE 4.1.1

Coordinate Rotation An example of a group is the set of counterclockwise coordinate rotations

$$|\mathbf{x}'\rangle = \begin{pmatrix} x' \\ y' \end{pmatrix} \equiv \mathsf{R}(\varphi)\begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} \cos\varphi & \sin\varphi \\ -\sin\varphi & \cos\varphi \end{pmatrix}\begin{pmatrix} x \\ y \end{pmatrix} \tag{4.1}$$

through an angle φ of the xy-coordinate system to a new orientation (see Fig. 2.20). The product of two rotations is defined by rotating first by the angle φ_2 and then by φ_1. According to Eqs. (3.36) and (3.37), the product of the orthogonal 2×2 matrices, $\mathsf{R}(\varphi_1)\mathsf{R}(\varphi_2)$, describes the product of two rotations

$$\begin{aligned} &\begin{pmatrix} \cos\varphi_1 & \sin\varphi_1 \\ -\sin\varphi_1 & \cos\varphi_1 \end{pmatrix}\begin{pmatrix} \cos\varphi_2 & \sin\varphi_2 \\ -\sin\varphi_2 & \cos\varphi_2 \end{pmatrix} \\ &\quad = \begin{pmatrix} \cos(\varphi_1+\varphi_2) & \sin(\varphi_1+\varphi_2) \\ -\sin(\varphi_1+\varphi_2) & \cos(\varphi_1+\varphi_2) \end{pmatrix}, \end{aligned} \tag{4.2}$$

using the addition formulas for the trigonometric functions. The product is clearly a rotation represented by the orthogonal matrix with angle $\varphi_1+\varphi_2$. The product is the associative matrix multiplication. It is **commutative** or **Abelian** because the order in which these rotations are performed does not matter. The inverse of the rotation with angle φ is that with angle $-\varphi$. The unit corresponds to the angle $\varphi = 0$. The group's name is SO(2), which stands for **special orthogonal rotations in two dimensions**, where special means the 2×2 rotation matrices have determinant $+1$, and the angle φ varies continuously from 0 to 2π, so that the group has infinitely many elements. The angle is the **group parameter**. ■

A **subgroup** G' of a group G is a group consisting of elements of G so that the product of any of its elements is again in the subgroup G'; that is, G' is **closed** under the multiplication of G. For example, the unit 1 of G always forms a subgroup of G, and the unity with angle $\varphi = 0$ and the rotation with $\varphi = \pi$ about some axis form a finite subgroup of the group of rotations about that axis.

If $gg'g^{-1}$ is an element of G' for any g of G and g' of G', then G' is called an **invariant subgroup** of G. If the group elements are matrices, then the element $gg'g^{-1}$ corresponds to a similarity transformation [see Eq. (3.108)] of g' in G' by an element g of G (discussed in Chapter 3). Of course, the unit 1 of G always forms an invariant subgroup of G because $g1g^{-1} = 1$. When an element g of G lies outside the subgroup G', then $gg'g^{-1}$ may also lie outside G'. Let us illustrate this by three-dimensional rotations.

EXAMPLE 4.1.2

Similarity Transformation Rotations of the coordinates through a finite angle φ counterclockwise about the z-axis in three-dimensional space are described as

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \mathsf{R}_z(\varphi)\begin{pmatrix} x \\ y \\ z \end{pmatrix} \equiv \begin{pmatrix} \cos\varphi & \sin\varphi & 0 \\ -\sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} x \\ y \\ z \end{pmatrix}, \tag{4.3}$$

which form a group by a generalization of Eq. (4.2) to our special 3×3 matrices that keep their special form on multiplication. Moreover, the order of the rotations in a product does not matter, just like in Eq. (4.2), so that the group is Abelian. A general rotation about the x-axis is given by the matrix

$$\mathsf{R}_x(\varphi) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\varphi & \sin\varphi \\ 0 & -\sin\varphi & \cos\varphi \end{pmatrix}.$$

Now consider a rotation R_x by 90° about the x-axis. Its matrix is

$$\mathsf{R}_x = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix},$$

and its inverse is

$$\mathsf{R}_x^{-1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix},$$

corresponding to the angle -90°. This can be checked by multiplying them: $\mathsf{R}_x\mathsf{R}_x^{-1} = 1$. Then

$$\begin{aligned} \mathsf{R}_x\mathsf{R}_z(\varphi)\mathsf{R}_x^{-1} &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\varphi & \sin\varphi \\ 0 & -\sin\varphi & \cos\varphi \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix} \\ &= \begin{pmatrix} \cos\varphi & 0 & -\sin\varphi \\ 0 & 1 & 0 \\ \sin\varphi & 0 & \cos\varphi \end{pmatrix}, \end{aligned}$$

which is a rotation by $-\varphi$ about the y-axis and no longer a rotation about the z-axis so that this element lies outside the subgroup of rotations about the z-axis, and this subgroup is not an invariant subgroup. The set of these elements for all φ form a group called **conjugate** to the group of rotations about the z-axis. ■

Orthogonal $n \times n$ matrices form the group $\mathrm{O}(n)$, and they form $\mathrm{SO}(n)$ if their determinants are $+1$ (S stands for "special" and O for "orthogonal"), with elements denoted by O_i. Because $\tilde{\mathsf{O}}_i = \mathsf{O}_i^{-1}$ (see Section 3.3 for orthogonal 3×3 matrices that preserve the lengths of vectors and distances between points in three-dimensional Euclidean space), we see that the product

$$\widetilde{\mathsf{O}_1\mathsf{O}_2} = \tilde{\mathsf{O}}_2\tilde{\mathsf{O}}_1 = \mathsf{O}_2^{-1}\mathsf{O}_1^{-1} = (\mathsf{O}_1\mathsf{O}_2)^{-1}$$

is also an orthogonal matrix in $\mathrm{O}(n)$ or $\mathrm{SO}(n)$. The inverse is the transpose (orthogonal) matrix. The unit of the group is 1_n. A real orthogonal $n \times n$ matrix

has $n(n-1)/2$ independent parameters. For $n = 2$, there is only one parameter: one angle in Eq. (4.1). For $n = 3$, there are three independent parameters: for example, the three Euler angles of Section 3.3, and SO(3) is related to rotations in three dimensions, just as SO(2) is in two dimensions. Because O(n) contains orthogonal transformations with determinant -1, this group includes reflections of coordinates or parity inversions. Likewise, unitary $n \times n$ matrices form the group U(n), and they form SU(n) if their determinants are $+1$. Because $U_i^\dagger = U_i^{-1}$ (see Section 3.4 for unitary matrices, which preserve the norm of vectors with complex components and distances between points in n-dimensional complex space), we see that

$$(U_1U_2)^\dagger = U_2^\dagger U_1^\dagger = U_2^{-1}U_1^{-1} = (U_1U_2)^{-1}$$

so that the product is unitary and an element of U(n) or SU(n). Each unitary matrix obviously has an inverse, which again is unitary. Orthogonal matrices are unitary matrices that are real so that SO(n) forms a subgroup of SU(n), as does O(n) of U(n).

EXAMPLE 4.1.3

Simple Unitary Groups The phase factors $e^{i\theta}$, with real angle θ, of quantum mechanical wave functions form a group under multiplication of complex numbers because the phase angles add on multiplying $e^{i\theta_1}e^{i\theta_2} = e^{i(\theta_1+\theta_2)}$. Moreover, $(e^{i\theta})^\dagger = e^{-i\theta}$ and $e^{i\theta}e^{-i\theta} = 1$ show unitarity and inverse, and $\theta = 0$ gives the unit. This group (of unitary 1×1 matrices) has one continuous real parameter and is therefore called U(1). The two elements ± 1 form a finite (unitary) subgroup, and the four elements ± 1, $\pm i$ form another subgroup.

A finite unitary group of 2×2 matrices is defined by the two-dimensional unit matrix and one of the three Pauli matrices, σ_i, using matrix multiplication. Because $\sigma_i^2 = 1_2$, the inverse $\sigma_i^{-1} = \sigma_i$ and $1_2^{-1} = 1_2$. ■

When a potential has spherical symmetry we choose polar coordinates, and the associated group of transformations is a rotation group. For problems with spin (or other internal properties such as isospin or flavor), unitary groups play a similar role. Therefore, in the following we discuss only the rotation groups SO(n) and the unitary group SU(2) among the classical Lie groups.

Biographical Data

Lie, Sophus. Lie, who was born in 1842 in Nordfjordeid, Norway, and died in 1899 in Kristiana (now Oslo), started his analysis of continuous groups of transformations in Paris and continued it throughout his life.

Wigner, Eugen Paul. Wigner, who was born in 1902 in Budapest, Hungary, and died in 1995 in Princeton, New Jersey, studied in Berlin, moved to the United States in the 1930s, and received the Nobel prize in 1963 for his contributions to nuclear theory and applications of fundamental principles of symmetry, such as the charge independence of nuclear forces. He developed the unitary representations of the Lorentz group.

Homomorphism and Isomorphism

There may be a correspondence between the elements of two groups: one-to-one, two-to-one, or many-to-one. If this correspondence preserves the group multiplication, the two groups are **homomorphic**. If the correspondence is one-to-one, still preserving the group multiplication,[3] then the groups are **isomorphic**. An example is the rotations of the coordinates through an angle φ counterclockwise about the z-axis in three-dimensional space described by Eq. (4.3). If we identify every rotation with its orthogonal 2×2 submatrix, we have a one-to-one map that preserves the group multiplication according to Eq. (4.2), an isomorphism or **faithful representation**. Of course, we can also identify each rotation with its 3×3 matrix in Eq. (4.3), which is also an isomorphism. Therefore, matrix representations are by no means unique, but each isomorphism is a group multiplication preserving faithful map.

Matrix Representations: Reducible and Irreducible

The isomorphisms between rotations and groups of matrices just discussed are examples of matrix representations of a group (of rotations). Such representations of group elements by matrices are a very powerful technique and have been almost universally adopted by physicists. The use of matrices imposes no significant restriction. It can be shown that the elements of any finite group and of the continuous groups of Sections 4.2–4.4 may be represented by matrices. In each case, matrix multiplication follows from group multiplication. The same group can be represented by matrices of different rank. Examples are the rotations about the z-axis described in Eqs. (4.1) and (4.3).

To illustrate how matrix representations arise from a symmetry, consider the time-independent Schrödinger equation (or some other eigenvalue equation, such as $\mathsf{I}v_i = I_i v_i$ for the principal moments of inertia of a rigid body in classical mechanics, for example)

$$H\psi = E\psi. \tag{4.4}$$

Let us assume that Eq. (4.4) stays invariant under a group G of transformations R in G. For example, for a spherically symmetric Hamiltonian H the group G would be SO(3). Consequently, H is the same in a rotated coordinate system, where the Hamiltonian is given by the similarity transformation $\mathsf{R}H\mathsf{R}^{-1}$ according to Eq. (3.108) of Chapter 3. Hence,

$$\mathsf{R}H\mathsf{R}^{-1} = H, \quad \text{or} \quad \mathsf{R}H = H\mathsf{R}, \tag{4.5}$$

that is, "rotations" from G and H commute. Now take a solution ψ of Eq. (4.4) and "rotate" it with R, an element from G: $\psi \to \mathsf{R}\psi$. Then $\mathsf{R}\psi$ has the **same**

[3] Suppose the elements of one group are labeled g_i, and the elements of a second group are labeled h_i. Then $g_i \leftrightarrow h_i$ is a one-to-one correspondence for all values of i. If $g_i g_j = g_k$ and $h_i h_j = h_k$, then g_k and h_k must be the corresponding group elements.

value of energy E because multiplying Eq. (4.4) by R and using Eq. (4.5) yields

$$\mathsf{R}H\psi = E(\mathsf{R}\psi) = H(\mathsf{R}\psi). \tag{4.6}$$

In other words, all rotated solutions $\mathsf{R}\psi$ are **degenerate** in energy or form a vector space that physicists call a **multiplet**. For example, the spin-up and -down states of an electron form a doublet, and the states with projection quantum numbers $m = -l, -l+1, \ldots, 0, 1, \ldots, l$ of orbital angular momentum l form a multiplet with $2l + 1$ basis states. (The magnetic field in the Zeeman effect lifts the degeneracy of these states and breaks the rotational symmetry because the magnetic field points in some direction.)

Let us now assume that this vector space V_ψ of transformed solutions has a finite dimension n. Let $\psi_1, \psi_2, \ldots, \psi_n$ be a basis. Since $\mathsf{R}\psi_j$ is a member of the multiplet, we can expand it in terms of its basis,

$$\mathsf{R}\psi_j = \sum_k r_{jk}\psi_k. \tag{4.7}$$

Thus, with each transformation R in G we can associate a matrix $\mathsf{r} = (r_{jk})$, and this **map** $\mathsf{R} \rightarrow (\mathsf{r})$ is defined as a **representation** of G. If we can take any element of V_ψ and by rotating with all elements R of G transform it into **all** other elements of V_ψ, then the representation is **irreducible**. The spin-up and -down states of the hydrogen ground state form an irreducible representation of SU(2) (they can be rotated into each other), but the $2s$ state and $2p$ states of principal quantum number $n = 2$ of the hydrogen atom have the same energy (i.e., they are degenerate) and form a reducible representation because the $2s$ state cannot be rotated into the $2p$ states and vice versa (angular momentum is conserved under rotations). With this case in mind, we see that if all elements of V_ψ are not reached, then V_ψ splits into a direct sum of two or more vector subspaces (see Chapter 3), $V_\psi = V_1 \oplus V_2 \oplus \ldots$, which are mapped into themselves by rotating their elements (e.g., 2s→2s, 2p→2p). The **direct sum** of two vector spaces is spanned by the basis vectors of both vector spaces. In this case, the representation is called **reducible**. Then we can find a unitary matrix U so that

$$\mathsf{U}(r_{jk})\mathsf{U}^\dagger = \begin{pmatrix} \mathbf{r}_1 & \mathbf{0} & \cdots \\ \mathbf{0} & \mathbf{r}_2 & \cdots \\ \vdots & \vdots & \end{pmatrix} \tag{4.8}$$

for **all** R of G and **all** matrices (r_{jk}). Here, $\mathbf{r}_1, \mathbf{r}_2, \ldots$, are matrices of lower dimension than (r_{jk}) that are lined up along the diagonal and the $\mathbf{0}$ are matrices made up of zeros, that is, r is **block-diagonal**.

For example, for the $2s$ states of hydrogen, $\mathbf{r}_1$ would be a unitary 2×2 matrix

$$\mathbf{r}_1 = \begin{pmatrix} a & b \\ c & d \end{pmatrix}.$$

If the electron spin is ignored, $\mathbf{r}_1 = 1$ of the $2s$ state would be a one-dimensional unit matrix. We may say that the representation $\mathbf{r}$ has been decomposed into $\mathbf{r} = \mathbf{r}_1 + \mathbf{r}_2 + \cdots$ along with $V_\psi = V_1 \oplus V_2 \oplus \cdots$, where the smaller $\mathbf{r}_i$ are irreducible. In any representation, each irreducible representation may be repeated a finite number of times, and some do not appear at all.

The irreducible representations play a role in group theory that is analogous to that of the unit vectors of vector analysis. They are the simplest representations—all others can be built from them.

SUMMARY

Often, groups occur in physics as sets of transformations of coordinates or symmetry transformations that leave a partial or ordinary differential equation unchanged, or group elements define changes of bases of some vector space. Therefore, matrix representations of groups are common in physics. The most important application in quantum mechanics is based on the fact that the degenerate states of multiplets in a spectrum reflect the symmetry group of the Hamiltonian. Multiplets correspond to representations of the symmetry group of a Hamiltonian.

EXERCISES

4.1.1 Show that an $n \times n$ orthogonal matrix has $n(n-1)/2$ independent parameters.
Hint. The orthogonality condition, Eq. (3.79), provides constraints.

4.1.2 The special linear group SL(2,**C**) consists of all 2×2 matrices (with complex elements) having a determinant of $+1$. Show that such matrices form a group.
Note. The SL(2,**C**) group can be related to the full Lorentz group in Section 4.4, much as the SU(2) group is related to SO(3).

4.1.3 Show that rotations about the z-axis form a subgroup of SO(3). Is it an invariant subgroup?

4.1.4 Show that if R, S, T are elements of a group G so that $RS = T$, and $R \to (r_{ik})$, $S \to (s_{ik})$ is a representation according to Eq. (4.7), then

$$(r_{ik})(s_{ik}) = \left(t_{ik} = \sum_n r_{in} s_{nk}\right),$$

that is, group multiplication translates into matrix multiplication for any group representation.

4.1.5 A subgroup H of G has elements h_i. Let x be a fixed element of the original group G and **not** a member of H. The transform

$$x h_i x^{-1}, \quad i = 1, 2, \ldots$$

generates a **conjugate subgroup** xHx^{-1}. Show that this conjugate subgroup satisfies each of the four group postulates and therefore is a group.

4.2 Generators of Continuous Groups

A characteristic of continuous groups known as Lie groups is that the elements are functions of parameters having derivatives of arbitrary orders such as $\cos\varphi$ and $\sin\varphi$ in Eq. (4.1). This unlimited differentiability of the functions allows us to develop the concept of generator and reduce the study of the whole group to a study of the group elements in the neighborhood of the identity element.

Lie's essential idea was to study elements R in a group G that are infinitesimally close to the unity of G. Let us consider the SO(2) group as a simple example. The 2×2 rotation matrices in Eq. (4.1) can be written in exponential form using the Euler identity [Eq. (3.183)] as

$$\mathsf{R}(\varphi)=\begin{pmatrix}\cos\varphi & \sin\varphi\\ -\sin\varphi & \cos\varphi\end{pmatrix}=1_2\cos\varphi+i\sigma_2\sin\varphi=\exp(i\sigma_2\varphi). \tag{4.9}$$

From the exponential form it is obvious that multiplication of these matrices is equivalent to addition of the arguments

$$\mathsf{R}(\varphi_2)\mathsf{R}(\varphi_1)=\exp(i\sigma_2\varphi_2)\exp(i\sigma_2\varphi_1)=\exp(i\sigma_2(\varphi_1+\varphi_2))=\mathsf{R}(\varphi_1+\varphi_2).$$

Of course, the rotations close to 1 have small angle $\varphi\approx 0$.

This suggests that we look for an exponential representation

$$\mathsf{R}=\exp(i\varepsilon\mathsf{S}),\qquad \varepsilon\to 0, \tag{4.10}$$

for group elements R in G close to the unity 1. The operators S of the infinitesimal transformations $i\epsilon\mathsf{S}$ are called generators of G. Therefore, σ_2 in Eq. (4.9) is the generator of rotations about the z-axis. Thus, for SO(2) as defined by Eq. (4.1) there is only one linearly independent generator, σ_2. In SO(3) there is a generator for rotations about each axis. These generators form a linear space because multiplication of the elements R of the group translates into addition of generators S; its dimension is defined as the **order** of G. Therefore, the order of SO(2) is 1, and it is 3 for SO(3). One can also show that the commutator of two generators is again a generator

$$[S_j,\,S_k]=i\sum_l c_{jk}^l S_l,$$

where the c's are defined as the **structure constants** of the group. The vector space of generators can be endowed with a multiplication by defining the commutator as the product of two generators. This way the vector space of generators becomes an algebra, the so-called **Lie algebra**.

Because R does not change the volume—that is, $\det(\mathsf{R})=1$—we use Eq. (3.184) to see that

$$\det(\mathsf{R})=\exp(\text{trace}(\ln\mathsf{R}))=\exp(i\varepsilon\,\text{trace}(\mathsf{S}))=1,$$

which implies that **generators are traceless**:

$$\text{tr}(\mathsf{S})=0. \tag{4.11}$$

This is the case for the rotation groups SO(n) and unitary groups SU(n).

If R of G in Eq. (4.10) is unitary, then $S^\dagger = S$ is Hermitian, which is also the case for SO(n) and SU(n). Hence the i in Eq. (4.10).

Returning to Eq. (4.5), we now emphasize the most important result from group theory. The inverse of R is just $\mathsf{R}^{-1} = \exp(-i\varepsilon\mathsf{S})$. We expand H_R according to the Baker–Hausdorff formula [Eq. (3.185)]; taking the Hamiltonian H and S to be operators or matrices we see that

$$H = H_R = \exp(i\varepsilon\mathsf{S})H\exp(-i\varepsilon\mathsf{S}) = H + i\varepsilon[\mathsf{S}, H] - \frac{1}{2}\varepsilon^2[\mathsf{S}[\mathsf{S}, H]] + \cdots. \quad (4.12)$$

We subtract H from Eq. (4.12), divide by ε, and let $\varepsilon \to 0$. Then Eq. (4.12) implies that for any rotation close to 1 in G the commutator

$$[\mathsf{S}, H] = 0. \quad (4.13)$$

We see that S **is a constant of the motion: A symmetry of the system has led to a conservation law**. If S and H are Hermitian matrices, Eq. (4.13) states that S and H can be simultaneously diagonalized; that is, the eigenvalues of S are constants of the motion. If S and H are differential operators like the Hamiltonian and orbital angular momentum $\mathbf{L}^2$, L_z in quantum mechanics, then Eq. (4.13) states that S and H have common eigenfunctions, and that the degenerate eigenvalues of H can be distinguished by the eigenvalues of the generators S. These eigenfunctions and eigenvalues, s, are solutions of separate differential equations, $\mathsf{S}\psi_s = s\psi_s$, so that group theory (i.e., symmetries) leads to a separation of variables for a partial differential equation that is invariant under the transformations of the group. For examples, see the separation of variables method for partial differential equations in Section 8.9 and special functions in Chapter 11. This is by far the most important application of group theory in quantum mechanics.

In the following sections, we study orthogonal and unitary groups as examples to understand better the general concepts of this section.

Rotation Groups SO(2) and SO(3)

For SO(2) as defined by Eq. (4.1) there is only one linearly independent generator, σ_2, and the order of SO(2) is 1. We get σ_2 from Eq. (4.9) by differentiation at the unity of SO(2) (i.e., $\varphi = 0$),

$$-i\frac{d\mathsf{R}(\varphi)}{d\varphi}\bigg|_{\varphi=0} = -i\begin{pmatrix} -\sin\varphi & \cos\varphi \\ -\cos\varphi & -\sin\varphi \end{pmatrix}\bigg|_{\varphi=0} = -i\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = \sigma_2. \quad (4.14)$$

For the rotations $\mathsf{R}_z(\varphi)$ about the z-axis described by 3×3 matrices in Eq. (4.3), the generator is given by

$$-i\frac{d\mathsf{R}_z(\varphi)}{d\varphi}\bigg|_{\varphi=0} = \mathsf{S}_z = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \quad (4.15)$$

Here, σ_2 is recognized in the upper left-hand corner of S_z. The rotation $\mathsf{R}_z(\delta\varphi)$ through an infinitesimal angle $\delta\varphi$ may then be expanded near the unity ($\varphi = 0$) as

$$\mathsf{R}_z(\delta\varphi) = 1_3 + i\delta\varphi \mathsf{S}_z, \tag{4.16}$$

with terms of order $(\delta\varphi)^2$ and higher omitted. A finite rotation $\mathsf{R}(\varphi)$ may be compounded of successive infinitesimal rotations

$$\mathsf{R}_z(\delta\varphi_1 + \delta\varphi_2) = (1_3 + i\delta\varphi_1 \mathsf{S}_z)(1_3 + i\delta\varphi_2 \mathsf{S}_z). \tag{4.17}$$

Let $\delta\varphi = \varphi/N$ for N rotations, with $N \to \infty$. Then,

$$\mathsf{R}_z(\varphi) = \lim_{N\to\infty} [\mathsf{R}_z(\varphi/N)]^N = \lim_{N\to\infty} [1_3 + (i\varphi/N)\mathsf{S}_z]^N = \exp(i\varphi \mathsf{S}_z), \tag{4.18}$$

which is another way of getting Eq. (4.10). This form identifies S_z as the generator of the group R_z, an Abelian subgroup of SO(3), the group of rotations in three dimensions with determinant +1. Each 3×3 matrix $\mathsf{R}_z(\varphi)$ is orthogonal (hence unitary), and trace$(\mathsf{S}_z) = 0$ in accordance with Eq. (4.11).

By differentiation of the coordinate rotations

$$\mathsf{R}_x(\psi) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\psi & \sin\psi \\ 0 & -\sin\psi & \cos\psi \end{pmatrix}, \quad \mathsf{R}_y(\theta) = \begin{pmatrix} \cos\theta & 0 & -\sin\theta \\ 0 & 1 & 0 \\ \sin\theta & 0 & \cos\theta \end{pmatrix}, \tag{4.19}$$

we get the generators

$$\mathsf{S}_x = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad \mathsf{S}_y = \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix} \tag{4.20}$$

of $\mathsf{R}_x(\mathsf{R}_y)$, the subgroup of rotations about the x- (y-)axis.

Rotation of Functions and Orbital Angular Momentum

In the foregoing discussion the group elements are matrices that rotate the coordinates. Any physical system being described is held fixed. Now let us hold the coordinates fixed and rotate a function $\psi(x, y, z)$ relative to our fixed coordinates. With R to rotate the coordinates,

$$\mathbf{x}' = \mathsf{R}\mathbf{x}, \tag{4.21}$$

we define R on ψ by

$$\mathsf{R}\psi(x, y, z) = \psi'(x, y, z) \equiv \psi(\mathbf{x}'). \tag{4.22}$$

In words, R operates on the function ψ, creating a **new function** ψ' that is numerically equal to $\psi(\mathbf{x}')$, where $\mathbf{x}'$ are the coordinates rotated by R. If R rotates the coordinates counterclockwise, the effect of R is to rotate the pattern of the function ψ counterclockwise, as shown in Fig. 2.20.

Returning to Eqs. (4.3), (4.15), and (4.20) consider an infinitesimal rotation again, $\varphi \to \delta\varphi$. Then, using R_z [Eq. (4.3)], we obtain

$$\mathsf{R}_z(\delta\varphi)\psi(x, y, z) = \psi(x + y\delta\varphi, y - x\delta\varphi, z). \tag{4.23}$$

The right side may be expanded to first order in $\delta\varphi$ to give

$$\begin{aligned}\mathsf{R}_z(\delta\varphi)\psi(x, y, z) &= \psi(x, y, z) - \delta\varphi\{x\partial\psi/\partial y - y\partial\psi/\partial x\} + O(\delta\varphi)^2 \\ &= (1 - i\delta\varphi L_z)\psi(x, y, z),\end{aligned} \tag{4.24}$$

where the differential expression in curly brackets is the orbital angular momentum iL_z (Exercise 1.7.12). This shows how the orbital angular momentum operator arises as a generator. Since a rotation of first φ and then $\delta\varphi$ about the z-axis is given by

$$\mathsf{R}_z(\varphi + \delta\varphi)\psi = \mathsf{R}_z(\delta\varphi)\mathsf{R}_z(\varphi)\psi = (1 - i\delta\varphi L_z)\mathsf{R}_z(\varphi)\psi, \tag{4.25}$$

we have (as an operator equation)

$$\frac{d\mathsf{R}_z}{d\varphi} = \lim_{\delta\varphi\to 0}\frac{\mathsf{R}_z(\varphi + \delta\varphi) - \mathsf{R}_z(\varphi)}{\delta\varphi} = -iL_z\mathsf{R}_z(\varphi). \tag{4.26}$$

In this form, Eq. (4.26) integrates immediately to

$$\mathsf{R}_z(\varphi) = \exp(-i\varphi L_z). \tag{4.27}$$

Note that $\mathsf{R}_z(\varphi)$ rotates functions (counterclockwise) relative to fixed coordinates [so Eqs. (4.27) and (4.10) are similar but not the same] and that L_z is the z-component of the orbital angular momentum $\mathbf{L}$. The constant of integration is fixed by the boundary condition $\mathsf{R}_z(0) = 1$.

If we recognize that the operator

$$L_z = (x, y, z)\mathsf{S}_z\begin{pmatrix}\partial/\partial x\\ \partial/\partial y\\ \partial/\partial z\end{pmatrix}, \tag{4.28}$$

it becomes clear why L_x, L_y, and L_z satisfy the same commutation relation

$$[L_i, L_j] = i\varepsilon_{ijk}L_k \tag{4.29}$$

as S_x, S_y, and S_z and yield the structure constants ε_{ijk} of SO(3).

Special Unitary Group SU(2)

Since unitary 2×2 matrices transform complex two-dimensional vectors preserving their norm, they represent the most general transformations of (a basis in the Hilbert space of) spin $\frac{1}{2}$ wave functions in nonrelativistic quantum mechanics. The basis states of this system are conventionally chosen to be

$$|\uparrow\rangle = \begin{pmatrix}1\\0\end{pmatrix}, \quad |\downarrow\rangle = \begin{pmatrix}0\\1\end{pmatrix},$$

corresponding to spin $\frac{1}{2}$ up and down states, respectively. We can show that the **special unitary** group SU(2) of such unitary 2×2 matrices with determinant

$+1$ has the three Pauli matrices σ_i as generators. Therefore, we expect SU(2) to be of order 3 and to depend on three real continuous parameters ξ, η, ζ, which are often called the **Cayley–Klein** parameters and are essentially the SU(2) analog of Euler angles. We start with the observation that orthogonal 2×2 matrices [Eq. (4.1)] are real unitary matrices, so they form a subgroup of SU(2). We also see that

$$\begin{pmatrix} e^{i\alpha} & 0 \\ 0 & e^{-i\alpha} \end{pmatrix}$$

is unitary for real angle α with determinant $+1$. Therefore, these simple and manifestly unitary matrices form another subgroup of SU(2) from which we can obtain all elements of SU(2)—that is, the general 2×2 unitary matrix of determinant $+1$. For a two-component spin $\frac{1}{2}$ wave function of quantum mechanics, this diagonal unitary matrix corresponds to multiplication of the spin-up wave function with a phase factor $e^{i\alpha}$ and the spin-down component with the inverse phase factor. Using the real angle η instead of φ for the rotation matrix and then multiplying by the diagonal unitary matrices, we construct a 2×2 unitary matrix that depends on three parameters and is clearly a more general element of SU(2):

$$\begin{aligned}
&\begin{pmatrix} e^{i\alpha} & 0 \\ 0 & e^{-i\alpha} \end{pmatrix}\begin{pmatrix} \cos\eta & \sin\eta \\ -\sin\eta & \cos\eta \end{pmatrix}\begin{pmatrix} e^{i\beta} & 0 \\ 0 & e^{-i\beta} \end{pmatrix} \\
&= \begin{pmatrix} e^{i\alpha}\cos\eta & e^{i\alpha}\sin\eta \\ -e^{-i\alpha}\sin\eta & e^{-i\alpha}\cos\eta \end{pmatrix}\begin{pmatrix} e^{i\beta} & 0 \\ 0 & e^{-i\beta} \end{pmatrix} \\
&= \begin{pmatrix} e^{i(\alpha+\beta)}\cos\eta & e^{i(\alpha-\beta)}\sin\eta \\ -e^{-i(\alpha-\beta)}\sin\eta & e^{-i(\alpha+\beta)}\cos\eta \end{pmatrix}.
\end{aligned}$$

Defining $\alpha + \beta \equiv \xi$, $\alpha - \beta \equiv \zeta$, we have in fact constructed the general element of SU(2):

$$\mathsf{U}_2(\xi, \eta, \zeta) = \begin{pmatrix} e^{i\xi}\cos\eta & e^{i\zeta}\sin\eta \\ -e^{-i\zeta}\sin\eta & e^{-i\xi}\cos\eta \end{pmatrix} = \begin{pmatrix} a & b \\ -b^* & a^* \end{pmatrix}, \tag{4.30}$$

where $|a|^2 + |b|^2 = 1$. It is easy to check that the determinant $\det(\mathsf{U}_2) = 1$ by the product theorem of Section 3.2 and that $\mathsf{U}_2^\dagger \mathsf{U}_2 = 1 = \mathsf{U}_2 \mathsf{U}_2^\dagger$ holds provided ξ, η, ζ are real numbers.

To get the generators, we differentiate

$$-i\frac{\partial \mathsf{U}_2}{\partial \xi}_{|\xi=0,\eta=0} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \sigma_3, \tag{4.31a}$$

$$-i\frac{\partial \mathsf{U}_2}{\partial \eta}_{|\eta=0,\zeta=0} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \sigma_2. \tag{4.31b}$$

To avoid a factor $1/\sin\eta$ for $\eta \to 0$ upon differentiating with respect to ζ, we use instead the right-hand side of Eq. (4.30) for U_2 for pure imaginary $b = i\beta$

with $\beta \to 0$. Differentiating such a U_2, we get the third generator

$$-i\frac{\partial}{\partial\beta}\begin{pmatrix}\sqrt{1-\beta^2} & i\beta\\ i\beta & \sqrt{1-\beta^2}\end{pmatrix}\bigg|_{\beta=0} = -i\begin{pmatrix}\frac{-\beta}{\sqrt{1-\beta^2}} & i\\ i & \frac{-\beta}{\sqrt{1-\beta^2}}\end{pmatrix}\bigg|_{\beta=0} = \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} = \sigma_1. \tag{4.31c}$$

Being generators, these Pauli matrices are all traceless and Hermitian. A correspondence with the physical world is obtained if we scale the SU(2) generators so that they yield the angular momentum commutators. With the Pauli matrices as generators, the elements U_1, U_2, U_3 of SU(2) may be generated by

$$\mathsf{U}_1 = \exp(-i\alpha\sigma_1/2), \quad \mathsf{U}_2 = \exp(-i\beta\sigma_2/2), \quad \mathsf{U}_3 = \exp(-i\gamma\sigma_3/2). \tag{4.32}$$

The three parameters are real, and we interpret them as angles. The extra scale factor 1/2 is present in the exponents because $\mathsf{S}_i = \sigma_i/2$ satisfy the same commutation relations,[4]

$$[\mathsf{S}_i, \mathsf{S}_j] = i\varepsilon_{ijk}\mathsf{S}_k, \tag{4.33}$$

as the orbital angular momentum in Eq. (4.29).

Using the angular momentum matrix S_3, we have as the corresponding rotation operator $\mathsf{R}_z(\varphi) = \exp(i\varphi\sigma_3/2)$ in two-dimensional (complex wave function) space, analogous to Eq. (4.3) that gives the operator for rotating the Cartesian coordinates in the three-space.

For rotating the two-component vector wave function (spinor) or a spin $\frac{1}{2}$ particle relative to fixed coordinates, the rotation operator is $\mathsf{R}_z(\varphi) = \exp(-i\varphi\sigma_3/2)$ according to Eq. (4.27).

Using in Eq. (4.32) the Euler identity [Eq. (3.183)] we obtain

$$\mathsf{U}_j = \cos(\alpha/2) - i\sigma_j \sin(\alpha/2), \tag{4.34}$$

etc. Here, the parameter α appears as an angle, the coefficient of an angular momentum matrix–like φ in Eq. (4.27). With this identification of the exponentials, the general form of the SU(2) matrix (for rotating functions rather than coordinates) may be written as

$$\mathsf{U}(\alpha, \beta, \gamma) = \exp(-i\gamma\sigma_3/2)\exp(-i\beta\sigma_2/2)\exp(-i\alpha\sigma_3/2), \tag{4.35}$$

where the SU(2) Euler angles α, β, γ differ from the α, β, γ used in the definition of the Cayley–Klein parameters ξ, η, ζ by a factor of 1/2. Further discussion of the relation between SO(3) and orbital angular momentum appears in Sections 4.3 and 11.7.

SUMMARY

The orbital angular momentum operators are the generators of the rotation group SO(3) and (1/2) the Pauli spin matrices are those for SU(2), the symmetry group of the Schrödinger equation for a spin $\frac{1}{2}$ particle such as the electron. Generators obey commutation relations characteristic of the group.

[4] The structure constants (ε_{ijk}) lead to the SU(2) representations of dimension $2J+1$ for generators of dimension $2J+1$, $J = 0, 1/2, 1, \ldots$. The **integral** J cases also lead to the representations of SO(3).

EXERCISES

4.2.1 (i) Show that the Pauli matrices are the generators of SU(2) without using the parameterization of the general unitary 2×2 matrix in Eq. (4.30).
Hint. Exploit the general properties of generators.

4.2.2 Prove that the general form of a 2×2 unitary, unimodular matrix is

$$\mathsf{U} = \begin{pmatrix} a & b \\ -b^* & a^* \end{pmatrix},$$

with $a^*a + b^*b = 1$. Based on this result, derive the parameterization of Eq. (4.30).

4.2.3 A **translation** operator $T(a)$ converts $\psi(x)$ to $\psi(x + a)$,

$$T(a)\psi(x) = \psi(x + a).$$

In terms of the (quantum mechanical) linear momentum operator $p_x = -id/dx$, show that $T(a) = \exp(iap_x)$ (i.e., p_x is the generator of translations).
Hint. Expand $\psi(x + a)$ as a Taylor series.

4.2.4 Consider the general SU(2) element Eq. (4.30) to be built up of three Euler rotations: (i) a rotation of $a/2$ about the z-axis, (ii) a rotation of $b/2$ about the new x-axis, and (iii) a rotation of $c/2$ about the new z-axis. (All rotations are counterclockwise.) Using the Pauli $\boldsymbol{\sigma}$ generators, show that these rotation angles are determined by

$$\begin{aligned} a &= \xi - \zeta + \pi/2 = \alpha + \pi/2 \\ b &= 2\eta \qquad\qquad\quad = \beta \\ c &= \xi + \zeta - \pi/2 = \gamma - \pi/2. \end{aligned}$$

Note. The angles a and b here are not the a and b of Eq. (4.30).

4.2.5 We know that any 2×2 matrix A can be expanded as $\mathsf{A} = a_0 \cdot 1 + \mathbf{a} \cdot \boldsymbol{\sigma}$, where 1 is the two-dimensional unit matrix. Determine a_0 and $\mathbf{a}$ for the general SU(2) matrix in Eq. (4.30).

4.2.6 Rotate a nonrelativistic wave function $\tilde{\psi} = (\psi_\uparrow, \psi_\downarrow)$ of spin $\frac{1}{2}$ about the z-axis by a small angle $d\theta$. Find the corresponding generator.

4.3 Orbital Angular Momentum

The classical concept of angular momentum $\mathbf{L}_{\text{class}} = \mathbf{r} \times \mathbf{p}$ is presented in Section 1.3 to introduce the cross product. Following the usual Schrödinger representation of quantum mechanics, the classical linear momentum $\mathbf{p}$ is replaced by the operator $-i\boldsymbol{\nabla}$. The quantum mechanical orbital angular

momentum **operator** becomes[5]

$$\mathbf{L}_{QM} = -i\mathbf{r} \times \boldsymbol{\nabla}. \tag{4.36}$$

This is used repeatedly in Sections 1.7, 1.8, and 2.4 to illustrate vector differential operators. From Exercise 1.7.13 the angular momentum components satisfy the commutation relations

$$[L_i, L_j] = i\varepsilon_{ijk}L_k. \tag{4.37}$$

The ε_{ijk} is the Levi–Civita symbol of Section 2.9. A summation over the index k is understood.

The differential operator corresponding to the square of the angular momentum

$$\mathbf{L}^2 = \mathbf{L} \cdot \mathbf{L} = L_x^2 + L_y^2 + L_z^2 \tag{4.38}$$

may be determined from

$$\mathbf{L} \cdot \mathbf{L} = (\mathbf{r} \times \mathbf{p}) \cdot (\mathbf{r} \times \mathbf{p}), \tag{4.39}$$

which is the subject of Exercises 1.8.6 and 2.5.12(c). Since $\mathbf{L}^2$ is invariant under rotations, $[\mathbf{L}^2, L_i] = 0$, which can also be verified directly.

Equation (4.37) presents the basic commutation relations of the components of the quantum mechanical angular momentum. Indeed, within the framework of quantum mechanics and group theory, these commutation relations define an angular momentum operator. We shall use them now to construct the angular momentum eigenstates and find the eigenvalues. For the orbital angular momentum, these are the spherical harmonics of Section 11.5.

Ladder Operator Approach

Let us start with a general approach, where the angular momentum $\mathbf{J}$ we consider may represent an orbital angular momentum $\mathbf{L}$, a spin $\boldsymbol{\sigma}/2$, a total angular momentum $\mathbf{L} + \boldsymbol{\sigma}/2$, etc. Thus,

1. $\mathbf{J}$ is an Hermitian operator whose components satisfy the commutation relations

$$[J_i, J_j] = i\varepsilon_{ijk}J_k, \quad [\mathbf{J}^2, J_i] = 0. \tag{4.40}$$

   Otherwise $\mathbf{J}$ is arbitrary. (See Exercise 4.3.1.)
2. $|\lambda m\rangle$ is a normalized eigenfunction (or eigenvector) of J_z with eigenvalue m and an eigenfunction[6] of $\mathbf{J}^2$,

$$J_z|\lambda m\rangle = m|\lambda m\rangle, \quad \mathbf{J}^2|\lambda m\rangle = \lambda|\lambda m\rangle. \tag{4.41}$$

[5] For simplicity, $\hbar$ is set equal to 1. This means that the angular momentum is measured in units of $\hbar$.

[6] That $|\lambda m\rangle$ is an eigenfunction of **both** J_z and $\mathbf{J}^2$ follows from $[J_z, \mathbf{J}^2] = 0$ in Eq. (4.40). Note also that eigenvalues are in small letters, whereas operators are in capitals.

We shall show that $\lambda = j(j+1)$, with j either integral or half-integral, and then find other properties of the $|\lambda m\rangle$. The treatment will illustrate the generality and power of operator techniques, particularly the use of ladder operators.[7]

The **ladder operators** are defined as

$$J_+ = J_x + iJ_y, \quad J_- = J_x - iJ_y. \tag{4.42}$$

In terms of these operators $\mathbf{J}^2$ may be rewritten as

$$\mathbf{J}^2 = \frac{1}{2}(J_+J_- + J_-J_+) + J_z^2. \tag{4.43}$$

From the commutation relations, Eq. (4.40), we find

$$[J_z, J_+] = +J_+, \quad [J_z, J_-] = -J_-, \quad [J_+, J_-] = 2J_z. \tag{4.44}$$

Since J_+ commutes with $\mathbf{J}^2$ (Exercise 4.3.1),

$$\mathbf{J}^2(J_+|\lambda m\rangle) = J_+(\mathbf{J}^2|\lambda m\rangle) = \lambda(J_+|\lambda m\rangle). \tag{4.45}$$

Therefore, $J_+|\lambda m\rangle$ is still an eigenfunction of $\mathbf{J}^2$ with eigenvalue λ, and similarly for $J_-|\lambda m\rangle$. However, from Eq. (4.44)

$$J_zJ_+ = J_+(J_z+1), \tag{4.46}$$

or

$$J_z(J_+|\lambda m\rangle) = J_+(J_z+1)|\lambda m\rangle = (m+1)J_+|\lambda m\rangle. \tag{4.47}$$

Therefore, $J_+|\lambda m\rangle$ is still an eigenfunction of J_z but with the eigenvalue $m+1$. J_+ has raised the eigenvalue by 1 and so is called a **raising operator**. Similarly, J_- lowers the eigenvalue by 1; it is a **lowering operator**.

Taking the diagonal matrix element (also called expectation value) and using $J_x^\dagger = J_x$, $J_y^\dagger = J_y$, we get

$$\langle\lambda m|\mathbf{J}^2 - J_z^2|\lambda m\rangle = \langle\lambda m|J_x^2 + J_y^2|\lambda m\rangle = |J_x|\lambda m\rangle|^2 + |J_y|\lambda m\rangle|^2 \geq 0$$

and see that $\lambda - m^2 \geq 0$, so m is bounded, and $\lambda \geq 0$. Let j be the **largest** m value. Then $J_+|\lambda j\rangle = 0$, which implies $J_-J_+|\lambda j\rangle = 0$. Hence, combining Eqs. (4.43) and (4.44) to get

$$\mathbf{J}^2 = J_-J_+ + J_z(J_z+1), \tag{4.48}$$

we find from Eq. (4.48) that

$$0 = J_-J_+|\lambda j\rangle = (\mathbf{J}^2 - J_z^2 - J_z)|\lambda j\rangle = (\lambda - j^2 - j)|\lambda j\rangle.$$

Therefore,

$$\lambda = j(j+1) \geq 0. \tag{4.49}$$

[7] Ladder operators can be developed for other mathematical functions. Compare Section 13.1 for Hermite polynomials.

We now relabel the states $|\lambda m\rangle \equiv |jm\rangle$. Similarly, let j' be the **smallest** m value. Then $J_-|jj'\rangle = 0$. From

$$\mathbf{J}^2 = J_+J_- + J_z(J_z - 1), \tag{4.50}$$

we see that

$$0 = J_+J_-|jj'\rangle = (\mathbf{J}^2 + J_z - J_z^2)|jj'\rangle = (\lambda + j' - j'^2)|jj'\rangle. \tag{4.51}$$

Hence,

$$\lambda = j(j+1) = j'(j'-1) = (-j)(-j-1).$$

Therefore, $j' = -j$, and $j \geq 0$ because $j' \leq j$. Moreover, m runs in **integer steps** from $-j$ to j,

$$-j \leq m \leq j, \tag{4.52}$$

so that $2j$ must be a positive integer. Thus, j is either an integer or half of an odd integer.

Starting from $|jj\rangle$ and applying J_- repeatedly, we reach all other states $|jm\rangle$. Hence, the $|jm\rangle$ form an irreducible representation; m varies and j is fixed.

Then using Eqs. (4.40), (4.48), and (4.50) we obtain

$$\begin{aligned} J_-J_+|jm\rangle &= [j(j+1) - m(m+1)]|jm\rangle = (j-m)(j+m+1)|jm\rangle, \\ J_+J_-|jm\rangle &= [j(j+1) - m(m-1)]|jm\rangle = (j+m)(j-m+1)|jm\rangle. \end{aligned} \tag{4.53}$$

Because J_+ and J_- are Hermitian conjugates,[8]

$$J_+^\dagger = J_-, \quad J_-^\dagger = J_+, \tag{4.54}$$

the eigenvalues in Eq. (4.53) must be positive or zero.[9] This follows from

$$\langle jm|J_-(J_+|jm\rangle) = (J_+|jm\rangle)^\dagger J_+|jm\rangle \geq 0. \tag{4.55}$$

Examples of Eq. (4.53) are provided by the matrices of Exercises 3.2.9 (spin $\frac{1}{2}$), 3.2.11 (spin 1), and 3.2.13 (spin $\frac{3}{2}$). For the orbital angular momentum ladder operators L_+ and L_-, explicit forms are given in Exercise 2.5.10.

Since J_+ raises the eigenvalue m to $m+1$, we relabel the resultant eigenfunction $|jm+1\rangle$. From Eqs. (4.47) and (4.53) we see that

$$J_+|jm\rangle = \sqrt{(j-m)(j+m+1)}\,|jm+1\rangle, \tag{4.56}$$

taking the positive square root and not introducing any phase factor. By the same arguments

$$J_-|jm\rangle = \sqrt{(j+m)(j-m+1)}\,|jm-1\rangle. \tag{4.57}$$

[8]The Hermitian conjugation or adjoint operation is defined for matrices in Section 3.4 and for operators in general in Section 9.1.

[9]For an excellent discussion of adjoint operators and Hilbert space, see Messiah, A. (1961). *Quantum Mechanics*, Chapter 7. Wiley, New York.

As shown later, orbital angular momentum is described with integral j. From the spins of some of the fundamental particles and of some nuclei, we get $j = 1/2, 3/2, 5/2, \ldots$. Our angular momentum is quantized, essentially as a result of the commutation relations.

EXAMPLE 4.3.1

Spin $\frac{1}{2}$ States The spin raising operator is given by

$$S_+ = \frac{1}{2}\sigma_+ = \frac{1}{2}(\sigma_x + i\sigma_y) = \frac{1}{2}\begin{pmatrix} 0 & 1+i(-i) \\ 1+i\cdot i & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix},$$

so that

$$S_+\chi_\downarrow = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \chi_\uparrow,$$

which is consistent with $\sqrt{[\frac{1}{2} - (-\frac{1}{2})](\frac{1}{2} - \frac{1}{2} + 1)} = 1$ of Eq. (4.56). ■

In spherical polar coordinates θ, φ the functions $\langle\theta, \varphi|lm\rangle = Y_l^m(\theta, \varphi)$ are the spherical harmonics of Section 11.5. Similarly, we can work out Eq. (4.57) for the orbital angular momentum lowering operator $L_- = L_x - iL_y = -e^{-i\varphi}(\frac{\partial}{\partial\theta} - i\cot\theta\frac{\partial}{\partial\varphi})$ from Exercise 2.5.10b acting on the spherical harmonic $\langle\theta, \varphi|11\rangle = -\sqrt{\frac{3}{8\pi}}\sin\theta e^{i\varphi} = Y_{11}(\theta, \varphi)$. We find

$$L_-Y_{11} = -e^{-i\varphi}\left(\frac{\partial}{\partial\theta} - i\cot\theta\frac{\partial}{\partial\varphi}\right)(-1)\sqrt{\frac{3}{8\pi}}\sin\theta e^{i\varphi}$$

$$= e^{-i\varphi}\sqrt{\frac{3}{8\pi}}(\cos\theta - i\cos\theta i)e^{i\varphi} = \sqrt{\frac{6}{4\pi}}\cos\theta = \sqrt{2}\langle\theta, \varphi|1, 0\rangle = \sqrt{2}Y_{10},$$

where $\sqrt{(1+1)(1-1+1)} = \sqrt{2}$. That is, the ladder formulas (Eqs. 4.55 and 4.56) apply to the spherical harmonics and are equivalent to using the differential operators for **L**.

SUMMARY

Generators for the classical Lie groups can be organized into those defining additive eigenvalues and ladder operators that raise or lower these eigenvalues. For the rotation group SO(3) these are L_z and $L_\pm$. Altogether, they define the selection rules of a symmetry group.

EXERCISES

4.3.1 Show that (a) $[J_+, \mathbf{J}^2] = 0$, (b) $[J_-, \mathbf{J}^2] = 0$.

4.3.2 Write down all matrix elements $\langle j'm'|\mathsf{O}|jm\rangle$ of the angular momentum operator $\mathsf{O} = \mathbf{J}^2$, $\mathsf{O} = J_z$, and $\mathsf{O} = J_\pm$.

4.3.3 Construct matrix representations for $J_\pm$ and J_z for angular momentum $J = 1, 3/2, 2, 5/2$.

4.3.4 Let $|a, b\rangle$ be a complete set of common eigenfunctions of the Hermitian operators A and B; that is,

$$\mathsf{A}|a, b\rangle = a|a, b\rangle, \quad \mathsf{B}|a, b\rangle = b|a, b\rangle.$$

Show that $[\mathsf{A}, \mathsf{B}] = 0$. Is the inverse conclusion valid?

4.3.5 The three 2×2 matrices σ_j' for $j = 1, 2, 3$ satisfy the same commutation relations as the Pauli matrices. Show that there is one matrix s so that $\sigma_j' = \mathsf{s}\sigma_j\mathsf{s}^{-1}$ for $j = 1, 2, 3$. Interpret this result in your own words.

4.3.6 Determine the eigenvalues of the orbital angular momentum operators $\mathbf{L}^2$ and L_z for the functions $e^{\mathbf{r}^2/a^2}\cos\theta$ and $e^{\mathbf{r}^2/a^2}\sin\theta e^{\pm i\varphi}$, where a is some constant length.

4.3.7 Derive the generators of SU(3). Determine the order of SU(3). Write down various raising and lowering operators.

4.3.8 Explain why the theorem of Exercise 4.3.5 does not hold for three corresponding 3×3 generator matrices of SU(3).

4.4 Homogeneous Lorentz Group

Generalizing the approach to vectors of Section 2.6, in special relativity we demand that our physical laws be covariant[10] under

- space and time translations,
- rotations in real, three-dimensional space, and
- Lorentz transformations.

The demand for covariance under translations is based on the homogeneity of space and time. Covariance under rotations is an assertion of the isotropy of space. The requirement of Lorentz covariance follows from special relativity.

Space rotations and pure Lorentz transformations together form the homogeneous Lorentz group, and they form the Poincaré group when translations are included as well.

We first generate a subgroup—the Lorentz transformations in which the relative velocity $\mathbf{v}$ is along the $x = x_1$ axis. The generator may be determined by considering space–time reference frames moving with a relative velocity δv, an infinitesimal.[11] The relations are similar to those for rotations in real space (Sections 2.6 and 3.3), except that here the angle of rotation is pure imaginary.

Lorentz transformations are linear not only in the space coordinates x_i but also in time t. They originate from Maxwell's equations of electrodynamics,

[10] To be covariant means to have the same form in different coordinate systems, often called inertial frames, so that there is no preferred reference system (compare Section 2.6).

[11] This derivation, with a slightly different metric, appears in an article by J. L. Strecker, *Am. J. Phys.* **35**, 12 (1967).

which are invariant under Lorentz transformations. Lorentz transformations leave the quadratic form

$$c^2t^2 - x_1^2 - x_2^2 - x_3^2 = x_0^2 - x_1^2 - x_2^2 - x_3^2$$

invariant, where $x_0 = ct$ and c is the velocity of light that is the same in all inertial frames. We see this invariance if we switch on a light source at the origin of the coordinate system. At time t light has traveled the distance $ct = \sqrt{\sum x_i^2}$ so that $c^2t^2 - x_1^2 - x_2^2 - x_3^2 = 0$. Special relativity requires that in any inertial frame whose coordinates are x_i' that moves with velocity $v \leq c$ in any direction relative to the x_i system and has the same origin at time $t = 0$,

$$c^2t'^2 - x_1'^2 - x_2'^2 - x_3'^2 = 0$$

holds also.

Four-dimensional space–time with the metric

$$x \cdot x = x^2 = x_0^2 - x_1^2 - x_2^2 - x_3^2$$

is called Minkowski space, with the scalar product of two four-vectors defined as

$$a \cdot b = a_0 b_0 - \mathbf{a} \cdot \mathbf{b}.$$

Using the metric tensor

$$(g_{\mu\nu}) = (g^{\mu\nu}) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \tag{4.58}$$

we can raise and lower the indices of a four-vector, such as the coordinates $x^\mu = (x_0, \mathbf{x})$, so that $x_\mu = g_{\mu\nu}x^\nu = (x_0, -\mathbf{x})$, $x^\mu g_{\mu\nu} x^\nu = x_0^2 - \mathbf{x}^2$, Einstein's summation convention being understood. It is a common convention to use Greek letters for four-vector indices and, because $x_0 = x^0$, we usually write x_0 for the time variable. For the gradient that is a covariant four-vector we have

$$\partial^\mu = \left(\frac{\partial}{\partial x_0}, -\boldsymbol{\nabla}\right) = \frac{\partial}{\partial x_\mu}, \quad \partial_\mu = \left(\frac{\partial}{\partial x_0}, \boldsymbol{\nabla}\right),$$

so that

$$\partial^2 = \left(\frac{\partial}{\partial x_0}\right)^2 - \boldsymbol{\nabla}^2$$

is a Lorentz scalar, just like the metric $x^2 = x_0^2 - \mathbf{x}^2$.

For $v \ll c$, in the nonrelativistic limit, a Lorentz transformation must be Galilean. Hence, to derive the form of a Lorentz transformation along the

x_1-axis, we start with a Galilean transformation for infinitesimal relative velocity δv:

$$x'^1 = x^1 - t\delta v = x^1 - x^0\delta\beta. \tag{4.59}$$

Here, as usual, $\beta = v/c$. By symmetry, we also write

$$x'^0 = x^0 + a\delta\beta x^1, \tag{4.60}$$

with a a parameter that is fixed by the requirement that $x_0^2 - x_1^2$ be invariant,

$$x_0'^2 - x_1'^2 = x_0^2 - x_1^2. \tag{4.61}$$

Remember that $x^\mu = (x^0, \mathbf{x})$ is the prototype four-dimensional vector in Minkowski space. Thus, Eq. (4.61) is simply a statement of the invariance of the square of the magnitude of the "distance" vector under Lorentz transformation in Minkowski space. Here is where the special relativity is brought into our transformation. Squaring and subtracting Eqs. (4.59) and (4.60) and discarding terms of order $(\delta\beta)^2$, we find $a = -1$. Equations (4.59) and (4.60) may be combined as a matrix equation

$$\begin{pmatrix} x'^0 \\ x'^1 \end{pmatrix} = (1_2 - \delta\beta\sigma_1)\begin{pmatrix} x^0 \\ x^1 \end{pmatrix}, \tag{4.62}$$

where σ_1 happens to be the Pauli matrix σ_1, and the parameter $\delta\beta$ represents an infinitesimal change. Using the same techniques as in Section 4.2, we repeat the transformation N times to develop a finite transformation with the velocity parameter $\rho = N\delta\beta$. Then

$$\begin{pmatrix} x'^0 \\ x'^1 \end{pmatrix} = \left(1_2 - \frac{\rho\sigma_1}{N}\right)^N \begin{pmatrix} x^0 \\ x^1 \end{pmatrix}. \tag{4.63}$$

In the limit as $N \to \infty$,

$$\lim_{N\to\infty}\left(1_2 - \frac{\rho\sigma_1}{N}\right)^N = \exp(-\rho\sigma_1). \tag{4.64}$$

As in Section 4.2, the exponential is expanded as a Maclaurin expansion

$$\exp(-\rho\sigma_1) = 1_2 - \rho\sigma_1 + \frac{1}{2!}(\rho\sigma_1)^2 - \frac{1}{3!}(\rho\sigma_1)^3 + \cdots. \tag{4.65}$$

Noting that $\sigma_1^2 = 1_2$,

$$\exp(-\rho\sigma_1) = 1_2\cosh\rho - \sigma_1\sinh\rho. \tag{4.66}$$

Hence, our finite Lorentz transformation is

$$\begin{pmatrix} x'^0 \\ x'^1 \end{pmatrix} = \begin{pmatrix} \cosh\rho & -\sinh\rho \\ -\sinh\rho & \cosh\rho \end{pmatrix}\begin{pmatrix} x^0 \\ x^1 \end{pmatrix}. \tag{4.67}$$

σ_1 has generated the representations of this pure Lorentz transformation. Cosh ρ and sinh ρ may be identified by considering the origin of the primed coordinate system, $x'^1 = 0$, or $x^1 = vt$. Substituting into Eq. (4.67), we have

$$0 = x^1 \cosh\rho - x^0 \sinh\rho. \tag{4.68}$$

With $x^1 = vt$ and $x^0 = ct$,

$$\tanh\rho = \beta = v/c. \tag{4.69}$$

Note that the **rapidity** $\rho \neq v/c$ except in the limit as $v \to 0$. The rapidity is the **additive** parameter of a pure Lorentz transformation ("boost") along some axis that plays the same role as the angle of a rotation about some axis.

Using $1 - \tanh^2\rho = (\cosh^2\rho)^{-1}$,

$$\cosh\rho = (1-\beta^2)^{-1/2} \equiv \gamma, \quad \sinh\rho = \beta\gamma. \tag{4.70}$$

The preceding special case of the velocity parallel to one space axis is easy, but it illustrates the infinitesimal velocity-exponentiation–generator technique. Now this exact technique may be applied to derive the Lorentz transformation for the relative velocity **v not** parallel to any space axis. The matrices given by Eq. (4.67) for the case of $\mathbf{v} = \hat{\mathbf{x}}v_x$ form a subgroup. The matrices in the general case do not. The product of two Lorentz transformation matrices, $\mathsf{L}(\mathbf{v}_1)$ and $\mathsf{L}(\mathbf{v}_2)$, yields a third Lorentz matrix $\mathsf{L}(\mathbf{v}_3)$ if the two velocities $\mathbf{v}_1$ and $\mathbf{v}_2$ are parallel. The resultant velocity $\mathbf{v}_3$ is related to $\mathbf{v}_1$ and $\mathbf{v}_2$ by the Einstein velocity addition law (Exercise 4.4.3). If $\mathbf{v}_1$ and $\mathbf{v}_2$ are not parallel, no such simple relation exists. Specifically, consider three reference frames S, S', and S'', with S and S' related by $\mathsf{L}(\mathbf{v}_1)$ and S' and S'' related by $\mathsf{L}(\mathbf{v}_2)$. If the velocity of S'' relative to the original system S is $\mathbf{v}_3$, S'' is not obtained from S by $\mathsf{L}(\mathbf{v}_3) = \mathsf{L}(\mathbf{v}_2)\mathsf{L}(\mathbf{v}_1)$. Rather, one can show that

$$\mathsf{L}(\mathbf{v}_3) = \mathsf{R}\mathsf{L}(\mathbf{v}_2)\mathsf{L}(\mathbf{v}_1), \tag{4.71}$$

where R is a 3×3 space rotation matrix. With $\mathbf{v}_1$ and $\mathbf{v}_2$ not parallel, the final system S'' is **rotated** relative to S. This rotation is the origin of the Thomas precession involved in spin-orbit coupling terms in atomic and nuclear physics. Because of its presence, the $\mathsf{L}(\mathbf{v})$ by themselves do not form a group.

Vector Analysis in Minkowski Space–Time

We have seen that the propagation of light determines the metric

$$\mathbf{r}^2 - c^2t^2 = 0 = \mathbf{r}'^2 - c^2t'^2,$$

where $x^\mu = (ct, \mathbf{r})$ is the coordinate four-vector. For a particle moving with velocity $\mathbf{v}$ the Lorentz invariant infinitesimal version

$$cd\tau \equiv \sqrt{dx^\mu dx_\mu} = \sqrt{c^2dt^2 - d\mathbf{r}^2} = dt\sqrt{c^2 - \mathbf{v}^2}$$

defines the invariant proper time τ on its track. Because of time dilation in moving frames, a proper time clock rides with the particle (in its rest frame)

and runs at the slowest possible rate compared to any other inertial frame (e.g., of an observer). The four-velocity of the particle can now be defined properly as

$$\frac{dx^\mu}{d\tau} = u^\mu = \left(\frac{c}{\sqrt{c^2 - \mathbf{v}^2}}, \frac{\mathbf{v}}{\sqrt{c^2 - \mathbf{v}^2}}\right)$$

so that $u^2 = 1$, and the four-momentum $p^\mu = cmu^\mu = (\frac{E}{c}, \mathbf{p})$ yields Einstein's famous energy relation

$$E = \frac{mc^2}{\sqrt{1 - \mathbf{v}^2/c^2}} = mc^2 + \frac{m}{2}\mathbf{v}^2 \pm \cdots.$$

A consequence of $u^2 = 1$ and its physical significance is that the particle is on its mass shell $p^2 = m^2c^2$.

Now we formulate Newton's equation for a **single particle** of mass m in special relativity as $\frac{dp^\mu}{d\tau} = K^\mu$, with K^μ denoting the force four-vector, so that its vector part of the equation coincides with the usual form. For $\mu = 1, 2, 3$ we use $d\tau = dt\sqrt{1 - \mathbf{v}^2/c^2}$ and find

$$\frac{1}{\sqrt{1 - \mathbf{v}^2/c^2}}\frac{d\mathbf{p}}{dt} = \frac{\mathbf{F}}{\sqrt{1 - \mathbf{v}^2/c^2}} = \mathbf{K}$$

determining $\mathbf{K}$ in terms of the usual force $\mathbf{F}$. Next, we need to find K^0. We proceed by analogy with the derivation of energy conservation, multiplying the force equation into the four-velocity

$$mu_\nu \frac{du^\nu}{d\tau} = \frac{m}{2}\frac{du^2}{d\tau} = 0,$$

because $u^2 = 1 = \text{const}$. The other side of Newton's equation yields

$$0 = u \cdot K = \frac{K^0}{\sqrt{1 - \mathbf{v}^2/c^2}} - \frac{\mathbf{F} \cdot \mathbf{v}/c}{\sqrt{1 - \mathbf{v}^2/c^2}},$$

so that $K^0 = \frac{\mathbf{F}\cdot\mathbf{v}/c}{\sqrt{1-\mathbf{v}^2/c^2}}$ is related to the work done by the force on the particle.

Now we turn to two-body collisions in which energy-momentum conservation takes the form $p_1 + p_2 = p_3 + p_4$, where p_i^μ are the particle four-momenta. Because the scalar product of any four-vector with itself is an invariant under Lorentz transformations, it is convenient to define the Lorentz invariant energy squared $s = (p_1 + p_2)^2 = P^2$, where P^μ is the total four-momentum, and use units where the velocity of light $c = 1$. The laboratory system (lab) is defined as the rest frame of the particle with four-momentum $p_2^\mu = (m_2, \mathbf{0})$ and the center of momentum frame (cms) by the total four-momentum $P^\mu = (E_1 + E_2, \mathbf{0})$. When the incident lab energy E_1^L is given, then

$$s = p_1^2 + p_2^2 + 2p_1 \cdot p_2 = m_1^2 + m_2^2 + 2m_2E_1^L$$

is determined. Now the cms energies of the four particles are obtained from scalar products

$$p_1 \cdot P = E_1(E_1 + E_2) = E_1\sqrt{s}$$

so that

$$E_1 = \frac{p_1 \cdot (p_1 + p_2)}{\sqrt{s}} = \frac{m_1^2 + p_1 \cdot p_2}{\sqrt{s}} = \frac{m_1^2 - m_2^2 + s}{2\sqrt{s}},$$
$$E_2 = \frac{p_2 \cdot (p_1 + p_2)}{\sqrt{s}} = \frac{m_2^2 + p_1 \cdot p_2}{\sqrt{s}} = \frac{m_2^2 - m_1^2 + s}{2\sqrt{s}},$$
$$E_3 = \frac{p_3 \cdot (p_3 + p_4)}{\sqrt{s}} = \frac{m_3^2 + p_3 \cdot p_4}{\sqrt{s}} = \frac{m_3^2 - m_4^2 + s}{2\sqrt{s}},$$
$$E_4 = \frac{p_4 \cdot (p_3 + p_4)}{\sqrt{s}} = \frac{m_4^2 + p_3 \cdot p_4}{\sqrt{s}} = \frac{m_4^2 - m_3^2 + s}{2\sqrt{s}},$$

by substituting

$$2p_1 \cdot p_2 = s - m_1^2 - m_2^2, \quad 2p_3 \cdot p_4 = s - m_3^2 - m_4^2.$$

Thus, all cms energies E_i depend only on the incident energy but not on the scattering angle. For elastic scattering $m_3 = m_1$, $m_4 = m_2$ so that $E_3 = E_1$, $E_4 = E_2$. The Lorentz invariant momentum transfer squared

$$t = (p_1 - p_3)^2 = m_1^2 + m_3^2 - 2p_1 \cdot p_3$$

depends linearly on the cosine of the scattering angle.

EXAMPLE 4.4.1

Kaon Decay and Pion Photoproduction Threshold Find the kinetic energies of the muon of mass 106 MeV and massless neutrino into which a K meson of mass 494 MeV decays in its rest frame.

Conservation of energy and momentum gives $m_K = E_\mu + E_\nu = \sqrt{s}$. Applying the relativistic kinematics described previously yields

$$E_\mu = \frac{p_\mu \cdot (p_\mu + p_\nu)}{m_K} = \frac{m_\mu^2 + p_\mu \cdot p_\nu}{m_K},$$
$$E_\nu = \frac{p_\nu \cdot (p_\mu + p_\nu)}{m_K} = \frac{p_\mu \cdot p_\nu}{m_K}.$$

Combining both results, we obtain $m_K^2 = m_\mu^2 + 2p_\mu \cdot p_\nu$ so that

$$E_\mu = T_\mu + m_\mu = \frac{m_K^2 + m_\mu^2}{2m_K} = 258.4 \text{ MeV},$$
$$E_\nu = T_\nu = \frac{m_K^2 - m_\mu^2}{2m_K} = 235.6 \text{ MeV}.$$

As another example, in the production of a neutral pion by an incident photon according to $\gamma + p \to \pi^0 + p'$ at threshold, the neutral pion and proton are created at rest in the cms. Therefore,

$$s = (p_\gamma + p)^2 = m_p^2 + 2m_p E_\gamma^L = (p_\pi + p')^2 = (m_\pi + m_p)^2$$

so that $E_\gamma^L = m_\pi + \frac{m_\pi^2}{2m_p} = 144.7$ MeV. ■

SUMMARY

The Lorentz group is the symmetry group of electrodynamics: It governs special relativity of the electroweak gauge theory and of the strong interactions described by quantum chromodynamics. The metric of Minkowski space–time is Lorentz invariant and expresses the propagation of light; that is, the velocity of light is the same in all inertial frames. Newton's equations of motion are straightforward to extend to special relativity. The kinematics of two-body collisions are important applications of vector algebra in Minkowski space–time.

Biographical Data

Lorentz, Hendrik Antoon. Lorentz, a Dutch physicist, was born in 1853 in Arnhem and died in 1928 in Haarlem. He obtained his Ph.D. in 1875 at Leiden University, where he returned 3 years later as a professor of theoretical physics and stayed until his death. He refined Maxwell's theory of radiation, and light in particular, attributing it to oscillations of charged particles within matter at a time when atoms were not universally recognized. These were later identified as electrons by J. J. Thomson and ions by Arrhenius. As proof, he suggested subjecting atoms to magnetic fields, predicting effects that were demonstrated by his student Zeeman in 1896. He also analyzed the physical consequences (Lorentz–Fitzgerald contraction) of the invariance of Maxwell's equations under transformations that depend on the relative velocity of the inertial frames (now named after him) and differ from those (Galilean transformations) of Newton's equations of motion. Thus, he was a forerunner of Einstein's special relativity.

EXERCISES

4.4.1 Two Lorentz transformations are carried out in succession: v_1 along the x-axis and then v_2 along the y-axis. Show that the resultant transformation (given by the product of these two successive transformations) **cannot** be put in the form of a single Lorentz transformation.
Note. The discrepancy corresponds to a rotation so that pure Lorentz transformations (boosts) do not form a group.

4.4.2 Rederive the Lorentz transformation working entirely in Minkowski space (x^0, x^1, x^2, x^3) with $x^0 = x_0 = ct$. Show that the Lorentz transformation may be written $L(\mathbf{v}) = \exp(\rho\sigma)$, with

$$\sigma = \begin{pmatrix} 0 & -\lambda & -\mu & -\nu \\ -\lambda & 0 & 0 & 0 \\ -\mu & 0 & 0 & 0 \\ -\nu & 0 & 0 & 0 \end{pmatrix},$$

and λ, μ, ν the direction cosines of the velocity $\mathbf{v}$.

4.4.3 Using the matrix relation, Eq. (4.67), let the rapidity ρ_1 relate the Lorentz reference frames (x'^0, x'^1) and (x^0, x^1). Let ρ_2 relate (x''^0, x''^1) and

(x'^0, x'^1). Finally, let ρ relate (x''^0, x''^1) and (x^0, x^1). From $\rho = \rho_1 + \rho_2$, derive the Einstein velocity addition law

$$v = \frac{v_1 + v_2}{1 + v_1 v_2/c^2}.$$

4.4.4 (a) A particle A decays into B and C. What is the energy of the particle B in the rest frame of A? An example is a neutral pion that decays into two photons. (b) Explain why a photon of sufficient energy can produce an electron–positron pair only in the presence of matter.
Note. The particle masses obey $m_A > m_B + m_C$.

4.4.5 Determine the minimum frequency of a γ-ray that disintegrates a deuteron into a neutron of mass $m_n = 939.565$ MeV/c^2 and a proton of mass $m_p = 938.272$ MeV/c^2. The deuteron has a binding energy of 2.226 MeV.
Hint. Ignore the Fermi motion; that is, take the neutron and proton at rest. Explain why this is a good approximation.

4.4.6 An observer moving with four-velocity u^μ measures the energy E of a particle with four-momentum p^μ. Show that $E = cp \cdot u$.

4.4.7 Derive the relativistic generalization of the equation of motion $\frac{d\mathbf{p}}{dt} = q\mathbf{E} + q\mathbf{v} \times \mathbf{B}$ of a charged particle in an electromagnetic field.

4.4.8 Show that the Lorentz covariant equation of motion $\frac{dp^\mu}{d\tau} = \frac{q}{\epsilon_0 mc} F^{\mu\nu} p_\nu$ of a charged particle in an electromagnetic field is consistent with (has as a solution) the on-mass-shell relation $p^2 = m^2c^2$. Here, m is the rest mass of the particle and τ its proper time (i.e., the Lorentz invariant time measured in its rest frame), $p^\mu = mcu^\mu$ is its four-momentum, and $F^{\mu\nu} = \partial^\mu A^\nu - \partial^\nu A^\mu$ is the electromagnetic field tensor.

Additional Reading

Buerger, M. J. (1956). *Elementary Crystallography*. Wiley, New York. A comprehensive discussion of crystal symmetries. Buerger develops all 32 point groups and all 230 space groups. Related books by this author include *Contemporary Crystallography*. McGraw-Hill, New York (1970); *Crystal Structure Analysis*. Krieger, New York (1979); and *Introduction to Crystal Geometry*. Krieger, New York (1971, reprint 1977).

Burns, G., and Glazer, A. M. (1978). *Space Groups for Solid State Scientists*. Academic Press, New York. A well-organized, readable treatment of groups and their application to the solid state.

de-Shalit, A., and Talmi, I. (1963). *Nuclear Shell Model*. Academic Press, New York. We adopt the Condon–Shortley phase conventions of this text.

Edmonds, A. R. (1957). *Angular Momentum in Quantum Mechanics*. Princeton Univ. Press, Princeton, NJ.

Falicov, L. M. (1966). *Group Theory and Its Physical Applications* [Notes compiled by A. Luehrmann]. Univ. of Chicago Press, Chicago. Group theory

with an emphasis on applications to crystal symmetries and solid-state physics.

Greiner, W., and Müller, B. (1989). *Quantum Mechanics Symmetries*. Springer, Berlin. We refer to this textbook for more details and numerous exercises that are worked out in detail.

Hamermesh, M. (1962). *Group Theory and Its Application to Physical Problems*. Addison-Wesley, Reading, MA. A detailed, rigorous account of both finite and continuous groups. The 32 point groups are developed. The continuous groups are treated with Lie algebra included. A wealth of applications to atomic and nuclear physics.

Heitler, W. (1947). *The Quantum Theory of Radiation*, 2nd ed. Oxford Univ. Press, Oxford. Reprinted, Dover, New York (1983).

Higman, B. (1955). *Applied Group–Theoretic and Matrix Methods*. Clarendon, Oxford. A complete and unusually intelligible development of matrix analysis and group theory.

Messiah, A. (1961). *Quantum Mechanics*, Vol. 2. North-Holland, Amsterdam.

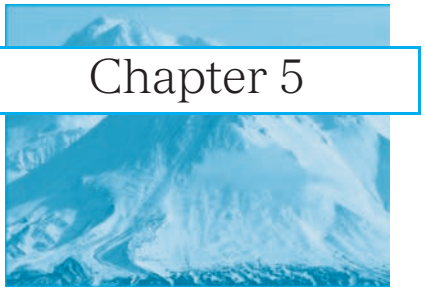
Panofsky, W. K. H., and Phillips, M. (1962). *Classical Electricity and Magnetism*, 2nd ed. Addison-Wesley, Reading, MA. The Lorentz covariance of Maxwell's equations is developed for both vacuum and material media. Panofsky and Phillips use contravariant and covariant tensors.

Park, D. (1968). Resource letter SP-1 on symmetry in physics. *Am. J. Phys.* **36**, 577–584. Includes a large selection of basic references on group theory and its applications to physics: atoms, molecules, nuclei, solids, and elementary particles.

Ram, B. (1967). Physics of the SU(3) symmetry model. *Am. J. Phys.* **35**, 16. An excellent discussion of the applications of SU(3) to the strongly interacting particles (baryons). For a sequel to this, see Young, R. D. (1973). Physics of the quark model. *Am. J. Phys.* **41**, 472.

Rose, M. E. (1957). *Elementary Theory of Angular Momentum*. Wiley, New York. Reprinted, Dover, New York (1995). As part of the development of the quantum theory of angular momentum, Rose includes a detailed and readable account of the rotation group.

Wigner, E. P. (1959). *Group Theory and Its Application to the Quantum Mechanics of Atomic Spectra* (translated by J. J. Griffin). Academic Press, New York. This is the classic reference on group theory for the physicist. The rotation group is treated in considerable detail. There is a wealth of applications to atomic physics.



Chapter 5

Infinite Series

5.1 Fundamental Concepts

Infinite series are summations of infinitely many real numbers. They occur frequently in both pure and applied mathematics as in accurate numerical approximations of constants such as $\sqrt{0.97} = (1 - 0.03)^{1/2} = 1 - 0.03/2 + \cdots \sim 0.985$, π, e, and periodic decimals by rational numbers. Elementary and transcendental functions may be defined by power series in a fundamental approach to the theory of functions in Section 5.6. In science and engineering infinite series are ubiquitous because they appear in the evaluation of integrals (Section 5.10), in the solution of differential equations (Sections 8.5 and 8.6), and as Fourier series (Chapter 14) and compete with integral representations for the description of a host of special functions (Chapters 11–13).

Right at the start we face the problem of attaching meaning to the sum of an infinite number of terms. The usual approach is by partial sums. If we have an infinite sequence of terms $u_1, u_2, u_3, u_4, u_5, \ldots$, we define the nth **partial sum** as

$$s_n = \sum_{i=1}^{n} u_i. \tag{5.1}$$

This is a **finite sum** and offers no difficulties.

Whenever the sequence of partial sums does not approach a finite limit, the infinite series is said to **diverge**.

EXAMPLE 5.1.1 **Diverging Partial Sums** The sum of positive integers

$$\sum_{i=1}^{n} i = \frac{n}{2}(n+1)$$

can be summed by pairing the first and last terms, whose sum is $n+1$, then the second and next to last term, whose sum is $n+1$ as well, etc. Because there are $n/2$ pairs, we get the result. Here, we have tacitly taken n to be even. However, for odd n, the same argument can be made including zero as the first term. We can also use **mathematical induction** by verifying that the result is valid for $n=1$, giving $1=\frac{1}{2}(1+1)$. The next step is to assume the result is true for n and then prove it for $n+1$ as follows:

$$s_n+(n+1)=\frac{n}{2}(n+1)+(n+1)=\left(\frac{n}{2}+1\right)(n+1)=\frac{n+1}{2}(n+2)=s_{n+1}.$$

Thus, it is valid for all natural numbers. Clearly, $s_n\to\infty$ as $n\to\infty$, and the series diverges. Moreover, the partial sums are independent of the order in which we sum the terms. ■

If the partial sums s_n approach a finite limit as $n\to\infty$,

$$\lim_{n\to\infty} s_n = S, \tag{5.2}$$

the infinite series $\sum_{n=1}^{\infty} u_n$ is defined to be **convergent** and to have the value S. Note that we reasonably, plausibly, but still arbitrarily **define** the infinite series as equal to S. Now consider one of the simplest convergent series.

EXAMPLE 5.1.2

The Geometric Series The geometrical sequence, starting with a and with a ratio r $(=u_{n+1}/u_n)$ independent of n, is given by

$$a+ar+ar^2+ar^3+\cdots+ar^{n-1}+\cdots.$$

The nth partial sum is given by[1]

$$s_n = a\frac{1-r^n}{1-r}. \tag{5.3}$$

Taking the limit as $n\to\infty$,

$$\lim_{n\to\infty} s_n = \frac{a}{1-r}, \quad \text{for } |r|<1. \tag{5.4}$$

Hence, by definition, the infinite geometric series converges for $|r|<1$ and has the value

$$a\sum_{n=1}^{\infty} r^{n-1} = \frac{a}{1-r}. \tag{5.5}$$

However, for

$$|r|>1, \quad \lim_{n\to\infty}|s_n| = \lim_{n\to\infty}\frac{|a||r|^n}{|1-r|}\to\infty,$$

so that the series diverges.

[1]Multiply and divide $s_n=a\sum_{m=0}^{n-1} r^m$ by $1-r$, which gives $(1+r+\cdots+r^{n-1})(1-r)=1+r+\cdots+r^{n-1}-r-r^2-\cdots-r^n=1-r^n$.

This exact series summation can be used to determine periodic decimals in terms of rational numbers as follows. Let us consider two typical cases

$$\begin{aligned} 1.11\cdots &= 1+10^{-1}+10^{-2}+\cdots=\frac{1}{1-10^{-1}}=\frac{10}{9},\\ 0.131313\cdots &= \frac{13}{100}+\frac{13}{10^4}+\cdots=\frac{13}{100}\left[1+10^{-2}+10^{-4}+\cdots\right]\\ &= \frac{13}{100}\frac{1}{1-10^{-2}}=\frac{13}{99}. \end{aligned}$$

■

These examples suggest that a **necessary condition** for the convergence to a limit is that $\lim_{n\to\infty} u_n = 0$. This condition is not sufficient to guarantee convergence. However, for special series it can be considerably sharpened, as shown in the following theorem:

If the $u_n > 0$ are monotonically decreasing to zero, that is, $u_n > u_{n+1}$ for all n, then $\sum_n u_n$ is converging to S if, and only if, $s_n - nu_n$ converges to S.

As the partial sums s_n converge to S, this theorem implies that $nu_n \to 0$, for $n \to \infty$.

To prove this theorem, we start by concluding from $0 < u_{n+1} < u_n$ and

$$s_{n+1} - (n+1)u_{n+1} = s_n - nu_{n+1} = s_n - nu_n + n(u_n - u_{n+1}) > s_n - nu_n$$

that $s_n - nu_n$ increases with $n \to \infty$. As a consequence of $s_n - nu_n < s_n \le S$, $s_n - nu_n$ converges to a value $s \le S$. Deleting the tail of positive terms $u_i - u_n$ from $i = \nu + 1$ to n, we infer from $s_n - nu_n > u_0 + (u_1 - u_n) + \cdots + (u_\nu - u_n) = s_\nu - \nu u_n$ that $s_n - nu_n \ge s_\nu$ for $n \to \infty$. Hence also $s \ge S$ so that $s = S$ and $nu_n \to 0$.

When this theorem is applied to the **harmonic series** $\sum_n \frac{1}{n}$ with $n\frac{1}{n} = 1$, it implies that it does not converge; it diverges to $+\infty$. This can also be verified as follows.

EXAMPLE 5.1.3 **Regrouping of the Harmonic Series**

$$\sum_{n=1}^{\infty}\frac{1}{n} = 1+\frac{1}{2}+\frac{1}{3}+\frac{1}{4}+\cdots+\frac{1}{n}+\cdots. \tag{5.6}$$

We have the $\lim_{n\to\infty} u_n = \lim_{n\to\infty} 1/n = 0$, but this is not sufficient to guarantee convergence, as we have just shown. To see this independently of the theorem, we sum the terms as indicated by the parentheses

$$1+\frac{1}{2}+\left(\frac{1}{3}+\frac{1}{4}\right)+\left(\frac{1}{5}+\frac{1}{6}+\frac{1}{7}+\frac{1}{8}\right)+\left(\frac{1}{9}+\cdots+\frac{1}{16}\right)+\cdots. \tag{5.7}$$

Then each pair of parentheses encloses p terms for $p = 2, 3, \ldots$ of the form

$$\frac{1}{p+1} + \frac{1}{p+2} + \cdots + \frac{1}{p+p} > \frac{p}{2p}. \tag{5.8}$$

Forming partial sums by adding the parenthetical groups one by one, we obtain

$$\begin{aligned} s_1 &= 1, \quad & s_4 &> \frac{5}{2}, \\ s_2 &= \frac{3}{2}, \quad & s_5 &> \frac{6}{2}, \cdots \\ s_3 &> \frac{4}{2}, \quad & s_n &> \frac{n+1}{2}. \end{aligned} \tag{5.9}$$

The harmonic series summed in this way is certainly divergent.[2] ■

The condition for the validity of Eq. (5.2) is usually written in formal mathematical notation as follows:

> The condition for the existence of a limit S is that for each $\varepsilon > 0$, there is a fixed $N = N(\varepsilon)$ such that
>
> $$|S - s_i| < \varepsilon, \quad \text{for } i > N.$$

Note that the size of the first few or any fixed finite number of terms does not matter for convergence; it is the **infinite tail** that **is decisive for convergence**. This convergence condition is often derived from the Cauchy criterion applied to the partial sums s_i. The **Cauchy criterion** is as follows:

> A necessary and sufficient condition that a sequence (s_i) converges is that for each $\varepsilon > 0$ there is a fixed number N such that
>
> $$|s_j - s_i| < \varepsilon \quad \text{for all } i, j > N.$$
>
> This means that the individual partial sums must cluster together as we move far out in the sequence, into the infinitely long tail of the series.

Addition and Subtraction of Series

If we have two convergent series $\sum_n u_n \to s$ and $\sum_n v_n \to S$, their sum and difference will also converge to $s \pm S$ because their partial sums satisfy

$$|s_j \pm S_j - (s_i \pm S_i)| = |s_j - s_i \pm (S_j - S_i)| \le |s_j - s_i| + |S_j - S_i| < 2\varepsilon$$

using the triangle inequality

$$|a| - |b| \le |a + b| \le |a| + |b|$$

for $a = s_j - s_i$, $b = S_j - S_i$.

A convergent series $\sum_n u_n \to S$ may be multiplied termwise by a real number a. The new series will converge to aS because

$$|as_j - as_i| = |a(s_j - s_i)| = |a||s_j - s_i| < |a|\varepsilon.$$

[2] The (finite) harmonic series appears in an interesting note on the maximum stable displacement of a stack of coins: Johnson, P. R. (1955). The leaning tower of Lire. *Am. J. Phys.* **23**, 240.

This multiplication by a constant can be generalized to a multiplication by terms c_n of a bounded sequence of numbers.

If $\sum_n u_n$ converges to S and $0 < c_n \le M$ are bounded, then $\sum_n u_n c_n$ is convergent. If $\sum_n u_n$ is divergent and $c_n > M > 0$, then $\sum_n u_n c_n$ diverges.

To prove this theorem, we take i, j sufficiently large so that $|s_j - s_i| < \varepsilon$. Then

$$\sum_{i+1}^{j} u_n c_n \le M \sum_{i+1}^{j} u_n = M|s_j - s_i| < M\varepsilon.$$

The divergent case follows from

$$\sum_n u_n c_n > M \sum_n u_n \to \infty.$$

Multiplication of two convergent series will be addressed in Section 5.4. Our partial sums s_n may not converge to a single limit but may oscillate, as demonstrated by the following example.

EXAMPLE 5.1.4 **Oscillatory Series**

$$\sum_{n=1}^{\infty} u_n = 1 - 1 + 1 - 1 + 1 + \cdots - (-1)^n + \cdots.$$

Clearly, $s_n = 1$ for n odd but 0 for n even. There is no convergence to a limit, and series such as this one are labeled **oscillatory** and cannot be assigned a value. However, using the geometric series,[3] we may expand the function

$$\frac{1}{1+x} = 1 - x + x^2 - x^3 + \cdots + (-x)^{n-1} + \cdots. \tag{5.10}$$

If we let $x \to 1$, this series becomes

$$1 - 1 + 1 - 1 + 1 - 1 + \cdots, \tag{5.11}$$

the same series that we just labeled oscillatory. Although it does not converge in the usual sense, meaning can be attached to this series. Euler, for example, assigned a value of 1/2 to this oscillatory sequence on the basis of the correspondence between this series and the well-defined function $(1+x)^{-1}$. Unfortunately, such correspondence between series and function is not unique and this approach must be refined (see Hardy, 1956, Additional Reading). Other methods of assigning a meaning to a divergent or oscillatory series, methods of defining a sum, have been developed.

In general, however, this aspect of infinite series is of relatively little interest to the scientist or the engineer. An exception to this statement, the very important asymptotic or semiconvergent series, is considered in Section 5.8. ■

[3] Actually, Eq. (5.10) may be taken as an identity and verified by multiplying both sides by $1 + x$, i.e., the geometric series of Eq. (5.5) with $a = 1$ and $r = -x$.

SUMMARY

In summary, infinite series often appear in physics by means of Taylor expansions or binomial or other expansions. Truncating appropriate series is central to the art of approximation in physics. The geometric series is the simplest that can be summed exactly and illustrates convergence properties.

EXERCISES

5.1.1 Find the fractions that correspond to the following decimals:

(a) $0.222\cdots$ (c) $0.123123\cdots$
(b) $0.0101\cdots$ (d) $0.45234523\cdots$.

5.1.2 Show that

$$\sum_{n=1}^{\infty} \frac{1}{(2n-1)(2n+1)} = \frac{1}{2}.$$

Hint. Show (by mathematical induction) that $s_m = m/(2m+1)$.

5.1.3 Show that

$$\sum_{n=1}^{\infty} \frac{1}{n(n+1)} = 1.$$

Find the partial sum s_m and verify its correctness by mathematical induction.
Note. The method of expansion in partial fractions (Section 15.8) offers an alternative way of solving Exercises 5.1.2 and 5.1.3.

5.2 Convergence Tests

It is important to be able to tell whether a given series is convergent. We shall develop a few tests, starting with the simple and relatively insensitive tests and then the more complicated but quite sensitive integral tests. For now, let us consider a **series of positive terms**, $a_n \geq 0$, postponing negative terms until the next section except when otherwise noted.

Comparison Test

We start with the theorem: If term by term a series of terms $0 \leq u_n \leq a_n$, in which the a_n form a convergent series, the series $\sum_n u_n$ is also convergent.

To prove it, assume that $u_n \leq a_n$ for all n; then $\sum_n u_n \leq \sum_n a_n$ and $\sum_n u_n$ therefore is **convergent**. Then, if term by term a series of terms $v_n \geq b_n$, in which the b_n form a divergent series, the series $\sum_n v_n$ is also **divergent**. If $v_n \geq b_n$ for all n, then $\sum_n v_n \geq \sum_n b_n$ and $\sum_n v_n$ therefore is divergent.

EXAMPLE 5.2.1

Riemann Zeta Function Series If we sum the inverse squares of all natural numbers, $1/n^2$, does the sum $\sum_n n^{-2}$ converge? This sum is the special case

of the Riemann zeta function

$$\zeta(x) = \sum_{n=1}^{\infty} \frac{1}{n^x} = 1 + \frac{1}{2^x} + \frac{1}{3^x} + \cdots \tag{5.12}$$

for $x = 2$, which plays a prominent role in analytic prime number theory. The harmonic series is $\zeta(x)$ for $x \to 1$, where the function diverges as $1/(x-1)$. Its special values at integer arguments occur in statistical mechanics. To see that it converges for $x = 2$, we use the convergent series $\sum_n 1/[n(n+1)]$ of Exercise 5.1.3 for comparison. Note that for $n \geq 1$, clearly $n + 1 > n$; hence, $(n+1)^2 > n(n+1)$ and, taking the inverse, $\frac{1}{(n+1)^2} < \frac{1}{n(n+1)}$. Therefore, our series converges and from the first two terms and the comparison sum, we find

$$\frac{5}{4} < 1 + \frac{1}{4} + \frac{1}{9} + \cdots < 1 + 1 = 2.$$

Its actual value, $\pi^2/6 \sim 1.6449\cdots$, was found by Euler along with $\zeta(4)$, $\zeta(6)$, $\cdots$ in terms of powers of π and Bernoulli numbers B_n that are related to the finite sums of powers of natural numbers $\sum_{i=1}^{N} i^n$. It takes approximately 200 terms in Eq. (5.12) to get the correct value of the second decimal place of $\zeta(2)$. ■

For the convergent comparison series a_n we already have the geometric series, whereas the harmonic series will serve as the divergent series b_n. As other series are identified as either convergent or divergent, they may be used for the known series in this comparison test. All tests developed in this section are essentially comparison tests.

Cauchy Root Test

If $0 \leq (a_n)^{1/n} \leq r < 1$ for all sufficiently large n, with r independent of n, then $\sum_n a_n$ is convergent. If $(a_n)^{1/n} \geq 1$ for all sufficiently large n, then $\sum_n a_n$ is divergent. The first part of this test is verified easily by raising $(a_n)^{1/n} \leq r$ to the nth power. We get

$$a_n \leq r^n < 1.$$

Since r^n is the nth term in a convergent geometric series, $\sum_n a_n$ is convergent by the comparison test. Conversely, if $(a_n)^{1/n} \geq 1$, then $a_n \geq 1$ and the series must diverge. This root test is particularly useful in establishing the properties of power series (Section 5.7).

d'Alembert or Cauchy Ratio Test

If $0 \leq a_{n+1}/a_n \leq r < 1$ for all sufficiently large n, and r is independent of n, then $\sum_n a_n$ is convergent. If $a_{n+1}/a_n \geq 1$ for all sufficiently large n, then $\sum_n a_n$ is divergent.

Convergence is proved by direct comparison with the geometric series $(1 + r + r^2 + \cdots)$, for which $r^{n+1}/r^n = r < 1$. In the second part, $a_{n+1} \geq a_n$ and divergence is obvious since not even $a_n \to 0$. Although not quite as sensitive as the Cauchy root test, the d'Alembert ratio test is one of the easiest to apply

and is widely used. An alternate statement of the ratio test is in the form of a limit: If

$$\lim_{n\to\infty} \frac{a_{n+1}}{a_n} \begin{cases} < 1, & \text{convergence,} \\ > 1, & \text{divergence,} \\ = 1, & \text{indeterminate.} \end{cases} \tag{5.13}$$

Because of this final indeterminate possibility, the ratio test is likely to fail at crucial points, and more delicate, sensitive tests are necessary. Let us illustrate how this indeterminacy arises. Actually, it is concealed in the first statement $a_{n+1}/a_n \le r < 1$. We might encounter $a_{n+1}/a_n < 1$ for all **finite** n but be unable to choose an $r < 1$ **and independent of** n such that $a_{n+1}/a_n \le r$ for all sufficiently large n. An example is provided by Example 5.2.2.

EXAMPLE 5.2.2 **Harmonic Series**

$$\frac{a_{n+1}}{a_n} = \frac{n}{n+1} < 1, \quad n = 1, 2, \ldots$$

because

$$\lim_{n\to\infty} \frac{a_{n+1}}{a_n} = 1. \tag{5.14}$$

No fixed ratio $r < 1$ exists and the ratio test fails. ■

Cauchy or Maclaurin Integral Test

This is the most common comparison test in which we compare a series with an integral. The test applies to $\sum_n a_n$, where $a_n = f(n)$ can be integrated in the (continuous) variable n and falls to zero monotonically. Geometrically, we compare the area of a series of unit-width rectangles with the area under a curve.

Let $f(x)$ be a continuous, **monotonically decreasing function** in which $f(n) = a_n$. Then $\sum_n a_n$ converges if $\int_1^\infty f(x)dx$ is finite and diverges if the integral is infinite. For the ith partial sum

$$s_i = \sum_{n=1}^{i} a_n = \sum_{n=1}^{i} f(n). \tag{5.15}$$

However,

$$s_i > \int_1^{i+1} f(x)dx \tag{5.16}$$

from Fig. 5.1a, with $f(x)$ being monotonically decreasing. On the other hand, from Fig. 5.1b,

$$s_i - a_1 < \int_1^{i} f(x)dx, \tag{5.17}$$

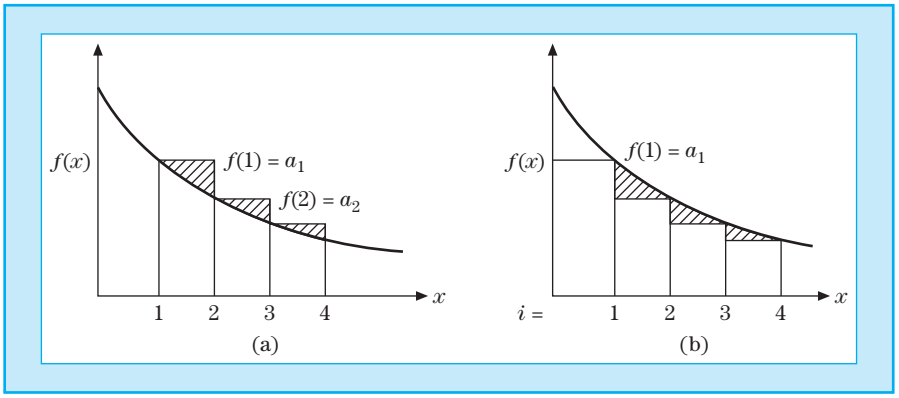


Figure 5.1

(a) Comparison of Integral and Sum-blocks Leading. (b) Comparison of Integral and Sum-blocks Lagging

in which the series is represented by the inscribed rectangles. Taking the limit as $i \to \infty$, we have

$$\int_1^\infty f(x)dx \le \sum_{n=1}^{\infty} a_n \le \int_1^\infty f(x)dx + a_1. \tag{5.18}$$

Hence, the infinite series converges or diverges as the corresponding integral converges or diverges. This integral test is particularly useful in setting upper and lower bounds on the remainder of a series after some number of initial terms have been summed. That is,

$$\sum_{n=1}^{\infty} a_n = \sum_{n=1}^{N} a_n + \sum_{n=N+1}^{\infty} a_n, \tag{5.19}$$

where

$$\int_{N+1}^\infty f(x)dx \le \sum_{n=N+1}^{\infty} a_n \le \int_{N+1}^\infty f(x)dx + a_{N+1}. \tag{5.20}$$

To free the integral test from the restrictive requirement that the interpolating function $f(x)$ be positive and monotonic, we show for any function $f(x)$ with a continuous derivative that

$$\sum_{n=N_i+1}^{N_f} f(n) = \int_{N_i}^{N_f} f(x)dx + \int_{N_i}^{N_f} (x - [x])f'(x)dx \tag{5.21}$$

holds. Here, $[x]$ denotes the largest integer below x so that $x - [x]$ varies sawtooth-like between 0 and 1. To derive Eq. (5.21), we observe that

$$\int_{N_i}^{N_f} xf'(x)dx = N_f f(N_f) - N_i f(N_i) - \int_{N_i}^{N_f} f(x)dx \tag{5.22}$$

using integration by parts. Next we evaluate the integral

$$\int_{N_i}^{N_f} [x]f'(x)dx = \sum_{n=N_i}^{N_f-1} n\int_n^{n+1} f'(x)dx = \sum_{n=N_i}^{N_f-1} n\{f(n+1)-f(n)\}$$

$$= -\sum_{n=N_i+1}^{N_f} f(n) - N_i f(N_i) + N_f f(N_f). \tag{5.23}$$

Subtracting Eq. (5.23) from Eq. (5.22), we arrive at Eq. (5.21). Note that $f(x)$ may go up or down and even change sign so that Eq. (5.21) applies to alternating series as well (see Section 5.3). Usually, $f'(x)$ falls faster than $f(x)$ for $x \to \infty$ so that the remainder term in Eq. (5.21) converges better. It is easy to improve Eq. (5.21) replacing $x-[x]$ by $x-[x]-\frac{1}{2}$, which varies between $-\frac{1}{2}$ and $\frac{1}{2}$:

$$\sum_{N_i<n\le N_f} f(n) = \int_{N_i}^{N_f} f(x)dx + \int_{N_i}^{N_f}\left(x-[x]-\frac{1}{2}\right)f'(x)dx + \frac{1}{2}\{f(N_f)-f(N_i)\}. \tag{5.24}$$

This formula was discovered independently by Euler and Maclaurin. Note that, as a periodic function, $x-[x]-\frac{1}{2} = -\sum_{n=1}^{\infty}\frac{\sin(2n\pi x)}{n\pi}$ has a Fourier expansion introduced in Chapter 14. The $f'(x)$ integral becomes even smaller if $f'(x)$ does not change sign too often. For an application of this integral test to an alternating series, see Example 5.3.2.

EXAMPLE 5.2.3 **Riemann Zeta Function** For the Riemann zeta function defined in Example 5.2.1 as

$$\zeta(p) = \sum_{n=1}^{\infty} n^{-p}, \tag{5.25}$$

we may take $f(n) = n^{-p}$ and then

$$\int_1^{\infty} n^{-p}dn = \left.\frac{n^{-p+1}}{-p+1}\right|_1^{\infty}, \quad p \neq 1$$

$$= \ln n\,|_{n=1}^{\infty}, \quad p = 1. \tag{5.26}$$

The integral and therefore the series are divergent for $p \le 1$ and convergent for $p > 1$. Hence, Eq. (5.25) should carry the condition $p > 1$. This, incidentally, is an independent proof that the harmonic series ($p = 1$) diverges logarithmically. The sum of the first million terms $\sum^{1,000,000} n^{-1}$ is only 14.392 726....

This integral comparison may also be used to set an upper limit to the Euler–Mascheroni constant[4] defined by

$$\gamma = \lim_{n\to\infty}\left(\sum_{m=1}^{n} m^{-1} - \ln n\right). \tag{5.27}$$

[4]This is the notation of the National Bureau of Standards (1972). *Handbook of Mathematical Functions*, Applied Mathematics Series 55 (AMS-55). Dover, New York.

Returning to partial sums, Eq. (5.17) yields

$$s_n = \sum_{m=1}^{n} m^{-1} - \ln n \le \int_1^n \frac{dx}{x} - \ln n + 1. \tag{5.28}$$

Evaluating the integral on the right, $s_n < 1$ for all n and therefore $\gamma \le 1$. Exercise 5.2.8 leads to more restrictive bounds. Actually, the Euler–Mascheroni constant is 0.577 215 66 . . . . ■

SUMMARY

The integral test is the workhorse for convergence. The ratio and root tests are based on comparison with the geometric series and simpler to apply, but they are far less sensitive and often indeterminate.

EXERCISES

5.2.1 (a) Show that if

$$\lim_{n\to\infty} n^p u_n \to A < \infty, \quad p > 1,$$

the series $\sum_{n=1}^{\infty} u_n$ converges.

(b) Show that if

$$\lim_{n\to\infty} n u_n = A > 0,$$

the series diverges. (The test fails for $A = 0$.)

These two tests, known as **limit tests**, are often convenient for establishing the convergence of a series. They may be treated as comparison tests, comparing with

$$\sum_n n^{-q}, \quad 1 \le q < p.$$

5.2.2 If

$$\lim_{n\to\infty} \frac{b_n}{a_n} = K,$$

a constant with $0 < K < \infty$, show that $\sum_n b_n$ converges or diverges with $\sum a_n$.

5.2.3 Test for convergence

(a) $\displaystyle\sum_{n=2}^{\infty} (\ln n)^{-1}$

(b) $\displaystyle\sum_{n=1}^{\infty} \frac{n!}{10^n}$

(c) $\displaystyle\sum_{n=1}^{\infty} \frac{1}{2n(2n+1)}$

(d) $\displaystyle\sum_{n=1}^{\infty} [n(n+1)]^{-1/2}$

(e) $\displaystyle\sum_{n=0}^{\infty} \frac{1}{2n+1}$.

5.2.4 Test for convergence

(a) $\displaystyle\sum_{n=1}^{\infty} \frac{1}{n(n+1)}$ (d) $\displaystyle\sum_{n=1}^{\infty} \ln\left(1+\frac{1}{n}\right)$

(b) $\displaystyle\sum_{n=2}^{\infty} \frac{1}{n\ln n}$ (e) $\displaystyle\sum_{n=1}^{\infty} \frac{1}{n\cdot n^{1/n}}$.

(c) $\displaystyle\sum_{n=1}^{\infty} \frac{1}{n2^n}$

5.2.5 For what values of p and q will the following series converge? $\sum_{n=2}^{\infty} \frac{1}{n^p(\ln n)^q}$.

ANS. Convergent for $\begin{cases} p>1, \text{ all } q, \\ p=1,\ q>1, \end{cases}$ divergent for $\begin{cases} p<1, \quad \text{all } q, \\ p=1,\ q\le 1. \end{cases}$

5.2.6 Determine the largest and smallest values of x, that is, the range of convergence for Gauss's **hypergeometric series**

$$F(\alpha,\beta,\gamma;x) = 1+\frac{\alpha\beta}{1!\gamma}x+\frac{\alpha(\alpha+1)\beta(\beta+1)}{2!\gamma(\gamma+1)}x^2+\cdots.$$

ANS. Convergent for $-1<x<1$ and $x=\pm 1$ if $\gamma>\alpha+\beta$.

5.2.7 Set upper and lower bounds on $\sum_{n=1}^{1,000,000} n^{-1}$, assuming that

(a) the Euler–Mascheroni constant [see Eq. (5.27)] is known.

ANS. $14.392726 < \sum_{n=1}^{1,000,000} n^{-1} < 14.392\,727.$

(b) The Euler–Mascheroni constant is unknown.

5.2.8 Given $\sum_{n=1}^{1,000} n^{-1} = 7.485\,470\ldots$, set upper and lower bounds on the Euler–Mascheroni constant [see Eq. (5.27)].

ANS. $0.5767 < \gamma < 0.5778.$

5.2.9 (From **Olbers's paradox**) Assume a static universe in which the stars are uniformly distributed. Divide all space into shells of constant thickness; the stars in any one shell by themselves subtend a solid angle of ω_0. **Allowing for the blocking out of distant stars by nearer stars**, show that the total net solid angle subtended by all stars, shells extending to infinity, is **exactly** 4π. [Therefore, the night sky should be ablaze with light. For historical and other details, see Harrison, E. (1987). *Darkness at Night: A Riddle of the Universe*. Harvard Univ. Press, Cambridge, MA.]

5.2.10 Test for convergence

$$\sum_{n=1}^{\infty}\left[\frac{1\cdot 3\cdot 5\cdots(2n-1)}{2\cdot 4\cdot 6\cdots(2n)}\right]^2 = \frac{1}{4}+\frac{9}{64}+\frac{25}{256}+\cdots.$$

Hint. Use Stirling's asymptotic formula for the factorials.

5.2.11 The Legendre series, $\sum_{j\ \text{even}} u_j(x)$, satisfies the recurrence relations

$$u_{j+2}(x) = \frac{(j+1)(j+2) - l(l+1)}{(j+2)(j+3)} x^2 u_j(x),$$

in which the index j is even and l is some constant (but, in this problem, **not** a nonnegative odd integer). Find the range of values of x for which this Legendre series is convergent. Test the end points carefully.

ANS. $-1 < x < 1$.

5.2.12 Show that the following series is convergent:

$$\sum_{s=0}^{\infty} \frac{(2s-1)!!}{(2s)!!(2s+1)}.$$

Note. $(2s-1)!! = (2s-1)(2s-3)\cdots 3\cdot 1$ with $(-1)!! = 1$; $(2s)!! = (2s)(2s-2)\cdots 4\cdot 2$ with $0!! = 1$. The series appears as a series expansion of $\sin^{-1}(1)$ and equals $\pi/2$, and $\sin^{-1} x \equiv \arcsin x \neq (\sin x)^{-1}$. Use Stirling's asymptotic formula for the factorials.

5.2.13 Catalan's constant [$\beta(2)$ of the National Bureau of Standards (1972). *Handbook of Mathematical Functions*, AMS-55, Chapter 23. Dover, New York] is defined by

$$\beta(2) = \sum_{k=0}^{\infty} (-1)^k (2k+1)^{-2} = \frac{1}{1^2} - \frac{1}{3^2} + \frac{1}{5^2} \cdots.$$

Calculate $\beta(2)$ to six-digit accuracy.
Hint. The rate of convergence is enhanced by pairing the terms:

$$(4k-1)^{-2} - (4k+1)^{-2} = 16k/(16k^2-1)^2.$$

If you have carried enough digits in your series summation, $\sum_{1\le k\le N} 16k/(16k^2-1)^2$, additional significant figures may be obtained by setting upper and lower bounds on the tail of the series, $\sum_{l=N+1}^{\infty}$. These bounds may be set by comparison with integrals as in the Maclaurin integral test.

ANS. $\beta(2) = 0.9159\ 6559\ 4177\cdots$.

5.3 Alternating Series

In Section 5.2, we limited ourselves to series of positive terms. Now, we consider infinite series in which the signs alternate. The partial cancellation due to changing signs makes convergence more rapid. We prove the Leibniz criterion, a fairly general condition for the convergence of an alternating series—that is, with **regular** sign changes. For series with irregular sign changes, such as Fourier series of Chapter 14 (see Example 5.3.3), the integral test of Eqs. (5.21) or (5.24) is often helpful.

Leibniz Criterion

Alternating series such as $\sum_n (-1)^n a_n$ with positive $a_n > 0$ involve summands that change sign at every term. Let us start with a typical example.

EXAMPLE 5.3.1

Alternating Harmonic Series We know from Example 5.1.3 and the $na_n \to 0$ criterion that the harmonic series $\sum_n n^{-1}$ diverges. However, the corresponding alternating series $\sum_n \frac{(-1)^n}{n}$ converges because we can cancel even against each subsequent odd term (without regrouping of the series) as follows:

$$\sum_{n=2}^{\infty} \frac{(-1)^n}{n} = \sum_{\nu=1}^{\infty} \left(\frac{1}{2\nu} - \frac{1}{2\nu+1} \right) = \sum_{\nu=1}^{\infty} \frac{1}{2\nu(2\nu+1)}.$$

We see from the integral test that the last positive sum converges

$$\begin{aligned} \sum_{\nu \geq \nu_0} \frac{1}{2\nu(2\nu+1)} &\approx \int_{\nu_0}^{\infty} \frac{d\nu}{2\nu(2\nu+1)} = \int_{\nu_0}^{\infty} \left(\frac{1}{2\nu} - \frac{1}{2\nu+1} \right) d\nu \\ &= \frac{1}{2} \ln \frac{2\nu}{2\nu+1} \Bigg|_{\nu_0}^{\infty} = -\frac{1}{2} \ln \frac{2\nu_0}{2\nu_0+1} \to 0, \quad \nu_0 \to \infty. \end{aligned}$$

■

More generally, consider the series $\sum_{n=1}^{\infty} (-1)^{n+1} a_n$ with $a_n > 0$. The **Leibniz criterion** states that if a_n is **monotonically decreasing** (for sufficiently large n) and $\lim_{n\to\infty} a_n = 0$, **then the series converges**.

To prove this theorem, we examine the even partial sums

$$\begin{aligned} s_{2n} &= a_1 - a_2 + a_3 - \cdots - a_{2n}, \\ s_{2n+2} &= s_{2n} + (a_{2n+1} - a_{2n+2}). \end{aligned} \tag{5.29}$$

Since $a_{2n+1} > a_{2n+2}$, we have

$$s_{2n+2} > s_{2n}. \tag{5.30}$$

On the other hand,

$$s_{2n+2} = a_1 - (a_2 - a_3) - (a_4 - a_5) - \cdots - a_{2n+2}. \tag{5.31}$$

Hence, with each pair of terms $a_{2p} - a_{2p+1} > 0$,

$$s_{2n+2} < a_1. \tag{5.32}$$

With the even partial sums bounded $s_{2n} < s_{2n+2} < a_1$ and the terms a_n decreasing monotonically and approaching zero, this alternating series converges.

One further important result can be extracted from the partial sums. From the difference between the series limit S and the partial sum s_n

$$\begin{aligned} S - s_n &= a_{n+1} - a_{n+2} + a_{n+3} - a_{n+4} + \cdots \\ &= a_{n+1} - (a_{n+2} - a_{n+3}) - (a_{n+4} - a_{n+5}) - \cdots \end{aligned} \tag{5.33}$$

or

$$S - s_n < a_{n+1}. \tag{5.34}$$

Equation (5.34) states that the **error in cutting off an alternating series after n terms is less than a_{n+1}, the first term dropped**. A knowledge of the error obtained in this way may be of great practical importance.

Absolute and Conditional Convergence

Given a series of terms u_n in which u_n may vary in sign, if $\sum |u_n|$ converges, then $\sum u_n$ is said to be **absolutely convergent**. If $\sum u_n$ converges but $\sum |u_n|$ diverges, the convergence is called **conditional**. In contrast to absolutely converging series whose terms can be summed in any order, **conditionally convergent series** must be manipulated more carefully. Its terms **must be summed in the prescribed order**.

The alternating harmonic series is a simple example of this conditional convergence, whereas the harmonic series has been shown to be divergent in Sections 5.1 and 5.2.

EXAMPLE 5.3.2

Rearrangement of Harmonic Series Let us continue with the alternating harmonic series to illustrate that conditionally converging alternating series cannot be rearranged arbitrarily without changing their limit or disrupting their convergence and hence must be handled carefully. If we write

$$1-\frac{1}{2}+\frac{1}{3}-\frac{1}{4}+\cdots=1-\left(\frac{1}{2}-\frac{1}{3}\right)-\left(\frac{1}{4}-\frac{1}{5}\right)-\cdots,$$

it is clear that the sum

$$\sum_{n=1}^{\infty}(-1)^{n-1}n^{-1}<1. \tag{5.35}$$

However, if we rearrange the terms, we may make the alternating harmonic series converge to $\frac{3}{2}$. We regroup the terms of Eq. (5.35), taking

$$\left(1+\frac{1}{3}+\frac{1}{5}\right)-\left(\frac{1}{2}\right)+\left(\frac{1}{7}+\frac{1}{9}+\frac{1}{11}+\frac{1}{13}+\frac{1}{15}\right)-\left(\frac{1}{4}\right)$$
$$+\left(\frac{1}{17}+\cdots+\frac{1}{25}\right)-\left(\frac{1}{6}\right)+\left(\frac{1}{27}+\cdots+\frac{1}{35}\right)-\left(\frac{1}{8}\right)+\cdots.$$

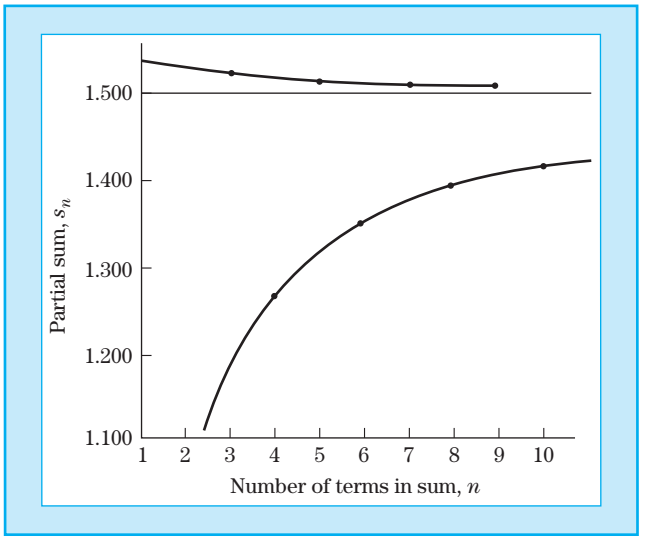
Of course, this rearrangement of terms does not omit any term but systematically postpones negative terms changing partial sums. Treating the terms grouped in parentheses as single terms for convenience, we obtain the partial sums

$$s_1=1.5333 \qquad s_2=1.0333$$
$$s_3=1.5218 \qquad s_4=1.2718$$
$$s_5=1.5143 \qquad s_6=1.3476$$
$$s_7=1.5103 \qquad s_8=1.3853$$
$$s_9=1.5078 \qquad s_{10}=1.4078.$$

From this tabulation of s_n and the plot of s_n versus n in Fig. 5.2 the convergence to $\frac{3}{2}$ is fairly clear. We have rearranged the terms, taking positive terms until the

Figure 5.2

Alternating Harmonic Series—Terms Rearranged to Give Convergence to 1.5



partial sum was equal to or greater than $\frac{3}{2}$, then adding in negative terms until the partial sum just fell below $\frac{3}{2}$, and so on. As the series extends to infinity, all original terms will eventually appear, but the partial sums of this rearranged alternating harmonic series converge to $\frac{3}{2}$.

By a suitable rearrangement of terms, a conditionally convergent series may be made to converge to any desired value or even to diverge. This statement is sometimes called **Riemann's theorem**. Obviously, conditionally convergent series must be treated with caution. ■

Note that most tests developed in Section 5.2 assume a series of positive terms and therefore guarantee absolute convergence.

EXAMPLE 5.3.3

Convergence of a Fourier Series For $0 < x < 2\pi$, the Fourier series (see Section 14.1 for an introduction)

$$\sum_{n=1}^{\infty} \frac{\cos(nx)}{n} = -\ln\left(2\sin\frac{x}{2}\right) \tag{5.36}$$

converges, having coefficients that change sign often but not at every term (except for $x = \pi$) so that Leibniz's convergence criterion cannot be used. Let us apply the integral test of Eq. (5.21). Using integration by parts we see immediately that

$$\int_1^{\infty} \frac{\cos(nx)}{n} dn = \left[\frac{\sin(nx)}{nx}\right]_{n=1}^{\infty} + \frac{1}{x}\int_1^{\infty} \frac{\sin(nx)}{n^2} dn \tag{5.37}$$

converges, and the integral on the right-hand side even converges absolutely. The derivative term in Eq. (5.21) has the form

$$\int_1^\infty (n-[n])\left\{-\frac{x}{n}\sin(nx)-\frac{\cos(nx)}{n^2}\right\}dn, \tag{5.38}$$

where the second term converges absolutely and need not be considered further. Next, we observe that $g(N)=\int_1^N (n-[n])\sin(nx)dn$ is bounded for $N\to\infty$, just as $\int^N \sin(nx)dn$ is bounded because of the periodic nature of $\sin(nx)$ and its regular sign changes. Using integration by parts again,

$$\int_1^\infty \frac{g'(n)}{n}dn=\left[\frac{g(n)}{n}\right]_{n=1}^\infty+\int_1^\infty \frac{g(n)}{n^2}dn, \tag{5.39}$$

we see that the second term is absolutely convergent, and the first goes to zero at the upper limit. Hence, the series in Eq. (5.36) converges, which is difficult to see from other convergence tests. ■

There are many conditionally convergent series with sign changes so irregular that it is sometimes extremely difficult to determine whether or not they converge. A prominent example is the inverse of the Riemann zeta function (see Example 5.2.1) $\zeta(s)$ for $s\to 1$, which can be defined by a product over all prime numbers p as

$$\left(1-\frac{1}{2^s}\right)\left(1-\frac{1}{3^s}\right)\left(1-\frac{1}{5^s}\right)\cdots,$$

where the exponent $s=1+\varepsilon$ for $\varepsilon\to 0$. Multiplying individual terms of the product yields the series $\sum_n \frac{\mu(n)}{n^s}$ with $\mu(1)=1$, $\mu(n)=(-1)^m$ if the integer $n=p_1p_2\cdots p_m$ is the product of m different primes p_i and $\mu(n)=0$ else; that is,

$$\frac{1}{\zeta(s)}=1-\frac{1}{2^s}-\frac{1}{3^s}-\frac{1}{5^s}+\frac{1}{6^s}+\cdots.$$

Proving that $1-\frac{1}{2}-\frac{1}{3}-\frac{1}{5}+\frac{1}{6}+\cdots$ converges to 0 is known to be equivalent to showing that there are $\frac{x}{\ln x}$ prime numbers $p\le x$. This asymptotic relation is known as the prime number theorem, which was conjectured first by Gauss and proved by two French mathematicians, J. Hadamard and Ch. de la Vallee-Poussin, in 1898 using the analytic properties of the zeta function as a function of the complex variable s.

SUMMARY

Sign changes are essential for the convergence of conditionally convergent series. Alternating series have regular sign changes with each term so that convergence can be easily tested by Leibniz's criterion. The integral test is sometimes applicable. Deciding the convergence of series with irregular sign changes can be extremely difficult. No general tests exist.

EXERCISES

5.3.1 (a) From the electrostatic two-hemisphere problem (Exercises 14.3.6, 14.3.7) we obtain the series

$$\sum_{s=0}^{\infty}(-1)^s(4s+3)\frac{(2s-1)!!}{(2s+2)!!}.$$

Test it for convergence.

(b) The corresponding series for the surface charge density is

$$\sum_{s=0}^{\infty}(-1)^s(4s+3)\frac{(2s-1)!!}{(2s)!!}.$$

Test it for convergence. The $n!!$ notation is defined in Exercise 5.2.12.
Hint. Use Stirling's asymptotic formula for the factorials.

5.3.2 Show by direct numerical computation that the sum of the first 10 terms of

$$\lim_{x\to 1}\ln(1+x)=\ln 2=\sum_{n=1}^{\infty}(-1)^{n-1}n^{-1}$$

differs from $\ln 2$ by less than the 11th term: $\ln 2 = 0.69314\,71806\cdots$.

5.3.3 In Exercise 5.2.6, the hypergeometric series is shown convergent for $x=\pm 1$, if $\gamma > \alpha+\beta$. Show that there is conditional convergence for $x=-1$ for γ down to $\gamma > \alpha+\beta-1$.
Hint. The asymptotic behavior of the factorial function is given by Stirling's formula.

5.3.4 If the u_n decrease monotonically to zero with $n\to\infty$, show that $\sum_n u_n(-1)^{[n/3]}$ converges, where $[n/3]$ is the largest integer below $n/3$.

5.4 Algebra of Series

The establishment of absolute convergence is important because it can be proved that absolutely convergent series can be reordered according to the familiar rules of algebra or arithmetic:

- If an infinite series is absolutely convergent, the series sum is independent of the order in which the terms are added.
- The series may be multiplied with another absolutely convergent series. The limit of the product will be the product of the individual series limits. The product series, a double series, will also converge absolutely.

No such guarantees can be given for conditionally convergent series, as we have seen in Example 5.3.2.

Multiplication of Series

The standard or Cauchy product of two series

$$\sum_n u_n \cdot \sum_n v_n = \sum_n c_n, \quad c_n = u_0 v_n + u_1 v_{n-1} + \cdots + u_n v_0, \tag{5.40}$$

which can be written as a double sum $\sum_n \sum_{m=0}^{n} u_m v_{n-m}$, where the sum of the indices is $m + (n - m) = n$ for the nth term c_n of the product series.

Absolutely convergent series can be multiplied without problems. This follows as a special case from the rearrangement of double series. However, conditionally convergent series cannot always be multiplied to yield convergent series, as the following example shows.

EXAMPLE 5.4.1

Square of a Conditionally Convergent Series May Diverge The series $\sum_{n=1}^{\infty} \frac{(-1)^{n-1}}{\sqrt{n}}$ converges by the Leibniz criterion. Its square

$$\left[\sum_n \frac{(-1)^{n-1}}{\sqrt{n}}\right]^2 = \sum_n (-1)^n \left[\frac{1}{\sqrt{1}}\frac{1}{\sqrt{n-1}} + \frac{1}{\sqrt{2}}\frac{1}{\sqrt{n-2}} + \cdots + \frac{1}{\sqrt{n-1}}\frac{1}{\sqrt{1}}\right]$$

has the general term in brackets consisting of $n - 1$ additive terms, each of which is $> \frac{1}{\sqrt{n-1}\sqrt{n-1}}$, so that the product term in brackets is $> \frac{n-1}{n-1}$ and does not go to zero. Hence, this product oscillates and therefore diverges. ■

Hence, for a product of two series to converge we have to demand as a sufficient condition that at least one of them converges absolutely. To prove this **product convergence theorem** that if $\sum_n u_n$ converges absolutely to U, $\sum_n v_n$ converges to V, then

$$\sum_n c_n, \quad c_n = \sum_{m=0}^{n} u_m v_{n-m}$$

converges to UV, it is sufficient to show that the difference terms $D_n \equiv c_0 + c_1 + \cdots + c_{2n} - U_n V_n \to 0$ for $n \to \infty$, where U_n, V_n are the partial sums of our series. As a result, the partial sum differences

$$\begin{aligned} D_n &= u_0 v_0 + (u_0 v_1 + u_1 v_0) + \cdots + (u_0 v_{2n} + u_1 v_{2n-1} + \cdots + u_{2n} v_0) \\ &\quad - (u_0 + u_1 + \cdots + u_n)(v_0 + v_1 + \cdots + v_n) \\ &= u_0(v_{n+1} + \cdots + v_{2n}) + u_1(v_{n+1} + \cdots + v_{2n-1}) + \cdots + u_{n+1} v_{n+1} \\ &\quad + v_{n+1}(v_0 + \cdots + v_{n-1}) + \cdots + u_{2n} v_0 \end{aligned}$$

so that for all sufficiently large n

$$|D_n| < \varepsilon(|u_0| + \cdots + |u_{n-1}|) + M(|u_{n+1}| + \cdots + |u_{2n}|) < \varepsilon(a + M)$$

because $|v_{n+1} + v_{n+2} + \cdots + v_{n+m}| < \varepsilon$ for sufficiently large n and all positive integers m as $\sum v_n$ converges, and the partial sums $V_n < B$ of $\sum_n v_n$ are bounded by M because the sum converges. Finally, we call $\sum_n |u_n| = a$, as $\sum u_n$ converges absolutely.

SUMMARY Two series can be multiplied provided one of them converges absolutely. Addition and subtraction of series are also valid termwise if one series converges absolutely.

EXERCISE

5.4.1 Given the series (derived in Section 5.6)

$$\ln(1+x) = x - \frac{x^2}{2} + \frac{x^3}{3} - \frac{x^4}{4}\cdots, \quad -1 < x \le 1,$$

show that

$$\ln\left(\frac{1+x}{1-x}\right) = 2\left(x + \frac{x^3}{3} + \frac{x^5}{5} + \cdots\right), \quad -1 < x < 1.$$

The original series, $\ln(1+x)$, appears in an analysis of binding energy in crystals. It is $\frac{1}{2}$ the Madelung constant $(2\ln 2)$ for a chain of atoms. The second series is useful in normalizing the Legendre polynomials (Section 11.3).

5.5 Series of Functions

We extend our concept of infinite series to include the possibility that each term u_n may be a function of some variable, $u_n = u_n(x)$. Numerous illustrations of such series of functions appear in Chapters 11–13. The partial sums become functions of the variable x,

$$s_n(x) = u_1(x) + u_2(x) + \cdots + u_n(x), \tag{5.41}$$

as does the series sum, defined as the limit of the partial sums

$$\sum_{n=1}^{\infty} u_n(x) = S(x) = \lim_{n\to\infty} s_n(x). \tag{5.42}$$

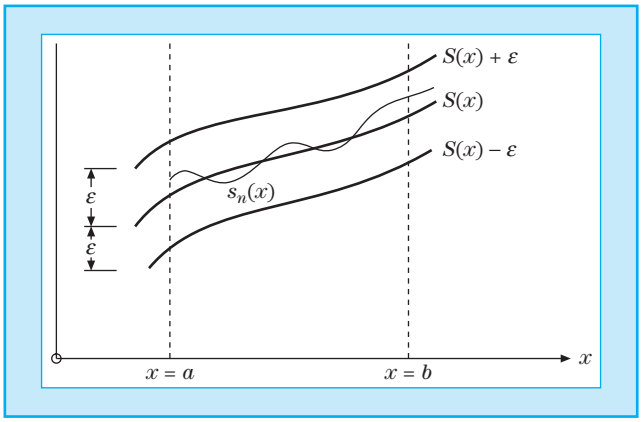
So far we have concerned ourselves with the behavior of the partial sums as a function of n. Now we consider how the foregoing quantities depend on x. The key concept here is that of uniform convergence.

Uniform Convergence

The concept of uniform convergence is related to a rate of convergence of a series of functions in an interval $[a, b]$ of the variable x that is independent of the location of x in that interval. Given uniform convergence, a series of continuous functions converges to a continuous function, limiting values of the sum exist at any point x of the interval, and even termwise differentiation of a series is valid under suitable conditions. Note that the interval must be closed, that is, include both end points.

Figure 5.3

Uniform Convergence



If for any small $\varepsilon > 0$ there exists a number N, **independent of** x in the interval $[a, b]$ (i.e., $a \le x \le b$), such that

$$|S(x) - s_n(x)| < \varepsilon, \quad \text{for all } n \ge N, \tag{5.43}$$

the series is defined to be **uniformly convergent** in the interval $[a, b]$. This states that for our series to be uniformly convergent, it must be possible to find a finite N so that the tail of the infinite series, $|\sum_{i=N+1}^{\infty} u_i(x)|$, will be less than an arbitrarily small ε for all x in the given interval.

This condition, Eq. (5.43), which defines uniform convergence, is illustrated in Fig. 5.3. The point is that no matter how small ε is taken to be, we can always choose n large enough so that the absolute magnitude of the difference between $S(x)$ and $s_n(x)$ is less than ε for all x, $a \le x \le b$. If this cannot be done, then $\sum u_n(x)$ is not uniformly convergent in $[a, b]$.

EXAMPLE 5.5.1 **Nonuniform Convergence**

$$\sum_{n=1}^{\infty} u_n(x) = \sum_{n=1}^{\infty} \frac{x}{[(n-1)x+1][nx+1]}. \tag{5.44}$$

A formula for the partial sum, $s_n(x) = nx(nx+1)^{-1}$, may be verified by mathematical induction. By inspection, this expression for $s_n(x)$ holds for $n = 1, 2$. We assume it holds for n terms and then prove it holds for $n+1$ terms:

$$\begin{aligned} s_{n+1}(x) &= s_n(x) + \frac{x}{[nx+1][(n+1)x+1]} \\ &= \frac{nx}{[nx+1]} + \frac{x}{[nx+1][(n+1)x+1]} \\ &= \frac{(n+1)x}{(n+1)x+1}, \end{aligned} \tag{5.45}$$

completing the proof.

Letting n approach infinity, we obtain

$$S(0) = \lim_{n\to\infty} s_n(0) = 0,$$
$$S(x \neq 0) = \lim_{n\to\infty} s_n(x \neq 0) = 1.$$

We have a discontinuity in our series limit at $x = 0$. However, $s_n(x)$ is a continuous function of x, for $0 \leq x \leq 1$, for all finite n. Equation (5.43) with ε sufficiently small will be violated for all **finite** n. Our series does not converge uniformly. ■

Weierstrass *M* (Majorant) Test

The most commonly encountered test for uniform convergence is the Weierstrass M test. If we can construct a series of numbers $\sum_1^\infty M_i$, in which $M_i \geq |u_i(x)|$ for all x in the interval $[a, b]$ and $\sum_1^\infty M_i$ is convergent, our series $u_i(x)$ will be **uniformly** convergent in $[a, b]$.

The proof of this Weierstrass M test is direct and simple. Since $\sum_i M_i$ converges, some number N exists such that for $n + 1 \geq N$,

$$\sum_{i=n+1}^{\infty} M_i < \varepsilon. \tag{5.46}$$

This follows from our definition of convergence. Then, with $|u_i(x)| \leq M_i$ for all x in the interval $a \leq x \leq b$,

$$\sum_{i=n+1}^{\infty} |u_i(x)| < \varepsilon. \tag{5.47}$$

Hence,

$$|S(x) - s_n(x)| = \left|\sum_{i=n+1}^{\infty} u_i(x)\right| < \varepsilon, \tag{5.48}$$

and by definition $\sum_{i=1}^\infty u_i(x)$ is uniformly convergent in $[a, b]$. Since we have specified absolute values in the statement of the Weierstrass M test, the series $\sum_{i=1}^\infty u_i(x)$ is also seen to be **absolutely** convergent. Note that uniform convergence and absolute convergence are independent properties. Neither implies the other. For specific examples,

$$\sum_{n=1}^{\infty} \frac{(-1)^n}{n + x^2}, \quad -\infty < x < \infty \tag{5.49}$$

and

$$\sum_{n=1}^{\infty} (-1)^{n-1} \frac{x^n}{n} = \ln(1 + x), \quad 0 \leq x \leq 1 \tag{5.50}$$

converge uniformly in the indicated intervals but do not converge absolutely. On the other hand,

$$\sum_{n=0}^{\infty}(1-x)x^n = 1, \quad 0 \le x < 1$$
$$= 0, \quad x = 1 \tag{5.51}$$

converges absolutely but does not converge uniformly in [0, 1].

From the definition of uniform convergence we may show that any series

$$f(x) = \sum_{n=1}^{\infty} u_n(x) \tag{5.52}$$

cannot converge uniformly in any interval that includes a discontinuity of $f(x)$.

Since the Weierstrass M test establishes both uniform and absolute convergence, it will necessarily fail for series that are uniformly but conditionally convergent.

Abel's Test

A more delicate test for uniform convergence has been given by Abel. If

$$u_n(x) = a_n f_n(x),$$
$$\sum a_n = A, \quad \text{convergent}$$

and the functions $f_n(x)$ are monotonic [$f_{n+1}(x) \le f_n(x)$] and bounded, $0 \le f_n(x) \le M$, for all x in $[a, b]$, then $\sum_n u_n(x)$ **converges uniformly** in $[a, b]$.

This test is especially useful in analyzing power series (compare Section 5.7). Details of the proof of Abel's test and other tests for uniform convergence are given in the Additional Reading section at the end of this chapter.

Uniformly convergent series have three particularly useful properties:

- If the individual terms $u_n(x)$ are continuous, the series sum

$$f(x) = \sum_{n=1}^{\infty} u_n(x) \tag{5.53}$$

  is also continuous.
- If the individual terms $u_n(x)$ are continuous, the series may be integrated term by term. The sum of the integrals is equal to the integral of the sum:

$$\int_a^b f(x)dx = \sum_{n=1}^{\infty} \int_a^b u_n(x)dx. \tag{5.54}$$

- The derivative of the series sum $f(x)$ equals the sum of the individual term derivatives,

$$\frac{d}{dx}f(x) = \sum_{n=1}^{\infty} \frac{d}{dx}u_n(x), \tag{5.55}$$

provided the following conditions are satisfied:

$u_n(x)$ and $\dfrac{du_n(x)}{dx}$ are continuous in $[a, b]$.

$\displaystyle\sum_{n=1}^{\infty} \frac{du_n(x)}{dx}$ is uniformly convergent in $[a, b]$.

SUMMARY

Term-by-term integration of a uniformly convergent series[5] requires only continuity of the individual terms. This condition is almost always satisfied in physical applications. Term-by-term differentiation of a series is often not valid because more restrictive conditions must be satisfied. Indeed, we shall encounter Fourier series in Chapter 14 in which term-by-term differentiation of a uniformly convergent series leads to a divergent series. Extracting values of series of functions for limiting values of the argument also requires uniform convergence.

Biographical Data

Abel, Niels Hendrik. Abel, a Norwegian mathematician, was born in 1802 on Finnoy Island and died in 1829 in Froland. Son of an alcoholic pastor, he lived in poverty and suffered professionally since he lived in Norway, far from the scientific mainstream in France and Germany. A teacher at the University of Christiania (now Oslo), where Abel studied, recognized his talents and supported him financially. In 1824, he showed the impossibility of solving algebraically for the roots of polynomials of 5th order. He sent his proof to Gauss, who, surprisingly, did not recognize his advance. He found the definitive form of the binomial expansion theorem and solved an integral equation now named after him. Recognition came so late (1829) that an appointment to a professorial position in Berlin arrived 2 days after his death at the age of 26.

EXERCISES

5.5.1 Find the range of **uniform** convergence of the Dirichlet series

(a) $\displaystyle\sum_{n=1}^{\infty} \frac{(-1)^{n-1}}{n^x}$ (b) $\zeta(x) = \displaystyle\sum_{n=1}^{\infty} \frac{1}{n^x}$.

ANS. (a) $1 \le x < \infty$. (b) $1 < s \le x < \infty$, with s arbitrary but fixed.

5.5.2 For what range of x is the geometric series $\sum_{n=0}^{\infty} x^n$ uniformly convergent?

ANS. $-1 < -s \le x \le s < 1$.

5.5.3 For what range of positive values of x is $\sum_{n=0}^{\infty} 1/(1 + x^n)$
(a) convergent? (b) uniformly convergent?

[5] Term-by-term integration may also be valid in the absence of uniform convergence.

5.5.4 If the series of the coefficients $\sum a_n$ and $\sum b_n$ are absolutely convergent, show that the Fourier series

$$\sum (a_n \cos nx + b_n \sin nx)$$

is **uniformly** convergent for $-\infty < x < \infty$.

5.6 Taylor's Expansion

This is an expansion of a function into an infinite series or into a finite series plus a remainder term. The coefficients of the successive terms of the series involve the successive derivatives of the function. We have already used Taylor's expansion in the establishment of a physical interpretation of divergence (Section 1.6) and in other sections of Chapters 1 and 2. Now we derive the Taylor expansion.

We assume that our function $f(x)$ has a continuous nth derivative[6] in the interval $a \le x \le b$. Then, integrating this nth derivative n times

$$\int_a^x f^{(n)}(x_1)dx_1 = f^{(n-1)}(x_1)\Big|_a^x = f^{(n-1)}(x) - f^{(n-1)}(a),$$

$$\begin{aligned}\int_a^x dx_2 \int_a^{x_2} dx_1 f^{(n)}(x_1) &= \int_a^x dx_2 [f^{(n-1)}(x_2) - f^{(n-1)}(a)] \\ &= f^{(n-2)}(x) - f^{(n-2)}(a) - (x-a)f^{(n-1)}(a).\end{aligned} \tag{5.56}$$

Continuing, we obtain

$$\begin{aligned}\int_a^x dx_3 \int_a^{x_3} dx_2 \int_a^{x_2} dx_1 f^{(n)}(x_1) &= f^{(n-3)}(x) - f^{(n-3)}(a) - (x-a)f^{(n-2)}(a) \\ &\quad - \frac{(x-a)^2}{2!} f^{(n-1)}(a).\end{aligned} \tag{5.57}$$

Finally, on integrating for the nth time,

$$\begin{aligned}\int_a^x dx_n \cdots \int_a^{x_2} dx_1 f^{(n)}(x_1) &= f(x) - f(a) - (x-a)f'(a) - \frac{(x-a)^2}{2!} f''(a) \\ &\quad - \cdots - \frac{(x-a)^{n-1}}{(n-1)!} f^{(n-1)}(a).\end{aligned} \tag{5.58}$$

Note that this expression is exact. No terms have been dropped and no approximations made. Now, solving for $f(x)$, we have

$$\begin{aligned}f(x) &= f(a) + (x-a)f'(a) \\ &\quad + \frac{(x-a)^2}{2!} f''(a) + \cdots + \frac{(x-a)^{n-1}}{(n-1)!} f^{(n-1)}(a) + R_n.\end{aligned} \tag{5.59}$$

[6] Taylor's expansion may be derived under slightly less restrictive conditions; compare Jeffreys, H., and Jeffreys, B. S. (1956). *Methods of Mathematical Physics*, 3rd ed., Section 1.133. Cambridge Univ. Press, Cambridge, UK.

In a first reading of this section, the remainder, R_n, can be ignored and the reader may continue with the infinite Taylor expansion series of Eq. (5.59).

The remainder, R_n, is given by the n-fold integral

$$R_n = \int_a^x dx_n \cdots \int_a^{x_2} dx_1 f^{(n)}(x_1). \tag{5.60}$$

This remainder may be put into a perhaps more practical form by using the **mean value theorem** of integral calculus:

$$\int_a^x g(x)dx = (x-a)g(\xi), \tag{5.61}$$

with $a \le \xi \le x$. By integrating n times we get the Lagrangian form[7] of the remainder:

$$R_n = \frac{(x-a)^n}{n!} f^{(n)}(\xi). \tag{5.62}$$

With Taylor's expansion in this form, we are not concerned with any questions of infinite series convergence. This series is finite, and the only question concerns the magnitude of the remainder.

When the function $f(x)$ is such that

$$\lim_{n\to\infty} R_n = 0, \tag{5.63}$$

Eq. (5.59) becomes Taylor's series[8]

$$\begin{aligned} f(x) &= f(a) + (x-a)f'(a) + \frac{(x-a)^2}{2!} f''(a) + \cdots \\ &= \sum_{n=0}^{\infty} \frac{(x-a)^n}{n!} f^{(n)}(a). \end{aligned} \tag{5.64}$$

Our Taylor series specifies the value of a function at one point, x, in terms of the value of the function and its derivatives at a reference point, a. It is an expansion in powers of the **change** in the variable, $\Delta x = x - a$ in this case. The notation may be varied at the user's convenience. With the substitution $x \to x + h$ and $a \to x$, we have an alternate form

$$f(x+h) = \sum_{n=0}^{\infty} \frac{h^n}{n!} f^{(n)}(x).$$

Biographical Data

Taylor, Brooke. Taylor, an English mathematician, was born in 1685 and died in 1731. He was educated in Cambridge and developed his famous theorem in the context of work on methods of finite differences (published

[7] An alternate form derived by Cauchy is

$$R_n = \frac{(x-\zeta)^{n-1}(x-a)}{(n-1)!} f^{(n)}(\zeta).$$

with $a \le \zeta \le x$.

[8] Note that $0! = 1$ (compare Section 10.1).

in 1715). He also discovered the method of integration by parts. The convergence of his series was not considered until a century later and then proved by Cauchy under suitable conditions. The theorem remained obscure until Lagrange recognized its importance and named it after Taylor.

Maclaurin Theorem

If we expand about the origin ($a = 0$), Eq. (5.64) is known as Maclaurin's series

$$f(x) = f(0) + xf'(0) + \frac{x^2}{2!}f''(0) + \cdots = \sum_{n=0}^{\infty} \frac{x^n}{n!} f^{(n)}(0). \tag{5.65}$$

An immediate application of the Maclaurin series (or the Taylor series) is in the expansion of various transcendental functions into infinite series.

EXAMPLE 5.6.1 **Exponential Function** Let $f(x) = e^x$. Differentiating, we have

$$f^{(n)}(0) = 1 \tag{5.66}$$

for all n, $n = 1, 2, 3, \ldots$. Then, by Eq. (5.65), we have

$$e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \cdots = \sum_{n=0}^{\infty} \frac{x^n}{n!}. \tag{5.67}$$

This is the series expansion of the exponential function. Some authors use this series to define the exponential function. The ratio test applied to this series, $x^{n+1}n!/[x^n(n+1)!] = x/(n+1) \to 0$ as $n \to \infty$, shows that it converges for any finite x. In a first reading, therefore, the reader may skip the analysis of the remainder and proceed to Example 5.6.2.

Although this series is clearly convergent for all x, we should check the remainder term, R_n. By Eq. (5.62) we have

$$R_n = \frac{x^n}{n!} f^{(n)}(\xi) = \frac{x^n}{n!} e^{\xi}, \quad 0 \le |\xi| \le x. \tag{5.68}$$

Therefore,

$$|R_n| \le \frac{x^n e^x}{n!} \tag{5.69}$$

and

$$\lim_{n\to\infty} R_n = 0 \tag{5.70}$$

for all **finite** values of x, which indicates that this Maclaurin expansion of e^x converges absolutely over the range $-\infty < x < \infty$.

Now we use the **operator** $\partial = d/dx$ in the Taylor expansion, which becomes

$$f(x+h) = \sum_{n=0}^{\infty} \frac{h^n \partial^n}{n!} f(x) = e^{h\partial} f(x).$$

As the argument x is shifted to $x+h$, the operator ∂ effects a **translation** in a differentiable function. An equivalent operator form of this Taylor expansion appears in Exercise 4.2.3. A derivation of the Taylor expansion in the context of complex variable theory appears in Section 6.5. ■

EXAMPLE 5.6.2 **Logarithm** Let $f(x) = \ln(1+x)$. By differentiating, we obtain

$$\begin{aligned} f'(x) &= (1+x)^{-1}, \\ f^{(n)}(x) &= (-1)^{n-1}(n-1)!(1+x)^{-n}. \end{aligned} \tag{5.71}$$

The Maclaurin expansion [Eq. (5.65)] yields

$$\begin{aligned} \ln(1+x) &= x - \frac{x^2}{2} + \frac{x^3}{3} - \frac{x^4}{4} + \cdots + R_n \\ &= \sum_{p=1}^{n} (-1)^{p-1} \frac{x^p}{p} + R_n. \end{aligned} \tag{5.72}$$

Again, in a first reading, the remainder may be ignored. We find that the infinite series

$$\ln(1+x) = \sum_{n=1}^{\infty} (-1)^{n-1} \frac{x^n}{n} \tag{5.73}$$

converges for $-1 < x \le 1$. The range $-1 < x < 1$ is established by the d'Alembert ratio test (Section 5.2). Convergence at $x = 1$ follows by the Leibniz criterion (Section 5.3). In particular, at $x = 1$, we have

$$\ln 2 = 1 - \frac{1}{2} + \frac{1}{3} - \frac{1}{4} + \frac{1}{5} - \cdots = \sum_{n=1}^{\infty} (-1)^{n-1} n^{-1}, \tag{5.74}$$

the conditionally convergent alternating harmonic series.

Returning to the remainder, in this case it is given by

$$\begin{aligned} R_n &= \frac{x^n}{n!} f^{(n)}(\xi), \quad 0 \le \xi \le x \\ &\le \frac{x^n}{n}, \quad 0 \le \xi \le x \le 1. \end{aligned} \tag{5.75}$$

Now the remainder approaches zero as n is increased indefinitely, provided $0 \le x \le 1$.[9] ■

Binomial Theorem

A second, extremely important application of the Taylor and Maclaurin expansions is the derivation of the binomial theorem for negative and/or nonintegral powers.

[9] This range can easily be extended to $-1 < x \le 1$ but not to $x = -1$.

Let $f(x) = (1+x)^m$, where m may be negative and is not limited to integral values. Direct application of Eq. (5.65) gives

$$(1+x)^m = 1 + mx + \frac{m(m-1)}{2!}x^2 + \cdots + R_n. \tag{5.76}$$

Ignoring the remainder at first, the binomial expansion leads to the infinite series

$$(1+x)^m = 1 + mx + \frac{m(m-1)}{2!}x^2 + \frac{m(m-1)(m-2)}{3!}x^3 + \cdots. \tag{5.77}$$

In other, equivalent notation

$$(1+x)^m = \sum_{n=0}^{\infty} \frac{m!}{n!(m-n)!}x^n = \sum_{n=0}^{\infty} \binom{m}{n} x^n. \tag{5.78}$$

The quantity $\binom{m}{n}$, which equals $m!/[n!(m-n)!]$, is called a **binomial coefficient**. Using the ratio and Leibniz tests, the series in Eq. (5.77) may actually be shown to be convergent for the extended range $-1 < x < 1$. For m an integer, $(m-n)! = \pm\infty$ if $n > m$ (Section 10.1), and the series automatically terminates at $n = m$.

We now return to the remainder for this function

$$R_n = \frac{x^n}{n!}(1+\xi)^{m-n} m(m-1)\cdots(m-n+1), \tag{5.79}$$

where ξ lies between 0 and x, $0 \le \xi \le x$. Now, for $n > m$, $(1+\xi)^{m-n}$ is a maximum for $\xi = 0$. Therefore,

$$R_n \le \frac{x^n}{n!} m(m-1)\cdots(m-n+1). \tag{5.80}$$

Note that the m-dependent factors do not yield a zero unless m is a nonnegative integer; R_n tends to zero as $n \to \infty$ if x is restricted to the range $0 \le x < 1$. Although we have only shown that the remainder vanishes,

$$\lim_{n\to\infty} R_n = 0,$$

for $0 \le x < 1$, the argument can be extended to $-1 < x \le 0$.

For polynomials we can generalize the binomial expansion to

$$(a_1 + a_2 + \cdots + a_m)^n = \sum \frac{n!}{n_1!n_2!\cdots n_m!} a_1^{n_1} a_2^{n_2} \cdots a_m^{n_m},$$

where the summation includes all different combinations of $n_1, n_2, \ldots, n_m$ with $\sum_{i=1}^{m} n_i = n$. Here, n_i and n are all integral. This generalization finds considerable use in statistical mechanics.

Maclaurin series may sometimes appear indirectly rather than by direct use of Eq. (5.65). For instance, the most convenient way to obtain the series expansion

$$\sin^{-1} x = \sum_{n=0}^{\infty} \frac{(2n-1)!!}{(2n)!!} \cdot \frac{x^{2n+1}}{(2n+1)} = x + \frac{x^3}{6} + \frac{3x^5}{40} + \cdots \tag{5.81}$$

is to make use of the relation (from $\sin y = x$, get $dy/dx = 1/\sqrt{1-x^2}$)

$$\sin^{-1} x = \int_0^x \frac{dt}{(1-t^2)^{1/2}}.$$

We expand $(1-t^2)^{-1/2}$ (binomial theorem) and then integrate term by term. This term-by-term integration is discussed in Section 5.7. The result is Eq. (5.81). Finally, we may take the limit as $x \to 1$. The series converges by the integral test.

Biographical Data

Maclaurin, Colin. Maclaurin, a Scottish mathematician, was born in 1698 in Kilmodan, County of Argyle, and died in 1746 in Edinburgh, Scotland. He entered the University of Glasgow at age 11 and obtained a degree in mathematics in 1715. In 1717, when he was 18, he was appointed professor of mathematics, enjoying Newton's recommendation. He extended and solidified Newton's calculus and was probably the greatest mathematician of the generation following Newton.

Taylor Expansion—More Than One Variable

If the function f has more than one independent variable, for example, $f = f(x, y)$, the Taylor expansion becomes

$$\begin{aligned} f(x, y) = {} & f(a, b) + (x-a)\frac{\partial f}{\partial x} + (y-b)\frac{\partial f}{\partial y} \\ & + \frac{1}{2!}\left[(x-a)^2\frac{\partial^2 f}{\partial x^2} + 2(x-a)(y-b)\frac{\partial^2 f}{\partial x \partial y} + (y-b)^2\frac{\partial^2 f}{\partial y^2}\right] \\ & + \frac{1}{3!}\left[(x-a)^3\frac{\partial^3 f}{\partial x^3} + 3(x-a)^2(y-b)\frac{\partial^3 f}{\partial x^2 \partial y}\right. \\ & \left. + 3(x-a)(y-b)^2\frac{\partial^3 f}{\partial x \partial y^2} + (y-b)^3\frac{\partial^3 f}{\partial y^3}\right] + \cdots, \end{aligned} \tag{5.82}$$

with all derivatives evaluated at the point (a, b). Using $\alpha_j = x_j - x_{j0}$, we may write the Taylor expansion for m independent variables in the form

$$f(x_1, \ldots, x_m) = \sum_{n=0}^{\infty} \frac{1}{n!}\left(\sum_{i=1}^{m} \alpha_i \frac{\partial}{\partial x_i}\right)^n f(x_k)\bigg|_{x_k = x_{k0}}.$$

A convenient (m-dimensional) vector form is

$$\psi(\mathbf{r} + \mathbf{a}) = \sum_{n=0}^{\infty} \frac{1}{n!}(\mathbf{a} \cdot \nabla)^n \psi(\mathbf{r}). \tag{5.83}$$

SUMMARY

The Taylor expansion generates all elementary functions and is of immense importance in physics applications, often, upon truncating it, serving as the start of controlled approximations. The Maclaurin series are special cases of Taylor expansions at the origin.

EXERCISES

5.6.1 Show that

(a) $\sin x = \sum_{n=0}^{\infty} (-1)^n \frac{x^{2n+1}}{(2n+1)!}$,

(b) $\cos x = \sum_{n=0}^{\infty} (-1)^n \frac{x^{2n}}{(2n)!}$,

In Section 6.1, e^{ix} is defined by a series expansion such that

$$e^{ix} = \cos x + i \sin x.$$

This is the basis for the polar representation of complex quantities. As a special case we find, with $x = \pi$,

$$e^{i\pi} = -1.$$

5.6.2 Derive a series expansion of $\cot x$ in increasing powers of x by dividing $\cos x$ by $\sin x$.

Note. The resultant series that starts with $1/x$ is actually a Laurent series (Section 6.5). Although the two series for $\sin x$ and $\cos x$ were valid for all x, the convergence of the series for $\cot x$ is limited by the zeros of the denominator, $\sin x$ (see Section 6.5).

5.6.3 Show by series expansion that

$$\frac{1}{2} \ln \frac{\eta_0 + 1}{\eta_0 - 1} = \coth^{-1} \eta_0, \quad |\eta_0| > 1.$$

This identity may be used to obtain a second solution for Legendre's equation.

5.6.4 Show that $f(x) = x^{1/2}$ (a) has no Maclaurin expansion but (b) has a Taylor expansion about any point $x_0 \neq 0$. Find the range of convergence of the Taylor expansion about $x = x_0$.

5.6.5 Let x be an approximation for a zero of $f(x)$ and Δx the correction. Show that by neglecting terms of order $(\Delta x)^2$

$$\Delta x = -\frac{f(x)}{f'(x)}.$$

This is Newton's formula for finding a root. Newton's method has the virtues of illustrating series expansions and elementary calculus but is very treacherous. See Appendix A1 for details and an alternative.

5.6.6 Expand a function $\Phi(x, y, z)$ by Taylor's expansion. Evaluate $\bar{\Phi}$, the average value of Φ, averaged over a small cube of side a centered on the origin and show that the Laplacian of Φ is a measure of deviation of Φ from $\Phi(0, 0, 0)$.

5.6.7 The ratio of two differentiable functions $f(x)$ and $g(x)$ takes on the indeterminate form $0/0$ at $x = x_0$. Using Taylor expansions prove

l'Hôpital's rule:

$$\lim_{x\to x_0}\frac{f(x)}{g(x)}=\lim_{x\to x_0}\frac{f'(x)}{g'(x)}.$$

5.6.8 With $n>1$, show that

$$\text{(a)}\ \frac{1}{n}-\ln\left(\frac{n}{n-1}\right)<0,\qquad \text{(b)}\ \frac{1}{n}-\ln\left(\frac{n+1}{n}\right)>0.$$

Use these inequalities to show that the limit defining the Euler–Mascheroni constant is finite.

5.6.9 Expand $(1-2tz+t^2)^{-1/2}$ in powers of t for any real number z so that $|-2tz+t^2|<1$. Assume that t is small. Collect the coefficients of t^0, t^1, and t^2.

ANS. $a_0=P_0(z)=1$,
$a_1=P_1(z)=z$,
$a_2=P_2(z)=\frac{1}{2}(3z^2-1)$,
where $a_n=P_n(z)$, the nth Legendre polynomial.

5.6.10 Using the double factorial notation of Exercise 5.2.12, show that

$$(1+x)^{-m/2}=\sum_{n=0}^{\infty}(-1)^n\frac{(m+2n-2)!!}{2^n!(m-2)!!}x^n,\quad m=1,2,3,\ldots.$$

5.6.11 Evaluate the Fresnel integral $\int_0^2\sin x^2dx$ by a Taylor expansion.

5.6.12 At CEBAF electrons are accelerated to relativistic energies in the GeV range. Determine v/c from $\frac{v}{c}=\sqrt{1-\frac{1}{4V^2}}$, where the accelerator voltage V is in millions of Volts. Truncate the binomial series at a suitable order to find v/c to one significant decimal place for $V=200$ million Volts.

5.6.13 Find the Taylor expansion of the function $\exp(\tan x)$.

5.6.14 Verify the relativistic energy formula

$$E=\frac{mc^2}{\sqrt{1-\mathbf{v}^2/c^2}}=mc^2+\frac{m}{2}\mathbf{v}^2+\cdots.$$

At what speed (in units of c) is there a 10% correction to the nonrelativistic kinetic energy?

5.6.15 How much time dilation occurs during a 2-hr trip tracking at 65 miles per hour?

5.6.16 A cosmic ray event is recorded with an energy of 3×10^{20} eV. If the particle is a proton (electron), calculate the difference between its speed and the velocity of light.

5.6.17 Using binomial expansions, compare the three Doppler shift formulas:

$$\text{(a)}\quad \nu' = \nu\left(1 \mp \frac{v}{c}\right)^{-1} \quad \text{moving source;}$$

$$\text{(b)}\quad \nu' = \nu\left(1 \pm \frac{v}{c}\right) \quad \text{moving observer;}$$

$$\text{(c)}\quad \nu' = \nu\left(1 \pm \frac{v}{c}\right)\left(1 - \frac{v^2}{c^2}\right)^{-1/2} \quad \text{relativistic.}$$

Note. The relativistic formula agrees with the classical formulas if terms of order v^2/c^2 can be neglected.

5.6.18 The relativistic sum w of two velocities u and v is given by

$$\frac{w}{c} = \frac{u/c + v/c}{1 + uv/c^2}.$$

If

$$\frac{v}{c} = \frac{u}{c} = 1 - \alpha,$$

where $0 \le \alpha \le 1$, find w/c in powers of α through terms in α^3.

5.6.19 The displacement x of a particle of rest mass m_0, resulting from a constant force $m_0 g$ along the x-axis, is

$$x = \frac{c^2}{g}\left\{\left[1 + \left(g\frac{t}{c}\right)^2\right]^{1/2} - 1\right\},$$

including relativistic effects. Find the displacement x as a power series in time t. Compare with the classical result

$$x = \frac{1}{2}gt^2.$$

5.6.20 With binomial expansions

$$\frac{x}{1-x} = \sum_{n=1}^{\infty} x^n, \qquad \frac{x}{x-1} = \frac{1}{1-x^{-1}} = \sum_{n=0}^{\infty} x^{-n}.$$

Adding these two series yields $\sum_{n=-\infty}^{\infty} x^n = 0$.
Hopefully, we can agree that this is nonsense, but what has gone wrong?

5.6.21 (a) Planck's theory of quantized oscillators leads to an average energy

$$\langle \varepsilon \rangle = \frac{\sum_{n=1}^{\infty} n\varepsilon_0 \exp(-n\varepsilon_0/kT)}{\sum_{n=0}^{\infty} \exp(-n\varepsilon_0/kT)},$$

where ε_0 is a fixed energy. Identify the numerator and denominator as binomial expansions and show that the ratio is

$$\langle \varepsilon \rangle = \frac{\varepsilon_0}{\exp(\varepsilon_0/kT) - 1}.$$

(b) Show that the $\langle \varepsilon \rangle$ of part (a) reduces to kT, the classical result, for $kT \gg \varepsilon_0$.

5.6.22 (a) Expand by the binomial theorem and integrate term by term to obtain the Gregory series for $y = \tan^{-1} x$ (note $\tan y = x$):

$$\tan^{-1} x = \int_0^x \frac{dt}{1+t^2} = \int_0^x \{1 - t^2 + t^4 - t^6 + \cdots\} dt$$
$$= \sum_{n=0}^{\infty} (-1)^n \frac{x^{2n+1}}{2n+1}, \quad -1 \le x \le 1.$$

(b) By comparing series expansions, show that

$$\tan^{-1} x = \frac{i}{2} \ln\left(\frac{1 - ix}{1 + ix}\right).$$

Hint. Compare Exercise 5.4.1.

5.6.23 In numerical analysis it is often convenient to approximate $d^2\psi(x)/dx^2$ by

$$\frac{d^2}{dx^2}\psi(x) \approx \frac{1}{h^2}[\psi(x+h) - 2\psi(x) + \psi(x-h)].$$

Find the error in this approximation.

ANS. Error $= \dfrac{h^2}{12}\psi^{(4)}(x)$.

5.6.24 You have a function $y(x)$ tabulated at equally spaced values of the argument

$$\begin{cases} y_n = y(x_n) \\ x_n = x + nh. \end{cases}$$

Show that the linear combination

$$\frac{1}{12h}\{-y_2 + 8y_1 - 8y_{-1} + y_{-2}\}$$

yields

$$y_0' - \frac{h^4}{30} y_0^{(5)} + \cdots.$$

Hence, this linear combination yields y_0' if $(h^4/30)y_0^{(5)}$ and higher powers of h and higher derivatives of $y(x)$ are negligible.

5.6.25 In a numerical integration of a partial differential equation the three-dimensional Laplacian is replaced by

$$\nabla^2\psi(x, y, z) \rightarrow h^{-2}[\psi(x+h, y, z) + \psi(x-h, y, z) + \psi(x, y+h, z) + \psi(x, y-h, z) + \psi(x, y, z+h) + \psi(x, y, z-h) - 6\psi(x, y, z)].$$

Determine the error in this approximation. Here, h is the step size, the distance between adjacent points in the x-, y-, or z-direction.

5.6.26 Find the Taylor expansion of the error function $\text{erf}(x) = \frac{2}{\sqrt{\pi}}\int_0^x e^{-t^2}dt$ and compare it to the asymptotic expansion of Section 5.10. How many terms are needed to obtain erf(0.1), erf(1), erf(2) for both cases? Use symbolic software or write a numerical program.

5.7 Power Series

The power series is a special and extremely useful type of infinite series of the form

$$f(x) = a_0 + a_1x + a_2x^2 + a_3x^3 + \cdots = \sum_{n=0}^{\infty} a_nx^n, \tag{5.84}$$

where the coefficients a_i are constants, independent of x.[10]

Convergence

Equation (5.84) may readily be tested for convergence by either the Cauchy root test or the d'Alembert ratio test (Section 5.2). If

$$\lim_{n\to\infty} \frac{a_{n+1}}{a_n} = R^{-1}, \tag{5.85}$$

the series converges for $-R < x < R$. This is the interval of convergence. Since the root and ratio tests fail when the limit is unity, the end points of the interval require special attention.

For instance, if $a_n = n^{-1}$, then $R = 1$ and, from Sections 5.1–5.3, the series converges for $x = -1$ but diverges for $x = +1$. If $a_n = n!$, then $R = 0$ and the series diverges for all $x \neq 0$.

Uniform and Absolute Convergence

Suppose our power series [Eq. (5.84)] has been found convergent for $-R < x < R$; then it will be uniformly and absolutely convergent in any **interior** interval, $-S \leq x \leq S$, where $0 < S < R$.

This may be proved directly by the Weierstrass M test (Section 5.5).

[10] Equation (5.84) may be generalized to $z = x + iy$, replacing x. Chapters 6 and 7 deal with uniform convergence, integrability, and differentiability in a region of a complex plane in place of an interval on the x-axis.

Continuity

Since each of the terms $u_n(x) = a_n x^n$ is a continuous function of x and $f(x) = \sum a_n x^n$ converges uniformly for $-S \le x \le S$, $f(x)$ must be a continuous function in the interval of uniform convergence.

This behavior is to be contrasted with the strikingly different behavior of the Fourier series (Chapter 14), in which the Fourier series is frequently used to represent discontinuous functions, such as sawtooth and square waves.

Differentiation and Integration

With $u_n(x)$ continuous and $\sum a_n x^n$ uniformly convergent, we find that the differentiated series is a power series with continuous functions and the same radius of convergence as the original series. The new factors introduced by differentiation (or integration) do not affect either the root or the ratio test. Therefore, our **power series may be differentiated or integrated as often as desired within the interval of uniform convergence** (Exercise 5.7.9).

In view of the severe restrictions placed on differentiation of series (Section 5.5), this is a remarkable and valuable result.

Uniqueness Theorem

In the preceding section, using the Maclaurin series, we expanded e^x and $\ln(1+x)$ into infinite series. In the succeeding chapters, functions are frequently represented or perhaps defined by infinite series. We now establish that the power-series representation is unique.

If

$$\begin{aligned} f(x) &= \sum_{n=0}^{\infty} a_n x^n, \quad -R_a < x < R_a \\ &= \sum_{n=0}^{\infty} b_n x^n, \quad -R_b < x < R_b, \end{aligned} \tag{5.86}$$

with overlapping intervals of convergence, including the origin, then

$$a_n = b_n \tag{5.87}$$

for all n; that is, we assume two (different) power-series representations and then proceed to show that the two are actually identical.

From Eq. (5.86),

$$\sum_{n=0}^{\infty} a_n x^n = \sum_{n=0}^{\infty} b_n x^n, \quad -R < x < R, \tag{5.88}$$

where R is the smaller of R_a, R_b. By setting $x = 0$, to eliminate all but the constant terms, we obtain

$$a_0 = b_0. \tag{5.89}$$

Now, exploiting the differentiability of our power series, we differentiate Eq. (5.88), obtaining

$$\sum_{n=1}^{\infty} n a_n x^{n-1} = \sum_{n=1}^{\infty} n b_n x^{n-1}, \tag{5.90}$$

We again set $x = 0$ to isolate the new constant terms and find

$$a_1 = b_1. \tag{5.91}$$

By repeating this process n times, we get

$$a_n = b_n, \tag{5.92}$$

which shows that the two series coincide. Therefore, our power-series representation is unique.

This will be a crucial point in Section 8.5, in which we use a power series to develop solutions of differential equations. This uniqueness of power series appears frequently in theoretical physics. The establishment of perturbation theory in quantum mechanics is one example. The power-series representation of functions is often useful in evaluating indeterminate forms, particularly when l'Hôpital's rule may be awkward to apply.

The uniqueness of power series means that the coefficients a_n may be identified with the derivatives in a Maclaurin series. From

$$f(x) = \sum_{n=0}^{\infty} a_n x^n = \sum_{n=0}^{\infty} \frac{1}{n!} f^{(n)}(0) x^n \tag{5.93}$$

we have

$$a_n = \frac{1}{n!} f^{(n)}(0). \tag{5.94}$$

Inversion of Power Series

Suppose we are given a series

$$y - y_0 = a_1(x - x_0) + a_2(x - x_0)^2 + \cdots = \sum_{n=1}^{\infty} a_n (x - x_0)^n. \tag{5.95}$$

This gives $(y - y_0)$ in terms of $(x - x_0)$. However, it may be desirable to have an explicit expression for $(x - x_0)$ in terms of $(y - y_0)$. We may solve Eq. (5.95) for $x - x_0$ by inversion of our series. Assume that

$$x - x_0 = \sum_{n=1}^{\infty} b_n (y - y_0)^n, \tag{5.96}$$

with the b_n to be determined in terms of the assumed known a_n. A brute-force approach, which is perfectly adequate for the first few coefficients, is simply to substitute Eq. (5.95) into Eq. (5.96). By equating coefficients of $(x - x_0)^n$ on

both sides of Eq. (5.96), since the power series is unique, we obtain

$$b_1 = \frac{1}{a_1}, \quad b_2 = -\frac{a_2}{a_1^3}, \quad b_3 = \frac{1}{a_1^5}(2a_2^2 - a_1 a_3), \tag{5.97}$$

$$b_4 = \frac{1}{a_1^7}(5a_1 a_2 a_3 - a_1^2 a_4 - 5a_2^3), \quad \text{and so on.}$$

Some of the higher coefficients are listed by Dwight.[11]

SUMMARY

Power series are Maclaurin series, that is, Taylor expansions at the origin. They can be integrated when they converge uniformly and differentiated when the differentiated series converges uniformly. Within the interval of convergence they can be added and subtracted. Multiplication is only safe when at least one of them converges absolutely.

EXERCISES

5.7.1 The classical Langevin theory of paramagnetism leads to an expression for the magnetic polarization

$$P(x) = c\left(\frac{\cosh x}{\sinh x} - \frac{1}{x}\right).$$

Expand $P(x)$ as a power series for small x (low fields, high temperature).

5.7.2 The analysis of the diffraction pattern of a circular opening involves

$$\int_0^{2\pi} \cos(c\cos\varphi)d\varphi.$$

Expand the integrand in a series and integrate by using

$$\int_0^{2\pi} \cos^{2n}\varphi\, d\varphi = \frac{(2n)!}{2^{2n}(n!)^2}\cdot 2\pi, \qquad \int_0^{2\pi} \cos^{2n+1}\varphi\, d\varphi = 0.$$

The result is 2π times the Bessel function $J_0(c)$.

5.7.3 Given that

$$\int_0^1 \frac{dx}{1+x^2} = \tan^{-1} x\Big|_0^1 = \frac{\pi}{4},$$

expand the integrand into a series and integrate term by term, obtaining[12]

$$\frac{\pi}{4} = 1 - \frac{1}{3} + \frac{1}{5} - \frac{1}{7} + \frac{1}{9} - \cdots + (-1)^n \frac{1}{2n+1} + \cdots,$$

[11] Dwight, H. B. (1961). *Tables of Integrals and Other Mathematical Data*, 4th ed. Macmillan, New York. (Compare Formula No. 50.)

[12] The series expansion of $\tan^{-1} x$ (upper limit 1 replaced by x) was discovered by James Gregory in 1671, 3 years before Leibniz. See Peter Beckmann's entertaining book, *A History of Pi*, 2nd ed. Golem Press, Boulder, CO (1971); and L. Berggren, J. Borwein, and P. Borwein, *Pi: A Source Book*. Springer, New York (1997).

which is Leibniz's formula for π. Compare the convergence (or lack of it) of the integrand series and the integrated series at $x = 1$.

5.7.4 Expand the incomplete factorial function

$$\int_0^x e^{-t} t^n dt$$

in a series of powers of x. What is the range of convergence of the resulting series?

$$ANS. \quad \int_0^x e^{-t} t^n dt = x^{n+1}\left[\frac{1}{n+1} - \frac{x}{n+2} + \frac{x^2}{2!(n+3)} - \cdots \frac{(-1)^p x^p}{p!(n+p+1)} + \cdots\right], \quad |x| < \infty.$$

5.7.5 Evaluate

$$\text{(a)} \lim_{x\to 0}[\sin(\tan x) - \tan(\sin x)]x^{-7}, \quad \text{(b)} \lim_{x\to 0} x^{-n} j_n(x), \quad n = 3,$$

where $j_n(x)$ is a spherical Bessel function (Section 12.4) defined by

$$j_n(x) = (-1)^n x^n \left(\frac{1}{x}\frac{d}{dx}\right)^n \left(\frac{\sin x}{x}\right).$$

$$ANS. \quad \text{(a)} -\frac{1}{30}, \quad \text{(b)} \frac{1}{1\cdot 3\cdot 5\cdots(2n+1)} \to \frac{1}{105} \quad \text{for } n = 3.$$

5.7.6 Neutron transport theory gives the following expression for the inverse neutron diffusion length of k:

$$\frac{a-b}{k}\tanh^{-1}\left(\frac{k}{a}\right) = 1.$$

By series inversion or otherwise, determine k^2 as a series of powers of b/a. Give the first two terms of the series.

$$ANS. \quad k^2 = 3ab\left(1 - \frac{4}{5}\frac{b}{a}\right).$$

5.7.7 Develop a series expansion of $y = \sinh^{-1} x$ (i.e., $\sinh y = x$) in powers of x by

(a) inversion of the series for $\sinh y$, and
(b) a direct Maclaurin expansion.

5.7.8 A function $f(z)$ is represented by a **descending** power series

$$f(z) = \sum_{n=0}^{\infty} a_n z^{-n}, \quad R \le z < \infty.$$

Show that this series expansion is unique; that is, if $f(z) = \sum_{n=0}^{\infty} b_n z^{-n}$, $R \le z < \infty$, then $a_n = b_n$ for all n.

5.7.9 A power series converges for $-R < x < R$. Show that the differentiated series and the integrated series have the same interval of convergence. (Do not bother with the end points $x = \pm R$.)

5.7.10 Assume that $f(x)$ may be expanded in a power series about the origin, $f(x) = \sum_{n=0}^{\infty} a_n x^n$, with some nonzero range of convergence. Use the techniques employed in proving uniqueness of series to show that your assumed series is a Maclaurin series:

$$a_n = \frac{1}{n!} f^{(n)}(0).$$

5.7.11 Show that each of the following integrals equals Catalan's constant:

$$\text{(a)} \int_0^1 \tan^{-1} t \frac{dt}{t}, \qquad \text{(b)} -\int_0^1 \ln x \frac{dx}{1+x^2}.$$

5.7.12 Use the integral test for the evaluation of finite series and show that

$$\text{(a)} \sum_{m=1}^{n} m = \frac{1}{2} n(n+1).$$

$$\text{(b)} \sum_{m=1}^{n} m^2 = \frac{1}{6} n(n+1)(2n+1).$$

$$\text{(c)} \sum_{m=1}^{n} m^3 = \frac{1}{4} n^2(n+1)^2.$$

$$\text{(d)} \sum_{m=1}^{n} m^4 = \frac{1}{30} n(n+1)(2n+1)(3n^2+3n-1).$$

5.8 Elliptic Integrals

Elliptic integrals are included here partly as an illustration of the use of power series and partly for their own intrinsic interest. This interest includes the occurrence of elliptic integrals in physical problems (Example 5.8.1 and Exercise 5.8.4) and applications in mathematical problems.

EXAMPLE 5.8.1

Period of a Simple Pendulum For small-amplitude oscillations our pendulum (Fig. 5.4) has simple harmonic motion with a period $T = 2\pi(l/g)^{1/2}$. For a maximum amplitude θ_M large enough so that $\sin\theta_M \neq \theta_M$, Newton's second law of motion (and Lagrange's equation) leads to a nonlinear differential equation ($\sin\theta$ is a nonlinear function of θ), so we turn to a different approach.

The swinging mass m has a kinetic energy of $ml^2(d\theta/dt)^2/2$ and a potential energy of $-mgl\cos\theta$ ($\theta = \pi/2$ taken for the arbitrary zero of potential energy). Since $d\theta/dt = 0$ at $\theta = \theta_M$, conservation of energy gives

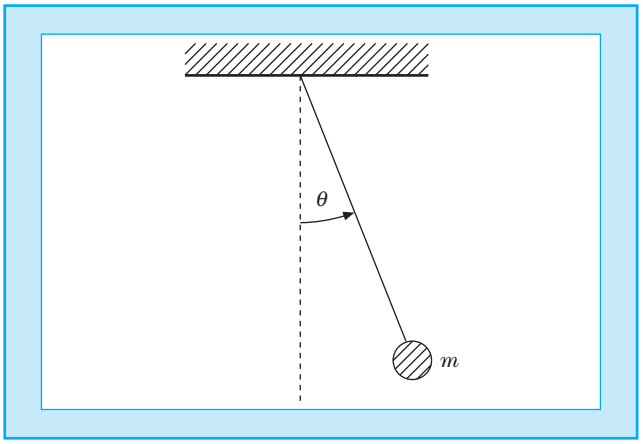
$$\frac{1}{2} ml^2 \left(\frac{d\theta}{dt}\right)^2 - mgl\cos\theta = -mgl\cos\theta_M. \tag{5.98}$$

Solving for $d\theta/dt$ we obtain

$$\frac{d\theta}{dt} = \pm\left(\frac{2g}{l}\right)^{1/2} (\cos\theta - \cos\theta_M)^{1/2} \tag{5.99}$$

Figure 5.4

Simple Pendulum



with the mass m canceling out. We take t to be zero, when $\theta = 0$ and $d\theta/dt > 0$. An integration from $\theta = 0$ to $\theta = \theta_M$ yields

$$\int_0^{\theta_M} (\cos\theta - \cos\theta_M)^{-1/2} d\theta = \left(\frac{2g}{l}\right)^{1/2} \int_0^t dt = \left(\frac{2g}{l}\right)^{1/2} t. \tag{5.100}$$

This is one-fourth of a cycle, and therefore the time t is one-fourth of the period, T. We note that $\theta \leq \theta_M$, and with a bit of clairvoyance we try the half-angle substitution

$$\sin\left(\frac{\theta}{2}\right) = \sin\left(\frac{\theta_M}{2}\right) \sin\varphi. \tag{5.101}$$

With this, Eq. (5.100) becomes

$$T = 4\left(\frac{l}{g}\right)^{1/2} \int_0^{\pi/2} \left(1 - \sin^2\left(\frac{\theta_M}{2}\right) \sin^2\varphi\right)^{-1/2} d\varphi. \tag{5.102}$$

Although not an obvious improvement over Eq. (5.100), the integral now defines the complete elliptic integral of the first kind, $K(\sin^2 \theta_M/2)$. From the series expansion, the period of our pendulum may be developed as a power series—powers of $\sin\theta_M/2$:

$$T = 2\pi\left(\frac{l}{g}\right)^{1/2} \left\{1 + \frac{1}{4}\sin^2\frac{\theta_M}{2} + \frac{9}{64}\sin^4\frac{\theta_M}{2} + \cdots\right\}. \tag{5.103}$$

Definitions

Generalizing Example 5.8.1 to include the upper limit as a variable, the **elliptic integral of the first kind** is defined as

$$F(\varphi\backslash\alpha) = \int_0^{\varphi} (1 - \sin^2\alpha \sin^2\theta)^{-1/2} d\theta \tag{5.104a}$$

or

$$F(x|m) = \int_0^x [(1-t^2)(1-mt^2)]^{-1/2} dt, \quad 0 \le m < 1. \tag{5.104b}$$

[This is the notation of the National Bureau of Standards (1972). *Handbook of Mathematical Functions*, AMS-55. Dover, New York.] For $\varphi = \pi/2$, $x = 1$, we have the **complete elliptic integral of the first kind**,

$$\begin{aligned} K(m) &= \int_0^{\pi/2} (1 - m\sin^2\theta)^{-1/2} d\theta \\ &= \int_0^1 [(1-t^2)(1-mt^2)]^{-1/2} dt, \end{aligned} \tag{5.105}$$

with $m = \sin^2\alpha$, $0 \le m < 1$.

The **elliptic integral of the second kind** is defined by

$$E(\varphi\backslash\alpha) = \int_0^{\varphi} (1 - \sin^2\alpha \sin^2\theta)^{1/2} d\theta \tag{5.106a}$$

or

$$E(x|m) = \int_0^x \left(\frac{1-mt^2}{1-t^2}\right)^{1/2} dt, \quad 0 \le m \le 1. \tag{5.106b}$$

Again, for the case $\varphi = \pi/2$, $x = 1$, we have the **complete elliptic integral of the second kind**:

$$\begin{aligned} E(m) &= \int_0^{\pi/2} (1 - m\sin^2\theta)^{1/2} d\theta \\ &= \int_0^1 \left(\frac{1-mt^2}{1-t^2}\right)^{1/2} dt, \quad 0 \le m \le 1. \end{aligned} \tag{5.107}$$

Exercise 5.8.1 is an example of its occurrence. Figure 5.5 shows the behavior of $K(m)$ and $E(m)$. Extensive tables are available in AMS-55.

Series Expansion

For our range $0 \le m < 1$, the denominator of $K(m)$ may be expanded by the binomial series

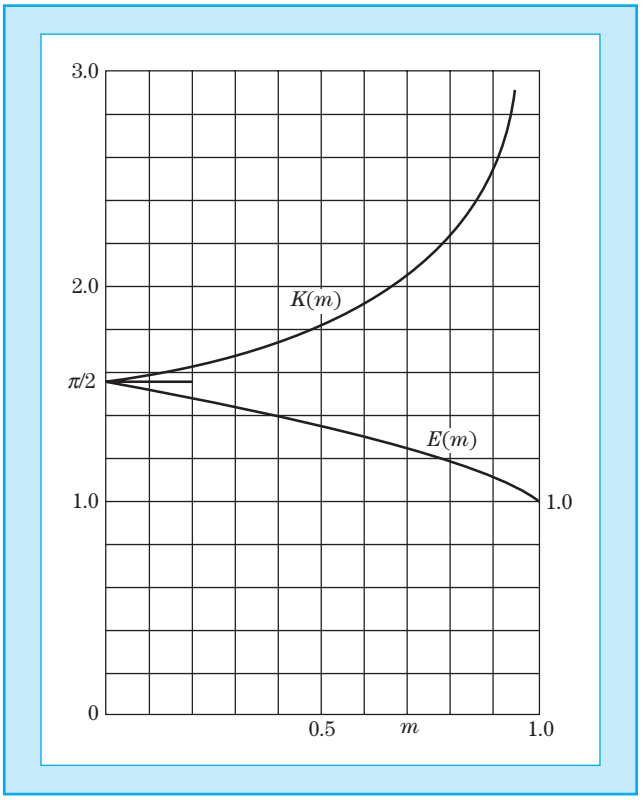
$$\begin{aligned} (1 - m\sin^2\theta)^{-1/2} &= 1 + \frac{1}{2} m\sin^2\theta + \frac{3}{8} m^2 \sin^4\theta + \cdots \\ &= \sum_{n=0}^{\infty} \frac{(2n-1)!!}{(2n)!!} m^n \sin^{2n}\theta. \end{aligned} \tag{5.108}$$

For any closed interval $[0, m_{\max}]$, $m_{\max} < 1$, this series is uniformly convergent and may be integrated term by term. From Exercise 5.7.2

$$\int_0^{\pi/2} \sin^{2n}\theta d\theta = \frac{(2n-1)!!}{(2n)!!} \cdot \frac{\pi}{2}. \tag{5.109}$$

Figure 5.5

Complete Elliptic Integrals, $K(m)$ and $E(m)$



Hence,

$$K(m) = \frac{\pi}{2}\left\{1 + \sum_{n=1}^{\infty}\left[\frac{(2n-1)!!}{(2n)!!}\right]^2 m^n\right\}. \tag{5.110}$$

Similarly,

$$E(m) = \frac{\pi}{2}\left\{1 - \sum_{n=1}^{\infty}\left[\frac{(2n-1)!!}{(2n)!!}\right]^2 \frac{m^n}{2n-1}\right\}. \tag{5.111}$$

(Exercise 5.8.2). These series are known as hypergeometric functions ${}_2F_1(a, b, c; x)$, and we have

$$K(m) = \frac{\pi}{2}{}_2F_1\left(\frac{1}{2}, \frac{1}{2}, 1; m\right), \tag{5.112}$$

$$E(m) = \frac{\pi}{2}{}_2F_1\left(-\frac{1}{2}, \frac{1}{2}, 1; m\right). \tag{5.113}$$

Limiting Values

From the series Eqs. (5.110) and (5.111), or from the defining integrals,

$$\lim_{m\to 0} K(m) = \frac{\pi}{2}, \tag{5.114}$$

$$\lim_{m\to 0} E(m) = \frac{\pi}{2}. \tag{5.115}$$

For $m \to 1$ the series expansions are of little use. However, the integrals yield

$$\lim_{m\to 1} K(m) = \infty, \tag{5.116}$$

the integral diverging logarithmically, and

$$\lim_{m\to 1} E(m) = 1. \tag{5.117}$$

The elliptic integrals have been used extensively for evaluating integrals. For instance, integrals of the form

$$I = \int_0^x R\left(t, \sqrt{a_4t^4 + a_3t^3 + a_2t^2 + a_1t^1 + a_0}\right)dt,$$

where R is a rational function of t and of the radical, may be expressed in terms of elliptic integrals. Jahnke and Emde, Dover (1943) (Chapter 5) discuss such transformations in-depth. With high-speed computers available for direct numerical evaluation, interest in these elliptic integral techniques has declined. However, elliptic integrals remain of interest because of their appearance in physical problems (Exercises 5.8.4 and 5.8.5).

For an extensive account of elliptic functions, integrals, and Jacobi theta functions, the reader is directed to Whittaker and Watson's treatise *A Course In Modern Analysis*, 4th ed. Cambridge Univ. Press, Cambridge, UK (1962).

EXERCISES

5.8.1 The ellipse $x^2/a^2 + y^2/b^2 = 1$ may be represented parametrically by $x = a\sin\theta$, $y = b\cos\theta$. Show that the length of arc within the first quadrant is

$$a\int_0^{\pi/2} (1 - m\sin^2\theta)^{1/2} d\theta = aE(m).$$

Here, $0 \le m = (a^2 - b^2)/a^2 \le 1$.

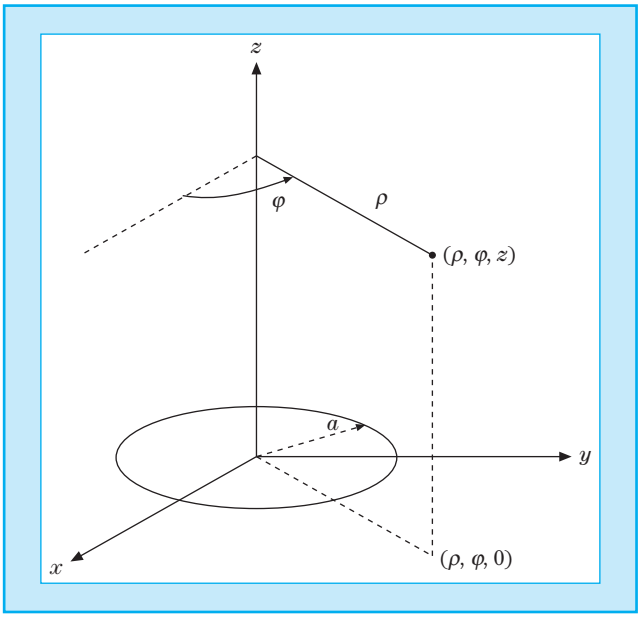
5.8.2 Derive the series expansion

$$E(m) = \frac{\pi}{2}\left\{1 - \left(\frac{1}{1}\right)^2 \frac{m}{1} - \left(\frac{1\cdot 3}{2\cdot 4}\right)^2 \frac{m^2}{3} - \cdots\right\}.$$

5.8.3 Show that

$$\lim_{m\to 0} \frac{(K - E)}{m} = \frac{\pi}{4}.$$

Figure 5.6
Circular Wire Loop



5.8.4 A circular loop of wire in the xy-plane, as shown in Fig. 5.6, carries a current I. Given that the vector potential is

$$A_\varphi(\rho, \varphi, z) = \frac{a\mu_0 I}{2\pi} \int_0^\pi \frac{\cos\alpha \, d\alpha}{(a^2 + \rho^2 + z^2 - 2a\rho\cos\alpha)^{1/2}},$$

show that

$$A_\varphi(\rho, \varphi, z) = \frac{\mu_0 I}{\pi k} \left(\frac{a}{\rho}\right)^{1/2} \left[\left(1 - \frac{k^2}{2}\right) K(k^2) - E\right],$$

where

$$k^2 = \frac{4a\rho}{(a+\rho)^2 + z^2}.$$

Note. For extension of Exercise 5.8.4 to **B** see Smythe.[13]

5.8.5 An analysis of the magnetic vector potential of a circular current loop leads to the expression

$$f(k^2) = k^{-2}[(2 - k^2)K(k^2) - 2E(k^2)],$$

where $K(k^2)$ and $E(k^2)$ are the complete elliptic integrals of the first and second kinds. Show that for $k^2 \ll 1$ ($r \gg$ radius of loop)

$$f(k^2) \approx \frac{\pi k^2}{16}.$$

[13]Smythe, W. R. (1969). *Static and Dynamic Electricity*, 3rd ed., p. 270. McGraw-Hill, New York.

5.8.6 Show that

(a) $$\frac{dE(k^2)}{dk} = \frac{1}{k}[E - K(k^2)],$$

(b) $$\frac{dK(k^2)}{dk} = \frac{E}{k(1-k^2)} - \frac{K}{k}.$$

Hint. For part (b) show that

$$E(k^2) = (1-k^2)\int_0^{\pi/2} (1 - k\sin^2\theta)^{-3/2} d\theta$$

by comparing series expansions.

5.8.7 (a) Write a function subroutine that will compute $E(m)$ from the series expansion, Eq. (5.111).

(b) Test your function subroutine by using it to calculate $E(m)$ over the range $m = 0.0(0.1)0.9$ and comparing the result with the values given by AMS-55.

5.8.8 Repeat Exercise 5.8.7 for $K(m)$.

Note. These series for $E(m)$ [Eq. (5.111)], and $K(m)$ [Eq. (5.110)], converge only very slowly for m near 1. More rapidly converging series for $E(m)$ and $K(m)$ exist. See Dwight's *Tables of Integrals*[14] Nos. 773.2 and 774.2. Your computer subroutine for computing E and K probably uses polynomial approximations (AMS-55, Chapter 17).

5.8.9 A simple pendulum is swinging with a maximum amplitude of θ_M. In the limit as $\theta_M \to 0$, the period is 1 sec. Using the elliptic integral, $K(k^2)$, $k = \sin(\theta_M/2)$, calculate the period T for $\theta_M = 0\ (10^\circ)\ 90^\circ$.

Caution. Some elliptic integral subroutines require $k = m^{1/2}$ as an input parameter, not m. **Check values**.

θ_M	10°	50°	90°
T(sec)	1.00193	1.05033	1.18258

5.8.10 Calculate the magnetic vector potential $\mathbf{A}(\rho, \varphi, z) = \hat{\boldsymbol{\varphi}} A_\varphi(\rho, \varphi, z)$ of a circular current loop (Exercise 5.8.4) for the ranges $\rho/a = 2, 3, 4$ and $z/a = 0, 1, 2, 3, 4$.

Note. This elliptic integral calculation of the magnetic vector potential may be checked by an associated Legendre function calculation.

Check value. For $\rho/a = 3$ and $z/a = 0$; $A_\varphi = 0.029023\mu_0 I$.

5.9 Bernoulli Numbers and the Euler–Maclaurin Formula

The Bernoulli numbers were introduced by Jacques Bernoulli. There are several equivalent definitions, but extreme care must be taken because some authors introduce variations in numbering or in algebraic signs. One relatively

[14] Dwight, H. B. (1947). *Tables of Integrals and Other Mathematical Data*. Macmillan, New York.

simple approach is to define the Bernoulli numbers by the series[15]

$$\frac{x}{e^x-1}=\sum_{n=0}^{\infty}\frac{B_n x^n}{n!}, \tag{5.118}$$

which converges for $|x|<2\pi$. By differentiating this power series repeatedly and then setting $x=0$, we obtain

$$B_n=\left[\frac{d^n}{dx^n}\left(\frac{x}{e^x-1}\right)\right]_{x=0}. \tag{5.119}$$

Specifically,

$$B_1=\frac{d}{dx}\left(\frac{x}{e^x-1}\right)\bigg|_{x=0}=\frac{1}{e^x-1}-\frac{xe^x}{(e^x-1)^2}\bigg|_{x=0}=-\frac{1}{2}, \tag{5.120}$$

as may be seen by series expansion of the denominators.

Using $B_0=1$ and $B_1=-\frac{1}{2}$, it is easy to verify that the function

$$\frac{x}{e^x-1}-1+\frac{x}{2}=\sum_{n=2}^{\infty}B_n\frac{x^n}{n!}=-\frac{x}{e^{-x}-1}-1-\frac{x}{2} \tag{5.121}$$

is even in x so that all $B_{2n+1}=0$.

To derive a recursion relation for the Bernoulli numbers, we multiply

$$\begin{aligned}\frac{e^x-1}{x}\frac{x}{e^x-1}=1&=\left\{\sum_{n=2}^{\infty}\frac{x^m}{(m+1)!}\right\}\left\{1-\frac{x}{2}+\sum_{n=1}^{\infty}B_{2n}\frac{x^{2n}}{(2n)!}\right\}\\&=1+\sum_{m=1}^{\infty}x^m\left\{\frac{1}{(m+1)!}-\frac{1}{2m!}\right\}\\&\quad+\sum_{N=2}^{\infty}x^N\sum_{1\le n\le N/2}\frac{B_{2n}}{(2n)!(N-2n+1)!}.\end{aligned} \tag{5.122}$$

For $N>0$ the coefficient of x^N is zero so that Eq. (5.122) yields

$$\frac{1}{2}(N+1)-1=\sum_{1\le n\le N/2}B_{2n}\binom{N+1}{2n}=\frac{1}{2}(N-1), \tag{5.123}$$

which is equivalent to

$$\begin{aligned}N-\frac{1}{2}&=\sum_{n=1}^{N}B_{2n}\binom{2N+1}{2n},\\N-1&=\sum_{n=1}^{N-1}B_{2n}\binom{2N}{2n}.\end{aligned} \tag{5.124}$$

[15]The function $x/(e^x-1)$ may be considered a **generating function** since it generates the Bernoulli numbers. Generating functions of the special functions of mathematical physics are discussed in Chapters 11–13.

Table 5.1

Bernoulli Numbers

Note: Additional values are given in the National Bureau of Standards Handbook of Mathematical Functions *(AMS-55).*

n	B_n	B_n
0	1	1.0000 00000
1	−1/2	−0.5000 00000
2	1/6	0.1666 66667
4	−1/30	−0.0333 33333
6	1/42	0.0238 09524
8	−1/30	−0.0333 33333
10	5/66	0.0757 57576

From Eq. (5.124) the Bernoulli numbers in Table 5.1 are readily obtained. If the variable x in Eq. (5.118) is replaced by $2ix$, we obtain an alternate (and equivalent) definition of B_{2n} (B_1 is set equal to $-\frac{1}{2}$) by the expression

$$x\cot x = \sum_{n=0}^{\infty}(-1)^n B_{2n}\frac{(2x)^{2n}}{(2n)!}, \qquad -\pi < x < \pi. \tag{5.125}$$

Using the method of residues (Section 7.2) or working from the infinite product representation of $\sin x$, we find that

$$B_{2n} = \frac{(-1)^{n-1}2(2n)!}{(2\pi)^{2n}}\sum_{p=1}^{\infty} p^{-2n}, \qquad n = 1, 2, 3, \ldots. \tag{5.126}$$

This representation of the Bernoulli numbers was discovered by Euler. It is readily seen from Eq. (5.126) that $|B_{2n}|$ increases without limit as $n \to \infty$. Numerical values have been calculated by Glaisher.[16] Illustrating the divergent behavior of the Bernoulli numbers, we have

$$B_{20} = -5.291 \times 10^{2}$$

$$B_{200} = -3.647 \times 10^{215}.$$

Some authors prefer to define the Bernoulli numbers with a modified version of Eq. (5.126) by using

$$\mathcal{B}_n = \frac{2(2n)!}{(2\pi)^{2n}}\sum_{p=1}^{\infty} p^{-2n}, \tag{5.127}$$

with the subscript being just half of our subscript and all signs are positive. Again, when using other texts or references the reader must check carefully to see how the Bernoulli numbers are defined.

The Bernoulli numbers occur frequently in number theory. The von Staudt–Clausen theorem states that

$$B_{2n} = A_n - \frac{1}{p_1} - \frac{1}{p_2} - \frac{1}{p_3} - \cdots - \frac{1}{p_k}, \tag{5.128}$$

[16] Glaisher, J. W. L. Table of the first 250 Bernoulli's numbers (to nine figures) and their logarithms (to ten figures). *Trans. Cambridge Philos. Soc.* **12**, 390 (1871–1879).

in which A_n is an integer and $p_1, p_2, \ldots, p_k$ are prime numbers so that $p_i - 1$ is a divisor of $2n$. It may readily be verified that this holds for

$$\begin{aligned} B_6(A_3 = 1, \quad p = 2, 3, 7), \\ B_8(A_4 = 1, \quad p = 2, 3, 5), \\ B_{10}(A_5 = 1, \quad p = 2, 3, 11), \end{aligned} \tag{5.129}$$

and other special cases.

The Bernoulli numbers appear in the summation of integral powers of the integers,

$$\sum_{j=1}^{N} j^p, \quad p \text{ integral},$$

and in numerous series expansions of the transcendental functions, including $\tan x$, $\cot x$, $\ln|\sin x|$, $(\sin x)^{-1}$, $\ln|\cos x|$, $\ln|\tan x|$, $(\cosh x)^{-1}$, $\tanh x$, and $\coth x$. For example,

$$\tan x = x + \frac{x^3}{3} + \frac{2}{15}x^5 + \cdots + \frac{(-1)^{n-1}2^{2n}(2^{2n}-1)B_{2n}}{(2n)!}x^{2n-1} + \cdots. \tag{5.130}$$

The Bernoulli numbers are likely to come in such series expansions because of the defining Eqs. (5.118) and (5.124) and because of their relation to the Riemann zeta function,

$$\zeta(2n) = \sum_{p=1}^{\infty} p^{-2n}. \tag{5.131}$$

Bernoulli Functions

If Eq. (5.118) is generalized slightly, we have

$$\frac{xe^{xs}}{e^x - 1} = \sum_{n=0}^{\infty} B_n(s)\frac{x^n}{n!} \tag{5.132}$$

defining the **Bernoulli functions**, $B_n(s)$. The first seven Bernoulli functions are given in Table 5.2.

From the generating function, Eq. (5.132),

$$B_n(0) = B_n, \quad n = 0, 1, 2, \ldots, \tag{5.133}$$

Table 5.2

Bernoulli Functions

$B_0 = 1$
$B_1 = x - \frac{1}{2}$
$B_2 = x^2 - x + \frac{1}{6}$
$B_3 = x^3 - \frac{3}{2}x^2 + \frac{1}{2}x$
$B_4 = x^4 - 2x^3 + x^2 - \frac{1}{30}$
$B_5 = x^5 - \frac{5}{2}x^4 + \frac{5}{3}x^3 - \frac{1}{6}x$
$B_6 = x^6 - 3x^5 + \frac{5}{2}x^4 - \frac{1}{2}x^2 + \frac{1}{42}$
$B_n(0) = B_n$, Bernoulli number

the Bernoulli function evaluated at zero equals the corresponding Bernoulli number. Two particularly important properties of the Bernoulli functions follow from the defining relation, Eq. (5.132): a differentiation relation

$$\frac{d}{ds}B_n(s) = nB_{n-1}(s), \quad n = 1, 2, 3, \ldots, \tag{5.134}$$

and a symmetry relation [replace $x \to -x$ in Eq. (5.132), then set $s = 1$]

$$B_n(1) = (-1)^n B_n(0), \quad n = 1, 2, 3, \ldots. \tag{5.135}$$

These relations are used next in the development of the Euler–Maclaurin integration formula.

Euler–Maclaurin Integration Formula

One use of the Bernoulli functions is in the derivation of the Euler–Maclaurin integration formula. This formula is used in Section 10.3 for the development of an asymptotic expression for the factorial function—Stirling's series.

The technique is repeated integration by parts using Eq. (5.134) to create new derivatives. We start with

$$\int_0^1 f(x)dx = \int_0^1 f(x)B_0(x)dx. \tag{5.136}$$

From Eq. (5.134),

$$B_1'(x) = B_0(x) = 1. \tag{5.137}$$

Substituting $B_1'(x)$ into Eq. (5.136) and integrating by parts, we obtain

$$\begin{aligned}\int_0^1 f(x)dx &= f(1)B_1(1) - f(0)B_1(0) - \int_0^1 f'(x)B_1(x)dx \\ &= \frac{1}{2}[f(1) + f(0)] - \int_0^1 f'(x)B_1(x)dx.\end{aligned} \tag{5.138}$$

Again, using Eq. (5.134), we have

$$B_1(x) = \frac{1}{2}B_2'(x), \tag{5.139}$$

and integrating by parts

$$\begin{aligned}\int_0^1 f(x)dx &= \frac{1}{2}[f(1) + f(0)] - \frac{1}{2!}[f'(1)B_2(1) - f'(0)B_2(0)] \\ &\quad + \frac{1}{2!}\int_0^1 f^{(2)}(x)B_2(x)dx.\end{aligned} \tag{5.140}$$

Using the relations

$$\begin{aligned} B_{2n}(1) &= B_{2n}(0) = B_{2n}, \quad n = 0, 1, 2, \ldots \\ B_{2n+1}(1) &= B_{2n+1}(0) = 0, \quad n = 1, 2, 3, \ldots \end{aligned} \tag{5.141}$$

and continuing this process, we have

$$\int_0^1 f(x)dx = \frac{1}{2}[f(1) + f(0)] - \sum_{p=1}^{q} \frac{1}{(2p)!} B_{2p}[f^{(2p-1)}(1) - f^{(2p-1)}(0)]$$
$$+ \frac{1}{(2q)!} \int_0^1 f^{(2q)}(x) B_{2q}(x)dx. \tag{5.142a}$$

This is the Euler–Maclaurin integration formula. It assumes that the function $f(x)$ has the required derivatives.

The range of integration in Eq. (5.142a) may be shifted from [0, 1] to [1, 2] by replacing $f(x)$ by $f(x + 1)$. Adding such results up to $[n - 1, n]$,

$$\int_0^n f(x)dx = \frac{1}{2}f(0) + f(1) + f(2) + \cdots + f(n-1) + \frac{1}{2}f(n)$$
$$- \sum_{p=1}^{q} \frac{1}{(2p)!} B_{2p}[f^{(2p-1)}(n) - f^{(2p-1)}(0)]$$
$$+ \frac{1}{(2q)!} \int_0^1 B_{2q}(x) \sum_{\nu=0}^{n-1} f^{(2q)}(x + \nu)dx. \tag{5.142b}$$

The terms $\frac{1}{2}f(0) + f(1) + \cdots + \frac{1}{2}f(n)$ appear exactly as in trapezoidal integration or quadrature. The summation over p may be interpreted as a correction to the trapezoidal approximation. Equation (5.142b) may be seen as a generalization of Eq. (5.22); it is the form used in Exercise 5.9.5 for summing positive powers of integers and in Section 10.3 for the derivation of Stirling's formula.

The Euler–Maclaurin formula is often useful in summing series by converting them to integrals.[17]

Improvement of Convergence

This section has so far been concerned with establishing convergence as an abstract mathematical property. In practice, the **rate** of convergence may be of considerable importance. Here, we present one method of improving the rate of convergence of a convergent series.

The basic principle of this method, due to Kummer, is to form a linear combination of our slowly converging series and one or more series whose

[17] For a number of examples, see Boas, R. P., and Stutz, C. (1971). Estimating sums with integrals. *Am. J. Phys.* **39**, 745.

sum is known. For the known series, the collection

$$\alpha_1 = \sum_{n=1}^{\infty} \frac{1}{n(n+1)} = 1$$

$$\alpha_2 = \sum_{n=1}^{\infty} \frac{1}{n(n+1)(n+2)} = \frac{1}{4}$$

$$\alpha_3 = \sum_{n=1}^{\infty} \frac{1}{n(n+1)(n+2)(n+3)} = \frac{1}{18}$$

$$\vdots \qquad \vdots \qquad \vdots$$

$$\alpha_p = \sum_{n=1}^{\infty} \frac{1}{n(n+1)\cdots(n+p)} = \frac{1}{p \cdot p!}$$

is particularly useful.[18] The series are combined term by term and the coefficients in the linear combination chosen to cancel the most slowly converging terms.

EXAMPLE 5.9.1

Riemann Zeta Function, $\zeta(3)$ Let the series to be summed be $\sum_{n=1}^{\infty} n^{-3}$. In Section 5.2, this is identified as the Riemann zeta function, $\zeta(3)$. We form a linear combination (using α_i defined above)

$$\sum_{n=1}^{\infty} n^{-3} + a_2\alpha_2 = \sum_{n=1}^{\infty} n^{-3} + \frac{a_2}{4}.$$

α_1 is not included, since it converges more slowly than $\zeta(3)$. Combining terms, we obtain on the left-hand side

$$\sum_{n=1}^{\infty} \left\{ \frac{1}{n^3} + \frac{a_2}{n(n+1)(n+2)} \right\} = \sum_{n=1}^{\infty} \frac{n^2(1+a_2) + 3n + 2}{n^3(n+1)(n+2)}.$$

If we choose $a_2 = -1$, the preceding equations yield

$$\zeta(3) = \sum_{n=1}^{\infty} n^{-3} = \frac{1}{4} + \sum_{n=1}^{\infty} \frac{3n+2}{n^3(n+1)(n+2)}. \tag{5.143}$$

The resulting series may not be beautiful, but it does converge as n^{-4}, faster than n^{-3}. A more convenient form is shown in Exercise 5.9.21. There, the symmetry leads to convergence as n^{-5}.

The method can be extended, including $a_3\alpha_3$ to get convergence as n^{-5}, $a_4\alpha_4$ to get convergence as n^{-6}, and so on. Eventually, you have to reach a compromise between how much algebra you do and how much arithmetic the computer does. As computers get faster, the balance is steadily shifting to less algebra for you and more arithmetic for them. ■

[18] These series sums may be verified by expanding the forms by partial fractions, writing out the initial terms, and inspecting the pattern of cancellation of positive and negative terms.

Improvement of Convergence by Rational Approximations

The series

$$\ln(1+x) = \sum_{n=1}^{\infty} (-1)^{n-1} \frac{x^n}{n}, \quad -1 < x \le 1, \tag{5.144}$$

converges very slowly as x approaches $+1$. The **rate** of convergence may be improved substantially by multiplying both sides of Eq. (5.144) by a polynomial and adjusting the polynomial coefficients to cancel the more slowly converging portions of the series. Consider the simplest possibility: Multiply $\ln(1+x)$ by $1 + a_1 x$:

$$(1 + a_1 x)\ln(1+x) = \sum_{n=1}^{\infty} (-1)^{n-1} \frac{x^n}{n} + a_1 \sum_{n=1}^{\infty} (-1)^{n-1} \frac{x^{n+1}}{n}. \tag{5.145}$$

Combining the two series on the right term by term, we obtain

$$\begin{aligned}(1 + a_1 x)\ln(1+x) &= x + \sum_{n=2}^{\infty} (-1)^{n-1} \left(\frac{1}{n} - \frac{a_1}{n-1} \right) x^n \\ &= x + \sum_{n=2}^{\infty} (-1)^{n-1} \frac{n(1-a_1) - 1}{n(n-1)} x^n. \end{aligned} \tag{5.146}$$

Clearly, if we take $a_1 = 1$, the n in the numerator disappears and our combined series converges as n^{-2}.

Continuing this process, we find that the general term of $(1 + 2x + x^2)\cdot \ln(1+x)$ vanishes as n^{-3} and that of $(1 + 3x + 3x^2 + x^3)\ln(1+x)$ vanishes as n^{-4}. In effect we are shifting from a simple series expansion of Eq. (5.144) to a rational fraction representation in which the function $\ln(1+x)$ is represented by the ratio of a series and a polynomial:

$$\ln(1+x) = \frac{x + \sum_{n=2}^{\infty} (-1)^n x^n / [n(n-1)]}{1+x}. \tag{5.147}$$

Such rational approximations may be both compact and accurate. Computer subroutines make extensive use of such methods.

If we are required to sum a convergent series $\sum_{n=1}^{\infty} a_n$ whose terms are rational functions of n, the convergence may be improved dramatically by introducing the Riemann zeta function.

EXAMPLE 5.9.2

Improvement of Convergence The problem is to evaluate the series $\sum_{n=1}^{\infty} 1/(1+n^2)$. Expanding $(1+n^2)^{-1} = n^{-2}(1+n^{-2})^{-1}$ by direct division, we have

$$\begin{aligned}(1+n^2)^{-1} &= n^{-2}\left(1 - n^{-2} + n^{-4} - \frac{n^{-6}}{1+n^{-2}}\right) \\ &= \frac{1}{n^2} - \frac{1}{n^4} + \frac{1}{n^6} - \frac{1}{n^8 + n^6}.\end{aligned}$$

Therefore,

$$\sum_{n=1}^{\infty} \frac{1}{1+n^2} = \zeta(2) - \zeta(4) + \zeta(6) - \sum_{n=1}^{\infty} \frac{1}{n^8 + n^6}.$$

The ζ values are tabulated and the remainder series converges as n^{-8}. Clearly, the process can be continued as desired. You make a choice between how much algebra you will do and how much arithmetic the computer will do. ■

EXERCISES

5.9.1 Show that

$$\tan x = \sum_{n=1}^{\infty} \frac{(-1)^{n-1} 2^{2n} (2^{2n} - 1) B_{2n}}{(2n)!} x^{2n-1}, \quad -\frac{\pi}{2} < x < \frac{\pi}{2}.$$

Hint. $\tan x = \cot x - 2 \cot 2x$.

5.9.2 Show that the first Bernoulli polynomials are

$$\begin{aligned} B_0(s) &= 1 \\ B_1(s) &= s - \frac{1}{2} \\ B_2(s) &= s^2 - s + \frac{1}{6}. \end{aligned}$$

Note that $B_n(0) = B_n$, the Bernoulli number.

5.9.3 Show that $B_n'(s) = nB_{n-1}(s), \ n = 1, 2, 3, \ldots$
Hint. Differentiate Eq. (5.132).

5.9.4 Show that

$$B_n(1) = (-1)^n B_n(0).$$

Hint. Go back to the generating function, Eq. (5.132) or Exercise 5.9.2.

5.9.5 The Euler–Maclaurin integration formula may be used for the evaluation of finite series:

$$\sum_{m=1}^{n} f(m) = \int_0^n f(x)dx + \frac{1}{2}f(1) + \frac{1}{2}f(n) + \frac{B_2}{2!}[f'(n) - f'(1)] + \cdots.$$

Show that

$$\text{(a)} \sum_{m=1}^{n} m = \frac{1}{2}n(n+1).$$

$$\text{(b)} \sum_{m=1}^{n} m^2 = \frac{1}{6}n(n+1)(2n+1).$$

$$\text{(c)} \sum_{m=1}^{n} m^3 = \frac{1}{4}n^2(n+1)^2.$$

$$\text{(d)} \sum_{m=1}^{n} m^4 = \frac{1}{30}n(n+1)(2n+1)(3n^2+3n-1).$$

5.9.6 From

$$B_{2n} = (-1)^{n-1}\frac{2(2n)!}{(2\pi)^{2n}}\zeta(2n),$$

show that

$$\text{(a) } \zeta(2) = \frac{\pi^2}{6} \qquad \text{(d) } \zeta(8) = \frac{\pi^8}{9{,}450}$$

$$\text{(b) } \zeta(4) = \frac{\pi^4}{90} \qquad \text{(e) } \zeta(10) = \frac{\pi^{10}}{93{,}555}.$$

$$\text{(c) } \zeta(6) = \frac{\pi^6}{945}$$

5.9.7 Planck's black-body radiation law involves the integral

$$\int_0^\infty \frac{x^3 dx}{e^x - 1}.$$

Show that this equals $6\zeta(4)$. From Exercise 5.9.6

$$\zeta(4) = \frac{\pi^4}{90}.$$

Hint. Make use of the gamma function (Chapter 10).

5.9.8 Prove that

$$\int_0^\infty \frac{x^n e^x dx}{(e^x-1)^2} = n!\zeta(n).$$

Assuming n to be real, show that each side of the equation diverges if $n = 1$. Hence, the preceding equation carries the condition $n > 1$. Integrals such as this appear in the quantum theory of transport effects—thermal and electrical conductivity.

5.9.9 The Bloch–Grüneissen approximation for the resistance in a monovalent metal is

$$\rho = C\frac{T^5}{\Theta^6}\int_0^{\Theta/T} \frac{x^5 dx}{(e^x-1)(1-e^{-x})},$$

where Θ is the Debye temperature characteristic of the metal.

(a) For $T \to \infty$, show that

$$\rho \approx \frac{C}{4} \cdot \frac{T}{\Theta^2}.$$

(b) For $T \to 0$, show that

$$\rho \approx 5!\zeta(5) C \frac{T^5}{\Theta^6}.$$

5.9.10 Show that

(a) $\displaystyle\int_0^1 \frac{\ln(1+x)}{x} dx = \frac{1}{2}\zeta(2), \qquad$ (b) $\displaystyle\lim_{a\to 1} \int_0^a \frac{\ln(1-x)}{x} dx = \zeta(2).$

From Exercise 5.9.6, $\zeta(2) = \pi^2/6$. Note that the integrand in part (b) diverges for $a = 1$, but that the **integrated** series is convergent.

5.9.11 The integral

$$\int_0^1 [\ln(1-x)]^2 \frac{dx}{x}$$

appears in the fourth-order correction to the magnetic moment of the electron. Show that it equals $2\zeta(3)$.
Hint. Let $1 - x = e^{-t}$.

5.9.12 Show that

$$\int_0^\infty \frac{(\ln z)^2}{1+z^2} dz = 4\left(1 - \frac{1}{3^3} + \frac{1}{5^3} - \frac{1}{7^3} + \cdots\right).$$

By contour integration (Exercises 7.2.16), this may be shown equal to $\pi^3/8$.

5.9.13 For "small" values of x,

$$\ln(x!) = -\gamma x + \sum_{n=2}^{\infty} (-1)^n \frac{\zeta(n)}{n} x^n,$$

where γ is the Euler–Mascheroni constant and $\zeta(n)$ the Riemann zeta function. For what values of x does this series converge?

ANS. $-1 < x \le 1$.

Note that if $x = 1$, we obtain

$$\gamma = \sum_{n=2}^{\infty} (-1)^n \frac{\zeta(n)}{n},$$

a series for the Euler–Mascheroni constant. The convergence of this series is exceedingly slow. For actual computation of γ, other, indirect approaches are far superior (see Exercises 5.10.11 and 10.5.16).

5.9.14 Show that the series expansion of $\ln(x!)$ (Exercise 5.9.13) may be written as

(a) $\displaystyle \ln(x!) = \frac{1}{2}\ln\left(\frac{\pi x}{\sin \pi x}\right) - \gamma x - \sum_{n=1}^{\infty} \frac{\zeta(2n+1)}{2n+1} x^{2n+1},$

(b) $$\ln(x!) = \frac{1}{2}\ln\left(\frac{\pi x}{\sin \pi x}\right) - \frac{1}{2}\ln\left(\frac{1+x}{1-x}\right) + (1-\gamma)x - \sum_{n=1}^{\infty}[\zeta(2n+1)-1]\frac{x^{2n+1}}{2n+1}.$$

Determine the range of convergence of each of these expressions.

5.9.15 Show that Catalan's constant, $\beta(2)$, may be written as

$$\beta(2) = 2\sum_{k=1}^{\infty}(4k-3)^{-2} - \frac{\pi^2}{8}.$$

Hint. $\pi^2 = 6\zeta(2)$.

5.9.16 Derive the following expansions of the Debye functions for $n \geq 1$:

$$\int_0^x \frac{t^n dt}{e^t - 1} = x^n\left[\frac{1}{n} - \frac{x}{2(n+1)} + \sum_{k=1}^{\infty}\frac{B_{2k}x^{2k}}{(2k+n)(2k)!}\right], \quad |x| < 2\pi,$$

$$\int_x^{\infty} \frac{t^n dt}{e^t - 1} = \sum_{k=1}^{\infty} e^{-kx}\left[\frac{x^n}{k} + \frac{nx^{n-1}}{k^2} + \frac{n(n-1)x^{n-2}}{k^3} + \cdots + \frac{n!}{k^{n+1}}\right]$$

for $x > 0$. The complete integral $(0, \infty)$ equals $n!\zeta(n+1)$.

5.9.17 (a) Show that the equation $\ln 2 = \sum_{s=1}^{\infty}(-1)^{s+1}s^{-1}$ (Exercise 5.4.1) may be rewritten as

$$\ln 2 = \sum_{s=2}^{\infty} 2^{-s}\zeta(s) + \sum_{p=1}^{\infty}(2p)^{-n-1}\left[1 - \frac{1}{2p}\right]^{-1}.$$

Hint. Take the terms in pairs.

(b) Calculate $\ln 2$ to six significant figures.

5.9.18 (a) Show that the equation $\pi/4 = \sum_{n=1}^{\infty}(-1)^{n+1}(2n-1)^{-1}$ (Exercise 5.7.3) may be rewritten as

$$\frac{\pi}{4} = 1 - 2\sum_{s=1}^{\infty} 4^{-2s}\zeta(2s) - 2\sum_{p=1}^{\infty}(4p)^{-2n-2}\left[1 - \frac{1}{(4p)^2}\right]^{-1}.$$

(b) Calculate $\pi/4$ to six significant figures.

Table 5.3

Riemann Zeta Function

s	$\zeta(s)$
2	1.6449340668
3	1.2020569032
4	1.0823232337
5	1.0369277551
6	1.0173430620
7	1.0083492774
8	1.0040773562
9	1.0020083928
10	1.0009945751

5.9.19 Write a function subprogram ZETA(N) that will calculate the Riemann zeta function for integer argument. Tabulate $\zeta(s)$ for $s = 2, 3, 4, \ldots, 20$. Check your values against Table 5.3 and AMS-55 (Chapter 23).
Hint. If you supply the function subprogram with the known values of $\zeta(2)$, $\zeta(3)$, and $\zeta(4)$, you avoid the more slowly converging series.

5.9.20 Calculate the logarithm (base 10) of $|B_{2n}|$, $n = 10, 20, \ldots, 100$.
Hint. Program $\zeta(n)$ as a function subprogram (Exercise 5.9.19).

Check values. $\log|B_{100}| = 78.45$
$\log|B_{200}| = 215.56$.

5.9.21 Determine the values of the coefficients a_1, a_2, and a_3 that will make $(1 + a_1x + a_2x^2 + a_3x^3)\ln(1 + x)$ converge as n^{-4}. Find the resulting series.

5.10 Asymptotic Series

Asymptotic series frequently occur in physics. In numerical computations they are employed for the accurate computation of a variety of functions. We consider here a type of integral that leads to asymptotic series—an integral of the form

$$I_1(x) = \int_x^\infty e^{-u} f(u)du,$$

where the variable x appears as the lower limit of an integral.

Asymptotic series often occur as solutions of differential equations. An example of this appears in Section 12.3, as a solution of Bessel's equation. One of the most useful and powerful methods of generating asymptotic expansions, the method of steepest descents, will be developed in Section 7.3. Applications include the derivation of Stirling's formula for the (complete) factorial function (Section 10.3) and the asymptotic forms of the various Bessel functions (Section 12.3). Asymptotic series occur fairly often in mathematical physics. One of the earliest and most important approximations of quantum mechanics, the **WKB expansion**, is an asymptotic series.

Error Function

The nature of an asymptotic series is perhaps best illustrated by a specific example. Let us start with the familiar error function $\text{erf}(x)$ and its complement $\text{erfc}(x)$,

$$\text{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt, \qquad \text{erfc}(x) = \frac{2}{\sqrt{\pi}} \int_x^\infty e^{-t^2} dt, \tag{5.148}$$

which have many applications in statistics, probability theory, and error analyses in physics and engineering and are normalized so that $\text{erf}(\infty) = 1$. Suppose we have to evaluate the error function for large values of x. Then we express $\text{erf}(x) = 1 - \text{erfc}(x)$, because $\text{erfc}(x)$ is better suited for an asymptotic expansion, which we now generate by repeated integration by parts of

$$\begin{aligned}
\int_x^\infty e^{-t^2} dt &= -\frac{1}{2} \int_x^\infty (-2t) e^{-t^2} \frac{dt}{t} = -\frac{e^{-t^2}}{2t}\bigg|_x^\infty - \frac{1}{2} \int_x^\infty e^{-t^2} \frac{dt}{t^2} \\
&= \frac{e^{-x^2}}{2x} + \frac{1}{4} \int_x^\infty (-2t) e^{-t^2} \frac{dt}{t^3} \\
&= \frac{e^{-x^2}}{2x} + \frac{e^{-t^2}}{4t^3}\bigg|_x^\infty + \frac{3}{4} \int_x^\infty e^{-t^2} \frac{dt}{t^4} = \cdots.
\end{aligned}$$

Once we recognize the emerging pattern

$$\int_x^\infty e^{-t^2}dt = \frac{e^{-x^2}}{2x}\left[1+\sum_{\nu=1}^{n}\frac{(2\nu-1)!!}{2^\nu x^{2\nu}}(-1)^\nu\right] - (-1)^n\frac{(2n+1)!!}{2^{n+1}}\int_x^\infty e^{-t^2}\frac{dt}{t^{2n+2}} \tag{5.149}$$

from the first two or three terms, we can prove it by mathematical induction by one more integration by parts of the last integral term

$$-\frac{1}{2}\int_x^\infty(-2t)e^{-t^2}\frac{dt}{t^{2n+3}} = -\frac{e^{-t^2}}{2t^{2n+3}}\bigg|_x^\infty - \frac{2n+3}{2}\int_x^\infty e^{-t^2}\frac{dt}{t^{2n+4}}.$$

Putting this result back into Eq. (5.149), we generate the integral term for $n \to n+1$ and the general term of the sum in Eq. (5.149) for $n \to n+1$, thus proving the expansion for all natural integers. Substituting Eq. (5.149) into Eq. (5.148), we obtain the error function

$$\begin{aligned}\operatorname{erf}(x) &= \frac{2}{\sqrt{\pi}}\int_0^x e^{-t^2}dt \\ &= 1-\frac{e^{-x^2}}{\sqrt{\pi}x}\left(1-\frac{1}{2x^2}+\frac{1\cdot 3}{2^2x^4}-\frac{1\cdot 3\cdot 5}{2^3x^6}+\cdots+(-1)^n\frac{(2n-1)!!}{2^n x^{2n}}\right) \\ &\quad +(-1)^n\frac{(2n+1)!!}{2^n\sqrt{\pi}}\int_x^\infty e^{-t^2}\frac{dt}{t^{2n+2}}\end{aligned} \tag{5.150}$$

in terms of a finite (partial) series and an integral as a remainder term.

This is a remarkable series. Checking the convergence by the d'Alembert ratio test,

$$\lim_{n\to\infty}\frac{|u_{n+1}|}{|u_n|} = \lim_{n\to\infty}\frac{2n+1}{2x^2} = \infty \tag{5.151}$$

for all values of x. Therefore, our series as an infinite series diverges everywhere. Before discarding it as worthless, let us see how well a given partial sum approximates the error function. When we substitute $t = x + v/x$ in the remainder, the integral becomes

$$\frac{1}{x}\int_0^\infty e^{-(x+v/x)^2}\frac{dv}{(x+v/x)^{2n+2}} = \frac{e^{-x^2}}{x^{2n+3}}\int_0^\infty e^{-2v-v^2/x^2}\frac{dv}{(1+v/x^2)^{2n+2}}.$$

For fixed n and large x, the integral is less than $\int_0^\infty e^{-2v}dv = 1/2$. Thus, the error function is equal to the partial sum up to an error that is less than

$$\frac{1}{\sqrt{\pi}}\frac{(2n+1)!!}{2^{n+1}}\frac{e^{-x^2}}{x^{2n+3}},$$

which goes to zero as $x \to \infty$ for all natural integers n. This means that if we take x large enough, our partial sum in Eq. (5.150) is an arbitrarily good approximation to the error function. Although formally divergent when extended to $n \to \infty$, any partial sum is perfectly good for computations. For this

reason, it is sometimes called a semiconvergent series. Note that such **asymptotic series are always finite sums and never infinite series.** Because the remainder integral in Eq. (5.150) alternates in sign, the successive partial sums give alternatively upper and lower bounds for the error function.

SUMMARY

Asymptotic series are approximations by one or more terms of a finite series of certain integrals (or integral representations of special functions) at special values of their argument. They are important tools for accurate approximations.

EXERCISES

5.10.1 Stirling's formula for the logarithm of the factorial function is

$$\ln(x!) = \frac{1}{2}\ln 2\pi + \left(x + \frac{1}{2}\right)\ln x - x + O(x^{-1}).$$

Show that Stirling's formula is an **asymptotic** expression.

5.10.2 Integrating by parts, develop asymptotic expansions of the Fresnel integrals:

$$\text{(a) } C(x) = \int_0^x \cos\frac{\pi u^2}{2}du \qquad \text{(b) } s(x) = \int_0^x \sin\frac{\pi u^2}{2}du.$$

These integrals appear in the analysis of a knife-edge diffraction pattern.

5.10.3 Derive the asymptotic expansions of $\text{Ci}(x)$ and $\text{si}(x)$ by repeated integration by parts.
Hint. $\text{Ci}\,(x) + i\,\text{si}\,(x) = -\int_x^\infty \frac{e^{it}}{t}dt$.

5.10.4 Evaluate the Gauss error function at $x = 1, 2, 3$ using the asymptotic series [Eq. (5.150)]. Choose n so as to obtain an accuracy of $1, 4, 8$ significant decimal places.

5.10.5 For $x > 1$

$$\frac{1}{1+x} = \sum_{n=0}^{\infty}(-1)^n\frac{1}{x^{n+1}}.$$

Test this series to determine if it is an asymptotic series.

5.10.6 Develop an asymptotic series for

$$\int_0^\infty e^{-xv}(1+v^2)^{-2}dv.$$

Take x to be real and positive.

$$\textit{ANS.}\quad \frac{1}{x} - \frac{2!}{x^3} + \frac{4!}{x^5} - \cdots + \frac{(-1)^n(2n)!}{x^{2n+1}}.$$

Additional Reading

Bender, C. M., and Orszag, S. (1978). *Advanced Mathematical Methods for Scientists and Engineers*. McGraw-Hill, New York. Particularly recommended for methods of accelerating convergence.

Davis, H. T. (1935). *Tables of Higher Mathematical Functions*. Principia Press, Bloomington, IN.

Dingle, R. B. (1973). *Asymptotic Expansions: Their Derivation and Interpretation*. Academic Press, New York.

Galambos, J. (1976). *Representations of Real Numbers by Infinite Series*. Springer, Berlin.

Gradshteyn, I. S., and Ryzhik, I. M. (1994). *Table of Integrals, Series and Products*, corrected and enlarged 5th edition prepared by Alan Jeffrey. Academic Press, New York.

Hamming, R. W. (1987). *Numerical Methods for Scientists and Engineers* (reprinted). Dover, New York.

Hansen, E. (1975). *A Table of Series and Products*. Prentice-Hall, Englewood Cliffs, NJ. A tremendous compilation of series and products.

Hardy, G. H. (1956). *Divergent Series*. Clarendon, Oxford. [2nd ed., Chelsea, 1992]. The standard, comprehensive work on methods of treating divergent series. Hardy includes instructive accounts of the gradual development of the concepts of convergence and divergence.

Jeffrey, A. (1995). *Handbook of Mathematical Formulas and Integrals*. Academic Press, San Diego.

Knopp, K. (1971). *Theory and Application of Infinite Series*, 2nd ed. Blackie, London. Hafner, New York. Reprinted, A. K. Peters Classics (1997). This is a thorough, comprehensive, and authoritative work that covers infinite series and products. Proofs of almost all of the statements not proved in Chapter 5 can be found in this book.

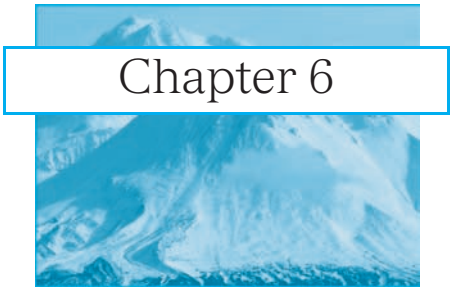
Mangulis, V. (1965). *Handbook of Series for Scientists and Engineers*. Academic Press, New York. A most convenient and useful collection of series. Includes algebraic functions, Fourier series, and series of the special functions: Bessel, Legendre, and so on.

Olver, F. W. J. (1974). *Asymptotics and Special Functions*. Academic Press, New York. A detailed, readable development of asymptotic theory. Considerable attention is paid to error bounds for use in computation.

Rainville, E. D. (1967). *Infinite Series*. Macmillan, New York. A readable and useful account of series-constants and functions.

Sokolnikoff, I. S., and Redheffer, R. M. (1966). *Mathematics of Physics and Modern Engineering*, 2nd ed. McGraw-Hill, New York. A long Chapter 2 (101 pages) presents infinite series in a thorough but very readable form. Extensions to the solutions of differential equations, to complex series, and to Fourier series are included.

The topic of infinite series is treated in many texts on advanced calculus.



Chapter 6

Functions of a Complex Variable I

Analytic Properties Mapping

> The imaginary numbers are a wonderful flight of God's spirit; they are almost an amphibian between being and not being.
>
> —Gottfried Wilhelm von Leibniz, 1702

The theory of functions of one complex variable contains some of the most powerful and widely useful tools in all of mathematical analysis. To indicate why complex variables are important, we mention briefly several areas of application.

First, for many pairs of functions u and v, both u and v satisfy Laplace's equation in two real dimensions

$$\nabla^2 u = \frac{\partial^2 u(x, y)}{\partial x^2} + \frac{\partial^2 u(x, y)}{\partial y^2} = 0.$$

For example, either u or v may be used to describe a two-dimensional electrostatic potential. The other function then gives a family of curves orthogonal to the equipotential curves of the first function and may be used to describe the electric field $\mathbf{E}$. A similar situation holds for the hydrodynamics of an ideal fluid in irrotational motion. The function u might describe the velocity potential, whereas the function v would then be the stream function.

In some cases in which the functions u and v are unknown, mapping or transforming complex variables permits us to create a (curved) coordinate system tailored to the particular problem.

Second, complex numbers are constructed (in Section 6.1) from pairs of real numbers so that the real number field is embedded naturally in the complex number field. In mathematical terms, the complex number field is an extension of the real number field, and the latter is complete in the sense that

any polynomial of order n has n (in general) complex zeros. This fact was first proved by Gauss and is called the fundamental theorem of algebra (see Sections 6.4 and 7.2). As a consequence, real functions, infinite real series, and integrals usually can be generalized naturally to complex numbers simply by replacing a real variable x, for example, by complex z.

In Chapter 8, we shall see that the second-order differential equations of interest in physics may be solved by power series. The same power series may be used by replacing x by the complex variable z. The dependence of the solution $f(z)$ at a given z_0 on the behavior of $f(z)$ elsewhere gives us greater insight into the behavior of our solution and a powerful tool (analytic continuation) for extending the region in which the solution is valid.

Third, the change of a parameter k from real to imaginary transforms the Helmholtz equation into the diffusion equation. The same change transforms the Helmholtz equation solutions (Bessel and spherical Bessel functions) into the diffusion equation solutions (modified Bessel and modified spherical Bessel functions).

Fourth, integrals in the complex plane have a wide variety of useful applications:

- Evaluating definite integrals (in Section 7.2)
- Inverting power series
- Infinite product representations of analytic functions (in Section 7.2)
- Obtaining solutions of differential equations for large values of some variable (asymptotic solutions in Section 7.3)
- Investigating the stability of potentially oscillatory systems
- Inverting integral transforms (in Chapter 15)

Finally, many physical quantities that were originally real become complex as a simple physical theory is made more general. The real index of refraction of light becomes a complex quantity when absorption is included. The real energy associated with an energy level becomes complex, $E = m \pm i\Gamma$, when the finite lifetime of the level is considered. Electric circuits with resistance R, capacitance C, and inductance L typically lead to a complex impedance $Z = R + i(\omega L - \frac{1}{\omega C})$.

We start with complex arithmetic in Section 6.1 and then introduce complex functions and their derivatives in Section 6.2. This leads to the fundamental Cauchy integral formula in Sections 6.3 and 6.4; analytic continuation, singularities, and Taylor and Laurent expansions of functions in Section 6.5; and conformal mapping, branch point singularities, and multivalent functions in Sections 6.6 and 6.7.

6.1 Complex Algebra

As we know from practice with solving real quadratic equations for their real zeros, they often fail to yield a solution. A case in point is the following example.

EXAMPLE 6.1.1 **Positive Quadratic Form** For all real x

$$y(x) = x^2 + x + 1 = \left(x + \frac{1}{2}\right)^2 + \frac{3}{4} > 0$$

is positive definite; that is, in the real number field $y(x) = 0$ has no solutions. Of course, if we use the **symbol** $i = \sqrt{-1}$, we can formally write the solutions of $y(x) = 0$ as $\frac{1}{2}(-1 \pm i\sqrt{3})$ and check that

$$\left[\frac{1}{2}(-1 \pm i\sqrt{3})\right]^2 + \frac{1}{2}(-1 \pm i\sqrt{3}) + 1 = \frac{1}{4}(1 - 3 \mp 2i\sqrt{3} - 2 \pm 2i\sqrt{3}) + 1 = 0.$$

Although we can do arithmetic with i subject to the rule $i^2 = -1$, this symbol does not tell us what imaginary numbers really are. ■

In order to make complex zeros visible we have to enlarge the real numbers on a line to complex numbers in a plane. **We define a complex number** such as a point with two coordinates in the Euclidean plane **as an ordered pair of two real numbers**, (a, b) as shown in Fig. 6.1. Similarly, **a complex variable is an ordered pair of two real variables**,

$$z \equiv (x, y). \tag{6.1}$$

The ordering is significant; x is called the **real part** of z and y the **imaginary part** of z. In general, (a, b) is not equal to (b, a) and (x, y) is not equal to (y, x). As usual, we continue writing a real number $(x, 0)$ simply as x, and call $i \equiv (0, 1)$ the imaginary unit. The x-axis is the real axis and the y-axis the imaginary axis of the complex number plane. Note that in electrical engineering the convention is $j = \sqrt{-1}$ and i is reserved for a current there. The complex numbers $\frac{1}{2}(-1 \pm i\sqrt{3})$ from Example 6.1.1 are the points $(-\frac{1}{2}, \pm\sqrt{3})$.

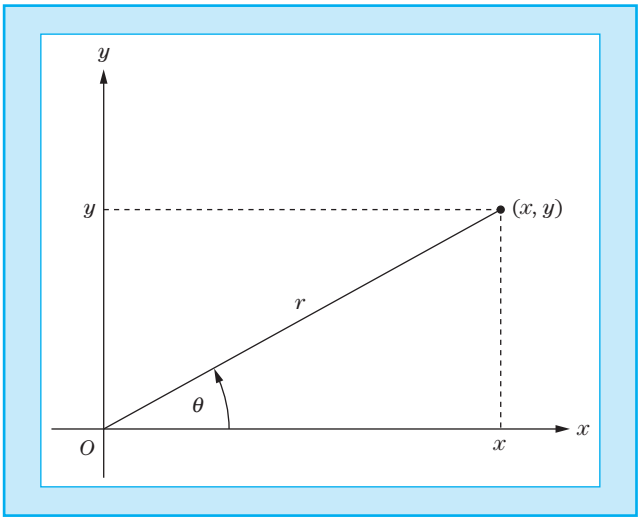


Figure 6.1
Complex Plane—Argand Diagram

A graphical representation is a powerful means to see a complex number or variable. By plotting x (the real part of z) as the abscissa and y (the imaginary part of z) as the ordinate, we have the complex plane or Argand plane shown in Fig. 6.1. If we assign specific values to x and y, then z corresponds to a point (x, y) in the plane. In terms of the ordering mentioned previously, it is obvious that the point (x, y) does not coincide with the point (y, x) except for the special case of $x = y$.

Complex numbers are points in the plane, and now we want to add, subtract, multiply, and divide them, just like real numbers. All our complex variable analyses can now be developed in terms of ordered pairs[1] of numbers (a, b), variables (x, y), and functions $(u(x, y), v(x, y))$.

We now define **addition** of complex numbers in terms of their Cartesian components as

$$z_1 + z_2 = (x_1, y_1) + (x_2, y_2) = (x_1 + x_2, y_1 + y_2) = z_2 + z_1, \tag{6.2}$$

that is, two-dimensional vector addition. In Chapter 1, the points in the xy-plane are identified with the two-dimensional displacement vector $\mathbf{r} = \hat{\mathbf{x}}x+\hat{\mathbf{y}}y$. As a result, two-dimensional vector analogs can be developed for much of our complex analysis. Exercise 6.1.2 is one simple example; Cauchy's theorem (Section 6.3) is another. Also, $-z + z = (-x, -y) + (x, y) = 0$ so that the negative of a complex number is uniquely specified. **Subtraction** of complex numbers then proceeds as addition: $z_1 - z_2 = (x_1 - x_2, y_1 - y_2)$.

Multiplication of complex numbers is defined as

$$z_1 z_2 = (x_1, y_1) \cdot (x_2, y_2) = (x_1 x_2 - y_1 y_2,\ x_1 y_2 + x_2 y_1). \tag{6.3}$$

Using Eq. (6.3) we verify that $i^2 = (0, 1) \cdot (0, 1) = (-1, 0) = -1$ so that we can also identify $i = \sqrt{-1}$ as usual, and further rewrite Eq. (6.1) as

$$z = (x, y) = (x, 0) + (0, y) = x + (0, 1) \cdot (y, 0) = x + iy. \tag{6.4}$$

Clearly, the i **is not necessary here but it is truly convenient and traditional**. It serves to keep pairs in order—somewhat like the unit vectors of vector analysis in Chapter 1.

With complex numbers at our disposal, we can determine the complex zeros of $z^2 + z + 1 = 0$ in Example 6.1.1 as $z = -\frac{1}{2} \pm \frac{i}{2}\sqrt{3}$ so that

$$z^2 + z + 1 = \left(z + \frac{1}{2} - \frac{i}{2}\sqrt{3}\right)\left(z + \frac{1}{2} + \frac{i}{2}\sqrt{3}\right)$$

factorizes completely.

Complex Conjugation

The operation of replacing i by $-i$ is called "taking the complex conjugate." The complex conjugate of z is denoted by z^*,[2] where

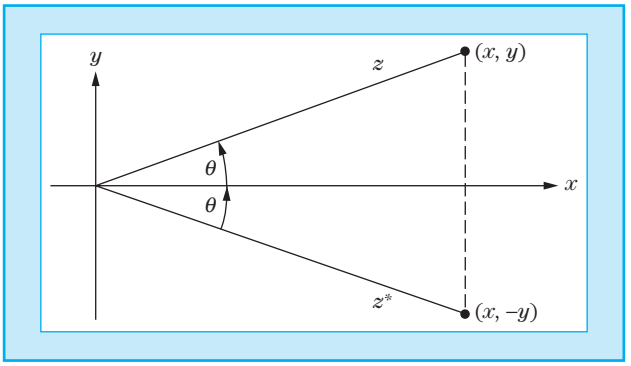
$$z^* = x - iy. \tag{6.5}$$

[1] This is precisely how a computer does complex arithmetic.

[2] The complex conjugate is often denoted by $\bar{z}$ in the mathematical literature.

Figure 6.2

Complex Conjugate Points



The complex variable z and its complex conjugate z^* are mirror images of each other reflected in the x-axis; that is, inversion of the y-axis (compare Fig. 6.2). The product zz^* leads to

$$zz^* = (x + iy)(x - iy) = x^2 + y^2 = r^2. \tag{6.6}$$

Hence,

$$(zz^*)^{1/2} = |z|$$

is defined as the **magnitude or modulus** of z.

Division of complex numbers is most easily accomplished by replacing the denominator by a positive number as follows:

$$\frac{z_1}{z_2} = \frac{x_1 + iy_1}{x_2 + iy_2} = \frac{(x_1 + iy_1)(x_2 - iy_2)}{(x_2 + iy_2)(x_2 - iy_2)} = \frac{(x_1x_2 + y_1y_2,\ x_2y_1 - x_1y_2)}{x_2^2 + y_2^2}, \tag{6.7}$$

which displays its real and imaginary parts as ratios of real numbers with the same positive denominator. Here, $|z_2|^2 = x_2^2 + y_2^2$ is the **absolute value (squared)** of z_2, and $z_2^* = x_2 - iy_2$ is called the **complex conjugate** of z_2. We write $|z_2|^2 = z_2^* z_2$, which is the squared length of the associated Cartesian vector in the complex plane.

Furthermore, from Fig. 6.1 we may write in plane polar coordinates

$$x = r\cos\theta, \quad y = r\sin\theta \tag{6.8}$$

and

$$z = r(\cos\theta + i\sin\theta). \tag{6.9}$$

In this representation r is the **modulus or magnitude** of

$$z\ (r = |z| = (x^2 + y^2)^{1/2})$$

and the angle θ $(= \tan^{-1}(y/x))$ is labeled the **argument or phase** of z. Using a result that is suggested (but not rigorously proved)[3] by Section 5.6, we have the very useful polar representation

$$z = re^{i\theta}. \tag{6.10}$$

In order to prove this identity, we use $i^3 = -i$, $i^4 = 1$, etc. in the Taylor expansion of the exponential and trigonometric functions and separate even and odd powers in

$$\begin{aligned} e^{i\theta} &= \sum_{n=0}^{\infty} \frac{(i\theta)^n}{n!} = \sum_{\nu=0}^{\infty} \frac{(i\theta)^{2\nu}}{(2\nu)!} + \sum_{\nu=0}^{\infty} \frac{(i\theta)^{2\nu+1}}{(2\nu+1)!} \\ &= \sum_{\nu=0}^{\infty} (-1)^{\nu} \frac{\theta^{2\nu}}{(2\nu)!} + i \sum_{\nu=0}^{\infty} (-1)^{\nu} \frac{\theta^{2\nu+1}}{(2\nu+1)!} = \cos\theta + i \sin\theta. \end{aligned} \tag{6.11}$$

For the special values $\theta = \pi/2$, and $\theta = \pi$, we obtain

$$e^{i\pi/2} = \cos(\pi/2) + i \sin(\pi/2) = i, \quad e^{i\pi} = \cos(\pi) = -1,$$

intriguing connections between e, i, and π. Moreover, the exponential function $e^{i\theta}$ is periodic with period 2π, just like $\sin\theta$ and $\cos\theta$. As an immediate application we can derive the trigonometric addition rules from

$$\begin{aligned} \cos(\theta_1 + \theta_2) + i \sin(\theta_1 + \theta_2) &= e^{i(\theta_1+\theta_2)} \\ &= e^{i\theta_1} e^{i\theta_2} = [\cos\theta_1 + i \sin\theta_1][\cos\theta_2 + i \sin\theta_2] \\ &= \cos\theta_1 \cos\theta_2 - \sin\theta_1 \sin\theta_2 \\ &\quad + i(\sin\theta_1 \cos\theta_2 + \sin\theta_2 \cos\theta_1). \end{aligned}$$

Let us now convert a ratio of complex numbers to polar form explicitly.

EXAMPLE 6.1.2

Conversion to Polar Form We start by converting the denominator of a ratio to a real number:

$$\frac{2+i}{3-2i} = \frac{(2+i)(3+2i)}{3^2+2^2} = \frac{6-2+i(3+4)}{13} = \frac{4+7i}{13} = \sqrt{\frac{5}{13}} e^{i\theta_0},$$

where $\frac{4^2+7^2}{13^2} = \frac{65}{13^2} = \frac{5}{13}$ and $\tan\theta_0 = \frac{7}{4}$. Because $\arctan(\theta)$ has two branches in the range from zero to 2π, we pick the solution $\theta_0 = 60.255^\circ$, $0 < \theta_0 < \pi/2$, because the second solution $\theta_0 + \pi$ gives $e^{i(\theta_0+\pi)} = -e^{i\theta_0}$ (i.e., the wrong sign).

Alternately, we can convert $2 + i = \sqrt{5} e^{i\alpha}$ and $3 - 2i = \sqrt{13} e^{i\beta}$ to polar form with $\tan\alpha = \frac{1}{2}$, $\tan\beta = -\frac{2}{3}$ and then divide them to get

$$\frac{2+i}{3-2i} = \sqrt{\frac{5}{13}} e^{i(\alpha-\beta)}. \quad \blacksquare$$

[3] Strictly speaking, Chapter 5 was limited to real variables. However, we can define e^z as $\sum_{n=0}^{\infty} z^n/n!$ for complex z. The development of power-series expansions for complex functions is taken up in Section 6.5 (Laurent expansion).

The choice of polar representation [Eq. (6.10)] or Cartesian representation [Eqs. (6.1) and (6.4)] is a matter of convenience. Addition and subtraction of complex variables are easier in the Cartesian representation [Eq. (6.2)]. Multiplication, division, powers, and roots are easier to handle in polar form [Eqs. (6.8)–(6.10)].

Let us examine the geometric meaning of multiplying a function by a complex constant.

EXAMPLE 6.1.3

Multiplication by a Complex Number When we multiply the complex variable z by $i = e^{i\pi/2}$, for example, it is rotated counterclockwise by 90° to $iz = ix - y = (-y, x)$. When we multiply $z = re^{i\theta}$ by $e^{i\alpha}$, we get $re^{i(\theta+\alpha)}$, which is z rotated by the angle α.

Similarly, curves defined by $f(z) = \text{const.}$ are rotated when we multiply a function by a complex constant. When we set

$$f(z) = (x + iy)^2 = (x^2 - y^2) + 2ixy = c = c_1 + ic_2 = \text{const.},$$

we define two hyperbolas

$$x^2 - y^2 = c_1, \quad 2xy = c_2.$$

Upon multiplying $f(z) = c$ by a complex number $Ae^{i\alpha}$, we obtain

$$\begin{aligned} Ae^{i\alpha} f(z) &= A(\cos\alpha + i\sin\alpha)(x^2 - y^2 + 2ixy) \\ &= A[i(2xy\cos\alpha + (x^2 - y^2)\sin\alpha) - 2xy\sin\alpha + (x^2 - y^2)\cos\alpha]. \end{aligned}$$

The hyperbolas are scaled by the modulus A and rotated by the angle α. ■

Analytically or graphically, using the vector analogy, we may show that the modulus of the sum of two complex numbers is no greater than the sum of the moduli and no less than the difference (Exercise 6.1.2):

$$|z_1| - |z_2| \le |z_1 + z_2| \le |z_1| + |z_2|. \tag{6.12}$$

Because of the vector analogy, these are called the **triangle** inequalities.

Using the polar form [Eq. (6.8)] we find that the magnitude of a product is the product of the magnitudes,

$$|z_1 \cdot z_2| = |z_1| \cdot |z_2|. \tag{6.13}$$

Also,

$$\arg(z_1 \cdot z_2) = \arg z_1 + \arg z_2. \tag{6.14}$$

From our complex variable z complex functions $f(z)$ or $w(z)$ may be constructed. These complex functions may then be resolved into real and imaginary parts

$$w(z) = u(x, y) + iv(x, y), \tag{6.15}$$

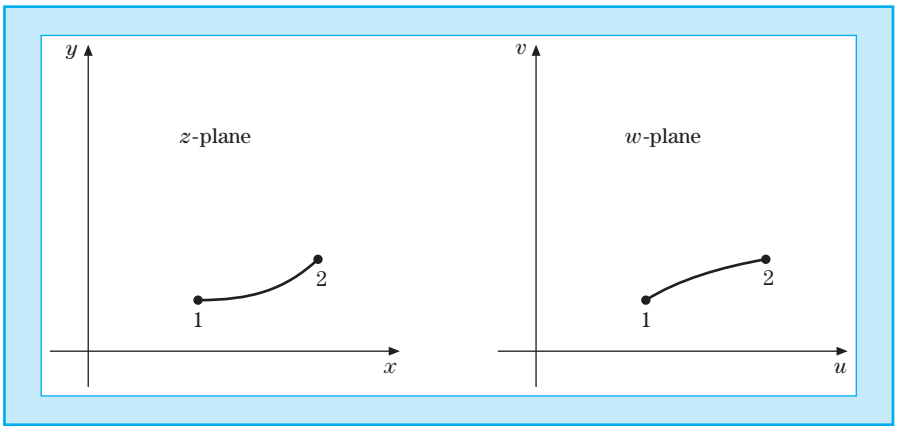


Figure 6.3

The Function $w(z) = u(x, y) + iv(x, y)$ Maps Points in the xy-Plane into Points in the uv-Plane

in which the separate functions $u(x, y)$ and $v(x, y)$ are pure real. For example, if $f(z) = z^2$, we have

$$f(z) = (x + iy)^2 = x^2 - y^2 + 2ixy.$$

The **real part** of a function $f(z)$ will be labeled $\Re f(z)$, whereas the **imaginary part** will be labeled $\Im f(z)$. In Eq. (6.15),

$$\Re w(z) = u(x, y), \qquad \Im w(z) = v(x, y). \tag{6.16}$$

The relationship between the independent variable z and the dependent variable w is perhaps best pictured as a mapping operation. A given $z = x + iy$ means a given point in the z-plane. The complex value of $w(z)$ is then a point in the w-plane. Points in the z-plane map into points in the w-plane, and curves in the z-plane map into curves in the w-plane, as indicated in Fig. 6.3.

Functions of a Complex Variable

All the elementary (real) functions of a real variable may be extended into the complex plane, replacing the real variable x by the complex variable z. This is an example of the analytic continuation mentioned in Section 6.5. The extremely important relations, Eqs. (6.4), (6.8), and (6.9), are illustrations. Moving into the complex plane opens up new opportunities for analysis.

EXAMPLE 6.1.4

De Moivre's Formula If Eq. (6.11) is raised to the nth power, we have

$$e^{in\theta} = (\cos\theta + i\sin\theta)^n. \tag{6.17}$$

Using Eq. (6.11) now with argument $n\theta$, we obtain

$$\cos n\theta + i\sin n\theta = (\cos\theta + i\sin\theta)^n. \tag{6.18}$$

This is De Moivre's formula.

Now if the right-hand side of Eq. (6.18) is expanded by the binomial theorem, we obtain $\cos n\theta$ as a series of powers of $\cos\theta$ and $\sin\theta$ (Exercise 6.1.5). Numerous other examples of relations among the exponential, hyperbolic, and trigonometric functions in the complex plane appear in the exercises. ■

Occasionally, there are complications. Taking the nth **root** of a complex number $z = re^{i\theta}$ gives $z^{1/n} = r^{1/n}e^{i\theta/n}$. This root is not the only solution, though, because $z = re^{i(\theta+2m\pi)}$ for any integer m yields $n-1$ additional roots $z^{1/n} = r^{1/n}e^{i\theta/n+2im\pi/n}$ for $m = 1, 2, \ldots, n-1$. Therefore, taking the nth **root is a multivalued function** or operation with n values, for a given complex number z. Let us look at a numerical example.

EXAMPLE 6.1.5

Square Root When we take the square root of a complex number of argument θ we get $\theta/2$. Starting from -1, which is $r = 1$ at $\theta = 180^\circ$, we end up with $r = 1$ at $\theta = 90^\circ$, which is i, or we get $\theta = -90^\circ$, which is $-i$ upon taking the root of $-1 = e^{-i\pi}$. Here is a more complicated ratio of complex numbers:

$$\sqrt{\frac{3-i}{4+2i}} = \sqrt{\frac{(3-i)(4-2i)}{4^2+2^2}} = \sqrt{\frac{12-2-i(4+6)}{20}} = \sqrt{\frac{1}{2}(1-i)}$$
$$= \sqrt{\frac{1}{\sqrt{2}}e^{-i(\pi/4-2n\pi)}} = \frac{1}{2^{1/4}}e^{-i\pi/8+in\pi} = \frac{\pm 1}{2^{1/4}}e^{-i\pi/8}$$

for $n = 0, 1$. ■

Another example is the logarithm of a complex variable z that may be expanded using the polar representation

$$\ln z = \ln re^{i\theta} = \ln r + i\theta. \tag{6.19}$$

Again, this is not complete due to the multiple branches of the inverse tangent function. To the phase angle, θ, we may add any integral multiple of 2π without changing z due to the period 2π of the tangent function. Hence, Eq. (6.19) should read

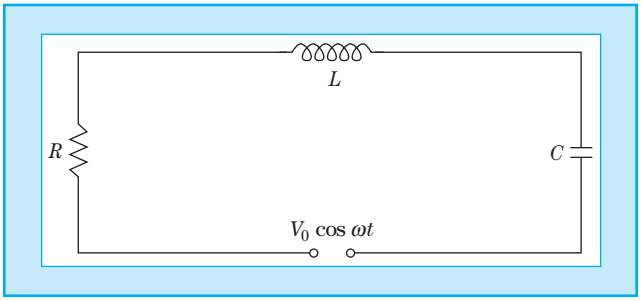
$$\ln z = \ln re^{i(\theta+2n\pi)} = \ln r + i(\theta + 2n\pi). \tag{6.20}$$

The parameter n may be any integer. This means that $\ln z$ is a **multivalued** function having an infinite number of values for a single pair of real values r and θ. To avoid ambiguity, we usually agree to set $n = 0$ and limit the phase to an interval of length 2π such as $(-\pi, \pi)$.[4] The line in the z-plane that is not crossed, the negative real axis in this case, is labeled a **cut line**. The value of $\ln z$ with $n = 0$ is called the **principal value** of $\ln z$. Further discussion of these functions, including the logarithm, appears in Section 6.6.

[4]There is no standard choice of phase: The appropriate phase depends on each problem.

Figure 6.4

Electric RLC Circuit with Alternating Current



EXAMPLE 6.1.6

Electric Circuits An electric circuit with a current I flowing through a resistor and driven by a voltage V is governed by Ohm's law, $V = IR$, where R is the resistance. If the resistance is replaced by an inductance L, then the voltage and current are related by $V = L\frac{dI}{dt}$. If the inductance is replaced by the capacitance C, then the voltage depends on the charge Q of the capacitor: $V = \frac{Q}{C}$. Taking the time derivative yields $C\frac{dV}{dt} = \frac{dQ}{dt} = I$. Therefore, a circuit with a resistor, a coil, and a capacitor in series (see Fig. 6.4) obeys the ordinary differential equation

$$L\frac{dI}{dt} + \frac{Q}{C} + IR = V = V_0 \cos \omega t \tag{6.21}$$

if it is driven by an alternating voltage with frequency ω. In electrical engineering it is a convention and tradition to use the complex voltage $V = V_0 e^{i\omega t}$ and a current $I = I_0 e^{i\omega t}$ of the same form, which is the steady-state solution of Eq. (6.21). This complex form will make the phase difference between current and voltage manifest. At the end, the physically observed values are taken to be the real parts (i.e., $V_0 \cos \omega t = V_0 \Re e^{i\omega t}$, etc.). If we substitute the exponential time dependence, use $dI/dt = i\omega I$, and integrate I once to get $Q = I/i\omega$ in Eq. (6.21), we find the following **complex form of Ohm's law**:

$$i\omega LI + \frac{I}{i\omega C} + RI = V \equiv ZI.$$

We define $Z = R + i(\omega L - \frac{1}{\omega C})$ as the impedance, a complex number, obtaining $V = ZI$, as shown.

More complicated electric circuits can now be constructed using the impedance alone—that is, without solving Eq. (6.21) anymore—according to the following combination rules:

- The resistance R of two resistors in series is $R = R_1 + R_2$.
- The inductance L of two inductors in series is $L = L_1 + L_2$.
- The resistance R of two parallel resistors obeys $\frac{1}{R} = \frac{1}{R_1} + \frac{1}{R_2}$.
- The inductance L of two parallel inductors obeys $\frac{1}{L} = \frac{1}{L_1} + \frac{1}{L_2}$.
- The capacitance of two capacitors in series obeys $\frac{1}{C} = \frac{1}{C_1} + \frac{1}{C_2}$.
- The capacitance of two parallel capacitors obeys $C = C_1 + C_2$.

In complex form these rules can be stated in a more compact form as follows:

- Two impedances in series combine as $Z = Z_1 + Z_2$;
- Two parallel impedances combine as $\frac{1}{Z} = \frac{1}{Z_1} + \frac{1}{Z_2}$. ■

SUMMARY

Complex numbers extend the real number axis to the complex number plane so that any polynomial can be completely factored. Complex numbers add and subtract like two-dimensional vectors in Cartesian coordinates:

$$z_1 + z_2 = (x_1 + iy_1) + (x_2 + iy_2) = x_1 + x_2 + i(y_1 + y_2).$$

They are best multiplied or divided in polar coordinates of the complex plane:

$$(x_1 + iy_1)(x_2 + iy_2) = r_1 e^{i\theta_1} r_2 e^{i\theta_2} = r_1 r_2 e^{i(\theta_1+\theta_2)}, \ r_j^2 = x_j^2 + y_j^2, \ \tan\theta_j = y_j/x_j.$$

The complex exponential function is given by $e^z = e^x(\cos y + i \sin y)$. For $z = x + i0 = x$, $e^z = e^x$. The trigonometric functions become

$$\cos z = \frac{1}{2}(e^{iz} + e^{-iz}) = \cos x \cosh y - i \sin x \sinh y,$$

$$\sin z = \frac{1}{2}(e^{iz} - e^{-iz}) = \sin x \cosh y + i \cos x \sinh y.$$

The hyperbolic functions become

$$\cosh z = \frac{1}{2}(e^z + e^{-z}) = \cos iz, \quad \sinh z = \frac{1}{2}(e^z - e^{-z}) = -i \sin iz.$$

The natural logarithm generalizes to $\ln z = \ln|z| + i(\theta + 2\pi n)$, $n = 0, \pm 1, \ldots$ and general powers are defined as $z^p = e^{p \ln z}$.

EXERCISES

6.1.1 (a) Find the reciprocal of $x + iy$, working entirely in the Cartesian representation.

(b) Repeat part (a), working in polar form but expressing the final result in Cartesian form.

6.1.2 Prove algebraically that

$$|z_1| - |z_2| \le |z_1 + z_2| \le |z_1| + |z_2|.$$

Interpret this result in terms of vectors. Prove that

$$|z - 1| < |\sqrt{z^2 - 1}| < |z + 1|, \quad \text{for} \quad \Re(z) > 0.$$

6.1.3 We may define a complex conjugation operator K such that $Kz = z^*$. Show that K is not a linear operator.

6.1.4 Show that complex numbers have square roots and that the square roots are contained in the complex plane. What are the square roots of i?

6.1.5 Show that

(a) $\cos n\theta = \cos^n\theta - \binom{n}{2}\cos^{n-2}\theta\sin^2\theta + \binom{n}{4}\cos^{n-4}\theta\sin^4\theta - \cdots$.

(b) $\sin n\theta = \binom{n}{1}\cos^{n-1}\theta\sin\theta - \binom{n}{3}\cos^{n-3}\theta\sin^3\theta + \cdots$.

Note. The quantities $\binom{n}{m}$ are the binomial coefficients (Chapter 5): $\binom{n}{m} = n!/[(n-m)!m!]$.

6.1.6 Show that

(a) $$\sum_{n=0}^{N-1}\cos nx = \frac{\sin(Nx/2)}{\sin x/2}\cos(N-1)\frac{x}{2},$$

(b) $$\sum_{n=0}^{N-1}\sin nx = \frac{\sin(Nx/2)}{\sin x/2}\sin(N-1)\frac{x}{2}.$$

Hint. Parts (a) and (b) may be combined to form a geometric series (compare Section 5.1).

6.1.7 For $-1 < p < 1$, show that

(a) $$\sum_{n=0}^{\infty} p^n\cos nx = \frac{1-p\cos x}{1-2p\cos x+p^2},$$

(b) $$\sum_{n=0}^{\infty} p^n\sin nx = \frac{p\sin x}{1-2p\cos x+p^2}.$$

These series occur in the theory of the Fabry–Perot interferometer.

6.1.8 Assume that the trigonometric functions and the hyperbolic functions are defined for complex argument by the appropriate power series

$$\begin{aligned}
\sin z &= \sum_{n=1,\text{odd}}^{\infty}(-1)^{(n-1)/2}\frac{z^n}{n!} = \sum_{s=0}^{\infty}(-1)^s\frac{z^{2s+1}}{(2s+1)!},\\
\cos z &= \sum_{n=0,\text{even}}^{\infty}(-1)^{n/2}\frac{z^n}{n!} = \sum_{s=0}^{\infty}(-1)^s\frac{z^{2s}}{(2s)!},\\
\sinh z &= \sum_{n=1,\text{odd}}^{\infty}\frac{z^n}{n!} = \sum_{s=0}^{\infty}\frac{z^{2s+1}}{(2s+1)!},\\
\cosh z &= \sum_{n=0,\text{even}}^{\infty}\frac{z^n}{n!} = \sum_{s=0}^{\infty}\frac{z^{2s}}{(2s)!}.
\end{aligned}$$

(a) Show that

$$i\sin z = \sinh iz,\ \sin iz = i\sinh z,$$
$$\cos z = \cosh iz,\ \cos iz = \cosh z.$$

(b) Verify that familiar functional relations such as

$$\cosh z = \frac{e^z + e^{-z}}{2},\ \sin(z_1+z_2) = \sin z_1\cos z_2 + \sin z_2\cos z_1$$

still hold in the complex plane.

6.1.9 Using the identities

$$\cos z = \frac{e^{iz} + e^{-iz}}{2}, \quad \sin z = \frac{e^{iz} - e^{-iz}}{2i},$$

established from comparison of power series, show that

(a) $\sin(x + iy) = \sin x \cosh y + i \cos x \sinh y$,
$\cos(x + iy) = \cos x \cosh y - i \sin x \sinh y$,

(b) $|\sin z|^2 = \sin^2 x + \sinh^2 y$, $|\cos z|^2 = \cos^2 x + \sinh^2 y$.

This demonstrates that we may have $|\sin z|, |\cos z| > 1$ in the complex plane.

6.1.10 From the identities in Exercises 6.1.8 and 6.1.9, show that

(a) $\sinh(x + iy) = \sinh x \cos y + i \cosh x \sin y$,
$\cosh(x + iy) = \cosh x \cos y + i \sinh x \sin y$,

(b) $|\sinh z|^2 = \sinh^2 x + \sin^2 y$, $|\cosh z|^2 = \sinh^2 x + \cos^2 y$.

6.1.11 Prove that

(a) $|\sin z| \geq |\sin x|$, (b) $|\cos z| \geq |\cos x|$.

6.1.12 Show that the exponential function e^z is periodic with a pure imaginary period of $2\pi i$.

6.1.13 Show that

(a) $\tanh(z/2) = \dfrac{\sinh x + i \sin y}{\cosh x + \cos y}$, (b) $\coth(z/2) = \dfrac{\sinh x - i \sin y}{\cosh x - \cos y}$.

6.1.14 Find all the zeros of

(a) $\sin z$, (b) $\cos z$, (c) $\sinh z$, (d) $\cosh z$.

6.1.15 Show that

(a) $\sin^{-1} z = -i \ln(iz \pm \sqrt{1 - z^2})$,

(b) $\cos^{-1} z = -i \ln(z \pm \sqrt{z^2 - 1})$,

(c) $\tan^{-1} z = \dfrac{i}{2} \ln\left(\dfrac{i + z}{i - z}\right)$,

(d) $\sinh^{-1} z = \ln(z + \sqrt{z^2 + 1})$,

(e) $\cosh^{-1} z = \ln(z + \sqrt{z^2 - 1})$,

(f) $\tanh^{-1} z = \dfrac{1}{2} \ln\left(\dfrac{1 + z}{1 - z}\right)$.

Hint. 1. Express the trigonometric and hyperbolic functions in terms of exponentials. 2. Solve for the exponential and then for the exponent. Note that $\sin^{-1} z = \arcsin z \neq (\sin z)^{-1}$, etc.

6.1.16 A plane wave of light of angular frequency ω is represented by

$$e^{i\omega(t - nx/c)}.$$

In a certain substance the simple real index of refraction n is replaced by the complex quantity $n - ik$. What is the effect of k on the wave? What does k correspond to physically? The generalization of a quantity from real to complex form occurs frequently in physics. Examples range from the complex Young's modulus of viscoelastic materials to the complex (optical) potential of the "cloudy crystal ball" model of the

atomic nucleus. See the chapter on the optical model in M. A. Preston, *Structure of the Nucleus*. Addison-Wesley, Reading, MA (1993).

6.1.17 A damped simple harmonic oscillator is driven by the complex external force $Fe^{i\omega t}$. Show that the steady-state amplitude is given by

$$A = \frac{F}{m(\omega_0^2 - \omega^2) + i\omega b}.$$

Explain the resonance condition and relate m, ω_0, b to the oscillator parameters.
Hint. Find a complex solution $z(t) = Ae^{i\omega t}$ of the ordinary differential equation.

6.1.18 We see that for the angular momentum components defined in Exercise 2.5.10,

$$L_x - iL_y \neq (L_x + iL_y)^*.$$

Explain why this happens.

6.1.19 Show that the **phase** of $f(z) = u + iv$ is equal to the imaginary part of the logarithm of $f(z)$. Exercise 10.2.13 depends on this result.

6.1.20 (a) Show that $e^{\ln z}$ always equals z.
(b) Show that $\ln e^z$ does not always equal z.

6.1.21 Verify the consistency of the combination rules of impedances with those of resistances, inductances, and capacitances by considering circuits with resistors only, etc. Derive the combination rules from Kirchhoff's laws. Describe the origin of Kirchhoff's laws.

6.1.22 Show that negative numbers have logarithms in the complex plane. In particular, find $\ln(-1)$.

ANS. $\ln(-1) = i\pi$.

6.2 Cauchy–Riemann Conditions

Having established complex functions of a complex variable, we now proceed to differentiate them. The derivative of $f(z) = u(x, y) + iv(x, y)$, like that of a real function, is defined by

$$\lim_{\delta z \to 0} \frac{f(z + \delta z) - f(z)}{z + \delta z - z} = \lim_{\delta z \to 0} \frac{\delta f(z)}{\delta z} = \frac{df}{dz} = f'(z), \tag{6.22}$$

provided that the limit is **independent** of the particular approach to the point z. For real variables we require that the right-hand limit ($x \to x_0$ from above) and the left-hand limit ($x \to x_0$ from below) be equal for the derivative $df(x)/dx$ to exist at $x = x_0$. Now, with z (or z_0) some point in a plane, our requirement that the limit be independent of the direction of approach is very restrictive. Consider increments δx and δy of the variables x and y, respectively. Then

$$\delta z = \delta x + i\delta y. \tag{6.23}$$

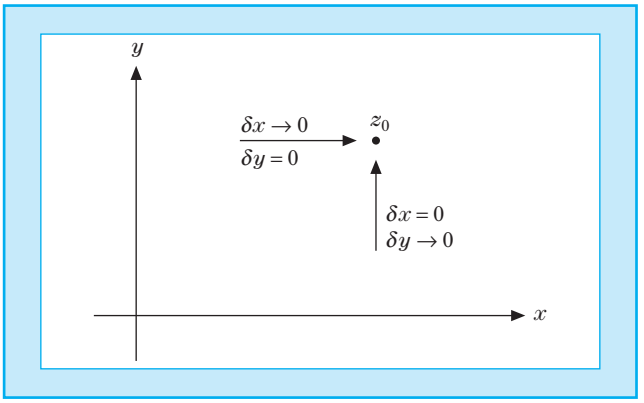


Figure 6.5

Alternate Approaches to z_0

Also,

$$\delta f = \delta u + i\delta v \tag{6.24}$$

so that

$$\frac{\delta f}{\delta z} = \frac{\delta u + i\delta v}{\delta x + i\delta y}. \tag{6.25}$$

Let us take the limit indicated by Eq. (6.23) by two different approaches as shown in Fig. 6.5. First, with $\delta y = 0$, we let $\delta x \to 0$. Equation (6.24) yields

$$\lim_{\delta z \to 0} \frac{\delta f}{\delta z} = \lim_{\delta x \to 0} \left(\frac{\delta u}{\delta x} + i\frac{\delta v}{\delta x} \right) = \frac{\partial u}{\partial x} + i\frac{\partial v}{\partial x}, \tag{6.26}$$

assuming the partial derivatives exist. For a second approach, we set $\delta x = 0$ and then let $\delta y \to 0$. This leads to

$$\lim_{\delta z \to 0} \frac{\delta f}{\delta z} = \lim_{\delta y \to 0} \left(-i\frac{\delta u}{\delta y} + \frac{\delta v}{\delta y} \right) = -i\frac{\partial u}{\partial y} + \frac{\partial v}{\partial y}. \tag{6.27}$$

If we are to have a derivative df/dz, Eqs. (6.26) and (6.27) must be identical. Equating real parts to real parts and imaginary parts to imaginary parts (like components of vectors), we obtain

$$\frac{\partial u}{\partial x} = \frac{\partial v}{\partial y}, \quad \frac{\partial u}{\partial y} = -\frac{\partial v}{\partial x}. \tag{6.28}$$

These are the famous **Cauchy–Riemann** conditions. They were discovered by Cauchy and used extensively by Riemann in his theory of analytic functions. These Cauchy–Riemann conditions are necessary for the existence of a derivative of $f(z)$; that is, if df/dz exists, the Cauchy–Riemann conditions must hold. They may be **interpreted geometrically** as follows. Let us write them as a product of ratios of partial derivatives

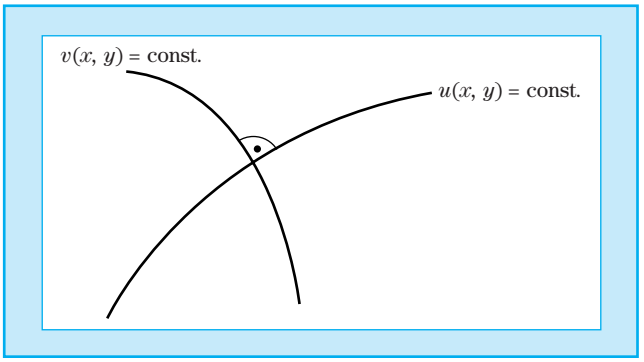
$$\frac{u_x}{u_y} \cdot \frac{v_x}{v_y} = -1, \tag{6.29}$$

with the abbreviations

$$\frac{\partial u}{\partial x} \equiv u_x, \quad \frac{\partial u}{\partial y} \equiv u_y, \quad \frac{\partial v}{\partial x} \equiv v_x, \quad \frac{\partial v}{\partial y} \equiv v_y.$$

Figure 6.6

Orthogonal Tangents to $u(x, y) = \text{const.}$ $v(x, y) = \text{const.}$ Lines



Now recall the geometric meaning of $-u_x/u_y$ as the slope of the tangent [see Eq. (1.54)] of each curve $u(x, y) = \text{const.}$ and similarly for $v(x, y) = \text{const.}$ (Fig. 6.6). Thus, Eq. (6.29) means that the $u = \text{const.}$ and $v = \text{const.}$ curves are mutually orthogonal at each intersection because $\sin\beta = \sin(\alpha + 90^\circ) = \cos\alpha$ and $\cos\beta = -\sin\alpha$ imply $\tan\beta \cdot \tan\alpha = -1$ by taking the ratio. Alternatively,

$$u_x\,dx + u_y\,dy = 0 = v_y\,dx - v_x\,dy$$

states that if (dx, dy) is tangent to the u-curve, then the orthogonal $(-dy, dx)$ is tangent to the v-curve at the intersection point $z = (x, y)$. Equivalently, $u_x v_x + u_y v_y = 0$ implies that the **gradient vectors** (u_x, u_y) and (v_x, v_y) **are perpendicular**. Conversely, if the Cauchy–Riemann conditions are satisfied and the partial derivatives of $u(x, y)$ and $v(x, y)$ are continuous, the derivative df/dz exists. This may be shown by writing

$$\delta f = \left(\frac{\partial u}{\partial x} + i\frac{\partial v}{\partial x}\right)\delta x + \left(\frac{\partial u}{\partial y} + i\frac{\partial v}{\partial y}\right)\delta y. \tag{6.30}$$

The justification for this expression depends on the continuity of the partial derivatives of u and v. Dividing by δz, we have

$$\begin{aligned}\frac{\delta f}{\delta z} &= \frac{(\partial u/\partial x + i(\partial v/\partial x))\delta x + (\partial u/\partial y + i(\partial u/\partial y))\delta y}{\delta x + i\delta y} \\ &= \frac{(\partial u/\partial x + i(\partial v/\partial x)) + (\partial u/\partial y + i(\partial v/\partial y))\delta y/\delta x}{1 + i(\delta y/\delta x)}.\end{aligned} \tag{6.31}$$

If $\delta f/\delta z$ is to have a unique value, the dependence on $\delta y/\delta x$ must be eliminated. Applying the Cauchy–Riemann conditions to the y derivatives, we obtain

$$\frac{\partial u}{\partial y} + i\frac{\partial v}{\partial y} = -\frac{\partial v}{\partial x} + i\frac{\partial u}{\partial x}. \tag{6.32}$$

Substituting Eq. (6.32) into Eq. (6.30), we may rewrite the δy and δx dependence as $\delta z = \delta x + i\delta y$ and obtain

$$\frac{\delta f}{\delta z} = \frac{\partial u}{\partial x} + i\frac{\partial v}{\partial x},$$

which shows that $\lim \delta f/\delta z$ is independent of the direction of approach in the complex plane as long as the partial derivatives are continuous.

It is worthwhile to note that the Cauchy–Riemann conditions guarantee that the curves $u = c_1 =$ constant will be orthogonal to the curves $v = c_2 =$ constant (compare Section 2.1). This property is fundamental in application to potential problems in a variety of areas of physics. If $u = c_1$ is a line of electric force, then $v = c_2$ is an equipotential line (surface) and vice versa. Also, it is easy to show from Eq. (6.28) that both u and v satisfy Laplace's equation. A further implication for potential theory is developed in Exercise 6.2.1.

We have already generalized the elementary functions to the complex plane by replacing the real variable x by complex z. Let us now check that their derivatives are the familiar ones.

EXAMPLE 6.2.1

Derivatives of Elementary Functions We define the elementary functions by their Taylor expansions (see Section 5.6, with $x \to z$, and Section 6.5)

$$e^z = \sum_{n=0}^{\infty} \frac{z^n}{n!},$$

$$\sin z = \sum_{n=0}^{\infty} (-1)^n \frac{z^{2n+1}}{(2n+1)!}, \qquad \cos z = \sum_{n=0}^{\infty} (-1)^n \frac{z^{2n}}{(2n)!},$$

$$\ln(1+z) = \sum_{n=1}^{\infty} (-1)^{n-1} \frac{z^n}{n}.$$

We differentiate termwise [which is justified by absolute convergence for e^z, $\cos z$, $\sin z$ for all z and for $\ln(1+z)$ for $|z| < 1$] and see that

$$\frac{d}{dz} z^n = \lim_{\delta z \to 0} \frac{(z+\delta z)^n - z^n}{\delta z}$$

$$= \lim_{\delta z \to 0} [z^n + n z^{n-1} \delta z + \cdots + (\delta z)^n - z^n]/\delta z = n z^{n-1},$$

$$\frac{de^z}{dz} = \sum_{n=1}^{\infty} \frac{n z^{n-1}}{n!} = e^z,$$

$$\frac{d \sin z}{dz} = \sum_{n=0}^{\infty} (-1)^n \frac{(2n+1) z^{2n}}{(2n+1)!} = \cos z,$$

$$\frac{d \cos z}{dz} = \sum_{n=1}^{\infty} (-1)^n \frac{2n z^{2n-1}}{(2n)!} = -\sin z,$$

$$\frac{d \ln(1+z)}{dz} = \frac{d}{dz} \sum_{n=1}^{\infty} (-1)^{n-1} \frac{z^n}{n} = \sum_{n=1}^{\infty} (-1)^{n-1} z^{n-1} = \frac{1}{1+z},$$

that is, the real derivative results all generalize to the complex field, simply replacing $x \to z$. ■

Biographical Data

Riemann, Bernhard Georg Friedrich. Riemann, a German mathematician, was born in 1826 in Hannover and died of tuberculosis in 1866 in Selasca, Italy. Son of a Lutheran pastor, he changed from studying theology to mathematics at the University of Göttingen where, in 1851, his Ph.D. thesis was approved by Gauss. He contributed to many branches of mathematics despite dying before the age of 40, the most famous being the development of metric (curved) spaces from their intrinsic geometric properties such as curvature. This topic was the subject of his Habilitation thesis, or venia legendi, which Gauss attended and deeply impressed him. Half a century later Riemannian geometry would become the basis for Einstein's General Relativity. Riemann's profound analysis of the complex zeta function laid the foundations for the first proof of the prime number theorem in 1898 by French mathematicians J. Hadamard and C. de la Vallée-Poussin and other significant advances in the theory of analytic functions of one complex variable. His hypothesis about the distribution of the nontrivial zeros of the zeta function, with many consequences in analytic prime number theory, remains the most famous unsolved problem in mathematics today.

Analytic Functions

Finally, if $f(z)$ is differentiable at $z = z_0$ and in some small region around z_0, we say that $f(z)$ is **analytic**[5] at $z = z_0$. If $f(z)$ is analytic everywhere in the (finite) complex plane, we call it an **entire** function. Our theory of complex variables is one of analytic functions of a complex variable, which indicates the crucial importance of the Cauchy–Riemann conditions. The concept of analyticity used in advanced theories of modern physics plays a crucial role in dispersion theory (of elementary particles or light). If $f'(z)$ does not exist at $z = z_0$, then z_0 is labeled a singular point and consideration of it is postponed until Section 7.1.

To illustrate the Cauchy–Riemann conditions, consider two very simple examples.

EXAMPLE 6.2.2

Let $f(z) = z^2$. Then the real part $u(x, y) = x^2 - y^2$ and the imaginary part $v(x, y) = 2xy$. Following Eq. (6.28),

$$\frac{\partial u}{\partial x} = 2x = \frac{\partial v}{\partial y}, \qquad \frac{\partial u}{\partial y} = -2y = -\frac{\partial v}{\partial x}.$$

We see that $f(z) = z^2$ satisfies the Cauchy–Riemann conditions throughout the complex plane. Since the partial derivatives are clearly continuous, we conclude that $f(z) = z^2$ is analytic. ■

[5]Some writers use the terms **holomorphic** or **regular**.

EXAMPLE 6.2.3

Let $f(z) = z^*$. Now $u = x$ and $v = -y$. Applying the Cauchy–Riemann conditions, we obtain

$$\frac{\partial u}{\partial x} = 1, \quad \text{whereas} \quad \frac{\partial v}{\partial y} = -1.$$

The Cauchy–Riemann conditions are not satisfied and $f(z) = z^*$ is not an analytic function of z. It is interesting to note that $f(z) = z^*$ is continuous, thus providing an example of a function that is everywhere continuous but nowhere differentiable. ■

SUMMARY

The derivative of a real function of a real variable is essentially a local characteristic in that it provides information about the function only in a local neighborhood—for instance, as a truncated Taylor expansion. The existence of a derivative of a function of a complex variable has much more far-reaching implications. The real and imaginary parts of analytic functions must separately satisfy Laplace's equation. This is Exercise 6.2.1. Furthermore, an analytic function is guaranteed derivatives of all orders (Section 6.4). In this sense the derivative not only governs the local behavior of the complex function but also controls the distant behavior.

EXERCISES

6.2.1 The functions $u(x, y)$ and $v(x, y)$ are the real and imaginary parts, respectively, of an analytic function $w(z)$.

(a) Assuming that the required derivatives exist, show that

$$\nabla^2 u = \nabla^2 v = 0.$$

Solutions of Laplace's equation, such as $u(x, y)$ and $v(x, y)$, are called **harmonic** functions.

(b) Show that

$$\frac{\partial u}{\partial x}\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\frac{\partial v}{\partial y} = 0$$

and give a geometric interpretation.

Hint. The technique of Section 1.5 allows you to construct vectors normal to the curve $u(x, y) = c_i$ and $v(x, y) = c_j$.

6.2.2 Show whether or not the function $f(z) = \Re(z) = x$ is analytic.

6.2.3 Having shown that the real part $u(x, y)$ and the imaginary part $v(x, y)$ of an analytic function $w(z)$ each satisfy Laplace's equation, show that $u(x, y)$ and $v(x, y)$ **cannot both have either a maximum or a minimum** in the interior of any region in which $w(z)$ is analytic. (They can have **saddle points**; see Section 7.3.)

6.2.4 Let $A = \partial^2 w/\partial x^2$, $B = \partial^2 w/\partial x \partial y$, $C = \partial^2 w/\partial y^2$. From the calculus of functions of two variables, $w(x, y)$, we have a **saddle point** if

$$B^2 - AC > 0.$$

With $f(z) = u(x, y) + iv(x, y)$, apply the Cauchy–Riemann conditions and show that both $u(x, y)$ and $v(x, y)$ do not have **a maximum or a minimum** in a finite region of the complex plane. (See also Section 7.3.)

6.2.5 Find the analytic function

$$w(z) = u(x, y) + iv(x, y)$$

if (a) $u(x, y) = x^3 - 3xy^2$, (b) $v(x, y) = e^{-y} \sin x$.

6.2.6 If there is some common region in which $w_1 = u(x, y) + iv(x, y)$ and $w_2 = w_1^* = u(x, y) - iv(x, y)$ are both analytic, prove that $u(x, y)$ and $v(x, y)$ are constants.

6.2.7 The function $f(z) = u(x, y) + iv(x, y)$ is analytic. Show that $f^*(z^*)$ is also analytic.

6.2.8 A proof of the Schwarz inequality (Section 9.4) involves minimizing an expression

$$f = \psi_{aa} + \lambda\psi_{ab} + \lambda^*\psi_{ab}^* + \lambda\lambda^*\psi_{bb} \geq 0.$$

The ψ are integrals of products of functions; ψ_{aa} and ψ_{bb} are real, ψ_{ab} is complex, and λ is a complex parameter.

(a) Differentiate the preceding expression with respect to λ^*, treating λ as an independent parameter, independent of λ^*. Show that setting the derivative $\partial f/\partial\lambda^*$ equal to zero yields

$$\lambda = -\psi_{ab}^*/\psi_{bb}.$$

(b) Show that $\partial f/\partial\lambda = 0$ leads to the same result.

(c) Let $\lambda = x + iy$, $\lambda^* = x - iy$. Set the x and y derivatives equal to zero and show that again

$$\lambda = \psi_{ab}^*/\psi_{bb}.$$

6.2.9 The function $f(z)$ is analytic. Show that the derivative of $f(z)$ with respect to z^* does not exist unless $f(z)$ is a constant.

Hint. Use the chain rule and take $x = (z + z^*)/2$, $y = (z - z^*)/2i$.

Note. This result emphasizes that our analytic function $f(z)$ is not just a complex function of two real variables x and y. It is a function of the complex variable $x + iy$.

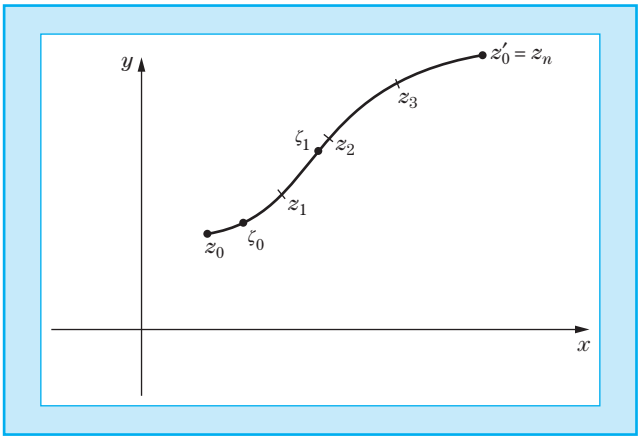
6.3 Cauchy's Integral Theorem

Contour Integrals

With differentiation under control, we turn to integration. The integral of a complex variable over a contour in the complex plane may be defined in close analogy to the (Riemann) integral of a real function integrated along the real x-axis and line integrals of vectors in Chapter 1. The contour integral may be

Figure 6.7

Integration Path



defined by

$$\int_{z_1}^{z_2} f(z)dz = \int_{x_1,y_1}^{x_2,y_2} [u(x, y) + iv(x, y)][dx + i\, dy]$$
$$= \int_{x_1,y_1}^{x_2,y_2} [u(x, y)dx - v(x, y)dy] + i \int_{x_1,y_1}^{x_2,y_2} [v(x, y)dx + u(x, y)dy] \tag{6.33}$$

with the path joining (x_1, y_1) and (x_2, y_2) specified. If the path C is parameterized as $x(s)$, $y(s)$, then $dx \to \frac{dx}{ds}ds$, and $dy \to \frac{dy}{ds}ds$. This reduces the complex integral to the complex sum of real integrals. It is somewhat analogous to the replacement of a vector integral by the vector sum of scalar integrals (Section 1.9).

We can also proceed by dividing the contour from z_0 to z_0' into n intervals by picking $n-1$ intermediate points $z_1, z_2, \ldots,$ on the contour (Fig. 6.7). Consider the sum

$$S_n = \sum_{j=1}^{n} f(\zeta_j)(z_j - z_{j-1}), \tag{6.34a}$$

where ζ_j is a point on the curve between z_j and z_{j-1}. Now let $n \to \infty$ with

$$|z_j - z_{j-1}| \to 0$$

for all j. If the $\lim_{n\to\infty} S_n$ exists and is independent of the details of choosing the points z_j and ζ_j as long as they lie on the contour, then

$$\lim_{n\to\infty} \sum_{j=1}^{n} f(\zeta_j)(z_j - z_{j-1}) = \int_{z_0}^{z_0'} f(z)dz. \tag{6.34b}$$

The right-hand side of Eq. (6.34b) is called the contour integral of $f(z)$ (along the specified contour C from $z = z_0$ to $z = z_0'$). When we **integrate** along

the contour **in the opposite direction**, dz changes sign and the **integral changes sign**.

An important example is the following contour integral.

EXAMPLE 6.3.1

Cauchy Integral for Powers Let us evaluate the contour integral $\int_C z^n\,dz$, where C is a **circle** of radius $r > 0$ around the origin $z = 0$ in the positive mathematical sense (counterclockwise). In polar coordinates of Eq. (6.10) we parameterize the circle as $z = re^{i\theta}$ and $dz = ire^{i\theta}d\theta$. For **integer** $n \neq -1$, we then obtain

$$\begin{aligned}\int_C z^n dz &= r^{n+1}\int_0^{2\pi} i\exp[i(n+1)\theta]d\theta \\ &= (n+1)^{-1}r^{n+1}[e^{i(n+1)\theta}]\big|_{\theta=0}^{2\pi} = 0 \end{aligned} \tag{6.35}$$

because 2π is a period of $e^{i(n+1)\theta}$, whereas for $n = -1$

$$\int_C \frac{dz}{z} = \int_0^{2\pi} i\,d\theta = 2\pi i, \tag{6.36}$$

again independent of r.

Alternatively, we can **integrate around a rectangle** with the corners z_1, z_2, z_3, z_4 to obtain for $n \neq -1$

$$\int z^n dz = \frac{z^{n+1}}{n+1}\bigg|_{z_1}^{z_2} + \frac{z^{n+1}}{n+1}\bigg|_{z_2}^{z_3} + \frac{z^{n+1}}{n+1}\bigg|_{z_3}^{z_4} + \frac{z^{n+1}}{n+1}\bigg|_{z_4}^{z_1} = 0$$

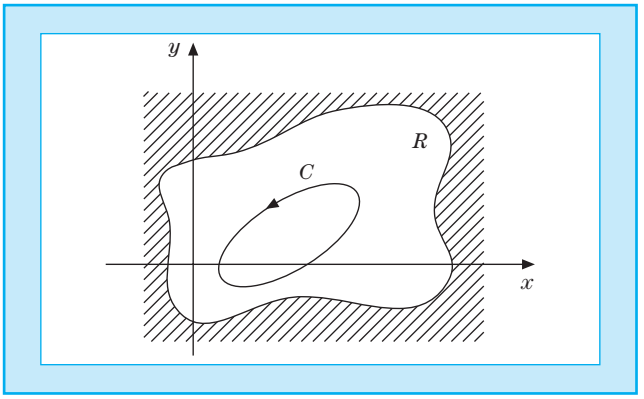
because each corner point appears once as an upper and a lower limit that cancel. For $n = -1$ the corresponding real parts of the logarithms cancel similarly, but their imaginary parts involve the increasing arguments of the points from z_1 to z_4 and, when we come back to the first corner z_1 its argument has increased by 2π due to the multivaluedness of the logarithm so that $2\pi i$ is left over as the value of the integral. Thus, **the value of the integral involving a multivalued function must be that which is reached in a continuous fashion on the path being taken**. These integrals are examples of Cauchy's integral theorem, which we prove for general functions in the next section. ■

Stokes's Theorem Proof of Cauchy's Integral Theorem

Cauchy's integral theorem is the first of two basic theorems in the theory of the behavior of functions of a complex variable. We present a proof under relatively restrictive conditions of physics applications—conditions that are intolerable to the mathematician developing a beautiful abstract theory but that are usually satisfied in physical problems. Cauchy's theorem states the following:

Figure 6.8

A Closed Contour C within a Simply Connected Region R



If a function $f(z)$ is analytic (therefore single-valued) and its partial derivatives are continuous throughout some simply connected region R,[6] for every closed path C (Fig. 6.8) in R the line integral of $f(z)$ around C is zero or

$$\oint_C f(z)dz = 0. \tag{6.37}$$

The symbol $\oint$ is used to emphasize that the path is closed.[7]

In this form the Cauchy integral theorem may be proved by direct application of Stokes's theorem (Section 1.11). With $f(z) = u(x, y) + iv(x, y)$ and $dz = dx + i\,dy$,

$$\begin{aligned}\oint_C f(z)dz &= \oint_C (u + iv)(dx + i\,dy)\\ &= \oint_C (u\,dx - v\,dy) + i\oint_C (v\,dx + u\,dy).\end{aligned} \tag{6.38}$$

These two line integrals may be converted to surface integrals by Stokes's theorem, a procedure that is justified if the partial derivatives are continuous within C. In applying Stokes's theorem, note that the final two integrals of Eq. (6.38) are real. Using

$$\mathbf{V} = \hat{\mathbf{x}}V_x + \hat{\mathbf{y}}V_y,$$

Stokes's (or Green's) theorem states that (A is area enclosed by C)

$$\oint_C (V_x\,dx + V_y\,dy) = \int_A \left(\frac{\partial V_y}{\partial x} - \frac{\partial V_x}{\partial y}\right) dx\,dy. \tag{6.39}$$

[6] A simply connected region or domain is one in which every closed contour in that region encloses only the points contained in it. If a region is not simply connected, it is called multiply connected. As an example of a multiply connected region, consider the z-plane with the interior of the unit circle **excluded**.

[7] Recall that in Section 1.12 such a function $f(z)$, identified as a force, was labeled conservative.

For the first integral in the last part of Eq. (6.38), let $u = V_x$ and $v = -V_y$.[8] Then

$$\oint_C (u\,dx - v\,dy) = \oint_C (V_x\,dx + V_y\,dy)$$
$$= \int_A \left(\frac{\partial V_y}{\partial x} - \frac{\partial V_x}{\partial y}\right) dx\,dy = -\int_A \left(\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y}\right) dx\,dy. \tag{6.40}$$

For the second integral on the right side of Eq. (6.38), we let $u = V_y$ and $v = V_x$. Using Stokes's theorem again, we obtain

$$\oint_C (v\,dx + u\,dy) = \int_A \left(\frac{\partial u}{\partial x} - \frac{\partial v}{\partial y}\right) dx\,dy. \tag{6.41}$$

On application of the Cauchy–Riemann conditions that must hold, since $f(z)$ is assumed analytic, each integrand vanishes and

$$\oint f(z)dz = -\int_A \left(\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y}\right) dx\,dy + i\int_A \left(\frac{\partial u}{\partial x} - \frac{\partial v}{\partial y}\right) dx\,dy = 0. \tag{6.42}$$

A consequence of the Cauchy integral theorem is that for analytic functions the line integral is a function only of its end points, independent of the path of integration,

$$\int_{z_1}^{z_2} f(z)dz = F(z_2) - F(z_1) = -\int_{z_2}^{z_1} f(z)dz, \tag{6.43}$$

again exactly like the case of a conservative force (Section 1.12).

In summary, a Cauchy integral around a closed contour $\oint f(z)dz = 0$ when the function $f(z)$ is analytic in the simply connected region whose boundary is the closed path of the integral. The Cauchy integral is a two-dimensional analog of line integrals of conservative forces.

Multiply Connected Regions

The original statement of our theorem demanded a simply connected region. This restriction may easily be relaxed by the creation of a barrier, a contour line. Consider the multiply connected region of Fig. 6.9, in which $f(z)$ is not defined for the interior R'. Cauchy's integral theorem is not valid for the contour C, as shown, but we can construct a contour C' for which the theorem holds. We draw a line from the interior forbidden region R' to the forbidden region exterior to R and then run a new contour C', as shown in Fig. 6.10. The new contour C' through $ABDEFGA$ never crosses the contour line that converts R into a simply connected region. The three-dimensional analog of this technique

[8] In the proof of Stokes's theorem (Section 1.12), V_x and V_y are any two functions (with continuous partial derivatives).

Figure 6.9

A Closed Contour C in a Multiply Connected Region

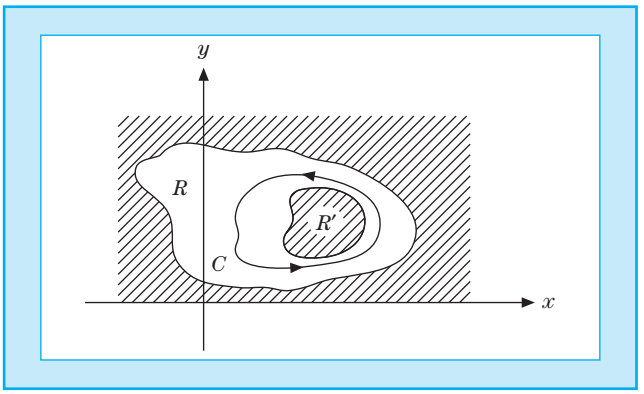
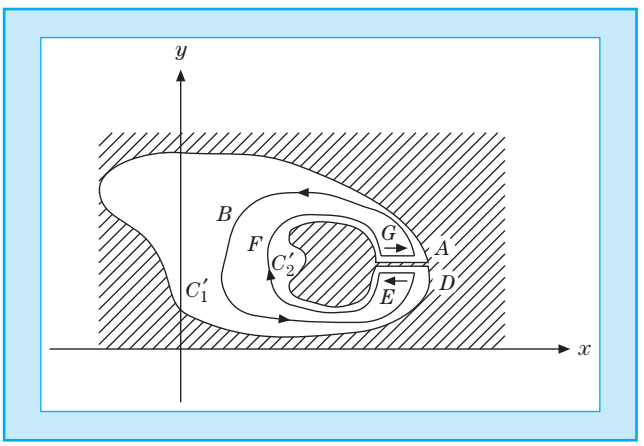


Figure 6.10

Conversion of a Multiply Connected Region into a Simply Connected Region



was used in Section 1.13 to prove Gauss's law. By Eq. (6.43),

$$\int_G^A f(z)dz = -\int_E^D f(z)dz, \tag{6.44}$$

with $f(z)$ having been continuous across the contour line and line segments DE and GA arbitrarily close together. Then

$$\oint_{C'} f(z)dz = \int_{ABD} f(z)dz + \int_{EFG} f(z)dz = 0 \tag{6.45}$$

by Cauchy's integral theorem, with region R now simply connected. Applying Eq. (6.43) once again with $ABD \to C_1'$ and $EFG \to -C_2'$, we obtain

$$\oint_{C_1'} f(z)dz = \oint_{C_2'} f(z)dz, \tag{6.46}$$

in which C_1' and C_2' are both traversed in the same (counterclockwise) direction.

Let us emphasize that the contour line here is a matter of mathematical convenience to permit the application of Cauchy's integral theorem. Since $f(z)$ is analytic in the annular region, it is necessarily single-valued and continuous across any such contour line.

Biographical Data

Cauchy, Augustin Louis, Baron. Cauchy, a French mathematician, was born in 1789 in Paris and died in 1857 in Sceaux, France. In 1805, he entered the Ecole Polytechnique, where Ampère was one of his teachers. In 1816, he replaced Monge in the Académie des Sciences, when Monge was expelled for political reasons. The father of modern complex analysis, his most famous contribution is his integral formula for analytic functions and their derivatives, but he also contributed to partial differential equations and the ether theory in electrodynamics.

EXERCISES

6.3.1 Show that $\int_{z_1}^{z_2} f(z)dz = -\int_{z_2}^{z_1} f(z)dz$.

6.3.2 Prove that

$$\left| \int_C f(z)dz \right| \leq |f|_{\max} \cdot L,$$

where $|f|_{\max}$ is the maximum value of $|f(z)|$ along the contour C and L is the length of the contour.

6.3.3 Verify that

$$\int_{0,0}^{1,1} z^* dz$$

depends on the path by evaluating the integral for the two paths shown in Fig. 6.11. Recall that $f(z) = z^*$ is not an analytic function of z and that Cauchy's integral theorem therefore does not apply.

6.3.4 Show that

$$\oint \frac{dz}{z^2 + z} = 0,$$

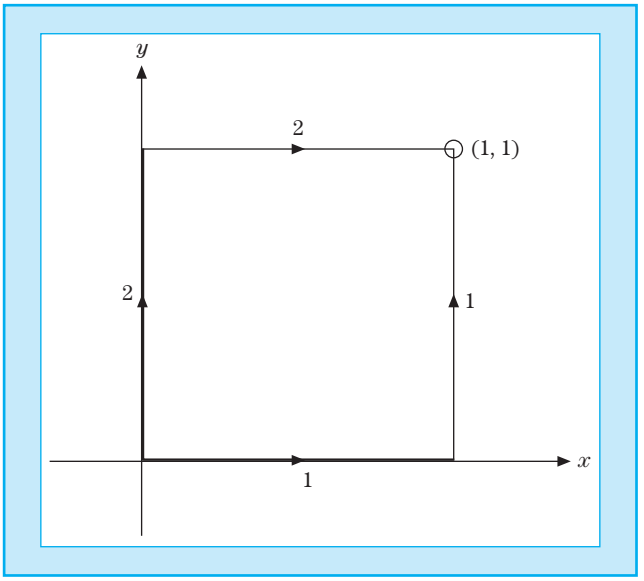
in which the contour C is (i) a circle defined by $|z| = R > 1$ and (ii) a square with the corners $\pm 2 \pm 2i$.

Hint. Direct use of the Cauchy integral theorem is illegal. Why? The integral may be evaluated by transforming to polar coordinates and using tables. The preferred technique is the calculus of residues (Section 7.2). This yields 0 for $R > 1$ and $2\pi i$ for $R < 1$.

6.3.5 Evaluate $\int_0^{2+i} |z|^2 \, dz$ along a straight line from the origin to $2 + i$ and on a second path along the real axis from the origin to 2 continuing from 2

Figure 6.11

Contour



to $2 + i$ parallel to the imaginary axis. Compare with the same integrals where $|z|^2$ is replaced by z^2. Discuss why there is path dependence in one case but not in the other.

6.4 Cauchy's Integral Formula

As in the preceding section, we consider a function $f(z)$ that is analytic on a closed contour C and within the interior region bounded by C. We seek to prove the Cauchy integral formula,

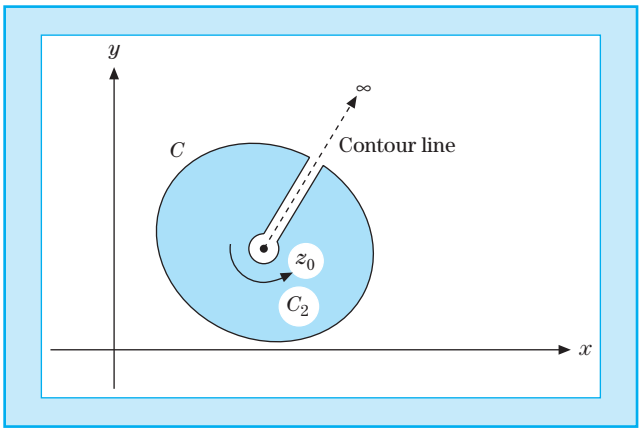
$$\frac{1}{2\pi i}\oint_C \frac{f(z)}{z - z_0}dz = f(z_0), \tag{6.47}$$

in which z_0 is some point in the interior region bounded by C. This is the second of the two basic theorems. Note that since z is on the contour C while z_0 is in the interior, $z - z_0 \neq 0$ and the integral Eq. (6.47) is well defined. Looking at the integrand $\frac{f(z)}{z-z_0}$, we realize that although $f(z)$ is analytic within C, the denominator vanishes at $z = z_0$. If $f(z_0) \neq 0$ and z_0 lies inside C, the **integrand is singular, and this singularity is defined as a first-order or simple pole**. The presence of the pole is essential for Cauchy's formula to hold and in the $n = -1$ case of Example 6.3.1 as well. If the contour is deformed as shown in Fig. 6.12 (or Fig. 6.10, Section 6.3), Cauchy's integral theorem applies. By Eq. (6.46),

$$\oint_C \frac{f(z)}{z - z_0}dz - \oint_{C_2} \frac{f(z)}{z - z_0}dz = 0, \tag{6.48}$$

Figure 6.12

Exclusion of a Singular Point



where C is the original outer contour and C_2 is the circle surrounding the point z_0 traversed in a **counterclockwise** direction. Let $z = z_0 + re^{i\theta}$, using the polar representation because of the circular shape of the path around z_0. Here, r is small and will eventually be made to approach zero. We have

$$\oint_{C_2} \frac{f(z)}{z - z_0} dz = \oint_{C_2} \frac{f(z_0 + re^{i\theta})}{re^{i\theta}} rie^{i\theta} d\theta.$$

Taking the limit as $r \to 0$, we obtain

$$\oint_{C_2} \frac{f(z)}{z - z_0} dz = if(z_0) \int_{C_2} d\theta = 2\pi i f(z_0) \tag{6.49}$$

since $f(z)$ is analytic and therefore continuous at $z = z_0$. This proves the Cauchy integral formula [Eq. (6.47)].

Here is a remarkable result. The value of an analytic function $f(z)$ is given at an interior point $z = z_0$ once the values on the boundary C are specified. This is closely analogous to a two-dimensional form of Gauss's law (Section 1.13) in which the magnitude of an interior line charge would be given in terms of the cylindrical surface integral of the electric field **E**. A further analogy is the determination of a function in real space by an integral of the function and the corresponding Green's function (and their derivatives) over the bounding surface. Kirchhoff diffraction theory is an example of this.

It has been emphasized that z_0 is an interior point. What happens if z_0 is exterior to C? In this case, the entire integrand is analytic on and within C. Cauchy's integral theorem (Section 6.3) applies and the integral vanishes. We have

$$\frac{1}{2\pi i} \oint_C \frac{f(z)dz}{z - z_0} = \begin{cases} f(z_0), & z_0 \quad \text{interior} \\ 0, & z_0 \quad \text{exterior.} \end{cases}$$

Derivatives

Cauchy's integral formula may be used to obtain an expression for the derivative of $f(z)$. From Eq. (6.47), with $f(z)$ analytic,

$$\frac{f(z_0+\delta z_0)-f(z_0)}{\delta z_0}=\frac{1}{2\pi i\delta z_0}\left(\oint\frac{f(z)}{z-z_0-\delta z_0}dz-\oint\frac{f(z)}{z-z_0}dz\right).$$

Then, by definition of derivative [Eq. (6.22)],

$$\begin{aligned}f'(z_0)&=\lim_{\delta z_0\to 0}\frac{1}{2\pi i\delta z_0}\oint\frac{\delta z_0 f(z)}{(z-z_0-\delta z_0)(z-z_0)}dz\\&=\frac{1}{2\pi i}\oint\frac{f(z)}{(z-z_0)^2}dz.\end{aligned}\tag{6.50}$$

This result could have been obtained by differentiating Eq. (6.47) under the integral sign with respect to z_0. This formal or turning-the-crank approach is valid, but the justification for it is contained in the preceding analysis. Again, the integrand $f(z)/(z-z_0)^2$ is singular at $z=z_0$ if $f(z_0)\neq 0$, and **this singularity is defined to be a second-order pole**.

This technique for constructing derivatives may be repeated. We write $f'(z_0+\delta z_0)$ and $f'(z_0)$ using Eq. (6.50). Subtracting, dividing by δz_0, and finally taking the limit as $\delta z_0\to 0$, we have

$$f^{(2)}(z_0)=\frac{2}{2\pi i}\oint\frac{f(z)dz}{(z-z_0)^3}.$$

Note that $f^{(2)}(z_0)$ is independent of the direction of δz_0 as it must be. If $f(z_0)\neq 0$, then $f(z)/(z-z_0)^3$ has **a singularity, which is defined to be a third-order pole**. Continuing, we get[9]

$$f^{(n)}(z_0)=\frac{n!}{2\pi i}\oint\frac{f(z)dz}{(z-z_0)^{n+1}};\tag{6.51}$$

that is, the requirement that $f(z)$ be analytic guarantees not only a first derivative but also derivatives of **all** orders. Note that **the integrand has a pole of order** $n+1$ at $z=z_0$ if $f(z_0)\neq 0$. The derivatives of $f(z)$ are automatically analytic. Notice that this statement assumes the Goursat version of the Cauchy integral theorem [assuming $f'(z)$ exists but need not be assumed to be continuous; for a proof, see 5th ed. of Arfken and Weber's *Math. Methods*]. This is also why Goursat's contribution is so significant in the development of the theory of complex variables.

Morera's Theorem

A further application of Cauchy's integral formula is in the proof of Morera's theorem, which is the converse of Cauchy's integral theorem. The theorem states the following:

[9]This expression is the starting point for defining derivatives of **fractional order**. See Erdelyi, A. (Ed.) (1954). *Tables of Integral Transforms*, Vol. 2. McGraw-Hill, New York. For recent applications to mathematical analysis, see Osler, T. J. (1972). An integral analogue of Taylor's series and its use in computing Fourier transforms. *Math. Comput.* **26**, 449.

If a function $f(z)$ is continuous in a simply connected region R and $\oint_C f(z)\,dz = 0$ for every closed contour C within R, then $f(z)$ is analytic throughout R.

Let us integrate $f(z)$ from z_1 to z_2. Since every closed path integral of $f(z)$ vanishes, the integral is independent of path and depends only on its end points. We label the result of the integration $F(z)$, with

$$F(z_2) - F(z_1) = \int_{z_1}^{z_2} f(z)dz. \tag{6.52}$$

As an identity,

$$\frac{F(z_2) - F(z_1)}{z_2 - z_1} - f(z_1) = \frac{\int_{z_1}^{z_2} [f(t) - f(z_1)]dt}{z_2 - z_1}, \tag{6.53}$$

using t as another complex variable. Now we take the limit as $z_2 \to z_1$:

$$\lim_{z_2 \to z_1} \frac{\int_{z_1}^{z_2} [f(t) - f(z_1)]dt}{z_2 - z_1} = 0 \tag{6.54}$$

since $f(t)$ is continuous.[10] Therefore,

$$\lim_{z_2 \to z_1} \frac{F(z_2) - F(z_1)}{z_2 - z_1} = F'(z)|_{z=z_1} = f(z_1) \tag{6.55}$$

by definition of derivative [Eq. (6.22)]. We have proved that $F'(z)$ at $z = z_1$ exists and equals $f(z_1)$. Since z_1 is any point in R, we see that $F(z)$ is analytic. Then by Cauchy's integral formula [compare Eq. (6.51)] $F'(z) = f(z)$ is also analytic, proving Morera's theorem.

Drawing once more on our electrostatic analog, we might use $f(z)$ to represent the electrostatic field $\mathbf{E}$. If the net charge within every closed region in R is zero (Gauss's law), the charge density is everywhere zero in R. Alternatively, in terms of the analysis of Section 1.12, $f(z)$ represents a conservative force (by definition of conservative), and then we find that it is always possible to express it as the derivative of a potential function $F(z)$.

An important application of Cauchy's integral formula is the following Cauchy inequality. If $f(z) = \sum a_n z^n$ is analytic and bounded, $|f(z)| \le M$ on a circle of radius r about the origin, then

$$|a_n| r^n \le M \qquad \textbf{(Cauchy's inequality)} \tag{6.56}$$

gives upper bounds for the coefficients of its Taylor expansion. To prove Eq. (6.56), let us define $M(r) = \max_{|z|=r} |f(z)|$ and use the Cauchy integral for a_n:

$$|a_n| = \frac{1}{2\pi} \left| \int_{|z|=r} \frac{f(z)}{z^{n+1}} dz \right| \le M(r) \frac{2\pi r}{2\pi r^{n+1}}.$$

[10] We can quote the mean value theorem of calculus here.

An immediate consequence of the inequality (6.56) is **Liouville's theorem**:

> If $f(z)$ is analytic and bounded in the complex plane, it is a constant.

In fact, if $|f(z)| \leq M$ for all z, then Cauchy's inequality [Eq. (6.56)] gives $|a_n| \leq Mr^{-n} \to 0$ as $r \to \infty$ for $n > 0$. Hence, $f(z) = a_0$.

Conversely, the slightest deviation of an analytic function from a constant value implies that there must be at least one singularity somewhere in the infinite complex plane. Apart from the trivial constant functions, then, singularities are a fact of life, and we must learn to live with them. However, we shall do more than that. We shall next expand a function in a Laurent series at a singularity, and we shall use singularities to develop the powerful and useful calculus of residues in Chapter 7.

A famous application of Liouville's theorem yields the **fundamental theorem of algebra** (due to C. F. Gauss), which states that any polynomial $P(z) = \sum_{\nu=0}^{n} a_\nu z^\nu$ with $n > 0$ and $a_n \neq 0$ has n roots. To prove this, suppose $P(z)$ has no zero. Then $f(z) = 1/P(z)$ is analytic and bounded as $|z| \to \infty$. Hence, $f(z) = 1/P$ is a constant by Liouville's theorem—a contradiction. Thus, $P(z)$ has at least one root that we can divide out. Then we repeat the process for the resulting polynomial of degree $n - 1$. This leads to the conclusion that $P(z)$ has exactly n roots.

SUMMARY

In summary, if an analytic function $f(z)$ is given on the boundary C of a simply connected region R, then the values of the function and all its derivatives are known at any point inside that region R in terms of Cauchy integrals

$$f(z_0) = \frac{1}{2\pi i} \oint_C \frac{f(z)dz}{z - z_0}, \qquad f^{(n)}(z_0) = \frac{n!}{2\pi i} \oint_C \frac{f(z)dz}{(z - z_0)^{n+1}}.$$

These Cauchy integrals are extremely important in numerous physics applications.

EXERCISES

6.4.1 Show that

$$\frac{1}{2\pi i} \oint z^{m-n-1} dz, \quad m \text{ and } n \text{ integers}$$

(with the contour encircling the origin once counterclockwise) is a representation of the Kronecker δ_{mn}.

6.4.2 Solve Exercise 6.3.4 by separating the integrand into partial fractions and then applying Cauchy's integral theorem for multiply connected regions. *Note.* Partial fractions are explained in Section 15.7 in connection with Laplace transforms.

6.4.3 Evaluate

$$\oint_C \frac{dz}{z^2-1},$$

where C is the circle $|z| = 2$. Alternatively, integrate around a square with corners $\pm 2 \pm 2i$.

6.4.4 Assuming that $f(z)$ is analytic on and within a closed contour C and that the point z_0 is within C, show that

$$\oint_C \frac{f'(z)}{z-z_0}dz = \oint_C \frac{f(z)}{(z-z_0)^2}dz.$$

6.4.5 You know that $f(z)$ is analytic on and within a closed contour C. You suspect that the nth derivative $f^{(n)}(z_0)$ is given by

$$f^{(n)}(z_0) = \frac{n!}{2\pi i}\oint_C \frac{f(z)}{(z-z_0)^{n+1}}dz.$$

Using mathematical induction, prove that this expression is correct.

6.4.6 (a) A function $f(z)$ is analytic within a closed contour C (and continuous on C). If $f(z) \neq 0$ within C and $|f(z)| \leq M$ on C, show that

$$|f(z)| \leq M$$

for all points within C.
Hint. Consider $w(z) = 1/f(z)$.

(b) If $f(z) = 0$ within the contour C, show that the foregoing result does not hold—that it is possible to have $|f(z)| = 0$ at one or more points in the interior with $|f(z)| > 0$ over the entire bounding contour. Cite a specific example of an analytic function that behaves this way.

6.4.7 Using the Cauchy integral formula for the nth derivative, convert the following Rodrigues's formulas into Cauchy integrals with appropriate contours:

(a) Legendre

$$P_n(x) = \frac{1}{2^n n!}\frac{d^n}{dx^n}(x^2-1)^n.$$

ANS. $$\frac{(-1)^n}{2^n}\cdot\frac{1}{2\pi i}\oint \frac{(1-z^2)^n}{(z-x)^{n+1}}dz.$$

(b) Hermite

$$H_n(x) = (-1)^n e^{x^2}\frac{d^n}{dx^n}e^{-x^2}.$$

(c) Laguerre

$$L_n(x) = \frac{e^x}{n!}\frac{d^n}{dx^n}(x^n e^{-x}).$$

Note. From these integral representations one can develop generating functions for these special functions. Compare Sections 11.4, 13.1, and 13.2.

6.4.8 Obtain $\oint_C z^* dz$, where C is the unit circle in the first quadrant. Compare with the integral from $z = 1$ parallel to the imaginary axis to $1 + i$ and from there to i parallel to the real axis.

6.4.9 Evaluate $\int_{2\pi}^{2\pi+i\infty} e^{iz} dz$ along two different paths of your choice.

6.5 Laurent Expansion

Taylor Expansion

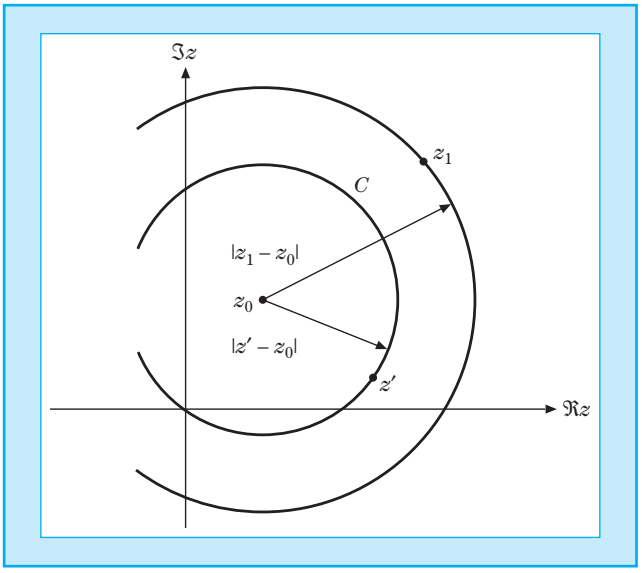
The Cauchy integral formula of the preceding section opens up the way for another derivation of Taylor's series (Section 5.6), but this time for functions of a complex variable. Suppose we are trying to expand $f(z)$ about $z = z_0$ and we have $z = z_1$ as the nearest point on the Argand diagram for which $f(z)$ is not analytic. We construct a circle C centered at $z = z_0$ with radius $|z' - z_0| < |z_1 - z_0|$ (Fig. 6.13). Since z_1 was assumed to be the nearest point at which $f(z)$ was not analytic, $f(z)$ is necessarily analytic on and within C.

From Eq. (6.47), the Cauchy integral formula,

$$\begin{aligned} f(z) &= \frac{1}{2\pi i} \oint_C \frac{f(z')dz'}{z' - z} \\ &= \frac{1}{2\pi i} \oint_C \frac{f(z')dz'}{(z' - z_0) - (z - z_0)} \\ &= \frac{1}{2\pi i} \oint_C \frac{f(z')dz'}{(z' - z_0)[1 - (z - z_0)/(z' - z_0)]}, \end{aligned} \tag{6.57}$$

Figure 6.13

Circular Domain for Taylor Expansion



where z' is a point on the contour C and z is any point interior to C. We expand the denominator of the integrand in Eq. (6.57) by the binomial theorem, which generalizes to complex variables as in Example 6.2.1 for other elementary functions. Or, we note the identity (for complex t)

$$\frac{1}{1-t} = 1 + t + t^2 + t^3 + \cdots = \sum_{n=0}^{\infty} t^n, \tag{6.58}$$

which may easily be verified by multiplying both sides by $1 - t$. The infinite series, following the methods of Section 5.2, is convergent for $|t| < 1$. Upon replacing the positive terms a_n in a real series by absolute values $|a_n|$ of complex numbers, the convergence criteria of Chapter 5 translate into valid convergence theorems for complex series.

Now for a point z interior to C, $|z - z_0| < |z' - z_0|$, and using Eq. (6.58), Eq. (6.57) becomes

$$f(z) = \frac{1}{2\pi i} \oint_C \sum_{n=0}^{\infty} \frac{(z - z_0)^n f(z')dz'}{(z' - z_0)^{n+1}}. \tag{6.59}$$

Interchanging the order of integration and summation [valid since Eq. (6.58) is uniformly convergent for $|t| < 1$], we obtain

$$f(z) = \frac{1}{2\pi i} \sum_{n=0}^{\infty} (z - z_0)^n \oint_C \frac{f(z')dz'}{(z' - z_0)^{n+1}}. \tag{6.60}$$

Referring to Eq. (6.51), we get

$$f(z) = \sum_{n=0}^{\infty} (z - z_0)^n \frac{f^{(n)}(z_0)}{n!}, \tag{6.61}$$

which is our desired Taylor expansion. Note that it is based only on the assumption that $f(z)$ is analytic for $|z - z_0| < |z_1 - z_0|$. Just as for real variable power series (Section 5.7), this expansion is unique for a given z_0.

From the Taylor expansion for $f(z)$ a binomial theorem may be derived (Exercise 6.5.2).

Schwarz Reflection Principle

From the binomial expansion of $g(z) = (z - x_0)^n$ for integral n we see that the complex conjugate of the function is the function of the complex conjugate, for real x_0

$$g^*(z) = (z - x_0)^{n*} = (z^* - x_0)^n = g(z^*). \tag{6.62}$$

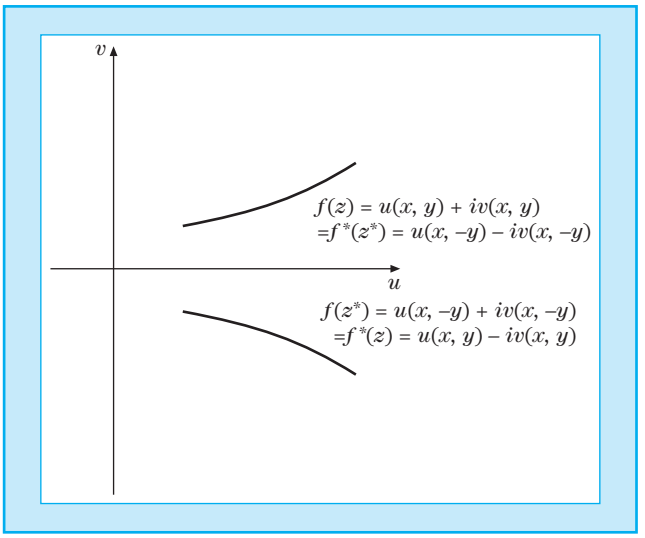
This leads us to the Schwarz reflection principle:

If a function $f(z)$ is (1) analytic over some region including the real axis and (2) real when z is real, then

$$f^*(z) = f(z^*). \tag{6.63}$$

Figure 6.14

Schwarz Reflection



(Fig. 6.14). It may be proved as follows. Expanding $f(z)$ about some (nonsingular) point x_0 on the real axis,

$$f(z) = \sum_{n=0}^{\infty} (z - x_0)^n \frac{f^{(n)}(x_0)}{n!} \tag{6.64}$$

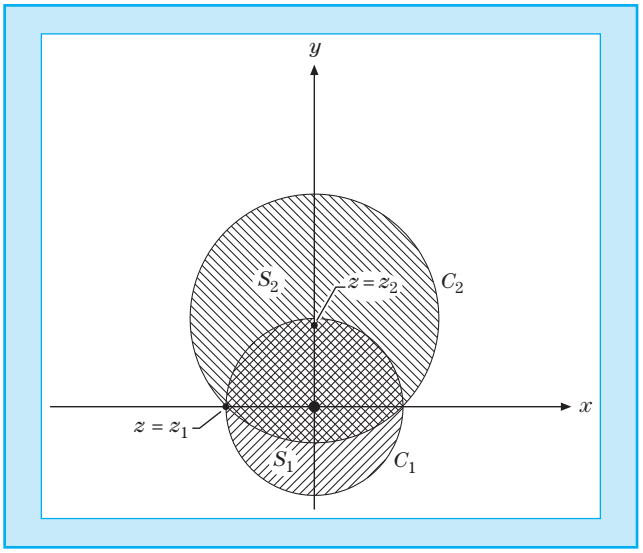
by Eq. (6.60). Since $f(z)$ is analytic at $z = x_0$, this Taylor expansion exists. Since $f(z)$ is real when z is real, $f^{(n)}(x_0)$ must be real for all n. Then when we use Eq. (6.62), Eq. (6.63) (the Schwarz reflection principle) follows immediately. Exercise 6.5.6 is another form of this principle. The Schwarz reflection principle applies to all elementary functions and those in Example 6.2.1 in particular.

Analytic Continuation

It is natural to think of the values $f(z)$ of an analytic function f as a single entity that is usually defined in some restricted region S_1 of the complex plane, for example, by a Taylor series (Fig. 6.15). Then f is analytic inside the **circle of convergence** C_1, whose radius is given by the distance r_1 from the center of C_1 to the **nearest singularity** of f at z_1 (in Fig. 6.15). If we choose a point inside C_1 that is farther than r_1 from the singularity z_1 and make a Taylor expansion of f about it (z_2 in Fig. 6.15), then the circle of convergence C_2 will usually extend beyond the first circle C_1. In the overlap region of both circles C_1, C_2 the function f is uniquely defined. In the region of the circle C_2 that extends beyond C_1, $f(z)$ is uniquely defined by the Taylor series about the center of C_2 and analytic there, although the Taylor series about the center of C_1 is no longer convergent there. After Weierstrass, this process is called **analytic continuation**. It defines the analytic functions in terms of its original definition (e.g., in C_1) and all its continuations.

Figure 6.15

Analytic Continuation



A specific example is the **meromorphic** function

$$f(z) = \frac{1}{1+z}, \tag{6.65}$$

which has a simple pole at $z = -1$ and is analytic elsewhere. The geometric series expansion

$$\frac{1}{1+z} = 1 - z + z^2 + \cdots = \sum_{n=0}^{\infty} (-z)^n \tag{6.66}$$

converges for $|z| < 1$ (i.e., inside the circle C_1 in Fig. 6.15).

Suppose we expand $f(z)$ about $z = i$ so that

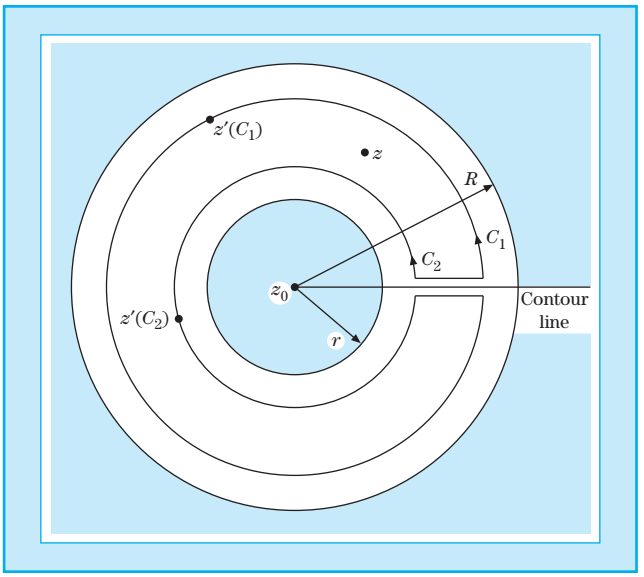
$$\begin{aligned} f(z) = \frac{1}{1+z} &= \frac{1}{1+i+(z-i)} = \frac{1}{(1+i)(1+(z-i)/(1+i))} \\ &= \left[1 - \frac{z-i}{1+i} + \frac{(z-i)^2}{(1+i)^2} - \cdots\right] \frac{1}{1+i} \end{aligned} \tag{6.67}$$

converges for $|z - i| < |1 + i| = \sqrt{2}$. Our circle of convergence is C_2 in Fig. 6.15. Now $f(z)$ is defined by the expansion [Eq. (6.67)] in S_2 that overlaps S_1 and extends further out in the complex plane.[11] This extension is an analytic

[11] One of the most powerful and beautiful results of the more abstract theory of functions of a complex variable is that if two analytic functions coincide in any region, such as the overlap of S_1 and S_2, or coincide on any line segment, they are the same function in the sense that they will coincide everywhere as long as they are both well defined. In this case, the agreement of the expansions [Eqs. (6.66) and (6.67)] over the region common to S_1 and S_2 would establish the identity of the functions these expansions represent. Then Eq. (6.67) would represent an analytic continuation or extension of $f(z)$ into regions not covered by Eq. (6.66). We could equally well say that $f(z) = 1/(1+z)$ is an analytic continuation of either of the series given by Eqs. (6.66) and (6.67).

Figure 6.16

$|z' - z_0|_{C_1} > |z - z_0|$; $|z' - z_0|_{C_2} < |z - z_0|$



continuation, and when we have only isolated singular points to contend with, the function can be extended indefinitely. Equations (6.65)–(6.67) are three different representations of the same function. Each representation has its own domain of convergence. Equation (6.66) is a Maclaurin series. Equation (6.67) is a Taylor expansion about $z = i$.

Analytic continuation may take many forms and the series expansion just considered is not necessarily the most convenient technique. As an alternate technique we shall use a recurrence relation in Section 10.1 to extend the factorial function around the isolated singular points, $z = -n$, $n = 1, 2, 3, \ldots$.

Laurent Series

We frequently encounter functions that are analytic in an annular region, for example, of inner radius r and outer radius R, as shown in Fig. 6.16. Drawing an imaginary contour line to convert our region into a simply connected region, we apply Cauchy's integral formula, and for two circles, C_2 and C_1, centered at $z = z_0$ and with radii r_2 and r_1, respectively, where $r < r_2 < r_1 < R$, we have[12]

$$f(z) = \frac{1}{2\pi i}\oint_{C_1} \frac{f(z')dz'}{z' - z} - \frac{1}{2\pi i}\oint_{C_2} \frac{f(z')dz'}{z' - z}. \tag{6.68}$$

Note that in Eq. (6.68) an explicit minus sign has been introduced so that contour C_2 (like C_1) is to be traversed in the positive (counterclockwise) sense. The treatment of Eq. (6.68) now proceeds exactly like that of Eq. (6.57) in the development of the Taylor series. Each denominator is written as $(z' - z_0) - (z - z_0)$

[12] We may take r_2 arbitrarily close to r and r_1 arbitrarily close to R, maximizing the area enclosed between C_1 and C_2.

and expanded by the binomial theorem, which now follows from the Taylor series [Eq. (6.61)].

Noting that for C_1, $|z'-z_0| > |z-z_0|$, whereas for C_2, $|z'-z_0| < |z-z_0|$, we find

$$f(z) = \frac{1}{2\pi i}\sum_{n=0}^{\infty}(z-z_0)^n \oint_{C_1} \frac{f(z')dz'}{(z'-z_0)^{n+1}} + \frac{1}{2\pi i}\sum_{n=1}^{\infty}(z-z_0)^{-n} \oint_{C_2} (z'-z_0)^{n-1} f(z')dz'. \tag{6.69}$$

The minus sign of Eq. (6.68) has been absorbed by the binomial expansion. Labeling the first series S_1 and the second S_2,

$$S_1 = \frac{1}{2\pi i}\sum_{n=0}^{\infty}(z-z_0)^n \oint_{C_1} \frac{f(z')dz'}{(z'-z_0)^{n+1}}, \tag{6.70}$$

which is the regular Taylor expansion, convergent for $|z-z_0| < |z'-z_0| = r_1$, that is, for all z **interior** to the larger circle, C_1. For the second series in Eq. (6.68), we have

$$S_2 = \frac{1}{2\pi i}\sum_{n=1}^{\infty}(z-z_0)^{-n} \oint_{C_2} (z'-z_0)^{n-1} f(z')dz' \tag{6.71}$$

convergent for $|z-z_0| > |z'-z_0| = r_2$, that is, for all z **exterior** to the smaller circle C_2. Remember, C_2 goes counterclockwise.

These two series are combined into one series[13] (a Laurent series) by

$$f(z) = \sum_{n=-\infty}^{\infty} a_n (z-z_0)^n, \tag{6.72}$$

where

$$a_n = \frac{1}{2\pi i}\oint_C \frac{f(z)dz}{(z-z_0)^{n+1}}. \tag{6.73}$$

Since, in Eq. (6.72), convergence of a binomial expansion is no problem, C may be any contour within the annular region $r < |z-z_0| < R$ encircling z_0 once in a counterclockwise sense. The integrals are independent of the contour, and Eq. (6.72) is the **Laurent series or Laurent expansion of** $f(z)$.

The use of the contour line (Fig. 6.16) is convenient in converting the annular region into a simply connected region. Since our function is analytic in this annular region (and therefore single-valued), the contour line is not essential and, indeed, does not appear in the final result [Eq. (6.72)]. For $n \geq 0$, the integrand $f(z)/(z-z_0)^{n+1}$ is singular at $z = z_0$ if $f(z_0) \neq 0$. The integrand has a pole of order $n+1$ at $z = z_0$. If f has a first-order zero at $z = z_0$, then $f(z)/(z-z_0)^{n+1}$ has a pole of order n, etc. The presence of poles is essential for the validity of the Laurent formula.

[13] Replace n by $-n$ in S_2 and add.

Laurent series coefficients need not come from evaluation of contour integrals (which may be very intractable). Other techniques such as ordinary series expansions often provide the coefficients.

Numerous examples of Laurent series appear in Chapter 7. We start here with a simple example to illustrate the application of Eq. (6.72).

EXAMPLE 6.5.1

Laurent Expansion by Integrals Let $f(z) = [z(z-1)]^{-1}$. If we choose $z_0 = 0$, then $r = 0$ and $R = 1$, $f(z)$ diverging at $z = 1$. From Eqs. (6.73) and (6.72),

$$a_n = \frac{1}{2\pi i}\oint \frac{dz'}{(z')^{n+2}(z'-1)}$$
$$= \frac{-1}{2\pi i}\oint \sum_{m=0}^{\infty}(z')^m \frac{dz'}{(z')^{n+2}}. \tag{6.74}$$

Again, interchanging the order of summation and integration (uniformly convergent series), we have

$$a_n = -\frac{1}{2\pi i}\sum_{m=0}^{\infty}\oint \frac{dz'}{(z')^{n+2-m}}. \tag{6.75}$$

If we employ the polar form, as before Eq. (6.35) (of Example 6.3.1),

$$a_n = -\frac{1}{2\pi i}\sum_{m=0}^{\infty}\oint \frac{rie^{i\theta}d\theta}{r^{n+2-m}e^{i(n+2-m)\theta}}$$
$$= -\frac{1}{2\pi i}\cdot 2\pi i\sum_{m=0}^{\infty}\delta_{n+2-m,1}. \tag{6.76}$$

In other words,

$$a_n = \begin{cases} -1 & \text{for } n \geq -1, \\ 0 & \text{for } n < -1. \end{cases} \tag{6.77}$$

The Laurent expansion about $z = 0$ [Eq. (6.72)] becomes

$$\frac{1}{z(z-1)} = -\frac{1}{z} - 1 - z - z^2 - z^3 - \cdots = -\sum_{n=-1}^{\infty} z^n. \tag{6.78}$$

For this simple function the Laurent series can, of course, be obtained by a direct binomial expansion or partial fraction and geometric series expansion as follows. We expand in partial fractions

$$f(z) = \frac{1}{z(z-1)} = \frac{b_0}{z} + \frac{b_1}{z-1},$$

where we determine b_0 at $z \to 0$,

$$\lim_{z\to 0} zf(z) = \lim_{z\to 0}\frac{1}{z-1} = -1 = b_0 + \lim_{z\to 0}\frac{b_1 z}{z-1} = b_0,$$

and b_1 at $z \to 1$ similarly,

$$\lim_{z\to 1}(z-1)f(z) = \lim_{z\to 1}\frac{1}{z} = 1 = b_1 + \lim_{z\to 1}\frac{b_0(z-1)}{z} = b_1.$$

Expanding $1/(z-1)$ in a geometric series yields the Laurent series [Eq. (6.78)]. ■

The Laurent series differs from the Taylor series by the obvious feature of negative powers of $(z - z_0)$. For this reason, the Laurent series will always diverge at least at $z = z_0$ and perhaps as far out as some distance r (Fig. 6.16).

EXAMPLE 6.5.2

Laurent Expansion by Series Expand $f(z) = \exp(z)\exp(1/z)$ in a Laurent series $f(z) = \sum_n a_n z^n$ about the origin.

This function is analytic in the complex plane except at $z = 0$ and $z \to \infty$. Moreover, $f(1/z) = f(z)$, so that $a_{-n} = a_n$. Multiplying the power series

$$e^z e^{\frac{1}{z}} = \sum_{m=0}^{\infty}\frac{z^m}{m!}\sum_{n=0}^{\infty}\frac{1}{z^n n!},$$

we get the constant term a_0 from the products of the $m = n$ terms as

$$a_0 = \sum_{m=0}^{\infty}\frac{1}{(m!)^2}.$$

The coefficient of z^k comes from the products of the terms $\frac{z^{m+k}}{(m+k)!}$ and $\frac{1}{z^m m!}$; that is,

$$a_k = a_{-k} = \sum_{m=0}^{\infty}\frac{1}{m!(m+k)!}.$$

From the ratio test or the absence of singularities in the finite complex plane for $z \neq 0$, this Laurent series converges for $|z| > 0$. ■

Biographical Data

Laurent, Pierre-Alphonse. Laurent, a French mathematician, was born in 1813 and died in 1854. He contributed to complex analysis, his famous theorem being published in 1843.

SUMMARY

The Taylor expansion of an analytic function about a regular point follows from Cauchy's integral formulas. The radius of convergence of a Taylor series around a regular point is given by its distance to the nearest singularity. An analytic function can be expanded in a power series with positive and negative (integer) exponents about an arbitrary point, which is called its Laurent series; it converges in an annular region around a singular point and becomes its Taylor series around a regular point. If there are infinitely many negative exponents in its Laurent series the function has an essential singularity; if the Laurent series breaks off with a finite negative exponent it has a pole of that order at the expansion point. Analytic continuation of an analytic function from some

neighborhood of a regular point to its natural domain by means of successive Taylor or Laurent series, an integral representation, or functional equation is a concept unique to the theory of analytic functions that highlights its power.

EXERCISES

6.5.1 Develop the Taylor expansion of $\ln(1+z)$.

ANS. $\displaystyle\sum_{n=1}^{\infty}(-1)^{n-1}\frac{z^n}{n}$.

6.5.2 Derive the binomial expansion

$$(1+z)^m = 1 + mz + \frac{m(m-1)}{1\cdot 2}z^2 + \cdots = \sum_{n=0}^{\infty}\binom{m}{n}z^n$$

for m any real number. The expansion is convergent for $|z| < 1$.

6.5.3 A function $f(z)$ is analytic on and within the unit circle. Also, $|f(z)| < 1$ for $|z| \le 1$ and $f(0) = 0$. Show that $|f(z)| < |z|$ for $|z| \le 1$.
Hint. One approach is to show that $f(z)/z$ is analytic and then express $[f(z_0)/z_0]^n$ by the Cauchy integral formula. Finally, consider absolute magnitudes and take the nth root. This exercise is sometimes called **Schwarz's theorem**.

6.5.4 If $f(z)$ is a real function of the complex variable $z = x + iy$ [i.e., $f(x) = f^*(x)$], and the Laurent expansion about the origin, $f(z) = \sum a_n z^n$, has $a_n = 0$ for $n < -N$, show that all of the coefficients, a_n, are real.
Hint. Show that $z^N f(z)$ is analytic (via Morera's theorem; Section 6.4).

6.5.5 A function $f(z) = u(x, y) + iv(x, y)$ satisfies the conditions for the Schwarz reflection principle. Show that
(a) u is an even function of y. (b) v is an odd function of y.

6.5.6 A function $f(z)$ can be expanded in a Laurent series about the origin with the coefficients a_n real. Show that the complex conjugate of this function of z is the same function of the complex conjugate of z; that is,

$$f^*(z) = f(z^*).$$

Verify this explicitly for
(a) $f(z) = z^n$, n an integer, (b) $f(z) = \sin z$.
If $f(z) = iz$, $(a_1 = i)$, show that the foregoing statement does not hold.

6.5.7 The function $f(z)$ is analytic in a domain that includes the real axis. When z is real $(z = x)$, $f(x)$ is pure imaginary.
(a) Show that

$$f(z^*) = -[f(z)]^*.$$

(b) For the specific case $f(z) = iz$, develop the Cartesian forms of $f(z)$, $f(z^*)$, and $f^*(z)$. Do not quote the general result of part (a).

6.5.8 Develop the first three nonzero terms of the Laurent expansion of

$$f(z) = (e^z - 1)^{-1}$$

about the origin.

6.5.9 Prove that the Laurent expansion of a given function about a given point is unique; that is, if

$$f(z) = \sum_{n=-N}^{\infty} a_n (z - z_0)^n = \sum_{n=-N}^{\infty} b_n (z - z_0)^n,$$

show that $a_n = b_n$ for all n.
Hint. Use the Cauchy integral formula.

6.5.10 (a) Develop a Laurent expansion of $f(z) = [z(z-1)]^{-1}$ about the point $z = 1$ valid for small values of $|z - 1|$. Specify the exact range over which your expansion holds. This is an analytic continuation of Eq. (6.78).
(b) Determine the Laurent expansion of $f(z)$ about $z = 1$ but for $|z-1|$ large.
Hint. Use partial fraction of this function and the geometric series.

6.5.11 (a) Given $f_1(z) = \int_0^\infty e^{-zt} dt$ (with t real), show that the domain in which $f_1(z)$ exists (and is analytic) is $\Re(z) > 0$.
(b) Show that $f_2(z) = 1/z$ equals $f_1(z)$ over $\Re(z) > 0$ and is therefore an analytic continuation of $f_1(z)$ over the entire z-plane except for $z = 0$.
(c) Expand $1/z$ about the point $z = i$. You will have $f_3(z) = \sum_{n=0}^{\infty} a_n (z - i)^n$. What is the domain of $f_3(z)$?

ANS. $$\frac{1}{z} = -i \sum_{n=0}^{\infty} i^n (z - i)^n, \quad |z - i| < 1.$$

6.5.12 Expand $f(z) = \sin(\frac{z}{1-z})$ in a Laurent series about $z = 1$.

6.5.13 Expand

$$f(z) = \frac{z^3 - 2z^2 + 1}{(z - 3)(z^2 + 3)}$$

in a Laurent series about (i) $z = 3$, (ii) $z = \pm i\sqrt{3}$, (iii) $z = 1$, and (iv) $z = \frac{1}{2}(1 \pm \sqrt{5})$.

6.5.14 Find the Laurent series of $\ln((1 + z^2)/(1 - z^2))$ at ∞.

6.5.15 Write z in polar form and set up the relations that have to be satisfied for $\ln z = \ln |z| + i \arg z$ and $\ln(1 + z)$ defined by its Maclaurin series to be consistent.

6.6 Mapping

In the preceding sections, we defined analytic functions and developed some of their main features. Now we introduce some of the more geometric aspects of functions of complex variables—aspects that will be useful in visualizing the integral operations in Chapter 7 and that are valuable in their own right in solving Laplace's equation in two-dimensional systems.

In ordinary analytic geometry we may take $y = f(x)$ and then plot y versus x. Our problem here is more complicated because z is a function of two real variables x and y. We use the notation

$$w = f(z) = u(x, y) + iv(x, y). \tag{6.79}$$

Then for a point in the z-plane (specific values for x and y) there may correspond specific values for $u(x, y)$ and $v(x, y)$ that then yield a point in the w-plane. As points in the z-plane transform or are mapped into points in the w-plane, lines or areas in the z-plane will be mapped into lines or areas in the w-plane. Our immediate purpose is to see how lines and areas map from the z-plane to the w-plane for a number of simple functions.

Translation

$$w = z + z_0. \tag{6.80}$$

The function w is equal to the variable z plus a constant, $z_0 = x_0 + iy_0$. By Eqs. (6.2) and (6.80),

$$u = x + x_0, \qquad v = y + y_0, \tag{6.81}$$

representing a pure translation of the coordinate axes as shown in Fig. 6.17.

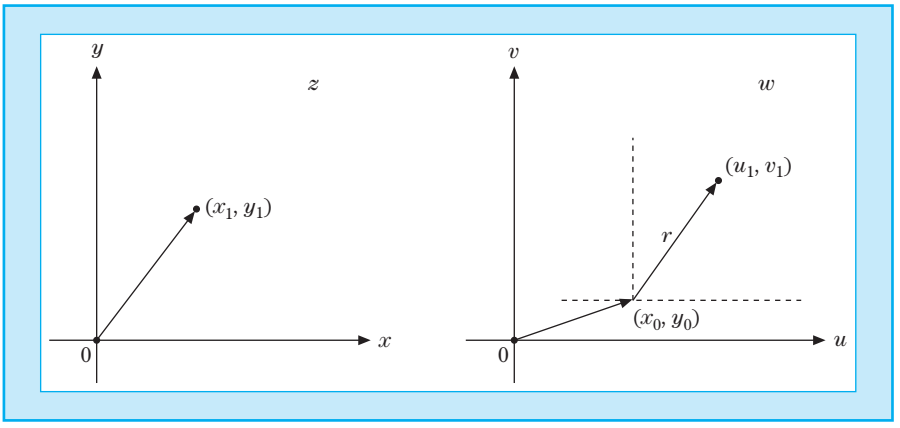
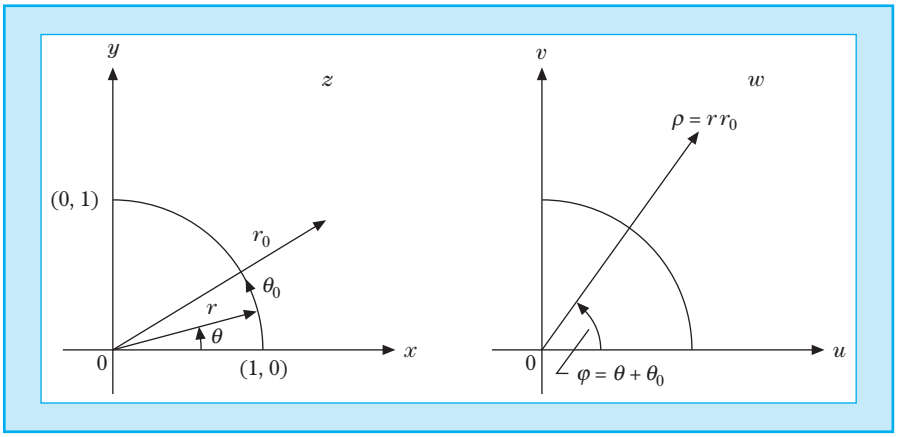


Figure 6.17
Translation

Figure 6.18

Rotation



Rotation

$$w = zz_0. \tag{6.82}$$

Here, it is convenient to return to the polar representation, using

$$w = \rho e^{i\varphi}, \quad z = re^{i\theta}, \quad \text{and} \quad z_0 = r_0 e^{i\theta_0}, \tag{6.83}$$

then

$$\rho e^{i\varphi} = rr_0 e^{i(\theta+\theta_0)} \tag{6.84}$$

or

$$\rho = rr_0, \qquad \varphi = \theta + \theta_0. \tag{6.85}$$

Two things have occurred. First, the modulus r has been modified, either expanded or contracted, by the factor r_0. Second, the argument θ has been increased by the additive constant θ_0 (Fig. 6.18). This represents a rotation of the complex variable through an angle θ_0. For the special case of $z_0 = i$, we have a pure rotation through $\pi/2$ radians.

Inversion

$$w = \frac{1}{z}. \tag{6.86}$$

Again, using the polar form, we have

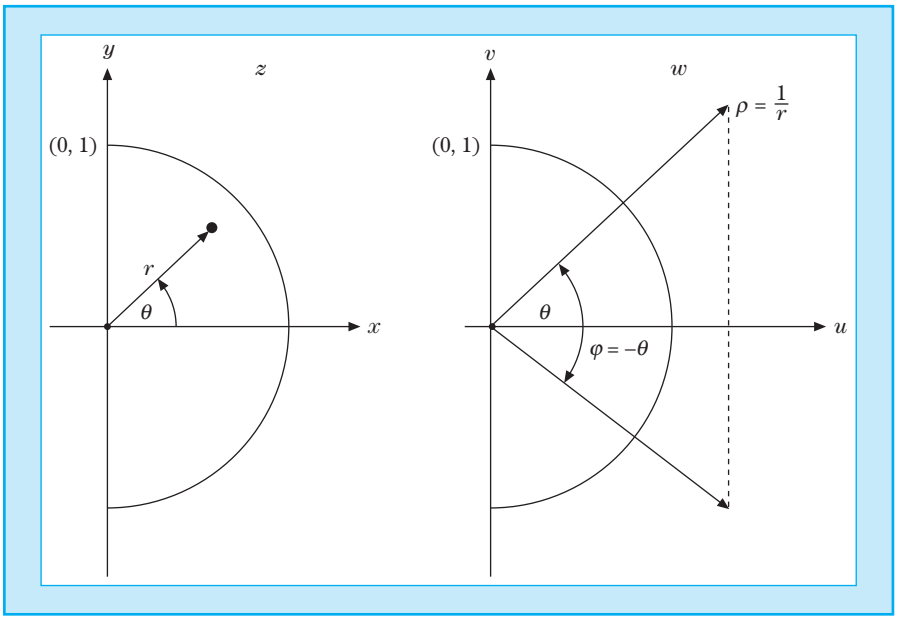
$$\rho e^{i\varphi} = \frac{1}{re^{i\theta}} = \frac{1}{r}e^{-i\theta}, \tag{6.87}$$

which shows that

$$\rho = \frac{1}{r}, \qquad \varphi = -\theta. \tag{6.88}$$

Figure 6.19

Inversion



The radial part of Eq. (6.87) shows that inversion clearly. The interior of the unit circle is mapped onto the exterior and vice versa (Fig. 6.19). In addition, the angular part of Eq. (6.87) shows that the polar angle is reversed in sign. Equation (6.86) therefore also involves a reflection of the y-axis (like the complex conjugate equation).

To see how lines in the z-plane transform into the w-plane, we simply return to the Cartesian form:

$$u + iv = \frac{1}{x + iy}. \tag{6.89}$$

Rationalizing the right-hand side by multiplying numerator and denominator by z^* and then equating the real parts and the imaginary parts, we have

$$\begin{aligned} u &= \frac{x}{x^2 + y^2}, \qquad x = \frac{u}{u^2 + v^2}, \\ v &= -\frac{y}{x^2 + y^2}, \qquad y = -\frac{v}{u^2 + v^2}. \end{aligned} \tag{6.90}$$

A circle centered at the origin in the z-plane has the form

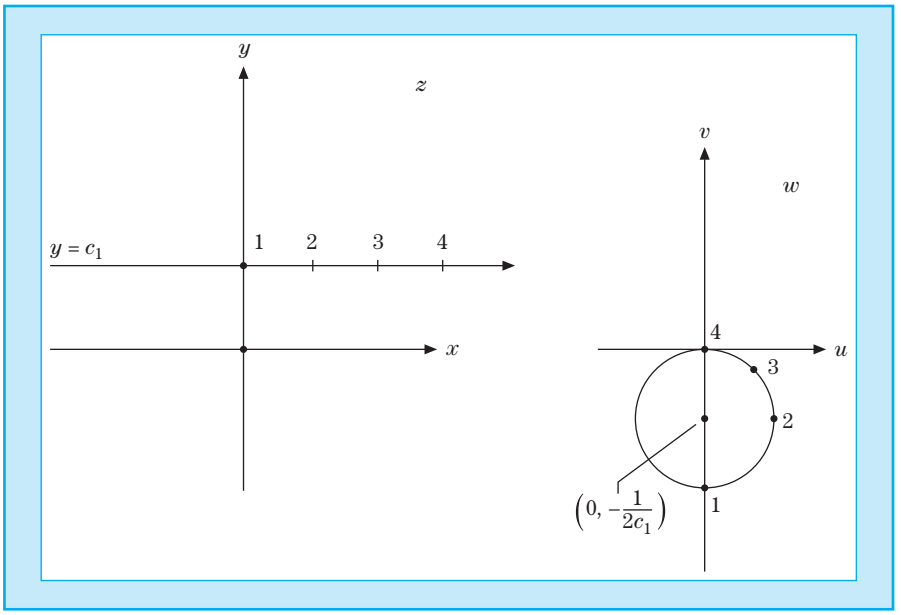
$$x^2 + y^2 = r^2 \tag{6.91}$$

and by Eq. (6.90) transforms into

$$\frac{u^2}{(u^2 + v^2)^2} + \frac{v^2}{(u^2 + v^2)^2} = r^2. \tag{6.92}$$

Figure 6.20

Inversion, Line ↔ Circle



Simplifying Eq. (6.92), we obtain

$$u^2 + v^2 = \frac{1}{r^2} = \rho^2, \tag{6.93}$$

which describes a circle in the w-plane also centered at the origin.

The horizontal line $y = c_1$ transforms into

$$\frac{-v}{u^2 + v^2} = c_1 \tag{6.94}$$

or

$$u^2 + \left(v + \frac{1}{2c_1}\right)^2 = \frac{1}{(2c_1)^2}, \tag{6.95}$$

which describes a circle in the w-plane of radius $(\frac{1}{2})c_1$ and centered at $u = 0$, $v = -\frac{1}{2}c_1$ (Fig. 6.20). We pick up the other three possibilities, $x = \pm c_1$, $y = -c_1$, by rotating the xy-axes. In general, any straight line or circle in the z-plane will transform into a straight line or a circle in the w-plane (compare Exercise 6.6.1).

Branch Points and Multivalent Functions

The three transformations just discussed all involved one-to-one correspondence of points in the z-plane to points in the w-plane. Now to illustrate the variety of transformations that are possible and the problems that can arise, we introduce first a two-to-one correspondence and then a many-to-one correspondence. Finally, we take up the inverses of these two transformations.

Consider first the transformation

$$w = z^2, \tag{6.96}$$

which leads to

$$\rho = r^2, \qquad \varphi = 2\theta. \tag{6.97}$$

Clearly, our transformation is nonlinear because the modulus is squared, but the significant feature of Eq. (6.96) is that the phase angle or argument is doubled. This means that the

- first quadrant of z, $0 \le \theta < \frac{\pi}{2} \rightarrow$ upper half-plane of w, $0 \le \varphi < \pi$,
- upper half-plane of z, $0 \le \theta < \pi \rightarrow$ whole plane of w, $0 \le \varphi < 2\pi$.

The lower half-plane of z maps into the already covered entire plane of w, thus covering the w-plane a second time. This is our two-to-one correspondence: two distinct points in the z-plane, z_0 and $z_0 e^{i\pi} = -z_0$, corresponding to the single point $w = z_0^2$.

In Cartesian representation,

$$u + iv = (x + iy)^2 = x^2 - y^2 + i2xy, \tag{6.98}$$

leading to

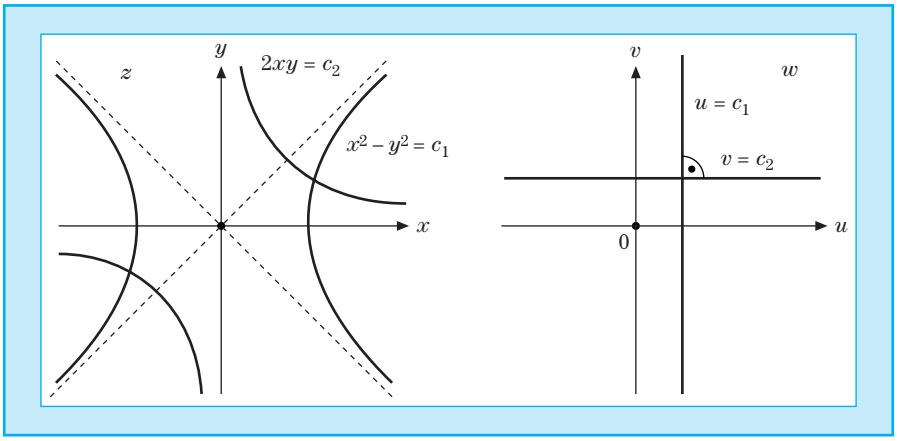
$$u = x^2 - y^2, \qquad v = 2xy. \tag{6.99}$$

Hence, the lines $u = c_1$, $v = c_2$ in the w-plane correspond to $x^2 - y^2 = c_1$, $2xy = c_2$, rectangular (and orthogonal) hyperbolas in the z-plane (Fig. 6.21). To every point on the hyperbola $x^2 - y^2 = c_1$ in the right half-plane, $x > 0$, one point on the line $u = c_1$ corresponds and vice versa. However, every point on the line $u = c_1$ also corresponds to a point on the hyperbola $x^2 - y^2 = c_1$ in the left half-plane, $x < 0$, as already explained.

It will be shown in Section 6.7 that if lines in the w-plane are orthogonal the corresponding lines in the z-plane are also orthogonal, as long as the transformation is analytic. Since $u = c_1$ and $v = c_2$ are constructed perpendicular

Figure 6.21

Mapping—Hyperbolic Coordinates



to each other, the corresponding hyperbolas in the z-plane are orthogonal. We have constructed a new orthogonal system of hyperbolic lines. Exercise 2.3.3 was an analysis of this system. Note that if the hyperbolic lines are electric or magnetic lines of force, then we have a quadrupole lens useful in focusing beams of high-energy particles.

The inverse of the fourth transformation [Eq. (6.96)] is

$$w = z^{1/2}. \tag{6.100}$$

From the relation

$$\rho e^{i\varphi} = r^{1/2} e^{i\theta/2}, \tag{6.101}$$

and

$$2\varphi = \theta, \tag{6.102}$$

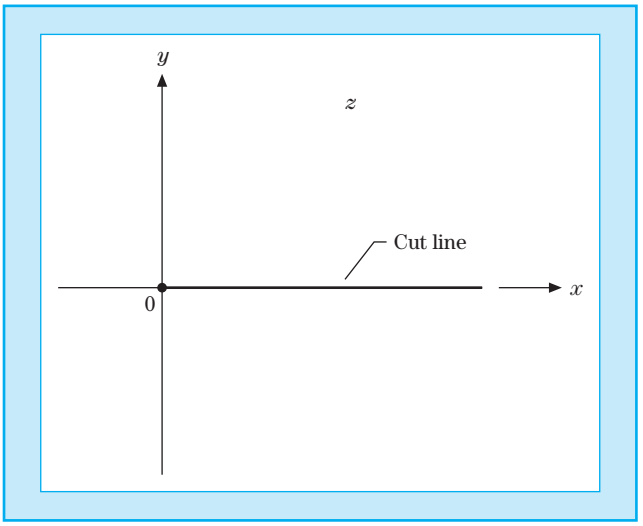
we now have two points in the w-plane (arguments φ and $\varphi + \pi$) corresponding to one point in the z-plane (except for the point $z = 0$). In other words, θ and $\theta + 2\pi$ correspond to φ and $\varphi + \pi$, two distinct points in the w-plane. This is the complex variable analog of the simple real variable equation $y^2 = x$, in which two values of y, plus and minus, correspond to each value of x. Replacing $z \to 1/z$ for $z \to 0$ in Eq. (6.100) shows that our function $w(z)$ behaves similarly around the point at infinity.

The important point here is that we can make the function w of Eq. (6.100) a single-valued function instead of a double-valued function if we agree to restrict θ to a range such as $0 \le \theta < 2\pi$. This may be done by agreeing never to cross the line $\theta = 0$ in the z-plane (Fig. 6.22). Such a line of demarcation is called a **cut line**.

The **cut line joins the two branch point singularities** at 0 and ∞, where the function is clearly not analytic. Any line from $z = 0$ to infinity would serve

Figure 6.22

A Cut Line



equally well. The purpose of the cut line is to restrict the argument of z. The points z and $z\exp(2\pi i)$ coincide in the z-plane but yield different points w and $-w = w\exp(\pi i)$ in the w-plane. Hence, in the absence of a cut line the function $w = z^{1/2}$ is ambiguous. Alternatively, since the function $w = z^{1/2}$ is double valued, we can also glue two sheets of the complex z-plane together along the cut line so that $\arg(z)$ increases beyond 2π along the cut line and steps down from 4π on the second sheet to the start on the first sheet. This construction is called the **Riemann surface** of $w = z^{1/2}$. We shall encounter branch points and cut lines frequently in Chapter 7.

The transformation

$$w = e^z \tag{6.103}$$

leads to

$$\rho e^{i\varphi} = e^{x+iy} \tag{6.104}$$

or

$$\rho = e^x, \qquad \varphi = y. \tag{6.105}$$

If y ranges from $0 \le y < 2\pi$ (or $-\pi < y \le \pi$), then φ covers the same range. However, this is the whole w-plane. In other words, a horizontal strip in the z-plane of width 2π maps into the entire w-plane. Furthermore, any point $x + i(y + 2n\pi)$, in which n is any integer, maps into the same point [by Eq. (6.104)], in the w-plane. We have a many-(infinitely many)-to-one correspondence.

Finally, as the inverse of the fifth transformation [Eq. (6.103)], we have

$$w = \ln z. \tag{6.106}$$

By expanding it, we obtain

$$u + iv = \ln re^{i\theta} = \ln r + i\theta. \tag{6.107}$$

For a given point z_0 in the z-plane, the argument θ is unspecified within an integral multiple of 2π. This means that

$$v = \theta + 2n\pi, \tag{6.108}$$

and, as in the exponential transformation, we have an infinitely many-to-one correspondence.

Equation (6.106) has a nice physical representation. If we go around the unit circle in the z-plane, $r = 1$, and by Eq. (6.107), $u = \ln r = 0$; however, $v = \theta$, and θ is steadily increasing and continues to increase as θ continues, past 2π.

The cut line joins the branch point at the origin with infinity. As θ increases past 2π, we glue a new sheet of the complex z-plane along the cut line, etc. Going around the unit circle in the z-plane is like the advance of a screw as it is rotated or the ascent of a person walking up a spiral staircase (Fig. 6.23), which is the **Riemann surface** of $w = \ln z$.

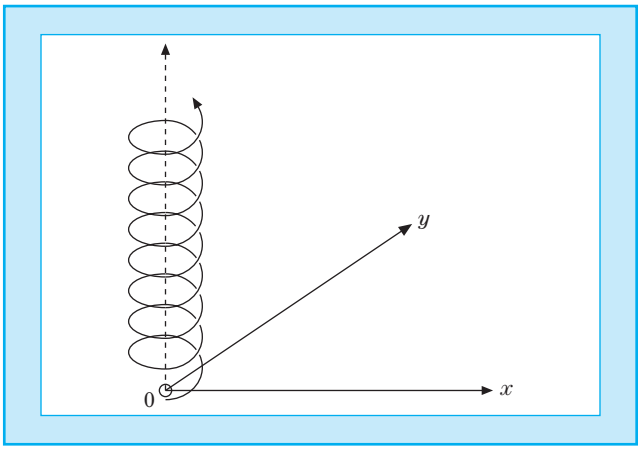


Figure 6.23

The Riemann Surface for $\ln z$, a Multivalued Function

As in the preceding example, we can also make the correspondence unique [and Eq. (6.106) unambiguous] by restricting θ to a range such as $0 \le \theta < 2\pi$ by taking the line $\theta = 0$ (positive real axis) as a cut line. This is equivalent to taking one and only one complete turn of the spiral staircase.

It is because of the multivalued nature of $\ln z$ that the contour integral

$$\oint \frac{dz}{z} = 2\pi i \neq 0,$$

integrating about the origin. This property appears in Exercise 6.4.1 and is the basis for the entire calculus of residues (Chapter 7).

SUMMARY

The concept of mapping is a very broad and useful one in mathematics. Our mapping from a complex z-plane to a complex w-plane is a simple generalization of one definition of function: a mapping of x (from one set) into y in a second set.

A more sophisticated form of mapping appears in Section 1.14, in which we use the Dirac delta function $\delta(x - a)$ to map a function $f(x)$ into its value at the point a. In Chapter 15, integral transforms are used to map one function $f(x)$ in x-space into a second (related) function $F(t)$ in t-space.

EXERCISES

6.6.1 How do circles centered on the origin in the z-plane transform for

$$\text{(a) } w_1(z) = z + \frac{1}{z}, \qquad \text{(b) } w_2(z) = z - \frac{1}{z}, \quad \text{for } z \neq 0?$$

What happens when $|z| \to 1$?

6.6.2 What part of the z-plane corresponds to the interior of the unit circle in the w-plane if

$$\text{(a) } w = \frac{z-1}{z+1}, \qquad \text{(b) } w = \frac{z-i}{z+i}?$$

6.6.3 Discuss the transformations

(a) $w(z) = \sin z$, (c) $w(z) = \sinh z$,
(b) $w(z) = \cos z$, (d) $w(z) = \cosh z$.

Show how the lines $x = c_1$, $y = c_2$ map into the w-plane. Note that the last three transformations can be obtained from the first one by appropriate translation and/or rotation.

6.6.4 Show that the function

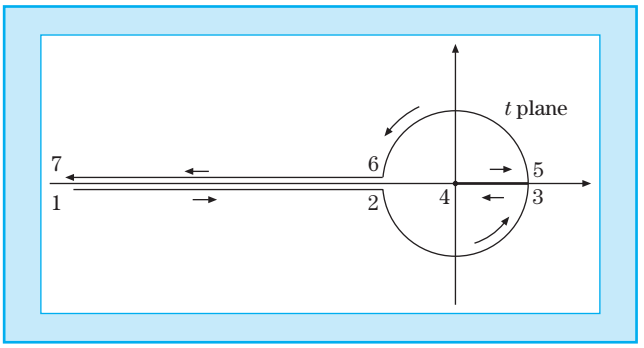
$$w(z) = (z^2 - 1)^{1/2}$$

is single-valued if we take $-1 \le x \le 1$, $y = 0$ as a cut line.

6.6.5 An integral representation of the Bessel function follows the contour in the t-plane shown in Fig. 6.24. Map this contour into the θ-plane with $t = e^{\theta}$. Many additional examples of mapping are given in Chapters 11–13.

Figure 6.24

Bessel Function Integration Contour



6.6.6 For noninteger m, show that the binomial expansion of Exercise 6.5.2 holds only for a suitably defined branch of the function $(1 + z)^m$. Show how the z-plane is cut. Explain why $|z| < 1$ may be taken as the circle of convergence for the expansion of this branch, in light of the cut you have chosen.

6.6.7 The Taylor expansion of Exercises 6.5.2 and 6.6.6 is **not** suitable for branches other than the one suitably defined branch of the function $(1+z)^m$ for noninteger m. [Note that other branches cannot have the same Taylor expansion since they must be distinguishable.] Using the same branch cut of the earlier exercises for all other branches, find the corresponding Taylor expansions detailing the phase assignments and Taylor coefficients.

6.7 Conformal Mapping

In Section 6.6, hyperbolas were mapped into straight lines and straight lines were mapped into circles. However, in all these transformations one feature, angles, stayed constant, which we now address. This constancy was a result of the fact that all the transformations of Section 6.6 were analytic.

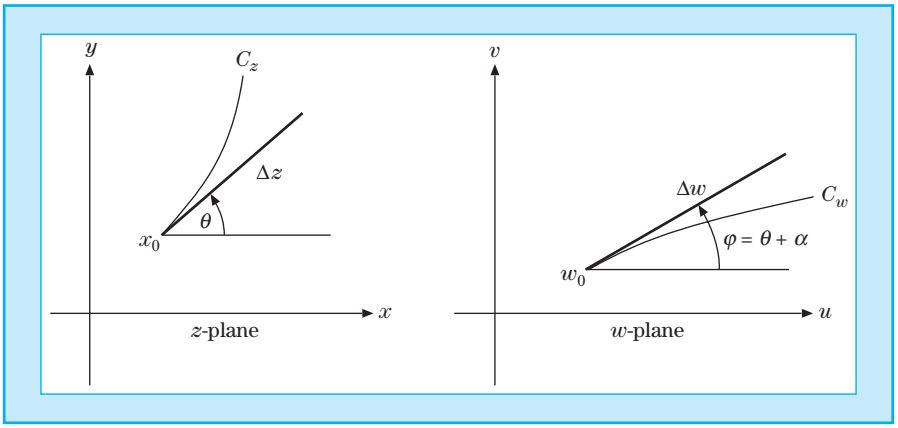


Figure 6.25

Conformal Mapping—Preservation of Angles

As long as $w = f(z)$ is an analytic function, we have

$$\frac{df}{dz} = \frac{dw}{dz} = \lim_{\Delta z \to 0} \frac{\Delta w}{\Delta z}. \tag{6.109}$$

Assuming that this equation is in polar form, we may equate modulus to modulus and argument to argument. For the latter (assuming that $df/dz \neq 0$),

$$\begin{aligned} \arg \lim_{\Delta z \to 0} \frac{\Delta w}{\Delta z} &= \lim_{\Delta z \to 0} \arg \frac{\Delta w}{\Delta z} \\ &= \lim_{\Delta z \to 0} \arg \Delta w - \lim_{\Delta z \to 0} \arg \Delta z = \arg \frac{df}{dz} = \alpha, \end{aligned} \tag{6.110}$$

where α, the argument of the derivative, may depend on z but is a constant for fixed z, independent of the direction of approach. To see the significance of this, consider two curves, C_z in the z-plane and the corresponding curve C_w in the w-plane (Fig. 6.25). The increment Δz is shown at an angle of θ relative to the real (x) axis, whereas the corresponding increment Δw forms an angle of φ with the real (u) axis. From Eq. (6.110),

$$\varphi = \theta + \alpha, \tag{6.111}$$

or any line in the z-plane is rotated through an angle α in the w-plane as long as w is an analytic transformation and the derivative is not zero.[14]

Since this result holds for any line through z_0, it will hold for a pair of lines. Then for the angle between these two lines

$$\varphi_2 - \varphi_2 = (\theta_2 + \alpha) - (\theta_1 + \alpha) = \theta_2 - \theta_1, \tag{6.112}$$

which shows that the included angle is preserved under an analytic transformation. Such **angle-preserving transformations are called conformal**. The rotation angle α will, in general, depend on z. In addition, $|f'(z)|$ will usually be a function of z.

[14]If $df/dz = 0$, its argument or phase is undefined and the (analytic) transformation will not necessarily preserve angles.

SUMMARY

Historically, conformal transformations have been of great importance to scientists and engineers in solving Laplace's equation for problems of electrostatics, hydrodynamics, heat flow, and so on. Unfortunately, the conformal transformation approach, however elegant, is limited to problems that can be reduced to two dimensions. The method is often beautiful if there is a high degree of symmetry present but often impossible if the symmetry is broken or absent.

Because of these limitations and primarily because high-speed electronic computers offer a useful alternative (iterative solution of the partial differential equation), the details and applications of conformal mappings are omitted.

EXERCISES

6.7.1 Expand $w(x)$ in a Taylor series about the point $z = z_0$, where $f'(z_0) = 0$. (Angles are not preserved.) Show that if the first $n-1$ derivatives vanish but $f^{(n)}(z_0) \neq 0$, then angles in the z-plane with vertices at $z = z_0$ appear in the w-plane multiplied by n.

6.7.2 In the transformation

$$e^z = \frac{a - w}{a + w},$$

how do the coordinate lines in the z-plane transform? What coordinate system have you constructed?

6.7.3 Develop a conformal transformation that maps a circle in the z-plane into a circle in the w-plane. Consider first circles with centers at the origin and then those with arbitrary centers. Plot several cases using graphical software.

6.7.4 Develop a conformal transformation that maps straight lines parallel to the coordinate axes in the z-plane into parabolas in the w-plane. Plot several parabolas using graphical software.

Additional Reading

Ahlfors, L. V. (1979). *Complex Analysis*, 3rd ed. McGraw-Hill, New York. This text is detailed, thorough, rigorous, and extensive.

Churchill, R. V., Brown, J. W., and Verkey, R. F. (1989). *Complex Variables and Applications*, 5th ed. McGraw-Hill, New York. This is an excellent text for both the beginning and advanced student. It is readable and quite complete. A detailed proof of the Cauchy–Goursat theorem is given in Chapter 5.

Greenleaf, F. P. (1972). *Introduction to Complex Variables*. Saunders, Philadelphia. This very readable book has detailed, careful explanations.

Kurala, A. (1972). *Applied Functions of a Complex Variable*. Wiley–Interscience, New York. An intermediate-level text designed for scientists and engineers. Includes many physical applications.

Levinson, N., and Redheffer, R. M. (1970). *Complex Variables*. Holden-Day, San Francisco. This text is written for scientists and engineers who are interested in applications.

Morse, P. M., and Feshbach, H. (1953). *Methods of Theoretical Physics*. McGraw-Hill, New York. Chapter 4 is a presentation of portions of the theory of functions of a complex variable of interest to theoretical physicists.

Remmert, R. (1991). *Theory of Complex Functions*. Springer, New York.

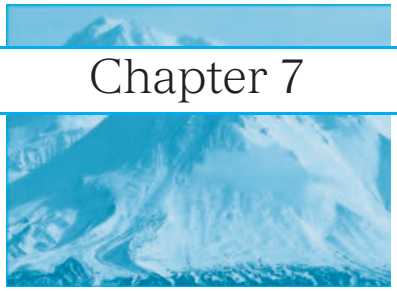
Sokolnikoff, I. S., and Redheffer, R. M. (1966). *Mathematics of Physics and Modern Engineering*, 2nd ed. McGraw-Hill, New York. Chapter 7 covers complex variables.

Spiegel, M. R. (1985). *Complex Variables*. McGraw-Hill, New York. An excellent summary of the theory of complex variables for scientists.

Titchmarsh, E. C. (1958). *The Theory of Functions*, 2nd ed. Oxford Univ. Press, New York. A classic.

Watson, G. N. (1917/1960). *Complex Integration and Cauchy's Theorem*. Hafner, New York. A short work containing a rigorous development of the Cauchy integral theorem and integral formula. Applications to the calculus of residues are included. *Cambridge Tracts in Mathematics, and Mathematical Physics*, No. 15.

Other references are given at the end of Chapter 15.



Chapter 7

Functions of a Complex Variable II

Calculus of Residues

7.1 Singularities

In this chapter we return to the line of analysis that started with the Cauchy–Riemann conditions in Chapter 6 and led to the Laurent expansion (Section 6.5). The Laurent expansion represents a generalization of the Taylor series in the presence of singularities. We define the point z_0 as an **isolated singular point** of the function $f(z)$ if $f(z)$ is not analytic at $z = z_0$ but is analytic and single valued in a punctured disk $0 < |z - z_0| < R$ for some positive R. For rational functions, which are quotients of polynomials, $f(z) = P(z)/Q(z)$, the only singularities arise from zeros of the denominator if the numerator is nonzero there. For example, $f(z) = \frac{z^3-2z^2+1}{(z-3)(z^2+3)}$ from Exercise 6.5.13 has simple poles at $z = \pm i\sqrt{3}$ and $z = 3$ and is regular everywhere else. A function that is analytic throughout the finite complex plane **except** for isolated poles is called **meromorphic**. Examples are **entire** functions that have no singularities in the finite complex plane, such as e^z, $\sin z$, $\cos z$, rational functions with a finite number of poles, or $\tan z$, $\cot z$ with infinitely many isolated simple poles at $z = n\pi$ and $z = (2n+1)\pi/2$ for $n = 0, \pm 1, \pm 2, \ldots$, respectively.

From Cauchy's integral we learned that a loop integral of a function around a simple pole gives a nonzero result, whereas higher order poles do not contribute to the integral (Example 6.3.1). We consider in this chapter the generalization of this case to meromorphic functions leading to the residue theorem, which has important applications to many integrals that physicists and engineers encounter, some of which we will discuss. Here, singularities, and simple poles in particular, play a dominant role.

Poles

In the Laurent expansion of $f(z)$ about z_0

$$f(z) = \sum_{n=-\infty}^{\infty} a_n (z - z_0)^n, \tag{7.1}$$

if $a_n = 0$ for $n < -m < 0$ and $a_{-m} \neq 0$, we say that z_0 is a pole of order m. For instance, if $m = 1$—that is, if $a_{-1}/(z - z_0)$ is the first nonvanishing term in the Laurent series—we have a pole of order 1, often called a simple pole. Example 6.5.1 is a relevant case: The function

$$f(z) = [z(z-1)]^{-1} = -\frac{1}{z} + \frac{1}{z-1}$$

has a simple pole at the origin and at $z = 1$. Its square, $f^2(z)$, has poles of order 2 at the same places and $[f(z)]^m$ has poles of order $m = 1, 2, 3 \ldots$. In contrast, the function

$$e^{\frac{1}{z}} = \sum_{n=0}^{\infty} \frac{1}{z^n n!}$$

from Example 6.5.2 has poles of any order at $z = 0$.

If there are poles of any order (i.e., the summation in the Laurent series at z_0 continues to $n = -\infty$), then z_0 is a pole of infinite order and is called an **essential singularity**. These essential singularities have many pathological features. For instance, we can show that in any small neighborhood of an essential singularity of $f(z)$ the function $f(z)$ comes arbitrarily close to any (and therefore every) preselected complex quantity w_0.[1] Literally, the entire w-plane is mapped into the neighborhood of the point z_0, the essential singularity. One point of fundamental difference between a pole of finite order and an essential singularity is that a pole of order m can be removed by multiplying $f(z)$ by $(z - z_0)^m$. This obviously cannot be done for an essential singularity.

The behavior of $f(z)$ as $z \to \infty$ is defined in terms of the behavior of $f(1/t)$ as $t \to 0$. Consider the function

$$\sin z = \sum_{n=0}^{\infty} \frac{(-1)^n z^{2n+1}}{(2n+1)!}. \tag{7.2}$$

As $z \to \infty$, we replace the z by $1/t$ to obtain

$$\sin\left(\frac{1}{t}\right) = \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)! t^{2n+1}}. \tag{7.3}$$

Clearly, from the definition, $\sin z$ has an essential singularity at infinity. This result could be anticipated from Exercise 6.1.9 since

$$\sin z = \sin iy = i \sinh y, \quad \text{when} \quad x = 0,$$

[1] This theorem is due to Picard. A proof is given by E. C. Titchmarsh, *The Theory of Functions*, 2nd ed. Oxford Univ. Press, New York (1939).

which approaches infinity exponentially as $y \to \infty$. Thus, although the absolute value of $\sin x$ for real x is equal to or less than unity, the absolute value of $\sin z$ is not bounded. The same applies to $\cos z$.

Branch Points

There is another sort of singularity that will be important in the later sections of this chapter and that we encountered in Chapter 6 in the context of inverting powers and the exponential function, namely roots and logarithms. Consider

$$f(z) = z^a,$$

in which a **is not an integer**.[2] As z moves around the unit circle from e^0 to $e^{2\pi i}$,

$$f(z) \to e^{2\pi a i} \neq e^{0i}$$

for nonintegral a. As in Section 6.6, we have a branch point at the origin and another at infinity. If we set $z = 1/t$, a similar analysis for $t \to 0$ shows that $t = 0$; that is, ∞ is also a branch point. The points e^{0i} and $e^{2\pi i}$ in the z-plane coincide but these **coincident points lead to different values** of $f(z)$; that is, $f(z)$ is a **multivalued function**. The problem is resolved by constructing a **cut line joining both branch points** so that $f(z)$ will be uniquely specified for a given point in the z-plane. For z^a the cut line can go out at any angle. Note that the point at infinity must be included here; that is, the cut line may join finite branch points via the point at infinity. The next example is a case in point. If $a = p/q$ is a rational number, then q is called the order of the branch point because one needs to go around the branch point q times before coming back to the starting point or, equivalently, the Riemann surface of $z^{1/q}$ and $z^{p/q}$ is made up of q sheets, as discussed in Chapter 6. If a is irrational, then the order of the branch point is infinite, just as for the logarithm.

Note that a function with a branch point and a required cut line will not be continuous across the cut line. In general, there will be a phase difference on opposite sides of this cut line. Exercise 7.2.23 is an example of this situation. Hence, line integrals on opposite sides of this branch point cut line will not generally cancel each other. Numerous examples of this case appear in the exercises.

The contour line used to convert a multiply connected region into a simply connected region (Section 6.3) is completely different. Our function is continuous across this contour line, and no phase difference exists.

EXAMPLE 7.1.1 **Function with Two Branch Points** Consider the function

$$f(z) = (z^2 - 1)^{1/2} = (z + 1)^{1/2}(z - 1)^{1/2}. \tag{7.4}$$

[2] $z = 0$ is technically a singular point because z^a has only a finite number of derivatives, whereas an analytic function is guaranteed an infinite number of derivatives (Section 6.4). The problem is that $f(z)$ is not single-valued as we encircle the origin. The Cauchy integral formula may not be applied.

The first factor on the right-hand side, $(z+1)^{1/2}$, has a branch point at $z=-1$. The second factor has a branch point at $z=+1$. Each branch point has order 2 because the Riemann surface is made up of two sheets. At infinity $f(z)$ has a simple pole. This is best seen by substituting $z=1/t$ and making a binomial expansion at $t=0$

$$(z^2-1)^{1/2}=\frac{1}{t}(1-t^2)^{1/2}=\frac{1}{t}\sum_{n=0}^{\infty}\binom{1/2}{n}(-1)^n t^{2n}=\frac{1}{t}-\frac{1}{2}t-\frac{1}{8}t^3+\cdots.$$

The **cut line has to connect both branch points** so that it is not possible to encircle either branch point completely. To check the possibility of taking the line segment joining $z=+1$ and $z=-1$ as a cut line, let us follow the phases of these two factors as we move along the contour shown in Fig. 7.1.

For convenience in following the changes of phase, let $z+1=re^{i\theta}$ and $z-1=\rho e^{i\varphi}$. Then the phase of $f(z)$ is $(\theta+\varphi)/2$. We start at point 1, where both $z+1$ and $z-1$ have a phase of zero. Moving from point 1 to point 2, φ, the phase of $z-1=\rho e^{i\varphi}$ increases by π. ($z-1$ becomes negative.) φ then stays constant until the circle is completed, moving from 6 to 7. θ, the phase of $z+1=re^{i\theta}$, shows a similar behavior increasing by 2π as we move from 3 to 5. The phase of the function $f(z)=(z+1)^{1/2}(z-1)^{1/2}=r^{1/2}\rho^{1/2}e^{i(\theta+\varphi)/2}$ is $(\theta+\varphi)/2$. This is tabulated in the final column of Table 7.1.

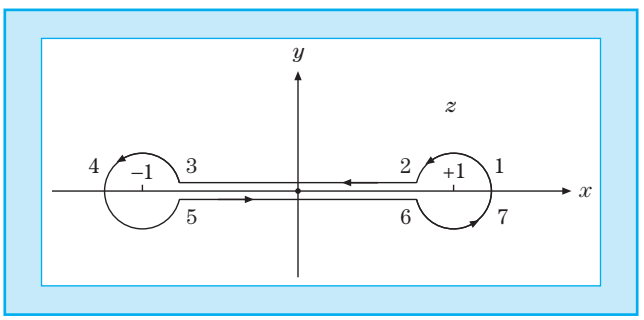
Table 7.1

Phase Angle

Point	θ	φ	$(\theta+\varphi)/2$
1	0	0	0
2	0	π	$\pi/2$
3	0	π	$\pi/2$
4	π	π	π
5	2π	π	$3\pi/2$
6	2π	π	$3\pi/2$
7	2π	2π	2π

Figure 7.1

Cut Line Joining Two Branch Points at ± 1



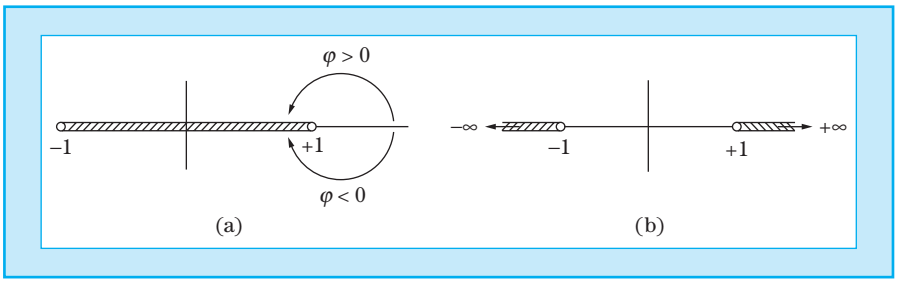


Figure 7.2

Branch Points Joined by (a) a Finite Cut Line and (b) Two Cut Lines from 1 to ∞ and −1 to −∞ that Form a Single Cut Line Through the Point at Infinity. Phase Angles are Measured as Shown in (a)

Two features emerge:

1. The phase at points 5 and 6 is not the same as the phase at points 2 and 3. This behavior can be expected at a branch point cut line.
2. The phase at point 7 exceeds that at point 1 by 2π and the function $f(z) = (z^2 - 1)^{1/2}$ is therefore **single-valued** for the contour shown, encircling **both** branch points.

If we take the x-axis $-1 \le x \le 1$ as a cut line, $f(z)$ is uniquely specified. Alternatively, the positive x-axis for $x > 1$ and the negative x-axis for $x < -1$ may be taken as cut lines. In this case, the branch points at ± 1 are joined by the cut line via the point at infinity. Again, the branch points cannot be encircled and the function remains single-valued. ■

Generalizing from this example, the phase of a function

$$f(z) = f_1(z) \cdot f_2(z) \cdot f_3(z) \cdots$$

is the algebraic sum of the phase of its individual factors:

$$\arg f(z) = \arg f_1(z) + \arg f_2(z) + \arg f_3(z) + \cdots .$$

The phase of an individual factor may be taken as the arctangent of the ratio of its imaginary part to its real part,

$$\arg f_i(z) = \tan^{-1}(v_i/u_i),$$

but one should be aware of the different branches of arctangent. For the case of a factor of the form

$$f_i(z) = (z - z_0),$$

the phase corresponds to the phase angle of a two-dimensional vector from $+z_0$ to z, with the phase increasing by 2π as the point $+z_0$ is encircled provided, it is measured without crossing a cut line ($z_0 = 1$ in Fig. 7.2a). Conversely, the traversal of any closed loop not encircling z_0 does not change the phase of $z - z_0$.

SUMMARY

Poles are the simplest singularities, and functions that have only poles besides regular points are called meromorphic. Examples are $\tan z$ and ratios

of polynomials. Branch points are singularities characteristic of multivalent functions. Examples are fractional powers of the complex variable z, whereas the logarithm has branch points of infinite order at the origin of the complex plane and at infinity. Essential singularities are the most complicated ones, and many functions have one, such as $\cos z$, $\sin z$ at infinity.

EXERCISES

7.1.1 The function $f(z)$ expanded in a Laurent series exhibits a pole of order m at $z = z_0$. Show that the coefficient of $(z - z_0)^{-1}$, a_{-1}, is given by

$$a_{-1} = \frac{1}{(m-1)!}\frac{d^{m-1}}{dz^{m-1}}[(z - z_0)^m f(z)]_{z=z_0},$$

with

$$a_{-1} = [(z - z_0)f(z)]_{z=z_0},$$

when the pole is a simple pole ($m = 1$). These equations for a_{-1} are extremely useful in determining the residue to be used in the residue theorem of the next section.
Hint. The technique that was so successful in proving the uniqueness of power series (Section 5.7) will work here also.

7.1.2 A function $f(z)$ can be represented by

$$f(z) = \frac{f_1(z)}{f_2(z)},$$

where $f_1(z)$ and $f_2(z)$ are analytic. The denominator $f_2(z)$ vanishes at $z = z_0$, showing that $f(z)$ has a pole at $z = z_0$. However, $f_1(z_0) \neq 0$, $f_2'(z_0) \neq 0$. Show that a_{-1}, the coefficient of $(z - z_0)^{-1}$ in a Laurent expansion of $f(z)$ at $z = z_0$, is given by

$$a_{-1} = \frac{f_1(z_0)}{f_2'(z_0)}.$$

This result leads to the Heaviside expansion theorem (Section 15.12).

7.1.3 In analogy with Example 7.1.1, consider in detail the phase of each factor and the resultant overall phase of $f(z) = (z^2 + 1)^{1/2}$ following a contour similar to that of Fig. 7.1 but encircling the new branch points.

7.1.4 As an example of an essential singularity, consider $e^{1/z}$ as z approaches zero. For any complex number z_0, $z_0 \neq 0$, show that

$$e^{1/z} = z_0$$

has an infinite number of solutions.

7.1.5 If the analytic function $f(z)$ goes to zero for $|z| \to \infty$, show that its residue (a_{-1} as defined in Exercise 7.1.1) at infinity is $-\lim_{z\to\infty} zf(z)$; if $f(z)$ has a finite (nonzero) limit at infinity, show that its residue at infinity is $-\lim_{z\to\infty} z^2 f'(z)$.

7.2 Calculus of Residues

Residue Theorem

If the Laurent expansion of a function $f(z) = \sum_{n=-\infty}^{\infty} a_n (z - z_0)^n$ is integrated term by term by using a closed contour that encircles one isolated singular point z_0 once in a counterclockwise sense, we obtain (Example 6.3.1)

$$a_n \oint (z - z_0)^n dz = a_n \frac{(z - z_0)^{n+1}}{n+1}\bigg|_{z_1}^{z_1} = 0, \quad n \neq -1. \tag{7.5}$$

However, if $n = -1$, using the polar form $z = z_0 + re^{i\theta}$ we find that

$$a_{-1} \oint (z - z_0)^{-1} dz = a_{-1} \oint \frac{ire^{i\theta} d\theta}{re^{i\theta}} = 2\pi i a_{-1}. \tag{7.6}$$

The first and simplest case of a residue occurred in Example 6.3.1 involving $\oint z^n dz = 2\pi n i \delta_{n,-1}$, where the integration is anticlockwise around a circle of radius r. Of all powers z^n, only $1/z$ contributes.

Summarizing Eqs. (7.5) and (7.6), we have

$$\frac{1}{2\pi i} \oint f(z)\, dz = a_{-1}. \tag{7.7}$$

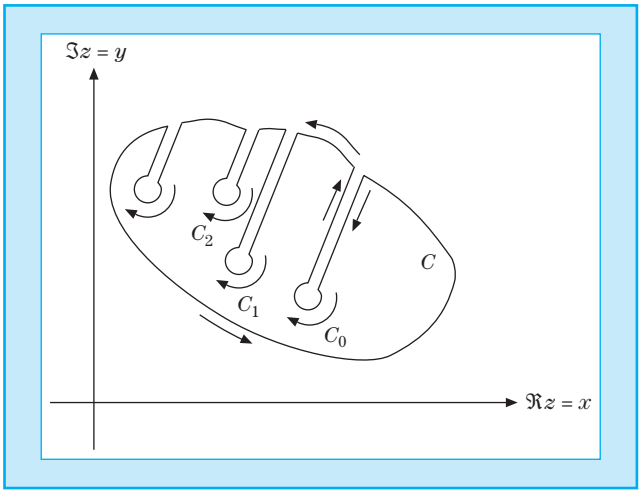
The constant a_{-1}, the coefficient of $(z - z_0)^{-1}$ in the Laurent expansion, is called the residue of $f(z)$ at $z = z_0$.

A set of isolated singularities can be handled by deforming our contour as shown in Fig. 7.3. Cauchy's integral theorem (Section 6.3) leads to

$$\oint_C f(z)\, dz + \oint_{C_0} f(z)\, dz + \oint_{C_1} f(z)\, dz + \oint_{C_2} f(z)\, dz + \cdots = 0. \tag{7.8}$$

Figure 7.3

Excluding Isolated Singularities



The circular integral around any given singular point is given by Eq. (7.7),

$$\oint_{C_i} f(z)\,dz = -2\pi i a_{-1z_i}, \tag{7.9}$$

assuming a Laurent expansion about the singular point $z = z_i$. The negative sign comes from the clockwise integration as shown in Fig. 7.3. Combining Eqs. (7.8) and (7.9), we have

$$\begin{aligned}\oint_C f(z)\,dz &= 2\pi i(a_{-1z_0} + a_{-1z_1} + a_{-1z_2} + \cdots)\\ &= 2\pi i \ \text{(sum of enclosed residues)}.\end{aligned} \tag{7.10}$$

This is the **residue theorem**. The problem of evaluating one or more contour integrals is replaced by the algebraic problem of computing residues at the enclosed singular points (poles of order 1). In the remainder of this section, we apply the residue theorem to a wide variety of definite integrals of mathematical and physical interest. The residue theorem will also be needed in Chapter 15 for a variety of integral transforms, particularly the inverse Laplace transform. We also use the residue theorem to develop the concept of the Cauchy principal value.

Using the transformation $z = 1/w$ for $w \to 0$, we can find the nature of a singularity at $z \to \infty$ and the residue of a function $f(z)$ with just isolated singularities and no branch points. In such cases, we know that

$$\sum\{\text{residues in the finite } z\text{-plane}\} + \{\text{residue at } z \to \infty\} = 0.$$

Evaluation of Definite Integrals

The calculus of residues is useful in evaluating a wide variety of definite integrals in both physical and purely mathematical problems. We consider, first, **integrals of the form**

$$I = \int_0^{2\pi} f(\sin\theta, \cos\theta)\,d\theta, \tag{7.11}$$

where f is finite for all values of θ. We also require f to be a rational function of $\sin\theta$ and $\cos\theta$ so that it will be single-valued. Let

$$z = e^{i\theta}, \quad dz = ie^{i\theta}d\theta.$$

From this,

$$d\theta = -i\frac{dz}{z}, \quad \sin\theta = \frac{z - z^{-1}}{2i}, \quad \cos\theta = \frac{z + z^{-1}}{2}. \tag{7.12}$$

Our integral becomes

$$I = -i\oint f\left(\frac{z - z^{-1}}{2i}, \frac{z + z^{-1}}{2}\right)\frac{dz}{z}, \tag{7.13}$$

with the path of integration the unit circle. By the residue theorem [Eq. (7.10)],

$$I = (-i)2\pi i \sum \text{residues within the unit circle.} \tag{7.14}$$

Note that we want to determine the residues of $f(z)/z$. Illustrations of integrals of this type are provided by Exercises 7.2.6–7.2.9.

EXAMPLE 7.2.1

Reciprocal Cosine Our problem is to evaluate the definite integral

$$I = \int_0^{2\pi} \frac{d\theta}{1+\varepsilon\cos\theta}, \quad |\varepsilon| < 1.$$

By Eq. (7.13), this becomes

$$I = -i \oint_{\text{unit circle}} \frac{dz}{z[1+(\varepsilon/2)(z+z^{-1})]}$$

$$= -i\frac{2}{\varepsilon} \oint \frac{dz}{z^2+(2/\varepsilon)z+1}.$$

The denominator has roots

$$z_- = -\frac{1}{\varepsilon} - \frac{1}{\varepsilon}\sqrt{1-\varepsilon^2} \qquad \text{and} \qquad z_+ = -\frac{1}{\varepsilon} + \frac{1}{\varepsilon}\sqrt{1-\varepsilon^2}$$

and can be written as $(z-z_+)(z-z_-)$. Here, z_+ is within the unit circle; z_- is outside. Near z_+ the denominator can be expanded as

$$z^2+\frac{2}{\epsilon}z+1 = 0+(z-z_+)\frac{d}{dz}\left(z^2+\frac{2}{\epsilon}z+1\right)\Big|_{z_+} = (z-z_+)\left(2z_+ + \frac{2}{\epsilon}\right)$$

so that the residue at z_+ is $\frac{1}{2z_+ + 2/\epsilon}$. (See Exercise 7.1.1.) Then by Eq. (7.14),

$$I = -i\frac{2}{\varepsilon}\cdot 2\pi i \frac{1}{2z+2/\varepsilon}\Big|_{z=-1/\varepsilon+(1/\varepsilon)\sqrt{1-\varepsilon^2}}.$$

Hence,

$$\int_0^{2\pi} \frac{d\theta}{1+\varepsilon\cos\theta} = \frac{2\pi}{\sqrt{1-\varepsilon^2}}, \quad |\varepsilon| < 1. \quad \blacksquare$$

Now consider a **class of definite integrals** that have the form

$$I = \int_{-\infty}^{\infty} f(x)\,dx \tag{7.15}$$

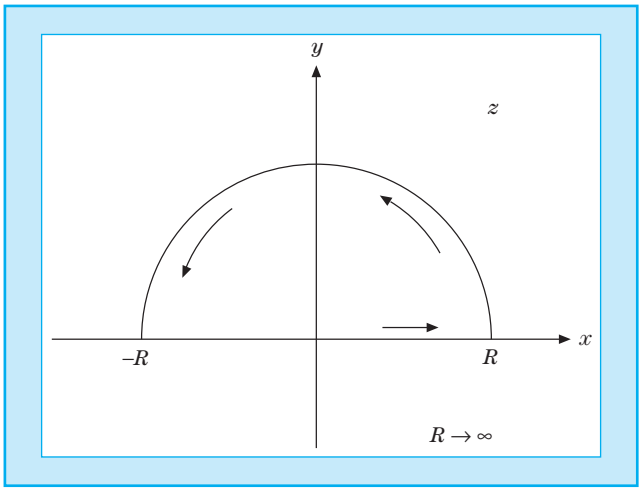
and satisfy the two conditions:

- $f(z)$ is analytic in the upper half-plane except for a finite number of poles. (It will be assumed that there are no poles on the real axis. If poles are present on the real axis, they may be included or excluded as discussed elsewhere.)
- $f(z)$ vanishes as strongly[3] as $1/z^2$ for $|z| \to \infty$, $\quad 0 \le \arg\ z \le \pi$.

[3]We could use $f(z)$ vanishes faster than $1/z$; that is, the second condition is overly sufficient, and we wish to have $f(z)$ single-valued.

Figure 7.4

Path of Integration is a Half Circle in the Upper Half Plane



With these conditions, we may take as a contour of integration the real axis and a semicircle in the upper half-plane as shown in Fig. 7.4. We let the radius R of the semicircle become infinitely large. Then

$$\oint f(z)\,dz = \lim_{R\to\infty}\int_{-R}^{R} f(x)\,dx + \lim_{R\to\infty}\int_{0}^{\pi} f(Re^{i\theta})iRe^{i\theta}\,d\theta$$

$$= 2\pi i \sum \text{residues (upper half-plane)} \tag{7.16}$$

From the second condition, the second integral (over the semicircle) vanishes and

$$\int_{-\infty}^{\infty} f(x)\,dx = 2\pi i \sum \text{residues (upper half-plane)}. \tag{7.17}$$

Note that a corresponding result is obtained when f is analytic in the lower half-plane and we use a contour in the lower half-plane. In that case, the contour will be tracked clockwise and the residues will enter with a minus sign.

EXAMPLE 7.2.2

Inverse Polynomial Evaluate

$$I = \int_{-\infty}^{\infty} \frac{dx}{1+x^2}. \tag{7.18}$$

From Eq. (7.16),

$$\int_{-\infty}^{\infty} \frac{dx}{1+x^2} = 2\pi i \sum \text{residues (upper half-plane)}.$$

Here and in every other similar problem, we have the question: Where are the poles? Rewriting the integrand as

$$\frac{1}{z^2+1} = \frac{1}{z+i}\cdot\frac{1}{z-i}, \tag{7.19}$$

we see that there are simple poles (order 1) at $z = i$ and $z = -i$.

A simple pole at $z = z_0$ indicates (and is indicated by) a Laurent expansion of the form

$$f(z) = \frac{a_{-1}}{z - z_0} + a_0 + \sum_{n=1}^{\infty} a_n (z - z_0)^n. \tag{7.20}$$

The residue a_{-1} is easily isolated as (Exercise 7.1.1)

$$a_{-1} = (z - z_0) f(z) \,|_{z=z_0}. \tag{7.21}$$

Using Eq. (7.21), we find that the residue at $z = i$ is $1/2i$, whereas that at $z = -i$ is $-1/2i$. Another way to see this is to write the partial fraction decomposition:

$$\frac{1}{z^2 + 1} = \frac{1}{2i}\left(\frac{1}{z - i} - \frac{1}{z + i}\right).$$

Then

$$\int_{-\infty}^{\infty} \frac{dx}{1 + x^2} = 2\pi i \cdot \frac{1}{2i} = \pi. \tag{7.22}$$

Here, we used $a_{-1} = 1/2i$ for the residue of the one included pole at $z = i$. Readers should satisfy themselves that it is possible to use the lower semicircle and that this choice will lead to the same result: $I = \pi$. ■

A more delicate problem is provided by the next example.

EXAMPLE 7.2.3

Evaluation of Definite Integrals Consider **definite integrals of the form**

$$I = \int_{-\infty}^{\infty} f(x) e^{iax} dx, \tag{7.23}$$

with a real and positive. This is a Fourier transform (Chapter 15). We assume the two conditions:

- $f(z)$ is analytic in the upper half-plane except for a finite number of poles.
- $\lim_{|z| \to \infty} f(z) = 0, \quad 0 \le \arg z \le \pi.$ (7.24)

Note that this is a less restrictive condition than the second condition imposed on $f(z)$ for integrating $\int_{-\infty}^{\infty} f(x)\, dx$.

We employ the contour shown in Fig. 7.4 because the exponential factor goes rapidly to zero in the upper half-plane. The application of the calculus of residues is the same as the one just considered, but here we have to work harder to show that the integral over the (infinite) semicircle goes to zero. This integral becomes

$$I_R = \int_0^{\pi} f(Re^{i\theta})\, e^{iaR\cos\theta - aR\sin\theta} iRe^{i\theta} d\theta. \tag{7.25}$$

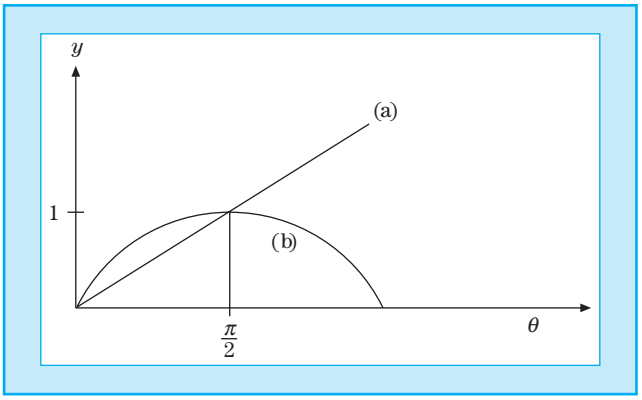


Figure 7.5
(a) $y = (2/\pi)\theta$;
(b) $y = \sin\theta$

Let R be so large that $|f(z)| = |f(Re^{i\theta})| < \varepsilon$. Then

$$|I_R| \le \varepsilon R \int_0^{\pi} e^{-aR\sin\theta}\, d\theta = 2\varepsilon R \int_0^{\pi/2} e^{-aR\sin\theta}\, d\theta. \tag{7.26}$$

In the range $[0, \pi/2]$,

$$\frac{2}{\pi}\theta \le \sin\theta.$$

Therefore (Fig. 7.5),

$$|I_R| \le 2\varepsilon R \int_0^{\pi/2} e^{-aR2\theta/\pi}\, d\theta. \tag{7.27}$$

Now, integrating by inspection, we obtain

$$|I_R| \le 2\varepsilon R \frac{1 - e^{-aR}}{aR2/\pi}.$$

Finally,

$$\lim_{R\to\infty} |I_R| \le \frac{\pi}{a}\varepsilon. \tag{7.28}$$

From condition (7.24), $\varepsilon \to 0$ as $R \to \infty$ and

$$\lim_{R\to\infty} |I_R| = 0. \tag{7.29}$$

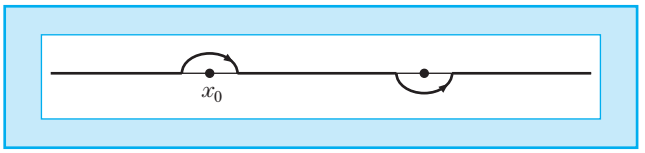
This useful result is sometimes called **Jordan's lemma**. With it, we are prepared to deal with Fourier integrals of the form shown in Eq. (7.23).

Using the contour shown in Fig. 7.4, we have

$$\int_{-\infty}^{\infty} f(x)e^{iax}dx + \lim_{R\to\infty} I_R = 2\pi i \sum \text{residues (upper half-plane)}.$$

Figure 7.6

Bypassing Singular Points



Since the integral over the upper semicircle I_R vanishes as $R \to \infty$ (Jordan's lemma),

$$\int_{-\infty}^{\infty} f(x)e^{iax}dx = 2\pi i \sum \text{residues (upper half-plane)} \quad (a > 0). \tag{7.30}$$

This result actually holds more generally for complex a with $\Re(a) > 0$. ■

Cauchy Principal Value

Occasionally, an isolated first-order pole will be directly on the contour of integration. In this case, we may deform the contour to include or exclude the residue as desired by including a semicircular detour of **infinitesimal radius**. This is shown in Fig. 7.6. The integration over the semicircle then gives, with $z - x_0 = \delta e^{i\varphi}$, $dz = i\delta e^{i\varphi}d\varphi$,

$$\int \frac{dz}{z - x_0} = i\int_{\pi}^{2\pi} d\varphi = i\pi, \text{ i.e., } \pi i a_{-1} \qquad \text{if counterclockwise,}$$

$$\int \frac{dz}{z - x_0} = i\int_{\pi}^{0} d\varphi = -i\pi, \text{ i.e., } -\pi i a_{-1} \text{ if clockwise.}$$

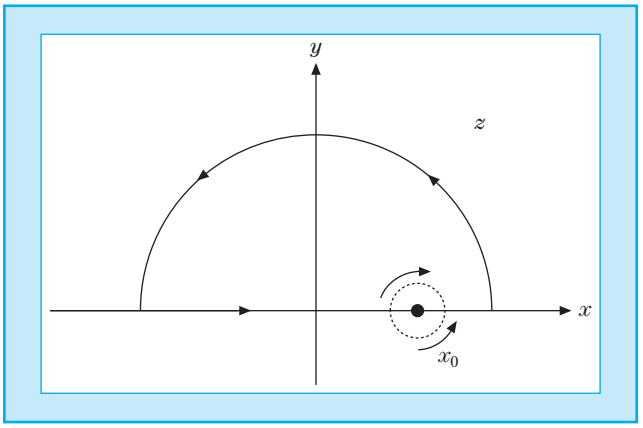
This contribution, $+$ or $-$, appears on the left-hand side of Eq. (7.10). If our detour were clockwise, the residue would not be enclosed and there would be no corresponding term on the right-hand side of Eq. (7.10). However, if our detour were counterclockwise, this residue would be enclosed by the contour C and a term $2\pi i a_{-1}$ would appear on the right-hand side of Eq. (7.10). The net result for either a clockwise or counterclockwise detour is that a simple pole on the contour is counted as one-half what it would be if it were within the contour.

For instance, let us suppose that $f(z)$ with a simple pole at $z = x_0$ is integrated over the entire real axis assuming $|f(z)| \to 0$ for $|z| \to \infty$ fast enough (faster than $1/|z|$) that the integrals in question are finite. The contour is closed with an infinite semicircle in the upper half-plane (Fig. 7.7). Then

$$\begin{aligned}\oint f(z)\,dz &= \int_{-\infty}^{x_0-\delta} f(x)\,dx + \int_{C_{x_0}} f(z)\,dz \\ &\quad + \int_{x_0+\delta}^{\infty} f(x)\,dx + \int_{C} f(z)\,dz \quad \text{infinite semicircle} \\ &= 2\pi i \sum \textbf{enclosed residues.}\end{aligned} \tag{7.31}$$

Figure 7.7

Closing the Contour with an Infinite Radius Semicircle



If the small semicircle C_{x_0} includes x_0 (by going below the x-axis; counterclockwise), x_0 is enclosed, and its contribution appears **twice**—as $\pi i a_{-1}$ in $\int_{C_{x_0}}$ and as $2\pi i a_{-1}$ in the term $2\pi i \sum$ enclosed residues—for a net contribution of $\pi i a_{-1}$ on the right-hand side of Eq. (7.31). If the upper small semicircle is selected, x_0 is excluded. The only contribution is from the **clockwise** integration over C_{x_0}, which yields $-\pi i a_{-1}$. Moving this to the extreme right of Eq. (7.11), we have $+\pi i a_{-1}$, as before.

The integrals along the x-axis may be combined and the semicircle radius permitted to approach zero. We therefore define

$$\lim_{\delta\to 0}\left\{\int_{-\infty}^{x_0-\delta} f(x)\,dx + \int_{x_0+\delta}^{\infty} f(x)\,dx\right\} = P\int_{-\infty}^{\infty} f(x)\,dx. \tag{7.32}$$

P indicates the Cauchy **principal value** and represents the preceding limiting process. Note that the Cauchy principal value is a balancing or canceling process; for even-order poles, $P\int_{-\infty}^{\infty} f(x)\,dx$ is not finite because there is no cancellation. In the vicinity of our singularity at $z = x_0$,

$$f(x) \approx \frac{a_{-1}}{x - x_0}. \tag{7.33}$$

This is odd, relative to x_0. The symmetric or even interval (relative to x_0) provides cancellation of the shaded areas (Fig. 7.8). The contribution of the singularity is in the integration about the semicircle.

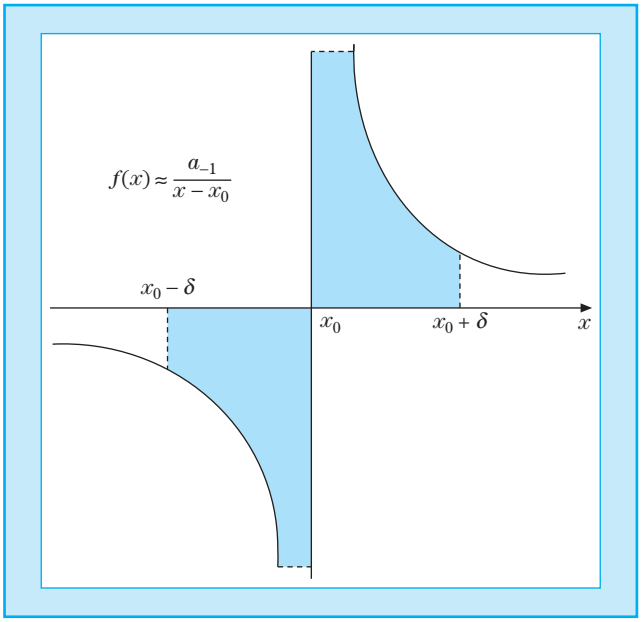
Sometimes, this same limiting technique is applied to the integration limits $\pm\infty$. If there is no singularity, we may define

$$P\int_{-\infty}^{\infty} f(x)\,dx = \lim_{a\to\infty}\int_{-a}^{a} f(x)\,dx. \tag{7.34}$$

An alternate treatment moves the pole off the contour and then considers the limiting behavior as it is brought back, in which the singular points are moved off the contour in such a way that the integral is forced into the form desired to satisfy the boundary conditions of the physical problem (for Green's functions this is often the case; see Examples 7.2.5 and 16.3.2). The principal value limit

Figure 7.8

Contour



is not necessary when a pole is removed by a zero of a numerator function. The integral

$$\int_{-\infty}^{\infty} \frac{\sin z}{z} dz = 2 \int_{0}^{\infty} \frac{\sin z}{z} dz = \pi,$$

evaluated next, is a case in point.

EXAMPLE 7.2.4

Singularity on Contour of Integration The problem is to evaluate

$$I = \int_{0}^{\infty} \frac{\sin x}{x} dx. \tag{7.35}$$

This may be taken as half the imaginary part[4] of

$$I_z = P \int_{-\infty}^{\infty} \frac{e^{iz} dz}{z}. \tag{7.36}$$

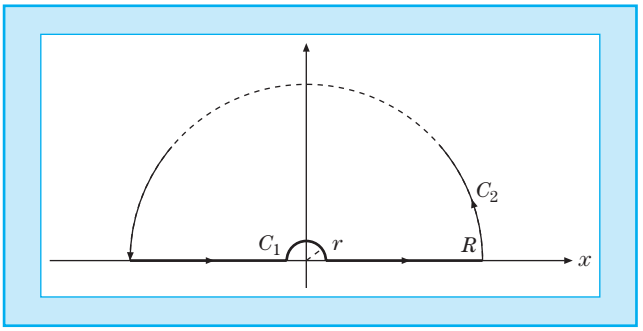
Now the only pole is a simple pole at $z = 0$ and the residue there by Eq. (7.21) is $a_{-1} = 1$. We choose the contour shown in Fig. 7.9 (i) to avoid the pole, (ii) to include the real axis, and (iii) to yield a vanishingly small integrand for $z = iy$, $y \to \infty$. Note that in this case a large (infinite) semicircle in the lower half-plane would be disastrous. We have

$$\oint \frac{e^{iz} dz}{z} = \int_{-R}^{-r} e^{ix} \frac{dx}{x} + \int_{C_1} \frac{e^{iz} dz}{z} + \int_{r}^{R} \frac{e^{ix} dx}{x} + \int_{C_2} \frac{e^{iz} dz}{z} = 0, \tag{7.37}$$

[4]One can use $\int [(e^{iz} - e^{-iz})/2iz] dz$, but then two different contours will be needed for the two exponentials.

Figure 7.9

Singularity on Contour



the final zero coming from the residue theorem [Eq. (7.10)]. By Jordan's lemma,

$$\int_{C_2} \frac{e^{iz}dz}{z} = 0, \tag{7.38}$$

and

$$\oint \frac{e^{iz}dz}{z} = \int_{C_1} \frac{e^{iz}dz}{z} + P\int_{-\infty}^{\infty} \frac{e^{ix}dx}{x} = 0. \tag{7.39}$$

The integral over the small semicircle yields $(-)\pi i$ times the residue of 1, the minus as a result of going clockwise. Taking the imaginary part,[5] we have

$$\int_{-\infty}^{\infty} \frac{\sin x}{x}dx = \pi \tag{7.40}$$

or

$$\int_{0}^{\infty} \frac{\sin x}{x}dx = \frac{\pi}{2}. \tag{7.41}$$

The contour of Fig. 7.9, although convenient, is not at all unique. Another choice of contour for evaluating Eq. (7.35) is presented as Exercise 7.2.14. ■

EXAMPLE 7.2.5

Quantum Mechanical Scattering The quantum mechanical analysis of scattering leads to the function

$$I(\sigma) = \int_{-\infty}^{\infty} \frac{x\sin x dx}{x^2 - \sigma^2}, \tag{7.42}$$

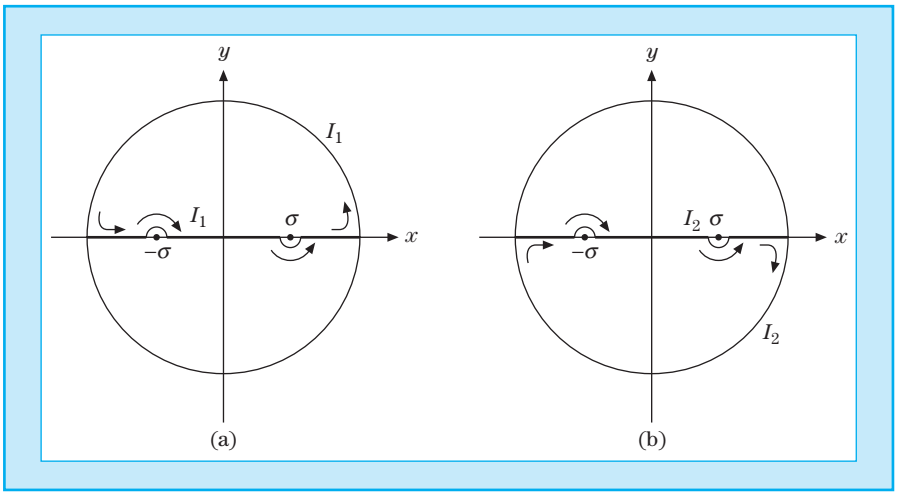
where σ is real and positive. From the physical conditions of the problem there is a further requirement: $I(\sigma)$ must have the form $e^{i\sigma}$ so that it will represent an outgoing scattered wave.

[5] Alternatively, we may combine the integrals of Eq. (7.37) as

$$\int_{-R}^{-r} e^{ix}\frac{dx}{x} + \int_{r}^{R} e^{ix}\frac{dx}{x} = \int_{r}^{R} (e^{ix} - e^{-ix})\frac{dx}{x} = 2i\int_{r}^{R} \frac{\sin x}{x}dx.$$

Figure 7.10

Contours



Using

$$\sin z = \frac{1}{2i}e^{iz} - \frac{1}{2i}e^{-iz}, \tag{7.43}$$

we write Eq. (7.42) in the complex plane as

$$I(\sigma) = I_1 + I_2, \tag{7.44}$$

with

$$I_1 = \frac{1}{2i}\int_{-\infty}^{\infty} \frac{ze^{iz}}{z^2 - \sigma^2}dz,$$

$$I_2 = -\frac{1}{2i}\int_{-\infty}^{\infty} \frac{ze^{-iz}}{z^2 - \sigma^2}dz. \tag{7.45}$$

Integral I_1 is similar to Example 7.2.2 and, as in that case, we may complete the contour by an infinite semicircle in the upper half-plane as shown in Fig. 7.10a. For I_2, the exponential is negative and we complete the contour by an infinite semicircle in the lower half-plane, as shown in Fig. 7.10b. As in Example 7.2.2, neither semicircle contributes anything to the integral–Jordan's lemma.

There is still the problem of locating the poles and evaluating the residues. We find poles at $z = +\sigma$ and $z = -\sigma$ **on the contour of integration**. The residues are (Exercises 7.1.1 and 7.2.1)

	$z = \sigma$	$z = -\sigma$
I_1	$\frac{e^{i\sigma}}{2}$	$\frac{e^{-i\sigma}}{2}$
I_2	$\frac{e^{-i\sigma}}{2}$	$\frac{e^{i\sigma}}{2}$

.

Detouring around the poles, as shown in Fig. 7.10 (it matters little whether we go above or below), we find that the residue theorem leads to

$$PI_1 - \pi i\left(\frac{1}{2i}\right)\frac{e^{-i\sigma}}{2} + \pi i\left(\frac{1}{2i}\right)\frac{e^{i\sigma}}{2} = 2\pi i\left(\frac{1}{2i}\right)\frac{e^{i\sigma}}{2} \tag{7.46}$$

because we have enclosed the singularity at $z = \sigma$ but excluded the one at $z = -\sigma$. In similar fashion, but noting that the contour for I_2 is clockwise,

$$PI_2 - \pi i\left(\frac{-1}{2i}\right)\frac{e^{i\sigma}}{2} + \pi i\left(\frac{-1}{2i}\right)\frac{e^{-i\sigma}}{2} = -2\pi i\left(\frac{-1}{2i}\right)\frac{e^{i\sigma}}{2}. \tag{7.47}$$

Adding Eqs. (7.46) and (7.47), we have

$$PI(\sigma) = PI_1 + PI_2 = \frac{\pi}{2}(e^{i\sigma} + e^{-i\sigma}) = \pi\cos\sigma. \tag{7.48}$$

This is a perfectly good evaluation of Eq. (7.42), but unfortunately the cosine dependence is appropriate for a standing wave and not for the outgoing scattered wave as specified.

To obtain the desired form, we try a different technique. We note that the integral, Eq. (7.42), is not absolutely convergent and its value will depend on the method of evaluation. Instead of dodging around the singular points, let us move them off the real axis. Specifically, let $\sigma \to \sigma + i\gamma$, $-\sigma \to -\sigma - i\gamma$, where γ is positive but small and will eventually be made to approach zero; that is, for I_1 we include one pole and for I_2 the other one:

$$I_+(\sigma) = \lim_{\gamma\to 0} I(\sigma + i\gamma). \tag{7.49}$$

With this simple substitution, the first integral I_1 becomes

$$I_1(\sigma + i\gamma) = 2\pi i\left(\frac{1}{2i}\right)\frac{e^{i(\sigma+i\gamma)}}{2} \tag{7.50}$$

by direct application of the residue theorem. Also,

$$I_2(\sigma + i\gamma) = -2\pi i\left(\frac{-1}{2i}\right)\frac{e^{i(\sigma+i\gamma)}}{2}. \tag{7.51}$$

Adding Eqs. (7.50) and (7.51) and then letting $\gamma \to 0$, we obtain

$$\begin{aligned} I_+(\sigma) &= \lim_{\gamma\to o}[I_1(\sigma + i\gamma) + I_2(\sigma + i\gamma)] \\ &= \lim_{\gamma\to 0} \pi e^{i(\sigma+i\gamma)} = \pi e^{i\sigma}, \end{aligned} \tag{7.52}$$

a result that does fit the boundary conditions of our scattering problem.

It is interesting to note that the substitution $\sigma \to \sigma - i\gamma$ would have led to

$$I_-(\sigma) = \pi e^{-i\sigma}, \tag{7.53}$$

which could represent an incoming wave. Our earlier result [Eq. (7.48)] is seen to be the arithmetic average of Eqs. (7.52) and (7.53). This average is

the Cauchy principal value of the integral. Note that we have these possibilities [Eqs. (7.48), (7.52), and (7.53)] because our integral is not uniquely defined until we specify the particular limiting process (or average) to be used. ■

Pole Expansion of Meromorphic Functions

Analytic functions $f(z)$ that have only separated poles as singularities are called **meromorphic**. Examples are ratios of polynomials, $\cot z$ (see Example 7.2.7) and $\frac{f'(z)}{f(z)}$ of entire functions. For simplicity, we assume that these poles at finite $z = z_n$ with $0 < |z_1| < |z_2| < \cdots$ are all simple, with residues b_n. Then an expansion of $f(z)$ in terms of $b_n(z - z_n)^{-1}$ depends only on **intrinsic properties** of $f(z)$, in contrast to the Taylor expansion about an arbitrary analytic point of $f(z)$ or the Laurent expansion about some singular point of $f(z)$.

EXAMPLE 7.2.6

Rational Functions Rational functions are ratios of polynomials that can be completely factored according to the fundamental theorem of algebra. A partial fraction expansion then generates the pole expansion. Let us consider a few simple examples. We check that the meromorphic function

$$f(z) = \frac{1}{z(z+1)} = \frac{1}{z} - \frac{1}{z+1}$$

has simple poles at $z = 0, z = -1$ with residues $\frac{z}{z(z+1)}|_{z=0} = \frac{1}{z+1}|_{z=0} = 1$ and $\frac{z+1}{z(z+1)}|_{z=-1} = \frac{1}{z} = -1$, respectively. At ∞, $f(z)$ has a second order zero. Similarly, the meromorphic function

$$f(z) = \frac{1}{z^2 - 1} = \frac{1}{2}\left(\frac{1}{z-1} - \frac{1}{z+1}\right)$$

has simple poles at $z = \pm 1$ with residues $\frac{z-1}{z^2-1}|_{z=1} = \frac{1}{z+1}|_{z=1} = \frac{1}{2}$ and $\frac{z+1}{z^2-1}|_{z=-1} = \frac{1}{z-1}|_{z=-1} = -\frac{1}{2}$. At infinity, $f(z)$ has a second-order zero also. ■

Let us consider a series of concentric circles C_n about the origin so that C_n includes $z_1, z_2, \ldots, z_n$ but no other poles, its radius $R_n \to \infty$ as $n \to \infty$. To guarantee convergence we assume that $|f(z)| < \varepsilon R_n$ for an arbitrarily small positive constant ε and all z on C_n, and f is regular at the origin. Then the series

$$f(z) = f(0) + \sum_{n=1}^{\infty} b_n\{(z - z_n)^{-1} + z_n^{-1}\} \tag{7.54}$$

converges to $f(z)$.

To prove this theorem (due to Mittag–Leffler) we use the residue theorem to evaluate the following contour integral for z inside C_n and not equal to a

singular point of $f(w)/w$:

$$I_n = \frac{1}{2\pi i}\int_{C_n} \frac{f(w)}{w(w-z)}dw$$
$$= \sum_{m=1}^{n} \frac{b_m}{z_m(z_m - z)} + \frac{f(z)-f(0)}{z}, \tag{7.55}$$

where w in the denominator is needed for convergence and $w - z$ to produce $f(z)$ via the residue theorem. On C_n we have for $n \to \infty$,

$$|I_n| \le 2\pi R_n \frac{\max_{w \text{ on } C_n} |f(w)|}{2\pi R_n(R_n - |z|)} < \frac{\varepsilon R_n}{R_n - |z|} \le \varepsilon$$

for $R_n \gg |z|$ so that $|I_n| \to 0$ as $n \to \infty$. Using $I_n \to 0$ in Eq. (7.55) proves Eq. (7.54).

If $|f(z)| < \varepsilon R_n^{p+1}$ for some positive integer p, then we evaluate similarly the integral

$$I_n = \frac{1}{2\pi i}\int \frac{f(w)}{w^{p+1}(w-z)}dw \to 0 \quad \text{as} \quad n \to \infty$$

and obtain the analogous pole expansion

$$f(z) = f(0) + zf'(0) + \cdots + \frac{z^p f^{(p)}(0)}{p!} + \sum_{n=1}^{\infty} \frac{b_n z^{p+1}/z_n^{p+1}}{z - z_n}. \tag{7.56}$$

Note that **the convergence of the series** in Eqs. (7.54) and (7.56) **is implied by the bound** of $|f(z)|$ for $|z| \to \infty$.

EXAMPLE 7.2.7

Pole Expansion of Cotangent The meromorphic function $f(z) = \pi \cot \pi z$ has simple poles at $z = \pm n$, for $n = 0, 1, 2, \ldots$ with residues $\frac{\pi \cos \pi z}{d \sin \pi z/dz}|_{z=n} = \frac{\pi \cos \pi n}{\pi \cos \pi n} = 1$. Before we apply the Mittag–Leffler theorem, we have to subtract the pole at $z = 0$. Then the pole expansion becomes

$$\pi \cot \pi z - \frac{1}{z} = \sum_{n=1}^{\infty}\left(\frac{1}{z-n} + \frac{1}{n} + \frac{1}{z+n} - \frac{1}{n}\right) = \sum_{n=1}^{\infty}\left(\frac{1}{z-n} + \frac{1}{z+n}\right)$$
$$= \sum_{n=1}^{\infty} \frac{2z}{z^2 - n^2}.$$

We check this result by taking the logarithm of the product for the sine [Eq. (7.60)] and differentiating

$$\pi \cot \pi z = \frac{1}{z} + \sum_{n=1}^{\infty}\left(\frac{-1}{n(1-\frac{z}{n})} + \frac{1}{n(1+\frac{z}{n})}\right) = \frac{1}{z} + \sum_{n=1}^{\infty}\left(\frac{1}{z-n} + \frac{1}{z+n}\right).$$

Finally, let us also compare the pole expansion of the rational functions of Example 7.2.6 with the earlier partial fraction forms. From the Mittag–Leffler theorem, we get

$$\frac{1}{z^2 - 1} = -1 + \frac{1}{2}\left(\frac{1}{z-1} + 1\right) - \frac{1}{2}\left(\frac{1}{z+1} - 1\right),$$

which is in agreement with our earlier result. In order to apply the Mittag–Leffler theorem to $\frac{1}{z(z+1)}$, we first must subtract the pole at $z = 0$. We obtain

$$\frac{1}{z(z+1)} - \frac{1}{z} = \frac{-1}{z+1} = -1 - \left(\frac{1}{z+1} - 1\right),$$

which again is consistent with Example 7.2.6. ■

Product Expansion of Entire Functions

A function $f(z)$ that is analytic for all finite z is called an **entire** function. The logarithmic derivative f'/f is a meromorphic function with a pole expansion, which can be used to get a product expansion of $f(z)$.

If $f(z)$ has a simple zero at $z = z_n$, then $f(z) = (z - z_n)g(z)$ with analytic $g(z)$ and $g(z_n) \neq 0$. Hence, the logarithmic derivative

$$\frac{f'(z)}{f(z)} = (z - z_n)^{-1} + \frac{g'(z)}{g(z)} \tag{7.57}$$

has a simple pole at $z = z_n$ with residue 1, and g'/g is analytic there. If f'/f satisfies the conditions that led to the pole expansion in Eq. (7.54), then

$$\frac{f'(z)}{f(z)} = \frac{f'(0)}{f(0)} + \sum_{n=1}^{\infty}\left[\frac{1}{z_n} + \frac{1}{z - z_n}\right] \tag{7.58}$$

holds. Integrating Eq. (7.58) yields

$$\begin{aligned}\int_0^z \frac{f'(z)}{f(z)}dz &= \ln f(z) - \ln f(0)\\ &= \frac{zf'(0)}{f(0)} + \sum_{n=1}^{\infty}\left\{\ln(z - z_n) - \ln(-z_n) + \frac{z}{z_n}\right\},\end{aligned}$$

and exponentiating we obtain the product expansion

$$f(z) = f(0)\exp\left(\frac{zf'(0)}{f(0)}\right)\prod_{n=1}^{\infty}\left(1 - \frac{z}{z_n}\right)e^{z/z_n}. \tag{7.59}$$

Examples are the product expansions for

$$\sin z = z\prod_{\substack{n=-\infty\\ n\neq 0}}^{\infty}\left(1 - \frac{z}{n\pi}\right)e^{z/n\pi} = z\prod_{n=1}^{\infty}\left(1 - \frac{z^2}{n^2\pi^2}\right),$$

$$\cos z = \prod_{n=1}^{\infty}\left\{1 - \frac{z^2}{(n - 1/2)^2\pi^2}\right\}. \tag{7.60}$$

Note that the sine-product expansion is derived by applying Eq. (7.59) to $f(z) = \sin z/z$ rather than to $\sin z$, so that $f(0) = 1$ and

$$f'(0) = \left(\frac{\cos z}{z} - \frac{\sin z}{z^2}\right)\bigg|_{z=0} = \left(\frac{1}{z} - \frac{z}{2} - \frac{1}{z} + \frac{z}{6} + \cdots\right)\bigg|_{z=0} = 0,$$

inserting the power expansions for $\sin z$ and $\cos z$. Another example is the product expansion of the gamma function, which will be discussed in Chapter 10.

As a consequence of Eq. (7.57), the contour integral of the logarithmic derivative may be used to count the number N_f of zeros (including their multiplicities) of the function $f(z)$ inside the contour C:

$$\frac{1}{2\pi i}\int_C \frac{f'(z)}{f(z)}dz = N_f. \tag{7.61}$$

This follows from the leading term of the Taylor expansion of f at a zero z_0, $f(z) = (z - z_0)f'(z_0)$, with $f'(z_0) \neq 0$, so that

$$\frac{f'(z_0)}{f(z)} = \frac{1}{z - z_0} \quad \text{with} \quad \frac{1}{2\pi i}\oint \frac{dz}{z - z_0} = 1,$$

where we integrate about a small circle around z_0. For a zero of order m (a positive integer), where $f^{(m)}(z_0) \neq 0$ is the lowest nonvanishing derivative, the leading term of the Taylor expansion becomes

$$f(z) = \frac{(z - z_0)^m}{m!}f^m(z_0), \qquad \frac{f'(z)}{f(z)} = \frac{m}{z - z_0}.$$

Thus, the logarithmic derivative counts the zero with its multiplicity m. Moreover, using

$$\int \frac{f'(z)}{f(z)}dz = \ln f(z) = \ln|f(z)| + i \arg\ f(z), \tag{7.62}$$

we see that the real part in Eq. (7.62) does not change as z moves once around the contour, whereas the corresponding change in $\arg f$, called $\Delta_C \arg(f)$, must be

$$\Delta_C \arg(f) = 2\pi N_f. \tag{7.63}$$

This leads to **Rouché's theorem**:

> If $f(z)$ and $g(z)$ are analytic inside and on a closed contour C, and $|g(z)| < |f(z)|$ on C, then $f(z)$ and $f(z) + g(z)$ have the same number of zeros inside C.

To show this we use

$$2\pi N_{f+g} = \Delta_C \arg(f + g) = \Delta_C \arg(f) + \Delta_C \arg\left(1 + \frac{g}{f}\right).$$

Since $|g| < |f|$ on C, the point $w = 1 + g(z)/f(z)$ is always an interior point of the circle in the w-plane with center at 1 and radius 1. Hence, $\arg(1 + g/f)$ must return to its original value when z moves around C (it passes to the right of the origin); it cannot decrease or increase by a multiple of 2π so that $\Delta_C \arg(1 + g/f) = 0$.

Rouché's theorem may be used for an alternative proof of the fundamental theorem of algebra: A polynomial $\sum_{m=0}^{n} a_m z^m$ with $a_n \neq 0$ has n zeros. We define $f(z) = a_n z^n$. Then f has an n-fold zero at the origin and no other zeros. Let $g(z) = \sum_{0}^{n-1} a_m z^m$. We apply Rouché's theorem to a circle C with center at the origin and radius $R > 1$. On C, $|f(z)| = |a_n| R^n$ and

$$|g(z)| \leq |a_0| + |a_1| R + \cdots + |a_{n+1}| R^{n-1} \leq \left(\sum_{m=0}^{n-1} |a_m| \right) R^{n-1}.$$

Hence, $|g(z)| < |f(z)|$ for z on C provided $R > (\sum_{m=0}^{n-1} |a_m|)/|a_n|$. For all sufficiently large circles C, therefore, $f + g = \sum_{m=0}^{n} a_m z^m$ has n zeros inside C according to Rouché's theorem.

SUMMARY

The residue theorem

$$\oint_C f(z) dz = 2\pi i \sum_{z_j \in C} [a_{-1 z_j}] = 2\pi i \sum (\text{residues enclosed by } C)$$

and its applications to definite integrals are of central importance for mathematicians and physicists. When it is applied to merophorphic functions it yields an intrinsic pole expansion that depends on the first-order pole locations and their residues provided the functions behave reasonably at $|z| \to \infty$. When it is applied to the logarithmic derivative of an entire function, it leads to its product expansion.

The residue theorem is the workhorse for solving definite integrals, at least for physicists and engineers. However, the mathematician also employs it to derive pole expansions for meromorphic functions and product expansions for entire functions. It forms part of the tool kit of every scientist.

EXERCISES

7.2.1 Determine the nature of the singularities of each of the following functions and evaluate the residues ($a > 0$):

(a) $\dfrac{1}{z^2 + a^2}$.

(b) $\dfrac{1}{(z^2 + a^2)^2}$.

(c) $\dfrac{z^2}{(z^2 + a^2)^2}$.

(d) $\dfrac{\sin 1/z}{z^2 + a^2}$.

(e) $\dfrac{z e^{+iz}}{z^2 + a^2}$.

(f) $\dfrac{z e^{+iz}}{z^2 + a^2}$.

(g) $\dfrac{e^{+iz}}{z^2 - a^2}$.

(h) $\dfrac{z^{-k}}{z + 1}$, $\quad 0 < k < 1$.

Hint. For the point at infinity, use the transformation $w = 1/z$ for $|z| \to 0$. For the residue, transform $f(z)\, dz$ into $g(w)\, dw$ and look at the behavior of $g(w)$.

7.2.2 The statement that the integral halfway around a singular point is equal to one-half the integral all the way around was limited to simple poles.

Show, by a specific example, that

$$\int_{\text{semicircle}} f(z)\,dz = \frac{1}{2}\oint_{\text{circle}} f(z)\,dz$$

does not necessarily hold if the integral encircles a pole of higher order. *Hint.* Try $f(z) = z^{-2}$.

7.2.3 A function $f(z)$ is analytic along the real axis except for a third-order pole at $z = x_0$. The Laurent expansion about $z = x_0$ has the form

$$f(z) = \frac{a_{-3}}{(z-x_0)^3} + \frac{a_{-1}}{(z-x_0)} + g(z),$$

with $g(z)$ analytic at $z = x_0$. Show that the Cauchy principal value technique is applicable in the sense that

(a) $\lim_{\delta\to 0}\left\{\int_{-\infty}^{x_0-\delta} f(x)\,dx + \int_{x_0+\delta}^{\infty} f(x)\,dx\right\}$ is well behaved.

(b) $\int_{C_{x_0}} f(z)\,dz = \pm i\pi a_{-1}$,

where C_{x_0} denotes a **small semicircle** about $z = x_0$.

7.2.4 The unit step function is defined as

$$u(s-a) = \begin{cases} 0, & s < a \\ 1, & s > a. \end{cases}$$

Show that $u(s)$ has the integral representations

(a) $u(s) = \lim_{\varepsilon\to 0^+} \frac{1}{2\pi i}\int_{-\infty}^{\infty} \frac{e^{ixs}}{x - i\varepsilon}dx$, (b) $u(s) = \frac{1}{2} + \frac{1}{2\pi i}P\int_{-\infty}^{\infty} \frac{e^{ixs}}{x}dx$.

Note. The parameter s is real.

7.2.5 Most of the special functions of mathematical physics may be generated (defined) by a generating function of the form

$$g(t, x) = \sum_n f_n(x)t^n.$$

Given the following integral representations, derive the corresponding generating function:

(a) Bessel

$$J_n(x) = \frac{1}{2\pi i}\oint e^{(x/2)(t-1/t)}t^{-n-1}dt.$$

(b) Legendre

$$P_n(x) = \frac{1}{2\pi i}\oint (1 - 2tx + t^2)^{-1/2}t^{-n-1}dt.$$

(c) Hermite

$$H_n(x) = \frac{n!}{2\pi i}\oint e^{-t^2+2tx}t^{-n-1}dt.$$

(d) Laguerre

$$L_n(x) = \frac{1}{2\pi i}\oint \frac{e^{-xt/(1-t)}}{(1-t)t^{n+1}}dt.$$

Each of the contours encircles the origin and no other singular points.

7.2.6 Generalizing Example 7.2.1, show that

$$\int_0^{2\pi}\frac{d\theta}{a\pm b\cos\theta} = \int_0^{2\pi}\frac{d\theta}{a\pm b\sin\theta} = \frac{2\pi}{(a^2-b^2)^{1/2}}, \quad \text{for } a > |b|.$$

What happens if $|b| > |a|$?

7.2.7 Show that

$$\int_0^{\pi}\frac{d\theta}{(a+\cos\theta)^2} = \frac{\pi a}{(a^2-1)^{3/2}}, \quad a > 1.$$

7.2.8 Show that

$$\int_0^{2\pi}\frac{d\theta}{1-2t\cos\theta+t^2} = \frac{2\pi}{1-t^2}, \quad \text{for } |t| < 1.$$

What happens if $|t| > 1$? What happens if $|t| = 1$?

7.2.9 With the calculus of residues show that

$$\int_0^{\pi}\cos^{2n}\theta d\theta = \pi\frac{(2n)!}{2^{2n}(n!)^2} = \pi\frac{(2n-1)!!}{(2n)}, \quad n = 0, 1, 2, \ldots.$$

(The double factorial notation is defined in Chapter 5 and Section 10.1.)
Hint. $\cos\theta = \frac{1}{2}(e^{i\theta}+e^{-i\theta}) = \frac{1}{2}(z+z^{-1}), \quad |z| = 1.$

7.2.10 Evaluate

$$\int_{-\infty}^{\infty}\frac{\cos bx-\cos ax}{x^2}dx, \quad a > b > 0.$$

ANS. $\pi(a-b)$.

7.2.11 Prove that

$$\int_{-\infty}^{\infty}\frac{\sin^2 x}{x^2}dx = \frac{\pi}{2}.$$

Hint. $\sin^2 x = \frac{1}{2}(1-\cos 2x)$.

7.2.12 A quantum mechanical calculation of a transition probability leads to the function $f(t,\omega) = 2(1-\cos\omega t)/\omega^2$. Show that

$$\int_{-\infty}^{\infty} f(t,\omega)\,d\omega = 2\pi t.$$

7.2.13 Show that ($a > 0$)

(a) $$\int_{-\infty}^{\infty} \frac{\cos x}{x^2 + a^2} dx = \frac{\pi}{a} e^{-a}.$$

How is the right side modified if $\cos x$ is replaced by $\cos kx$?

(b) $$\int_{-\infty}^{\infty} \frac{x \sin x}{x^2 + a^2} dx = \pi e^{-a}.$$

How is the right side modified if $\sin x$ is replaced by $\sin kx$?

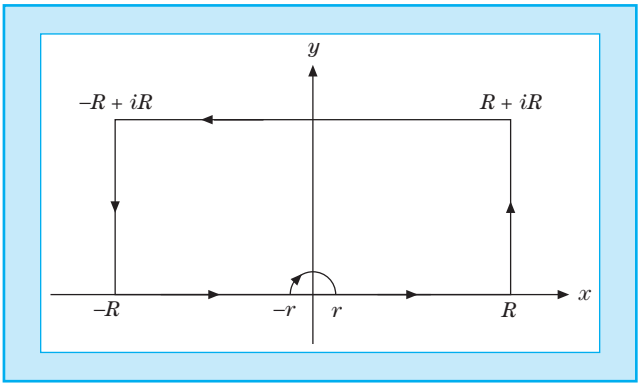
These integrals may also be interpreted as Fourier cosine and sine transforms (Chapter 15).

7.2.14 Use the contour shown in Fig. 7.11 with $R \to \infty$ to prove that

$$\int_{-\infty}^{\infty} \frac{\sin x}{x} dx = \pi.$$

Figure 7.11

Contour



7.2.15 In the quantum theory of atomic collisions we encounter the integral

$$I = \int_{-\infty}^{\infty} \frac{\sin t}{t} e^{ipt} dt,$$

in which p is real. Show that

$$I = 0, \quad |p| > 1$$
$$I = \pi, \quad |p| < 1.$$

What happens if $p = \pm 1$?

7.2.16 Evaluate

$$\int_0^{\infty} \frac{(\ln x)^2}{1 + x^2} dx.$$

(a) by appropriate series expansion of the integrand to obtain

$$4 \sum_{n=0}^{\infty} (-1)^n (2n + 1)^{-3},$$

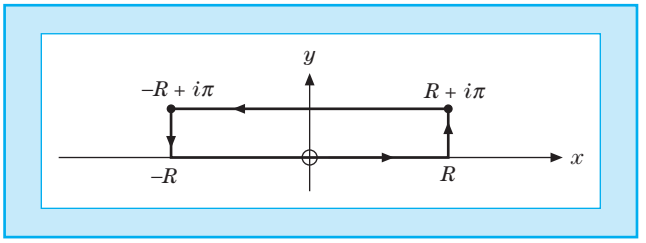
(b) and by contour integration to obtain

$$\frac{\pi^3}{8}.$$

Hint. $x \to z = e^t$. Try the contour shown in Fig. 7.12, letting $R \to \infty$.

Figure 7.12

Contour



7.2.17 Show that

$$\int_0^\infty \frac{dx}{(x^2+a^2)^2} = \frac{\pi}{4a^3}, \quad a > 0.$$

7.2.18 Evaluate

$$\int_{-\infty}^{\infty} \frac{x^2}{1+x^4}dx.$$

ANS. $\pi/\sqrt{2}$.

7.2.19 Show that

$$\int_0^\infty \cos(t^2)dt = \int_0^\infty \sin(t^2)dt = \frac{\sqrt{\pi}}{2\sqrt{2}}.$$

Hint. Try the contour shown in Fig. 7.13.
Note. These are the Fresnel integrals for the special case of infinity as the upper limit. For the general case of a varying upper limit, asymptotic expansions of the Fresnel integrals are the topic of Exercise 5.10.2. Spherical Bessel expansions are the subject of Exercise 12.4.13.

7.2.20 Several of the Bromwich integrals (Section 15.12) involve a portion that may be approximated by

$$I(y) = \int_{a-iy}^{a+iy} \frac{e^{zt}}{z^{1/2}}dz,$$

where a and t are positive and finite. Show that

$$\lim_{y\to\infty} I(y) = 0.$$

7.2.21 Show that

$$\int_0^\infty \frac{1}{1+x^n}dx = \frac{\pi/n}{\sin(\pi/n)}.$$

Hint. Try the contour shown in Fig. 7.14.

Figure 7.13

Contour

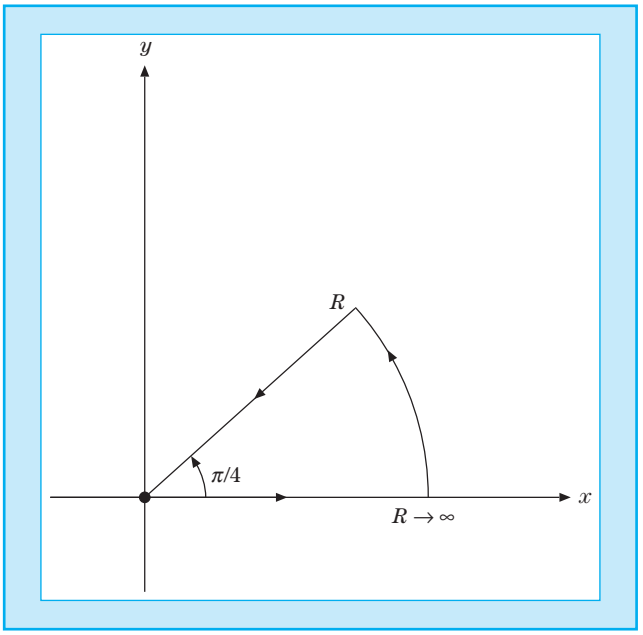
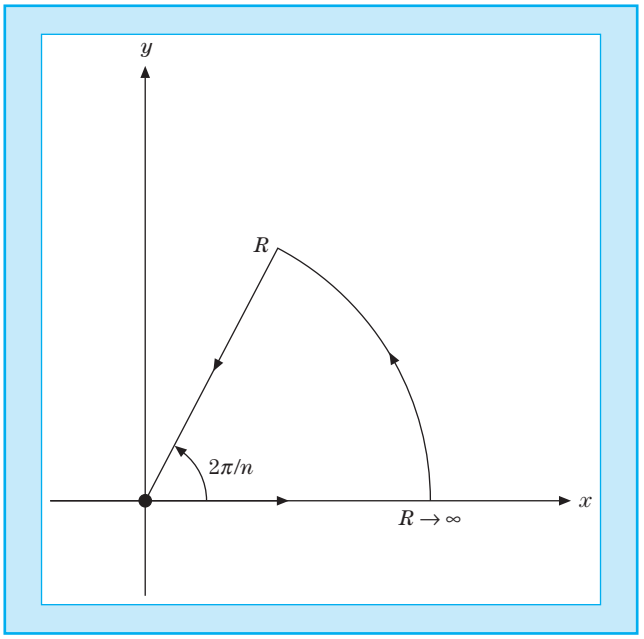


Figure 7.14

Contour



7.2.22 (a) Show that

$$f(z) = z^4 - 2\cos 2\theta z^2 + 1$$

has zeros at $e^{i\theta}$, $e^{-i\theta}$, $-e^{i\theta}$, and $-e^{-i\theta}$.

(b) Show that

$$\int_{-\infty}^{\infty} \frac{dx}{x^4 - 2\cos 2\theta x^2 + 1} = \frac{\pi}{2\sin\theta} = \frac{\pi}{2^{1/2}(1-\cos 2\theta)^{1/2}}.$$

Exercise 7.2.21 ($n = 4$) is a special case of this result.

7.2.23 Evaluate the integral

$$\int_{-\infty}^{\infty} \frac{x^2 dx}{x^4 - 2\cos 2\theta x^2 + 1}$$

by contour integration.

7.2.24 The integral in Exercise 7.2.16 may be transformed into

$$\int_0^{\infty} e^{-y} \frac{y^2}{1+e^{-2y}} dy = \frac{\pi^3}{16}.$$

Evaluate this integral by the Gauss–Laguerre quadrature and compare your numerical result with $\pi^3/16$.

ANS. Integral = 1.93775 (10 points).

7.3 Method of Steepest Descents

Analytic Landscape

In analyzing problems in mathematical physics, one often finds it desirable to know the behavior of a function for large values of the variable or some parameter s, that is, the asymptotic behavior of the function. Specific examples are furnished by the gamma function (Chapter 10) and various Bessel functions (Chapter 12). All these analytic functions [$I(s)$] are defined by integrals

$$I(s) = \int_C F(z, s)\, dz, \tag{7.64}$$

where F is analytic in z and depends on a real parameter s. We write $F(z)$ simply whenever possible.

So far, we have evaluated such definite integrals of analytic functions along the real axis (the initial path C) by deforming the path C to C' in the complex plane so that $|F|$ becomes small for all z on C'. [See Example 7.2.3 for $I(a)$.] This method succeeds as long as only isolated singularities occur in the area between C and C'. Their contributions are taken into account by applying the residue theorem of Section 7.2. The residues (from the simple pole part) give a measure of the singularities, where $|F| \to \infty$, which usually dominate and determine the value of the integral.

The behavior of an integral as in Eq. (7.64) clearly depends on the absolute value $|F|$ of the integrand. Moreover, the contours of $|F|$ at constant steps $\Delta|F|$ often become more closely spaced as s becomes large. Let us focus on a plot of $|F(x+iy)|^2 = U^2(x, y) + V^2(x, y)$ rather than the real part $\Re F = U$ and the imaginary part $\Im F = V$ separately. Such a plot of $|F|^2$ over the complex plane is called the **analytic landscape** after Jensen, who, in 1912, proved that it has **only saddle points and troughs, but no peaks**. Moreover, the troughs reach down all the way to the complex plane, that is, go to $|F| = 0$. **In the absence of singularities, saddle points** are next in line to **dominate the integral** in Eq. (7.64). Jensen's theorem explains why only saddle points (and singularities) of the integrand are so important for integrals. Hence the name saddle point method for finding the asymptotic behavior of $I(s)$ for $s \to \infty$ that we describe now. At a saddle point the real part U of F has a local maximum, for example, which implies that

$$\frac{\partial U}{\partial x} = \frac{\partial U}{\partial y} = 0,$$

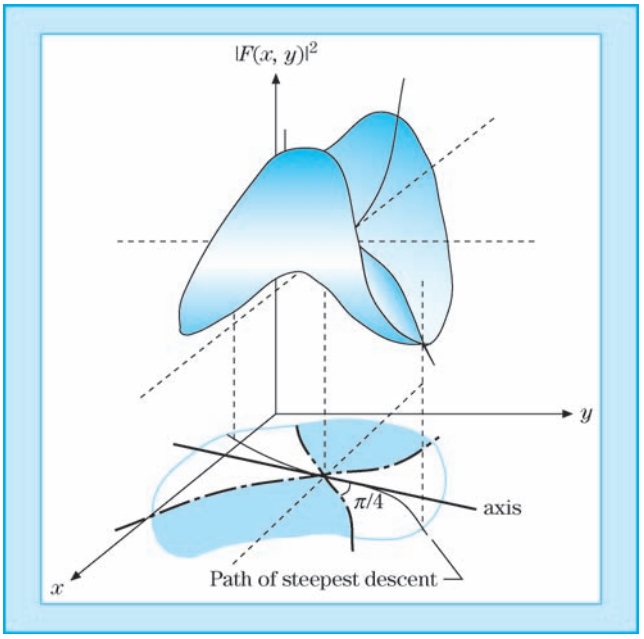
and therefore, by the use of the Cauchy–Riemann conditions of Section 6.2,

$$\frac{\partial V}{\partial x} = \frac{\partial V}{\partial y} = 0,$$

so that V has a minimum or vice versa, and $F'(z) = 0$. **Jensen's theorem prevents U and V from having both a maximum or minimum**. See Fig. 7.15 for a typical shape (and Exercises 6.2.3 and 6.2.4). We will **choose the path C so that it runs over the saddle point and in the valleys elsewhere**

Figure 7.15

A Saddle Point



so that the saddle point dominates the value of $I(s)$. This deformation of the path is analogous to the applications of the residue theorem to integrals over functions with poles. In the rare case that there are several saddle points, we treat each alike, and their contributions will add to $I(s)$ for large s.

To prove that there are no peaks, assume there is one at z_0. That is, $|F(z_0)|^2 > |F(z)|^2$ for all z of a neighborhood $|z - z_0| \le r$. If

$$F(z) = \sum_{n=0}^{\infty} a_n (z - z_0)^n$$

is the Taylor expansion at z_0, the mean value $m(F)$ on the circle $z = z_0 + r\exp(i\varphi)$ becomes

$$\begin{aligned} m(F) &\equiv \frac{1}{2\pi}\int_0^{2\pi} |F(z_0 + re^{i\varphi})|^2 d\varphi \\ &= \frac{1}{2\pi}\int_0^{2\pi} \sum_{m,n=0}^{\infty} a_m^* a_n r^{m+n} e^{i(n-m)\varphi} d\varphi \\ &= \sum_{n=0}^{\infty} |a_n|^2 r^{2n} \ge |a_0|^2 = |F(z_0)|^2, \end{aligned} \tag{7.65}$$

using orthogonality, $\frac{1}{2\pi}\int_0^{2\pi} \exp[i(n-m)\varphi]d\varphi = \delta_{nm}$. Since $m(F)$ is the mean value of $|F|^2$ on the circle of radius r, there must be a point z_1 on it so that $|F(z_1)|^2 \ge m(F) \ge |F(z_0)|^2$, which contradicts our assumption. Hence, there can be no such peak.

Next, let us assume there is a minimum at z_0 so that $0 < |F(z_0)|^2 < |F(z)|^2$ for all z of a neighborhood of z_0. In other words, the dip in the valley does not go down to the complex plane. Then $|F(z)|^2 > 0$ and since $1/F(z)$ is analytic there, it has a Taylor expansion and z_0 would be a peak of $1/|F(z)|^2$, which is impossible. This proves Jensen's theorem. We now turn our attention to the integral in Eq. (7.64).

Saddle Point Method

Since a saddle point z_0 of $|F(z)|^2$ lies above the complex plane, that is, $|F(z_0)|^2 > 0$, so $F(z_0) \ne 0$, we write F in exponential form, $F(z) = e^{f(z,s)}$, in its vicinity without loss of generality. Note that having no zero in the complex plane is a characteristic property of the exponential function. Moreover, any saddle point with $F(z) = 0$ becomes a trough of $|F(z)|^2$ because $|F(z)|^2 \ge 0$. A case in point is the function z^2 at $z = 0$ where $2z = 0$. Here $z^2 = (x+iy)^2 = x^2 - y^2 + 2ixy$, and $2xy$ has a saddle point at $z = 0$, as well as at $x^2 - y^2$, but $|z|^4$ has a trough there. The phase of $F(z_0)$ is given by $\Im f(z_0)$. At z_0 the tangential plane is horizontal; that is,

$$\left.\frac{\partial F}{\partial z}\right|_{z=z_0} = 0, \qquad \text{or equivalently} \qquad \left.\frac{\partial f}{\partial z}\right|_{z=z_0} = 0.$$

This condition locates the saddle point.

Our next goal is to determine the **direction of steepest descent**, the heart of the saddle point method. To this end, we use the power-series expansion of f at z_0,

$$f(z) = f(z_0) + \frac{1}{2}f''(z_0)(z - z_0)^2 + \cdots, \tag{7.66}$$

or

$$f(z) = f(z_0) + \frac{1}{2}(f''(z_0) + \varepsilon)(z - z_0)^2, \tag{7.67}$$

upon collecting all higher powers in the (small) ε. Let us take $f''(z_0) \neq 0$ for simplicity. Then

$$f''(z_0)(z - z_0)^2 = -t^2, \quad t \quad \text{real} \tag{7.68}$$

defines a line through z_0 (**saddle point axis** in Fig. 7.15). At z_0, $t = 0$. Along the axis $\Im f''(z_0)(z-z_0)^2$ is zero and $v = \Im f(z) \approx \Im f(z_0)$ is constant if ε in Eq. (7.67) is neglected. Thus, F has **constant phase along the axis**. Equation (7.68) can also be expressed in terms of angles,

$$\arg(z - z_0) = \frac{\pi}{2} - \frac{1}{2}\arg f''(z_0) = \text{constant}. \tag{7.69}$$

Since $|F(z)|^2 = \exp(2\Re f)$ varies monotonically with $\Re f$, $|F(z)|^2 \sim \exp(-t^2)$ falls off exponentially from its maximum at $t = 0$ along this axis. Hence the name **steepest descent** for this method of extracting the asymptotic behavior of $I(s)$ for $s \to \infty$. The line through z_0 defined by

$$f''(z_0)(z - z_0)^2 = +t^2 \tag{7.70}$$

is orthogonal to this axis (**dashed** line in Fig. 7.15), which is evident from its angle

$$\arg(z - z_0) = -\frac{1}{2}\arg f''(z_0) = \text{constant}, \tag{7.71}$$

when compared with Eq. (7.69). Here, $|F(z)|^2$ grows exponentially.

The curves $\Re f(z) = \Re f(z_0)$ go through z_0 so that $\Re[(f''(z_0)+\varepsilon)(z-z_0)^2] = 0$, or $(f''(z_0) + \varepsilon)(z - z_0)^2 = it$ for real t. Expressing this in angles as

$$\arg(z - z_0) = \frac{\pi}{4} - \frac{1}{2}\arg(f''(z_0) + \varepsilon), \ t > 0 \tag{7.72a}$$

$$\arg(z - z_0) = -\frac{\pi}{4} - \frac{1}{2}\arg(f''(z_0) + \varepsilon), \ t < 0, \tag{7.72b}$$

and comparing with Eqs. (7.69) and (7.71), we note that these curves (**dot-dashed** line in Fig. 7.15) divide the saddle point region into four sectors—two with $\Re f(z) > \Re f(z_0)$ (hence $|F(z)| > |F(z_0)|$) shown shaded in Fig. 7.15 and two with $\Re f(z) < \Re f(z_0)$ (hence $|F(z)| < |F(z_0)|$). They are at $\pm\frac{\pi}{4}$ angles from the axis. Thus, the integration path has to avoid the shaded areas where $|F|$ rises. If a path is chosen to run up the slopes above the saddle point,

large imaginary parts of $f(z)$ are involved that lead to rapid oscillations of $F(z) = e^{f(z)}$ and cancelling contributions to the integral. So far, our treatment has been general, except for $f''(z_0) \neq 0$, which can be relaxed.

Now we are ready to **specialize the integrand** F further in order to tie up the path selection with the **asymptotic behavior** as $s \to \infty$. We assume that the parameter s appears linearly in the exponent; that is, we replace $\exp f(z, s) \to \exp(sf(z))$. This dependence on s often occurs in physics applications and ensures that the saddle point at z_0 grows with $s \to \infty$ [if $\Re f(z_0) > 0$]. In order to account for the region far away from the saddle point that is not influenced by s, we include another analytic function $g(z)$ that varies slowly near the saddle point and is independent of s. Altogether, our integral has the more appropriate and **specific form**

$$I(s) = \int_C g(z) e^{sf(z)} dz. \tag{7.73}$$

Our **goal now is to estimate the integral** $I(s)$ near the saddle point. **The path of steepest descent is the saddle point axis** when we neglect the higher order terms, ε, in Eq. (7.67). With ε, the path of steepest descent is the curve close to the axis within the unshaded sectors, where the phase $v = \Im f(z)$ is strictly constant, whereas $\Im f(z)$ is only approximately constant on the axis. We approximate $I(s)$ by the integral along the piece of the axis inside the patch in Fig. 7.15, where [compare with Eq. (7.68)]

$$z = z_0 + xe^{i\alpha}, \quad \alpha = \frac{\pi}{2} - \frac{1}{2} \arg f''(z_0), \quad a \leq x \leq b. \tag{7.74}$$

Here, the interval $[a, b]$ will be given below. We find

$$I(s) \approx e^{i\alpha} \int_a^b g(z_0 + xe^{i\alpha}) \exp[sf(z_0 + xe^{i\alpha})] dx, \tag{7.75a}$$

and the omitted part is small and can be estimated because $\Re(f(z) - f(z_0))$ has an upper negative bound (e.g., $-R$) that depends on the size of the saddle point patch in Fig. 7.15 [i.e., the values of a, b in Eq. (7.74)] that we choose. In Eq. (7.75a) we use the Taylor expansions

$$\begin{aligned} f(z_0 + xe^{i\alpha}) &= f(z_0) + \frac{1}{2} f''(z_0) e^{2i\alpha} x^2 + \cdots, \\ g(z_0 + xe^{i\alpha}) &= g(z_0) + g'(z_0) e^{i\alpha} x + \cdots, \end{aligned} \tag{7.75b}$$

and recall from Eq. (7.74) that

$$\frac{1}{2} f''(z_0) e^{2i\alpha} = -\frac{1}{2} |f''(z_0)| < 0.$$

We find for the leading term

$$I(s) = g(z_0) e^{sf(z_0) ti\alpha} \int_a^b e^{-\frac{1}{2} s|f''(z_0)|x^2} dx. \tag{7.76}$$

Since the integrand in Eq. (7.76) is essentially zero when x departs appreciably from the origin, we let $b \to \infty$ and $a \to -\infty$. The small error involved is

straightforward to estimate. Noting that the remaining integral is just a Gauss error integral,

$$\int_{-\infty}^{\infty} e^{-\frac{1}{2}c^2x^2}dx = \frac{1}{c}\int_{-\infty}^{\infty} e^{-\frac{1}{2}x^2}dx = \frac{\sqrt{2\pi}}{c},$$

we obtain the asymptotic formula

$$I(s) = \frac{\sqrt{2\pi}\,g(z_0)e^{sf(z_0)}e^{i\alpha}}{|sf''(z_0)|^{1/2}} \tag{7.77}$$

for the case in which one saddle point dominates. Here, the phase α was introduced in Eqs. (7.74) and (7.69).

One note of warning: We assumed that the only significant contribution to the integral came from the immediate vicinity of the saddle point $z = z_0$. This condition must be checked for each new problem (Exercise 7.3.3).

EXAMPLE 7.3.1

Asymptotic Form of the Hankel Function, $H_\nu^{(1)}(s)$ In Section 12.3, it is shown that the Hankel functions, which satisfy Bessel's equation, may be defined by

$$H_\nu^{(1)}(s) = \frac{1}{\pi i}\int_{C_1(0)}^{\infty e^{i\pi}} e^{(s/2)(z-1/z)}\frac{dz}{z^{\nu+1}}, \tag{7.78}$$

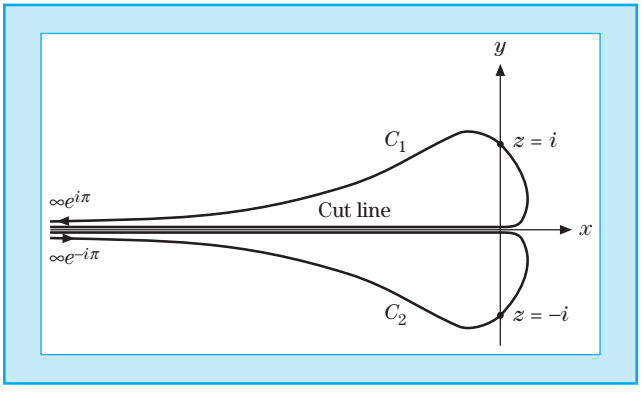
$$H_\nu^{(2)}(s) = \frac{1}{\pi i}\int_{C_2(\infty e^{-i\pi})}^{0} e^{(s/2)(z-1/z)}\frac{dz}{z^{\nu+1}}, \tag{7.79}$$

where $\infty e^{i\pi} = -\infty$ and the contour C_1 is the curve in the upper half-plane of Fig. 7.16 that starts at the origin and ends at $-\infty$. The contour C_2 is in the lower half-plane, starting at $\infty e^{-i\pi}$ and ending at the origin. We apply the method of steepest descents to the first Hankel function, $H_\nu^{(1)}(s)$, which is conveniently in the form specified by Eq. (7.73), with $g(z) = 1/(i\pi z^{\nu+1})$ and $f(z)$ given by

$$f(z) = \frac{1}{2}\left(z - \frac{1}{z}\right). \tag{7.80}$$

Figure 7.16

Hankel Function Contours



By differentiating, we obtain

$$f'(z) = \frac{1}{2} + \frac{1}{2z^2}, \quad f''(z) = -\frac{1}{z^3}. \tag{7.81}$$

Setting $f'(z) = 0$, we obtain

$$z = i, -i. \tag{7.82}$$

Hence, there are saddle points at $z = +i$ and $z = -i$. At $z = i$, $f''(i) = -i$, or $\arg f''(i) = -\pi/2$, so that the saddle point direction is given by Eq. (7.74) as $\alpha = \frac{\pi}{2} + \frac{\pi}{4} = \frac{3}{4}\pi$. For the integral for $H_\nu^{(1)}(s)$ we must choose the contour through the point $z = +i$ so that it starts at the origin, moves out tangentially to the positive real axis, and then moves around through the saddle point at $z = +i$ in the direction given by the angle $\alpha = 3\pi/4$ and then on out to minus infinity, asymptotic with the negative real axis. The path of steepest ascent that we must avoid has the phase $-\frac{1}{2}\arg f''(i) = \frac{\pi}{4}$ according to Eq. (7.71) and is orthogonal to the axis, our path of steepest descent.

Direct substitution into Eq. (7.77) with $\alpha = 3\pi/4$ yields

$$\begin{aligned} H_\nu^{(1)}(s) &= \frac{1}{\pi i} \frac{\sqrt{2\pi i^{-\nu-1}} e^{(s/2)(i-1/i)} e^{3\pi i/4}}{|(s/2)(-2/i^3)|^{1/2}} \\ &= \sqrt{\frac{2}{\pi s}} e^{(i\pi/2)(-\nu-2)} e^{is} e^{i(3\pi/4)}. \end{aligned} \tag{7.83}$$

By combining terms, we finally obtain

$$H_\nu^{(1)}(s) \approx \sqrt{\frac{2}{\pi s}} e^{i(s-\nu(\pi/2)-\pi/4)} \tag{7.84}$$

as the leading term of the asymptotic expansion of the Hankel function $H_\nu^{(1)}(s)$. Additional terms, if desired, may be picked up from the power series of f and g in Eq. (7.75b). The other Hankel function can be treated similarly using the saddle point at $z = -i$. ■

EXAMPLE 7.3.2

Asymptotic Form of the Factorial Function In many physical problems, particularly in the field of statistical mechanics, it is desirable to have an accurate approximation of the gamma or factorial function of very large numbers. As developed in Section 10.1, the factorial function may be defined by the Euler integral

$$s! = \int_0^\infty \rho^s e^{-\rho} d\rho = s^{s+1} \int_0^\infty e^{s(\ln z - z)} dz. \tag{7.85}$$

Here, we have made the substitution $\rho = zs$ in order to put the integral into the form required by Eq. (7.73). As before, we assume that s is real and positive, from which it follows that the integrand vanishes at the limits 0 and ∞. By

differentiating the z dependence appearing in the exponent, we obtain

$$f'(z) = \frac{d}{dz}(\ln z - z) = \frac{1}{z} - 1, \quad f''(z) = -\frac{1}{z^2}, \tag{7.86}$$

which shows that the point $z = 1$ is a saddle point, and $\arg f''(1) = \arg(-1) = \pi$. According to Eq. (7.74) we let

$$z - 1 = xe^{i\alpha}, \quad \alpha = \frac{\pi}{2} - \frac{1}{2}\arg f''(1) = \frac{\pi}{2} - \frac{\pi}{2}, \tag{7.87}$$

with x small to describe the contour in the vicinity of the saddle point. From this we see that the direction of steepest descent is along the real axis, a conclusion that we could have reached more or less intuitively.

Direct substitution into Eq. (7.77) with $\alpha = 0$ gives

$$s! \approx \frac{\sqrt{2\pi}s^{s+1}e^{-s}}{|s(-1^{-2})|^{1/2}}. \tag{7.88}$$

Thus, the first term in the asymptotic expansion of the factorial function is

$$s! \approx \sqrt{2\pi s}s^s e^{-s}. \tag{7.89}$$

This result is the first term in Stirling's expansion of the factorial function. The method of steepest descent is probably the easiest way of obtaining this first term. If more terms in the expansion are desired, then the method of Section 10.3 is preferable. ■

In the foregoing example the calculation was carried out by assuming s to be real. This assumption is not necessary. We may show that Eq. (7.89) also holds when s is replaced by the complex variable w, provided only that the real part of w is required to be large and positive.

SUMMARY

Asymptotic limits of integral representations of functions are extremely important in many approximations and applications in physics:

$$\int_C g(z)e^{sf(z)}dz \sim \frac{\sqrt{2\pi}g(z_0)e^{sf(z_0)}e^{i\alpha}}{\sqrt{|sf''(z_0)|}}.$$

The saddle point method is one method of choice for deriving them and belongs in the tool kit of every physicist and engineer.

EXERCISES

7.3.1 Using the method of steepest descents, evaluate the second Hankel function given by

$$H_\nu^{(2)}(s) = \frac{1}{\pi i}\int_{-\infty C_2}^{0} e^{(s/2)(z-1/z)}\frac{dz}{z^{\nu+1}},$$

with contour C_2 as shown in Fig. 7.16.

ANS. $H_\nu^{(2)}(s) \approx \sqrt{\dfrac{2}{\pi s}}e^{-i(s-\pi/4-\nu\pi/2)}$.

7.3.2 Find the steepest path and leading asymptotic expansion for the Fresnel integrals $\int_0^s \cos x^2 dx$, $\int_0^s \sin x^2 dx$.
Hint. Use $\int_0^1 e^{isz^2} dz$.

7.3.3 (a) In applying the method of steepest descent to the Hankel function $H_\nu^{(1)}(s)$, show that

$$\Re[f(z)] < \Re[f(z_0)] = 0$$

for z on the contour C_1 but away from the point $z = z_0 = i$.

(b) Show that

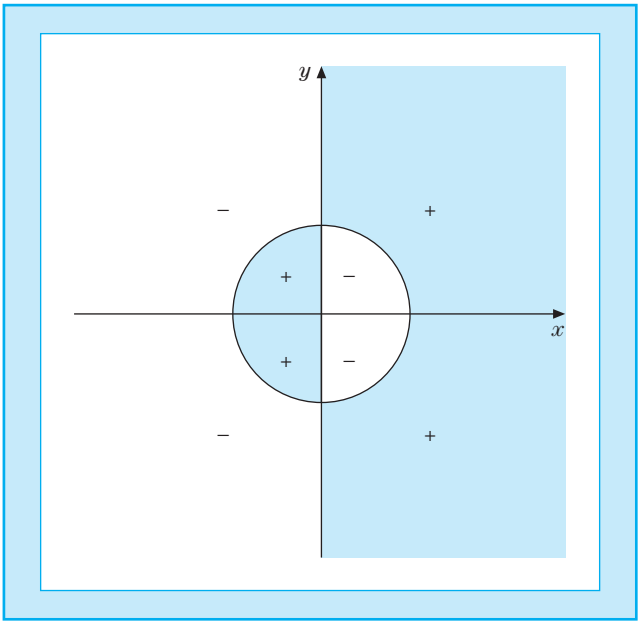
$$\Re[f(z)] > 0 \qquad \text{for} \quad 0 < r < 1, \quad \begin{cases} \dfrac{\pi}{2} < \theta \le \pi \\ -\pi \le \theta < \dfrac{\pi}{2} \end{cases}$$

and

$$\Re[f(z)] < 0 \qquad \text{for} \quad r > 1, \quad -\frac{\pi}{2} < \theta < \frac{\pi}{2}$$

(Fig. 7.17). This is why C_1 may not be deformed to pass through the second saddle point $z = -i$. Compare with and verify the dot-dashed lines in Fig. 7.15 for this case.

Figure 7.17
Saddle Points of Hankel Function



7.3.4 Show that Stirling's formula

$$s! \approx \sqrt{2\pi s} s^s e^{-s}$$

holds for complex values of s [with $\Re(s)$ large and positive].

Hint. This involves assigning a phase to s and then demanding that $\Im[sf(z)] =$ constant in the vicinity of the saddle point.

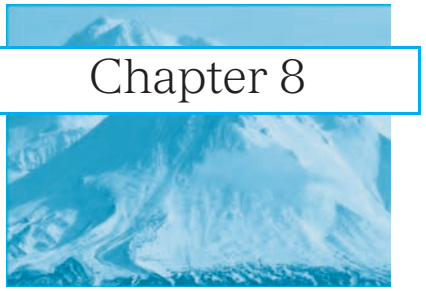
7.3.5 Assume $H_\nu^{(1)}(s)$ to have a negative power-series expansion of the form

$$H_\nu^{(1)}(s) = \sqrt{\frac{2}{\pi s}} e^{i(s-\nu(\pi/2)-\pi/4)} \sum_{n=0}^{\infty} a_{-n} s^{-n},$$

with the coefficient of the summation obtained by the method of steepest descent. Substitute into Bessel's equation and show that you reproduce the asymptotic series for $H_\nu^{(1)}(s)$ given in Section 12.3.

Additional Reading

Wyld, H. W. (1976). *Mathematical Methods for Physics*. Benjamin/Cummings, Reading, MA. Reprinted, Perseus, Cambridge, MA. (1999). This is a relatively advanced text.



Chapter 8

Differential Equations

8.1 Introduction

In physics, the knowledge of the force in an equation of motion usually leads to a differential equation, with time as the independent variable, that governs dynamical changes in space. Almost all the elementary and numerous advanced parts of theoretical physics are formulated in terms of differential equations. Sometimes these are ordinary differential equations in one variable (**ODE**). More often, the equations are partial differential equations (**PDE**) in combinations of space and time variables. In fact, PDEs motivate physicists' interest in ODEs. The term **ordinary** is applied when the only derivatives dy/dx, d^2y/dx^2, ... are ordinary or total derivatives. An ODE is **first order** if it contains the first and no higher derivatives of the unknown function $y(x)$, **second order** if it contains d^2y/dx^2 and no higher derivatives, etc.

Recall from calculus that the operation of taking an ordinary derivative is a **linear operation** ($\mathcal{L}$)[1]

$$\frac{d(a\varphi(x)+b\psi(x))}{dx}=a\frac{d\varphi}{dx}+b\frac{d\psi}{dx}.$$

In general,

$$\mathcal{L}(a\varphi+b\psi)=a\mathcal{L}(\varphi)+b\mathcal{L}(\psi), \tag{8.1}$$

where a and b are constants. An ODE is called **linear** if it is **linear in the unknown function and its derivatives**. Thus, linear ODEs appear as linear operator equations

$$\mathcal{L}\psi=F,$$

[1] We are especially interested in linear operators because in quantum mechanics physical quantities are represented by linear operators operating in a complex, infinite dimensional Hilbert space.

where ψ is the unknown function or general solution, the source F is a known function of one variable (for ODEs) and independent of ψ, and $\mathcal{L}$ is a linear combination of derivatives acting on ψ. If $F \neq 0$, the ODE is called **inhomogeneous**; if $F \equiv 0$, the ODE is called **homogeneous**. The solution of the homogeneous ODE can be multiplied by an arbitrary constant. If ψ_p is a **particular solution** of the inhomogeneous ODE, then $\psi_h = \psi - \psi_p$ is a solution of the homogeneous ODE because $\mathcal{L}(\psi - \psi_p) = F - F = 0$. Thus, the general solution is given by $\psi = \psi_p + \psi_h$. For the homogeneous ODE, any linear combination of solutions is again a solution, provided the differential equation is linear in the unknown function ψ_h; this is the **superposition principle**. We usually have to solve the homogeneous ODE first before searching for particular solutions of the inhomogeneous ODE.

Since the dynamics of many physical systems involve second-order derivatives (e.g., acceleration in classical mechanics and the kinetic energy operator, $\sim\nabla^2$, in quantum mechanics), differential equations of **second order** occur most frequently in physics. [Maxwell's and Dirac's equations are first order but involve two unknown functions. Eliminating one unknown yields a second-order differential equation for the other (compare Section 1.9).] Similarly, any higher order (linear) ODE can be reduced to a system of coupled first-order ODEs.

Nonetheless, there are many physics problems that involve first-order ODEs. Examples are resistance–inductance electrical circuits, radioactive decays, and special second-order ODEs that can be reduced to first-order ODEs. These cases and **separable ODEs** will be discussed first. ODEs of second order are more common and treated in subsequent sections, involving the special class of **linear ODEs with constant coefficients**. The important power-series expansion method of solving ODEs is demonstrated using second-order ODEs.

8.2 First-Order ODEs

Certain physical problems involve first-order differential equations. Moreover, sometimes second-order ODEs can be reduced to first-order ODEs, which then have to be solved. Thus, it seems desirable to start with them. We consider here differential equations of the general form

$$\frac{dy}{dx} = f(x, y) = -\frac{P(x, y)}{Q(x, y)}. \tag{8.2}$$

Equation (8.2) is clearly a first-order ODE; it may or may not be **linear**, although we shall treat the linear case explicitly later, starting with Eq. (8.12).

Separable Variables

Frequently, Eq. (8.2) will have the special form

$$\frac{dy}{dx} = f(x, y) = -\frac{P(x)}{Q(y)}. \tag{8.3}$$

Then it may be rewritten as

$$P(x)dx + Q(y)dy = 0.$$

Integrating from (x_0, y_0) to (x, y) yields

$$\int_{x_0}^{x} P(X)dX + \int_{y_0}^{y} Q(Y)dY = 0. \tag{8.4}$$

Here we have used capitals to distinguish the integration variables from the upper limits of the integrals, a practice that we will continue without further comment. Since the lower limits x_0 and y_0 contribute constants, we may ignore the lower limits of integration and write a constant of integration on the right-hand side instead of zero, which can be used to satisfy an initial condition. Note that this separation of variables technique does **not** require that the differential equation be linear.

EXAMPLE 8.2.1

Radioactive Decay The decay of a radioactive sample involves an event that is repeated at a constant rate λ. If the observation time dt is small enough so that the emission of two or more particles is negligible, then the probability that one particle is emitted is $\lambda\, dt$, with $\lambda\, dt \ll 1$. The decay law is given by

$$\frac{dN(t)}{dt} = -\lambda N(t), \tag{8.5}$$

where $N(t)$ is the number of radioactive atoms in the sample at time t. This ODE is separable

$$dN/N = -\lambda\, dt \tag{8.6}$$

and can be integrated to give

$$\ln N = -\lambda t + \ln N_0, \quad \text{or} \quad N(t) = N_0 e^{-\lambda t}, \tag{8.7}$$

where we have written the integration constant in logarithmic form for convenience; N_0 is fixed by an initial condition $N(0) = N_0$. ■

In the next example from classical mechanics, the ODE is separable but not linear in the unknown, which poses no problem.

EXAMPLE 8.2.2

Parachutist We want to find the velocity of the falling parachutist as a function of time and are particularly interested in the constant limiting velocity, v_0, that comes about by air resistance taken to be quadratic, $-bv^2$, and opposing the force of the gravitational attraction, mg, of the earth. We choose a coordinate system in which the positive direction is downward so that the gravitational force is positive. For simplicity we assume that the parachute opens immediately, that is, at time $t = 0$, where $v(t = 0) = 0$, our initial condition. Newton's law applied to the falling parachutist gives

$$m\dot{v} = mg - bv^2,$$

where m includes the mass of the parachute.

The terminal velocity v_0 can be found from the equation of motion as $t \to \infty$, when there is no acceleration, $\dot{v} = 0$, so that

$$bv_0^2 = mg, \quad \text{or} \quad v_0 = \sqrt{mg/b}.$$

The variables t and v separate

$$\frac{dv}{g - \frac{b}{m}v^2} = dt,$$

which we integrate by decomposing the denominator into partial fractions. The roots of the denominator are at $v = \pm v_0$. Hence,

$$\left(g - \frac{b}{m}v^2\right)^{-1} = \frac{m}{2v_0 b}\left(\frac{1}{v + v_0} - \frac{1}{v - v_0}\right).$$

Integrating both terms yields

$$\int^v \frac{dV}{g - \frac{b}{m}V^2} = \frac{1}{2}\sqrt{\frac{m}{gb}} \ln \frac{v_0 + v}{v_0 - v} = t.$$

Solving for the velocity yields

$$v = \frac{e^{2t/T} - 1}{e^{2t/T} + 1} v_0 = v_0 \frac{\sinh \frac{t}{T}}{\cosh \frac{t}{T}} = v_0 \tanh \frac{t}{T},$$

where $T = \sqrt{\frac{m}{gb}}$ is the time constant governing the asymptotic approach of the velocity to the limiting velocity v_0.

Putting in numerical values, $g = 9.8$ m/sec^2 and taking $b = 700$ kg/m, $m = 70$ kg, gives $v_0 = \sqrt{9.8/10} \sim 1$ m/sec, ~ 3.6 km/hr, or ~ 2.23 miles/hr, the walking speed of a pedestrian at landing, and $T = \sqrt{\frac{m}{bg}} = 1/\sqrt{10 \cdot 9.8} \sim 0.1$ sec. Thus, the constant speed v_0 is reached within 1 sec. Finally, because **it is always important to check the solution**, we verify that our solution satisfies

$$\dot{v} = \frac{\cosh t/T}{\cosh t/T}\frac{v_0}{T} - \frac{\sinh^2 t/T}{\cosh^2 t/T}\frac{v_0}{T} = \frac{v_0}{T} - \frac{v^2}{Tv_0} = g - \frac{b}{m}v^2,$$

that is, Newton's equation of motion. The more realistic case, in which the parachutist is in free fall with an initial speed $v_i = v(0) \neq 0$ before the parachute opens, is addressed in Exercise 8.2.16. ■

Exact Differential Equations

We rewrite Eq. (8.2) as

$$P(x, y)dx + Q(x, y)dy = 0. \tag{8.8}$$

This equation is said to be **exact** if we can match the left-hand side of it to a differential $d\varphi$,

$$d\varphi = \frac{\partial \varphi}{\partial x}dx + \frac{\partial \varphi}{\partial y}dy. \tag{8.9}$$

Since Eq. (8.8) has a zero on the right, we look for an unknown function $\varphi(x, y) = \text{constant}$ and $d\varphi = 0$.

We have [if such a function $\varphi(x, y)$ exists]

$$P(x, y)dx + Q(x, y)dy = \frac{\partial \varphi}{\partial x}dx + \frac{\partial \varphi}{\partial y}dy \tag{8.10a}$$

and

$$\frac{\partial \varphi}{\partial x} = P(x, y), \quad \frac{\partial \varphi}{\partial y} = Q(x, y). \tag{8.10b}$$

The necessary and sufficient condition for our equation to be exact is that the second, mixed partial derivatives of $\varphi(x, y)$ (assumed continuous) are independent of the order of differentiation:

$$\frac{\partial^2 \varphi}{\partial y \partial x} = \frac{\partial P(x, y)}{\partial y} = \frac{\partial Q(x, y)}{\partial x} = \frac{\partial^2 \varphi}{\partial x \partial y}. \tag{8.11}$$

Note the resemblance to Eq. (1.124) of Section 1.12. If Eq. (8.8) corresponds to a curl (equal to zero), then a potential, $\varphi(x, y)$, must exist.

If $\varphi(x, y)$ exists then, from Eqs. (8.8) and (8.10a), our solution is

$$\varphi(x, y) = C.$$

We may construct $\varphi(x, y)$ from its partial derivatives, just as we construct a magnetic vector potential from its curl. See Exercises 8.2.7 and 8.2.8.

It may well turn out that Eq. (8.8) is not exact and that Eq. (8.11) is not satisfied. However, there always exists at least one and perhaps many more integrating factors, $\alpha(x, y)$, such that

$$\alpha(x, y)P(x, y)dx + \alpha(x, y)Q(x, y)dy = 0$$

is exact. Unfortunately, an integrating factor is not always obvious or easy to find. Unlike the case of the linear first-order differential equation to be considered next, there is no systematic way to develop an integrating factor for Eq. (8.8).

A differential equation in which the variables have been separated is automatically exact. An exact differential equation is not necessarily separable.

Linear First-Order ODEs

If $f(x, y)$ in Eq. (8.2) has the form $-p(x)y + q(x)$, then Eq. (8.2) becomes

$$\frac{dy}{dx} + p(x)y = q(x). \tag{8.12}$$

Equation (8.12) is the most general **linear** first-order ODE. If $q(x) = 0$, Eq. (8.12) is **homogeneous** (in y). A nonzero $q(x)$ may be regarded as a **source** or a **driving term** for the **inhomogeneous ODE**. In Eq. (8.12), each term is

linear in y or dy/dx. There are no higher powers, such as y^2, and no products, such as $y(dy/dx)$. Note that the **linearity** refers to the y and dy/dx; $p(x)$ and $q(x)$ need not be linear in x. Equation (8.12), the most important for physics of these first-order ODEs, may be solved exactly.

Let us look for an **integrating factor** $\alpha(x)$ so that

$$\alpha(x)\frac{dy}{dx} + \alpha(x)p(x)y = \alpha(x)q(x) \tag{8.13}$$

may be rewritten as

$$\frac{d}{dx}[\alpha(x)y] = \alpha(x)q(x). \tag{8.14}$$

The purpose of this is to make the left-hand side of Eq. (8.12) a derivative so that it can be integrated by inspection. It also, incidentally, makes Eq. (8.12) exact. Expanding Eq. (8.14), we obtain

$$\alpha(x)\frac{dy}{dx} + \frac{d\alpha}{dx}y = \alpha(x)q(x).$$

Comparison with Eq. (8.13) shows that we must require

$$\frac{d\alpha}{dx} = \alpha(x)p(x). \tag{8.15}$$

Here is a differential equation for $\alpha(x)$, with the variables α and x **separable**. We separate variables, integrate, and obtain

$$\alpha(x) = \exp\left[\int^x p(X)dX\right] \tag{8.16}$$

as our integrating factor. The lower limit is not written because it only multiplies α and the ODE by a constant, which is irrelevant.

With $\alpha(x)$ known we proceed to integrate Eq. (8.14). This, of course, was the point of introducing α in the first place. We have

$$\int^x \frac{d}{dX}[\alpha(X)y(X)]dX = \int^x \alpha(X)q(X)dX.$$

Now integrating by inspection, we have

$$\alpha(x)y(x) = \int^x \alpha(X)q(X)dX + C.$$

The constants from a constant lower limit of integration are absorbed in the constant C. Dividing by $\alpha(x)$, we obtain

$$y(x) = [\alpha(x)]^{-1}\left\{\int^x \alpha(X)q(X)dX + C\right\}.$$

Finally, substituting in Eq. (8.16) for α yields

$$y(x) = \exp\left[-\int^x p(X)dX\right]\left\{\int^x \exp\left[\int^Z p(Y)dY\right]q(Z)dZ + C\right\}. \tag{8.17}$$

Here the (dummy) variables of integration have been rewritten as capitals. Equation (8.17) is the complete general solution of the linear, first-order ODE, Eq. (8.12). The portion

$$y_h(x) = C \exp\left[-\int^x p(X)dX\right] \tag{8.18}$$

corresponds to the case $q(x) = 0$ and is a **general solution of the homogeneous ODE** because it contains the integration constant. The other term in Eq. (8.17),

$$y_p(x) = \exp\left[-\int^x p(X)dX\right]\int^x \exp\left[\int^Z p(Y)dY\right]q(Z)dZ, \tag{8.19}$$

is a **particular solution of the inhomogeneous ODE corresponding to the specific source term** $q(x)$.

Let us summarize this solution of the inhomogeneous ODE in terms of a method called **variation of the constant** as follows. In the first step, we solve the homogeneous ODE by separation of variables as before, giving

$$\frac{y'}{y} = -p, \quad \ln y = -\int^x p(X)dX + \ln C, \quad y(x) = Ce^{-\int^x p(X)dX}.$$

In the second step, we let the integration constant become x-dependent, that is, $C \to C(x)$. This is the variation of the constant used to solve the inhomogeneous ODE. Differentiating $y(x)$ we obtain

$$y' = -pCe^{-\int p(x)dx} + C'(x)e^{-\int p(x)dx} = -py(x) + C'(x)e^{-\int p(x)dx}.$$

Comparing with the inhomogeneous ODE we find the ODE for C:

$$C'e^{-\int p(x)dx} = q, \quad \text{or} \quad C(x) = \int^x e^{\int^X p(Y)dY}q(X)dX.$$

Substituting this C into $y = C(x)e^{-\int^x p(X)dX}$ reproduces Eq. (8.19).

Now we prove the *theorem* that **the solution of the inhomogeneous ODE is unique up to an arbitrary multiple of the solution of the homogeneous ODE**.

To show this, suppose y_1, y_2 both solve the inhomogeneous ODE [Eq. (8.12)]; then

$$y_1' - y_2' + p(x)(y_1 - y_2) = 0$$

follows by subtracting the ODEs and states that $y_1 - y_2$ is a solution of the homogeneous ODE. The solution of the homogeneous ODE can always be multiplied by an arbitrary constant. ■

We also prove the *theorem* that **a first-order linear homogeneous ODE has only one linearly independent solution**. This is meant in the following sense. If two solutions are **linearly dependent**, by definition they satisfy $ay_1(x) + by_2(x) = 0$ with nonzero constants a, b for all values of x. If the only solution of this linear relation is $a = 0 = b$, then our solutions y_1 and y_2 are said to be **linearly independent**.

To prove this theorem, suppose y_1, y_2 both solve the homogeneous ODE. Then

$$\frac{y_1'}{y_1} = -p(x) = \frac{y_2'}{y_2} \text{ implies } W(x) \equiv y_1'y_2 - y_1y_2' \equiv 0. \tag{8.20}$$

The functional determinant W is called the **Wronskian** of the pair y_1, y_2. We now show that $W \equiv 0$ is the condition for them to be linearly dependent. Assuming linear dependence, that is,

$$ay_1(x) + by_2(x) = 0$$

with nonzero constants a, b for all values of x, we differentiate this linear relation to get another linear relation

$$ay_1'(x) + by_2'(x) = 0.$$

The condition for these two homogeneous linear equations in the unknowns a, b to have a nontrivial solution is that their determinant be zero, which is $W = 0$.

Conversely, from $W = 0$, there follows linear dependence because we can find a nontrivial solution of the relation

$$\frac{y_1'}{y_1} = \frac{y_2'}{y_2}$$

by integration, which gives

$$\ln y_1 = \ln y_2 + \ln C, \quad \text{or} \quad y_1 = Cy_2.$$

Linear dependence and the Wronskian are generalized to three or more functions in Section 8.3. ■

EXAMPLE 8.2.3

Linear Independence The solutions of the linear oscillator equation $y'' + \omega^2 y(x) = 0$ are $y_1 = \sin \omega x$, $y_2 = \cos \omega x$, which we check by differentiation. The Wronskian becomes

$$\begin{vmatrix} \sin \omega x & \cos \omega x \\ \omega \cos \omega x & -\omega \sin \omega x \end{vmatrix} = -\omega \neq 0.$$

These two solutions, y_1 and y_2, are therefore linearly independent. For just two functions this means that one is not a multiple of the other, which is obviously true in this case.

You know that

$$\sin \omega x = \pm(1 - \cos^2 \omega x)^{1/2},$$

but this is **not** a **linear** relation. ■

Note that if our linear first-order differential equation is homogeneous ($q = 0$), then it is separable. Otherwise, apart from special cases such as $p =$ constant, $q =$ constant, or $q(x) = ap(x)$, Eq. (8.12) is not separable.

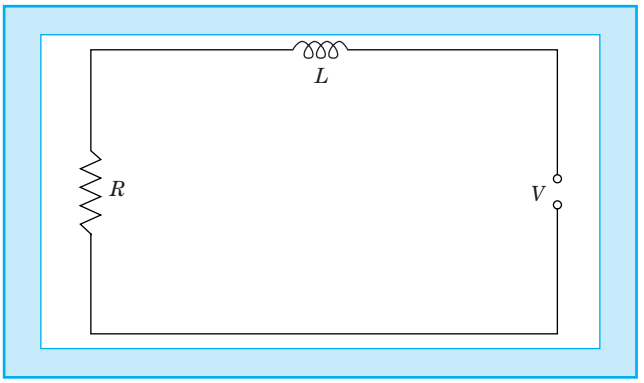


Figure 8.1
Circuit with Resistance R and Inductance L in Series

EXAMPLE 8.2.4 **RL Circuit** For a resistance–inductance circuit (Fig. 8.1 and Example 6.1.6) Kirchhoff's first law leads to

$$L\frac{dI(t)}{dt} + RI(t) = V(t) \tag{8.21}$$

for the current $I(t)$, where L is the inductance and R the resistance, both constant. Here, $V(t)$ is the time-dependent input voltage.

From Eq. (8.16), our integrating factor $\alpha(t)$ is

$$\alpha(t) = \exp \int^t \frac{R}{L} dT = e^{Rt/L}.$$

Then by Eq. (8.17),

$$I(t) = e^{-Rt/L}\left[\int^t e^{RT/L}\frac{V(T)}{L}dT + C\right], \tag{8.22}$$

with the constant C to be determined by an initial condition (a boundary condition).

For the special case $V(t) = V_0$, a constant,

$$I(t) = e^{-Rt/L}\left[\frac{V_0}{L}\cdot\frac{L}{R}e^{Rt/L} + C\right] = \frac{V_0}{R} + Ce^{-Rt/L}.$$

For a first-order ODE one initial condition has to be given. If it is $I(0) = 0$, then $C = -V_0/R$ and

$$I(t) = \frac{V_0}{R}[1 - e^{-Rt/L}]. \quad \blacksquare$$

ODEs of Special Type

Let us mention a few more types of ODEs that can be integrated analytically.

EXAMPLE 8.2.5

First-Order ODEs, with *y/x* Dependence The ODE $y' = f(y/x)$ is not of the form of Eq. (8.12) in general but is homogeneous in y. The substitution $z(x) = y(x)/x$, suggested by the form of the ODE, leads via $y' = xz' + z$ to the ODE $xz' + z = f(z)$, which is not of the type in Eq. (8.12). However, it is separable and can be integrated as follows:

$$z' = \frac{f(z) - z}{x}, \quad \int \frac{dz}{f(z) - z} = \int \frac{dx}{x} = \ln x + \ln C.$$

An explicit case is the ODE

$$xyy' = y^2 - x^2, \quad \text{or} \quad y' = \frac{y}{x} - \frac{x}{y}.$$

In terms of $z(x) = y/x$, we obtain $xz' + z = z - \frac{1}{z}$, or $zdz = -dx/x$, which has separated variables. We integrate it to get $z^2 = C - 2\ln x$, where C is the integration constant. We check that our solution $y = x\sqrt{C - 2\ln x}$ satisfies

$$y' = \sqrt{C - 2\ln x} - 1/\sqrt{C - 2\ln x}, \quad \text{or} \quad \frac{yy'}{x} = \frac{y^2}{x^2} - 1.$$

The constant C is determined by the initial condition. If, for example, $y(1) = 1$, we obtain $C = 1$. ■

Clairaut's ODE $y = xy' + f(y')$ can be solved in closed form despite the general nature of the function f in it.

Replacing y' by a constant C, we verify that each straight line $y = Cx + f(C)$ is a solution. The slope of each straight line coincides with the direction of the tangent prescribed by the ODE. A systematic method to find this class of solutions starts by setting $y' = u(x)$ in the ODE so that $y = xu + f(u)$ with the differential $udx = dy = udx + xdu + f'(u)du$. Dropping the udx term we find

$$[x + f'(u)]du = 0.$$

Setting each factor equal to zero, $du = 0$ yields $u = C = \text{const.}$ and the straight lines again. Next, eliminating u from the other factor set to zero,

$$x + f'(u) = 0, \quad \text{and} \quad y = xu + f(u)$$

generates another solution of Clairaut's ODE, a curve $(x(u), y(u))$ that no longer contains the arbitrary constant C. From $y' = u$, we verify $y = xu + f(u) = xy' + f(y')$. The pair of coordinates $x(u)$, $y(u)$ given previously represents a curve parameterized by the variable u; it represents the **envelope of the class of straight lines** $y = Cx + f(C)$ for various values of C that are tangents to this curve. The envelope of a class of solutions of an ODE is called its **singular solution**; it does not involve an integration constant (and cannot be adapted to initial conditions).

In general, **geometric problems in which a curve is to be determined from properties of its tangent at** x, y **lead to Clairaut's ODE** as follows. The **tangent equation** is given by

$$Y - y = y'(X - x), \quad \text{or} \quad Y = y'X + (y - xy'),$$

where X, Y are the coordinates of the tangent and y' is its slope. A property of the tangent can be expressed as some functional relation $F(y', y - xy') = 0$. Solving this relation for $y - xy'$ yields Clairaut's ODE. Let us illustrate this by the following example.

EXAMPLE 8.2.6

Envelope of Tangents as Singular Solution of Clairaut's ODE Determine a curve so that the length of the line segment T_1T_2 in Fig. 8.2 cut out of its tangent by the coordinate axes X, Y is a constant a. Setting $X = 0$ in the previous tangent equation gives the length OT_1 from the origin to T_1 on the Y-axis as $y - xy'$, and setting $Y = 0$ gives the OT_2 length on the X-axis as $(xy' - y)/y'$. The right-angle triangle with corners OT_1T_2 yields the tangent condition

$$(y - xy')^2 + \frac{(y - xy')^2}{y'^2} = a^2, \quad \text{or} \quad y = xy' \pm \frac{ay'}{\sqrt{y'^2 + 1}},$$

a Clairaut ODE with the general solution $y = xC \pm \frac{aC}{\sqrt{C^2+1}}$, which are straight lines. The envelope of this class of straight lines is obtained by eliminating u from

$$y = xu \pm \frac{au}{\sqrt{u^2 + 1}}, \quad x \pm a\left(\frac{1}{\sqrt{u^2 + 1}} - \frac{u^2}{\sqrt{u^2 + 1}^3}\right) = 0.$$

The second equation simplifies to $x \pm \frac{a}{\sqrt{u^2+1}^3} = 0$. Substituting $u = \tan\varphi$ yields $x \pm a\cos^3\varphi = 0$ and

$$y = \mp a\cos^3\varphi \pm a\sin\varphi = \pm a\sin^3\varphi$$

from the first equation. Eliminating the parameter φ from $x(\varphi)$, $y(\varphi)$ yields the astroid $x^{2/3} + y^{2/3} = a^{2/3}$, plotted in Fig. 8.2. ■

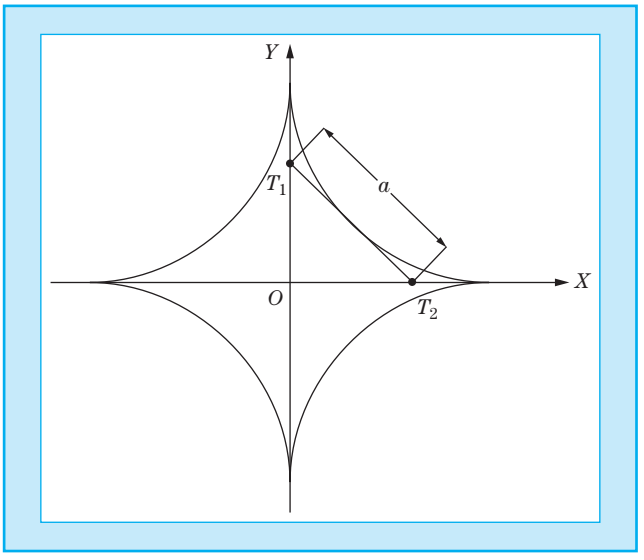


Figure 8.2

Astroid as Envelope of Tangents of Constant Length $T_1T_2 = a$

First-order differential equations will be discussed again in Chapter 15 in connection with Laplace transforms, in Chapter 18 with regard to the Euler equation of the calculus of variations, and in Chapter 19 with regard to nonlinear (Riccati and Bernoulli's) ODEs. Numerical techniques for solving first-order differential equations are examined in Section 8.7.

SUMMARY

In summary, **first-order** ODEs of the implicit form $F(x, y, y') = 0$ (as discussed in the context of Clairaut's ODE) or explicit form $y' = f(x, y)$ contain the variable x, the unknown function $y(x)$, and its derivative $\frac{dy}{dx} = y'(x)$. The general solution contains one arbitrary constant, called the integration constant, which often is determined by an initial condition $y(x_0) = y_0$ involving given constants x_0, y_0. Such ODEs are sometimes called initial value problems.

Among the simplest ODEs are separable equations $y' = f(x, y) = -\frac{P(x)}{Q(y)}$ of Section 8.2. Their general solution is obtained by the integration $\int_{x_0}^{x} P(X)dX + \int_{y_0}^{y} Q(Y)dY = \text{const}$.

Closely related are the more general **exact** differential equations

$$P(x, y)dx + Q(x, y)dy = d\varphi = \frac{\partial \varphi}{\partial x}dx + \frac{\partial \varphi}{\partial y}dy$$

with the integrability condition $\frac{\partial P}{\partial y} = \frac{\partial Q}{\partial x}$. If the **integrability condition** is not satisfied, a solution $\varphi(x, y)$ does not exist. In that case, one has to search for an **integrating factor** $\alpha(x, y)$ so that $\frac{\partial(\alpha P)}{\partial y} = \frac{\partial(\alpha Q)}{\partial x}$ holds.

Linear first-order equations $y' + p(x)y = q(x)$ are common ODEs. The radioactive decay law and electrical circuits are prime examples. The homogeneous ODE $y' + py = 0$ is separable and integrated first, yielding $\ln y + \int^{x} p\,dX = \ln C$; then the integration constant $C \to C(x)$ is varied to find the solution of the inhomogeneous ODE.

EXERCISES

8.2.1 From Kirchhoff's law, the current I in an RC (resistance–capacitance) circuit [change L to C in Fig. 8.1 and remove $V(t)$; that is, short out the circuit] obeys the equation

$$R\frac{dI}{dt} + \frac{1}{C}I = 0.$$

(a) Find $I(t)$.

(b) For a capacitance of 10,000 μF charged to 100 V and discharging through a resistance of 1 mΩ, find the current I for $t = 0$ and for $t = 100$ sec.

Note. The initial voltage is I_0R or Q/C, where $Q = \int_0^{\infty} I(t)dt$.

8.2.2 The Laplace transform of Bessel's equation ($n = 0$) leads to

$$(s^2 + 1)f'(s) + sf(s) = 0.$$

Solve for $f(s)$.

8.2.3 The decay of a population by catastrophic two-body collisions is described by

$$\frac{dN}{dt} = -kN^2$$

for $t \geq 0$. This is a first-order, **nonlinear** differential equation. Derive the solution

$$N(t) = N_0\left(1 + \frac{t}{\tau_0}\right)^{-1},$$

where $\tau_0 = (kN_0)^{-1}$ and N_0 is the population at time $t = 0$. This implies an infinite population at $t = -\tau_0$, which is irrelevant because the initial value problem starts at $t = 0$ with $N(0) = N_0$.

8.2.4 The rate of a particular chemical reaction $A + B \rightarrow C$ is proportional to the concentrations of the reactants A and B:

$$\frac{dC(t)}{dt} = \alpha[A(0) - C(t)][B(0) - C(t)],$$

where $A(0) - C(t)$ is the amount of A left to react at time t, and similarly for B.

(a) Find $C(t)$ for $A(0) \neq B(0)$.

(b) Find $C(t)$ for $A(0) = B(0)$.

The initial condition is that $C(0) = 0$.

8.2.5 A boat coasting through the water experiences a resisting force proportional to v^n, where v is the boat's instantaneous velocity and n an integer. Newton's second law leads to

$$m\frac{dv}{dt} = -kv^n.$$

With $v(t = 0) = v_0$, $x(t = 0) = 0$, integrate to find v as a function of time and v as a function of distance.

8.2.6 The differential equation

$$P(x, y)dx + Q(x, y)dy = 0$$

is **exact**. Verify that

$$\varphi(x, y) = \int_{x_0}^{x} P(X, Y)dX + \int_{y_0}^{y} Q(X, Y)dY = \text{constant}$$

is a solution.

8.2.7 The differential equation

$$P(x, y)dx + Q(x, y)dy = 0$$

is **exact**. If

$$\varphi(x, y) = \int_{x_0}^{x} P(X, Y)dX + \int_{y_0}^{y} Q(x, Y)dY,$$

show that

$$\frac{\partial \varphi}{\partial x} = P(x, y), \qquad \frac{\partial \varphi}{\partial y} = Q(x, y).$$

Hence, $\varphi(x, y) =$ constant is a solution of the original differential equation.

8.2.8 Prove that Eq. (8.13) is exact in the sense of Eq. (8.8), provided that $\alpha(x)$ satisfies Eq. (8.15).

8.2.9 A certain differential equation has the form

$$f(x)dx + g(x)h(y)dy = 0,$$

with none of the functions $f(x)$, $g(x)$, $h(y)$ identically zero. Show that a necessary and sufficient condition for this equation to be exact is that $g(x) =$ constant.

8.2.10 Show that

$$y(x) = \exp\left[-\int^x p(t)dt\right]\left\{\int^x \exp\left[\int^s p(t)dt\right]q(s)ds + C\right\}$$

is a solution of

$$\frac{dy}{dx} + p(x)y(x) = q(x)$$

by differentiating the expression for $y(x)$ and substituting into the differential equation.

8.2.11 The motion of a body falling in a resisting medium may be described by

$$m\frac{dv}{dt} = mg - bv$$

when the retarding force is proportional to the velocity, v. Find the velocity. Evaluate the constant of integration by demanding that $v(0) = 0$. Explain the signs of the terms mg and bv.

8.2.12 The rate of evaporation from a particular spherical drop of liquid (constant density) is proportional to its surface area. Assuming this to be the sole mechanism of mass loss, find the radius of the drop as a function of time.

8.2.13 In the linear homogeneous differential equation

$$\frac{dv}{dt} = -av$$

the variables are separable. When the variables are separated the equation is exact. Solve this differential equation subject to $v(0) = v_0$ by the following three methods:

(a) separating variables and integrating;
(b) treating the separated variable equation as exact; and
(c) using the result for a linear homogeneous differential equation.

ANS. $v(t) = v_0e^{-at}$.

8.2.14 Bernoulli's equation,

$$\frac{dy}{dt} + f(x)y = g(x)y^n$$

is nonlinear for $n \neq 0$ or 1. Show that the substitution $u = y^{1-n}$ reduces Bernoulli's equation to a linear equation.

ANS. $\dfrac{du}{dx} + (1-n)f(x)u = (1-n)g(x).$

8.2.15 Solve the linear, first-order equation, Eq. (8.12), by assuming $y(x) = u(x)v(x)$, where $v(x)$ is a solution of the corresponding homogeneous equation $[q(x) = 0]$.

8.2.16 (a) Rework Example 8.2.2 with an initial speed $v_i = 60$ miles/hr, when the parachute opens. Find $v(t)$.
(b) For a skydiver in free fall (no parachute) use the much smaller friction coefficient $b = 0.25$ kg/m and $m = 70$ kg. What is the limiting velocity in this case?

ANS. $v_0 = 52$ m/sec $= 187$ km/hr.

8.2.17 The flow lines of a fluid are given by the hyperbolas $xy = C = \text{const.}$ Find the orthogonal trajectories (equipotential lines) and plot them along with the flow lines using graphical software.
Hint. Start from $y' = \tan\alpha$ for the hyperbolas.

8.2.18 Heat flows in a thin plate in the xy-plane along the hyperbolas $xy = \text{const.}$ What are the lines of constant temperature (isotherms)?

8.2.19 Solve the ODE $y' = ay/x$ for real a and initial condition $y(0) = 1$.

8.2.20 Solve the ODE $y' = y + y^2$ with $y(0) = 1$.

8.2.21 Solve the ODE $y' = \frac{1}{x+y}$ with $y(0) = 0$.

ANS. $x(y) = e^y - 1 - y.$

8.2.22 Find the general solution of $y'^3 - 4xyy' + 8y^2 = 0$ and its singular solution. Plot them.

ANS. $y = C(x - C)^2$. The singular solution is $y = \frac{4}{27}x^3$.

8.3 Second-Order ODEs

Linear ODEs of second order are most common in physics and engineering applications because of dynamics: In classical mechanics the acceleration is a second-order derivative and so is the kinetic energy in quantum mechanics. Thus, any problem of classical mechanics, where we describe the motion of a particle subject to a force, involves an ODE. Specifically, a force or driving term leads to an inhomogeneous ODE. In quantum mechanics we are led to the Schrödinger equation, a PDE. We will develop methods to find **particular solutions of the inhomogeneous ODE** and the **general solution of the homogeneous ODE**, such as the variation of constants, power-series expansion, and Green's functions. Special classes of ODEs are those with **constant**

coefficients that occur in RLC electrical circuits and harmonic oscillators in classical mechanics. The simple harmonic oscillator of quantum mechanics is treated in Chapter 13. Nonlinear ODEs are addressed in Chapter 19. We start this section with examples of special classes of ODEs. We use the standard notation[2] $dy/dx = y'$, $d^2y/dx^2 = y''$.

In Examples 8.3.1 and 8.3.2, we encounter a general feature. **Because the solution of a second-order ODE involves two integrations, the general solution will contain two integration constants that may be adjusted to initial or boundary conditions.**

When one variable is missing in the ODE, such as x or y, the ODE can be reduced to a first-order ODE.

EXAMPLE 8.3.1

Second-Order ODEs, Missing Variable y If the unknown function y **is absent from the ODE**, as in

$$y'' = f(y', x), \tag{8.23}$$

then it becomes a first-order ODE for $z(x) = y'(x)$, $z' = f(z, x)$. If $z(x, C_1)$ is a solution of this ODE depending on an integration constant C_1, then

$$y(x) = \int^x z(X, C_1)dX + C_2$$

is the general solution of the second-order ODE.

A simple example is the ODE $y'' = y'$ with boundary conditions $y(0) = 1$, $y(-\infty) = 0$.

Setting $z = y'$, we solve $\frac{dz}{dx} = z$ by integrating

$$\int^z \frac{dZ}{Z} = \ln z = \int^x dX = x + \ln C_1.$$

Exponentiating we obtain

$$z = C_1 e^x = \frac{dy}{dx}.$$

Integrating again we find

$$y = C_1 \int^x e^X dX + C_2 = C_1 e^x + C_2.$$

We check our solution by differentiating it twice: $y' = C_1 e^x$, $y'' = C_1 e^x = y'$. The boundary conditions $y(0) = 1$, $y(-\infty) = 0$ determine the integration constants C_1, C_2. They give $C_1 + C_2 = 1$ and $C_2 = 0$ so that $C_1 = 1$ results, and the solution is $y = e^x$.

Another specific case is $y'' = y'^2$ with initial conditions $y(0) = 2$, $y'(0) = -1$.

[2]This prime notation y' was introduced by Lagrange in the late 18th century as an abbreviation for Leibniz's more explicit but more cumbersome dy/dx.

We start by integrating $z' = z^2$, or

$$\int^z \frac{dZ}{Z^2} = -1/z = \int^x dX + C_1.$$

This yields $z = y' = \frac{-1}{x+C_1}$. Integrating again we find

$$y(x) = -\ln(x + C_1) + C_2.$$

Checking this solution gives $y'' = (x+C_1)^{-2} = y'^2$. The initial conditions yield $2 = -\ln C_1 + C_2$, $-1 = -1/C_1$ so that $C_1 = 1$, implying $C_2 = 2$. The solution is $y = -\ln(x + 1) + 2$.

A third case is the ODE $y'' = (xy')^2$. We solve $z' = (xz)^2$ by separating variables:

$$\int^z \frac{dZ}{Z^2} = \frac{-1}{z} = \int^x X^2\, dX = \frac{1}{3}(x^3 - C_1^3).$$

We have chosen the integration constant in this special cubic form so that we can factorize the third-order polynomial

$$x^3 - C_1^3 = (x - C_1)(x^2 + C_1x + C_1^2)$$

and, in the ODE,

$$z = y' = \frac{-3}{x^3 - C_1^3}$$

decompose the inverse polynomial into partial fractions

$$\frac{1}{x^3 - C_1^3} = \frac{1}{x - C_1} + \frac{i}{C_1\sqrt{3}}\left(\frac{1}{x + \frac{C_1}{2}(1 + i\sqrt{3})} - \frac{1}{x + \frac{C_1}{2}(1 - i\sqrt{3})}\right).$$

Integrating the ODE yields the solution

$$y(x) = -3\ln(x - C_1) + \ln C_2$$
$$-i\frac{\sqrt{3}}{C_1}[\ln(x + C_1(1 + i\sqrt{3})/2) - \ln(x + C_1(1 - i\sqrt{3})/2)]. \quad \blacksquare$$

EXAMPLE 8.3.2 **Second-Order ODEs, Missing Variable x** If the variable x does not appear in the ODE, as in

$$y'' = f(y', y), \tag{8.24}$$

then we seek a solution $y' = z(y)$ instead of searching for $y(x)$ directly. Using the chain rule we obtain

$$y'' = \frac{dz}{dy}\frac{dy}{dx} = z\frac{dz}{dy} = f(z, y),$$

which is a first-order ODE for $z(y)$. If we can find a solution $z(y, C_1)$, then we can integrate $y' = z(y)$ to get

$$\int^y \frac{dY}{z(Y, C_1)} = \int^x dX = x + C_2. \quad \blacksquare$$

EXAMPLE 8.3.3

y″ + f(x)y′ + g(y)y′² = 0 This more general and nonlinear ODE is a combination of the types treated in Examples 8.3.1 and 8.3.2 so that we try a product solution $y' = v(x)w(y)$ incorporating the previous solution types. Differentiating this ansatz (trial solution) and substituting into the ODE we find

$$y'' = v'w + v\frac{dw}{dy}y' = v'w + v^2w\frac{dw}{dy} = -fvw - gv^2w^2.$$

Here, we divide by an overall factor v^2w without loss of generality because we reject $y' = 0$ as a trivial solution. We can solve the resulting ODE

$$\frac{v' + f(x)v}{v^2} + \frac{dw}{dy} + g(y)w(y) = 0$$

by choosing $v(x)$ as a solution of the first-order ODE $v' + f(x)v(x) = 0$ from the first term alone and $w(y)$ as a solution of the first-order ODE $\frac{dw}{dy} + g(y)w(y) = 0$ from the second term alone. Both ODEs can be solved by separating variables

$$\int^v \frac{dV}{V} = -\int^x f(X)dX = \ln v, \quad \int^w \frac{dW}{W} = -\int^y g(Y)dY = \ln w.$$

Alternatively, integrating the ODE written in the form

$$\frac{y''}{y'} + f(x) + g(y)y' = 0$$

yields

$$\ln y' + \int^x f(X)dX + \int^y g(Y)dY = C,$$

where C is an integration constant. Exponentiating this result gives the same solution.

Let us illustrate a more specific example:

$$xyy'' + yy' - xy'^2 = 0.$$

where $f(x) = \frac{1}{x}$ and $g(y) = -\frac{1}{y}$ so that $\ln v = -\ln x + \ln C_1$ [i.e., $v(x) = \frac{C_1}{x}$] and $\ln w = \ln y + \ln C_2$ [i.e., $w(y) = C_2y$]. Therefore, $y' = C_1C_2y/x$, which we integrate as

$$\ln y = C_1C_2 \ln x + \ln C_3$$

so that finally $y(x) = C_3x^{C_1C_2}$, a power law that indeed satisfies the ODE. ■

EXAMPLE 8.3.4

Euler's ODE Euler's ODE,

$$ax^2y'' + bxy' + cy = 0, \tag{8.25}$$

is a **homogeneous linear** ODE that can be solved with a power ansatz $y = x^p$. This power law is a natural guess because the reduction of the exponent by differentiation is restored by the coefficients x, x^2 of the y' and y'' terms, each producing the same power.

Substituting $y' = px^{p-1}$, $y'' = p(p-1)x^{p-2}$ into the ODE yields

$$[ap(p-1) + bp + c]x^p = 0,$$

an **algebraic equation for the exponent** but only for the homogeneous ODE. Now we drop the factor x^p to find two roots p_1, p_2 from the quadratic equation. If both exponents p_i are real, the **general solution** is

$$C_1 x^{p_1} + C_2 x^{p_2}.$$

If the **exponents are complex conjugates** $p_{1,2} = r \pm iq$, then the Euler identity for $x^{iq} = e^{iq \ln x}$ yields the **general solution**

$$y(x) = x^r [C_1 \cos(q \ln x) + C_2 \sin(q \ln x)].$$

If there is a **degenerate** solution $p_1 = p_2 = p$ for the exponent, we approach the degenerate case by letting the exponents become equal in the linear combination $(x^{p+\varepsilon} - x^p)/\varepsilon$, which is a solution of the ODE for $\varepsilon \to 0$. This may be achieved by slightly varying the coefficients a, b, c of the ODE so that the degenerate exponent p splits into $p + \varepsilon$ and p. Thus, we are led to differentiate x^p with respect to p. This yields the second solution $x^p \ln x$ and the **general solution**

$$y = x^p (C_1 + C_2 \ln x).$$

A specific example is the ODE

$$x^2 y'' + 3xy' + y = 0 \quad \text{with} \quad p(p-1) + 3p + 1 = 0 = (p+1)^2$$

so that $p = -1$ is a degenerate exponent. Thus, the solution is $y(x) = \frac{C_1}{x} + C_2 \frac{\ln x}{x}$. ■

EXAMPLE 8.3.5

ODEs with Constant Coefficients ODEs with constant coefficients

$$ay'' + by' + cy = 0 \tag{8.26}$$

are solved with the exponential ansatz $y = e^{px}$. This is a natural guess because differentiation reproduces the exponential up to a multiplicative constant $y' = py$ and $y'' = p^2 y$. Hence, substituting **the exponential ansatz reduces the ODE to the quadratic equation**

$$ap^2 + bp + c = 0$$

for the exponent. If there are **two real roots** p_1, p_2, then

$$y = C_1 e^{p_1 x} + C_2 e^{p_2 x}$$

is the general solution. If $p_1 > 0$, or $p_2 > 0$, we have an exponentially growing solution. When $p_1 < 0$, and $p_2 < 0$, we have the **overdamped** solution displayed in Fig. 8.3.

Figure 8.3

Typical Solution of ODE with Constant Coefficients: Two Negative Exponents

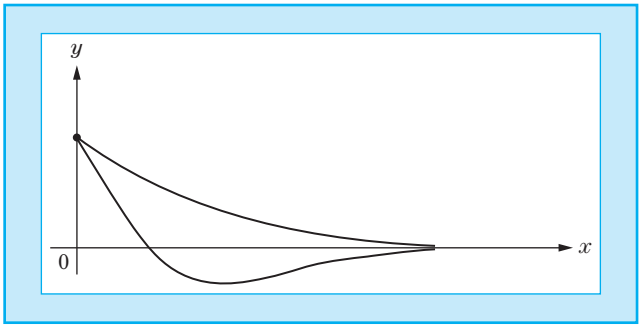
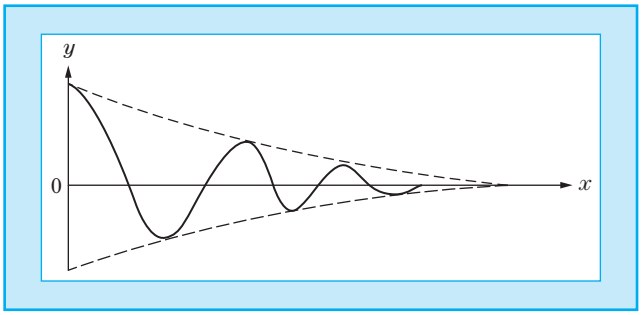


Figure 8.4

Typical Solution of ODE with Constant Coefficients: Two Complex Conjugate Exponents



If there are **two complex conjugate roots**, then Euler's identity yields

$$p_{1,2} = r \pm iq, \qquad y(x) = e^{rx}(C_1 \cos qx + C_2 \sin qx)$$

as the **general oscillatory or underdamped solution** (Fig. 8.4).

If there is **one degenerate exponent**, we approach the degenerate case with two slightly different exponents $p + \varepsilon$ and p for $\varepsilon \to 0$ in the solution $[e^{(p+\varepsilon)x} - e^{px}]/\varepsilon$ of the ODE. Again, as in Example 8.3.4, this leads us to differentiate e^{px} with respect to p to find the **second solution** xe^{px}, giving the general **critically damped solution** $y = e^{px}(C_1 + C_2 x)$ for the double-root case (Fig. 8.5). See also Examples 15.8.1, 15.9.1, and 15.10.1 for a solution by Laplace transform. ■

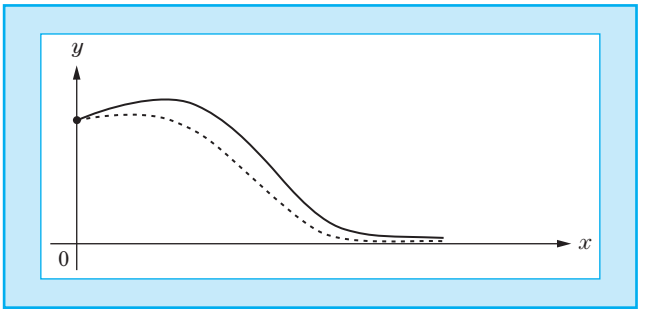
Because ODEs with constant coefficients and Euler's ODEs are linear in the unknown function y and homogeneous, we have used the **superposition principle** in Examples 8.3.4 and 8.3.5: If y_1, y_2 are two solutions of the homogeneous ODE, so is the linear combination $C_1 y_1 + C_2 y_2$ with constants C_1, C_2 that are fixed by initial or boundary conditions as usual.

The same exponential form $y(x) = e^{px}$ leads to the solutions of nth-order ODEs

$$a_0 y^{(n)} + a_1 y^{(n-1)} + \cdots + a_{n-1} y' + a_n y = 0$$

Figure 8.5

Typical Solutions of ODE with Constant Coefficients: Two Equal Exponents



with constant coefficients a_i in terms of exponents p_i that are roots of the polynomial equation

$$a_0 p^n + a_1 p^{n-1} + \cdots + a_{n-1} p + a_n = 0.$$

The general solution is the linear combination

$$y(x) = \sum_{i=1}^{n} b_i e^{p_i x},$$

where the constants b_i are determined by initial or boundary conditions.

Other generalizations are coupled ODEs with constant coefficients. Several cases are treated in Chapter 19 (Examples 19.4.6–19.4.10) in the context of linear approximations to nonlinear ODEs.

Inhomogeneous Linear ODEs and Particular Solutions

We have already discussed inhomogeneous first-order ODEs, such as Eq. (8.12). The general solution $y(x) = y_h(x) + y_p(x)$ is a sum of the general solution y_h of the homogeneous ODE and a particular solution y_p of the inhomogeneous ODE, which can be immediately verified by substituting y into the inhomogeneous ODE. This theorem generalizes to nth-order linear ODEs, the general solution being $y(x) = y_p(x) + \sum_{i=1}^{n} c_i y_i(x)$, where y_i are the independent solutions of the homogeneous ODE with constants c_i. The particular solution y_p usually inherits its form from the driving term $q(x)$ provided differentiations produce the same types of functions that $q(x)$ contains. The next few examples are cases in point, where we treat special types of functions $q(x)$, such as power laws, periodic functions, exponentials, and their combinations.

Inhomogeneous Euler ODE

Let us look at the inhomogeneous Euler ODE with a power law driving term

$$ax^2 y'' + bxy' + cy = Dx^d,$$

where the exponent d and strength D are known numbers. The power law is the natural form for the Euler ODE because each term retains its exponent. Substituting the ansatz $y_p = Ax^d$ into the Euler ODE, we realize that each

term contains the same power x^d, which we can drop. We obtain

$$A[ad(d-1)+bd+c]=D,$$

which determines A provided d is not an exponent of the homogeneous ODE.

If d is an exponent of the homogeneous ODE, that is, $ad(d-1)+bd+c=0$, then our solution $y_p=x^d(A+B\ln x)$ is a linear combination of both contributions of the degenerate case in Example 8.3.4. Substituting this trial solution into Euler's ODE yields

$$\begin{aligned} Dx^d &= ax^2y''+bxy'+cy \\ &= x^d[a(d-1)dA+a(d-1)dB\ln x+a(2d-1)B+bdA \\ &\quad +bdB\ln x+bB+cA+cB\ln x] \\ &= x^d(A[a(d-1)d+bd+c]+B[a(2d-1)+b] \\ &\quad +B[a(d-1)d+bd+c]\ln x), \end{aligned}$$

where the terms containing a come from y_p'', those containing b from y_p', and those containing c from y_p. Now we drop x^d and use $ad(d-1)+bd+c=0$, obtaining

$$D=B[a(2d-1)+b],$$

thereby getting B in terms of D, whereas A is not determined by the source term; A can be used to satisfy an initial or boundary condition. The source can also have the more general form $x^d(D+E\ln x)$ in the degenerate case.

For an exponential driving term

$$ax^2y''+bxy'+cy=De^{-x},$$

the powers of x in the ODE force us to a more complicated trial solution $y_p=e^{-x}\sum_{n=0}^{\infty}a_nx^n$. Substituting this ansatz into Euler's ODE yields recursion relations for the coefficients a_n. Such power series solutions are treated more systematically in Section 8.5. Similar complications arise for a periodic driving term, such as $\sin\omega x$, which shows that these forms are not natural for Euler's ODE.

Inhomogeneous ODE with Constant Coefficients

We start with a natural driving term of exponential form

$$ay''+by'+cy=De^{-dx},$$

where the strength D and exponent d are known numbers. We choose a particular solution $y_p=Ae^{-dx}$ of the same form as the source, because the derivatives preserve it. Substituting this y_p into the ODE with constant coefficients a, b, c yields

$$A[ad^2-bd+c]=D,$$

determining A in terms of D, provided d is not an exponent of the homogeneous ODE.

If the latter is the case, that is, $ad^2 - bd + c = 0$, we have to start from the more general form $y_p = e^{-dx}(A + Bx)$ appropriate for the degenerate case of Example 8.3.5. Substituting this y_p into the ODE yields

$$\begin{aligned} D &= ad^2(A + Bx) - 2adB - bd(A + Bx) + bB + c(A + Bx) \\ &= A[ad^2 - bd + c] + Bx[ad^2 - bd + c] + B(b - 2ad), \end{aligned}$$

where the terms containing a come from y_p'', those containing b from y_p' and c from y_p. Now we drop the terms containing $ad^2 - bd + c = 0$ to obtain

$$B(b - 2ad) = D,$$

determining B in terms of D, while A remains free to be adjusted to an initial or boundary condition.

A source term of polynomial form is solved by a particular solution of polynomial form of the same degree if the coefficient of the y term in the ODE is nonzero; if not, the degree of y increases by one, etc.

Periodic source terms, such as $\cos \omega x$ or $\sin \omega x$, are also natural and lead to particular solutions of the form $y_p = A \cos \omega x + B \sin \omega x$, where both the sine and cosine have to be included because the derivative of the sine gives the cosine and vice versa. We deal with such a case in the next example.

EXAMPLE 8.3.6

Electrical Circuit Let us take Example 8.2.4, include a capacitance C and an external AC voltage $V(t) = V_0 \sin \omega t$ in series to form an RLC circuit (Fig. 8.6). Here, the $\sin \omega t$ driving term leads to a particular solution $y_p \sim \sin(\omega t - \varphi)$, a sine shape with the same frequency ω as the driving term.

The voltage drop across the resistor is RI, across the inductor it is given by the instantaneous rate of change of the current $L\frac{dI}{dt}$, and across the capacitor it is given by Q/C with the charge $Q(t)$ giving

$$L\frac{dI}{dt} + RI + \frac{Q}{C} = V_0 \sin \omega t.$$

Because $I(t) = \frac{dQ}{dt}$, we differentiate both sides of this equation to obtain the ODE with constant coefficients

$$L\frac{d^2I}{dt^2} + R\frac{dI}{dt} + \frac{I}{C} = \omega V_0 \cos \omega t.$$

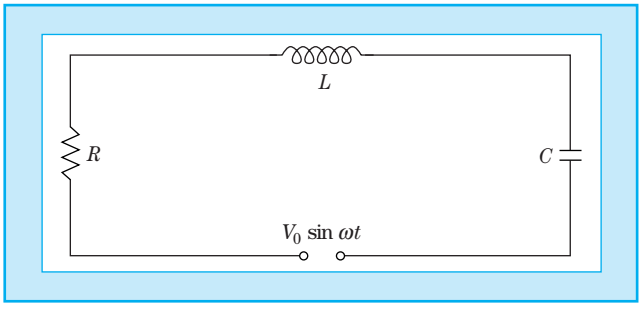


Figure 8.6

Electrical Circuit: Resistance, Inductance, and Capacitance in Series

Comparing this ODE with the harmonic oscillator ODE in classical mechanics, we see that the inductance L is the electrical analog of the mass, the resistance R is the analog of the damping, and the inverse of the capacitance $1/C$ is the analog of a spring constant, whereas the current I is the analog of the mechanical displacement $x(t)$. The general solution of the **homogeneous** ODE is

$$I_h = C_1 e^{p_1 t} + C_2 e^{p_2 t},$$

where $p = p_1$ and $p = p_2$ are the roots of the quadratic equation

$$p^2 + \frac{R}{L}p + \frac{1}{LC} = 0, \quad p = -\frac{R}{2L} \pm \frac{1}{2L}\sqrt{R^2 - \frac{4L}{C}}.$$

Because of the dominant negative term $-R/2L$ in p (note the negative sign in the radicand), I_h is a **transient current that decays exponentially with time**.

We now look for the **particular solution** with the same harmonic form as the driving voltage $I_p = A\cos\omega t + B\sin\omega t$. This is called the **steady-state current** with the same frequency as the input, which survives after a sufficiently long time ($-p_2 t \gg 1$). This is seen from the general solution $I = I_p + I_h$. In this sense, the steady-state current is an asymptotic form, but it is a particular solution that is present from the initial time onward. We differentiate I_p twice, substitute into the ODE, and compare the coefficients of the $\sin\omega t$ and $\cos\omega t$ terms. This yields

$$-\omega^2 L(A\cos\omega t + B\sin\omega t) + R\omega(-A\sin\omega t + B\cos\omega t) + \frac{1}{C}(A\cos\omega t + B\sin\omega t) = \omega V_0 \cos\omega t$$

so that

$$-\omega^2 LA + \omega RB + \frac{A}{C} = \omega V_0, \quad -\omega^2 LB - \omega RA + \frac{B}{C} = 0.$$

From the second of these equations we find

$$A = -B\frac{S}{R}, \quad S = \omega L - \frac{1}{\omega C},$$

where S is defined as the reactance by electrical engineers. Substituting this expression A into the first equation yields

$$B = \frac{V_0 R}{R^2 + S^2} \quad \text{so that} \quad A = -\frac{V_0 S}{R^2 + S^2}.$$

The steady-state current may also be written as

$$I_p = I_0 \sin(\omega t - \varphi), \quad I_0 = \sqrt{A^2 + B^2} = \frac{V_0}{\sqrt{R^2 + S^2}}, \quad \tan\varphi = -\frac{A}{B} = \frac{S}{R},$$

where $\sqrt{R^2 + S^2}$ is the impedance. ■

More examples of coupled and nonlinear ODEs are given in Chapter 19, particularly Examples 19.4.6–19.4.10.

Finally, let us address the **uniqueness and generality** of our solutions. If we have found **a particular solution of a linear inhomogeneous second-order ODE**

$$y'' + P(x)y' + Q(x)y = f(x), \tag{8.27}$$

then it **is unique up to an additive solution of the homogeneous ODE.** To show this theorem, suppose y_1, y_2 are two solutions. Subtracting both ODEs it follows that $y_1 - y_2$ is a solution of the homogeneous ODE

$$y'' + P(x)y' + Q(x)y = 0 \tag{8.28}$$

because of linearity of the ODE in y, y', y'' and $f(x)$ cancels. ■

The general solution of the homogeneous ODE [Eq. (8.28)] **is a linear combination of two linearly independent solutions.** To prove this theorem we assume there are three solutions and show that there is a linear relation between them. The analysis will lead us to the generalization of the Wronskian of two solutions of a first-order ODE in Section 8.2. Therefore, now we consider the question of linear independence of a set of functions.

Linear Independence of Solutions

Given a set of functions, φ_λ, the criterion for linear dependence is the existence of a relation of the form

$$\sum_\lambda k_\lambda \varphi_\lambda = 0, \tag{8.29}$$

in which **not all the coefficients k_λ are zero**. On the other hand, if the only solution of Eq. (8.29) is $k_\lambda = 0$ for all λ, the set of functions φ_λ is said to be linearly **independent**. In other words, functions are linearly independent if they cannot be obtained as solutions of linear relations that hold for all x.

It may be helpful to think of linear dependence of vectors. Consider **A**, **B**, and **C** in three-dimensional space with $\mathbf{A} \cdot \mathbf{B} \times \mathbf{C} \neq 0$. Then no nontrivial relation of the form

$$a\mathbf{A} + b\mathbf{B} + c\mathbf{C} = 0 \tag{8.30}$$

exists. **A**, **B**, and **C** are linearly independent. On the other hand, any fourth vector **D** may be expressed as a linear combination of **A**, **B**, and **C** (see Section 2.1). We can always write an equation of the form

$$\mathbf{D} - a\mathbf{A} - b\mathbf{B} - c\mathbf{C} = 0, \tag{8.31}$$

and the four vectors are **not** linearly independent. The three noncoplanar vectors **A**, **B**, and **C** span our real three-dimensional space.

Let us assume that the functions φ_λ are differentiable as needed. Then, differentiating Eq. (8.29) repeatedly, we generate a set of equations

$$\sum_\lambda k_\lambda \varphi'_\lambda(x) = 0, \tag{8.32}$$

$$\sum_\lambda k_\lambda \varphi''_\lambda(x) = 0, \tag{8.33}$$

and so on. This gives us a set of homogeneous linear equations in which k_λ are the unknown quantities. By Section 3.1 there is a solution $k_\lambda \neq 0$ only if the determinant of the coefficients of the k_λs vanishes for all values of x. This means that the **Wronskian** of $\varphi_1, \varphi_2, \ldots, \varphi_n$,

$$W(\varphi_1, \varphi_2, \ldots, \varphi_n) \equiv \begin{vmatrix} \varphi_1 & \varphi_2 & \cdots & \varphi_n \\ \varphi_1' & \varphi_2' & \cdots & \varphi_n' \\ \cdots & \cdots & \cdots & \cdots \\ \varphi_1^{(n-1)} & \varphi_2^{(n-1)} & \cdots & \varphi_n^{(n-1)} \end{vmatrix}, \tag{8.34}$$

a function of x, vanishes for all x.

1. If the Wronskian is not equal to zero, then Eq. (8.29) has no solution other than $k_\lambda = 0$. The set of functions φ_λ is therefore linearly independent.
2. If the Wronskian vanishes at isolated values of the argument, this does not necessarily prove linear dependence (unless the set of functions has only two functions). However, if the Wronskian is zero over the entire range of the variable, the functions φ_λ are linearly dependent over this range.[3]

EXAMPLE 8.3.7

Linear Dependence For an illustration of linear dependence of three functions, consider the solutions of the one-dimensional diffusion equation $y'' = y$. We have $\varphi_1 = e^x$ and $\varphi_2 = e^{-x}$, and we add $\varphi_3 = \cosh x$, also a solution. The Wronskian is

$$\begin{vmatrix} e^x & e^{-x} & \cosh x \\ e^x & -e^{-x} & \sinh x \\ e^x & e^{-x} & \cosh x \end{vmatrix} = 0.$$

The determinant vanishes for all x because the first and third rows are identical. Hence, e^x, e^{-x}, and $\cosh x$ are linearly dependent, and indeed, we have a relation of the form of Eq. (8.29):

$$e^x + e^{-x} - 2\cosh x = 0 \qquad \text{with} \quad k_\lambda \neq 0. \quad \blacksquare$$

Now we are ready to prove the **theorem that a second-order homogeneous ODE has two linearly independent solutions**.

Suppose y_1, y_2, y_3 are three solutions of the homogeneous ODE [Eq. (8.28)]. Then we form the Wronskian $W_{jk} = y_j y_k' - y_j' y_k$ of any pair y_j, y_k of them and recall that $W_{jk}' = y_j y_k'' - y_j'' y_k$. Next we divide each ODE by y, getting $-Q$ on the right-hand side so that

$$\frac{y_j''}{y_j} + P\frac{y_j'}{y_j} = -Q(x) = \frac{y_k''}{y_k} + P\frac{y_k'}{y_k}.$$

Multiplying by $y_j y_k$, we find

$$(y_j y_k'' - y_j'' y_k) + P(y_j y_k' - y_j' y_k) = 0, \quad \text{or} \quad W_{jk}' = -PW_{jk} \tag{8.35}$$

[3]For proof, see H. Lass (1957), *Elements of Pure and Applied Mathematics*, p. 187. McGraw-Hill, New York. It is assumed that the functions have continuous derivatives and that at least one of the minors of the bottom row of Eq. (8.34) (Laplace expansion) does not vanish in $[a, b]$, the interval under consideration.

for any pair of solutions. Finally, we evaluate the Wronskian of all three solutions expanding it along the second row and using the ODEs for the W_{jk}:

$$W = \begin{vmatrix} y_1 & y_2 & y_3 \\ y_1' & y_2' & y_3' \\ y_1'' & y_2'' & y_3'' \end{vmatrix} = -y_1' W_{23}' + y_2' W_{13}' - y_3' W_{12}'$$

$$= P(y_1' W_{23} - y_2' W_{13} + y_3' W_{12}) = -P \begin{vmatrix} y_1 & y_2 & y_3 \\ y_1' & y_2' & y_3' \\ y_1' & y_2' & y_3' \end{vmatrix} = 0.$$

The vanishing Wronskian, $W = 0$, because of two identical rows is the condition for linear dependence of the solutions y_j. Thus, there are at most two linearly independent solutions of the homogeneous ODE. Similarly, one can prove that a linear homogeneous nth-order ODE has n linearly independent solutions y_j so that the general solution $y(x) = \sum c_j y_j(x)$ is a linear combination of them. ■

Biographical Data
Wrónski, Jozef Maria. Wrónski, a Polish mathematician (1778–1853) who changed his name from Höne, introduced the determinants named after him.

SUMMARY

In summary, second-order ODEs require two integrations and therefore contain two integration constants, and there are two linearly independent solutions. The general solution $y_p + c_1 y_1 + c_2 y_2$ of the inhomogeneous ODE consists of a particular solution y_p and the general solution of the homogeneous ODE. If an ODE $y'' = f(y', y)$ does not contain the variable x, then a solution of the form $y' = z(y)$ reduces the second-order ODE to a first-order ODE. An ODE where the unknown function $y(x)$ does not appear can be reduced to first order similarly, and combinations of these types can also be treated. Euler's ODE involving $x^2 y''$, xy', y linearly is solved by a linear combination of the power x^p, where the exponent p is a solution of a quadratic equation, to which the ODE reduces. ODEs with constant coefficients are solved by exponential functions e^{px}, where the exponent p is a solution of a quadratic equation, to which the ODE reduces.

EXERCISES

8.3.1 You know that the three unit vectors $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$, and $\hat{\mathbf{z}}$ are mutually perpendicular (orthogonal). Show that $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$, and $\hat{\mathbf{z}}$ are linearly independent. Specifically, show that no relation of the form of Eq. (8.30) exists for $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$, and $\hat{\mathbf{z}}$.

8.3.2 The criterion for the linear **independence** of three vectors **A**, **B**, and **C** is that the equation

$$a\mathbf{A} + b\mathbf{B} + c\mathbf{C} = 0$$

[analogous to Eq. (8.30)] has no solution other than the trivial $a = b = c = 0$. Using components $\mathbf{A} = (A_1, A_2, A_3)$, and so on, set up the determinant criterion for the existence or nonexistence of a nontrivial solution for the coefficients a, b, and c. Show that your criterion is equivalent to the scalar product $\mathbf{A} \cdot \mathbf{B} \times \mathbf{C} \neq 0$.

8.3.3 Using the Wronskian determinant, show that the set of functions

$$\left\{1, \frac{x^n}{n!}(n = 1, 2, \ldots, N)\right\}$$

is linearly independent.

8.3.4 If the Wronskian of two functions y_1 and y_2 is identically zero, show by direct integration that

$$y_1 = cy_2;$$

that is, y_1 and y_2 are linearly dependent. Assume the functions have continuous derivatives and that at least one of the functions does not vanish in the interval under consideration.

8.3.5 The Wronskian of two functions is found to be zero at $x = x_0$ and all x in a small neighborhood of x_0. Show that this Wronskian vanishes for all x and that the functions are linearly dependent. If x_0 is an isolated zero of the Wronskian, show by giving a counterexample that linear dependence is not a valid conclusion in general.

8.3.6 The three functions $\sin x$, e^x, and e^{-x} are linearly independent. No one function can be written as a linear combination of the other two. Show that the Wronskian of $\sin x$, e^x, and e^{-x} vanishes but only at isolated points.

ANS. $W = 4 \sin x$,
$W = 0$ for $x = \pm n\pi$, $n = 0, 1, 2, \ldots$.

8.3.7 Consider two functions $\varphi_1 = x$ and $\varphi_2 = |x| = x \operatorname{sgn} x$ (Fig. 8.7). The function $\operatorname{sgn} x$ is the sign of x. Since $\varphi_1' = 1$ and $\varphi_2' = \operatorname{sgn} x$, $W(\varphi_1, \varphi_2) = 0$ for any interval including $[-1, +1]$. Does the vanishing of the Wronskian over $[-1, +1]$ prove that φ_1 and φ_2 are linearly dependent? Clearly, they are not. What is wrong?

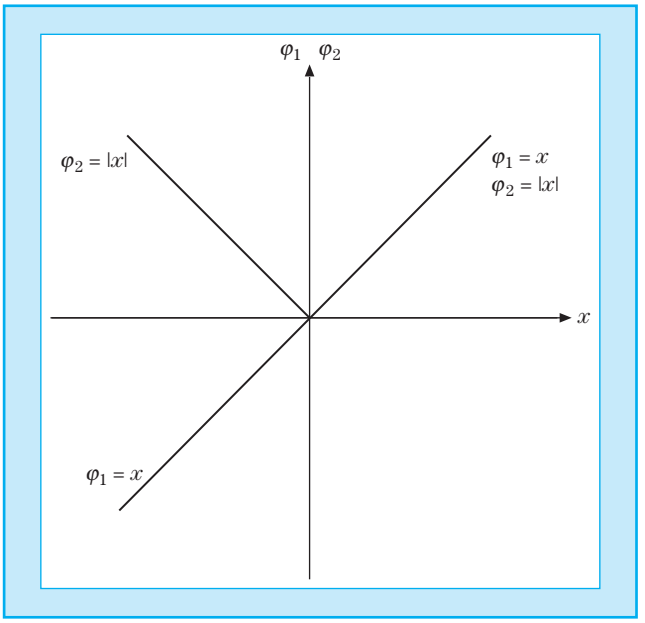
8.3.8 Explain that **linear independence** does not mean the absence of any dependence. Illustrate your argument with $y_1 = \cosh x$ and $y_2 = e^x$.

8.3.9 Find and plot the solution of the ODE satisfying the given initial conditions:
1. $y'' + 3y' - 4y = 0$ with $y(0) = 1$, $y'(0) = 0$,
2. $y'' + 2y' - 3y = 0$ with $y(0) = 0$, $y'(0) = 1$,
3. $y'' + 2y' + 3y = 0$ with $y(0) = 0$, $y'(0) = 1$.

8.3.10 Find the general solution of the ODEs in Exercise 8.3.9.

Figure 8.7

***x* and $|x|$**



8.3.11 Find and plot the solution of the ODE satisfying the given boundary conditions:
1. $y'' + 3y' - 4y = 0$ with $y(0) = 1$, $y(\infty) = 0$,
2. $y'' + 2y' - 3y = 0$ with $y(0) = 1$, $y(-\infty) = 0$,
3. $y'' + 4y' - 12y = 0$ with $y(0) = 1$, $y(1) = 2$.

8.3.12 Find and plot a particular solution of the inhomogeneous ODE
1. $y'' + 3y' - 4y = \sin \omega x$,
2. $y'' + 3y' - 4y = \cos \omega x$.

8.3.13 Find the general solution of the ODE $x^2 y'' + xy' - n^2 y = 0$ for integer n.

8.3.14 Solve the ODE $y'' + 9y = 0$ using the ansatz $y' = z(y)$ as the ODE does not contain the variable x. Compare your result with the standard solution of an ODE with constant coefficients.

8.3.15 Find and plot a particular solution of the following ODEs and give all details for the general solution of the corresponding homogeneous ODEs

1. $y'' + 3y = 2\cos x - 3\sin 2x$,
2. $y'' + 4y' + 20y = \sin x + \frac{1}{19}\cos x$,
3. $y'' + y' - 2y = e^x/x$.

8.3.16 The sun moves along the x-axis with constant velocity $c \neq 0$. A planet moves around it so that its velocity is always perpendicular to the radius vector from the sun to the planet, but no other force is acting

(i.e., no gravitational force). Show that Kepler's area law is valid and the planet's orbit is an ellipse with the sun in a focus.

8.3.17 A small massive sphere is elastically coupled to the origin moving in a straight line through the origin in a massless glass tube that rotates at a constant angular velocity ω around the origin. Describe the orbit of the mass if it is at $r = a$, $\dot{r} = 0$ at time $t = 0$.

ANS. The rosetta curve $r = a\cos N\varphi$, $N = \sqrt{(\omega_0/\omega)^2 - 1}$ for $\omega_0^2 = k/m > \omega^2$; for $\omega_0 = \omega$ a circle, and for $\omega_0 < \omega$ a hyperbolic cosine spiral $r = a\cosh n\varphi$, $n = \sqrt{(1 - (\omega_0/\omega)^2}$.

8.3.18 A charged particle of mass m and charge e is moving in a constant electric field in the positive x-direction and a constant magnetic field in the positive z-direction. At time $t = 0$ the particle is located at the origin with velocity v in the y-direction. Determine the motion $\mathbf{r}(t)$ and orbits for the cases $B = 0$, $E \neq 0$; $E = 0$, $B \neq 0$; $E \neq 0$, $B \neq 0$, $v = 0$; $E \neq 0$, $B \neq 0$, $v \neq 0$. Plot the orbits.

8.3.19 Two small masses m_1, m_2 are suspended at the ends of a rope of constant length L over a pulley. Find their motion $z_i(t)$ under the influence of the constant gravitational acceleration $g = 9.8$ m/sec^2. Discuss various initial conditions.

8.3.20 Find the general solution of the ODE $x^2y'' - 4xy' + 6y = 14x^{-4}$, showing all steps of your calculations.

8.3.21 Find the steady-state current of the RLC circuit in Example 8.3.6 for $R = 7\,\Omega$, $L = 10$ H, $C = 10^{-4}$ F, $V = 220\sin 60t$ V.

8.3.22 Find the transient current for Exercise 8.3.21.

8.4 Singular Points

In this section, the concept of a singular point or singularity (as applied to a differential equation) is introduced. The interest in this concept stems from its usefulness in (i) classifying ODEs and (ii) investigating the feasibility of a series solution. This feasibility is the topic of Fuchs's theorem (Section 8.5). First, we give a definition of ordinary and singular points of ODEs.

All the ODEs listed in Sections 8.2 and 8.3 may be solved for d^2y/dx^2. We have

$$y'' = f(x, y, y'). \tag{8.36}$$

Now, if in Eq. (8.36), y and y' can take on all finite values at $x = x_0$ and y'' remains finite, point $x = x_0$ is an **ordinary** point. On the other hand, if y'' **becomes infinite** for any finite choice of y and y', point $x = x_0$ is labeled a **singular point**. We need to understand if the solution $y(x_0)$ is still well defined at such a point.

Another way of presenting this definition of a singular point is to write our second-order, homogeneous, linear differential equation (in y) as

$$y'' + P(x)y' + Q(x)y = 0. \tag{8.37}$$

Now, if the functions $P(x)$ and $Q(x)$ remain finite at $x = x_0$, point $x = x_0$ is an **ordinary point**. However, if $P(x)$ or $Q(x)$ (or both) diverges as $x \to x_0$, point x_0 is a **singular point**. Using Eq. (8.37), we may distinguish between two kinds of singular points.

1. If either $P(x)$ or $Q(x)$ diverges as $x \to x_0$ but $(x-x_0)P(x)$ and $(x-x_0)^2Q(x)$ remain finite as $x \to x_0$, then $x = x_0$ is a **regular** or nonessential singular point. We shall see that a power series solution is possible at ordinary points and regular singularities.
2. If $P(x)$ diverges faster than $1/(x-x_0)$ so that $(x-x_0)P(x)$ goes to infinity as $x \to x_0$, or $Q(x)$ diverges faster than $1/(x-x_0)^2$ so that $(x-x_0)^2Q(x)$ goes to infinity as $x \to x_0$, then point $x = x_0$ is an **irregular or essential singularity**. We shall see that at such essential singularities a solution usually does not exist.

These definitions hold for all finite values of x_0. The analysis of point $x \to \infty$ is similar to the treatment of functions of a complex variable (Chapters 6 and 7). We set $x = 1/z$, substitute into the differential equation, and then let $z \to 0$. By changing variables in the derivatives, we have

$$\frac{dy(x)}{dx} = \frac{dy(z^{-1})}{dz}\frac{dz}{dx} = -\frac{1}{x^2}\frac{dy(z^{-1})}{dz} = -z^2\frac{dy(z^{-1})}{dz} \tag{8.38}$$

$$\begin{aligned}\frac{d^2y(x)}{dx^2} = \frac{d}{dz}\left[\frac{dy(x)}{dx}\right]\frac{dz}{dx} &= (-z^2)\left[-2z\frac{dy(z^{-1})}{dz} - z^2\frac{d^2y(z^{-1})}{dz^2}\right] \\ &= 2z^3\frac{dy(z^{-1})}{dz} + z^4\frac{d^2y(z^{-1})}{dz^2}.\end{aligned} \tag{8.39}$$

Using these results, we transform Eq. (8.37) into

$$z^4\frac{d^2y}{dz^2} + [2z^3 - z^2P(z^{-1})]\frac{dy}{dz} + Q(z^{-1})y = 0. \tag{8.40}$$

The behavior at $x = \infty\,(z = 0)$ then depends on the behavior of the new coefficients

$$\frac{2z - P(z^{-1})}{z^2} \quad \text{and} \quad \frac{Q(z^{-1})}{z^4},$$

as $z \to 0$. If these two expressions remain finite, point $x = \infty$ is an ordinary point. If they diverge no more rapidly than $1/z$ and $1/z^2$, respectively, point $x = \infty$ is a **regular singular point**; otherwise, it is an **irregular singular point** (an essential singularity).

EXAMPLE 8.4.1

Bessel Singularity Bessel's equation is

$$x^2y'' + xy' + (x^2 - n^2)y = 0. \tag{8.41}$$

Comparing it with Eq. (8.37) we have

$$P(x) = \frac{1}{x}, \quad Q(x) = 1 - \frac{n^2}{x^2},$$

which shows that point $x = 0$ is a regular singularity. By inspection we see that there are no other singular points in the finite range. As $x \to \infty\,(z \to 0)$, from Eq. (8.41) we have the coefficients

$$\frac{2z - z}{z^2} \quad \text{and} \quad \frac{1 - n^2z^2}{z^4}.$$

Since the latter expression diverges as z^4, point $x = \infty$ is an irregular or essential singularity.

More examples of ODEs with regular and irregular singularities are discussed in Section 8.5. ■

EXERCISES

8.4.1 Show that Legendre's equation has regular singularities at $x = -1, 1$, and ∞.

8.4.2 Show that Laguerre's equation, like the Bessel equation, has a regular singularity at $x = 0$ and an irregular singularity at $x = \infty$.

8.4.3 Show that the substitution

$$x \to \frac{1 - x}{2}, \quad a = -l, \quad b = l + 1, \quad c = 1$$

converts the hypergeometric equation into Legendre's equation.

8.5 Series Solutions—Frobenius's Method

In this section, we develop a method of obtaining one solution of the linear, second-order, homogeneous ODE. The method, a power series expansion, will always work, provided the point of expansion is no worse than a regular singular point, a gentle condition that is almost always satisfied in physics.

A **linear, second-order, homogeneous** ODE may be put in the form

$$\frac{d^2y}{dx^2} + P(x)\frac{dy}{dx} + Q(x)y = 0. \tag{8.42}$$

The equation is **homogeneous** because each term contains $y(x)$ or a derivative, and it is **linear** because each y, dy/dx, or d^2y/dx^2 appears as the first power—and no products.

Here, we develop (at least) one solution of Eq. (8.42). In Section 8.6, we develop the **second, independent solution. We have proved that no third, independent solution exists**. Therefore, the **most general solution of the homogeneous ODE**, Eq. (8.42), may be written as

$$y_h(x) = c_1 y_1(x) + c_2 y_2(x) \tag{8.43}$$

as a consequence of the superposition principle for linear ODEs. Our physical problem may involve a driving term and lead to a **nonhomogeneous**, linear, second-order ODE

$$\frac{d^2y}{dx^2} + P(x)\frac{dy}{dx} + Q(x)y = F(x). \tag{8.44}$$

The function on the right, $F(x)$, represents a source (such as electrostatic charge) or a driving force (as in a driven oscillator). These are also explored in detail in Chapter 15 with a Laplace transform technique. Calling this a particular solution y_p, we may add to it any solution of the corresponding homogeneous equation [Eq. (8.42)]. Hence, the **most general solution of the inhomogeneous ODE** [Eq. (8.44)] is

$$y(x) = c_1 y_1(x) + c_2 y_2(x) + y_p(x). \tag{8.45}$$

The constants c_1 and c_2 will eventually be fixed by boundary or initial conditions.

For now, we assume that $F(x) = 0$—that our differential equation is homogeneous. We shall attempt to develop a solution of our linear, second-order, homogeneous differential equation [Eq. (8.42)] by substituting in a power series with undetermined coefficients. Also available as a parameter is the power of the lowest nonvanishing term of the series. To illustrate, we apply the method to two important differential equations. First, the linear oscillator equation

$$\frac{d^2y}{dx^2} + \omega^2 y = 0, \tag{8.46}$$

with known solutions $y = \sin\omega x, \cos\omega x$. Now we try

$$\begin{aligned} y(x) &= x^k(a_0 + a_1x + a_2x^2 + a_3x^3 + \cdots) \\ &= \sum_{\lambda=0}^{\infty} a_\lambda x^{k+\lambda}, \quad a_0 \neq 0, \end{aligned} \tag{8.47}$$

with the exponent k and all the coefficients a_λ still undetermined. Note that k need not be an integer. By differentiating twice, we obtain

$$\begin{aligned} \frac{dy}{dx} &= \sum_{\lambda=0}^{\infty} a_\lambda (k+\lambda) x^{k+\lambda-1}, \\ \frac{d^2y}{dx^2} &= \sum_{\lambda=0}^{\infty} a_\lambda (k+\lambda)(k+\lambda-1) x^{k+\lambda-2}. \end{aligned}$$

By substituting the series for y and y'' into the ODE [Eq. (8.46)], we have

$$\sum_{\lambda=0}^{\infty} a_\lambda (k+\lambda)(k+\lambda-1)x^{k+\lambda-2} + \omega^2 \sum_{\lambda=0}^{\infty} a_\lambda x^{k+\lambda} = 0. \tag{8.48}$$

From our analysis of the uniqueness of power series (Chapter 5) the coefficients of each power of x on the left-hand side of Eq. (8.48) must vanish individually.

The lowest power of x appearing in Eq. (8.48) is x^{k-2}, for $\lambda = 0$ in the first summation. The requirement that the coefficient vanish[4] yields

$$a_0 k(k-1) = 0.$$

We had chosen a_0 as the coefficient of the lowest nonvanishing term of the series [Eq. (8.48)]; hence, by definition, $a_0 \neq 0$. Therefore, we have

$$k(k-1) = 0. \tag{8.49}$$

This equation, coming from the coefficient of the lowest power of x, we call the **indicial equation**. The indicial equation and its roots are of critical importance to our analysis. The coefficient $a_1(k+1)k$ of x^{k-1} must also vanish. This is satisfied if $k = 0$; if $k = 1$, then $a_1 = 0$. Clearly, in this example we must require that either $k = 0$ or $k = 1$.

Before considering these two possibilities for k, we return to Eq. (8.48) and demand that the remaining coefficients, viz., the coefficient of $x^{k+j}(j \geq 0)$, vanish. We set $\lambda = j+2$ in the first summation and $\lambda = j$ in the second. (They are independent summations and λ is a dummy index.) This results in

$$a_{j+2}(k+j+2)(k+j+1) + \omega^2 a_j = 0$$

or

$$a_{j+2} = -a_j \frac{\omega^2}{(k+j+2)(k+j+1)}. \tag{8.50}$$

This is a two-term **recurrence relation**.[5] Given a_j, we may compute a_{j+2} and then a_{j+4}, a_{j+6}, and so on as far as desired. Note that for this example, if we start with a_0, Eq. (8.50) leads to the even coefficients a_2, a_4, and so on and ignores a_1, a_3, a_5, and so on. Since a_1 is arbitrary if $k = 0$ and necessarily zero if $k = 1$, let us set it equal to zero (compare Exercises 8.5.3 and 8.5.4) and then by Eq. (8.50)

$$a_3 = a_5 = a_7 = \cdots = 0,$$

and all the odd-numbered coefficients vanish. The odd powers of x will actually reappear when the **second** root of the indicial equation is used.

[4] See the uniqueness of power series (Section 5.7).

[5] Recurrence relations may involve three or more terms; that is, a_{j+2}, depending on a_j and a_{j-2}, etc. An unusual feature is that it goes in steps of two rather than the more common steps of one. This feature will be explained by a symmetry of the ODE called parity.

Returning to Eq. (8.49), our indicial equation, we first try the solution $k = 0$. The recurrence relation [Eq. (8.50)] becomes

$$a_{j+2} = -a_j \frac{\omega^2}{(j+2)(j+1)}, \tag{8.51}$$

which leads to

$$\begin{aligned} a_2 &= -a_0 \frac{\omega^2}{1 \cdot 2} = -\frac{\omega^2}{2!} a_0, \\ a_4 &= -a_2 \frac{\omega^2}{3 \cdot 4} = +\frac{\omega^4}{4!} a_0, \\ a_6 &= -a_4 \frac{\omega^2}{5 \cdot 6} = -\frac{\omega^6}{6!} a_0, \quad \text{and so on.} \end{aligned}$$

By inspection (or mathematical induction),

$$a_{2n} = (-1)^n \frac{\omega^{2n}}{(2n)!} a_0, \tag{8.52}$$

and our solution is

$$y(x)_{k=0} = a_0 \left[1 - \frac{(\omega x)^2}{2!} + \frac{(\omega x)^4}{4!} - \frac{(\omega x)^6}{6!} + \cdots \right] = a_0 \cos \omega x. \tag{8.53}$$

If we choose the indicial equation root $k = 1$ [Eq. (8.49)], the recurrence relation becomes

$$a_{j+2} = -a_j \frac{\omega^2}{(j+3)(j+2)}. \tag{8.54}$$

Substituting in $j = 0, 2, 4$, successively, we obtain

$$\begin{aligned} a_2 &= -a_0 \frac{\omega^2}{2 \cdot 3} = -\frac{\omega^2}{3!} a_0, \\ a_4 &= -a_2 \frac{\omega^2}{4 \cdot 5} = +\frac{\omega^4}{5!} a_0, \\ a_6 &= -a_4 \frac{\omega^2}{6 \cdot 7} = -\frac{\omega^6}{7!} a_0, \quad \text{and so on.} \end{aligned}$$

Again, by inspection and mathematical induction,

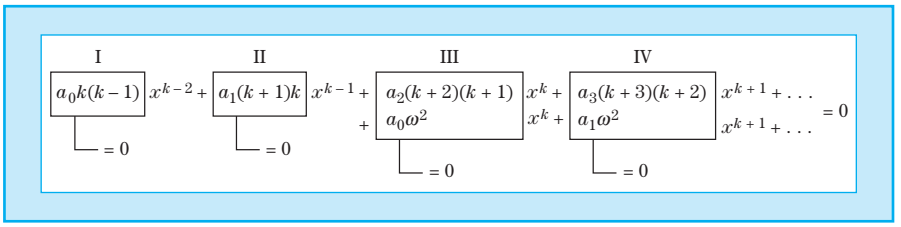
$$a_{2n} = (-1)^n \frac{\omega^{2n}}{(2n+1)!} a_0. \tag{8.55}$$

For this choice, $k = 1$, we obtain

$$\begin{aligned} y(x)_{k=1} &= a_0 x \left[1 - \frac{(\omega x)^2}{3!} + \frac{(\omega x)^4}{5!} - \frac{(\omega x)^6}{7!} + \cdots \right] \\ &= \frac{a_0}{\omega} \left[(\omega x) - \frac{(\omega x)^3}{3!} + \frac{(\omega x)^5}{5!} - \frac{(\omega x)^7}{7!} + \cdots \right] \\ &= \frac{a_0}{\omega} \sin \omega x. \end{aligned} \tag{8.56}$$

Figure 8.8

Schematic Power Series



SUMMARY

To summarize this power series approach, we may write Eq. (8.48) schematically as shown in Fig. 8.8. From the uniqueness of power series (Section 5.7), the total coefficient of each power of x must vanish all by itself. The requirement that the first coefficient vanish leads to the indicial equation [Eq. (8.49)]. The second coefficient is handled by setting $a_1 = 0$. The vanishing of the coefficient of x^k (and higher powers, taken one at a time) leads to the recurrence relation [Eq. (8.50)].

This series substitution, known as Frobenius's method, has given us two series solutions of the linear oscillator equation. However, there are two points about such series solutions that must be strongly emphasized:

- The series solution should always be substituted back into the differential equation, to see if it works, as a precaution against algebraic and logical errors. If it works, it is a solution.
- The acceptability of a series solution depends on its convergence (including asymptotic convergence). It is quite possible for Frobenius's method to give a series solution that satisfies the original differential equation, when substituted in the equation, but that does **not** converge over the region of interest.

Expansion about x_0

Equation (8.47) is an expansion about the origin, $x_0 = 0$. It is perfectly possible to replace Eq. (8.47) with

$$y(x) = \sum_{\lambda=0}^{\infty} a_\lambda (x - x_0)^{k+\lambda}, \quad a_0 \neq 0. \tag{8.57}$$

The point x_0 should not be chosen at an essential singularity—or our Frobenius method will probably fail. The resultant series (x_0 an ordinary point or regular singular point) will be valid where it converges. You can expect a divergence of some sort when $|x - x_0| = |z_s - x_0|$, where z_s is the closest singularity to x_0 in the complex plane.

Symmetry of ODE and Solutions

Note that for the ODE in Eq. (8.46) we obtained one solution of **even symmetry**, defined as $y_1(x) = y_1(-x)$, and one of **odd symmetry**, defined as $y_2(x) = -y_2(-x)$. This is not just an accident but a direct consequence of the

form of the ODE. Writing a general ODE as

$$\mathcal{L}(x)y(x) = 0, \tag{8.58}$$

where $\mathcal{L}(x)$ is the differential operator, we see that for the linear oscillator equation [Eq. (8.46)], upon reversing the coordinate $x \to -x$ (defined as parity transformation),

$$\mathcal{L}(x) = \mathcal{L}(-x) \tag{8.59}$$

is **even under parity**. Whenever the differential operator has a specific parity or symmetry, either even or odd, we may interchange $+x$ and $-x$, and Eq. (8.58) becomes

$$\pm\mathcal{L}(x)y(-x) = 0. \tag{8.60}$$

It is $+$ if $\mathcal{L}(x)$ is even and $-$ if $\mathcal{L}(x)$ is odd. Clearly, if $y(x)$ is a solution of the differential equation, $y(-x)$ is also a solution. Then any solution may be resolved into even and odd parts,

$$y(x) = \frac{1}{2}[y(x) + y(-x)] + \frac{1}{2}[y(x) - y(-x)], \tag{8.61}$$

the first bracket on the right giving an even solution and the second an odd solution. Such a combination of solutions of definite parity has no definite parity.

Many other ODEs of importance in physics exhibit this even parity; that is, their $P(x)$ in Eq. (8.42) is odd and $Q(x)$ even. Solutions of all of them may be presented as series of even powers of x and separate series of odd powers of x. Parity is particularly important in quantum mechanics. We find that wave functions are usually either even or odd, meaning that they have a definite parity. For example, the Coulomb potential in the Schrödinger equation for hydrogen has positive parity. As a result, its solutions have definite parity.

Limitations of Series Approach—Bessel's Equation

The power series solution for the linear oscillator equation was perhaps a bit too easy. By substituting the power series [Eq. (8.47)] into the differential equation [Eq. (8.46)], we obtained two independent solutions with no trouble at all.

To get some idea of what can happen, we try to solve Bessel's equation,

$$x^2y'' + xy' + (x^2 - n^2)y = 0. \tag{8.62}$$

Again, assuming a solution of the form

$$y(x) = \sum_{\lambda=0}^{\infty} a_\lambda x^{k+\lambda},$$

we differentiate and substitute into Eq. (8.62). The result is

$$\sum_{\lambda=0}^{\infty} a_\lambda (k+\lambda)(k+\lambda-1)x^{k+\lambda} + \sum_{\lambda=0}^{\infty} a_\lambda (k+\lambda)x^{k+\lambda} + \sum_{\lambda=0}^{\infty} a_\lambda x^{k+\lambda+2} - \sum_{\lambda=0}^{\infty} a_\lambda n^2 x^{k+\lambda} = 0. \tag{8.63}$$

By setting $\lambda = 0$, we get the coefficient of x^k, the lowest power of x appearing on the left-hand side,

$$a_0[k(k-1)+k-n^2] = 0, \tag{8.64}$$

and again $a_0 \neq 0$ by definition. Equation (8.64) therefore yields the **indicial** equation

$$k^2 - n^2 = 0, \tag{8.65}$$

with solutions $k = \pm n$.

It is of interest to examine the coefficient of x^{k+1}. Here, we obtain

$$a_1[(k+1)k+k+1-n^2] = 0$$

or

$$a_1(k+1-n)(k+1+n) = 0. \tag{8.66}$$

For $k = \pm n$, neither $k+1-n$ nor $k+1+n$ vanishes and we **must** require $a_1 = 0$.[6]

Proceeding to the coefficient of x^{k+j} for $k = n$, we set $\lambda = j$ in the first, second, and fourth terms of Eq. (8.63) and $\lambda = j-2$ in the third term. By requiring the resultant coefficient of x^{k+1} to vanish, we obtain

$$a_j[(n+j)(n+j-1)+(n+j)-n^2] + a_{j-2} = 0.$$

When j is replaced by $j+2$, this can be rewritten for $j \geq 0$ as

$$a_{j+2} = -a_j \frac{1}{(j+2)(2n+j+2)}, \tag{8.67}$$

which is the desired recurrence relation. Repeated application of this recurrence relation leads to

$$a_2 = -a_0 \frac{1}{2(2n+2)} = -\frac{a_0 n!}{2^2 1!(n+1)!},$$

$$a_4 = -a_2 \frac{1}{4(2n+4)} = \frac{a_0 n!}{2^4 2!(n+2)!},$$

$$a_6 = -a_4 \frac{1}{6(2n+6)} = -\frac{a_0 n!}{2^6 3!(n+3)!}, \quad \text{and so on,}$$

[6] $k = \pm n = -\frac{1}{2}$ are exceptions.

and in general,

$$a_{2p} = (-1)^p \frac{a_0 n!}{2^{2p} p!(n+p)!}. \tag{8.68}$$

Inserting these coefficients in our assumed series solution, we have

$$y(x) = a_0 x^n \left[1 - \frac{n! x^2}{2^2 1!(n+1)!} + \frac{n! x^4}{2^4 2!(n+2)!} - \cdots\right]. \tag{8.69}$$

In summation form

$$\begin{aligned} y(x) &= a_0 \sum_{j=0}^{\infty} (-1)^j \frac{n! x^{n+2j}}{2^{2j} j!(n+j)!} \\ &= a_0 2^n n! \sum_{j=0}^{\infty} (-1)^j \frac{1}{j!(n+j)!} \left(\frac{x}{2}\right)^{n+2j}. \end{aligned} \tag{8.70}$$

In Chapter 12, the final summation is identified as the Bessel function $J_n(x)$. Notice that this solution $J_n(x)$ has either even or odd symmetry,[7] as might be expected from the form of Bessel's equation.

When $k = -n$, and n is not an integer, we may generate a second distinct series to be labeled $J_{-n}(x)$. However, when $-n$ is a negative integer, trouble develops. The recurrence relation for the coefficients a_j is still given by Eq. (8.67), but with $2n$ replaced by $-2n$. Then, when $j + 2 = 2n$ or $j = 2(n-1)$, the coefficient a_{j+2} blows up and we have no series solution. This catastrophe can be remedied in Eq. (8.70), as it is done in Chapter 12, with the result that

$$J_{-n}(x) = (-1)^n J_n(x), \qquad n \text{ an integer.} \tag{8.71}$$

The second solution simply reproduces the first. We have failed to construct a second independent solution for Bessel's equation by this series technique when n is an integer.

SUMMARY

By substituting in an infinite series, we have obtained two solutions for the linear oscillator equation and one for Bessel's equation (two if n is not an integer). To the questions "Can we always do this? Will this method always work?" the answer is no. This method of power series solution will not always work, as we explain next.

Biographical Data

Frobenius, Georg. Frobenius, a German mathematician (1849–1917), contributed to matrices, groups, and algebra as well as differential equations.

Regular and Irregular Singularities

The success of the series substitution method depends on the roots of the indicial equation and the degree of singularity of the coefficients in the differential equation. To understand better the effect of the equation coefficients on this

[7] $J_n(x)$ is an even function if n is an even integer, and it is an odd function if n is an odd integer. For nonintegral n the x^n has no such simple symmetry.

naive series substitution approach, consider four simple equations:

$$y'' - \frac{6}{x^2}y = 0, \tag{8.72a}$$

$$y'' - \frac{6}{x^3}y = 0, \tag{8.72b}$$

$$y'' + \frac{1}{x}y' - \frac{a^2}{x^2}y = 0, \tag{8.72c}$$

$$y'' + \frac{1}{x^2}y' - \frac{a^2}{x^2}y = 0. \tag{8.72d}$$

You may show that for Eq. (8.72a) the indicial equation is

$$k^2 - k - 6 = 0,$$

giving $k = 3, -2$. Since the equation is homogeneous in x (counting d^2/dx^2 as x^{-2}), there is no recurrence relation. However, we are left with two perfectly good solutions, x^3 and x^{-2}.

Equation (8.72b) differs from Eq. (8.72a) by only one power of x, but this changes the indicial equation to

$$-6a_0 = 0,$$

with no solution at all because we have agreed that $a_0 \neq 0$. Our series substitution worked for Eq. (8.72a), which had only a regular singularity, but broke down in Eq. (8.72b), which has an **irregular singular point** at the origin.

Continuing with Eq. (8.72c), we have added a term y'/x. The indicial equation is

$$k^2 - a^2 = 0,$$

but again there is no recurrence relation. The solutions are $y = x^a, x^{-a}$—both perfectly acceptable one-term series. Despite the regular singularity at the origin, two independent solutions exist in this case.

When we change the power of x in the coefficient of y' from -1 to -2 [Eq. (8.72d)], there is a drastic change in the solution. The indicial equation (with only the y' term contributing) becomes

$$k = 0.$$

There is a recurrence relation

$$a_{j+1} = +a_j \frac{a^2 - j(j-1)}{j+1}.$$

Unless the parameter a is selected to make the series terminate, we have

$$\lim_{j\to\infty} \left| \frac{a_{j+1}}{a_j} \right| = \lim_{j\to\infty} \frac{j(j+1)}{j+1}$$

$$= \lim_{j\to\infty} \frac{j^2}{j} = \infty.$$

Hence, our series solution diverges for all $x \neq 0$. Again, our method worked for Eq. (8.72c) with a regular singularity but failed when we had the irregular singularity of Eq. (8.72d).

Fuchs's Theorem

The answer to the basic question as to when the method of series substitution can be expected to work is given by Fuchs's theorem, which asserts that **we can always obtain at least one power series solution, provided we are expanding about a point that is an ordinary point or at worst a regular singular point**.

If we attempt an expansion about an irregular or essential singularity, our method may fail as it did for Eqs. (8.72b) and (8.72d). Fortunately, the more important equations of mathematical physics have no irregular singularities in the finite plane. Further discussion of Fuchs's theorem appears in Section 8.6.

Summary

If we are expanding about an ordinary point or, at worst, about a regular singularity, the series substitution approach will yield at least one solution (**Fuchs's theorem**).

Whether we get one or two distinct solutions depends on the roots of the indicial equation:

- If the two roots of the indicial equation are equal, we can obtain only one solution by this series substitution method.
- If the two roots differ by a nonintegral number, two independent solutions may be obtained.
- If the two roots differ by an integer, the larger of the two will yield a solution.

The smaller may or may not give a solution, depending on the behavior of the coefficients. In the linear oscillator equation we obtain two solutions; for Bessel's equation, only one solution is obtained.

The usefulness of the series solution in terms of what is the solution (i.e., numbers) depends on the rapidity of convergence of the series and the availability of the coefficients. Many ODEs will not yield simple recurrence relations for the coefficients. In general, the available series will probably be useful when $|x|$ (or $|x-x_0|$) is very small. Computers can be used to determine additional series coefficients using a symbolic language, such as Mathematica,[8] Maple,[9] or Reduce.[10] Often, however, for numerical work a direct numerical integration will be preferred (Section 8.7).

[8]Wolfram, S. (1991). *Mathematica, A System for Doing Mathematics by Computer*. Addison Wesley, New York.
[9]Heck, A. (1993). *Introduction to Maple*. Springer, New York.
[10]Rayna, G. (1987). *Reduce Software for Algebraic Computation*. Springer, New York.

EXERCISES

8.5.1 Uniqueness theorem. The function $y(x)$ satisfies a second-order, linear, homogeneous differential equation. At $x = x_0$, $y(x) = y_0$ and $dy/dx = y'_0$. Show that $y(x)$ is unique in that no other solution of this differential equation passes through the points (x_0, y_0) with a slope of y'_0.
Hint. Assume a second solution satisfying these conditions and compare the Taylor series expansions.

8.5.2 A series solution of Eq. (8.47) is attempted, expanding about the point $x = x_0$. If x_0 is an ordinary point, show that the indicial equation has roots $k = 0, 1$.

8.5.3 In the development of a series solution of the simple harmonic oscillator (SHO) equation the second series coefficient a_1 was neglected except to set it equal to zero. From the coefficient of the next to the lowest power of x, x^{k-1}, develop a second indicial-type equation.
(a) SHO equation with $k = 0$: Show that a_1 may be assigned any finite value (including zero).
(b) SHO equation with $k = 1$: Show that a_1 must be set equal to zero.

8.5.4 Analyze the series solutions of the following differential equations to see when a_1 **may** be set equal to zero without irrevocably losing anything and when a_1 **must** be set equal to zero.
(a) Legendre, (b) Bessel, (c) Hermite.

ANS. (a) Legendre and (c) Hermite: For $k = 0$, a_1 **may** be set equal to zero; for $k = 1$, a_1 **must** be set equal to zero.
(b) Bessel: a_1 **must** be set equal to zero (except for $k = \pm n = -\frac{1}{2}$).

8.5.5 Solve the Legendre equation

$$(1 - x^2)y'' - 2xy' + n(n+1)y = 0$$

by direct series substitution and plot the solution for $n = 0, 1, 2, 3$.
(a) Verify that the indicial equation is

$$k(k-1) = 0.$$

(b) Using $k = 0$, obtain a series of even powers of x, ($a_1 = 0$).

$$y_{\text{even}} = a_0\left[1 - \frac{n(n+1)}{2!}x^2 + \frac{n(n-2)(n+1)(n+3)}{4!}x^4 + \cdots\right],$$

where

$$a_{j+2} = \frac{j(j+1) - n(n+1)}{(j+1)(j+2)}a_j.$$

(c) Using $k = 1$, develop a series of odd powers of $x (a_1 = 0)$.

$$y_{\text{odd}} = a_0 \left[x - \frac{(n-1)(n+2)}{3!} x^3 + \frac{(n-1)(n-3)(n+2)(n+4)}{5!} x^5 + \cdots \right],$$

where

$$a_{j+2} = \frac{(j+1)(j+2) - n(n+1)}{(j+2)(j+3)} a_j.$$

(d) Show that both solutions, y_{even} and y_{odd}, diverge for $x = \pm 1$ **if the series continue to infinity**.

(e) Finally, show that by an appropriate choice of n, one series at a time may be converted into a polynomial, thereby avoiding the divergence catastrophe. In quantum mechanics this restriction of n to integral values corresponds to **quantization of angular momentum**.

8.5.6 Develop series solutions for Hermite's differential equation

(a) $y'' - 2xy' + 2\alpha y = 0$.

ANS. $k(k-1) = 0$, indicial equation.

For $k = 0$

$$a_{j+2} = 2a_j \frac{j - \alpha}{(j+1)(j+2)} \quad (j \text{ even}),$$

$$y_{\text{even}} = a_0 \left[1 + \frac{2(-\alpha)x^2}{2!} + \frac{2^2(-\alpha)(2-\alpha)x^4}{4!} + \cdots \right].$$

For $k = 1$

$$a_{j+2} = 2a_j \frac{j + 1 - \alpha}{(j+2)(j+3)} \quad (j \text{ even}),$$

$$y_{\text{even}} = a_0 \left[x + \frac{2(1-\alpha)x^3}{3!} + \frac{2^2(1-\alpha)(3-\alpha)x^5}{5!} + \cdots \right].$$

(b) Show that both series solutions are convergent for all x, the ratio of successive coefficients behaving, for large index, like the corresponding ratio in the expansion of $\exp(2x^2)$.

(c) Show that by appropriate choice of α the series solutions may be cut off and converted to finite polynomials. (These polynomials, properly normalized, become the Hermite polynomials in Section 13.1.)

8.5.7 Laguerre's ODE is

$$xL_n''(x) + (1-x)L_n'(x) + nL_n(x) = 0.$$

Develop a series solution selecting the parameter n to make your series a polynomial and plot the partial series for the three lowest values of n and enough terms to demonstrate convergence.

8.5.8 A quantum mechanical analysis of the Stark effect (parabolic coordinates) leads to the differential equation

$$\frac{d}{d\xi}\left(\xi\frac{du}{d\xi}\right)+\left(\frac{1}{2}E\xi+\alpha-\frac{m^2}{4\xi}-\frac{1}{4}F\xi^2\right)u=0,$$

where α is a separation constant, E is the total energy, and F is a constant; Fz is the potential energy added to the system by the introduction of an electric field.

Using the larger root of the indicial equation, develop a power series solution about $\xi=0$. Evaluate the first three coefficients in terms of a_0, the lowest coefficient in the power series for $u(\xi)$ below.

$$\text{Indicial equation}\quad k^2-\frac{m^2}{4}=0,$$

$$u(\xi)=a_0\xi^{m/2}\left\{1-\frac{\alpha}{m+1}\xi+\left[\frac{\alpha^2}{2(m+1)(m+2)}-\frac{E}{4(m+2)}\right]\xi^2+\cdots\right\}.$$

Note that the perturbation F does not appear until a_3 is included.

8.5.9 For the special case of no azimuthal dependence, the quantum mechanical analysis of the hydrogen molecular ion leads to the equation

$$\frac{d}{d\eta}\left[(1-\eta^2)\frac{du}{d\eta}\right]+\alpha u+\beta\eta^2u=0.$$

Develop a power series solution for $u(\eta)$. Evaluate the first three nonvanishing coefficients in terms of a_0.

$$\text{Indicial equation}\quad k(k-1)=0.$$

$$u_{k=1}=a_0\eta\left\{1+\frac{2-\alpha}{6}\eta^2+\left[\frac{(2-\alpha)(12-\alpha)}{120}-\frac{\beta}{20}\right]\eta^4+\cdots\right\}.$$

8.5.10 To a good approximation, the interaction of two nucleons may be described by a mesonic potential

$$V=\frac{Ae^{-ax}}{x},$$

attractive for A negative. Develop a series solution of the resultant Schrödinger wave equation

$$\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+(E-V)\psi=0$$

through the first three nonvanishing coefficients:

$$\psi_{k=1}=a_0\left\{x+\frac{1}{2}A'x^2+\frac{1}{6}\left[\frac{1}{2}A'^2-E'-aA'\right]x^3+\cdots\right\},$$

where the prime indicates multiplication by $2m/\hbar^2$. Plot the solution for $a=0.7\ \text{fm}^{-1}$ and $A=-0.1$.

8.5.11 Near the nucleus of a complex atom the potential energy of one electron is given by

$$V = -\frac{Ze^2}{r}(1 + b_1 r + b_2 r^2),$$

where the coefficients b_1 and b_2 arise from screening effects. For the case of zero angular momentum determine the first three terms of the solution of the Schrödinger equation; that is, write out the first three terms in a series expansion of the wave function. Plot the potential and wave function.

8.5.12 If the parameter a^2 in Eq. (8.72d) is equal to 2, Eq. (8.72d) becomes

$$y'' + \frac{1}{x^2}y' - \frac{2}{x^2}y = 0.$$

From the indicial equation and the recurrence relation, **derive** a solution $y = 1 + 2x + 2x^2$. Verify that this is indeed a solution by substituting back into the differential equation.

8.6 A Second Solution

In Section 8.5, a solution of a second-order homogeneous ODE was developed by substituting in a power series. By Fuchs's theorem this is possible, provided the power series is an expansion about an ordinary point or a nonessential singularity.[11] There is no guarantee that this approach will yield the two independent solutions we expect from a linear second-order ODE. Indeed, the technique gives only one solution for Bessel's equation (n an integer). In this section, we develop two methods of obtaining a second independent solution: an integral method and a power series containing a logarithmic term.

Returning to our linear, second-order, homogeneous ODE of the general form

$$y'' + P(x)y' + Q(x)y = 0, \tag{8.73}$$

let y_1 and y_2 be two independent solutions. Then the Wronskian, by definition, is

$$W = y_1 y_2' - y_1' y_2. \tag{8.74}$$

By differentiating the Wronskian, we obtain

$$\begin{aligned} W' &= y_1' y_2' + y_1 y_2'' - y_1'' y_2 - y_1' y_2' \\ &= y_1[-P(x)y_2' - Q(x)y_2] - y_2[-P(x)y_1' - Q(x)y_1] \\ &= -P(x)(y_1 y_2' - y_1' y_2). \end{aligned} \tag{8.75}$$

The expression in parentheses is just W, the Wronskian, and we have

$$W' = -P(x)W. \tag{8.76}$$

[11] This is why the classification of singularities in Section 8.4 is of vital importance.

In the special case that $P(x) = 0$, that is,

$$y'' + Q(x)y = 0, \tag{8.77}$$

the Wronskian

$$W = y_1 y_2' - y_1' y_2 = \text{constant}. \tag{8.78}$$

Since our original differential equation is homogeneous, we may multiply the solutions y_1 and y_2 by whatever constants we wish and arrange to have the Wronskian equal to unity (or -1). This case, $P(x) = 0$, appears more frequently than might be expected. Recall that ∇^2 in Cartesian coordinates contains no first derivative. Similarly, the radial dependence of $\nabla^2(r\psi)$ in spherical polar coordinates lacks a first derivative. Finally, every linear second-order differential equation can be transformed into an equation of the form of Eq. (8.77) (compare Exercise 8.6.3).

For the general case, let us assume that we have one solution of Eq. (8.73) by a series substitution (or by guessing). We now proceed to develop a second, independent solution for which $W \neq 0$. Rewriting Eq. (8.76) as

$$\frac{dW}{W} = -P\,dx_1,$$

we integrate from $x_1 = a$ to $x_1 = x$ to obtain

$$\ln \frac{W(x)}{W(a)} = -\int_a^x P(x_1)dx_1$$

or[12]

$$W(x) = W(a)\exp\left[-\int_a^x P(x_1)dx_1\right]. \tag{8.79}$$

However,

$$W(x) = y_1 y_2' - y_1' y_2 = y_1^2 \frac{d}{dx}\left(\frac{y_2}{y_1}\right). \tag{8.80}$$

By combining Eqs. (8.79) and (8.80), we have

$$\frac{d}{dx}\left(\frac{y_2}{y_1}\right) = W(a)\frac{\exp\left[-\int_a^x P(x_1)dx_1\right]}{y_1^2(x)}. \tag{8.81}$$

Finally, by integrating Eq. (8.81) from $x_2 = b$ to $x_2 = x$ we get

$$y_2(x) = y_1(x)W(a)\int_b^x \frac{\exp\left[-\int_a^{x_2} P(x_1)dx_1\right]}{[y_1(x_2)]^2}dx_2, \tag{8.82}$$

[12] If $P(x_1)$ remains finite, $a \le x_1 \le x$, $W(x) \neq 0$ unless $W(a) = 0$. That is, the Wronskian of our two solutions is either identically zero or never zero.

where a and b are arbitrary constants and a term $y_1(x)y_2(b)/y_1(b)$ has been dropped because it leads to nothing new. Since $W(a)$, the Wronskian evaluated at $x = a$, is a constant and our solutions for the homogeneous differential equation always contain an unknown normalizing factor, we set $W(a) = 1$ and write

$$y_2(x) = y_1(x) \int^x \frac{\exp\left[-\int^{x_2} P(x_1)dx_1\right]}{[y_1(x_2)]^2} dx_2. \tag{8.83}$$

Note that the lower limits $x_1 = a$ and $x_2 = b$ have been omitted. If they are retained, they simply make a contribution equal to a constant times the known first solution, $y_1(x)$, and hence add nothing new.

If we have the important special case of $P(x) = 0$, Eq. (8.83) reduces to

$$y_2(x) = y_1(x) \int^x \frac{dx_2}{[y_1(x_2)]^2}. \tag{8.84}$$

This means that by using either Eq. (8.77) or Eq. (8.78), we can take one known solution and by integrating can generate a second independent solution of Eq. (8.73). As we shall see later, this technique to generate the second solution from the power series of the first solution $y_1(x)$ can be tedious.

EXAMPLE 8.6.1 **A Second Solution for the Linear Oscillator Equation** From $d^2y/dx^2 + y = 0$ with $P(x) = 0$, let one solution be $y_1 = \sin x$. By applying Eq. (8.84), we obtain

$$y_2(x) = \sin x \int^x \frac{dx_2}{\sin^2 x_2} = \sin x(-\cot x) = -\cos x,$$

which is clearly independent (not a linear multiple) of $\sin x$. ■

Series Form of the Second Solution

Further insight into the nature of the second solution of our differential equation may be obtained by the following sequence of operations:

1. Express $P(x)$ and $Q(x)$ in Eq. (8.77) as

$$P(x) = \sum_{i=-1}^{\infty} p_i x^i, \qquad Q(x) = \sum_{j=-2}^{\infty} q_j x^j. \tag{8.85}$$

   The lower limits of the summations are selected to create the strongest possible **regular** singularity (at the origin). These conditions just satisfy Fuchs's theorem and thus help us gain a better understanding of that theorem.
2. Develop the first few terms of a power series solution, as in Section 8.5.
3. Using this solution as y_1, obtain a second series-type solution, y_2, with Eq. (8.77), integrating term by term.

Proceeding with step 1, we have

$$y'' + (p_{-1}x^{-1} + p_0 + p_1x + \cdots)y' + (q_{-2}x^{-2} + q_{-1}x^{-1} + \cdots)y = 0, \quad (8.86)$$

in which point $x = 0$ is at worst a regular singular point. If $p_{-1} = q_{-1} = q_{-2} = 0$, it reduces to an ordinary point. Substituting

$$y = \sum_{\lambda=0}^{\infty} a_\lambda x^{k+\lambda}$$

(step 2), we obtain

$$\sum_{\lambda=0}^{\infty} (k+\lambda)(k+\lambda-1)a_\lambda k^{k+\lambda-2} + \sum_{i=-1}^{\infty} p_i x^i \sum_{\lambda=0}^{\infty} (k+\lambda)a_\lambda x^{k+\lambda-1}$$
$$+ \sum_{j=-2}^{\infty} q_j x^j \sum_{\lambda=0}^{\infty} a_\lambda x^{k+\lambda} = 0. \quad (8.87)$$

Our indicial equation is

$$k(k-1) + p_{-1}k + q_{-2} = 0,$$

which sets the coefficient of x^{k-2} equal to zero. This reduces to

$$k^2 + (p_{-1} - 1)k + q_{-2} = 0. \quad (8.88)$$

We denote the two roots of this indicial equation by $k = \alpha$ and $k = \alpha - n$, where n is zero or a positive integer. (If n is not an integer, we expect two independent series solutions by the methods of Section 8.6 and we are done.) Then

$$(k - \alpha)(k - \alpha + n) = 0$$

or

$$k^2 + (n - 2\alpha)k + \alpha(a - n) = 0, \quad (8.89)$$

and equating coefficients of k in Eqs. (8.88) and (8.89), we have

$$p_{-1} - 1 = n - 2\alpha. \quad (8.90)$$

The known series solution corresponding to the larger root $k = \alpha$ may be written as

$$y_1 = x^\alpha \sum_{\lambda=0}^{\infty} a_\lambda x^\lambda.$$

Substituting this series solution into Eq. (8.77) (step 3), we are faced with the formidable-looking expression,

$$y_2(x) = y_1(x) \int^x \frac{\exp\left(-\int_a^{x_2} \sum_{i=-1}^{\infty} p_i x_1^i \, dx_1\right)}{x_2^{2\alpha}\left(\sum_{\lambda=0}^{\infty} a_\lambda x_2^\lambda\right)^2} \, dx_2, \quad (8.91)$$

where the solutions y_1 and y_2 have been normalized so that the Wronskian $W(a) = 1$. Handling the exponential factor first, we have

$$\int_a^{x_2} \sum_{i=-1}^{\infty} p_i x_1^i \, dx_1 = p_{-1} \ln x_2 + \sum_{k=0}^{\infty} \frac{p_k}{k+1} x_2^{k+1} + f(a), \tag{8.92}$$

where $f(a) = -p_{-1} \ln a$ is an integration constant from the $i = -1$ term that leads to an unimportant overall factor and can be dropped. Hence,

$$\exp\left(-\int_a^{x_2} \sum_i p_i x_1^i dx_1\right) = \exp[-f(a)] x_2^{-p_{-1}} \exp\left(-\sum_{k=0}^{\infty} \frac{p_k}{k+1} x_2^{k+1}\right)$$

$$= \exp[-f(a)] x_2^{-p_{-1}} \left[1 - \sum_{k=0}^{\infty} \frac{p_k}{k+1} x_2^{k+1} + \frac{1}{2!}\left(-\sum_{k=0}^{\infty} \frac{p_k}{k+1} x_2^{k+1}\right)^2 + \cdots\right]. \tag{8.93}$$

This final series expansion of the exponential is certainly convergent if the original expansion of the coefficient $P(x)$ was convergent.

The denominator in Eq. (8.91) may be handled by writing

$$\left[x_2^{2\alpha}\left(\sum_{\lambda=0}^{\infty} a_\lambda x_2^\lambda\right)^2\right]^{-1} = x_2^{-2\alpha}\left(\sum_{\lambda=0}^{\infty} a_\lambda x_2^\lambda\right)^{-2} = x_2^{-2\alpha} \sum_{\lambda=0}^{\infty} b_\lambda x_2^\lambda, \tag{8.94}$$

provided $a_0 \neq 0$. Neglecting constant factors that will be picked up anyway by the requirement that $W(a) = 1$, we obtain

$$y_2(x) = y_1(x) \int^x x_2^{-p_{-1}-2\alpha} \left(\sum_{\lambda=0}^{\infty} c_\lambda x_2^\lambda\right) dx_2. \tag{8.95}$$

By Eq. (8.90),

$$x_2^{-p_{-1}-2\alpha} = x_2^{-n-1}, \tag{8.96}$$

where $n \geq 0$ is an integer. Substituting this result into Eq. (8.95), we obtain

$$y_2(x) = y_1(x) \int^x \left(c_0 x_2^{-n-1} + c_1 x_2^{-n} + c_2 x_2^{-n+1} + \cdots + c_n x_2^{-1} + \cdots\right) dx_2. \tag{8.97}$$

The integration indicated in Eq. (8.97) leads to a coefficient of $y_1(x)$ consisting of two parts:

1. A power series starting with x^{-n}.
2. A logarithm term from the integration of x^{-1} (when $\lambda = n$). This term always appears when n is an integer **unless** c_n fortuitously happens to vanish.[13]

EXAMPLE 8.6.2

A Second Solution of Bessel's Equation From Bessel's equation, Eq. (8.62) [divided by x^2 to agree with Eq. (8.73)], we have

$$P(x) = x^{-1} \qquad Q(x) = 1 \qquad \text{for the case} \quad n = 0.$$

[13] For parity considerations, $\ln x$ is taken to be $\ln |x|$, even.

Hence, $p_{-1} = 1, q_0 = 1$ in Eq. (8.85); all other p_i and q_j vanish. The Bessel indicial equation is

$$k^2 = 0$$

[Eq. (8.65) with $n = 0$]. Hence, we verify Eqs. (8.88)–(8.90) with n and $\alpha = 0$.

Our first solution is available from Eq. (8.69). Relabeling it to agree with Chapter 12 (and using $a_0 = 1$), we obtain[14]

$$y_1(x) = J_0(x) = 1 - \frac{x^2}{4} + \frac{x^4}{64} - O(x^6), \tag{8.98a}$$

valid for all x because of the absolute convergence of the series. Now, substituting all this into Eq. (8.83), we have the specific case corresponding to Eq. (8.91):

$$y_2(x) = J_0(x) \int^x \frac{\exp\left[-\int^{x_2} x_1^{-1} dx_1\right]}{\left[1 - x_2^2/4 + x_2^4/64 - \cdots\right]^2} dx_2. \tag{8.98b}$$

From the numerator of the integrand

$$\exp\left[-\int^{x_2} \frac{dx_1}{x_1}\right] = \exp[-\ln x_2] = \frac{1}{x_2}.$$

This corresponds to the $x_2^{-p_{-1}}$ in Eq. (8.93). From the denominator of the integrand, using a binomial expansion, we obtain

$$\left[1 - \frac{x_2^2}{4} + \frac{x_2^4}{64}\right]^{-2} = 1 + \frac{x_2^2}{2} + \frac{5x_2^4}{32} + \cdots.$$

Corresponding to Eq. (8.85), we have

$$\begin{aligned} y_2(x) &= J_0(x) \int^x \frac{1}{x_2} \left[1 + \frac{x_2^2}{2} + \frac{5x_2^4}{32} + \cdots\right] dx_2 \\ &= J_0(x) \left\{\ln x + \frac{x^2}{4} + \frac{5x^4}{128} + \cdots\right\}. \end{aligned} \tag{8.98c}$$

Let us check this result. From Eqs. (12.60) and (12.62), which give the standard form of the second solution,

$$Y_0(x) = \frac{2}{\pi}[\ln x - \ln 2 + \gamma] J_0(x) + \frac{2}{\pi} \left\{\frac{x^2}{4} - \frac{3x^4}{128} + \cdots\right\}. \tag{8.98d}$$

Two points arise. First, since Bessel's equation is homogeneous, we may multiply $y_2(x)$ by any constant. To match $Y_0(x)$, we multiply our $y_2(x)$ by $2/\pi$. Second, to our second solution $(2/\pi)y_2(x)$, we may add any constant multiple

[14]The capital O (order of) as written here means terms proportional to x^6 and possibly higher powers of x.

of the first solution. Again, to match $Y_0(x)$ we add

$$\frac{2}{\pi}[-\ln 2 + \gamma]J_0(x),$$

where γ is the Euler–Mascheroni constant (Section 5.2).[15] Our new, modified second solution is

$$y_2(x) = \frac{2}{\pi}[\ln x - \ln 2 + \gamma]J_0(x) + \frac{2}{\pi}J_0(x)\left\{\frac{x^2}{4} - \frac{5x^4}{128} + \cdots\right\}. \tag{8.98e}$$

Now the comparison with $Y_0(x)$ becomes a simple multiplication of $J_0(x)$ from Eq. (8.98a) and the curly bracket of Eq. (8.98c). The multiplication checks, through terms of order x^2 and x^4, which is all we carried. Our second solution from Eqs. (8.83) and (8.91) agrees with the standard second solution, the Neumann function, $Y_0(x)$. ■

From the preceding analysis, the second solution of Eq. (8.83), $y_2(x)$, may be written as

$$y_2(x) = y_1(x)\ln x + \sum_{j=-n}^{\infty} d_j x^{j+\alpha}, \tag{8.98f}$$

the first solution times $\ln x$ and another power series, this one starting with $x^{\alpha-n}$, which means that we may look for a logarithmic term when the indicial equation of Section 8.5 gives only one series solution. With the form of the second solution specified by Eq. (8.98f), we can substitute Eq. (8.98f) into the original differential equation and determine the coefficients d_j exactly as in Section 8.5. It is worth noting that no series expansion of $\ln x$ is needed. In the substitution $\ln x$ will drop out; its derivatives will survive.

The second solution will usually diverge at the origin because of the logarithmic factor and the negative powers of x in the series. For this reason, $y_2(x)$ is often referred to as the **irregular solution**. The first series solution, $y_1(x)$, which usually converges at the origin, is the regular solution. The question of behavior at the origin is discussed in more detail in Chapters 11 and 12, in which we take up Legendre functions and Bessel functions.

SUMMARY

The two solutions of both sections (together with the exercises) provide a **complete solution** of our linear, homogeneous, second-order ODE—assuming that the point of expansion is no worse than a regular singularity. At least one solution can always be obtained by series substitution (Section 8.5). A **second, linearly independent solution** can be constructed by the **Wronskian** double integral [Eq. (8.83)]. **No third, linearly independent solution exists**.

The **inhomogeneous**, linear, second-order ODE has an **additional** solution: the **particular solution**. This particular solution may be obtained by the method of variation of parameters.

[15] The Neumann function Y_0 is defined as it is in order to achieve convenient asymptotic properties (Section 12.3).

EXERCISES

8.6.1 Legendre's differential equation

$$(1-x^2)y''-2xy'+n(n+1)y=0$$

has a regular solution $P_n(x)$ and an irregular solution $Q_n(x)$. Show that the Wronskian of P_n and Q_n is given by

$$P_n(x)Q_n'(x)-P_n'(x)Q_n(x)=\frac{A_n}{1-x^2},$$

with A_n **independent** of x.

8.6.2 Show, by means of the Wronskian, that a linear, second-order, homogeneous ODE of the form

$$y''(x)+P(x)y'(x)+Q(x)y(x)=0$$

cannot have three independent solutions. (Assume a third solution and show that the Wronskian vanishes for all x.)

8.6.3 Transform our linear, second-order ODE

$$y''+P(x)y'+Q(x)y=0$$

by the substitution

$$y=z\exp\left[-\frac{1}{2}\int^x P(t)\,dt\right]$$

and show that the resulting differential equation for z is

$$z''+q(x)z=0,$$

where

$$q(x)=Q(x)-\frac{1}{2}P'(x)-\frac{1}{4}P^2(x).$$

8.6.4 Use the result of Exercise 8.6.3 to show that the replacement of $\varphi(r)$ by $r\varphi(r)$ may be expected to eliminate the first derivative from the Laplacian in spherical polar coordinates. See also Exercise 2.5.15(b).

8.6.5 By direct differentiation and substitution show that

$$y_2(x)=y_1(x)\int^x \frac{\exp\left[-\int^s P(t)\,dt\right]}{[y_1(s)]^2}\,ds$$

satisfies

$$y_2''(x)+P(x)y_2'(x)+Q(x)y_2(x)=0.$$

Note. The Leibniz formula for the derivative of an integral is

$$\frac{d}{d\alpha}\int_{g(\alpha)}^{h(\alpha)} f(x,\alpha)\,dx=\int_{g(\alpha)}^{h(\alpha)}\frac{\partial f(x,\alpha)}{\partial\alpha}\,dx + f[h(\alpha),\alpha]\frac{dh(\alpha)}{d\alpha}-f[g(\alpha),\alpha]\frac{dg(\alpha)}{d\alpha}.$$

8.6.6 In the equation

$$y_2(x) = y_1(x) \int^x \frac{\exp\left[-\int^s P(t)\,dt\right]}{[y_1(s)]^2}\,ds,$$

$y_1(x)$ satisfies

$$y_1'' + P(x)y_1' + Q(x)y_1 = 0.$$

The function $y_2(x)$ is a linearly **independent** second solution of the same equation. Show that the inclusion of lower limits on the two integrals leads to nothing new; that is, it adds only overall factors and/or a multiple of the known solution $y_1(x)$.

8.6.7 Given that one solution of

$$R'' + \frac{1}{r}R' - \frac{m^2}{r^2}R = 0$$

is $R = r^m$, show that Eq. (8.83) predicts a second solution, $R = r^{-m}$.

8.6.8 Using $y_1(x) = \sum_{n=0}^{\infty}(-1)^n x^{2n+1}/(2n+1)!$ as a solution of the linear oscillator equation, follow the analysis culminating in Eq. (8.98f) and show that $c_1 = 0$ so that the second solution does not, in this case, contain a logarithmic term.

8.6.9 Show that when n is **not** an integer the second solution of Bessel's equation, obtained from Eq. (8.83), does **not** contain a logarithmic term.

8.6.10 (a) One solution of Hermite's differential equation

$$y'' - 2xy' + 2\alpha y = 0$$

for $\alpha = 0$ is $y_1(x) = 1$. Find a second solution $y_2(x)$ using Eq. (8.83). Show that your second solution is equivalent to y_{odd} (Exercise 8.5.6).

(b) Find a second solution for $\alpha = 1$, where $y_1(x) = x$, using Eq. (8.83). Show that your second solution is equivalent to y_{even} (Exercise 8.5.6).

8.6.11 One solution of Laguerre's differential equation

$$xy'' + (1-x)y' + ny = 0$$

for $n = 0$ is $y_1(x) = 1$. Using Eq. (8.83), develop a second, linearly independent solution. Exhibit the logarithmic term explicitly.

8.6.12 For Laguerre's equation with $n = 0$

$$y_2(x) = \int^x \frac{e^s}{s}\,ds.$$

(a) Write $y_2(x)$ as a logarithm plus a power series.

(b) Verify that the integral form of $y_2(x)$, previously given, is a solution of Laguerre's equation ($n = 0$) by direct differentiation of the integral and substitution into the differential equation.

(c) Verify that the series form of $y_2(x)$, part (a), is a solution by differentiating the series and substituting back into Laguerre's equation.

8.6.13 The radial Schrödinger wave equation has the form

$$\left\{-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}+l(l+1)\frac{\hbar^2}{2mr^2}+V(r)\right]y(r)=Ey(r).$$

The potential energy $V(r)$ may be expanded about the origin as

$$V(r)=\frac{b_{-1}}{r}+b_0+b_1r+\cdots.$$

(a) Show that there is one (regular) solution starting with r^{l+1}.
(b) From Eq. (8.83) show that the irregular solution diverges at the origin as r^{-l}.

8.6.14 Show that if a second solution, y_2, is assumed to have the form $y_2(x)=y_1(x)f(x)$, substitution back into the original equation

$$y_2''+P(x)y_2'+Q(x)y_2=0$$

leads to

$$f(x)=\int^x\frac{\exp\left[-\int^s P(t)\,dt\right]}{[y_1(s)]^2}\,ds,$$

in agreement with Eq. (8.83).

8.6.15 If our linear, second-order ODE is nonhomogeneous—that is, of the form of Eq. (8.44)—the **most general solution is**

$$y(x)=y_1(x)+y_2(x)+y_p(x).$$

(y_1 and y_2 are independent solutions of the homogeneous equation.) Show that

$$y_p(x)=y_2(x)\int^x\frac{y_1(s)F(s)\,ds}{W\{y_1(s),\,y_2(s)\}}-y_1(x)\int^x\frac{y_2(s)F(s)\,ds}{W\{y_1(s),\,y_2(s)\}},$$

where $W\{y_1(x),\,y_2(x)\}$ is the Wronskian of $y_1(s)$ and $y_2(s)$.
Hint. Let $y_p(x)=y_1(x)v(x)$ and develop a first-order ODE for $v'(x)$.

8.6.16 (a) Show that

$$y''+\frac{1-\alpha^2}{4x^2}y=0$$

has two solutions:

$$y_1(x)=a_0x^{(1+\alpha)/2}$$

$$y_2(x)=a_0x^{(1-\alpha)/2}.$$

(b) For $\alpha=0$ the two linearly independent solutions of part (a) reduce to $y_{10}=a_0x^{1/2}$. Using Eq. (8.83) derive a second solution

$$y_{20}(x)=a_0x^{1/2}\ln x.$$

Verify that y_{20} is indeed a solution.

(c) Show that the second solution from part (b) may be obtained as a limiting case from the two solutions of part (a):

$$y_{20}(x) = \lim_{\alpha \to 0} \left(\frac{y_1 - y_2}{\alpha} \right).$$

8.7 Numerical Solutions

The analytic solutions and approximate solutions to differential equations in this chapter and in succeeding chapters may suffice to solve the problem at hand, particularly if there is some symmetry present. The power series solutions show how the solution behaves at small values of x. The asymptotic solutions show how the solution behaves at large values of x. These limiting cases and also the possible resemblance of our differential equation to the standard forms with known solutions (Chapters 11–13) are invaluable in helping us gain an understanding of the general behavior of our solution.

However, the usual situation is that we have a **different** equation, perhaps a different potential in the Schrödinger wave equation, and we want a reasonably exact solution. So we turn to numerical techniques.

First-Order Differential Equations

The differential equation involves a continuity of points. The independent variable x is continuous. The (unknown) dependent variable $y(x)$ is assumed continuous. The concept of differentiation demands continuity. Numerical processes replace these continua by discrete sets. We take x to have only specific values on a uniform grid, such as at

$$x_0, \qquad x_0 + h, \qquad x_0 + 2h, \qquad x_0 + 3h, \qquad \text{and so on,}$$

where h is some small interval. The smaller h is, the better the approximation is in principle. However, if h is made too small, the demands on machine time will be excessive, and accuracy may actually decline because of accumulated round-off errors. In practice, therefore, one chooses a step size by trial and error or the code adapts the step size optimally that minimizes round-off errors. We refer to the successive discrete values of x as x_n, x_{n+1}, and so on, and the corresponding values of $y(x)$ as $y(x_n) = y_n$. If x_0 and y_0 are given, the problem is to find y_1, then to find y_2, and so on.

Taylor Series Solution

Consider the ordinary (possibly nonlinear) first-order differential equation

$$\frac{d}{dx} y(x) = f(x, y), \tag{8.99}$$

with the initial condition $y(x_0) = y_0$. In principle, a step-by-step solution of the first-order equation [Eq. (8.99)] may be developed to any degree of accuracy

by a Taylor expansion

$$y(x_0 + h) = y(x_0) + hy'(x_0) + \frac{h^2}{2!}y''(x_0) + \cdots + \frac{h^n}{n!}y^{(n)}(x_0) + \cdots, \quad (8.100)$$

assuming the derivatives exist and the series is convergent. The initial value $y(x_0)$ is known and $y'(x_0)$ is given as $f(x_0, y_0)$. In principle, the higher derivatives may be obtained by differentiating $y'(x) = f(x, y)$. In practice, this differentiation may be tedious. Now, however, this differentiation can be done by computer using symbolic software, such as Mathematica, Maple, or Reduce, or numerical packages. For equations of the form encountered in this chapter, a computer has no trouble generating and evaluating 10 or more derivatives.

The Taylor series solution is a form of analytic continuation (Section 6.5). If the right-hand side of Eq. (8.100) is truncated after two terms, we have

$$y_1 = y_0 + hy_0' = y_0 + hf(x_0, y_0), \ldots, y_{n+1} = y_n + hf(x_n, y_n), \quad (8.101)$$

neglecting the terms of order h^2. Equation (8.101) is often called the **Euler solution**. Clearly, it is subject to serious error with the neglect of terms of order h^2. Let us discuss a specific case.

EXAMPLE 8.7.1

Taylor Series Approximation for First-Order ODE Because there is no general method for solving first-order ODEs, we often resort to numerical approximations. From $y' = f(x, y)$, we obtain by differentiation of the ODE

$$y'' = \frac{\partial f}{\partial x}(x, y) + \frac{\partial f}{\partial y}(x, y)y', \quad y''' = \frac{\partial^2 f}{\partial x^2}(x, y) + \cdots + \frac{\partial f}{\partial y}(x, y)y'',$$

etc. Starting from the point (x_0, y_0), we determine $y(x_0), y'(x_0), y''(x_0), \ldots$ from these derivatives of the ODE and plug them into the Taylor expansion in order to get to a neighboring point, from which we continue the process.

To be specific, consider the ODE $y' + y^2 = 0$, whose analytic solution through the point $(x = 1, y = 1)$ is the hyperbola $y(x) = 1/x$. Following the approximation method we just outlined, we find

$$y'' = -2yy', \quad y''' = -2(yy'' + y'^2), \quad y^{(IV)} = -2(yy''' + 3y'y''), \ldots.$$

The resulting Taylor series

$$\begin{aligned} y(x) &= y(1) + (x-1)y'(1) + \frac{(x-1)^2}{2}y''(1) + \frac{(x-1)^3}{3!}y'''(1) + \cdots \\ &= 1 - (x-1) + (x-1)^2 - (x-1)^3 + (x-1)^4 + \cdots = \frac{1}{1 + (x-1)} = \frac{1}{x}, \end{aligned}$$

for $0 < x < 2$ indeed confirms the exact solution and extends its validity beyond the interval of convergence. ■

Runge–Kutta Method

The Runge–Kutta method is a refinement of Euler's approximation [Eq. (8.101)]. The fourth-order Runge–Kutta approximation has an error of order h^5. The relevant formulas are

$$y_{n+1} = y_n + \frac{1}{6}[k_0 + 2k_1 + 2k_2 + k_3], \tag{8.102}$$

where

$$\begin{aligned} k_0 &= hf(x_n, y_n), \\ k_1 &= hf\left(x_n + \frac{1}{2}h, y_n + \frac{1}{2}k_0\right), \\ k_2 &= hf\left(x_n + \frac{1}{2}h, y_n + \frac{1}{2}k_1\right), \\ k_3 &= hf(x_n + h, y_n + k_2). \end{aligned} \tag{8.103}$$

The basic idea of the Runge–Kutta method is to eliminate the error terms order by order. A derivation of these equations appears in Ralston and Wilf[16] (see Chapter 9 by M. J. Romanelli) and in Press *et al.*[17]

Equations (8.102) and (8.103) define what might be called the classic fourth-order Runge–Kutta method (accurate through terms of order h^4). This is the form followed in Sections 15.1 and 15.2 of Press *et al.* Many other Runge–Kutta methods exist. Lapidus and Seinfeld (see Additional Reading) analyze and compare other possibilities and recommend a fifth-order form due to Butcher as slightly superior to the classic method. However, for applications not demanding high precision and for not so smooth ODEs the fourth-order Runge–Kutta method **with adaptive step size control** (see Press *et al.*, Chapter 15) is the method of choice for numerical solutions of ODEs. In general, but not always, fourth-order Runge–Kutta is superior to second-order **and higher order** Runge–Kutta schemes. From this Taylor expansion viewpoint the Runge–Kutta method is also an example of analytic continuation.

For the special case in which dy/dx is a function of x alone [$f(x, y)$ in Eq. (8.99) $\rightarrow f(x)$], the last term in Eq. (8.102) reduces to a Simpson rule numerical integration from x_n to x_{n+1}.

The Runge–Kutta method is stable, meaning that small errors do not get amplified. It is self-starting, meaning that we just take the x_0 and y_0 and away we go. However, it has disadvantages. Four separate calculations of $f(x, y)$ are required at each step. The errors, although of order h^5 per step, are not known. One checks the numerical solution by cutting h in half and repeating the calculation. If the second result agrees with the first, then h was small enough. Finally, the Runge–Kutta method can be extended to a set of coupled

[16] Ralston, A., and Wilf, H. S. (Eds.) (1960). *Mathematical Methods for Digital Computers*. Wiley, New York.

[17] Press, W. H., Flannery, B. P., Teukolsky, S. A., and Vetterling, W. T. (1992). *Numerical Recipes*, 2nd ed. Cambridge Univ. Press, Cambridge, UK.

first-order equations:

$$\frac{du}{dx} = f_1(x, u, v), \qquad \frac{dv}{dx} = f_2(x, u, v), \quad \text{and so on,} \tag{8.104}$$

with as many **dependent** variables as desired. Again, Eq. (8.104) may be nonlinear, an advantage of the numerical solution.

For high-precision applications one can also use either Richardson's extrapolation in conjunction with the Burlish–Stoer method[18] or the predictor–corrector method described later. Richardson's extrapolation is based on approximating the numerical solution by a rational function that can then be evaluated in the limit of step size $h \to 0$. This often allows for a large actual step size in applications.

Predictor–Corrector Methods

As an alternate attack on Eq. (8.99), we might estimate or **predict** a tentative value of y_{n+1} by

$$\bar{y}_{n+1} = y_{n-1} + 2hy'_n = y_{n-1} + 2hf(x_n, y_n). \tag{8.105}$$

This is not quite the same as Eq. (8.101). Rather, it may be interpreted as

$$y'_n \approx \frac{\Delta y}{\Delta x} = \frac{y_{n+1} - y_{n-1}}{2h}, \tag{8.106}$$

the derivative as a tangent being replaced by a chord. Next, we **calculate**

$$y'_{n+1} = f(x_{n+1}, \bar{y}_{n+1}). \tag{8.107}$$

Then to correct for the crudeness of Eq. (8.105), we take

$$y_{n+1} = y_n + \frac{h}{2}(\bar{y}_{n+1} + y'_n). \tag{8.108}$$

Here, the finite difference ratio $\Delta y/h$ is approximated by the average of the two derivatives. This technique—a prediction followed by a correction (and iteration until agreement is reached)—is the heart of the predictor–corrector method. It should be emphasized that the preceding set of equations is intended only to illustrate the predictor–corrector method. The accuracy of this set (to order h^3) is usually inadequate.

The iteration [substituting y_{n+1} from Eq. (8.108) back into Eq. (8.107) and recycling until y_{n+1} settles down to some limit] is time-consuming in a computer run. Consequently, the iteration is usually replaced by an intermediate step (the **modifier**) between Eqs. (8.105) and (8.107). This modified predictor–corrector method has the major advantage over the Runge–Kutta method of requiring only two computations of $f(x, y)$ per step instead of four. Unfortunately, the method as originally developed was unstable—small errors (round-off and truncation) tended to propagate and become amplified.

[18]See Section 15.4 of Press *et al.* and also Stoer, J., and Burlirsch, R. (1980). *Introduction to Numerical Analysis* (Chap. 7). Springer-Verlag, New York.

This very serious problem of instability has been overcome in a version of the predictor–corrector method devised by Hamming. The formulas (which are moderately involved), a partial derivation, and detailed instructions for starting the solution are all given by Ralston (Chapter 8 of Ralston and Wilf). Hamming's method is accurate to order h^4. It is stable for all reasonable values of h and provides an estimate of the error. Unlike the Runge–Kutta method, it is **not** self-starting. For example, Eq. (8.105) requires both y_{n-1} and y_n. Starting values (y_0, y_1, y_2, y_3) for the Hamming predictor–corrector method may be computed by series solution (power series for small x and asymptotic series for large x) or by the Runge–Kutta method. The Hamming predictor–corrector method may be extended to cover a set of coupled first-order ODEs—that is, Eq. (8.104).

Second-Order ODEs

Any second-order differential equation,

$$y''(x) + P(x)y'(x) + Q(x)y(x) = F(x), \tag{8.109}$$

may be split into two first-order ODEs by writing

$$y'(x) = z(x) \tag{8.110}$$

and then

$$z'(x) + P(x)z(x) + Q(x)y(x) = F(x). \tag{8.111}$$

These coupled first-order ODEs may be solved by either the Runge–Kutta or Hamming predictor–corrector techniques previously described. The Runge–Kutta–Nyström method for second-order ODEs is a more accurate version that proceeds via an intermediate auxiliary y'_{n+1}. The form of Eqs. (8.102) and (8.103) is assumed and the parameters are adjusted to fit a Taylor expansion through h^4.

As a final note, a thoughtless "turning the crank" application of these powerful numerical techniques is an invitation to disaster. The solution of a new and different differential equation will usually involve a combination of analysis and numerical calculation. There is little point in trying to force a Runge–Kutta solution through a singular point (see Section 8.4) where the solution (or y' or y'') may blow up. For a more extensive treatment of computational methods we refer the reader to Garcia (see Additional Reading).

EXERCISES

8.7.1 The Runge–Kutta method, Eq. (8.102), is applied to a first-order ODE $dy/dx = f(x)$. Note that this function $f(x)$ is independent of y. Show that in this special case the Runge–Kutta method reduces to Simpson's rule for numerical quadrature.

8.7.2 (a) A body falling through a resisting medium is described by

$$\frac{dv}{dt} = g - av$$

(for a retarding force proportional to the velocity). Take the constants to be $g = 9.80$ (m/sec^2) and $a = 0.2$ (sec^{-1}). The initial conditions are $t = 0$, $v = 0$. Integrate this equation out to $t = 20.0$ in steps of 0.1 sec. Tabulate the value of the velocity for each whole second, $v(1.0)$, $v(2.0)$, and so on. If a plotting routine is available, plot $v(t)$ versus t.

(b) Calculate the ratio of $v(20.0)$ to the terminal velocity $v(\infty)$.
Check value. $v(10) = 42.369$ m/sec.

ANS. (b) 0.9817.

8.7.3 Integrate Legendre's differential equation (Exercise 8.5.5) from $x = 0$ to $x = 1$ with the initial conditions $y(0) = 1$, $y'(0) = 0$ (even solution). Tabulate $y(x)$ and dy/dx at intervals of 0.05. Take $n = 2$.

8.7.4 The Lane–Emden equation of astrophysics is

$$\frac{d^2y}{dx^2} + \frac{2}{x}\frac{dy}{dx} + y^s = 0.$$

Take $y(0) = 1$, $y'(0) = 0$, and investigate the behavior of $y(x)$ for $s = 0, 1, 2, 3, 4, 5$, and 6. In particular, locate the first zero of $y(x)$.
Hint. From a power series solution $y''(0) = -\frac{1}{3}$.
Note. For $s = 0$, $y(x)$ is a parabola; for $s = 1$, a spherical Bessel function, $j_0(x)$. As $s \to 5$, the first zero moves out to ∞, and for $s > 5$, $y(x)$ never crosses the positive x-axis.

ANS. For $y(x_s) = 0$, $x_0 = 2.45(\approx\sqrt{6})$, $x_1 = 3.14(\approx\pi)$, $x_2 = 4.35$, $x_3 = 6.90$.

8.7.5 As a check on Exercise 8.6.10(a), integrate Hermite's equation ($x = 0$)

$$\frac{d^2y}{dx^2} - 2x\frac{dy}{dx} = 0$$

from $x = 0$ out to $x = 3$. The initial conditions are $y(0) = 0$, $y'(0) = 1$. Tabulate $y(1)$, $y(2)$, and $y(3)$.

ANS. $y(1) = 1.463$, $y(2) = 16.45$, $y(3) = 1445$.

8.7.6 Solve numerically ODE 3 of Exercise 8.3.15 using the Euler method, then compare with the Runge–Kutta method. For several fixed x, plot on a log–log scale $|y(x) - y_{\text{num}}(x)|$ versus step size, where $y(x)$ is your analytic and y_{num} your numerical solution. Find the best step size.

8.7.7 Solve numerically Bessel's ODE in Eq. (8.62) for $n = 0, 1, 2$ and calculate the location of the first two roots $J_n(\alpha_{ns}) = 0$.
Check value. $\alpha_{12} = 7.01559$.

8.7.8 Solve numerically the pendulum ODE

$$l\frac{d^2\theta}{dt^2} = -(g + a\sin\omega t)\sin\theta$$

with a harmonically driven pivot. Choose your step size according to the driving frequency ω and pick suitable parameters l, a, ω. Include and discuss the case $g \ll a$.

8.7.9 Solve numerically the ODE of Exercise 8.2.20. Compare with a Runge–Kutta result.

8.7.10 Solve numerically the ODE of Exercise 8.2.21.

8.7.11 Solve numerically the ODE of Exercise 8.2.22.

8.8 Introduction to Partial Differential Equations

The dynamics of many physical systems involve second-order derivatives, such as the acceleration in classical mechanics and the kinetic energy, $\sim\nabla^2$, in quantum mechanics, and lead to partial differential equations (PDEs) in time and one or more spatial variables.

Partial derivatives are linear operators:

$$\frac{\partial(a\varphi(x,y)+b\psi(x,y))}{\partial x}=a\frac{\partial\varphi(x,y)}{\partial x}+b\frac{\partial\psi(x,y)}{\partial x},$$

where a, b are constants. Similarly, if $\mathcal{L}$ is an operator consisting of (partial) derivatives, and the operator $\mathcal{L}$ is linear,

$$\mathcal{L}(a\psi_1+b\psi_2)=a\mathcal{L}\psi_1+b\mathcal{L}\psi_2,$$

and the PDE may be cast in the form

$$\mathcal{L}\psi=F,$$

where F is the external source, independent of $\psi(t,\mathbf{r})$, the unknown function. If $F\equiv 0$ the PDE is called **homogeneous**; if $F\neq 0$ the PDE is **inhomogeneous**. For homogeneous PDEs the **superposition principle** is valid: If ψ_1, ψ_2 are solutions of the PDE, so is any linear combination $a\psi_1+b\psi_2$. If $\mathcal{L}$ contains first-order partial derivatives at most, the PDE is called **first order**; if $\mathcal{L}$ contains second-order derivatives, such as ∇^2, but no higher derivatives, we have a second-order PDE, etc. Second-order PDEs with constant coefficients occur often in physics. They are classified further into **elliptic** PDEs if they involve ∇^2 or $\nabla^2+c^{-2}\partial^2/\partial t^2$, **parabolic** with $a\partial/\partial t+\nabla^2$, and **hyperbolic** with operators such as $c^{-2}\partial^2/\partial t^2-\nabla^2$. Hyperbolic (and some parabolic) PDEs have waves as solutions.

8.9 Separation of Variables

Our first technique for solving PDEs splits the PDE of n variables into n ordinary differential equations. Each separation introduces an arbitrary constant of separation. If we have n variables, we have to introduce $n-1$ constants, determined by the conditions imposed in the problem being solved. Let us

start with the heat flow equation for a rectangular metal slab. The geometry suggests using Cartesian coordinates.[19]

Cartesian Coordinates

In a homogeneous medium at temperature $\psi(\mathbf{r})$ that varies with location, heat flows from sites at high temperature to lower temperature in the direction of negative temperature gradient. We assume that appropriate heat sources are present on the boundaries to produce the boundary conditions. The heat flow must be of the form $\mathbf{j} = -\kappa\nabla\psi$, where the proportionality constant κ measures the heat conductivity of the medium, a rectangular metal slab in our case. The current density is proportional to the velocity of the heat flow. If the temperature increases somewhere, this is due to more heat flowing into that particular volume element d^3r than leaves it. From Section 1.6, we know that the difference is given by the negative divergence of the heat flow; that is, $-\nabla\cdot\mathbf{j}d^3r = \kappa\nabla^2\psi d^3r$. On the other hand, the increase of energy with time is proportional to the change of temperature with time, the specific heat σ, and the mass ρd^3r, where ρ is the density, taken to be constant in space and time. In the absence of sources, we obtain the **heat flow equation**

$$\frac{\partial\psi}{\partial t} = \frac{\kappa}{\sigma\rho}\nabla^2\psi, \tag{8.112}$$

a parabolic PDE. For the simplest, **time-independent steady-state** case we have $\partial\psi/\partial t = 0$, and the Laplace equation results. In Cartesian coordinates the Laplace equation becomes

$$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2} = 0, \tag{8.113}$$

using Eq. (2.5) for the Laplacian. Perhaps the simplest way of treating a PDE such as Eq. (8.113) is to split it into a set of ODEs. This may be done with a product ansatz, or trial form, for

$$\psi(x, y, z) = X(x)Y(y)Z(z), \tag{8.114}$$

and then substitute it back into Eq. (8.113). How do we know Eq. (8.114) is valid? We are proceeding with trial and error. If our attempt succeeds, then Eq. (8.114) will be justified. If it does not succeed, we shall find out soon enough and then we try another attack. With ψ assumed given by Eq. (8.114), Eq. (8.113) becomes

$$YZ\frac{d^2X}{dx^2} + XZ\frac{d^2Y}{dy^2} + XY\frac{d^2Z}{dz^2} = 0. \tag{8.115}$$

Dividing by $\psi = XYZ$ and rearranging terms, we obtain

$$\frac{1}{X}\frac{d^2X}{dx^2} = -\frac{1}{Y}\frac{d^2Y}{dy^2} - \frac{1}{Z}\frac{d^2Z}{dz^2}. \tag{8.116}$$

[19]Boundary conditions are part of the geometry, assumed Euclidean as well, and will be discussed later and in Chapter 16 in more detail.

Equation (8.116) exhibits one separation of variables. The left-hand side is a function of the variable x alone, whereas the right-hand side depends only on y and z. However, x, y, and z are all independent coordinates. This independence means that the recipe of Eq. (8.114) worked; the left-hand side of Eq. (8.116) depends on x only, etc. That is, the behavior of x as an independent variable is not determined by y and z. Therefore, each side must be equal to a constant—a **constant of separation**.

The choice of sign, completely arbitrary here, will be fixed in specific problems by the need to satisfy **specific boundary conditions**, which we need to discuss now. Let us put one corner of the slab in the coordinate origin with its sides along the coordinate axes and its bottom sitting at $z = 0$ with a given temperature distribution $\psi(x, y, z = 0) = \psi_0(x, y)$. To simplify the problem further, we assume that the slab is finite in the x- and y-directions but infinitely long in the z-direction with zero temperature as $z \to +\infty$. This is a reasonable assumption, as long as we are not interested in the temperature near the end of the slab ($z \to \infty$). We take the lengths of the slab in the transverse x, y-directions to be the same, 2π. Now we choose

$$\frac{1}{X}\frac{d^2X}{dx^2} = -l^2 \tag{8.117}$$

because the $\sin lx$, $\cos lx$ solutions with integer l implied by the boundary condition allow for a Fourier expansion to fit the x-dependence of the temperature distribution ψ_0 at $z = 0$ and fixed y. [Note that if a is the length of the slab in the x-direction, we write the separation constant as $-(2\pi l/a)^2$ with integer l, and this boundary condition gives the solutions $a_l \sin(2\pi lx/a) + b_l \cos(2\pi lx/a)$. If the temperature at $x = 0$, $x = a$ and $z = 0$ is zero, then all $b_l = 0$ and the cosine solutions are ruled out.]

Returning to the other half of Eq. (8.116), it becomes

$$-\frac{1}{Y}\frac{d^2Y}{dy^2} - \frac{1}{Z}\frac{d^2Z}{dz^2} = -l^2. \tag{8.118}$$

Rewriting it so as to separate the y- and z-dependent parts, we obtain

$$\frac{1}{Y}\frac{d^2Y}{dy^2} = l^2 - \frac{1}{Z}\frac{d^2Z}{dz^2}, \tag{8.119}$$

and a second separation has been achieved. Here we have a function of y equated to a function of z as before. We resolve the situation as before by equating each side to another (negative) constant of separation, $-m^2$,

$$\frac{1}{Y}\frac{d^2Y}{dy^2} = -m^2, \tag{8.120}$$

$$\frac{1}{Z}\frac{d^2Z}{dz^2} = l^2 + m^2 = n^2, \tag{8.121}$$

introducing a positive constant n^2 by $n^2 = l^2 + m^2$ to produce a symmetric set of equations in x, y. As a consequence, the separation constant in the z-direction is positive, which implies that its solution is exponential, $e^{\pm nz}$.

We discard solutions containing e^{+nz} because they violate the boundary condition for large values of z, where the temperature goes to zero. Now we have three ODEs [Eqs. (8.117), (8.120), and (8.121)] to replace the PDE [Eq. (8.113)]. Our assumption [Eq. (8.114)] has succeeded and is thereby justified.

Our solution should be labeled according to the choice of our constants l, m, and n; that is,

$$\psi_{lm}(x, y, z) = X_l(x)Y_m(y)Z_n(z), \tag{8.122}$$

subject to the conditions of the problem being solved and to the condition $n^2 = l^2 + m^2$. We may choose l and m as we like and Eq. (8.122) will still be a solution of Eq. (8.113), provided $X_l(x)$ is a solution of Eq. (8.117), and so on. We may develop **the most general solution** of Eq. (8.113) by taking a **linear combination of solutions** ψ_{lm}, **by the superposition principle**

$$\Psi(x, y, z) = \sum_{l,m} a_{lm}\psi_{lm}, \tag{8.123}$$

because the Laplace equation is homogeneous and linear. The constant coefficients a_{lm} are chosen to permit Ψ to satisfy the **boundary condition** of the problem at $z = 0$, where all Z_n are normalized to $Z_n(0) = 1$, so that

$$\psi_0(x, y) = \sum_{l,m} a_{lm}X_l(x)Y_m(y). \tag{8.124}$$

In other words, the expansion coefficients a_{lm} of our solution Ψ in Eq. (8.123) are uniquely determined as Fourier coefficients of the given temperature distribution at the boundary $z = 0$ of the metal slab. A specific case is treated in the next example.

EXAMPLE 8.9.1

Cartesian Boundary Conditions Let us consider a case in which, at $z = 0$, $\psi(x, y, 0) = \psi_0(x, y) = 100°\text{C}$ (the boiling point of water) in the area $-1 < x < 1, -1 < y < 1$, an input temperature distribution on the $z = 0$ plane. Moreover, the temperature ψ is held at zero, $\psi = 0$ (the freezing point of water) at the end points $x = \pm 1$ for all y and z, and at $y = \pm 1$ for all x and z, a boundary condition that restricts the temperature spread to the finite area of the slab in the x, y-directions. Also, $\psi(x, y, z) \to 0$ for $z \to \infty$ for all x, y. The entire slab, except the $z = 0$ plane, is in contact with a constant-temperature heat bath, whose temperature can be taken as the zero of ψ; Eq. (8.113) is invariant with respect to the addition of a constant to ψ.

Because of the adopted boundary conditions, we choose the solutions $\cos\frac{\pi l x}{2}$ with integer l that vanish at the end points $x = \pm 1$ and the corresponding ones in the y-direction, excluding $l = 0$ and $X, Y = \text{const}$. Inside the interval at $z = 0$, therefore, we have the (Fourier) expansion

$$X(x) = \sum_{l=1}^{\infty} a_l \cos\left(\frac{\pi l x}{2}\right) = 1, \quad -1 < x < 1,$$

with coefficients (see Section 14.1)

$$a_l = \int_{-1}^{1} 100 \cdot \cos\frac{\pi l x}{2} dx = \frac{200}{l\pi} \sin\frac{\pi l x}{2}\bigg|_{x=-1}^{1}$$
$$= \frac{400}{\pi l} \sin\frac{l\pi}{2} = \frac{400(-1)^{\mu}}{(2\mu+1)\pi}, \quad l = 2\mu + 1;$$
$$a_l = 0, \quad l = 2\mu$$

for integer μ. The same Fourier expansion (now without the factor 100) applies to the y-direction involving the integer summation index ν in $Y(y)$, whereas the z-dependence is given by Eq. (8.121), so that the complete solution becomes

$$\psi(x, y, z) = XYZ = 100 \sum_{\mu=0}^{\infty} \frac{4(-1)^{\mu}}{(2\mu+1)\pi} \cos\left((2\mu+1)\frac{\pi x}{2}\right)$$
$$\times \sum_{\nu=0}^{\infty} \frac{4(-1)^{\nu}}{(2\nu+1)\pi} \cos\left((2\nu+1)\frac{\pi y}{2}\right) e^{-\pi n z/2},$$
$$n^2 = (2\mu+1)^2 + (2\nu+1)^2.$$

For $z > 0$ this solution converges absolutely, but at $z = 0$ there is only conditional convergence for each sum that is caused by the discontinuity at $z = 0$, $x = \pm 1$, $y = \pm 1$. ■

Circular Cylindrical Coordinates

Let us now consider a cylindrical, infinitely long metal rod with a heat source at $z = 0$ that generates a given steady-state temperature distribution $\psi_0(\rho, \varphi) = \psi(\rho, \varphi, 0)$ at $z = 0$ in a circular area about the origin and zero temperature at large values of z for all ρ and φ. For the method of separation of variables to apply, the radial boundary condition needs to be independent of z and φ. Choices that lead to reasonable physical situations are (i) zero temperature at $\rho = a$ (radius of the rod, corresponding to immersion of the rod in a constant-temperature bath) and (ii) zero gradient of temperature at $\rho = a$ (corresponding to no lateral flow out of the rod). This choice will lead to a situation in which the lateral temperature distribution for large z will approach a uniform value equal to the average temperature of the area at $z = 0$. We want to find the temperature distribution for $z > 0$ for all ρ and φ under such conditions.

With our unknown function ψ dependent on ρ, φ, and z, the Laplace equation becomes (see Section 2.2 for ∇^2)

$$\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial\psi}{\partial\rho}\right) + \frac{1}{\rho^2}\frac{\partial^2\psi}{\partial\varphi^2} + \frac{\partial^2\psi}{\partial z^2} = 0. \tag{8.125}$$

As before, we assume a factored form for ψ,

$$\psi(\rho, \varphi, z) = P(\rho)\Phi(\varphi)Z(z). \tag{8.126}$$

Substituting into Eq. (8.125), we have

$$\frac{\Phi Z}{\rho}\frac{d}{d\rho}\left(\rho\frac{dP}{d\rho}\right) + \frac{PZ}{\rho^2}\frac{d^2\Phi}{d\varphi^2} + P\Phi\frac{d^2Z}{dz^2} = 0. \tag{8.127}$$

All the partial derivatives have become ordinary derivatives because each function depends on a single variable. Dividing by the product $P\Phi Z$ and moving the z derivative to the right-hand side yields

$$\frac{1}{\rho P}\frac{d}{d\rho}\left(\rho\frac{dP}{d\rho}\right)+\frac{1}{\rho^2\Phi}\frac{d^2\Phi}{d\varphi^2}=-\frac{1}{Z}\frac{d^2Z}{dz^2}. \tag{8.128}$$

Again, a function of z on the right depends on a function of ρ and φ on the left. We resolve this paradox by setting each side of Eq. (8.128) equal to the same constant. Let us choose $-n^2$. Then

$$\frac{d^2Z}{dz^2}=n^2Z, \tag{8.129}$$

and

$$\frac{1}{\rho P}\frac{d}{d\rho}\left(\rho\frac{dP}{d\rho}\right)+\frac{1}{\rho^2\Phi}\frac{d^2\Phi}{d\varphi^2}=-n^2. \tag{8.130}$$

From Eq. (8.130) we find the already familiar exponential solutions $Z\sim e^{\pm nz}$, from which we discard e^{+nz} again because the temperature goes to zero at large values of $z\geq 0$.

Returning to Eq. (8.131), multiplying by ρ^2 and rearranging terms, we obtain[20]

$$\frac{\rho}{P}\frac{d}{d\rho}\left(\rho\frac{dP}{d\rho}\right)+n^2\rho^2=-\frac{1}{\Phi}\frac{d^2\Phi}{d\varphi^2}. \tag{8.131}$$

We then set the right-hand side to the positive constant m^2 to obtain

$$\frac{d^2\Phi(\varphi)}{d\varphi^2}=-m^2\Phi(\varphi). \tag{8.132}$$

Finally, as an illustration of how the constant m in Eq. (8.133) is restricted, we note that φ in cylindrical and spherical polar coordinates is an azimuth angle. If this is a classical problem, we shall certainly require that the azimuthal solution $\Phi(\varphi)$ be single-valued; that is,

$$\Phi(\varphi+2\pi)=\Phi(\varphi), \tag{8.133}$$

which yields the periodic solutions $\Phi(\varphi)\sim e^{\pm im\varphi}$ for integer m. This is equivalent to requiring the azimuthal solution to have a period of 2π or some integral multiple of it.[21] Therefore, m must be an integer. Which integer it is depends on the details of the boundary conditions of the problem. This is discussed later and in Chapter 9. Whenever a coordinate corresponds to an azimuth angle the separated equation always has the form of Eq. (8.132).

Finally, for the ρ dependence we have

$$\rho\frac{d}{d\rho}\left(\rho\frac{dP}{d\rho}\right)+(n^2\rho^2-m^2)P=0. \tag{8.134}$$

[20]The choice of sign of the separation constant is arbitrary. However, a minus sign is chosen for the axial coordinate z in expectation of a possible exponential dependence on $z\geq 0$. A positive sign is chosen for the azimuthal coordinate φ in expectation of a periodic dependence on φ.

[21]This also applies in most quantum mechanical problems but the argument is much more involved. If m is not an integer, or half an integer for spin $\frac{1}{2}$ particles, rotation group relations and ladder operator relations (Section 4.3) are disrupted. Compare Merzbacher, E. (1962). Single valuedness of wave functions. *Am. J. Phys.* **30**, 237.

This is Bessel's ODE. The solutions and their properties are presented in Chapter 12. We emphasize here that we can rescale the variable ρ by a constant in Eq. (8.134) so that P must be a function of $n\rho$ and also depend on the parameter m; hence the notation $P_m(n\rho)$. Because the temperature is finite at the center of the rod, $\rho = 0$, P_m must be the regular solution J_m of Bessel's ODE rather than the irregular solution, the Neumann function Y_m. In case of boundary condition (i), $J_m(na) = 0$ will require na to be a zero of the Bessel function, thereby restricting n to a discrete set of values. The alternative (ii) requires $dJ_m/d\rho|_{n\rho=a} = 0$ instead. To fit the solution to a distribution ψ_0 at $z = 0$ one needs an expansion in Bessel functions and to use the associated orthogonality relations.

The separation of variables of Laplace's equation in parabolic coordinates also gives rise to Bessel's equation. The Bessel equation is notorious for the variety of disguises it may assume. For an extensive tabulation of possible forms the reader is referred to *Tables of Functions* by Jahnke and Emde.[22]

The original Laplace equation, a three-dimensional PDE, has been replaced by three ODEs [Eqs. (8.129), (8.132), and (8.134)]. A solution of the Laplace equation is

$$\psi_{mn}(\rho, \varphi, z) = P_m(n\rho)\Phi_m(\varphi)Z_n(z). \tag{8.135}$$

Identifying the specific P, Φ, Z solutions by subscripts, we see that the **most general solution of the Laplace equation** is a linear combination of the product solutions:

$$\Psi(\rho, \varphi, z) = \sum_{m,n} a_{mn}P_m(n\rho)\Phi_m(\varphi)Z_n(z). \tag{8.136}$$

Here, the coefficients a_{mn} are determined by the Bessel–Fourier expansion of the boundary condition at $z = 0$, where the given temperature distribution ψ_0 has to obey

$$\psi_0(\rho, \varphi) = \sum_{m,n} a_{mn}P_m(n\rho)\Phi_m(\varphi) \tag{8.137}$$

because all $Z_n(z = 0) = 1$. Recall that na is restricted to a discrete set of values by the radial boundary condition, and m are integers.

Spherical Polar Coordinates

For a large metal sphere and spherical boundary conditions, with a temperature distribution on the surface $\psi(r = a, \theta, \varphi) = \psi_0(\theta, \varphi)$ generated by a heat source at the surface $r = a$, let us separate the Laplace equation in spherical

[22] Jahnke, E., and Emde, F. (1945). *Tables of Functions*, 4th rev. ed. (p. 146). Dover, New York; also, Jahnke, E., Emde, F., and Lösch, F. (1960). *Tables of Higher Functions*, 6th ed. McGraw-Hill, New York.

polar coordinates. Using Eq. (2.77), we obtain

$$\frac{1}{r^2\sin\theta}\left[\sin\theta\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right)+\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right)+\frac{1}{\sin\theta}\frac{\partial^2\psi}{\partial\varphi^2}\right]=0. \tag{8.138}$$

Now, in analogy with Eq. (8.114) we try a product solution

$$\psi(r,\theta,\varphi)=R(r)\Theta(\theta)\Phi(\varphi). \tag{8.139}$$

By substituting back into Eq. (8.138) and dividing by $R\Theta\Phi$, we have

$$\frac{1}{Rr^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\frac{1}{\Theta r^2\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)+\frac{1}{\Phi r^2\sin^2\theta}\frac{d^2\Phi}{d\varphi^2}=0. \tag{8.140}$$

Note that all derivatives are now ordinary derivatives rather than partials. By multiplying by $r^2\sin^2\theta$, we can isolate $(1/\Phi)(d^2\Phi/d\varphi^2)$ to obtain[23]

$$\frac{1}{\Phi}\frac{d^2\Phi}{d\varphi^2}=r^2\sin^2\theta\left[-\frac{1}{r^2R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)-\frac{1}{r^2\sin\theta\Theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)\right]. \tag{8.141}$$

Equation (8.141) relates a function of φ alone to a function of r and θ alone. Since r, θ, and φ are independent variables, we equate each side of Eq. (8.141) to a constant. In almost all physical problems φ will appear as an azimuth angle. This suggests a periodic solution rather than an exponential so that Φ is single-valued. With this in mind, let us use $-m^2$ as the separation constant. Then

$$\frac{1}{\Phi}\frac{d^2\Phi(\varphi)}{d\varphi^2}=-m^2 \tag{8.142}$$

and

$$\frac{1}{r^2R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\frac{1}{r^2\sin\theta\Theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)-\frac{m^2}{r^2\sin^2\theta}=0. \tag{8.143}$$

Multiplying Eq. (8.143) by r^2 and rearranging terms, we obtain

$$\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)=-\frac{1}{\sin\theta\Theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)+\frac{m^2}{\sin^2\theta}. \tag{8.144}$$

Again, the variables are separated. We equate each side to a constant Q and finally obtain

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)-\frac{m^2}{\sin^2\theta}\Theta+Q\Theta=0, \tag{8.145}$$

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)-\frac{QR}{r^2}=0. \tag{8.146}$$

Once more we have replaced a PDE of three variables by three ODEs. The solutions of these ODEs are discussed in Chapters 11 and 12. In Chapter 11, for example, Eq. (8.145) is identified as the **associated Legendre equation** in which the constant Q becomes $l(l+1)$; l is a positive integer. The radial

[23]The order in which the variables are separated here is not unique. Many quantum mechanics texts show the r dependence split off first.

Eq. (8.146) has powers $R \sim r^l, r^{-l-1}$ for solutions so that $Q = l(l+1)$ is maintained. These power solutions occur in the multipole expansions of electrostatic and gravitational potentials, the most important physical applications. The corresponding positive power solutions are called harmonic polynomials, but the negative powers are required for a complete solution. The boundary conditions usually determine whether or not the negative powers are retained as (irregular) solutions.

Again, our most general solution may be written as

$$\psi(r, \theta, \varphi) = \sum_{l,m} a_{lm} R_l(r) \Theta_{lm}(\theta) \Phi_m(\varphi). \tag{8.147}$$

The great importance of this separation of variables in spherical polar coordinates stems from the fact that the method covers a tremendous amount of physics—many of the theories of gravitation, electrostatics, atomic, nuclear, and particle physics, where the **angular dependence** is isolated in the **same** Eqs. (8.142) and (8.145), **which can be solved exactly**. In the hydrogen atom problem, one of the most important examples of the Schrödinger wave equation with a closed form solution, the analog of Eq. (8.146) for the hydrogen atom becomes the associated Laguerre equation.

Whenever a coordinate z corresponds to an axis of translation the separated equation always has the form

$$\frac{d^2 Z(z)}{dz^2} = \pm a^2 Z(z)$$

in one of the cylindrical coordinate systems. The solutions, of course, are $\sin az$ and $\cos az$ for $-a^2$ and the corresponding hyperbolic function (or exponentials) $\sinh az$ and $\cosh az$ for $+a^2$.

Other occasionally encountered ODEs include the Laguerre and associated Laguerre equations from the supremely important hydrogen atom problem in quantum mechanics:

$$x\frac{d^2 y}{dx^2} + (1-x)\frac{dy}{dx} + \alpha y = 0, \tag{8.148}$$

$$x\frac{d^2 y}{dx^2} + (1+k-x)\frac{dy}{dx} + \alpha y = 0. \tag{8.149}$$

From the quantum mechanical theory of the linear oscillator we have Hermite's equation,

$$\frac{d^2 y}{dx^2} - 2x\frac{dy}{dx} + 2\alpha y = 0. \tag{8.150}$$

Finally, occasionally we find the Chebyshev differential equation

$$(1-x^2)\frac{d^2 y}{dx^2} - x\frac{dy}{dx} + n^2 y = 0. \tag{8.151}$$

More ODEs and two generalizations of them will be examined and systematized in Chapter 16. General properties following from the form of the differential equations are discussed in Chapter 9. The individual solutions are developed and applied in Chapters 11–13.

The practicing physicist probably will encounter other second-order ODEs, some of which may possibly be transformed into the examples studied here. Some of these ODEs may be solved by the techniques of Sections 8.5 and 8.6. Others may require a computer for a numerical solution.

- To put the separation method of solving PDEs in perspective, let us view it as a consequence of a symmetry of the PDE. Take the stationary Schrödinger equation $H\psi = E\psi$ as an example with a potential $V(r)$ depending only on the radial distance r. Then this PDE is invariant under rotations that comprise the group SO(3). Its diagonal generator is the orbital angular momentum operator $L_z = -i\frac{\partial}{\partial\varphi}$, and its quadratic (Casimir) invariant is $\mathbf{L}^2$. Since both commute with H (see Section 4.3), we end up with three separate eigenvalue equations:

$$H\psi = E\psi, \qquad \mathbf{L}^2\psi = l(l+1)\psi, \qquad L_z\psi = m\psi.$$

  Upon replacing L_z^2 in $\mathbf{L}^2$ by its eigenvalue m^2, the $\mathbf{L}^2$ PDE becomes Legendre's ODE (see Exercise 2.5.12), and similarly $H\psi = E\psi$ becomes the radial ODE of the separation method in spherical polar coordinates upon substituting the eigenvalue $l(l+1)$ for $\mathbf{L}^2$.
- For cylindrical coordinates the PDE is invariant under rotations about the z-axis only, which form a subgroup of SO(3). This invariance yields the generator $L_z = -i\partial/\partial\varphi$ and separate azimuthal ODE $L_z\psi = m\psi$ as before. Invariance under translations along the z-axis with the generator $-i\partial/\partial z$ gives the separate ODE in the z-variable provided the boundary conditions obey the same symmetry. The potential $V = V(\rho)$ or $V = V(z)$ depends on one variable, as a rule.
- In general, there are n mutually commuting generators H_i with eigenvalues m_i of the (classical) Lie group G of rank n and the corresponding Casimir invariants C_i with eigenvalues c_i, which yield the separate ODEs

$$H_i\psi = m_i\psi, \qquad C_i\psi = c_i\psi$$

  in addition to the radial ODE $H\psi = E\psi$.

EXERCISES

8.9.1 An atomic (quantum mechanical) particle is confined inside a rectangular box of sides a, b, and c. The particle is described by a wave function ψ that satisfies the Schrödinger wave equation

$$-\frac{\hbar^2}{2m}\nabla^2\psi = E\psi.$$

The wave function is required to vanish at each surface of the box (but not to be identically zero). This condition imposes constraints on the separation constants and therefore on the energy E. What is the smallest value of E for which such a solution can be obtained?

ANS. $E = \dfrac{\pi^2\hbar^2}{2m}\left(\dfrac{1}{a^2}+\dfrac{1}{b^2}+\dfrac{1}{c^2}\right)$.

8.9.2 The quantum mechanical angular momentum operator is given by $L = -i(\mathbf{r} \times \boldsymbol{\nabla})$. Show that

$$\mathbf{L} \cdot \mathbf{L}\psi = l(l+1)\psi$$

leads to the associated Legendre equation.
Hint. Exercises 1.8.6 and 2.5.13 may be helpful.

8.9.3 The one-dimensional Schrödinger wave equation for a particle in a potential field $V = \frac{1}{2}kx^2$ is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2}kx^2\psi = E\psi(x).$$

(a) Using $\xi = ax$ and a constant λ, we have

$$a = \left(\frac{mk}{\hbar^2}\right)^{1/4}, \qquad \lambda = \frac{2E}{\hbar}\left(\frac{m}{k}\right)^{1/2}.$$

Show that

$$\frac{d^2\psi(\xi)}{d\xi^2} + (\lambda - \xi^2)\psi(\xi) = 0.$$

(b) Substituting

$$\psi(\xi) = y(\xi)e^{-\xi^2/2},$$

show that $y(\xi)$ satisfies the Hermite differential equation.

8.9.4 Verify that the following are solutions of Laplace's equation:

(a) $\psi_1 = 1/r$, (b) $\psi_2 = \dfrac{1}{2r}\ln\dfrac{r+z}{r-z}$.

Note. The z derivatives of $1/r$ generate the Legendre polynomials, $P_n(\cos\theta)$ (Exercise 11.1.7). The z derivatives of $(1/2r)\ln[(r+z)/(r-z)]$ generate the Legendre functions, $Q_n(\cos\theta)$.

8.9.5 If Ψ is a solution of Laplace's equation, $\boldsymbol{\nabla}^2\Psi = 0$, show that $\partial\Psi/\partial z$ is also a solution.

Additional Reading

Cohen, H. (1992). *Mathematics for Scientists and Engineers*. Prentice-Hall, Englewood Cliffs, NJ.

Davis, P. J., and Rabinowitz, P. (1967). *Numerical Integration*. Blaisdell, Waltham, MA. This book covers a great deal of material in a relatively easy-to-read form. Appendix 1 (*On the Practical Evaluation of Integrals* by M. Abramowitz) is excellent as an overall view.

Garcia, A. L. (1994). *Numerical Methods for Physics*. Prentice-Hall, Englewood Cliffs, NJ.

Hamming, R. W. (1973). *Numerical Methods for Scientists and Engineers*, 2nd ed. McGraw-Hill, New York. Reprinted, Dover (1987). This well-written text discusses a wide variety of numerical methods from zeros of functions

to the fast Fourier transform. All topics are selected and developed with a modern high-speed computer in mind.

Hubbard, J., and West, B. H. (1995). *Differential Equations*. Springer, Berlin.

Ince, E. L. (1956). *Ordinary Differential Equations*. Dover, New York. The classic work on the theory of ordinary differential equations.

Lapidus, L., and Seinfeld, J. H. (1971). *Numerical Solutions of Ordinary Differential Equations*. Academic Press, New York. A detailed and comprehensive discussion of numerical techniques with emphasis on the Runge–Kutta and predictor–corrector methods. Work on the improvement of characteristics such as stability is clearly presented.

Margenau, H., and Murphy, G. M. (1956). *The Mathematics of Physics and Chemistry*, 2nd ed. Van Nostrand, Princeton, NJ. Chapter 5 covers curvilinear coordinates and 13 specific coordinate systems.

Miller, R. K., and Michel, A. N. (1982). *Ordinary Differential Equations*. Academic Press, New York.

Morse, P. M., and Feshbach, H. (1953). *Methods of Theoretical Physics*. McGraw-Hill, New York. Chapter 5 includes a description of several different coordinate systems. Note that Morse and Feshbach are not above using left-handed coordinate systems even for Cartesian coordinates. Elsewhere in this excellent (and difficult) book there are many examples of the use of the various coordinate systems in solving physical problems. Eleven additional fascinating but seldom encountered orthogonal coordinate systems are discussed in the second edition of *Mathematical Methods for Physicists* (1970).

Murphy, G. M. (1960). *Ordinary Differential Equations and Their Solutions*. Van Nostrand, Princeton, NJ. A thorough, relatively readable treatment of ordinary differential equations, both linear and nonlinear.

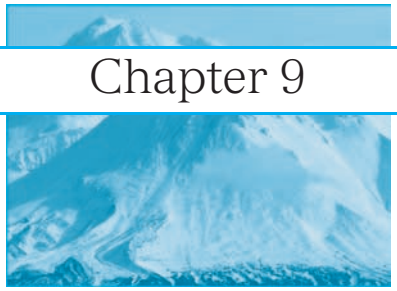
Press, W. H., Flannery, B. P., Teukolsky, S. A., and Vetterling, W. T. (1992). *Numerical Recipes*, 2nd ed. Cambridge Univ. Press, Cambridge, UK.

Ralston, A., and Wilf, H. (Eds.) (1960). *Mathematical Methods for Digital Computers*. Wiley, New York.

Ritger, P. D., and Rose, N. J. (1968). *Differential Equations with Applications*. McGraw-Hill, New York.

Stoer, J., and Burlirsch, R. (1992). *Introduction to Numerical Analysis*. Springer-Verlag, New York.

Stroud, A. H. (1974). *Numerical Quadrature and Solution of Ordinary Differential Equations*, Applied Mathematics Series Vol. 10. Springer-Verlag, New York. A balanced, readable, and very helpful discussion of various methods of integrating differential equations. Stroud provides numerous references.



Chapter 9

Sturm–Liouville Theory—Orthogonal Functions

In the preceding chapter, we developed two linearly independent solutions of the second-order linear homogeneous differential equation and proved that no third linearly independent solution existed. In this chapter, the emphasis shifts from solving the differential equation to developing and understanding general properties of the set of solutions. There is a close analogy between the concepts in this chapter and those of linear algebra in Chapter 3. Functions here play the role of vectors there, and linear operators play that of matrices in Chapter 3. The diagonalization of a real symmetric matrix in Chapter 3 corresponds here to the solution of an ordinary differential equation (ODE), defined by a **self-adjoint** operator $\mathcal{L}$, in terms of its eigenfunctions, which are the "continuous" analog of the eigenvectors in Chapter 3, and real eigenvalues that correspond to physically observable quantities in the laboratory. Just as a column eigenvector vector $\mathbf{a}$ is written as $|a\rangle$ in the Dirac notation of Chapter 3, we now write an eigenfunction as $|\varphi\rangle$. In the Cartesian component $a_i = \hat{\mathbf{x}}_i \cdot \mathbf{a}$, the discrete index i of the coordinate unit vectors is now replaced by the continuous variable x in $\varphi(x)$.

In Section 9.1, the concepts of self-adjoint operator, eigenfunction, eigenvalue, and Hermitian operator are presented. The concept of adjoint operator, given first in terms of differential equations, is then redefined in accordance with usage in quantum mechanics. The vital properties of reality of eigenvalues and orthogonality of eigenfunctions are derived in Section 9.2. In Section 9.3, we discuss the Gram–Schmidt procedure for systematically constructing sets of orthogonal functions. Finally, the general property of the completeness of a set of eigenfunctions is explored in Section 9.4.

9.1 Self-Adjoint ODEs

In Chapter 8, we studied, classified, and solved linear, second-order ODEs corresponding to linear, second-order differential operators of the general form

$$\mathcal{L} = p_0(x)\frac{d^2}{dx^2} + p_1(x)\frac{d}{dx} + p_2(x), \tag{9.1}$$

defined over the region $a \le x \le b$. A number of restrictions apply. The coefficients $p_0(x)$, $p_1(x)$, and $p_2(x)$ are real functions of x, and the first $2 - i$ derivatives of $p_i(x)$ are continuous. Reference to Eqs. (8.42) and (8.44) shows that $P(x) = p_1(x)/p_0(x)$ and $Q(x) = p_2(x)/p_0(x)$. Hence, $p_0(x)$ must not vanish for $a < x < b$. The zeros of $p_0(x)$ are singular points (Section 8.4), and the preceding statement means that our interval $[a, b]$ must be such that there are no singular points in the interior of the interval. There may be and often are singular points on the boundaries. Moreover, $b \to \infty$ and/or $a \to -\infty$ are possible in certain problems.

For a linear operator $\mathcal{L}$, the analog of a quadratic form for a matrix in Chapter 3 is the integral in Dirac's notation of Section 3.2:

$$\begin{aligned}\langle u|\mathcal{L}|u\rangle \equiv \langle u|\mathcal{L}u\rangle &\equiv \int_a^b u^*(x)\mathcal{L}u(x)\,dx \\ &= \int_a^b u(p_0u'' + p_1u' + p_2u)\,dx,\end{aligned} \tag{9.2}$$

taking $u = u^*$ to be real. This integral is the continuous analog of the **inner product** of vectors in Chapter 1 and here of u and $\mathcal{L}u$. Two vectors $u(x)$, $v(x)$ are **orthogonal** if their inner product vanishes,

$$\langle v|u\rangle \equiv \int_a^b v^*(x)u(x)\,dx = 0.$$

If we shift the derivatives to the first factor u in Eq. (9.2) by integrating by parts once or twice, we are led to the equivalent expression

$$\begin{aligned}\langle u|\mathcal{L}u\rangle &= [u(x)(p_1 - p_0')u(x)]_{x=a}^b \\ &\quad + \int_a^b \left[\frac{d^2}{dx^2}(p_0u) - \frac{d}{dx}(p_1u) + p_2u\right]u\,dx \\ &= [u(x)(p_1 - p_0')u(x)]_{x=a}^b + \left\langle \left[\frac{d^2}{dx^2}(p_0u) - \frac{d}{dx}(p_1u) + p_2u\right] \middle| u \right\rangle.\end{aligned} \tag{9.3}$$

For Eqs. (9.2) and (9.3) to agree for all u, the integrands have to be equal. The comparison yields

$$u(p_0'' - p_1')u + 2u(p_0' - p_1)u' = 0$$

or

$$p_0'(x) = p_1(x). \tag{9.4}$$

The terms at the boundary $x = a$ and $x = b$ in Eq. (9.3) then also vanish.

Because of the analogy with the transpose matrix in Chapter 3, it is convenient to define the linear operator in Eq. (9.3)

$$\begin{aligned}\bar{\mathcal{L}}u &= \frac{d^2}{dx^2}(p_0u) - \frac{d}{dx}(p_1u) + p_2u \\ &= p_0\frac{d^2u}{dx^2} + (2p_0' - p_1)\frac{du}{dx} + (p_0'' - p_1' + p_2)u\end{aligned} \tag{9.5}$$

as the **adjoint**[1] **operator** $\bar{\mathcal{L}}$ so that $\langle u|\mathcal{L}u\rangle = \langle\bar{\mathcal{L}}u|u\rangle$ for all u. The necessary and sufficient condition that $\bar{\mathcal{L}} = \mathcal{L}$, or $\langle u|\mathcal{L}u\rangle = \langle\mathcal{L}u|u\rangle$, is that Eq. (9.4) be satisfied for all u. When this condition is satisfied,

$$\bar{\mathcal{L}}u = \mathcal{L}u = \frac{d}{dx}\left[p(x)\frac{du(x)}{dx}\right] + q(x)u(x), \tag{9.6}$$

where $p(x) = p_0(x)$ and $q(x) = p_2(x)$, and the operator $\mathcal{L}$ is said to be **self-adjoint**. The importance of the form of Eq. (9.6) is that we will be able to carry out two integrations by parts in Eq. (9.3).[2]

The ODEs introduced in Section 8.3, Legendre's equation, and the linear oscillator equation are self-adjoint, but others, such as the Laguerre and Hermite equations, are not. However, the theory of linear, second-order, self-adjoint differential equations is perfectly general because we can **always** transform the non-self-adjoint operator into the required self-adjoint form. Consider Eq. (9.1) with $p_0' \neq p_1$. If we multiply $\mathcal{L}$ by[3]

$$\frac{1}{p_0(x)}\exp\left[\int^x \frac{p_1(t)}{p_0(t)}dt\right],$$

[1]The **adjoint** operator bears a somewhat forced relationship to the **transpose** matrix. A better justification for the nomenclature is found in a comparison of the **self-adjoint** operator (plus appropriate boundary conditions) with the **symmetric** matrix. These significant properties are developed in Section 9.2. Because of these properties, we are interested in **self-adjoint** operators. When adjoint or self-adjoint operators are discussed in the context of a Hilbert space, all functions of that space will satisfy the boundary conditions.

[2]The importance of the self-adjoint form (plus boundary conditions) will become apparent in Section 9.2, Eq. (9.22) and after.

[3]If we multiply $\mathcal{L}$ by $f(x)/p_0(x)$ and then demand that

$$f'(x) = \frac{fp_1}{p_0}$$

so that the new operator will be self-adjoint, we obtain

$$f(x) = \exp\left[\int^x \frac{p_1(t)}{p_0(t)}dt\right].$$

we obtain

$$\frac{1}{p_0(x)}\exp\left[\int^x \frac{p_1(t)}{p_0(t)}dt\right]\mathcal{L}u(u) = \frac{d}{dx}\left\{\exp\left[\int^x \frac{p_1(t)}{p_0(t)}dt\right]\frac{du(x)}{dx}\right\} + \frac{p_2(x)}{p_0(x)}\cdot\exp\left[\int^x \frac{p_1(t)}{p_0(t)}dt\right]u, \quad (9.7)$$

which is clearly self-adjoint [see Eq. (9.6)]. Notice the $p_0(x)$ in the denominator. This is why we require $p_0(x) \neq 0$, $a < x < b$. In the following development, we assume that $\mathcal{L}$ has been put into self-adjoint form.

Eigenfunctions and Eigenvalues

Schrödinger's time-independent wave equation for a single-particle system,

$$H\psi(x) = E\psi(x),$$

is a major example of an eigenvalue equation in physics; here, the differential operator $\mathcal{L}$ is defined by the Hamiltonian H and the eigenvalue is the total energy E of the system. The eigenfunction $\psi(x)$ is usually called a wave function. A variational derivation of this Schrödinger equation appears in Section 18.5. Based on spherical, cylindrical, or some other symmetry properties, a three- or four-dimensional partial differential equation (PDE) or eigenvalue equation, such as the Schrödinger equation, often separates into three (or more) eigenvalue equations in a single variable. In this context, an eigenvalue equation sometimes takes the more general self-adjoint form,

$$\mathcal{L}u(x) + \lambda w(x)u(x) = 0, \quad \text{or} \quad \mathcal{L}|u\rangle + \lambda w|u\rangle = 0, \quad (9.8)$$

where the constant λ is the eigenvalue, $\mathcal{L}$ is self-adjoint, and $w(x)$ is a known **weight** or density function; $w(x) > 0$ except possibly at isolated points at which $w(x) = 0$. The Schrödinger equation for the simple harmonic oscillator is a particular case of Eq. (9.8) with $w = 1$. The analysis of Eq. (9.8) with $\mathcal{L}$ as defined in Eq. (9.6) and its solutions is called **Sturm–Liouville theory**. For a given choice of the parameter λ, a function $u_\lambda(x)$, which satisfies Eq. (9.8) **and the imposed boundary conditions** discussed later, is called an **eigenfunction** corresponding to λ. The constant λ is then called an eigenvalue. There is no guarantee that an eigenfunction $u_\lambda(x)$ will exist for an arbitrary choice of the parameter λ. Indeed, the requirement that there be an eigenfunction often restricts the acceptable values of λ to a discrete set.

The **inner product** (or overlap integral) of two functions

$$\langle v|u\rangle \equiv \int v^*(x)u(x)w(x)dx$$

depends on the weight function and generalizes our previous definition for $w = 1$ to $w \neq 1$. The latter also modifies the definition of **orthogonality** of two eigenfunctions: They are orthogonal if their overlap integral vanishes, $\langle u_{\lambda'}|u_\lambda\rangle = 0$. Examples of eigenvalues for the Legendre and Hermite equations appear in the exercises of Section 8.5. Here, we have the mathematical approach to the process of quantization in quantum mechanics.

Table 9.1

Equation	$p(x)$	$q(x)$	λ	$w(x)$
Legendre	$1-x^2$	0	$l(l+1)$	1
Shifted Legendre	$x(1-x)$	0	$l(l+1)$	1
Associated Legendre	$1-x^2$	$-m^2/(1-x^2)$	$l(l+1)$	1
Bessel[a]	x	$-\frac{n^2}{x}$	a^2	x
Laguerre	xe^{-x}	0	α	e^{-x}
Associated Laguerre	$x^{k+1}e^{-x}$	0	$\alpha-k$	$x^k e^{-x}$
Hermite	e^{-x^2}	0	2α	e^{-x^2}
Simple harmonic oscillator[b]	1	0	n^2	1

[a] Orthogonality of Bessel functions is special. Compare Section 12.1 for details.
[b] This will form the basis for Chapter 14, Fourier series.

The extra weight function $w(x)$ sometimes appears as an asymptotic wave function ψ_∞ that is a common factor in all solutions of a PDE, such as the Schrödinger equation, for example, when the potential $V(x) \to 0$ as $x \to \infty$ in $H = T + V$. We find ψ_∞ when we set $V = 0$ in the Schrödinger equation. Another source for $w(x)$ may be a nonzero angular momentum barrier of the form $l(l+1)/x^2$ in a PDE or separated ODE that has a regular singularity and dominates at $x \to 0$. In such a case the indicial equation, such as Eqs. (8.65) or (8.88), shows that the wave function has x^l as an overall factor. Since the wave function enters twice in matrix elements $\langle v|Hu\rangle$ and orthogonality relations $\langle v|u\rangle$, the weight functions in Table 9.1 come from these common factors in both radial wave functions. This is the physical reason why the $\exp(-x)$ for Laguerre polynomials and $x^k \exp(-x)$ for associated Laguerre polynomials in Table 9.1 arise and is explained in more detail in the next example. The mathematical reason is that the weight function is needed to make the ODE self-adjoint.

EXAMPLE 9.1.1

Asymptotic Behavior, Weight Function Let us look at the asymptotic forms for small and large r of the radial Schrödinger equation for a particle of mass m moving in a spherically symmetric potential $V(r)$,

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2} + V(r) - E\right) u_l(r) = 0,$$

where $R_l(r) = u_l(r)/r$ is the radial wave function, E is the energy eigenvalue, and l is the orbital angular momentum (see Exercises 2.5.12 and 2.5.14). From the asymptotic ODEs we derive the asymptotic forms of the radial wave function. The boundary conditions are that $u_l(0) = 0$ and $u_l(r) \to 0$ for large r. Let us explain these boundary conditions for $l = 0$. We ask that $u_0 \to 0$ as $r \to 0$ because if $u_0(0)$ diverged the wave function could not be normalized; that is, $\langle u_0|u_0\rangle = 1$ cannot be enforced. If $u_0(0)$ is a finite nonzero constant, then $R_0(r) \sim 1/r$ for $r \to 0$. In that case, the kinetic energy, $\sim \nabla^2 \frac{1}{r} \sim \delta(\mathbf{r})$, would generate a singularity at the origin in the Schrödinger equation.

First, we explore how the angular momentum barrier ($\sim\frac{l(l+1)}{r^2}$) affects the solution for r close to zero, when $l \neq 0$. We assume that the potential is no more singular than a Coulomb potential, that is, $r^2V(r) \to 0$ as $r \to 0$, so that the potential and the energy eigenvalue are negligible compared to the angular momentum barrier for small r. Then the regular solution of the (asymptotic, meaning approximate for small r) radial ODE

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}+\frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}\right)u_l(r)=0$$

is $u_l(r) \sim r^{l+1}$ for small r, the regular solution of this radial ODE, whereas the irregular solution $u_l(r) \sim r^{-l}$ is not finite at small r and is not an acceptable solution. Thus, for $r \to 0$, the radial wave function $R_l(r) \sim r^l$ due to the barrier.

Now we turn our attention to large $r \to \infty$, assuming $V(r) \to 0$, so that we have to solve the asymptotic ODE

$$-\frac{\hbar^2}{2m}\frac{d^2u_l(r)}{dr^2}=Eu_l(r)$$

because the angular momentum barrier is also negligible at large r. For bound states $E < 0$, the solution is $u_l(r) \sim e^{-\kappa r}$ for large r with $E = -\hbar^2\kappa^2/2m$, whereas the other independent solution $e^{\kappa r} \to \infty$ for large r.

This settles the asymptotic behavior of the wave functions, which must have these limiting forms, r^l at small r and $e^{-\kappa r}$ at large r. In Chapter 13, the complete solution will be given in terms of associated Laguerre polynomials $L(r)$ so that $R_l(r) \sim r^l e^{-\kappa r}L(r)$. Therefore, orthonormality integrals $\langle\psi|\psi\rangle$ will contain the weight function $r^{2l+2}e^{-2\kappa r}$ along with a product of Laguerre polynomials, as shown in Table 9.1, except for scaling $2\kappa r \to x$ and renaming $2l+2 \to k$, and the corresponding ODEs are self-adjoint. ■

EXAMPLE 9.1.2

Legendre's Equation Legendre's equation is given by

$$(1-x^2)y''-2xy'+n(n+1)y=0, \tag{9.9}$$

over the interval $-1 \le x \le 1$ and with boundary condition that $y(\pm1)$ is finite. From Eqs. (9.1), (9.8), and (9.9),

$$\begin{aligned} p_0(x) &= 1-x^2 = p, \quad w(x)=1,\\ p_1(x) &= -2x = p', \quad \lambda = n(n+1),\\ p_2(x) &= 0 = q. \end{aligned}$$

Recall that our series solutions of Legendre's equation (Exercise 8.5.5)[4] diverged, unless n was restricted to an integer. This also represents a quantization of the eigenvalue λ. ■

[4]Compare also Exercise 5.2.11.

When the equations of Chapter 8 are transformed into the self-adjoint form, we find the values of the coefficients and parameters (Table 9.1). The coefficient $p(x)$ is the coefficient of the second derivative of the eigen-function. The eigenvalue λ is the parameter that is available in a term of the form $\lambda w(x)y(x)$; any x dependence apart from the eigenfunction becomes the weighting function $w(x)$. If there is another term containing the eigenfunction (not the derivatives), the coefficient of the eigenfunction in this additional term is identified as $q(x)$. If no such term is present, $q(x)$ is simply zero.

EXAMPLE 9.1.3

Deuteron Further insight into the concepts of eigenfunction and eigenvalue may be provided by an extremely simple model of the deuteron. The neutron–proton nuclear interaction is represented by a square well potential: $V = V_0 < 0$ for $0 \le r < a$, $V = 0$ for $r \ge a$. The Schrödinger wave equation is

$$-\frac{\hbar^2}{2M}\nabla^2\psi + V\psi = E\psi, \tag{9.10}$$

where $\psi = \psi(r)$ is the probability amplitude for finding a neutron–proton pair at relative distance r. The boundary conditions are $\psi(0)$ finite and $\psi(r) \to 0$ for large r.

We may write $u(r) = r\psi(r)$, and using Exercises 2.5.12 and 2.5.14 the radial wave equation becomes

$$\frac{d^2u}{dr^2} + k_1^2 u = 0, \tag{9.11}$$

with

$$k_1^2 = \frac{2M}{\hbar^2}(E - V_0) > 0 \tag{9.12}$$

for the interior range, $0 \le r < a$. Here, M is the reduced mass of the neutron–proton system. Note that $V_0 < E < 0$ for a bound state, leading to the sign of k_1^2 in Eq. (9.11). For $a \le r < \infty$, we have

$$\frac{d^2u}{dr^2} - k_2^2 u = 0, \tag{9.13}$$

with

$$k_2^2 = -\frac{2ME}{\hbar^2} > 0 \tag{9.14}$$

because $E < 0$ for a bound state with $V \to 0$ as $r \to \infty$. From the boundary condition that ψ remain finite, $u(0) = 0$, and

$$u_{\text{in}}(r) = \sin k_1 r, \quad 0 \le r < a. \tag{9.15}$$

In the range outside the potential well, we have a linear combination of the two exponentials,

$$u_{\text{ex}}(r) = A\exp k_2 r + B\exp(-k_2 r), \quad a \le r < \infty. \tag{9.16}$$

At $r = a$ the solution to the ODE must be continuous, with a continuous derivative, demanding that $u_{\text{in}}(a) = u_{\text{ex}}(a)$ and that $u'_{\text{in}}(a) = u'_{\text{ex}}(a)$. These **joining or matching conditions** give

$$\begin{aligned} \sin k_1 a &= A \exp k_2 a + B \exp(-k_2 a), \\ k_1 \cos k_1 a &= k_2 A \exp k_2 a - k_2 B \exp(-k_2 a). \end{aligned} \tag{9.17}$$

The boundary condition for large r means that $A = 0$. Dividing the preceding pair of equations (to cancel B), we obtain

$$\tan k_1 a = -\frac{k_1}{k_2} = -\sqrt{\frac{E - V_0}{-E}}, \tag{9.18}$$

a transcendental equation for the energy E with only certain discrete solutions. If E is such that Eq. (9.18) can be satisfied, our solutions $u_{\text{in}}(r)$ and $u_{\text{ex}}(r)$ can satisfy the boundary conditions. If Eq. (9.18) is not satisfied, **no acceptable solution exists**. The values of E, for which Eq. (9.18) is satisfied, are the eigenvalues; the corresponding function $\psi(r) = u_{in}/r$ for $r < a$ and $\psi(r) = u_{\text{ex}}/r$ for $r > a$ is the eigenfunction. For the actual deuteron problem, there is one (and only one) negative value of E satisfying Eq. (9.18); that is, the deuteron has one and only one bound state.

Now, what happens if E does not satisfy Eq. (9.18) (i.e., $E \neq E_0$ is not an eigenvalue)? In graphical form, imagine that E and therefore k_1 are varied slightly. For $E = E_1 < E_0$, k_1 is reduced, and $\sin k_1 a$ has not turned down enough to match $\exp(-k_2 a)$. The joining conditions, Eq. (9.17), require $A > 0$ and the wave function goes to $+\infty$, exponentially. For $E = E_2 > E_0$, k_1 is larger, $\sin k_1 a$ peaks sooner and has descended more rapidly at $r = a$. The joining conditions demand $A < 0$, and the wave function goes to $-\infty$ exponentially. Only for $E = E_0$, an eigenvalue, will the wave function have the required negative exponential asymptotic behavior (Fig. 9.1). ■

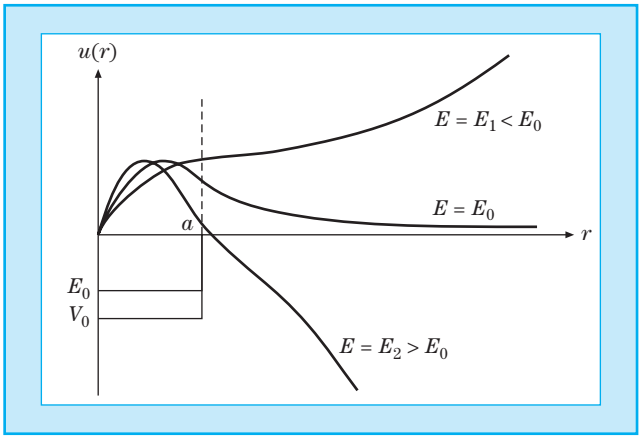


Figure 9.1

Deuteron Wave Functions; Eigenfunction for $E = E$

Boundary Conditions

In the foregoing definition of eigenfunction, it was noted that the eigenfunction $u_\lambda(x)$ was required to satisfy certain imposed boundary conditions. The term boundary conditions includes as a special case the concept of initial conditions, for instance, specifying the initial position x_0 and the initial velocity v_0 in some dynamical problem. The only difference in the present usage of boundary conditions in these one-dimensional problems is that we are going to apply the conditions on **both** ends of the allowed range of the variable to ensure a self-adjoint ODE.

Usually, the form of the differential equation or the boundary conditions on the eigenfunctions will guarantee that, at the ends of our interval (i.e., at the boundary), the following products will vanish:

$$p(x)v^*(x)\frac{du(x)}{dx}\bigg|_{x=a} = 0 \qquad \text{and} \qquad p(x)v^*(x)\frac{du(x)}{dx}\bigg|_{x=b} = 0. \tag{9.19}$$

Here, $u(x)$ and $v(x)$ are solutions of the particular ODE [Eq. (9.8)] being considered. A reason for the particular form of Eq. (9.19) is suggested later. If we recall the radial wave function u of the hydrogen atom in Example 9.1.1 with $u(0) = 0$ and $du/dr \sim e^{-kr} \to 0$ as $r \to \infty$, then both boundary conditions are satisfied. Similarly, in the deuteron Example 9.1.3, $\sin k_1 r \to 0$ as $r \to 0$ and $d(e^{-k_2 r})/dr \to 0$ as $r \to \infty$, both boundary conditions are obeyed.

We can, however, work with a less restrictive set of boundary conditions,

$$v^* pu'\,|_{x=a} = v^* pu'\,|_{x=b}, \tag{9.20}$$

in which $u(x)$ and $v(x)$ are solutions of the differential equation corresponding to the same or to different eigenvalues. Equation (9.20) might well be satisfied if we were dealing with a periodic physical system, such as a crystal lattice.

Equations (9.19) and (9.20) are written in terms of v^*, complex conjugate. When the solutions are real, $v = v^*$ and the asterisk may be ignored. However, in Fourier exponential expansions and in quantum mechanics the functions will be complex and the complex conjugate will be needed.

Hermitian Operators

We now prove an important property of the combination self-adjoint, second-order differential operator [Eq. (9.6)], with functions $u(x)$ and $v(x)$ that satisfy boundary conditions given by Eq. (9.20) and explain the special form of the latter.

By integrating v^* (complex conjugate) times the second-order self-adjoint differential operator $\mathcal{L}$ (operating on u) over the range $a \le x \le b$, we obtain

$$\int_a^b v^* \mathcal{L}u\, dx = \int_a^b v^*(pu')'dx + \int_a^b v^* qu\, dx \tag{9.21}$$

using Eq. (9.6), or in Dirac notation,

$$\langle v|\mathcal{L}u\rangle = \langle v|\left(\frac{d}{dx}p\frac{d}{dx}+q\right)u\rangle.$$

Integrating by parts, we have

$$\int_a^b v^*(pu')'dx = v^*pu'\Big|_a^b - \int_a^b v'^*pu'dx. \tag{9.22}$$

The integrated part vanishes on application of the boundary conditions [Eq. (9.20)]. Integrating the remaining integral by parts a second time, we have

$$-\int_a^b v'^*pu'dx = -v'^*pu\Big|_a^b + \int_a^b u(pv'^*)'dx. \tag{9.23}$$

Again, the integrated part vanishes in an application of Eq. (9.20). A combination of Eqs. (9.21)–(9.23) gives us

$$\langle v|\mathcal{L}u\rangle = \int_a^b v^*\mathcal{L}u\,dx = \int_a^b u\mathcal{L}v^*dx = \langle \mathcal{L}v|u\rangle. \tag{9.24}$$

This property, given by Eq. (9.24), is expressed by stating that the operator $\mathcal{L}$ is Hermitian with respect to the functions $u(x)$ and $v(x)$, which satisfy the boundary conditions specified by Eq. (9.20). Note that if this Hermitian property follows from self-adjointness in a Hilbert space, then it includes that boundary conditions are imposed on all functions of that space. The integral in Eq. (9.24) may also be recognized as **inner product**, $\langle v|\mathcal{L}u\rangle$, of $|v\rangle$ and $|\mathcal{L}u\rangle$.

These properties [Eqs. (9.19) or (9.20)] are so important for the concept of Hermitian operator (discussed next) and the consequences (Section 9.2) that the interval (a, b) must be so as to ensure that either Eq. (9.19) or Eq. (9.20) is **satisfied**. The boundary conditions of the problem determine the range of integration. If our solutions are polynomials, the coefficient $p(x)$ may restrict the range of integration. Note that $p(x)$ also determines the singular points of the differential equation (Section 8.4). For nonpolynomial solutions, for example, $\sin nx$, $\cos nx$; $(p = 1)$, the range of integration is determined by the boundary conditions of each problem, as explained in the next example.

EXAMPLE 9.1.4

Integration Interval, $[a, b]$ For $\mathcal{L} = d^2/dx^2$ a possible eigenvalue equation is

$$\frac{d^2}{dx^2}y(x) + n^2y(x) = 0, \tag{9.25}$$

with eigenfunctions

$$u_n = \cos nx, \qquad v_m = \sin mx.$$

Equation (9.20) becomes

$$-n\sin mx\sin nx\,|_a^b = 0, \qquad \text{or} \quad m\cos mx\cos nx\,|_a^b = 0,$$

interchanging u_n and v_m. Since $\sin mx$ and $\cos nx$ are periodic with period 2π (for n and m integral), Eq. (9.20) is clearly satisfied if $a = x_0$ and $b = x_0 + 2\pi$. If a problem prescribes a different interval, the eigenfunctions and eigenvalues will change along with the boundary conditions. The functions must always be so that the boundary conditions [Eq. (9.20), etc.] are satisfied. For this case (Fourier series), the usual cases are $x_0 = 0$, leading to $(0, 2\pi)$, and $x_0 = -\pi$ leading to $(-\pi, \pi)$. Here and throughout the following several chapters, the relevant functions will satisfy the boundary conditions prescribed by the integration interval [Eq. (9.20)]. The interval $[a, b]$ and the weighting factor $w(x)$ for the most commonly encountered second-order ODEs are listed in Table 9.2. ■

Table 9.2

Equation	a	b	$w(x)$
Legendre	-1	1	1
Shifted Legendre	0	1	1
Associated Legendre	-1	1	1
Laguerre	0	∞	e^{-x}
Associated Laguerre	0	∞	$x^k e^{-x}$
Hermite	$-\infty$	∞	e^{-x^2}
Simple harmonic oscillator	0	2π	1
	$-\pi$	π	1

[1]The orthogonality interval $[a, b]$ is determined by the boundary conditions of Section 9.1. $p(x)$, $q(x)$ are given in Table 9.1.
[2]The weighting function is established by putting the ODE in self-adjoint form.

Hermitian Operators in Quantum Mechanics

The preceding discussion focused on the classical second-order differential operators of mathematical physics. Generalizing our Hermitian operator theory, as required in quantum mechanics, we have an extension: The operators need be neither second-order differential operators nor real. For example, the linear momentum operator $p_x = -i\hbar(\partial/\partial x)$ represents a real physical observable and will be an Hermitian operator. We simply assume (as is customary in quantum mechanics) that the wave functions satisfy appropriate boundary conditions in one or three (or other number of) dimensions, vanishing sufficiently strongly at infinity or having periodic behavior (as in a crystal lattice or unit intensity for waves). In practice, this means that the wave functions are in a given Hilbert space. The operator $\mathcal{L}$ is called **Hermitian** if

$$\langle \psi_1 | \mathcal{L}\psi_2 \rangle = \int \psi_1^* \mathcal{L}\psi_2 d\tau = \int (\mathcal{L}\psi_1)^* \psi_2 d\tau = \langle \mathcal{L}\psi_1 | \psi_2 \rangle \tag{9.26}$$

for all ψ_1, ψ_2 of a given Hilbert space. Apart from the simple extension to complex quantities, this definition is identical to Eq. (9.24).

The **adjoint** $A^\dagger$ of an operator A is defined by

$$\langle\psi_1|A^\dagger\psi_2\rangle = \int \psi_1^* A^\dagger \psi_2 d\tau \equiv \int (A\psi_1)^* \psi_2 d\tau = \langle A\psi_1|\psi_2\rangle. \tag{9.27}$$

Comparing with our classical, second derivative operator-oriented Eq. (9.5) defining $\tilde{\mathcal{L}}$, we see that $\mathcal{L}^\dagger = \tilde{\mathcal{L}}^*$ so that we have generalized the adjoint operator to the complex domain (of quantum mechanics). Here, the adjoint is defined in terms of the resultant integral, with the $A^\dagger$ as part of the integrand. Clearly, if $A = A^\dagger$ (**self-adjoint**) and the (space of) functions, on which it acts, satisfy the previously mentioned boundary conditions, then A is Hermitian.

The **expectation value** of an operator $\mathcal{L}$ is defined as

$$\langle\mathcal{L}\rangle = \int \psi^* \mathcal{L}\psi \, d\tau = \langle\psi|\mathcal{L}\psi\rangle. \tag{9.28a}$$

In the framework of quantum mechanics $\langle\mathcal{L}\rangle$ corresponds to the theoretical value of the physical observable represented by $\mathcal{L}$, if the physical system is in a state described by the wave function ψ. When this property is measured experimentally, $\langle\mathcal{L}\rangle$ may be obtained as the mean or average of many measurements of the observable $\mathcal{L}$ of the physical system in the state ψ.

If we require $\mathcal{L}$ to be Hermitian, it is easy to show that $\langle\mathcal{L}\rangle$ is real (as would be expected from a measurement in a physical theory). Taking the complex conjugate of Eq. (9.28a), we obtain

$$\langle\mathcal{L}\rangle^* = \left[\int \psi^* \mathcal{L}\psi \, d\tau\right]^* = \int \psi \mathcal{L}^* \psi^* d\tau.$$

Rearranging the factors in the integrand, we have

$$\langle\mathcal{L}\rangle^* = \int (\mathcal{L}\psi)^* \psi d\tau = \langle\mathcal{L}\psi|\psi\rangle.$$

Then, applying our definition of Hermitian operator [Eq. (9.26)], we get

$$\langle\mathcal{L}\rangle^* = \int \psi^* \mathcal{L}\psi d\tau = \langle\mathcal{L}\rangle, \tag{9.28b}$$

or $\langle\mathcal{L}\rangle$ is real. It is worth noting that ψ is not necessarily an eigenfunction of $\mathcal{L}$.

EXERCISES

9.1.1 Show that Laguerre's equation may be put into self-adjoint form by multiplying by e^{-x} and that $w(x) = e^{-x}$ is the weighting function.

9.1.2 Show that the Hermite equation may be put into self-adjoint form by multiplying by e^{-x^2} and that this gives $w(x) = e^{-x^2}$ as the appropriate density function.

9.1.3 Show the following when the linear second-order differential equation is expressed in self-adjoint form:

(a) The Wronskian is equal to a constant divided by the initial coefficient p.

$$W[y_1, y_2] = \frac{C}{p(x)}.$$

(b) A second solution is given by

$$y_2(x) = Cy_1(x)\int^x \frac{dt}{p[y_1(t)]^2}.$$

9.1.4 For the very special case $\lambda = 0$ and $q(x) = 0$, the self-adjoint eigenvalue equation becomes

$$\frac{d}{dx}\left[p(x)\frac{du(x)}{dx}\right] = 0,$$

satisfied by

$$\frac{du}{dx} = \frac{1}{p(x)}.$$

Use this to obtain a "second" solution of the following:
(a) Legendre's equation;
(b) Laguerre's equation; and
(c) Hermite's equation.

ANS. (a) $u_2(x) = \frac{1}{2}\ln\frac{1+x}{1-x}$,

(b) $u_2(x) - u_2(x_0) = \int_{x_0}^{x} e^t \frac{dt}{t}$,

(c) $u_2(x) = \int_0^x e^{t^2} dt$.

These second solutions illustrate the divergent behavior usually found in a second solution.
Note. In all three cases $u_1(x) = 1$.

9.1.5 Given that $\mathcal{L}u = 0$ and $g\mathcal{L}u$ is self-adjoint, show that for the adjoint operator $\tilde{\mathcal{L}}$, $\tilde{\mathcal{L}}(gu) = 0$.

9.1.6 For a second-order differential operator $\mathcal{L}$ that is self-adjoint show that

$$\langle y_2|\mathcal{L}y_1\rangle - \langle y_1|\mathcal{L}y_2\rangle = \int_a^b [y_2\mathcal{L}y_1 - y_1\mathcal{L}y_2]dx = p(y_1'y_2 - y_1y_2')\,|_a^b\,.$$

9.1.7 Show that if a function ψ is required to satisfy Laplace's equation in a finite region of space and to satisfy Dirichlet boundary conditions over the entire closed bounding surface, then ψ is unique.
Hint. One of the forms of Green's theorem (Section 1.10) will be helpful.

9.1.8 Consider the solutions of the Legendre, Hermite, and Laguerre equations to be polynomials. Show that the ranges of integration that guarantee that the Hermitian operator boundary conditions will be satisfied are
(a) Legendre $[-1, 1]$, (b) Hermite $(-\infty, \infty)$, (c) Laguerre $[0, \infty)$.

9.1.9 Within the framework of quantum mechanics [Eq. (9.26) and following], show that the following are Hermitian operators:

(a) momentum $\mathbf{p} = -i\hbar\nabla \equiv -i\dfrac{h}{2\pi}\nabla$; and

(b) angular momentum $\mathbf{L} = -i\hbar\mathbf{r}\times\nabla \equiv -i\dfrac{h}{2\pi}\mathbf{r}\times\nabla$.

Hint. In Cartesian form $\mathbf{L}$ is a linear combination of noncommuting Hermitian operators.

9.1.10 (a) A is a non-Hermitian operator. In the sense of Eqs. (9.26) and (9.27), show that

$$A + A^\dagger \qquad \text{and} \qquad i(A - A^\dagger)$$

are Hermitian operators.

(b) Using the preceding result, show that every non-Hermitian operator may be written as a linear combination of two Hermitian operators.

9.1.11 U and V are two arbitrary operators, not necessarily Hermitian. In the sense of Eq. (9.27), show that

$$(UV)^\dagger = V^\dagger U^\dagger.$$

Note the resemblance to Hermitian adjoint matrices.
Hint. Apply the definition of adjoint operator [Eq. (9.27)].

9.1.12 Prove that the product of two Hermitian operators is Hermitian [Eq. (9.26)] if and only if the two operators commute.

9.1.13 A and B are noncommuting quantum mechanical operators:

$$AB - BA = iC.$$

Show that C is Hermitian. Assume that appropriate boundary conditions are satisfied.

9.1.14 The operator $\mathcal{L}$ is Hermitian. Show that $\langle\mathcal{L}^2\rangle \geq 0$.

9.1.15 A quantum mechanical expectation value is defined by

$$\langle A\rangle = \int \psi^*(x)A\psi(x)dx = \langle\psi|A\psi\rangle,$$

where A is a linear operator. Show that demanding that $\langle A\rangle$ be real means that A must be Hermitian with respect to $\psi(x)$.

9.1.16 From the definition of adjoint [Eq. (9.27)], show that $A^{\dagger\dagger} = A$ in the sense that $\int \psi_1^* A^{\dagger\dagger}\psi_2 d\tau = \int \psi_1^* A\psi_2 d\tau$. The adjoint of the adjoint is the original operator.
Hint. The functions ψ_1 and ψ_2 of Eq. (9.27) represent a class of functions. The subscripts 1 and 2 may be interchanged or replaced by other subscripts.

9.1.17 For a quantum particle moving in a potential well, $V(x) = \frac{1}{2}m\omega^2x^2$, the Schrödinger wave equation is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + \frac{1}{2}m\omega^2x^2\psi(x) = E\psi(x)$$

or

$$\frac{d^2\psi(z)}{dz^2} - z^2\psi(z) = -\frac{2E}{\hbar\omega}\psi(z),$$

where $z = (m\omega/\hbar)^{1/2}x$. Since this operator is even, we expect solutions of definite parity. For the initial conditions that follow, integrate out from the origin and determine the minimum constant $2E/\hbar\omega$ that will lead to $\psi(\infty) = 0$ in each case. (You may take $z = 6$ as an approximation of infinity.)

(a) For an even eigenfunction,

$$\psi(0) = 1, \qquad \psi'(0) = 0.$$

(b) For an odd eigenfunction,

$$\psi(0) = 0, \qquad \psi'(0) = 1.$$

Note. Analytical solutions appear in Section 13.1.

9.2 Hermitian Operators

Hermitian or self-adjoint operators with appropriate boundary conditions have the following properties that are of extreme importance in classical and quantum physics:

1. The eigenvalues of an Hermitian operator are real.
2. The eigenfunctions of an Hermitian operator are orthogonal.
3. The eigenfunctions of an Hermitian operator form a complete set, meaning that under suitable conditions a function can be expanded in a series of eigenfunctions.[5]

Real Eigenvalues

We proceed to prove the first two of these three properties. Let

$$\mathcal{L}u_i + \lambda_i w u_i = 0, \quad \text{or} \quad \mathcal{L}|u_i\rangle + \lambda_i w|u_i\rangle = 0. \tag{9.29}$$

Assuming the existence of a second eigenvalue and eigenfunction

$$\mathcal{L}u_j + \lambda_j w u_j = 0, \quad \text{or} \quad \mathcal{L}|u_j\rangle + \lambda_j w|u_j\rangle = 0. \tag{9.30}$$

[5]This property is not universal. It **does** hold for our linear, second-order differential operators in Sturm–Liouville (self-adjoint) form. Completeness is defined and discussed in more detail in Section 9.4. A proof that the eigenfunctions of our linear, second-order, self-adjoint, differential equations form a complete set may be developed from the calculus of variations of Section 18.6.

Then, taking the Hermitian adjoint, using $\mathcal{L}^\dagger = \mathcal{L}$ we obtain

$$\mathcal{L}u_j^* + \lambda_j^* w u_j^* = 0, \quad \text{or} \quad \langle u_j|\mathcal{L} + \langle u_j|\lambda_j^* w = 0, \tag{9.31}$$

where p and q are real functions of x, and $w(x)$ is a real function. However, we permit λ_k, the eigenvalues, and u_k, the eigenfunctions, to be complex. Multiplying Eq. (9.29) by u_j^* (or $\langle u_j|$) and Eq. (9.31) by u_i (or $|u_i\rangle$) and then subtracting, we have

$$u_j^*\mathcal{L}u_i - u_i\mathcal{L}u_j^* = (\lambda_j^* - \lambda_i)wu_iu_j^*. \tag{9.32}$$

We integrate over the range $a \le x \le b$,

$$\int_a^b u_j^*\mathcal{L}u_i dx - \int_a^b u_i\mathcal{L}u_j^* dx = (\lambda_j^* - \lambda_i)\int_a^b u_iu_j^* w\, dx, \tag{9.33}$$

or in Dirac notation,

$$\langle u_j|\mathcal{L}u_i\rangle - \langle \mathcal{L}u_j|u_i\rangle = (\lambda_j^* - \lambda_i)\langle u_j|u_i\rangle.$$

Since $\mathcal{L}$ is Hermitian, the left-hand side vanishes by Eq. (9.27) and

$$(\lambda_j^* - \lambda_i)\int_a^b u_iu_j^* w\, dx = (\lambda_j^* - \lambda_i)\langle u_j|u_i\rangle = 0. \tag{9.34}$$

If $i = j$, the integral cannot vanish [$w(x) > 0$, apart from isolated points], except in the trivial case $u_i = 0$. Hence, the coefficient $(\lambda_i^* - \lambda_i)$ must be zero,

$$\lambda_i^* = \lambda_i, \tag{9.35}$$

which states that the eigenvalue is real. Since λ_i can represent any one of the eigenvalues, this proves the first property. This is an exact analog of the nature of the eigenvalues of real symmetric (and Hermitian) matrices (compare Sections 3.3 and 3.4).

Real eigenvalues of Hermitian operators have a fundamental significance in quantum mechanics. In quantum mechanics the eigenvalues correspond to observable (precisely measurable or sharp) quantities, such as energy and angular momentum. When a single measurement of an observable $\mathcal{L}$ is made, the result must be one of its eigenvalues. With the theory formulated in terms of Hermitian operators, this proof of real eigenvalues guarantees that the theory will predict real numbers for these measurable physical quantities. In Section 18.6, it will be seen that for some operators, such as Hamiltonians, the set of real eigenvalues has a lower bound. Physically important Hermitian operators are real potentials $V^* = V$ and the momentum operator $-id/dx$. The latter is Hermitian because upon using integration by parts and discarding the integrated term, we have

$$\left\langle \psi_1 \middle| -i\frac{d\psi_2}{dx}\right\rangle = \int_{-\infty}^{\infty} \psi_1^*\left(-i\frac{d\psi_2}{dx}\right)dx = -i\psi_2\psi_1^*|_{-\infty}^{\infty} + i\int_{-\infty}^{\infty}\frac{d\psi_1^*}{dx}\psi_2 dx$$
$$= \int_{-\infty}^{\infty}\left(-i\frac{d\psi_1}{dx}\right)^*\psi_2 dx = \left\langle -i\frac{d\psi_1}{dx}\middle|\psi_2\right\rangle.$$

Orthogonal Eigenfunctions

If we take $i \neq j$ and if $\lambda_i \neq \lambda_j$ in Eq. (9.34), the integral of the product of the two different eigenfunctions must vanish:

$$\langle u_j | u_i \rangle = \int_a^b u_j^* u_i w \, dx = 0. \tag{9.36}$$

This condition, called **orthogonality, is the continuum analog of the vanishing of a scalar (or inner) product of two vectors**.[6] We say that the eigenfunctions $u_i(x)$ and $u_j(x)$ are orthogonal with respect to the weighting function $w(x)$ over the interval $[a, b]$. Equation (9.36) constitutes a partial proof of the second property of our Hermitian operators. Again, the precise analogy with matrix analysis should be noted. Indeed, we can establish a one-to-one correspondence between this Sturm–Liouville theory of differential equations and the treatment of Hermitian matrices. Historically, this correspondence has been significant in establishing the mathematical equivalence of matrix mechanics developed by Heisenberg and wave mechanics developed by Schrödinger. Today, the two diverse approaches are merged into the theory of quantum mechanics, and the mathematical formulation that is more convenient for a particular problem is used for that problem. Actually, the mathematical alternatives do not end here. Integral equations form a third equivalent and sometimes more convenient or more powerful approach. Similarly, any two functions u, v, not necessarily eigenfunctions, are orthogonal if $\langle v | u \rangle = \int_a^b v^* u w dx = 0$.

This proof of orthogonality is not quite complete. There is a loophole because we may have $u_i \neq u_j$ but still have $\lambda_i = \lambda_j$. Such eigenvalues are labeled **degenerate**. Illustrations of degeneracy are given at the end of this section. If $\lambda_i = \lambda_j$, the integral in Eq. (9.34) need not vanish. This means that linearly independent eigenfunctions corresponding to the same eigenvalue are not automatically orthogonal and that some other method must be sought to obtain an orthogonal set. Although the eigenfunctions in this degenerate case may not be orthogonal, they can always be made orthogonal. One method is developed in the next section. See also the discussion after Eq. (4.13) for degeneracy due to symmetry.

We shall see in succeeding chapters that it is just as desirable to have a given set of functions orthogonal as it is to have an orthogonal coordinate system. We can work with nonorthogonal functions, but they are likely to prove as messy as an oblique coordinate system.

[6] From the definition of Riemann integral,

$$\int_a^b f(x)g(x)\,dx = \lim_{N\to\infty} \left(\sum_{i=1}^{N} f(x_i)g(x_i)\Delta x \right),$$

where $x_0 = a$, $x_N = b$, and $x_i - x_{i-1} = \Delta x$. If we interpret $f(x_i)$ and $g(x_i)$ as the ith components of an N component vector, then this sum (and therefore this integral) corresponds directly to a scalar product of vectors, Eq. (1.11). The vanishing of the scalar product is the condition for **orthogonality** of the vectors—or functions.

EXAMPLE 9.2.1

Fourier Series—Orthogonality To continue Example 9.1.4 with the interval $-\pi \le x \le \pi$, the eigenvalue equation [Eq. (9.25)],

$$\frac{d^2}{dx^2}y(x) + n^2 y(x) = 0,$$

subject to Eq. (9.20), may describe a vibrating violin string with eigenfunctions—$\sin nx$ subject to the boundary conditions $\sin(\pm n\pi) = 0$ so that n is an integer, and the orthogonality integrals become

$$\text{(a)} \int_{x_0-\pi}^{x_0+\pi} \sin mx \sin nx\, dx = C_n \delta_{nm}, \quad x_0 = 0.$$

For an interval of length 2π the preceding analysis guarantees the Kronecker delta in (a). Our Sturm–Liouville theory says nothing about the values of C_n.

Similarly, a quantum mechanical particle in a box may have eigenfunctions $\cos nx$ subject to the boundary conditions $\frac{d\cos nx}{dx}|_{x=\pm\pi} = 0$ giving integer n again. Then

$$\text{(b)} \int_{x_0-\pi}^{x_0+\pi} \cos mx \cos nx\, dx = D_n \delta_{nm}, \quad x_0 = 0,$$

where D_n remains undetermined. Actual calculation yields

$$C_n = \begin{cases} \pi, & n \neq 0, \\ 0, & n = 0, \end{cases} \qquad D_n = \begin{cases} \pi, & n \neq 0, \\ 2\pi, & n = 0. \end{cases}$$

Finally, inspection shows that

$$\text{(c)} \int_{x_0-\pi}^{x_0+\pi} \sin mx \cos nx\, dx = 0$$

always vanishes for all integral m and n. ■

Expansion in Orthogonal Eigenfunctions

Starting from some Hamiltonian and its eigenvalue equation $H|\psi\rangle = E|\psi\rangle$, we determine the set of eigenvalues E_j and eigenfunctions $|\varphi_j\rangle$ taking the latter to be orthonormal; that is,

$$\langle\varphi_k|\varphi_j\rangle = \delta_{jk}.$$

The property of completeness of the set $|\varphi_j\rangle$ means that certain classes of (e.g., sectionally or piecewise continuous) functions may be represented by a series of orthogonal eigenfunctions to any desired degree of accuracy. We now assume $|\psi\rangle$ is in that class and expand it as

$$|\psi\rangle = \sum_j a_j |\varphi_j\rangle.$$

We determine the coefficient a_k by projection

$$\left\langle \varphi_k \middle| H \sum_j a_j \varphi_j \right\rangle = E \left\langle \varphi_k \middle| \sum_j a_j \varphi_j \right\rangle = E \sum_j a_j \langle\varphi_k|\varphi_j\rangle = E \sum_j a_j \delta_{kj} = E a_k.$$

Calling $\langle \varphi_k | H \varphi_j \rangle \equiv H_{k,j}$ the **matrix elements of the Hamiltonian**, we have the eigenvalue equations

$$\sum_j H_{k,j} a_j = E a_k, \tag{9.37}$$

from which the column vector of admixture coefficients a_j may be determined, along with the eigenvalue E. This usually infinite set of linear equations is truncated in practice.

The choice of eigenfunction is made on the basis of convenience. To illustrate the expansion technique, let us choose the eigenfunctions of Example 9.2.1, $\cos nx$ and $\sin nx$. The eigenfunction series is conveniently (and conventionally) written as the Fourier series

$$f(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty} (a_n \cos nx + b_n \sin nx).$$

From the orthogonality integrals of Example 9.2.1 the coefficients are given by

$$a_n = \frac{1}{\pi} \int_{-\pi}^{\pi} f(t) \cos nt \, dt, \quad b_n = \frac{1}{\pi} \int_{-\pi}^{\pi} f(t) \sin nt \, dt, \qquad n = 0, 1, 2 \ldots .$$

EXAMPLE 9.2.2

Square Wave Now consider the square wave

$$f(x) = \begin{cases} \dfrac{h}{2}, & 0 < x < \pi, \\ -\dfrac{h}{2}, & -\pi < x < 0. \end{cases}$$

Direct substitution of $\pm h/2$ for $f(t)$ yields

$$a_n = 0,$$

which is expected because of the antisymmetry, $f(-x) = -f(x)$, and

$$b_n = \frac{h}{n\pi}(1 - \cos n\pi) = \begin{cases} 0, & n \text{ even}, \\ \dfrac{2h}{n\pi}, & n \text{ odd}. \end{cases}$$

Hence, the eigenfunction (Fourier) expansion of the square wave is

$$f(x) = \frac{2h}{\pi} \sum_{n=0}^{\infty} \frac{\sin(2n+1)x}{2n+1}. \tag{9.38}$$

Additional examples, using other eigenfunctions, appear in Chapters 11–13. ■

Degeneracy

The concept of degeneracy was introduced earlier. If N linearly independent eigenfunctions correspond to the same eigenvalue, the eigenvalue is said to be N-fold degenerate. A particularly simple illustration is provided by the eigenvalues and eigenfunctions of the linear oscillator equation of classical mechanics (Example 9.2.1). For each value of the eigenvalue n, there are two possible solutions: $\sin nx$ and $\cos nx$ (and any linear combination). We may say the eigenfunctions are degenerate or the eigenvalue is degenerate.

When an underlying symmetry, such as rotational invariance, is causing the degeneracies, states belonging to the same energy eigenvalue will then form a multiplet or representation of the symmetry group. The powerful group–theoretical methods are treated in Chapter 4 in detail.

In Section 9.3, we show an alternative method of how such functions may be made orthogonal.

Biographical Data

Sturm, Jacques Charles. Sturm, who was born in 1803 in Geneva, Switzerland and died in 1855, was Poisson's successor at the Sorbonne and worked with his friend Liouville on heat flow, from which the eigenvalue problems arose now named after both.

Liouville, Joseph. Liouville (1809–1882), a professor at the Collège de France, made contributions to elliptic functions, analytic functions, and quadratic forms.

EXERCISES

9.2.1 The functions $u_1(x)$ and $u_2(x)$ are eigenfunctions of the same Hermitian operator but for distinct eigenvalues λ_1 and λ_2. Show that $u_1(x)$ and $u_2(x)$ are linearly independent.

9.2.2 (a) The vectors $\mathbf{e}_n$ are orthogonal to each other: $\mathbf{e}_n \cdot \mathbf{e}_m = 0$ for $n \neq m$. Show that they are linearly independent.

(b) The functions $\psi_n(x)$ are orthogonal to each other over the interval $[a, b]$ and with respect to the weighting function $w(x)$. Show that the $\psi_n(x)$ are linearly independent.

9.2.3 Given that

$$P_1(x) = x \qquad \text{and} \qquad Q_0(x) = \tfrac{1}{2}\ln\left(\frac{1+x}{1-x}\right)$$

are solutions of Legendre's differential equation corresponding to different eigenvalues:

(a) Evaluate their orthogonality integral

$$\int_{-1}^{1} \frac{x}{2}\ln\left(\frac{1+x}{1-x}\right) dx.$$

(b) Explain why these two functions are not orthogonal, that is, why the proof of orthogonality does not apply.

9.2.4 $T_0(x) = 1$ and $V_1(x) = (1 - x^2)^{1/2}$ are solutions of the Chebyshev differential equation corresponding to different eigenvalues. Explain, in terms of the boundary conditions, why these two functions are not orthogonal.

9.2.5 (a) Show that the first derivatives of the Legendre polynomials satisfy a self-adjoint differential equation with eigenvalue $\lambda = n(n+1) - 2$.

(b) Show that these Legendre polynomial derivatives satisfy an orthogonality relation

$$\int_{-1}^{1} P_m'(x) P_n'(x)(1 - x^2)\,dx = 0, \qquad m \neq n.$$

Note. In Section 11.5, $(1 - x^2)^{1/2} P_n'(x)$ will be labeled an associated Legendre polynomial, $P_n^1(x)$.

9.2.6 A set of functions $u_n(x)$ satisfies the Sturm–Liouville equation

$$\frac{d}{dx}\left[p(x)\frac{d}{dx}u_n(x)\right] + \lambda_n w(x) u_n(x) = 0.$$

The functions $u_m(x)$ and $u_n(x)$ satisfy boundary conditions that lead to orthogonality. The corresponding eigenvalues λ_m and λ_n are distinct. Prove that for appropriate boundary conditions $u_m'(x)$ and $u_n'(x)$ are orthogonal with $p(x)$ as a weighting function.

9.2.7 A linear operator A has n distinct eigenvalues and n corresponding eigenfunctions: $A\psi_i = \lambda_i \psi_i$. Show that the n eigenfunctions are linearly independent. A is not necessarily Hermitian.
Hint. Assume linear dependence—that $\psi_n = \sum_{i=1}^{n-1} a_i \psi_i$. Use this relation and the operator–eigenfunction equation first in one order and then in the reverse order. Show that a contradiction results.

9.2.8 With $\mathcal{L}$ **not** self-adjoint, $\tilde{\mathcal{L}} \neq \mathcal{L}$,

$$\mathcal{L}u_i + \lambda_i w u_i = 0$$

and

$$\tilde{\mathcal{L}}v_j + \lambda_j w v_j = 0.$$

(a) Show that

$$\int_a^b v_j \mathcal{L} u_i\,dx = \int_a^b u_i \tilde{\mathcal{L}} v_j\,dx,$$

provided

$$u_i p_0 v_j' \Big|_a^b = v_j p_0 u_i' \Big|_a^b$$

and

$$u_i(p_1 - p_0')v_j\Big|_a^b = 0.$$

(b) Show that the orthogonality integral for the eigenfunctions u_i and v_j becomes

$$\int_a^b u_i v_j w\, dx = 0 \qquad (\lambda_i \neq \lambda_j).$$

9.3 Gram–Schmidt Orthogonalization

The Gram–Schmidt orthogonalization is a method that takes a nonorthogonal set of linearly independent functions[7] and constructs an orthogonal set over an arbitrary interval and with respect to an arbitrary weight or density factor w that may or may not originate from our basic Eq. (9.8). The choice of these weights gives a particular set of **orthonormal** functions in the end (orthogonal plus unit normalization). In the language of linear algebra, the process is equivalent to a matrix transformation relating an orthogonal set of basis vectors (functions) to a nonorthogonal set. The functions involved may be real or complex. Here, for convenience they are assumed to be real. The generalization to more than one dimension or to complex cases offers no difficulty.

Before taking up orthogonalization, we should consider normalization of functions. So far, no normalization has been specified. This means that

$$\langle \varphi_i | \varphi_i \rangle = \int_a^b \varphi_i^2 w\, dx = N_i^2,$$

but no attention has been paid to the value of N_i. We now demand that each function $\varphi_i(x)$ be multiplied by N_i^{-1} so that the new (normalized) φ_i will satisfy

$$\langle \varphi_i | \varphi_i \rangle = \int_a^b \varphi_i^2(x) w(x) dx = 1 \tag{9.39}$$

and

$$\langle \varphi_j | \varphi_i \rangle = \int_a^b \varphi_i(x)\varphi_j(x) w(x) dx = \delta_{ij}. \tag{9.40}$$

Equation (9.39) states that we have normalized to unity. Including the property of orthogonality, we have Eq. (9.40). Functions satisfying this equation are said to be **orthonormal** (orthogonal plus unit normalization). Other normalizations are certainly possible, and indeed, by historical convention, each of the special functions of mathematical physics treated in Chapters 12 and 13 will be normalized differently.

[7] Such a set of functions might well arise from the solutions of a PDE, in which the eigenvalue was independent of one or more of the constants of separation. Note, however, that the origin of the set of functions is irrelevant to the Gram–Schmidt orthogonalization procedure.

We consider three sets of functions: an original, linearly independent given set $u_n(x)$, $n = 0, 1, 2, \ldots$; an orthogonalized set $\psi_n(x)$ to be constructed; and a final set of functions $\varphi_n(x)$ that are the normalized ψ_n. The original u_n may be degenerate eigenfunctions, but this is not necessary. We shall have

$u_n(x)$	$\psi_n(x)$	$\varphi_n(x)$
Linearly independent	*Linearly independent*	*Linearly independent*
Nonorthogonal	*Orthogonal*	*Orthogonal*
Unnormalized	Unnormalized	*Normalized*
		(Orthonormal)

The Gram–Schmidt procedure takes the nth ψ function, ψ_n, to be $u_n(x)$ plus an unknown linear combination of the previous φ. The presence of the new $u_n(x)$ will guarantee linear independence. The requirement that $\psi_n(x)$ be orthogonal to each of the previous φ yields just enough constraints to determine each of the unknown coefficients. Then the fully determined ψ_n will be normalized to unity, yielding $\varphi_n(x)$. Then the sequence of steps is repeated for $\psi_{n+1}(x)$.

We start with $n = 0$, letting

$$\psi_0(x) = u_0(x) \tag{9.41}$$

with no "previous" φ to worry about. Then normalize

$$\varphi_0(x) = \frac{\psi_0(x)}{[\int_a^b \psi_0^2 w\, dx]^{1/2}}, \quad \text{or} \quad |\varphi_0\rangle = \frac{|\psi_0\rangle}{[\langle\psi_0|\psi_0\rangle]^{1/2}}. \tag{9.42}$$

For $n = 1$, let

$$\psi_1(x) = u_1(x) + a_{10}\varphi_0(x). \tag{9.43}$$

We demand that $\psi_1(x)$ be orthogonal to $\varphi_0(x)$. [At this stage the normalization of $\psi_1(x)$ is irrelevant.] This demand of orthogonality leads to

$$\int_a^b \psi_1\varphi_0 w\, dx = \int_a^b u_1\varphi_0 w\, dx + a_{10}\int \varphi_0^2 w\, dx = 0. \tag{9.44}$$

Since φ_0 is normalized to unity [Eq. (9.42)], we have

$$a_{10} = -\int_a^b u_1\varphi_0 w\, dx = -\langle\varphi_0|u_1\rangle, \tag{9.45}$$

fixing the value of a_{10}. In Dirac notation we write Eq. (9.43) as

$$|\psi_1\rangle = |u_1\rangle - \langle\varphi_0|u_1\rangle|\varphi_0\rangle \tag{9.43a}$$

and Eq. (9.44) as

$$0 = \langle\varphi_0|\psi_1\rangle = \langle\varphi_0|u_1\rangle + a_{10}\langle\varphi_0|\varphi_0\rangle. \tag{9.44a}$$

In this form we recognize that the coefficient a_{10} is determined by projection, similar to expanding a vector $\mathbf{u}$ in terms of Cartesian coordinate or basis vectors $\hat{\mathbf{x}}_i$ as

$$\mathbf{u} = (\mathbf{u}\cdot\hat{\mathbf{x}}_1)\hat{\mathbf{x}}_1 + (\mathbf{u}\cdot\hat{\mathbf{x}}_2)\hat{\mathbf{x}}_2 + (\mathbf{u}\cdot\hat{\mathbf{x}}_3)\hat{\mathbf{x}}_3 = \sum_i u_i\hat{\mathbf{x}}_i. \tag{9.45a}$$

Normalizing, we define

$$\varphi_1(x) = \frac{\psi_1(x)}{\left(\int \psi_1^2 w\, dx\right)^{1/2}}, \quad \text{or} \quad |\varphi_1\rangle = \frac{|\psi_1\rangle}{[\langle\psi_1|\psi_1\rangle]^{1/2}}. \tag{9.46}$$

Finally, we generalize so that

$$\varphi_i(x) = \frac{\psi_i(x)}{\left(\int \psi_i^2(x)w(x)dx\right)^{1/2}}, \tag{9.47}$$

where

$$\psi_i(x) = u_i + a_{i0}\varphi_0 + a_{i1}\varphi_1 + \cdots + a_{ii-1}\varphi_{i-1}. \tag{9.48}$$

The coefficients a_{ij} are again given by projection (using orthogonality)

$$a_{ij} = -\int u_i\varphi_j w\, dx = -\langle\varphi_j|u_i\rangle. \tag{9.49}$$

Equation (9.49) holds for unit normalization. If some other normalization is selected,

$$\int_a^b [\varphi_j(x)]^2 w(x)dx = N_j^2,$$

then Eq. (9.47) is replaced by

$$\varphi_i(x) = N_i\frac{\psi_i(x)}{\left(\int \psi_i^2 w\, dx\right)^{1/2}} \tag{9.47a}$$

and a_{ij} becomes

$$a_{ij} = -\frac{\int u_i\varphi_j w\, dx}{N_j^2}. \tag{9.49a}$$

Equations (9.48) and (9.49) may be rewritten in terms of **projection operators**, P_j. If we consider the $\varphi_n(x)$ to form a linear vector space, then the integral in Eq. (9.49) may be interpreted as the projection of u_i into the φ_j "coordinate" or the jth component of u_i. With

$$P_j u_i(x) = \left\{\int u_i(t)\varphi_j(t)w(t)dt\right\}\varphi_j(x) = |\varphi_j\rangle\langle\varphi_j|u_i\rangle,$$

that is, $P_j = |\varphi_j\rangle\langle\varphi_j|$. Equation (9.48) becomes

$$\psi_i(x) = \left\{1 - \sum_{j=1}^{i-1} P_j\right\} u_i(x). \tag{9.48a}$$

Subtracting off the jth components, $j = 1$ to $i - 1$, leaves $\psi_i(x)$ orthogonal to all the $\varphi_j(x)$.

Note that although this Gram–Schmidt procedure is one possible way of constructing an orthogonal or orthonormal set, the functions $\varphi_i(x)$ are not unique. There is an infinite number of possible orthonormal sets for a given interval and a given density function. As an illustration of the freedom involved, consider two (nonparallel) vectors **A** and **B** in the xy-plane. We may normalize **A** to unit magnitude and then form $\mathbf{B}' = a\mathbf{A} + \mathbf{B}$ so that $\mathbf{B}'$ is perpendicular to **A**. By normalizing $\mathbf{B}'$ we have completed the Gram–Schmidt orthogonalization for two vectors. However, any two perpendicular unit vectors, such as $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$, could have been chosen as our orthonormal set. Again, with an infinite number of possible rotations of $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ about the z-axis, we have an infinite number of possible orthonormal sets.

EXAMPLE 9.3.1

Legendre Polynomials by Gram–Schmidt Orthogonalization Let us form an orthonormal set from the set of functions $u_n(x) = x^n$, $n = 0, 1, 2 \ldots$. The interval is $-1 \le x \le 1$ and the density function is $w(x) = 1$.

In accordance with the Gram–Schmidt orthogonalization process described,

$$u_0 = 1, \qquad \text{hence} \qquad \varphi_0 = \frac{1}{\sqrt{2}}. \tag{9.50}$$

Then

$$\psi_1(x) = x + a_{10}\frac{1}{\sqrt{2}} \tag{9.51}$$

and

$$a_{10} = -\int_{-1}^{1} \frac{x}{\sqrt{2}} dx = 0 \tag{9.52}$$

by symmetry. We normalize ψ_1 to obtain

$$\varphi_1(x) = \sqrt{\frac{3}{2}}x. \tag{9.53}$$

Then continue the Gram–Schmidt process with

$$\psi_2(x) = x^2 + a_{20}\frac{1}{\sqrt{2}} + a_{21}\sqrt{\frac{3}{2}}x, \tag{9.54}$$

where

$$a_{20} = -\int_{-1}^{1} \frac{x^2}{\sqrt{2}} dx = -\frac{\sqrt{2}}{3}, \tag{9.55}$$

$$a_{21} = -\int_{-1}^{1} \sqrt{\frac{3}{2}}x^3 dx = 0, \tag{9.56}$$

again by symmetry. Therefore,

$$\psi_2(x) = x^2 - \frac{1}{3}, \tag{9.57}$$

and, on normalizing to unity, we have

$$\varphi_2(x) = \sqrt{\frac{5}{2}} \cdot \frac{1}{2}(3x^2 - 1). \tag{9.58}$$

The next function $\varphi_3(x)$ becomes

$$\varphi_3(x) = \sqrt{\frac{7}{2}} \cdot \frac{1}{2}(5x^3 - 3x). \tag{9.59}$$

Reference to Chapter 11 will show that

$$\varphi_n(x) = \sqrt{\frac{2n+1}{2}} P_n(x), \tag{9.60}$$

where $P_n(x)$ is the nth-order Legendre polynomial. Our Gram–Schmidt process provides a possible, but very cumbersome, method of generating the Legendre polynomials. It illustrates how a power series expansion in $u_n(x) = x^n$, which is not orthogonal, can be converted into an orthogonal series over the finite interval $[-1, 1]$.

The equations for Gram–Schmidt orthogonalization tend to be ill conditioned because of the subtractions. A technique for avoiding this difficulty using the polynomial recurrence relation is discussed by Hamming.[8]

In Example 9.3.1, we have specified an orthogonality interval $[-1, 1]$, a unit weighting function, and a set of functions, x^n, to be taken one at a time in increasing order. Given all these specifications the Gram–Schmidt procedure is unique (to within a normalization factor and an overall sign as discussed subsequently). Our resulting orthogonal set, the Legendre polynomials, P_0 through P_n, forms a complete set for the description of polynomials of order $\leq n$ over $[-1, 1]$. This concept of completeness is taken up in detail in Section 9.4. Expansions of functions in series of Legendre polynomials are discussed in Section 11.3. ■

Orthogonal Polynomials

The previous example was chosen strictly to illustrate the Gram–Schmidt procedure. Although it has the advantage of introducing the Legendre polynomials, the initial functions $u_n = x^n$ are not degenerate eigenfunctions and are not solutions of Legendre's equation. They are simply a set of functions that we have rearranged to create an orthonormal set for the given interval and

[8] Hamming, R. W. (1973). *Numerical Methods for Scientists and Engineers*, 2nd ed. McGraw-Hill, New York. See Section 27.2 and references given there.

Table 9.3

Orthogonal Polynomials Generated by Gram–Schmidt Orthogonalization of $u_n(x) = x^n, n = 0, 1, 2, \ldots$

Polynomials	Interval	Weighting Function $w(x)$	Standard Normalization
Legendre	$-1 \le x \le 1$	1	$\int_{-1}^{1} [P_n(x)]^2 dx = \frac{2}{2n+1}$
Shifted Legendre	$0 \le x \le 1$	1	$\int_{0}^{1} [P_n^*(x)]^2 dx = \frac{1}{2n+1}$
Laguerre	$0 \le x < \infty$	e^{-x}	$\int_{0}^{\infty} [L_n(x)]^2 e^{-x} dx = 1$
Associated Laguerre	$0 \le x < \infty$	$x^k e^{-x}$	$\int_{0}^{\infty} [L_n^k(x)]^2 x^k e^{-x} dx = \frac{(n+k)!}{n!}$
Hermite	$-\infty < x < \infty$	e^{-x^2}	$\int_{-\infty}^{\infty} [H_n(x)]^2 e^{-x^2} dx = 2^n \pi^{1/2} n!$

given weighting function. The fact that we obtained the Legendre polynomials is not quite magic but a direct consequence of the choice of interval and weighting function. The use of $u_n(x) = x^n$, but with other choices of interval and weighting function or a different ordering of the functions, leads to other sets of orthogonal polynomials as shown in Table 9.3. We consider these polynomials in detail in Chapters 11 and 13 as solutions of particular differential equations.

An examination of this orthogonalization process reveals two arbitrary features. First, as emphasized previously, it is not necessary to normalize the functions to unity. In the example just given, we could have required

$$\int_{-1}^{1} \varphi_n(x)\varphi_m(x)\,dx = \frac{2}{2n+1}\delta_{nm}, \tag{9.61}$$

and the resulting set would have been the actual Legendre polynomials. Second, the sign of φ_n is always indeterminate. In the example, we chose the sign by requiring the coefficient of the highest power of x in the polynomial to be positive. For the Laguerre polynomials, on the other hand, we would require the coefficient of the highest power to be $(-1)^n/n!$.

EXERCISES

9.3.1 Rework Example 9.3.1 by replacing $\varphi_n(x)$ by the conventional Legendre polynomial, $P_n(x)$:

$$\int_{-1}^{1} [P_n(x)]^2 dx = \frac{2}{2n+1}.$$

Using Eqs. (9.47a) and (9.49a), construct P_0, $P_1(x)$, and $P_2(x)$.

ANS. $P_0 = 1, \quad P_1 = x, \quad P_2 = \frac{3}{2}x^2 - \frac{1}{2}.$

9.3.2 Following the Gram–Schmidt procedure, construct a set of polynomials $P_n^*(x)$ orthogonal (unit weighting factor) over the range $[0, 1]$ from the set $[1, x]$. Normalize so that $P_n^*(1) = 1$.

$$\begin{aligned} \textit{ANS.}\quad & P_n^*(x) = 1, \\ & P_1^*(x) = 2x - 1, \\ & P_2^*(x) = 6x^2 - 6x + 1, \\ & P_3^*(x) = 20x^3 - 30x^2 + 12x - 1. \end{aligned}$$

These are the first four **shifted** Legendre polynomials.
Note. The asterisk is the standard notation for "shifted": $[0, 1]$ instead of $[-1, 1]$. It does **not** mean complex conjugate.

9.3.3 Apply the Gram–Schmidt procedure to form the first three Laguerre polynomials, using

$$u_n(x) = x^n, \qquad n = 0, 1, 2, \ldots, \quad 0 \le x < \infty, \quad w(x) = e^{-x}.$$

The conventional normalization is

$$\langle L_m | L_n \rangle = \int_0^\infty L_m(x) L_n(x) e^{-x} dx = \delta_{mn}.$$

$$\textit{ANS.}\quad L_0 = 1, \quad L_1 = (1 - x), \quad L_2 = \frac{2 - 4x + x^2}{2}.$$

9.3.4 You are given
(a) a set of functions $u_n(x) = x^n$, $n = 0, 1, 2, \ldots$,
(b) an interval $(0, \infty)$, and
(c) a weighting function $w(x) = xe^{-x}$. Use the Gram–Schmidt procedure to construct the first **three orthonormal** functions from the set $u_n(x)$ for this interval and this weighting function.

$$\textit{ANS.}\quad \varphi_0(x) = 1, \quad \varphi_1(x) = (x - 2)/\sqrt{2}, \quad \varphi_2(x) = (x^2 - 6x + 6)/2\sqrt{3}.$$

9.3.5 Using the Gram–Schmidt orthogonalization procedure, construct the lowest three Hermite polynomials, using

$$u_n(x) = x^n, \quad n = 0, 1, 2, \ldots, \quad -\infty < x < \infty, \quad w(x) = e^{-x^2}.$$

For this set of polynomials the usual normalization is

$$\langle H_m | H_n \rangle = \int_{-\infty}^{\infty} H_m(x) H_n(x) w(x) dx = \delta_{mn} 2^m m! \pi^{1/2}.$$

$$\textit{ANS.}\quad H_0 = 1, \quad H_1 = 2x, \quad H_2 = 4x^2 - 2.$$

9.3.6 As a modification of Exercise 9.3.5, apply the Gram–Schmidt orthogonalization procedure to the set $u_n(x) = x^n$, $n = 0, 1, 2, \ldots, 0 \le x < \infty$. Take $w(x)$ to be $\exp[-x^2]$. Find the first two nonvanishing polynomials. Normalize so that the coefficient of the highest power of x is unity. In Exercise 9.3.5, the interval $(-\infty, \infty)$ led to the Hermite polynomials. These are certainly not the Hermite polynomials.

$$\textit{ANS.}\quad \varphi_0 = 1, \quad \varphi_1 = x - \pi^{-1/2}.$$

9.3.7 Form an orthogonal set over the interval $0 \le x < \infty$, using $u_n(x) = e^{-nx}$, $n = 1, 2, 3, \ldots$. Take the weighting factor, $w(x)$, to be unity. These functions are solutions of $u_n'' - n^2 u_n = 0$, which is clearly already in Sturm–Liouville (self-adjoint) form. Why doesn't the Sturm–Liouville theory guarantee the orthogonality of these functions?

9.4 Completeness of Eigenfunctions

The third important property of an Hermitian operator is that its eigenfunctions form a complete set. This completeness means that any well-behaved (at least piecewise continuous) function $F(x)$ can be approximated by a series

$$F(x) = \sum_{n=0}^{\infty} a_n \varphi_n(x) \tag{9.62}$$

to any desired degree of accuracy.[9] More precisely, the set $\varphi_n(x)$ is called complete[10] if the limit of the mean square error vanishes:

$$\lim_{m\to\infty} \int_a^b \left[F(x) - \sum_{n=0}^{m} a_n \varphi_n(x) \right]^2 w(x)\,dx = 0. \tag{9.63}$$

We have not required that the error vanish identically in $[a, b]$ but only that the integral of the error squared go to zero. This convergence in the mean [Eq. (9.63)] should be compared with uniform convergence [Section 5.5, Eq. (5.43)]. Clearly, uniform convergence implies convergence in the mean, but the converse does not hold; convergence in the mean is less restrictive. Specifically, Eq. (9.63) is not upset by piecewise continuous functions with only a finite number of finite discontinuities. Equation (9.63) is perfectly adequate for our purposes and is far more convenient than Eq. (5.43). Indeed, since we frequently use expansions in eigenfunctions to describe discontinuous functions, convergence in the mean is all we can expect.

In the language of linear algebra, we have a linear space, a function vector space. The linearly independent, orthonormal functions $\varphi_n(x)$ form the basis for this (infinite-dimensional) space. Equation (9.62) is a statement that the functions $\varphi_n(x)$ span this linear space. With an inner product defined by Eq. (9.36), our linear space is a **Hilbert space** spanned by the complete set of basis states $\varphi_n(x)$; it contains all square-integrable functions F that can be expanded in the sense of Eq. (9.63).

The question of completeness of a set of functions is often determined by comparison with a Laurent series (Section 6.5). In Section 14.1, this is done for Fourier series, thus establishing the completeness of Fourier series. For all orthogonal polynomials mentioned in Section 9.3, it is possible to find a

[9] If we have a finite set, as with vectors, the summation is over the number of linearly independent members of the set.

[10] Many authors use the term *closed* here.

polynomial expansion of each power of z,

$$z^n = \sum_{i=0}^{n} a_i P_i(z), \tag{9.64}$$

where $P_i(z)$ is the ith polynomial. Exercises 11.4.6, 13.1.8, and 13.2.5 are specific examples of Eq. (9.64). Using Eq. (9.64), we may reexpress the Laurent expansion of $f(z)$ in terms of the polynomials, showing that the polynomial expansion exists (when it exists, it is unique; Exercise 9.4.1). The limitation of this Laurent series development is that it requires the function to be analytic. Equations (9.62) and (9.63) are more general. $F(x)$ may be only piecewise continuous. Numerous examples of the representation of such piecewise continuous functions appear in Chapter 14 (Fourier series). A proof that our Sturm–Liouville eigenfunctions form complete sets appears in Courant and Hilbert.[11]

In Eq. (9.62) the expansion coefficients a_m may be determined by

$$a_m = \int_a^b F(x)\varphi_m(x)w(x)\,dx = \langle \varphi_m | F \rangle. \tag{9.65}$$

This follows from multiplying Eq. (9.62) by $\varphi_m(x)w(x)$ and integrating. In Dirac notation,

$$|F\rangle = \sum_n a_n |\varphi_n\rangle \quad \text{implies} \quad \langle \varphi_m | F\rangle = \sum_n a_n \langle \varphi_m | \varphi_n \rangle = \sum_n a_n \delta_{mn} = a_m$$

provided the $|\varphi_n\rangle$ are normalized to unity. From the orthogonality of the eigenfunctions, $\varphi_n(x)$, only the mth term survives. Here, we see the value of orthogonality. Equation (9.65) may be compared with the dot or inner product of vectors (Section 1.2) and a_m interpreted as the mth projection of the function $F(x)$. Often, the coefficient a_m is called a generalized Fourier coefficient.

For a known function $F(x)$, Eq. (9.65) gives a_m as a **definite** integral that can always be evaluated, by computer if not analytically.

For examples of particular eigenfunction expansions, see the following: Fourier series, Chapter 14; Legendre series, Section 11.3; Laplace series, Section 11.6; Bessel and Fourier–Bessel expansions, Section 12.1; Hermite series, Section 13.1; and Laguerre series, Section 13.2. An explicit case of a Fourier expansion is the square wave (Example 9.2.2). The corresponding Hilbert space contains only periodic functions that can be expanded in a series of $\sin nx$, $\cos nx$, the eigenfunctions of one-dimensional square-well potentials in quantum mechanics under suitable boundary conditions.

It may also happen that the eigenfunction expansion [Eq. (9.62)] is the expansion of an unknown $F(x)$ in a series of known eigenfunctions $\varphi_n(x)$ with unknown coefficients a_n. An example is the quantum chemist's attempt to describe an (unknown) molecular wave function as a linear combination of known atomic wave functions. The unknown coefficients a_n would be determined by a variational technique, Rayleigh–Ritz (Section 18.6).

[11] Courant, R., and Hilbert, D. (1953). *Methods of Mathematical Physics* (English translation), Vol. 1. Interscience, New York. Reprinted, Wiley (1989), Chap. 6, Section 3.

Bessel's Inequality

If the set of functions $\varphi_n(x)$ does not form a complete set, possibly because we have not included the required infinite number of members of an infinite set, we are led to an inequality. First, consider the case of a finite sum of components. Let A be an n component vector,

$$\mathbf{A} = \mathbf{e}_1 a_1 + \mathbf{e}_2 a_2 + \cdots + \mathbf{e}_n a_n, \tag{9.66}$$

in which $\mathbf{e}_i$ form a set of orthonormal unit vectors and a_i is the corresponding component (projection) of $\mathbf{A}$; that is,

$$a_i = \mathbf{A} \cdot \mathbf{e}_i. \tag{9.67}$$

Then

$$\left(\mathbf{A} - \sum_{i=1}^{n} \mathbf{e}_i a_i \right)^2 \geq 0. \tag{9.68}$$

If we sum over all n components, clearly the summation equals $\mathbf{A}$ by Eq. (9.66) and the equality holds. If, however, the summation does not include all n components, the inequality results. By expanding Eq. (9.68) and remembering that the orthogonal unit vectors satisfy orthogonality relations

$$\mathbf{e}_i \cdot \mathbf{e}_j = \delta_{ij}, \tag{9.69}$$

we have

$$A^2 \geq \sum_i a_i^2. \tag{9.70}$$

This is **Bessel's inequality**.

For functions we consider the integral

$$\int_a^b \left[f(x) - \sum_{i=1}^{n} a_i \varphi_i(x) \right]^2 w(x)\, dx \geq 0. \tag{9.71}$$

This is the continuum analog of Eq. (9.68), letting $n \to \infty$ and replacing the summation by an integration. Again, with the weighting factor $w(x) > 0$, the integrand is nonnegative. The integral vanishes by Eq. (9.62) if we have a complete set. Otherwise it is positive. Expanding the squared term, we obtain

$$\int_a^b [f(x)]^2 w(x) dx - 2 \sum_{i=1}^{n} a_i \int_a^b f(x) \varphi_i(x) w(x) dx + \sum_{i=1}^{n} a_i^2 \geq 0. \tag{9.72}$$

Applying Eq. (9.65), we have

$$\int_a^b [f(x)]^2 w(x) dx \geq \sum_{i=1}^{n} a_i^2. \tag{9.73}$$

Hence, the sum of the squares of the expansion coefficients a_i is less than or equal to the weighted integral of $[f(x)]^2$, the equality holding if and only if the expansion is exact—that is, if the set of functions $\varphi_n(x)$ is a complete set and $n \to \infty$.

In later chapters, when we consider eigenfunctions that form complete sets (such as Legendre polynomials), Eq. (9.73) with the equal sign holding is called a Parseval relation.

Bessel's inequality has a variety of uses, including proof of convergence of the Fourier series.

Schwarz Inequality

The frequently used Schwarz inequality is similar to the Bessel inequality. Consider the quadratic equation with unknown x:

$$\sum_{i=1}^{n}(a_i x + b_i)^2 = \sum_{i=1}^{n} a_i^2 \left(x + \frac{b_i}{a_i}\right)^2 = 0. \tag{9.74}$$

If $b_i/a_i =$ constant c, then the solution is $x = -c$. If b_i/a_i is not a constant, all terms cannot vanish simultaneously for real x. Therefore, the solution must be complex. Expanding, we find that

$$x^2 \sum_{i=1}^{n} a_i^2 + 2x \sum_{i=1}^{n} a_i b_i + \sum_{i=1}^{n} b_i^2 = 0, \tag{9.75}$$

and since x is complex (or $= -b_i/a_i$), the quadratic formula[12] for x leads to

$$\left(\sum_{i=1}^{n} a_i b_i\right)^2 \le \left(\sum_{i=1}^{n} a_i^2\right)\left(\sum_{i=1}^{n} b_i^2\right), \tag{9.76}$$

the equality holding when b_i/a_i equals a constant.

Once more, in terms of vectors, we have

$$(\mathbf{a} \cdot \mathbf{b})^2 = a^2 b^2 \cos^2\theta \le a^2 b^2, \tag{9.77}$$

where θ is the angle included between $\mathbf{a}$ and $\mathbf{b}$.

The analogous Schwarz inequality for functions has the form

$$\left|\int_a^b f^*(x) g(x) w(x)\, dx\right|^2 \le \int_a^b f^*(x) f(x) w(x)\, dx \int_a^b g^*(x) g(x) w(x)\, dx, \tag{9.78}$$

the equality holding if and only if $g(x) = \alpha f(x)$, with α being a constant. To prove this function form of the Schwarz inequality,[13] consider a complex function $\psi(x) = f(x) + \lambda g(x)$ with λ a complex constant. The functions $f(x)$ and $g(x)$ are any two functions (for which the integrals exist). Multiplying by

[12] With discriminant $b^2 - 4ac$ negative (or zero).

[13] An alternate derivation is provided by the inequality $\int\int [f(x)g(y) - f(y)g(x)]^*[f(x)g(y) - f(y)g(x)]w(x)w(y)dx\,dy \ge 0$.

the complex conjugate and integrating, we obtain

$$\int_a^b \psi^*\psi w(x)dx \equiv \int_a^b f^*f w(x)dx + \lambda \int_a^b f^*g w(x)dx + \lambda^* \int_a^b g^*f w(x)dx + \lambda\lambda^* \int_a^b g^*g w(x)dx \geq 0. \tag{9.79}$$

The ≥ 0 appears since $\psi^*\psi$ is nonnegative, the equal ($=$) sign holding only if $\psi(x)$ is identically zero. Noting that λ and λ^* are linearly independent, we differentiate with respect to one of them and set the derivative equal to zero to minimize $\int_a^b \psi^*\psi dx$:

$$\frac{\partial}{\partial\lambda^*}\int_a^b \psi^*\psi w(x)dx = \int_a^b g^*f w(x)dx + \lambda\int_a^b g^*g w(x)dx = 0.$$

This yields

$$\lambda = -\frac{\int_a^b g^*f w(x)dx}{\int_a^b g^*g w(x)dx}. \tag{9.80a}$$

Taking the complex conjugate, we obtain

$$\lambda^* = -\frac{\int_a^b f^*g w(x)dx}{\int_a^b g^*g w(x)dx}. \tag{9.80b}$$

Substituting these values of λ and λ^* back into Eq. (9.79), we obtain Eq. (9.78), the Schwarz inequality.

In quantum mechanics $f(x)$ and $g(x)$ might each represent a state or configuration of a physical system. Then the Schwarz inequality guarantees that the inner product $\int_a^b f^*(x)g(x)w(x)dx$ exists. In some texts, the Schwarz inequality is a key step in the derivation of the Heisenberg uncertainty principle.

The function notation of Eqs. (9.78) and (9.79) is relatively cumbersome. In advanced mathematical physics, and especially in quantum mechanics, it is common to use the Dirac bra-ket notation:

$$\langle f|g\rangle \equiv \int_a^b f^*(x)g(x)w(x)dx.$$

Using this new notation, we simply understand the range of integration, (a, b), and any weighting function. In this notation the Schwarz inequality becomes

$$|\langle f|g\rangle|^2 \leq \langle f|f\rangle\langle g|g\rangle. \tag{9.78a}$$

If $g(x)$ is a normalized eigenfunction, $\varphi_i(x)$, Eq. (9.78) yields

$$a_i^*a_i \leq \int_a^b f^*(x)f(x)w(x)dx, \tag{9.81}$$

a result that also follows from Eq. (9.73).

Summary of Vector Spaces—Completeness

Here we summarize some properties of vector space, first with the vectors taken to be the familiar real vectors of Chapter 1 and then with the vectors taken to be ordinary functions—polynomials. The concept of completeness is developed for finite vector spaces and carried over into infinite vector spaces.

1v. We shall describe our vector space with a set of n linearly independent vectors $\mathbf{e}_i$, $i = 1, 2, \ldots, n$. If $n = 3$, $\mathbf{e}_1 = \hat{\mathbf{x}}$, $\mathbf{e}_2 = \hat{\mathbf{y}}$, and $\mathbf{e}_3 = \hat{\mathbf{z}}$. The n $\mathbf{e}_i$ **span** the linear vector space and are defined to be a **basis**.

1f. We shall describe our vector (function) space with a set of n linearly independent functions, $\varphi_i(x)$, $i = 0, 1, \ldots, n-1$. The index i starts with 0 to agree with the labeling of the classical polynomials. Here, $\varphi_i(x)$ is assumed to be a polynomial of degree i. The n $\varphi_i(x)$ span the linear vector (function) space forming a **basis**.

2v. The vectors in our vector space satisfy the following relations (Section 1.2; the vector components are numbers):

a. Vector addition is commutative	$\mathbf{u} + \mathbf{v} = \mathbf{v} + \mathbf{u}$
b. Vector addition is associative	$[\mathbf{u} + \mathbf{v}] + \mathbf{w} = \mathbf{u} + [\mathbf{v} + \mathbf{w}]$
c. There is a null vector	$\mathbf{0} + \mathbf{v} = \mathbf{v}$
d. Multiplication by a scalar	
Distributive	$a[\mathbf{u} + \mathbf{v}] = a\mathbf{u} + a\mathbf{v}$
Distributive	$(a + b)\mathbf{u} = a\mathbf{u} + b\mathbf{u}$
Associative	$a[b\mathbf{u}] = (ab)\mathbf{u}$
e. Multiplication	
By unit scalar	$1\mathbf{u} = \mathbf{u}$
By zero	$0\mathbf{u} = 0$
f. Negative vector	$(-1)\mathbf{u} = -\mathbf{u}$.

2f. The functions in our linear function space satisfy the properties listed for vectors (substitute "function" for "vector"):

a. $$f(x) + g(x) = g(x) + f(x)$$

b. $$[f(x) + g(x)] + h(x) = f(x) + [g(x) + h(x)]$$

c. $$0 + f(x) = f(x)$$

d. $$a[f(x) + g(x)] = af(x) + ag(x)$$
$$(a + b)f(x) = af(x) + bf(x)$$
$$a[bf(x)] = (ab)f(x)$$

e. $$1 \cdot f(x) = f(x)$$
$$0 \cdot f(x) = 0$$

f. $$(-1) \cdot f(x) = -f(x).$$

3v. In n-dimensional vector space an arbitrary vector $\mathbf{c}$ is described by its n components $(c_1, c_2, \ldots, c_n)$ or

$$\mathbf{c} = \sum_{i=1}^{n} c_i \mathbf{e}_i, \quad c_i = \hat{\mathbf{e}}_i \cdot \mathbf{c}.$$

When (i) n $\mathbf{e}_i$ are linearly independent and (ii) span the n-dimensional vector space, then the $\mathbf{e}_i$ form a basis and constitute a **complete** set.

3f. In n-dimensional function space a polynomial of degree $m \leq n-1$ is described by

$$f(x) = \sum_{i=0}^{n-1} c_i \varphi_i(x), \quad c_i = \frac{\langle \varphi_i | f \rangle}{\langle \varphi_i | \varphi_i \rangle}.$$

When (i) the $n\varphi_i(x)$ are linearly independent and (ii) span the n-dimensional function space, then the $\varphi_i(x)$ form a basis and constitute a **complete** set (for describing polynomials of degree $m \leq n-1$).

4v. An inner product (scalar, dot product) is defined by

$$\mathbf{c} \cdot \mathbf{d} = \sum_{i=1}^{n} c_i d_i.$$

If $\mathbf{c}$ and $\mathbf{d}$ have complex components, the inner product is defined as $\sum_{i=1}^{n} c_i^* d_i$. The inner product has the properties of

a. Distributive law of addition $\quad \mathbf{c} \cdot (\mathbf{d} + \mathbf{e}) = \mathbf{c} \cdot \mathbf{d} + \mathbf{c} \cdot \mathbf{e}$

b. Scalar multiplication $\quad \mathbf{c} \cdot a\mathbf{d} = a\mathbf{c} \cdot \mathbf{d}$

c. Complex conjugation $\quad \mathbf{c} \cdot \mathbf{d} = (\mathbf{d} \cdot \mathbf{c})^*$.

4f. An inner product is defined by

$$\langle f | g \rangle = \int_a^b f^*(x) g(x) w(x) dx.$$

The choice of the weighting function $w(x)$ and the interval (a, b) follows from the differential equation satisfied by $\varphi_i(x)$ and the boundary conditions (Section 9.1). In matrix terminology (Section 3.2), $|g\rangle$ is a column vector and $\langle f|$ is a row vector, the adjoint of $|f\rangle$.

The inner product has the properties listed for vectors:

a. $\langle f | g + h \rangle = \langle f | g \rangle + \langle f | h \rangle$

b. $\langle f | ag \rangle = a \langle f | g \rangle$

c. $\langle f | g \rangle = \langle g | f \rangle^*$.

5v. Orthogonality:

$$\mathbf{e}_j \cdot \mathbf{e}_j = 0, \quad i \neq j.$$

If the n $\mathbf{e}_i$ are not already orthogonal, the Gram–Schmidt process may be used to create an orthogonal set.

5f. Orthogonality:

$$\langle \varphi_i | \varphi_j \rangle = \int_a^b \varphi_i^*(x) \varphi_j(x) w(x) dx = 0, \quad i \neq j.$$

If the n $\varphi_i(x)$ are not already orthogonal, the Gram–Schmidt process (Section 9.3) may be used to create an orthogonal set.

6v. Definition of norm:

$$|\mathbf{c}| = (\mathbf{c}\cdot\mathbf{c})^{1/2} = \left(\sum_{i=1}^{n} c_i^2\right)^{1/2}.$$

The basis vectors $\mathbf{e}_i$ are taken to have unit norm (length) $\mathbf{e}_i \cdot \mathbf{e}_i = 1$. The components of $\mathbf{c}$ are given by

$$c_i = \mathbf{e}_i \cdot \mathbf{c}, \quad i = 1, 2, \ldots, n.$$

6f. Definition of norm:

$$\|f\| = \langle f|f\rangle^{1/2} = \left[\int_a^b |f(x)|^2 w(x)\,dx\right]^{1/2} = \left[\sum_{i=0}^{n-1} |c_i|^2\right]^{1/2},$$

Parseval's identity: $\|f\| > 0$ unless $f(x)$ is identically zero. The basis functions $\varphi_i(x)$ may be taken to have unit norm (unit normalization)

$$\|\varphi_i\| = 1.$$

Note that Legendre polynomials are not normalized to unity.

The expansion coefficients of our polynomial $f(x)$ are given by

$$c_i = \langle \varphi_i|f\rangle, \quad i = 0, 1, \ldots, n-1.$$

7v. Bessel's inequality:

$$\mathbf{c}\cdot\mathbf{c} \geq \sum_i c_i^2.$$

If the equal sign holds for all $\mathbf{c}$, it indicates that the $\mathbf{e}_i$ span the vector space; that is, they are complete.

7f. Bessel's inequality:

$$\langle f|f\rangle = \int_a^b |f(x)|^2 w(x)\,dx \geq \sum_i |c_i|^2.$$

If the equal sign holds for all allowable f, it indicates that the $\varphi_i(x)$ span the function space; that is, they are complete.

8v. Schwarz inequality:

$$\mathbf{c}\cdot\mathbf{d} \leq |\mathbf{c}|\cdot|\mathbf{d}|.$$

The equal sign holds when $\mathbf{c}$ is a multiple of $\mathbf{d}$. If the angle included between $\mathbf{c}$ and $\mathbf{d}$ is θ, then $|\cos\theta| \leq 1$.

8f. Schwarz inequality:

$$|\langle f|g\rangle| \leq \langle f|f\rangle^{1/2}\langle g|g\rangle^{1/2} = \|f\|\cdot\|g\|.$$

The equals sign holds when $f(x)$ and $g(x)$ are linearly dependent; that is, when $f(x)$ is a multiple of $g(x)$.

9v. Now, let $n \to \infty$, forming an infinite-dimensional linear vector space, l^2.

In an infinite-dimensional space our vector $\mathbf{c}$ is

$$\mathbf{c} = \sum_{i=1}^{\infty} c_i \mathbf{e}_i.$$

We require that

$$\sum_{i=1}^{\infty} c_i^2 < \infty.$$

The components of $\mathbf{c}$ are given by

$$c_i = \mathbf{e}_i \cdot \mathbf{c}, \quad i = 1, 2, \ldots, \infty,$$

exactly as in a finite-dimensional vector space.

9f. Then let $n \to \infty$, forming an infinite-dimensional vector (function) space, L^2. Then the superscript 2 stands for the quadratic norm [i.e., the 2 in $|f(x)|^2$]. Our functions need no longer be polynomials, but we do require that $f(x)$ be at least piecewise continuous (Dirichlet conditions for Fourier series) and that $\langle f|f\rangle = \int_a^b |f(x)|^2 w(x)dx$ exist. This latter condition is often stated as a requirement that $f(x)$ be square integrable.

Cauchy sequence: Let

$$f_n(x) = \sum_{i=0}^{n} c_i \varphi_i(x).$$

If

$$\|f(x) - f_n(x)\| \to 0 \quad \text{as} \quad n \to \infty$$

or

$$\lim_{n\to\infty} \int \left| f(x) - \sum_{i=0}^{n} c_i \varphi_i x \right|^2 w(x)dx = 0,$$

then we have convergence in the mean. This is analogous to the partial sum–Cauchy sequence criterion for the convergence of an infinite series (Section 5.1).

If every Cauchy sequence of allowable vectors (square integrable, piecewise continuous functions) converges to a limit vector in our linear space, the space is said to be complete. Then

$$f(x) = \sum_{i=0}^{\infty} c_i \varphi_i(x) \quad \text{(almost everywhere)}$$

in the sense of convergence in the mean. As noted previously, this is a weaker requirement than pointwise convergence (fixed value of x) or uniform convergence.

Expansion (Fourier) Coefficients

For a function f its Fourier coefficients are defined as

$$c_i = \langle \varphi_i | f \rangle, \quad i = 0, 1, \ldots, \infty,$$

exactly as in a finite-dimensional vector space. Hence,

$$f(x) = \sum_i \langle \varphi_i | f \rangle \varphi_i(x).$$

A linear space (finite- or infinite-dimensional) that (i) has an inner product defined, $\langle f \mid g \rangle$, and (ii) is complete is a **Hilbert space**.

Infinite-dimensional Hilbert space provides a natural mathematical framework for modern quantum mechanics because bound-state wave functions are normalized (square-integrable) and usually are eigenfunctions of some Hamiltonian that provides a basis of the Hilbert space. A physical state may be expanded in a set of basis vectors, which are eigenstates of some observable. The expansion coefficients squared give the probabilities of the different eigenvalues of the observable in the given state. Apart from quantum mechanics, Hilbert space retains its abstract mathematical power and beauty, but the necessity for its use is reduced.

SUMMARY

The Sturm–Liouville theory of second-order ODEs with boundary conditions leads to eigenvalue problems whose solutions are eigenfunctions with orthogonality properties. Special functions, such as Legendre polynomials, Bessel functions, and Laguerre polynomials, arise in this context. Eigenfunction expansions are important in quantum mechanics and many other areas of physics and engineering.

Biographical Data

Hilbert, David. Hilbert, a German mathematician, was born in 1862 in Königsberg, Prussia (now Russia), and died in 1943 in Göttingen, Germany. Son of a judge, he obtained his Ph.D. in mathematics at the University of Königsberg in 1885 and became a professor at Göttingen in 1895. In 1899, in his *Foundations of Geometry* he established the first consistent set of geometric axioms, which helped the axiomatic method for the foundation of mathematics to gain general recognition. He contributed to most active branches of mathematics and, with Poincaré, is considered one of the greatest mathematicians of the 20th century. He solved Waring's problem in number theory, developed solutions for integral equations, and is famous for an influential list of unsolved mathematics problems presented in 1900 at the International Congress of Mathematicians in Paris, which deeply influenced the development of mathematics in the 20th century.

EXERCISES

9.4.1 A function $f(x)$ is expanded in a series of orthonormal eigenfunctions

$$f(x) = \sum_{n=0}^{\infty} a_n \varphi_n(x).$$

Show that the series expansion is unique for a given set of $\varphi_n(x)$. The functions $\varphi_n(x)$ are being taken here as the **basis** vectors in an infinite-dimensional Hilbert space.

9.4.2 A function $f(x)$ is represented by a finite set of basis functions $\varphi_i(x)$,

$$f(x) = \sum_{i=1}^{N} c_i \varphi_i(x).$$

Show that the components c_i are unique; that no different set c_i' exists.
Note. Your basis functions are automatically linearly independent. They are not necessarily orthogonal.

9.4.3 A function $f(x)$ is approximated by a power series $\sum_{i=0}^{n-1} c_i x^i$ over the interval [0, 1]. Show that minimizing the mean square error leads to a set of linear equations

$$\mathsf{A}\mathbf{c} = \mathbf{b},$$

where

$$A_{ij} = \int_0^1 x^{i+j} dx = \frac{1}{i+j+1}, \quad i, j = 0, 1, 2, \ldots, n-1$$

and

$$b_i = \int_0^1 x^i f(x) dx, \quad i = 0, 1, 2, \ldots, n-1.$$

Note. The A_{ij} are the elements of the Hilbert matrix of order n. The determinant of this Hilbert matrix is a rapidly decreasing function of n. For $n = 5$, $\det \mathsf{A} = 3.7 \times 10^{-12}$ and the set of equations $\mathsf{A}\mathbf{c} = \mathbf{b}$ is becoming ill conditioned and unstable.

9.4.4 In place of the expansion of a function $F(x)$ given by

$$F(x) = \sum_{n=0}^{\infty} a_n \varphi_n(x),$$

with

$$a_n = \int_a^b F(x) \varphi_n(x) w(x) dx,$$

take the **finite** series approximation

$$F(x) \approx \sum_{n=0}^{m} c_n \varphi_n(x).$$

Show that the mean square error

$$\int_a^b \left[F(x) - \sum_{n=0}^{m} c_n \varphi_n(x) \right]^2 w(x) dx$$

is minimized by taking $c_n = a_n$.
Note. The values of the coefficients are independent of the number of terms in the finite series. This independence is a consequence of orthogonality and would not hold for a least-squares fit using powers of x.

9.4.5 From Example 9.2.2,

$$f(x) = \left\{ \begin{array}{ll} h/2, & 0 < x < \pi \\ -h/2, & -\pi < x < 0 \end{array} \right\} = \frac{2h}{\pi} \sum_{n=0}^{\infty} \frac{\sin(2n+1)x}{2n+1}.$$

(a) Show that

$$\int_{-\pi}^{\pi} [f(x)]^2 dx = \frac{\pi}{2} h^2 = \frac{4h^2}{\pi} \sum_{n=0}^{\infty} (2n+1)^{-2}.$$

For a finite upper limit, this would be Bessel's inequality. For the upper limit, ∞, this is Parseval's identity.

(b) Verify that

$$\frac{\pi}{2} h^2 = \frac{4h^2}{\pi} \sum_{n=0}^{\infty} (2n+1)^{-2}$$

by evaluating the series.

Hint. The series can be expressed as the Riemann zeta function.

9.4.6 Differentiate Eq. (9.79),

$$\langle \psi | \psi \rangle = \langle f | f \rangle + \lambda \langle f | g \rangle + \lambda^* \langle g | f \rangle + \lambda \lambda^* \langle g | g \rangle,$$

with respect to λ^* and show that you get the Schwarz inequality [Eq. (9.78)].

9.4.7 Derive the Schwarz inequality from the identity

$$\left[\int_a^b f(x) g(x) dx \right]^2 = \int_a^b [f(x)]^2 dx \int_a^b [g(x)]^2 dx - \frac{1}{2} \int_a^b \int_a^b [f(x)g(y) - f(y)g(x)]^2 dx\, dy.$$

9.4.8 If the functions $f(x)$ and $g(x)$ of the Schwarz inequality [Eq. (9.78)] may be expanded in a series of eigenfunctions $\varphi_i(x)$, show that Eq. (9.78) reduces to Eq. (9.76) (with n possibly infinite).

Note the description of $f(x)$ as a vector in a function space in which $\varphi_i(x)$ corresponds to the unit vector $\mathbf{e}_1$.

9.4.9 The operator H is Hermitian and positive definite; that is,

$$\int_a^b f^* H f \, dx > 0.$$

Prove the generalized Schwarz inequality:

$$\left| \int_a^b f^* H g \, dx \right|^2 \le \int_a^b f^* H f \, dx \int_a^b g^* H g \, dx.$$

9.4.10 A normalized wave function $\psi(x) = \sum_{n=0}^{\infty} a_n \varphi_n(x)$. The expansion coefficients a_n are known as probability amplitudes. We may define a density matrix ρ with elements $\rho_{ij} = a_i a_j^*$. Show that

$$(\rho^2)_{ij} = \rho_{ij}$$

or

$$\rho^2 = \rho.$$

This result, by definition, makes ρ a projection operator.
Hint: Use

$$\int \psi^* \psi \, dx = 1.$$

9.4.11 Show that

(a) the operator

$$|\varphi_i\rangle\langle\varphi_i|$$

operating on

$$f(t) = \sum_j c_j \langle t|\varphi_j\rangle$$

yields $c_i|\varphi_i(t)\rangle, \quad \langle t|\varphi_j\rangle \equiv \varphi_j(t).$

(b) $\displaystyle\sum_i |\varphi_i\rangle\langle\varphi_i| = 1.$

(c) For $\langle x|\varphi_p\rangle = e^{ipx}/\sqrt{2\pi}$ derive from (a) the Fourier integral of the function $f(t)$ and from (b) the Fourier integral representation of Dirac's δ function (see Chapter 1). Note that p is a continuous variable (momentum) replacing the discrete index i.

This operator is a **projection operator** projecting $f(x)$ onto the ith coordinate, selectively picking out the ith component $c_i|\varphi_i\rangle$ of $f(x)$.

Hint. The operator operates via the well-defined inner product. In the coordinate representation you actually have to work with $\langle x|\varphi_i\rangle\langle\varphi_i|t\rangle = \varphi_i(x)^\dagger \varphi_i(t)$.

Additional Reading

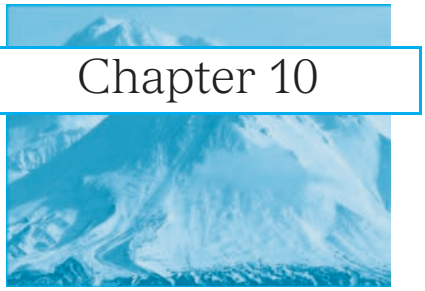
Byron, F. W., Jr., and Fuller, R. W. (1969). *Mathematics of Classical and Quantum Physics*. Addison-Wesley, Reading, MA.

Dennery, P., and Krzywicki, A. (1996). *Mathematics for Physicists* (reprinted). Dover, New York.

Hirsch, M. (1974). *Differential Equations, Dynamical Systems, and Linear Algebra*. Academic Press, San Diego.

Miller, K. S. (1963). *Linear Differential Equations in the Real Domain*. Norton, New York.

Titchmarsh, E. C. (1962). *Eigenfunction Expansions Associated with Second Order Differential Equations*, 2nd ed., Vol. 1. Oxford Univ. Press, London.



Chapter 10

The Gamma Function (Factorial Function)

The gamma function appears in physical problems of all kinds, such as the normalization of Coulomb wave functions and the computation of probabilities in statistical mechanics. Its importance stems from its usefulness in developing other functions that have direct physical application. The gamma function, therefore, is included here. A discussion of the numerical evaluation of the gamma function appears in Section 10.3. Closely related functions, such as the error integral, are presented in Section 10.4.

10.1 Definitions and Simple Properties

At least three different, convenient definitions of the gamma function are in common use. Our first task is to state these definitions, to develop some simple, direct consequences, and to show the equivalence of the three forms.

Infinite Limit (Euler)

The first definition, due to Euler, is

$$\Gamma(z) \equiv \lim_{n\to\infty} \frac{1\cdot 2\cdot 3\cdots n}{z(z+1)(z+2)\cdots(z+n)} n^z, \quad z \neq 0, -1, -2, -3, \ldots. \tag{10.1}$$

This definition of $\Gamma(z)$ is useful in developing the Weierstrass infinite-product form of $\Gamma(z)$ [Eq. (10.17)] and in obtaining the derivative of $\ln \Gamma(z)$ (Section 10.2). Here and elsewhere in this chapter, z may be either real or complex.

Replacing z with $z+1$, we have

$$\begin{aligned}\Gamma(z+1) &= \lim_{n\to\infty} \frac{1\cdot 2\cdot 3\cdots n}{(z+1)(z+2)(z+3)\cdots(z+n+1)} n^{z+1} \\ &= \lim_{n\to\infty} \frac{nz}{z+n+1} \cdot \frac{1\cdot 2\cdot 3\cdots n}{z(z+1)(z+2)\cdots(z+n)} n^{z} \\ &= z\Gamma(z). \end{aligned} \tag{10.2}$$

This is the basic functional relation for the gamma function. It should be noted that it is a **difference** equation. The gamma function is one of a general class of functions that do not satisfy any differential equation with rational coefficients. Specifically, the gamma function is one of the very few functions of mathematical physics that does not satisfy any of the ordinary differential equations (ODEs) common to physics. In fact, it does not satisfy any useful or practical differential equation.

Also, from the definition

$$\Gamma(1) = \lim_{n\to\infty} \frac{1\cdot 2\cdot 3\cdots n}{1\cdot 2\cdot 3\cdots n(n+1)} n = 1. \tag{10.3}$$

Now, application of Eq. (10.2) gives

$$\begin{aligned}&\Gamma(2) = 1, \\ &\Gamma(3) = 2\Gamma(2) = 2, \ldots \\ &\Gamma(n) = 1\cdot 2\cdot 3\cdots(n-1) = (n-1)!\end{aligned} \tag{10.4}$$

We see that the gamma function interpolates the factorials by a continuous function that returns the factorials at integer arguments.

Definite Integral (Euler)

A second definition, also frequently called the Euler integral, is

$$\Gamma(z) \equiv \int_0^\infty e^{-t} t^{z-1} dt, \quad \Re(z) > 0. \tag{10.5}$$

The restriction on z is necessary to avoid divergence of the integral at $t = 0$. When the gamma function does appear in physical problems, it is often in this form or some variation, such as

$$\Gamma(z) = 2\int_0^\infty e^{-t^2} t^{2z-1} dt, \quad \Re(z) > 0 \tag{10.6}$$

or

$$\Gamma(z) = \int_0^1 \left[\ln\left(\frac{1}{t}\right)\right]^{z-1} dt, \quad \Re(z) > 0.$$

EXAMPLE 10.1.1

The Euler Integral Interpolates the Factorials The Euler integral for positive integer argument, $z = n + 1$ with $n > 0$, yields the factorials. Using integration by parts repeatedly we find

$$\begin{aligned}\int_0^\infty e^{-t}t^n dt &= -t^n e^{-t}\Big|_0^\infty + n\int_0^\infty e^{-t}t^{n-1}dt = n\int_0^\infty e^{-t}t^{n-1}dt \\ &= n\left[-t^{n-1}e^{-t}\Big|_0^\infty + (n-1)\int_0^\infty e^{-t}t^{n-2}dt\right] \\ &= n(n-1)\int_0^\infty e^{-t}t^{n-2}dt = \cdots = n!\end{aligned}$$

because $\int_0^\infty e^{-t}dt = 1$. Thus, the Euler integral also interpolates the factorials. ■

When $z = \frac{1}{2}$, Eq. (10.6) contains the Gauss error integral, and we have the interesting result

$$\Gamma\left(\tfrac{1}{2}\right) = \sqrt{\pi}. \tag{10.7}$$

The value $\Gamma(\frac{1}{2})$ can be derived directly from the square of Eq. (10.6) for $z = \frac{1}{2}$ by introducing plane polar coordinates ($x^2 + y^2 = \rho^2$, $dx\,dy = \rho\,d\rho\,d\varphi$) in the product of integrals

$$\begin{aligned}\Gamma\left(\frac{1}{2}\right)^2 &= 4\int_0^\infty\int_0^\infty e^{-x^2-y^2}dx\,dy \\ &= 4\int_{\varphi=0}^{\pi/2}\int_{\rho=0}^\infty e^{-\rho^2}\rho\,d\rho\,d\varphi = -\pi e^{-\rho^2}\Big|_0^\infty = \pi.\end{aligned}$$

Generalizations of Eq. (10.7), the Gaussian integrals, are

$$\int_0^\infty x^{2s+1}\exp(-ax^2)\,dx = \frac{s!}{2a^{s+1}}, \tag{10.8}$$

$$\int_0^\infty x^{2s}\exp(-ax^2)\,dx = \frac{(s-\frac{1}{2})!}{2a^{s+1/2}} = \frac{(2s-1)!!}{2^{s+1}a^s}\sqrt{\frac{\pi}{a}}, \tag{10.9}$$

which are of major importance in statistical mechanics. A proof is left to the reader in Exercise 10.1.11. The double factorial notation is explained in Exercise 5.2.12 and Eq. (10.33b).

To show the equivalence of the two definitions, Eqs. (10.1) and (10.5), consider the function of two variables

$$F(z, n) = \int_0^n \left(1 - \frac{t}{n}\right)^n t^{z-1}\,dt, \quad \Re(z) > 0, \tag{10.10}$$

with n a positive integer. Since

$$\lim_{n\to\infty}\left(1 - \frac{t}{n}\right)^n \equiv e^{-t}, \tag{10.11}$$

from the definition of the exponential

$$\lim_{n\to\infty} F(z,n) = F(z,\infty) = \int_0^\infty e^{-t}t^{z-1}dt \equiv \Gamma(z) \tag{10.12}$$

by Eq. (10.5).

Returning to $F(z,n)$, we evaluate it in successive integrations by parts. For convenience let $u = t/n$. Then

$$F(z,n) = n^z \int_0^1 (1-u)^n u^{z-1}du. \tag{10.13}$$

Integrating by parts, we obtain for $\Re(z) > 0$,

$$\frac{F(z,n)}{n^z} = (1-u)^n \frac{u^z}{z}\bigg|_0^1 + \frac{n}{z}\int_0^1 (1-u)^{n-1}u^z du. \tag{10.14}$$

Repeating this, with the integrated part vanishing at both end points each time, we finally get

$$\begin{aligned} F(z,n) &= n^z \frac{n(n-1)\cdots 1}{z(z+1)\cdots(z+n-1)}\int_0^1 u^{z+n-1}du \\ &= \frac{1\cdot 2\cdot 3\cdots n}{z(z+1)(z+2)\cdots(z+n)}n^z. \end{aligned} \tag{10.15}$$

This is identical to the expression on the right side of Eq. (10.1). Hence,

$$\lim_{n\to\infty} F(z,n) = F(z,\infty) \equiv \Gamma(z) \tag{10.16}$$

by Eq. (10.1), completing the proof.

Using the functional equation (10.2) we can extend $\Gamma(z)$ from positive to negative arguments. For example, starting with Eq. (10.2) we define

$$\Gamma\left(-\frac{1}{2}\right) = -\frac{1}{0.5}\Gamma\left(\frac{1}{2}\right) = -2\sqrt{\pi},$$

and Eq. (10.2) for $z \to 0$ implies that $\Gamma(z\to 0)\to\infty$. Moreover, $z\Gamma(z)\to 1$ for $z\to 0$ [Eq. (10.2)] shows that $\Gamma(z)$ has a simple pole at the origin. Similarly, we find simple poles of $\Gamma(z)$ at all negative integers.

Infinite Product (Weierstrass)

The third definition (Weierstrass's form) is

$$\frac{1}{\Gamma(z)} \equiv ze^{\gamma z}\prod_{n=1}^{\infty}\left(1+\frac{z}{n}\right)e^{-z/n}, \tag{10.17}$$

where γ is the Euler–Mascheroni constant [Eq. (5.27)]

$$\gamma = \lim_{n\to\infty}\left(\sum_{m=1}^{n}\frac{1}{m} - \ln n\right) = 0.5772156\cdots. \tag{10.18}$$

This infinite product form may be used to develop the reflection identity, Eq. (10.24a), and applied in the exercises, such as Exercise 10.1.17. This form can be derived from the original definition [Eq. (10.1)] by rewriting it as

$$\Gamma(z) = \lim_{n\to\infty} \frac{1\cdot 2\cdot 3\cdots n}{z(z+1)\cdots(z+n)} n^z = \lim_{n\to\infty} \frac{1}{z}\prod_{m=1}^{n}\left(1+\frac{z}{m}\right)^{-1} n^z. \quad (10.19)$$

Inverting Eq. (10.19) and using

$$n^{-z} = e^{-z\ln n}, \quad (10.20)$$

we obtain

$$\frac{1}{\Gamma(z)} = z\lim_{n\to\infty} e^{(-\ln n)z}\prod_{m=1}^{n}\left(1+\frac{z}{m}\right). \quad (10.21)$$

Multiplying and dividing by

$$\exp\left[\left(1+\frac{1}{2}+\frac{1}{3}+\cdots+\frac{1}{n}\right)z\right] = \prod_{m=1}^{n} e^{z/m}, \quad (10.22)$$

we get

$$\frac{1}{\Gamma(z)} = z\left\{\lim_{n\to\infty}\exp\left[\left(1+\frac{1}{2}+\frac{1}{3}+\cdots+\frac{1}{n}-\ln n\right)z\right]\right\} \times\left[\lim_{n\to\infty}\prod_{m=1}^{n}\left(1+\frac{z}{m}\right)e^{-z/m}\right]. \quad (10.23)$$

As shown in Section 5.2, the infinite series in the exponent converges and defines γ, the Euler–Mascheroni constant. Hence, Eq. (10.17) follows.

The Weierstrass infinite product definition of $\Gamma(z)$ leads directly to an important identity,

$$\Gamma(z)\Gamma(1-z) = \frac{\pi}{\sin z\pi}, \quad (10.24a)$$

using the infinite product formulas for $\Gamma(z)$, $\Gamma(1-z)$, and $\sin z$ [Eq. (7.60)].

Alternatively, we can start from the product of Euler integrals

$$\Gamma(z+1)\Gamma(1-z) = \int_0^\infty s^z e^{-s}ds\int_0^\infty t^{-z}e^{-t}dt = \int_0^\infty v^z\frac{dv}{(v+1)^2}\int_0^\infty e^{-u}u\,du = \frac{\pi z}{\sin\pi z},$$

transforming from the variables s, t to $u = s+t$, $v = s/t$, as suggested by combining the exponentials and the powers in the integrands. The Jacobian is

$$J = -\begin{vmatrix} 1 & 1 \\ \frac{1}{t} & -\frac{s}{t^2}\end{vmatrix} = \frac{s+t}{t^2} = \frac{(v+1)^2}{u},$$

where $(v+1)t = u$. The integral $\int_0^\infty e^{-u}u\,du = 1$, whereas that over v may be derived by contour integration, giving $\frac{\pi z}{\sin\pi z}$. Similarly, one can establish

Legendre's duplication formula

$$\Gamma(1+z)\Gamma\left(z+\tfrac{1}{2}\right) = 2^{-2z}\sqrt{\pi}\,\Gamma(2z+1).$$

Setting $z = \frac{1}{2}$ in Eq. (10.24a), we obtain

$$\Gamma\left(\tfrac{1}{2}\right) = \sqrt{\pi}, \tag{10.24b}$$

(taking the positive square root) in agreement with Eqs. (10.7) and (10.9).

The Weierstrass definition shows immediately that $\Gamma(z)$ has simple poles at $z = 0, -1, -2, -3, \ldots$, and that $[\Gamma(z)]^{-1}$ has no poles in the finite complex plane, which means that $\Gamma(z)$ has no zeros. This behavior may also be seen in Eq. (10.24a), in which we note that $\pi/(\sin \pi z)$ is never equal to zero.

Actually, the infinite product definition of $\Gamma(z)$ may be derived from the Weierstrass factorization theorem with the specification that $[\Gamma(z)]^{-1}$ have simple zeros at $z = 0, -1, -2, -3, \ldots$. The Euler–Mascheroni constant is fixed by requiring $\Gamma(1) = 1$. See also the product expansions of entire functions in Chapter 7.

In mathematical probability theory the gamma distribution (probability density) is given by

$$f(x) = \begin{cases} \dfrac{1}{\beta^{\alpha}\Gamma(\alpha)} x^{\alpha-1} e^{-x/\beta}, & x > 0 \\ 0, & x \le 0. \end{cases} \tag{10.25a}$$

The constant $[\beta^{\alpha}\Gamma(\alpha)]^{-1}$ is included so that the total (integrated) probability will be unity. For $x \to E$, kinetic energy, $\alpha \to \frac{3}{2}$ and $\beta \to kT$, Eq. (10.25a) yields the classical Maxwell–Boltzmann statistics.

Biographical Data

Weierstrass, Karl Theodor Wilhelm. Weierstrass, a German mathematician, was born in 1815 in Ostenfelde, Germany, and died in 1897 in Berlin. He obtained a degree in mathematics in 1841 and studied Abel's and Jacobi's work on elliptical functions and extended their work on analytic functions while living as a schoolteacher. After being recognized as the father of modern analysis, he became a professor at the University of Berlin and a member of the Academy of Sciences in 1856.

Factorial Notation

So far, this discussion has been presented in terms of the classical notation. As pointed out by Jeffreys and others, the -1 of the $z - 1$ exponent in our second definition [Eq. (10.5)] is a continual nuisance. Accordingly, Eq. (10.5) is rewritten as

$$\int_0^{\infty} e^{-t} t^z dt \equiv z!, \quad \Re(z) > 1, \tag{10.25b}$$

to **define** a factorial function $z!$. Occasionally, we may even encounter Gauss's notation, $\prod(z)$, for the factorial function

$$\prod(z) = z!. \tag{10.26}$$

The Γ notation is due to Legendre. The factorial function of Eq. (10.25a) is, of course, related to the gamma function by

$$\Gamma(z) = (z-1)!, \qquad \text{or} \qquad \Gamma(z+1) = z!. \tag{10.27}$$

If $z = n$, a positive integer [Eq. (10.4)] shows that

$$z! = n! = 1 \cdot 2 \cdot 3 \cdots n, \tag{10.28}$$

the familiar factorial. However, it should be noted that since $z!$ is now defined by Eq. (10.25b) [or equivalently by Eq. (10.27)] **the factorial function is no longer limited to positive integral values of the argument** (Fig. 10.1). The difference relation [Eq. (10.2)] becomes

$$(z-1)! = \frac{z!}{z}. \tag{10.29}$$

This shows immediately that

$$0! = 1 \tag{10.30}$$

Figure 10.1

The Factorial Function—Extension to Negative Arguments

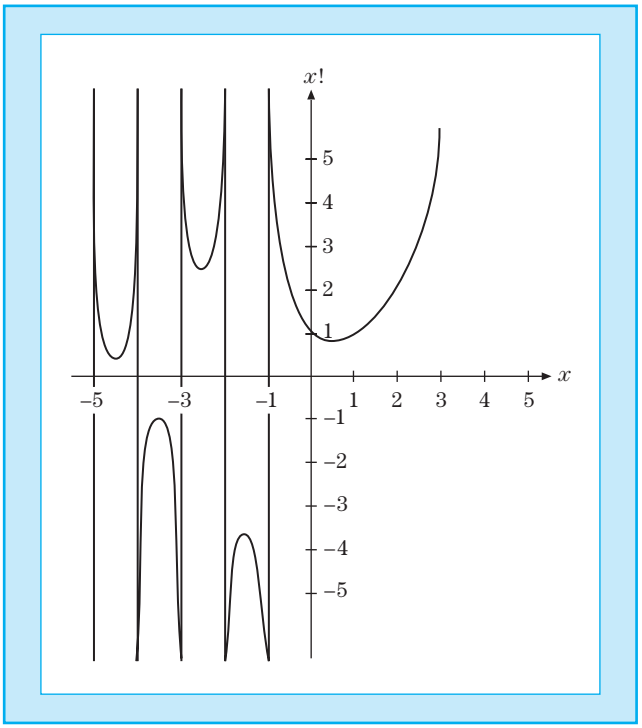
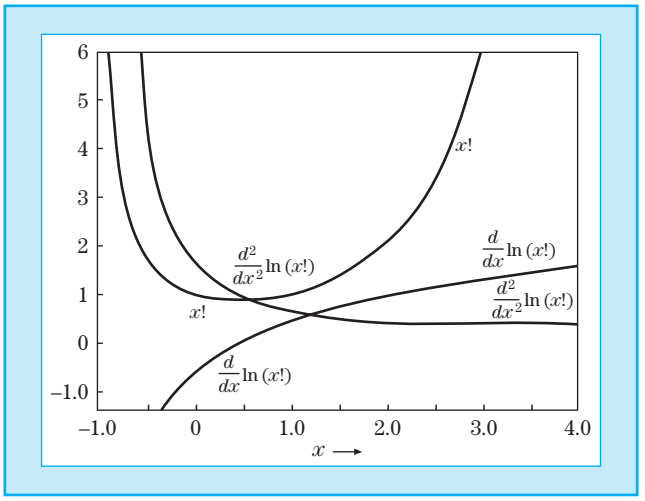


Figure 10.2

The Factorial Function and the First Two Derivatives of $\ln(x!)$



and

$$n! = \pm\infty \quad \text{for } n, \text{ a } \textbf{negative} \text{ integer.} \tag{10.31}$$

In terms of the factorial, Eq. (10.24a) becomes

$$z!(-z)! = \frac{\pi z}{\sin \pi z} \tag{10.32}$$

because

$$\Gamma(z)\Gamma(1-z) = (z-1)!(1-z-1)! = (z-1)!(-z)! = \frac{1}{z}z!(-z)!.$$

By restricting ourselves to the real values of the argument, we find that $x!$ defines the curve shown in Fig. 10.2. The minimum of the curve in Fig. 10.1 is

$$x! = (0.46163\cdots)! = 0.88560\cdots. \tag{10.33a}$$

Double Factorial Notation

In many problems of mathematical physics, particularly in connection with Legendre polynomials (Chapter 11), we encounter products of the odd positive integers and products of the even positive integers. For convenience, these are given special labels as double factorials:

$$\begin{aligned} 1\cdot 3\cdot 5\cdots(2n+1) &= (2n+1)!! \\ 2\cdot 4\cdot 6\cdots(2n) &= (2n)!!. \end{aligned} \tag{10.33b}$$

Clearly, these are related to the regular factorial functions by

$$(2n)!! = 2^n n! \quad \text{and} \quad (2n+1)!! = \frac{(2n+1)!}{2^n n!}. \tag{10.33c}$$

Integral Representation

An integral representation that is useful in developing asymptotic series for the Bessel functions is

$$\int_C e^{-z} z^{\nu} dz = (e^{2\pi i\nu} - 1)\nu!, \tag{10.34}$$

where C is the contour shown in Fig. 10.3. This contour integral representation is only useful when ν is not an integer, $z = 0$ then being a **branch point**. Equation (10.34) may be verified for $\nu > -1$ by deforming the contour as shown in Fig. 10.4. The integral from ∞ to $\epsilon > 0$ in Fig. 10.4 yields $-(\nu!)$, placing the phase of z at 0. The integral from ϵ to ∞ (in the fourth quadrant) then yields $e^{2\pi i\nu}\nu!$, the phase of z having increased to 2π. Since the circle of radius ϵ around the origin contributes nothing as $\epsilon \to 0$, when $\nu > -1$, Eq. (10.34) follows.

It is often convenient to put this result into a more symmetrical form

$$\int_C e^{-z}(-z)^{\nu} dz = 2i \sin(\nu\pi)\nu!, \tag{10.35}$$

multiplying both sides of Eq. (10.34) by $(-1)^{\nu} = e^{-\pi i\nu}$.

This analysis establishes Eqs. (10.34) and (10.35) for $\nu > -1$. It is relatively simple to extend the range to include all nonintegral ν. First, we note that the integral exists for $\nu < -1$, as long as we stay away from the origin. Second, integrating by parts we find that Eq. (10.35) yields the familiar difference relation [Eq. (10.29)]. If we take the difference relation to define the factorial

Figure 10.3

Factorial Function Contour

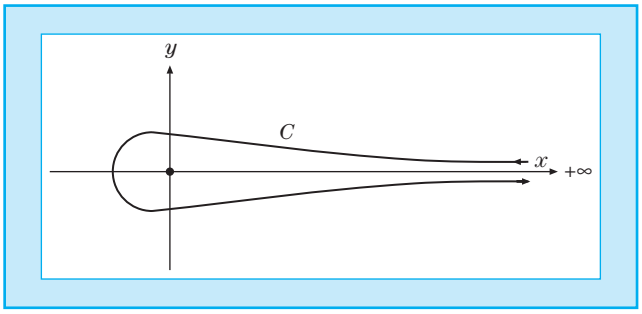
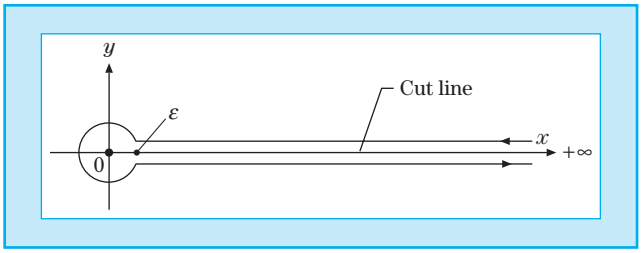


Figure 10.4

The Contour of Fig. 10.3 Deformed



function of $\nu < -1$, then Eqs. (10.34) and (10.35) are verified for all ν (except negative integers).

EXERCISES

10.1.1 Derive the recurrence relations

$$\Gamma(z+1) = z\Gamma(z)$$

from the Euler integral [Eq. (10.5)]

$$\Gamma(z) = \int_0^\infty e^{-t} t^{z-1} dt.$$

10.1.2 In a power series solution for the Legendre functions of the second kind, we encounter the expression

$$\frac{(n+1)(n+2)(n+3)\cdots(n+2s-1)(n+2s)}{2\cdot 4\cdot 6\cdot 8\cdots(2s-2)(2s)\cdot(2n+3)(2n+5)(2n+7)\cdots(2n+2s+1)},$$

in which s is a positive integer. Rewrite this expression in terms of factorials.

10.1.3 Show that

$$\frac{(s-n)!}{(2s-2n)!} = \frac{(-1)^{n-s}(2n-2s)!}{(n-s)!},$$

where s and n are integers with $s < n$. This result can be used to avoid negative factorials such as in the series representations of the spherical Neumann functions and the Legendre functions of the second kind.

10.1.4 Show that $\Gamma(z)$ may be written

$$\Gamma(z) = 2\int_0^\infty e^{-t^2} t^{2z-1} dz, \quad \Re(z) > 0,$$

$$\Gamma(z) = \int_0^1 \left[\ln\left(\frac{1}{t}\right)\right]^{z-1} dt, \quad \Re(z) > 0.$$

10.1.5 In a Maxwellian distribution the fraction of particles with speed between v and $v + dv$ is

$$\frac{dN}{N} = 4\pi\left(\frac{m}{2\pi kT}\right)^{3/2} \exp\left(-\frac{mv^2}{2kT}\right) v^2 dv,$$

where N is the total number of particles. The average or expectation value of v^n is defined as $\langle v^n\rangle = N^{-1}\int v^n dN$. Show that

$$\langle v^n\rangle = \left(\frac{2kT}{m}\right)^{n/2} \left(\frac{n+1}{2}\right)! \Big/ \frac{1}{2}!.$$

10.1.6 By transforming the integral into a gamma function, show that

$$-\int_0^1 x^k \ln x\, dx = \frac{1}{(k+1)^2}, \quad k > -1.$$

10.1.7 Show that

$$\int_0^\infty e^{-x^4} dx = \left(\frac{1}{4}\right)!.$$

10.1.8 Show that

$$\lim_{x\to 0} \frac{(ax-1)!}{(x-1)!} = \frac{1}{a}.$$

10.1.9 Locate the poles of $\Gamma(z)$. Show that they are simple poles and determine the residues.

10.1.10 Show that the equation $x! = k$, $k \neq 0$, has an infinite number of real roots.

10.1.11 Show that

(a) $\displaystyle\int_0^\infty x^{2s+1} \exp(-ax^2)\, dx = \frac{s!}{2a^{s+1}}.$

(b) $\displaystyle\int_0^\infty x^{2s} \exp(-ax^2)\, dx = \frac{(s-\frac{1}{2})!}{2a^{s+1/2}} = \frac{(2s-1)!!}{2^{s+1}a^s}\sqrt{\frac{\pi}{a}}.$

These Gaussian integrals are of major importance in statistical mechanics.

10.1.12 (a) Develop recurrence relations for $(2n)!!$ and for $(2n+1)!!$.

(b) Use these recurrence relations to calculate (or define) $0!!$ and $(-1)!!$.

ANS. $0!! = 1, \quad (-1)!! = 1.$

10.1.13 For s a nonnegative integer, show that

$$(-2s-1)!! = \frac{(-1)^s}{(2s-1)!!} = \frac{(-1)^s 2^s s!}{(2s)!}.$$

10.1.14 Express the coefficient of the nth term of the expansion of $(1+x)^{1/2}$

(a) in terms of factorials of integers; and

(b) in terms of the double factorial (!!) functions.

ANS. $a_n = (-1)^{n+1}\dfrac{(2n-3)!}{2^{2n-2}n!(n-2)!} = (-1)^{n+1}\dfrac{(2n-3)!!}{(2n)!!}, \; n = 2, 3, \cdots.$

10.1.15 Express the coefficient of the nth term of the expansion of $(1+x)^{1/2}$

(a) in terms of the factorials of integers; and

(b) in terms of the double factorial (!!) functions.

ANS. $\quad a_n = (-1)^n\dfrac{(2n)!}{2^{2n}(n!)^2} = (-1)^n\dfrac{(2n-1)!!}{(2n)!!}, \quad n = 1, 2, 3\cdots.$

10.1.16 The Legendre polynomial may be written as

$$P_n(\cos\theta) = 2\frac{(2n-1)!!}{(2n)!!}\left\{\cos n\theta + \frac{1}{1}\cdot\frac{n}{2n-1}\cos(n-2)\theta + \frac{1\cdot 3}{1\cdot 2}\frac{n(n-1)}{(2n-1)(2n-3)}\cos(n-4)\theta + \frac{1\cdot 3\cdot 5}{1\cdot 2\cdot 3}\frac{n(n-1)(n-2)}{(2n-1)(2n-3)(2n-5)}\cos(n-6)\theta + \cdots\right\}.$$

Let $n = 2s+1$. Then

$$P_n(\cos\theta) = P_{2s+1}(\cos\theta) = \sum_{m=0}^{s} a_m \cos(2m+1)\theta.$$

Find a_m in terms of factorials and double factorials.

10.1.17 (a) Show that

$$\Gamma\left(\frac{1}{2}-n\right)\Gamma\left(\frac{1}{2}+n\right) = (-1)^n\pi,$$

where n is an integer.

(b) Express $\Gamma(\frac{1}{2}+n)$ and $\Gamma(\frac{1}{2}-n)$ separately in terms of $\pi^{1/2}$ and a !! function.

ANS. $\Gamma\left(\frac{1}{2}+n\right) = \frac{(2n-1)!!}{2^n}\pi^{1/2}.$

10.1.18 From one of the definitions of the factorial or gamma function, show that

$$|(ix)!|^2 = \frac{\pi x}{\sinh \pi x}.$$

10.1.19 Prove that

$$|\Gamma(\alpha+i\beta)| = |\Gamma(\alpha)|\prod_{n=0}^{\infty}\left[1+\frac{\beta^2}{(\alpha+n)^2}\right]^{-1/2}.$$

This equation has been useful in calculations of beta decay theory.

10.1.20 Show that

$$|(n+ib)!| = \left(\frac{\pi b}{\sinh \pi b}\right)^{1/2}\prod_{s=1}^{n}(s^2+b^2)^{1/2}$$

for n, a positive integer.

10.1.21 Show that

$$|x!| \geq |(x+iy)!|$$

for all x. The variables x and y are real.

10.1.22 Show that

$$\left|\left(-\frac{1}{2}+iy\right)!\right|^2 = \frac{\pi}{\cosh \pi y}.$$

10.1.23 The probability density associated with the normal distribution of statistics is given by

$$f(x) = \frac{1}{\sigma(2\pi)^{1/2}} \exp\left[-\frac{(x-\mu)^2}{2\sigma^2}\right]$$

with $(-\infty, \infty)$ for the range of x. Show that
(a) the mean value of x, $\langle x\rangle$ is equal to μ; and
(b) the standard deviation $(\langle x^2\rangle - \langle x\rangle^2)^{1/2}$ is given by σ.

10.1.24 From the gamma distribution

$$f(x) = \begin{cases} \dfrac{1}{\beta^\alpha \Gamma(\alpha)} x^{\alpha-1} e^{-x/\beta}, & x > 0 \\ 0, & x \le 0, \end{cases}$$

show that
(a) $\langle x\rangle$ (mean) $= \alpha\beta$, (b) σ^2 (variance) $\equiv \langle x^2\rangle - \langle x\rangle^2 = \alpha\beta^2$.

10.1.25 The wave function of a particle scattered by a Coulomb potential is $\psi(r, \theta)$. At the origin the wave function becomes

$$\psi(0) = e^{-\pi\gamma/2}\Gamma(1 + i\gamma),$$

where $\gamma = Z_1 Z_2 e^2/\hbar v$. Show that

$$|\psi(0)|^2 = \frac{2\pi\gamma}{e^{2\pi\gamma} - 1}.$$

10.1.26 Derive the contour integral representation of Eq. (10.34)

$$(2i)^\nu \nu! \sin \nu\pi = \int_C e^{-z}(-z)^\nu dz.$$

10.2 Digamma and Polygamma Functions

Digamma Function

As may be noted from the definitions in Section 10.1, it is inconvenient to deal with the derivatives of the gamma or factorial function directly. Instead, it is customary to take the natural logarithm of the factorial function [Eq. (10.1)], convert the product to a sum, and then differentiate; that is, we start from

$$z! = z\Gamma(z) = \lim_{n\to\infty} \frac{n!}{(z+1)(z+2)\cdots(z+n)} n^z. \tag{10.36}$$

Then, because the logarithm of the limit is equal to the limit of the logarithm, we have

$$\ln(z!) = \lim_{n\to\infty} [\ln(n!) + z\ln n - \ln(z+1) - \ln(z+2) - \cdots - \ln(z+n)]. \tag{10.37}$$

Differentiating with respect to z, we obtain and define

$$\frac{d}{dz}\ln(z!) \equiv \psi(z+1) = \lim_{n\to\infty}\left(\ln n - \frac{1}{z+1} - \frac{1}{z+2} - \cdots - \frac{1}{z+n}\right), \tag{10.38}$$

which defines $\psi(z+1)$, the digamma function. From the definition of the Euler–Mascheroni constant,[1] Eq. (10.38) may be rewritten as

$$\begin{aligned}\psi(z+1) &= -\gamma - \sum_{n=1}^{\infty}\left(\frac{1}{z+n} - \frac{1}{n}\right)\\ &= -\gamma + \sum_{n=1}^{\infty}\frac{z}{n(n+z)}.\end{aligned} \tag{10.39}$$

Clearly,

$$\psi(1) = -\gamma = -0.577\,215\,664\,901\cdots.^{2} \tag{10.40}$$

Another, even more useful, expression for $\psi(z)$ is derived in Section 10.3.

Polygamma Function

The digamma function may be differentiated repeatedly, giving rise to the polygamma function:

$$\begin{aligned}\psi^{(m)}(z+1) &\equiv \frac{d^{m+1}}{dz^{m+1}}\ln(z!)\\ &= (-1)^{m+1}m!\sum_{n=1}^{\infty}\frac{1}{(z+n)^{m+1}}, \quad m = 1, 2, 3, \ldots.\end{aligned} \tag{10.41}$$

A plot of $\psi(x+1)$ and $\psi'(x+1)$ is included in Fig. 10.2. Since the series in Eq. (10.41) defines the Riemann zeta function,[3] when z is set to zero,

$$\zeta(m) \equiv \sum_{n=1}^{\infty}\frac{1}{n^{m}}, \tag{10.42}$$

we have

$$\psi^{(m)}(1) = (-1)^{m+1}m!\zeta(m+1), \quad m = 1, 2, 3, \ldots. \tag{10.43}$$

The values of the polygamma functions of positive integral argument, $\psi^{(m)}(n)$, may be calculated using Exercise 10.2.6.

In terms of the more common Γ notation,

$$\frac{d^{n+1}}{dz^{n+1}}\ln\Gamma(z) = \frac{d^{n}}{dz^{n}}\psi(z) = \psi^{(n)}(z). \tag{10.44a}$$

[1] Compare Section 5.2, Eq. (5.27). We add and subtract $\sum_{s=1}^{n} s^{-1}$.

[2] γ has been computed to 1271 places by D. E. Knuth, *Math. Comput.* **16**, 275 (1962) and to 3566 decimal places by D. W. Sweeney, *Math. Comput.* **17**, 170 (1963). It may be of interest that the fraction 228/395 gives γ accurate to six places.

[3] See Chapter 5. For $z \neq 0$ this series may be used to define a generalized zeta function.

Maclaurin Expansion, Computation

It is now possible to write a Maclaurin expansion for $\ln(z!)$:

$$\ln(z!) = \sum_{n=1}^{\infty} \frac{z^n}{n!} \psi^{(n-1)}(1) = -\gamma z + \sum_{n=2}^{\infty} (-1)^n \frac{z^n}{n} \zeta(n) \tag{10.44b}$$

convergent for $|z| < 1$; for $z = x$, the range is $-1 < x \leq 1$. Equation (10.44b) is a possible means of computing $z!$ for real or complex z, but Stirling's series (Section 10.3) is usually better. In addition, an excellent table of values of the gamma function for complex arguments based on the use of Stirling's series and the recurrence relation [Eq. (10.29)] is available[4] and can be accessed by symbolic software, such as Mathematica, Maple, Mathcad, and Reduce.

Series Summation

The digamma and polygamma functions may also be used in summing series. If the general term of the series has the form of a rational fraction (with the highest power of the index in the numerator at least two less than the highest power of the index in the denominator), it may be transformed by the method of partial fractions. The infinite series may then be expressed as a finite sum of digamma and polygamma functions. The usefulness of this method depends on the availability of tables of digamma and polygamma functions. Such tables and examples of series summation are given in AMS-55, Chapter 6.

EXAMPLE 10.2.1 **Catalan's Constant** Catalan's constant, Exercise 5.2.13, or $\beta(2)$, is given by

$$K = \beta(2) = \sum_{k=0}^{\infty} \frac{(-1)^k}{(2k+1)^2}. \tag{10.44c}$$

Grouping the positive and negative terms separately and starting with unit index [to match the form of $\psi^{(2)}$; Eq. (10.41)], we obtain

$$K = 1 + \sum_{n=1}^{\infty} \frac{1}{(4n+1)^2} - \frac{1}{9} - \sum_{n=1}^{\infty} \frac{1}{(4n+3)^2}.$$

Now, quoting Eq. (10.41), we get

$$K = \tfrac{8}{9} + \tfrac{1}{16}\psi^{(1)}\left(1 + \tfrac{1}{4}\right) - \tfrac{1}{16}\psi^{(1)}\left(1 + \tfrac{3}{4}\right). \tag{10.44d}$$

Using the values of $\psi^{(1)}$ from Table 6.1 of AMS-55, we obtain

$$K = 0.91596559\ldots.$$

Compare this calculation of Catalan's constant with the calculations of Chapter 5, using either direct summation by computer or a modification using Riemann zeta functions and then a (shorter) computer code. ■

[4] *Table of the Gamma Function for Complex Arguments*, Applied Mathematics Series No. 34. National Bureau of Standards, Washington, DC (1954).

EXERCISES

10.2.1 Verify that the following two forms of the digamma function,

$$\psi(x+1) = \sum_{r=1}^{x} \frac{1}{r} - \gamma$$

and

$$\psi(x+1) = \sum_{r=1}^{\infty} \frac{x}{r(r+x)} - \gamma,$$

are equal to each other (for x a positive integer).

10.2.2 Show that $\psi(z+1)$ has the series expansion

$$\psi(z+1) = -\gamma + \sum_{n=2}^{\infty} (-1)^n \zeta(n) z^{n-1}.$$

10.2.3 For a power series expansion of $\ln(z!)$, AMS-55 lists

$$\ln(z!) = -\ln(1+z) + z(1-\gamma) + \sum_{n=2}^{\infty} (-1)^n [\zeta(n) - 1] z^n/n.$$

(a) Show that this agrees with Eq. (10.44b) for $|z| < 1$.
(b) What is the range of convergence of this new expression?

10.2.4 Show that

$$\frac{1}{2} \ln\left(\frac{\pi z}{\sin \pi z}\right) = \sum_{n=1}^{\infty} \frac{\zeta(2n)}{2n} z^{2n}, \quad |z| < 1.$$

Hint. Try Eq. (10.32).

10.2.5 Write out a Weierstrass infinite product definition of $z!$. Without differentiating, show that this leads directly to the Maclaurin expansion of $\ln(z!)$ [Eq. (10.44b)].

10.2.6 Derive the difference relation for the polygamma function

$$\psi^{(m)}(z+2) = \psi^{(m)}(z+1) + (-1)^m \frac{m!}{(z+1)^{m+1}}, \quad m = 0, 1, 2, \ldots.$$

10.2.7 Show that if

$$\Gamma(x+iy) = u + iv$$

then

$$\Gamma(x-iy) = u - iv.$$

This is a special case of the Schwarz reflection principle (Section 6.5).

10.2.8 The Pochhammer symbol $(a)_n$ is defined as

$$(a)_n = a(a+1)\cdots(a+n-1), \qquad (a)_0 = 1$$

(for integral n).

(a) Express $(a)_n$ in terms of factorials.
(b) Find $(d/da)(a)_n$ in terms of $(a)_n$ and digamma functions.

$$\textit{ANS.} \quad \frac{d}{da}(a)_n = (a)_n[4(a+n) - 4(a)].$$

(c) Show that

$$(a)_{n+k} = (a+n)_k \cdot (a)_n.$$

10.2.9 Verify the following special values of the ψ form of the di- and polygamma functions:

$$\psi(1) = -\gamma, \qquad \psi^{(1)}(1) = \zeta(2), \qquad \psi^{(2)}(1) = -2\zeta(3).$$

10.2.10 Derive the polygamma function recurrence relation

$$\psi^{(m)}(1+z) = \psi^{(m)}(z) + (-1)^m m!/z^{m+1}, \quad m = 0, 1, 2, \ldots.$$

10.2.11 Verify

(a) $\displaystyle\int_0^\infty e^{-r} \ln r \, dr = -\gamma.$

(b) $\displaystyle\int_0^\infty re^{-r} \ln r \, dr = 1 - \gamma.$

(c) $\displaystyle\int_0^\infty r^n e^{-r} \ln r \, dr = (n-1)! + n\int_0^\infty r^{n-1} e^{-r} \ln r \, dr, \quad n = 1, 2, 3, \ldots.$

Hint. These may be verified by integration by parts, three parts, or differentiating the integral form of $n!$ with respect to n.

10.2.12 Dirac relativistic wave functions for hydrogen involve factors such as $[2(1-\alpha^2Z^2)^{1/2}]!$, where α, the fine structure constant, is $\frac{1}{137}$, and Z is the atomic number. Expand $[2(1-\alpha^2Z^2)^{1/2}]!$ in a series of powers of α^2Z^2.

10.2.13 The quantum mechanical description of a particle in a Coulomb field requires a knowledge of the phase of the complex factorial function. Determine the phase of $(1+ib)!$ for small b.

10.2.14 The total energy radiated by a black body is given by

$$u = \frac{8\pi k^4 T^4}{c^3 h^3} \int_0^\infty \frac{x^3}{e^x - 1} dx.$$

Show that the integral in this expression is equal to $3!\zeta(4)$ [$\zeta(4) = \pi^4/90 = 1.0823\ldots$]. The final result is the Stefan–Boltzmann law.

10.2.15 As a generalization of the result in Exercise 10.2.14, show that

$$\int_0^\infty \frac{x^s dx}{e^x - 1} = s!\zeta(s+1), \quad \Re(s) > 0.$$

10.2.16 The neutrino energy density (Fermi distribution) in the early history of the universe is given by

$$\rho_\nu = \frac{4\pi}{h^3} \int_0^\infty \frac{x^3}{\exp(x/kT) + 1} dx.$$

Show that

$$\rho_\nu = \frac{7\pi^5}{30h^3}(kT)^4.$$

10.2.17 Prove that

$$\int_0^\infty \frac{x^s dx}{e^x + 1} = s!(1 - 2^{-s})\zeta(s+1), \quad \Re(s) > 0.$$

Exercises 10.2.15 and 10.2.17 actually constitute Mellin integral transforms.

10.2.18 Prove that

$$\psi^{(n)}(z) = (-1)^{n+1} \int_0^\infty \frac{t^n e^{-zt}}{1 - e^{-t}}\, dt, \quad \Re(z) > 0.$$

10.2.19 Using di- and polygamma functions sum the series

(a) $\displaystyle\sum_{n=1}^{\infty} \frac{1}{n(n+1)}$, (b) $\displaystyle\sum_{n=2}^{\infty} \frac{1}{n^2 - 1}$.

Note. You can use Exercise 10.2.6 to calculate the needed digamma functions.

10.2.20 Show that

$$\sum_{n=1}^{\infty} \frac{1}{(n+a)(n+b)} = \frac{1}{(b-a)}\{\psi(a+1) - \psi(a+1)\},$$

$a \neq b$, and neither a nor b is a negative integer. It is of interest to compare this summation with the corresponding integral

$$\int_1^\infty \frac{dx}{(x+a)(x+b)} = \frac{1}{b-a}\{\ln(1+b) - \ln(1+a)\}.$$

10.3 Stirling's Series

For computation of $\ln(z!)$ for very large z (statistical mechanics) and for numerical computations at nonintegral values of z, a series expansion of $\ln(z!)$ in negative powers of z is desirable. Perhaps the most elegant way of deriving such an expansion is by the method of steepest descents (Section 7.3). The following method, starting with a numerical integration formula, does not require knowledge of contour integration and is particularly direct.

Derivation from Euler–Maclaurin Integration Formula

The Euler–Maclaurin formula (Section 5.9) for evaluating a definite integral[5] is

$$\int_0^n f(x)\, dx = \tfrac{1}{2}f(0) + f(1) + f(2) + \cdots + \tfrac{1}{2}f(n) - b_2[f'(n) - f'(0)] - b_4[f'''(n) - f'''(0)] - \cdots, \quad (10.45)$$

[5]This is obtained by repeated integration by parts.

in which the b_{2n} are related to the Bernoulli numbers B_{2n} by

$$(2n)!b_{2n} = B_{2n}, \tag{10.46}$$

$$\begin{aligned} B_0 &= 1, & B_6 &= \tfrac{1}{42}, \\ B_2 &= \tfrac{1}{6}, & B_8 &= -\tfrac{1}{30}, \\ B_4 &= -\tfrac{1}{30}, & B_{10} &= \tfrac{5}{66}, \quad \text{and so on.} \end{aligned} \tag{10.47}$$

By applying Eq. (10.45) to the elementary definite integral

$$\int_0^\infty \frac{dx}{(z+x)^2} = \frac{1}{z}, \quad f(x) = \frac{1}{(z+x)^2}, \tag{10.48}$$

(for z not on the negative real axis), we obtain for $n \to \infty$,

$$\frac{1}{z} = \frac{1}{2z^2} + \psi^{(1)}(z+1) - \frac{2!b_2}{z^3} - \frac{4!b_4}{z^5} - \cdots. \tag{10.49}$$

This is the reason for using Eq. (10.48). The Euler–Maclaurin evaluation yields $\psi'(z+1)$, which is $d^2 \ln(z!)/dz^2 = \sum_{n=1}^{\infty} \frac{1}{(z+n)^2}$ from Eq. (10.41).

Using Eq. (10.46) and solving for $\psi^{(1)}(z+1)$, we have

$$\begin{aligned} \psi'(z+1) = \frac{d}{dz}\psi(z+1) &= \frac{1}{z} - \frac{1}{2z^2} + \frac{B_2}{z^3} + \frac{B_4}{z^5} + \cdots \\ &= \frac{1}{z} - \frac{1}{2z^2} + \sum_{n=1}^{\infty} \frac{B_{2n}}{z^{2n+1}}. \end{aligned} \tag{10.50}$$

Since the Bernoulli numbers diverge strongly, this series does not converge. It is a semiconvergent or asymptotic series (Section 5.10), in which the sum always has a finite number of terms (compare Section 5.10).

Integrating once, we get the digamma function

$$\begin{aligned} \psi(z+1) &= C_1 + \ln z + \frac{1}{2z} - \frac{B_2}{2z^2} - \frac{B_4}{4z^4} - \cdots \\ &= C_1 + \ln z + \frac{1}{2z} - \sum_{n=1}^{\infty} \frac{B_{2n}}{2nz^{2n}}. \end{aligned} \tag{10.51}$$

Integrating Eq. (10.51) with respect to z from $z-1$ to z and then letting z approach infinity, C_1, the constant of integration may be shown to vanish. This gives us a second expression for the digamma function, often more useful than Eq. (10.39).

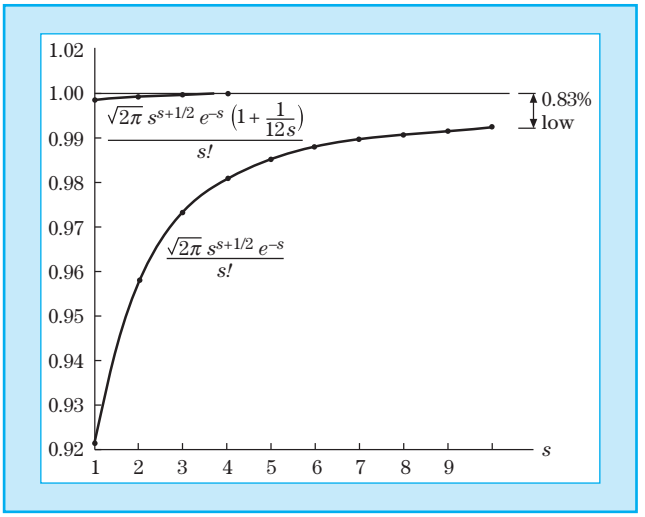
Stirling's Series

The indefinite integral of the digamma function [Eq. (10.51)] is

$$\ln(z!) = C_2 + \left(z + \frac{1}{2}\right)\ln z - z + \frac{B_2}{2z} + \cdots + \frac{B_{2n}}{2n(2n-1)z^{2n-1}} + \cdots, \tag{10.52}$$

Figure 10.5

Accuracy of Stirling's Formula



in which C_2 is another constant of integration. To fix C_2, we start from the asymptotic formula [Eq. (7.89) from Example 7.3.2]

$$z! \sim \sqrt{2\pi} z^{z+1/2} e^{-z}.$$

This gives for large enough $|z|$

$$\ln(z!) \sim \tfrac{1}{2}\ln 2\pi + (z+1/2)\ln z - z, \tag{10.53}$$

and comparing with Eq. (10.52), we find that C_2 is

$$C_2 = \tfrac{1}{2}\ln 2\pi, \tag{10.54}$$

giving for $|z| \to \infty$

$$\ln(z!) = \frac{1}{2}\ln 2\pi + \left(z+\frac{1}{2}\right)\ln z - z + \frac{1}{12z} - \frac{1}{360z^3} + \frac{1}{1260z^5} - \cdots. \tag{10.55}$$

This is Stirling's series, an asymptotic expansion. The absolute value of the error is less than the absolute value of the first term neglected. For large enough $|z|$, the simplest approximation $\ln(z!) \sim z\ln z - z$ may be sufficient.

To help convey a sense of the remarkable precision of Stirling's series for $s!$, the ratio of the first term of Stirling's approximation to $s!$ is plotted in Fig. 10.5. A tabulation gives the ratio of the first term in the expansion to $s!$ and the ratio of the first two terms in the expansion to $s!$ (Table 10.1). The derivation of these forms is Exercise 10.3.1.

Numerical Computation

The possibility of using the Maclaurin expansion [Eq. (10.44b)] for the numerical evaluation of the factorial function is mentioned in Section 10.2. However, for large x, Stirling's series [Eq. (10.55)] gives much more accuracy. The

Table 10.1

Stirling's Formula Compared with Stirling's Series for $n = 2$

s	$\frac{1}{s!}\sqrt{2\pi}s^{s+1/2}e^{-s}$	$\frac{1}{s!}\sqrt{2\pi}s^{s+1/2}e^{-s}\left(1+\frac{1}{12s}\right)$
1	0.92213	0.99898
2	0.95950	0.99949
3	0.97270	0.99972
4	0.97942	0.99983
5	0.98349	0.99988
6	0.98621	0.99992
7	0.98817	0.99994
8	0.98964	0.99995
9	0.99078	0.99996
10	0.99170	0.99998

Table of the Gamma Function for Complex Arguments, Applied Mathematics Series No. 34, National Bureau of Standards, is based on the use of Stirling's series for $z = x + iy$, $9 \le x \le 10$. Lower values of x are reached with the recurrence relation [Eq. (10.29)]. Now suppose the numerical value of $x!$ is needed for some particular value of x in a computer code. How shall we instruct the computer to do $x!$? Stirling's series followed by the recurrence relation is a good possibility. An even better possibility is to fit $x!$, $0 \le x \le 1$, by a short power series (polynomial) and then calculate $x!$ directly from this empirical fit. Presumably, the computer has been told the values of the coefficients of the polynomial. Such polynomial fits have been made by Hastings[6] for various accuracy requirements. For example,

$$x! = 1 + \sum_{n=1}^{8} b_n x^n + \varepsilon(x), \tag{10.56a}$$

with

$$\begin{aligned} b_1 &= -0.57719\ 1652 & b_5 &= -0.75670\ 4078 \\ b_2 &= 0.98820\ 5891 & b_6 &= 0.48219\ 9394 \\ b_3 &= -0.89705\ 6937 & b_7 &= -0.19352\ 7818 \\ b_4 &= 0.91820\ 6857 & b_8 &= 0.03586\ 8343 \end{aligned} \tag{10.56b}$$

with the magnitude of the error $|\varepsilon(x)| < 3 \times 10^{-7}$, $0 \le x \le 1$.

This is **not** a least-squares fit. Hastings employed a Chebyshev polynomial technique to minimize the maximum value of $|\varepsilon(x)|$ in Eq. (10.56a).

SUMMARY

The Euler integral

$$n! = \int_0^\infty e^{-t} t^n dt = \Gamma(n+1), \quad n = 0, 1, \ldots$$

gives the most direct entry to the gamma function. The functional equation $\Gamma(z+1) = z\Gamma(z)$ is its characteristic property that leads to the infinite product representation of its inverse, an entire function, and to the pole expansion

[6]Hastings, C., Jr. (1955). *Approximations for Digital Computers*. Princeton Univ. Press, Princeton, NJ.

of its logarithmic derivative, a meromorphic function. The asymptotic expansion, known as Stirling's series, is widely applied in statistical mechanics and leads to similar asymptotic expansions for the error integral and other related functions.

EXERCISES

10.3.1 Rewrite Stirling's series to give $z!$ instead of $\ln(z!)$.

$$ANS.\ z! = \sqrt{2\pi}\, z^{z+1/2} e^{-z}\left(1 + \frac{1}{12z} + \frac{1}{288z^2} - \frac{139}{51840z^3} + \cdots\right).$$

10.3.2 Use Stirling's formula to estimate 52!, the number of possible rearrangements of cards in a standard deck of playing cards.

10.3.3 By integrating Eq. (10.51) from $z-1$ to z and then letting $z \to \infty$, evaluate the constant C_1 in the asymptotic series for the digamma function $\psi(z+1)$.

10.3.4 Show that the constant C_2 in Stirling's formula Eq. (10.52) equals $\frac{1}{2}\ln 2\pi$ by using the logarithm of the doubling formula.

10.3.5 By direct expansion verify the doubling formula for $z = n + \frac{1}{2}$; n is an integer.

10.3.6 Without using Stirling's series show that

$$\text{(a) } \ln(n!) < \int_1^{n+1} \ln x\, dx, \quad \text{(b) } \ln(n!) > \int_1^{n} \ln x\, dx;\ n \text{ is an integer} \geq 2.$$

Notice that the arithmetic mean of these two integrals gives a good approximation for Stirling's series.

10.3.7 Test for convergence

$$\sum_{p=0}^{\infty}\left[\frac{(p-\frac{1}{2})!}{p!}\right]^2 \cdot \frac{2p+1}{2p+2} = \pi \sum_{p=0}^{\infty} \frac{(2p-1)!!(2p+1)!!}{(2p)!!(2p+2)!!}.$$

This series arises in an attempt to describe the magnetic field created by and enclosed by a current loop.

10.3.8 Show that

$$\lim_{x\to\infty} x^{b-a}\frac{(x+a)!}{(x+b)!} = 1.$$

10.3.9 Show that

$$\lim_{n\to\infty} \frac{(2n-1)!!}{(2n)!!} n^{1/2} = \pi^{-1/2}.$$

10.3.10 Calculate the binomial coefficient $\binom{2n}{n} = \frac{(2n)!}{n!n!}$ (see Chapter 5) to six significant figures for $n = 10$, 20, and 30. Check your values by

(a) a Stirling series approximation through terms in n^{-1}; and

(b) a double precision calculation.

ANS. $\binom{20}{10} = 1.84756 \times 10^5$, $\binom{40}{20} = 1.37846 \times 10^{11}$, $\binom{60}{30} = 1.18264 \times 10^{17}$.

10.3.11 Truncate the Stirling formula for $\ln n!$ so that the error is less than 10% for $n > 1$, <1% for $n > 10$, and <0.1% for $n > 100$.

10.3.12 Derive $\frac{d}{dz} \ln \Gamma(z) \sim \ln z - \frac{1}{2z}$ from Stirling's formula.

10.4 The Incomplete Gamma Functions and Related Functions

Generalizing the Euler definition of the gamma function [Eq. (10.5)], we define the incomplete gamma functions by the variable limit integrals

$$\gamma(a, x) = \int_0^x e^{-t} t^{a-1} dt, \quad \Re(a) > 0 \tag{10.57}$$

and

$$\Gamma(a, x) = \int_x^\infty e^{-t} t^{a-1} dt. \tag{10.58}$$

Clearly, the two functions are related because

$$\gamma(a, x) + \Gamma(a, x) = \Gamma(a). \tag{10.59}$$

These functions are useful for the error integrals discussed later. The choice of employing $\gamma(a, x)$ or $\Gamma(a, x)$ is purely a matter of convenience. If the parameter a is a positive integer, Eq. (10.58) may be integrated completely to yield

$$\begin{aligned} \gamma(n, x) &= (n-1)! \left(1 - e^{-x} \sum_{s=0}^{n-1} \frac{x^s}{s!}\right) \\ \Gamma(n, x) &= (n-1)! e^{-x} \sum_{s=0}^{n-1} \frac{x^s}{s!}, \quad n = 1, 2, \ldots. \end{aligned} \tag{10.60}$$

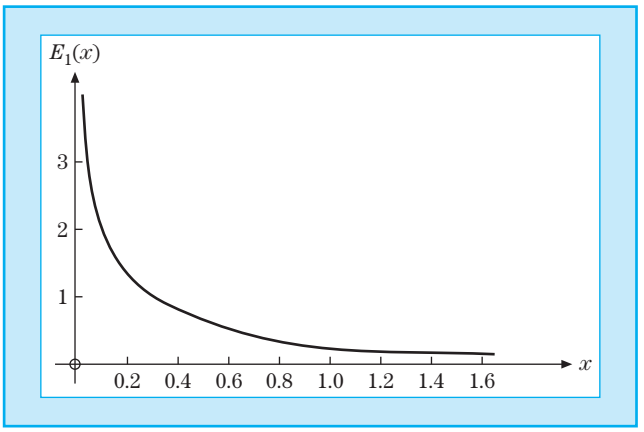
For nonintegral a, a power series expansion of $\gamma(a, x)$ for small x and an asymptotic expansion of $\Gamma(a, x)$ are developed in terms of the error function in Section 5.10 [see also Eq. (10.70b)]:

$$\begin{aligned} \gamma(a, x) &= x^a \sum_{n=0}^\infty (-1)^n \frac{x^n}{n!(a+n)}, \\ \Gamma(a, x) &= x^{a-1} e^{-x} \sum_{n=0}^\infty \frac{(a-1)!}{(a-1-n)!} \cdot \frac{1}{x^n} \\ &= x^{a-1} e^{-x} \sum_{n=0}^\infty (-1)^n \frac{(n-a)!}{(-a)!} \cdot \frac{1}{x^n}. \end{aligned} \tag{10.61}$$

These incomplete gamma functions may also be expressed elegantly in terms of confluent hypergeometric functions.

Figure 10.6

The Exponential Integral, $E_1(x) = -\text{Ei}(-x)$



Exponential Integral

Although the incomplete gamma function $\Gamma(a, x)$ in its general form [Eq. (10.61)] is only infrequently encountered in physical problems, a special case is very useful. We define the exponential integral by[7]

$$-\text{Ei}(-x) \equiv \int_x^\infty \frac{e^{-t}}{t} dt = E_1(x) \tag{10.62}$$

(Fig. 10.6). To obtain a series expansion for small x, we start from

$$E_1(x) = \Gamma(0, x) = \lim_{a\to 0}[\Gamma(a) - \gamma(a, x)]. \tag{10.63}$$

Caution is needed here because the integral in Eq. (10.62) diverges logarithmically as $x \to 0$. We may split the divergent term in the series expansion for $\gamma(a, x)$,

$$E_1(x) = \lim_{a\to 0}\left[\frac{a\Gamma(a) - x^a}{a}\right] - \sum_{n=1}^{\infty} \frac{(-1)^n x^n}{n \cdot n!}. \tag{10.64a}$$

Using l'Hôpital's rule (Exercise 5.6.7) and

$$\frac{d}{da}\{a\Gamma(a)\} = \frac{d}{da}a! = \frac{d}{da}e^{\ln(a!)} = a!\psi(a + 1), \tag{10.64b}$$

and then Eq. (10.39),[8] we obtain the rapidly converging series

$$E_1(x) = -\gamma - \ln x - \sum_{n=1}^{\infty} \frac{(-1)^n x^n}{n \cdot n!} \tag{10.65}$$

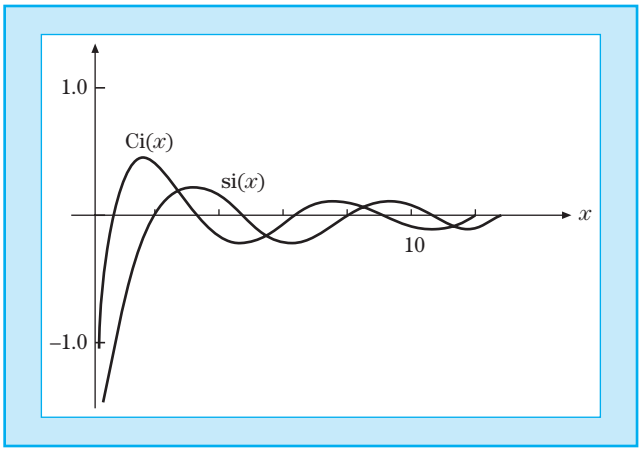
(Fig. 10.6). An asymptotic expansion is given in Section 5.10.

[7] The appearance of the two minus signs in $-\text{Ei}(-x)$ is an historical monstrosity. This integral is generally referred to as $E_1(x)$.

[8] $dx^a/da = x^a \ln x$.

Figure 10.7

Sine and Cosine Integrals



Further special forms related to the exponential integral are the sine integral, cosine integral (Fig. 10.7), and logarithmic integral defined by[9]

$$\begin{aligned} \mathrm{si}(x) &= -\int_x^\infty \frac{\sin t}{t}\,dt \\ \mathrm{Ci}(x) &= -\int_x^\infty \frac{\cos t}{t}\,dt \\ \mathrm{li}(x) &= \int_0^x \frac{du}{\ln u} = \mathrm{Ei}(\ln x). \end{aligned} \tag{10.66}$$

By transforming from real to imaginary argument, we can show that

$$\mathrm{si}(x) = \frac{1}{2i}[\mathrm{Ei}(ix) - \mathrm{Ei}(-ix)] = \frac{1}{2i}[E_1(ix) - E_1(-ix)], \tag{10.67}$$

whereas

$$\mathrm{Ci}(x) = \frac{1}{2}[\mathrm{Ei}(ix) + \mathrm{Ei}(-ix)] = -\frac{1}{2}[E_1(ix) + E_1(-ix)], \quad |\arg x| < \frac{\pi}{2}. \tag{10.68}$$

Adding these two relations, we obtain

$$\mathrm{Ei}(ix) = \mathrm{Ci}(x) + i\,\mathrm{si}(x) \tag{10.69}$$

to show that the relation among these integrals is exactly analogous to that among e^{ix}, $\cos x$, and $\sin x$. In terms of E_1,

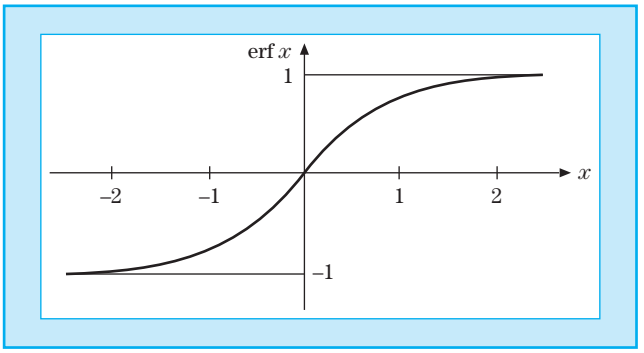
$$E_1(ix) = -\mathrm{Ci}(x) + i\,\mathrm{si}(x).$$

Asymptotic expansions of $\mathrm{Ci}(x)$ and $\mathrm{si}(x)$ may be developed similar to those for the error functions in Section 5.10. Power series expansions about the origin for $\mathrm{Ci}(x)$, $\mathrm{si}(x)$, and $\mathrm{li}(x)$ may be obtained from those for the exponential

[9] Another sine integral is given by $\mathrm{Si}(x) = \mathrm{si}(x) + \pi/2$.

Figure 10.8

Error Function erf *x*



integral, $E_1(x)$, or by direct integration. The exponential, sine, and cosine integrals are tabulated in AMS-55, Chapter 5, and can also be accessed by symbolic packages such as Mathematica, Maple, Mathcad, and Reduce.

Error Integrals

The error integrals

$$\operatorname{erf} z = \frac{2}{\sqrt{\pi}} \int_0^z e^{-t^2} dt, \qquad \operatorname{erfc} z = 1 - \operatorname{erf} z = \frac{2}{\sqrt{\pi}} \int_z^\infty e^{-t^2} dt \tag{10.70a}$$

(normalized so that $\operatorname{erf} \infty = 1$) are introduced in Section 5.10 (Fig. 10.8). Asymptotic forms are developed there. From the general form of the integrands and Eq. (10.6) we expect that erf z and erfc z may be written as incomplete gamma functions with $a = \frac{1}{2}$. The relations are

$$\operatorname{erf} z = \pi^{-1/2} \gamma\left(\tfrac{1}{2}, z^2\right), \qquad \operatorname{erfc} z = \pi^{-1/2} \Gamma\left(\tfrac{1}{2}, z^2\right). \tag{10.70b}$$

The power series expansion of erf z follows directly from Eq. (10.61).

EXERCISES

10.4.1 Show that

$$\gamma(a, x) = e^{-x} \sum_{n=0}^{\infty} \frac{(a-1)!}{(a+n)!} x^{a+n},$$

(a) by repeatedly integrating by parts; and
(b) demonstrate this relation by transforming it into Eq. (10.61).

10.4.2 Show that

(a) $$\frac{d^m}{dx^m}[x^{-a}\gamma(a, x)] = (-1)^m x^{-a-m} \gamma(a+m, x),$$

(b) $$\frac{d^m}{dx^m}[e^x \gamma(a, x)] = e^x \frac{\Gamma(a)}{\Gamma(a-m)} \gamma(a-m, x).$$

10.4.3 Show that $\gamma(a, x)$ and $\Gamma(a, x)$ satisfy the recurrence relations
(a) $\gamma(a+1, x) = a\gamma(a, x) - x^a e^{-x}$,
(b) $\Gamma(a-1, x) = a\Gamma(a, x) + x^a e^{-x}$.

10.4.4 The potential produced by a $1s$ hydrogen electron (Exercise 10.4.11) is given by

$$V(r) = \frac{q}{4\pi\varepsilon_0 a_0}\left\{\frac{1}{2r}\gamma(3, 2r) + \Gamma(2, 2r)\right\}.$$

(a) For $r \ll 1$, show that

$$V(r) = \frac{q}{4\pi\varepsilon_0 a_0}\left\{1 - \frac{2}{3}r^2 + \cdots\right\}.$$

(b) For $r \gg 1$, show that

$$V(r) = \frac{q}{4\pi\varepsilon_0 a_0}\cdot\frac{1}{r}.$$

Here, r is a pure number, the number of Bohr radii, a_0.
Note. For computation at intermediate values of r, Eqs. (10.60) are convenient.

10.4.5 The potential of a $2p$ hydrogen electron is found to be

$$V(r) = \frac{1}{4\pi\varepsilon_0}\cdot\frac{q}{24a_0}\left\{\frac{1}{r}\gamma(5, r) + \Gamma(4, r)\right\}$$
$$- \frac{1}{4\pi\varepsilon_0}\cdot\frac{q}{120a_0}\left\{\frac{1}{r^3}\gamma(7, r) + r^2\Gamma(2, r)\right\}P_2(\cos\theta).$$

Here, r is expressed in units of a_0, the Bohr radius. $P_2(\cos\theta)$ is a Legendre polynomial (Section 11.1).
(a) For $r \ll 1$, show that

$$V(r) = \frac{1}{4\pi\varepsilon_0}\cdot\frac{q}{a_0}\left\{\frac{1}{4} - \frac{1}{120}r^2 P_2(\cos\theta) + \cdots\right\}.$$

(b) For $r \gg 1$, show that

$$V(r) = \frac{1}{4\pi\varepsilon_0}\cdot\frac{q}{a_0 r}\left\{1 - \frac{6}{r^2}P_2(\cos\theta) + \cdots\right\}.$$

10.4.6 Prove the expansion

$$\int_x^\infty \frac{e^{-t}}{t}dt = -\gamma - \ln x - \sum_{n=1}^{\infty}\frac{(-1)^n x^n}{n\cdot n!}$$

for the exponential integral. Here, γ is the Euler–Mascheroni constant.

10.4.7 Show that $E_1(z)$ may be written as

$$E_1(z) = e^{-z}\int_0^\infty \frac{e^{-zt}}{1+t}\,dt.$$

Show also that we must impose the condition $|\arg z| \le \pi/2$.

10.4.8 Related to the exponential integral [Eq. (10.62)] is the function

$$E_n(x) = \int_1^\infty \frac{e^{-xt}}{t^n} dt.$$

Show that $E_n(x)$ satisfies the recurrence relation

$$E_{n+1}(x) = \frac{1}{n} e^{-x} - \frac{x}{n} E_n(x), \quad n = 1, 2, 3, \ldots.$$

10.4.9 With $E_n(x)$ defined in Exercise 10.4.8, show that $E_n(0) = 1/(n-1)$, $n > 1$.

10.4.10 Using the relation

$$\Gamma(a) = \gamma(a, x) + \Gamma(a, x),$$

show that if $\gamma(a, x)$ satisfies the relations of Exercise 10.4.2, then $\Gamma(a, x)$ must satisfy the same relations.

10.4.11 Calculate the potential produced by a 1*s* hydrogen electron (Exercise 10.4.4) (Fig. 10.9). Tabulate $V(r)/(q/4\pi\varepsilon_0 a_0)$ for $0.0 \le x \le 4.0$, x in steps of 0.1. Check your calculations for $r \ll 1$ and for $r \gg 1$ by calculating the limiting forms given in Exercise 10.4.4.

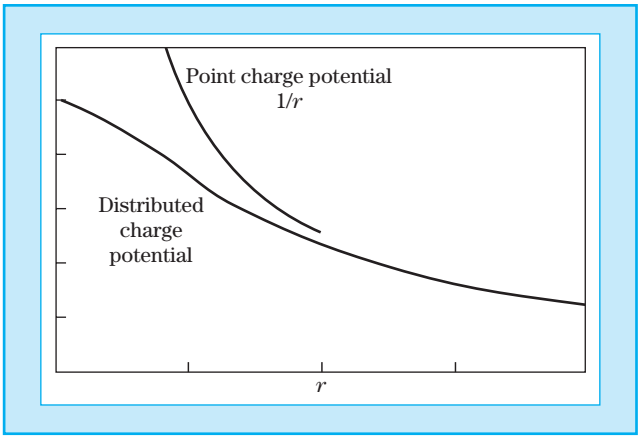


Figure 10.9

Distributed Charge Potential Produced by a 1*s* Hydrogen Electron (Exercise 10.4.11)

Additional Reading

Abramowitz, M., and Stegun, I. A. (Eds.) (1972). *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables* (AMS-55). National Bureau of Standards, Washington, DC. Reprinted, Dover (1974). Contains a wealth of information about gamma functions, incomplete gamma functions, exponential integrals, error functions, and related functions (Chapters 4–6).

Artin, E. (1964). *The Gamma Function* (M. Butler, Trans.). Holt, Rinehart & Winston, New York. Demonstrates that if a function $f(x)$ is smooth (log convex) and equal to $(n-1)!$ when $x = n =$ integer, it is the gamma function.

Davis, H. T. (1933). *Tables of the Higher Mathematical Functions*. Principia, Bloomington, IN. Volume 1 contains extensive information on the gamma function and the polygamma functions.

Gradshteyn, I. S., and Ryzhik, I. M. (2000). *Table of Integrals, Series, and Products*, 6th ed. Academic Press, New York.

Luke, Y. L. (1969). *The Special Functions and Their Approximations*, Vol. 1. Academic Press, New York.

Luke, Y. L. (1975). *Mathematical Functions and Their Approximations*. Academic Press, New York. This is an updated supplement to *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables* (AMS-55). Chapter 1 deals with the gamma function. Chapter 4 treats the incomplete gamma function and a host of related functions.

Chapter 11

Legendre Polynomials and Spherical Harmonics

11.1 Introduction

Legendre polynomials appear in many different mathematical and physical situations:

- They originate as solutions of the Legendre ordinary differential equation (ODE), which we have already encountered in the separation of variables (Section 8.9) for Laplace's equation, and similar ODEs in spherical polar coordinates.
- They arise as a consequence of demanding a complete, orthogonal set of functions over the interval $[-1, 1]$ (Gram–Schmidt orthogonalization; Section 9.3).
- In quantum mechanics, they (really the spherical harmonics; Section 11.5) represent angular momentum eigenfunctions. They also appear naturally in problems with azimuthal symmetry, which is the case in the next point.
- They are defined by a generating function: We introduce Legendre polynomials here by way of the electrostatic potential of a point charge, which acts as the generating function.

Physical Basis: Electrostatics

Legendre polynomials appear in an expansion of the electrostatic potential in inverse radial powers. Consider an electric charge q placed on the z-axis at $z = a$. As shown in Fig. 11.1, the electrostatic potential of charge q is

$$\varphi = \frac{1}{4\pi\varepsilon_0} \cdot \frac{q}{r_1} \quad \text{(SI units)}. \tag{11.1}$$

We want to express the electrostatic potential in terms of the spherical polar coordinates r and θ (the coordinate φ is absent because of azimuthal symmetry,

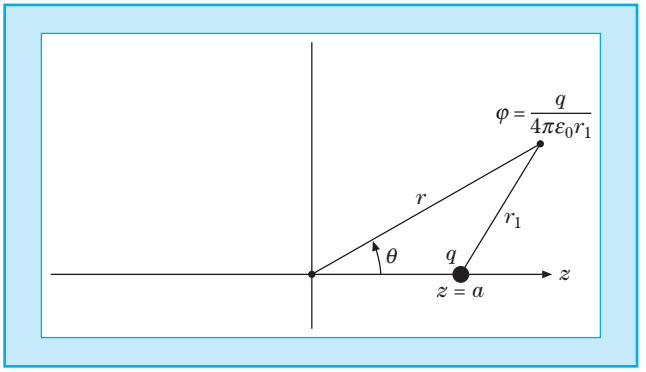


Figure 11.1

Electrostatic Potential. Charge q Displaced from Origin

that is, invariance under rotations about the z-axis). Using the law of cosines in Fig. 11.1, we obtain

$$\varphi = \frac{q}{4\pi\varepsilon_0}(r^2 + a^2 - 2ar\cos\theta)^{-1/2}. \tag{11.2}$$

Generating Function

Consider the case of $r > a$. The radical in Eq. (11.2) may be expanded in a binomial series (see Exercise 5.6.9) for $r^2 > |a^2 - 2ar\cos\theta|$ and then rearranged in powers of (a/r). This yields the coefficient 1 of $(a/r)^0 = 1$, $\cos\theta$ as coefficient of a/r, etc. The **Legendre polynomial** $P_n(\cos\theta)$ (Fig. 11.2) **is defined as the coefficient of** $(a/r)^n$ so that

$$\varphi = \frac{q}{4\pi\varepsilon_0 r}\sum_{n=0}^{\infty} P_n(\cos\theta)\left(\frac{a}{r}\right)^n. \tag{11.3}$$

Dropping the factor $q/4\pi\varepsilon_0 r$ and using $x = \cos\theta$ and $t = a/r$, respectively, we have

$$g(t, x) = (1 - 2xt + t^2)^{-1/2} = \sum_{n=0}^{\infty} P_n(x)t^n, \quad |t| < 1, \tag{11.4}$$

defining $g(t, x)$ as the **generating function for the** $P_n(x)$. These polynomials $P_n(x)$, shown in Table 11.1, are the same as those generated in Example 9.3.1 by Gram–Schmidt orthogonalization of powers x^n over the interval $-1 \le x \le 1$. This is no coincidence because $\cos\theta$ varies between the limits ± 1. In the next section, it is shown that $|P_n(\cos\theta)| \le 1$, which means that the series expansion [Eq. (11.4)] is convergent for $|t| < 1$.[1] Indeed, the series is convergent for $|t| = 1$ except for $x = \pm 1$, where $|P_n(\pm 1)| = 1$.

[1] Note that the series in Eq. (11.3) is convergent for $r > a$ even though the binomial expansion involved is valid only for $r > (a^2+2ar)^{1/2} \ge |a^2-2ar\cos\theta|^{1/2}$ so that $r^2 > a^2 + 2ar$, $(r-a)^2 > 2a^2$, or $r > a(1+\sqrt{2})$.

Figure 11.2

Legendre Polynomials $P_2(x)$, $P_3(x)$, $P_4(x)$, and $P_5(x)$

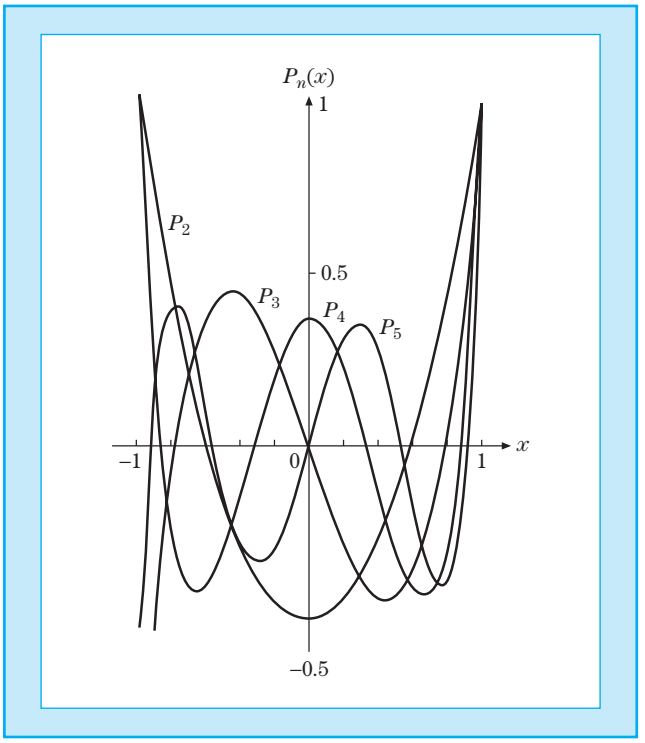


Table 11.1

Legendre Polynomials

$$
\begin{aligned}
&P_0(x) = 1\\
&P_1(x) = x\\
&P_2(x) = \tfrac{1}{2}(3x^2 - 1)\\
&P_3(x) = \tfrac{1}{2}(5x^3 - 3x)\\
&P_4(x) = \tfrac{1}{8}(35x^4 - 30x^2 + 3)\\
&P_5(x) = \tfrac{1}{8}(63x^5 - 70x^3 + 15x)\\
&P_6(x) = \tfrac{1}{16}(231x^6 - 315x^4 + 105x^2 - 5)\\
&P_7(x) = \tfrac{1}{16}(429x^7 - 693x^5 + 315x^3 - 35x)\\
&P_8(x) = \tfrac{1}{128}(6435x^8 - 12012x^6 + 6930x^4 - 1260x^2 + 35)
\end{aligned}
$$

In physical applications, such as the Coulomb or gravitational potentials, Eq. (11.4) often appears in the vector form

$$\frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} = \left[r_1^2 + r_2^2 - 2\mathbf{r}_1 \cdot \mathbf{r}_2\right]^{-1/2} = \frac{1}{r_1}\left[1 + \left(\frac{r_2}{r_1}\right)^2 - 2\left(\frac{r_2}{r_1}\right)\cos\theta\right]^{-1/2}.$$

The last equality is obtained by factoring $r_1 = |\mathbf{r}_1|$ from the denominator, which then, for $r_1 > r_2$, we can expand according to Eq. (11.4). In this way, we obtain

$$\frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} = \frac{1}{r_>} \sum_{n=0}^{\infty} \left(\frac{r_<}{r_>}\right)^n P_n(\cos\theta), \tag{11.4a}$$

where

$$\left.\begin{aligned} r_> &= |\mathbf{r}_1| \\ r_< &= |\mathbf{r}_2| \end{aligned}\right\} \quad \text{for} \quad |\mathbf{r}_1| > |\mathbf{r}_2|, \tag{11.4b}$$

and

$$\left.\begin{aligned} r_> &= |\mathbf{r}_2| \\ r_< &= |\mathbf{r}_1| \end{aligned}\right\} \quad \text{for} \quad |\mathbf{r}_2| > |\mathbf{r}_1|. \tag{11.4c}$$

EXAMPLE 11.1.1

Special Values A simple and powerful application of the generating function g is to use it for special values (e.g., $x = \pm 1$) where g can be evaluated explicitly. If we set $x = 1$, that is, point $z = a$ on the positive z-axis, where the potential has a simple form, Eq. (11.4) becomes

$$\frac{1}{(1 - 2t + t^2)^{1/2}} = \frac{1}{1 - t} = \sum_{n=0}^{\infty} t^n, \tag{11.5}$$

using a binomial expansion or the geometric series (Example 5.1.2). However, Eq. (11.4) for $x = 1$ defines

$$\frac{1}{(1 - 2t + t^2)^{1/2}} = \sum_{n=0}^{\infty} P_n(1) t^n.$$

Comparing the two series expansions (uniqueness of power series; Section 5.7), we have

$$P_n(1) = 1. \tag{11.6}$$

If we let $x = -1$ in Eq. (11.4), that is, point $z = -a$ on the negative z-axis in Fig. 11.1, where the potential is simple, then we sum similarly

$$\frac{1}{(1 + 2t + t^2)^{1/2}} = \frac{1}{1 + t} = \sum_{n=0}^{\infty} (-t)^n \tag{11.7}$$

so that

$$P_n(-1) = (-1)^n. \tag{11.8}$$

These general results are more difficult to develop from other formulas for Legendre polynomials.

If we take $x = 0$ in Eq. (11.4), using the binomial expansion

$$(1 + t^2)^{-1/2} = 1 - \tfrac{1}{2}t^2 + \tfrac{3}{8}t^4 + \cdots + (-1)^n \frac{1 \cdot 3 \cdots (2n-1)}{2^n n!} t^{2n} + \cdots, \tag{11.9}$$

we have[2]

$$P_{2n}(0) = (-1)^n \frac{1 \cdot 3 \cdots (2n-1)}{2^n n!} = (-1)^n \frac{(2n-1)!!}{(2n)!!} = \frac{(-1)^n (2n)!}{2^{2n}(n!)^2} \tag{11.10}$$

$$P_{2n+1}(0) = 0, \quad n = 0, 1, 2 \ldots . \tag{11.11}$$

These results can also be verified by inspection of Table 11.1. ■

EXAMPLE 11.1.2

Parity If we replace x by $-x$ and t by $-t$, the generating function is unchanged. Hence,

$$g(t, x) = g(-t, -x) = [1 - 2(-t)(-x) + (-t)^2]^{-1/2}$$

$$= \sum_{n=0}^{\infty} P_n(-x)(-t)^n = \sum_{n=0}^{\infty} P_n(x) t^n. \tag{11.12}$$

Comparing these two series, we have

$$P_n(-x) = (-1)^n P_n(x); \tag{11.13}$$

that is, the polynomial functions are odd or even (with respect to $x = 0$) according to whether the index n is odd or even. This is the parity[3] or reflection property that plays such an important role in quantum mechanics. Parity is conserved when the Hamiltonian is invariant under the reflection of the coordinates $\mathbf{r} \to -\mathbf{r}$. For central forces the index n is the orbital angular momentum [and $n(n+1)$ is the eigenvalue of $\mathbf{L}^2$], thus linking parity and orbital angular momentum. This parity property will be confirmed by the series solution and for the special cases tabulated in Table 11.1. ■

Power Series

Using the binomial theorem (Section 5.6) and Exercise 10.1.15, we expand the generating function as

$$(1 - 2xt + t^2)^{-1/2} = \sum_{n=0}^{\infty} \frac{(2n)!}{2^{2n}(n!)^2} (2xt - t^2)^n$$

$$= 1 + \sum_{n=1}^{\infty} \frac{(2n-1)!!}{(2n)!!} (2xt - t^2)^n. \tag{11.14}$$

Before we expand $(2xt - t^2)^n$ further, let us inspect the lowest powers of t.

[2]The double factorial notation is defined in Section 10.1:

$$(2n)!! = 2 \cdot 4 \cdot 6 \cdots (2n), \quad (2n-1)!! = 1 \cdot 3 \cdot 5 \cdots (2n-1).$$

[3]In spherical polar coordinates the inversion of the point (r, θ, φ) through the origin is accomplished by the transformation [$r \to r$, $\theta \to \pi - \theta$, and $\varphi \to \varphi \pm \pi$]. Then, $\cos\theta \to \cos(\pi - \theta) = -\cos\theta$, corresponding to $x \to -x$.

EXAMPLE 11.1.3

Lowest Legendre Polynomials For the first few Legendre polynomials (e.g., P_0, P_1, and P_2), we need the coefficients of t^0, t^1, and t^2 in Eq. (11.14). These powers of t appear only in the terms $n = 0$, 1, and 2; hence, we may limit our attention to the first three terms of the infinite series:

$$\frac{0!}{2^0(0!)^2}(2xt - t^2)^0 + \frac{2!}{2^2(1!)^2}(2xt - t^2)^1 + \frac{4!}{2^4(2!)^2}(2xt - t^2)^2$$
$$= 1t^0 + xt^1 + \left(\frac{3}{2}x^2 - \frac{1}{2}\right)t^2 + \mathcal{O}(t^3).$$

Then, from Eq. (11.4) (and uniqueness of power series) we obtain

$$P_0(x) = 1, \quad P_1(x) = x, \quad P_2(x) = \frac{3}{2}x^2 - \frac{1}{2}, \tag{11.15}$$

confirming the entries of Table 11.1. We repeat this limited development in a vector framework later in this section. ■

In employing a general treatment, we find that the binomial expansion of the $(2xt - t^2)^n$ factor yields the double series

$$(1 - 2xt + t^2)^{-1/2} = \sum_{n=0}^{\infty} \frac{(2n)!}{2^{2n}(n!)^2} t^n \sum_{k=0}^{n} (-1)^k \frac{n!}{k!(n-k)!}(2x)^{n-k}t^k$$
$$= \sum_{n=0}^{\infty} \sum_{k=0}^{n} (-1)^k \frac{(2n)!}{2^{2n}n!k!(n-k)!} \cdot (2x)^{n-k}t^{n+k}. \tag{11.16}$$

By rearranging the order of summation (valid by absolute convergence), Eq. (11.16) becomes

$$(1-2xt+t^2)^{-1/2} = \sum_{n=0}^{\infty} \sum_{k=0}^{[n/2]} (-1)^k \frac{(2n-2k)!}{2^{2n-2k}k!(n-k)!(n-2k)!} \cdot (2x)^{n-2k}t^n, \tag{11.17}$$

with the t^n independent of the index k.[4] Now, equating our two power series [Eqs. (11.4) and (11.17)] term by term, we have[5]

$$P_n(x) = \sum_{k=0}^{[n/2]} (-1)^k \frac{(2n-2k)!}{2^n k!(n-k)!(n-2k)!} x^{n-2k}. \tag{11.18}$$

We read off this formula, from $k = 0$, that the highest power of $P_n(x)$ is x^n, and the lowest power is $x^0 = 1$ for even n and x for odd n. This is consistent with Example 11.1.3 and Table 11.1. Also, for n even, P_n has only even powers of x and thus even parity [see Eq. (11.13)] and odd powers and odd parity for odd n.

[4] $[n/2] = n/2$ for n even, $(n-1)/2$ for n odd.

[5] Equation (11.18) starts with x^n. By changing the index, we can transform it into a series that starts with x^0 for n even and x^1 for n odd.

Biographical Data

Legendre, Adrien Marie. Legendre, a French mathematician who was born in Paris in 1752 and died there in 1833, made major contributions to number theory, elliptic integrals before Abel and Jacobi, and analysis. He tried in vain to prove the parallel axiom of Euclidean geometry. His taste in selecting research problems was remarkably similar to that of his contemporary Gauss, but nobody could match Gauss's depth and perfection. His great textbooks had enormous impact.

Linear Electric Multipoles

Returning to the electric charge on the z-axis, we demonstrate the usefulness and power of the generating function by adding a charge $-q$ at $z = -a$, as shown in Fig. 11.3, using the superposition principle of electric fields. The potential becomes

$$\varphi = \frac{q}{4\pi\varepsilon_0}\left(\frac{1}{r_1} - \frac{1}{r_2}\right), \tag{11.19}$$

and by using the law of cosines, we have for $r > a$

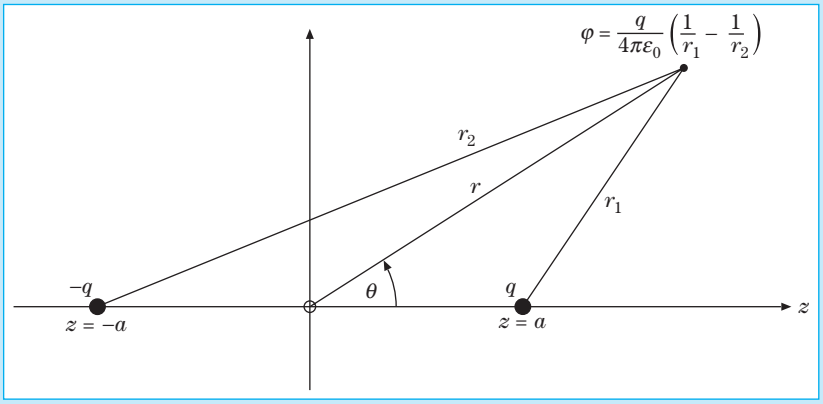
$$\varphi = \frac{q}{4\pi\varepsilon_0 r}\left\{\left[1 - 2\frac{a}{r}\cos\theta + \left(\frac{a}{r}\right)^2\right]^{-1/2} - \left[1 + 2\frac{a}{r}\cos\theta + \left(\frac{a}{r}\right)^2\right]^{-1/2}\right\},$$

where the second radical is like the first, except that a has been replaced by $-a$. Then, using Eq. (11.4), we obtain

$$\begin{aligned}\varphi &= \frac{q}{4\pi\varepsilon_0 r}\left[\sum_{n=0}^{\infty} P_n(\cos)\left(\frac{a}{r}\right)^n - \sum_{n=0}^{\infty} P_n(\cos\theta)(-1)^n\left(\frac{a}{r}\right)^n\right] \\ &= \frac{2q}{4\pi\varepsilon_0 r}\left[P_1(\cos\theta)\frac{a}{r} + P_3(\cos\theta)\left(\frac{a}{r}\right)^3 + \cdots\right].\end{aligned} \tag{11.20}$$

Figure 11.3

Electric Dipole



The first term (and dominant term for $r \gg a$) is the **electric dipole** potential

$$\varphi = \frac{2aq}{4\pi\varepsilon_0} \cdot \frac{P_1(\cos\theta)}{r^2}, \tag{11.21}$$

with $2aq$ the **electric dipole moment** (Fig. 11.3). If the potential in Eq. (11.19) is taken to be the dipole potential, then Eq. (11.21) gives its asymptotic behavior for large r. This analysis may be extended by placing additional charges on the z-axis so that the P_1 term, as well as the P_0 (monopole) term, is canceled. For instance, charges of q at $z = a$ and $z = -a$, $-2q$ at $z = 0$ give rise to a potential whose series expansion starts with $P_2(\cos\theta)$. This is a linear electric quadrupole. Two linear quadrupoles may be placed so that the quadrupole term is canceled, but the P_3, the electric octupole term, survives, etc. These expansions are special cases of the general multipole expansion of the electric potential.

Vector Expansion

We consider the electrostatic potential produced by a distributed charge $\rho(\mathbf{r}_2)$:

$$\varphi(\mathbf{r}_1) = \frac{1}{4\pi\varepsilon_0} \int \frac{\rho(\mathbf{r}_2)}{|\mathbf{r}_1 - \mathbf{r}_2|} d\tau_2. \tag{11.22a}$$

Taking the denominator of the integrand, using first the law of cosines and then a binomial expansion, yields

$$\begin{aligned} \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} &= \left(r_1^2 - 2\mathbf{r}_1 \cdot \mathbf{r}_2 + r_2^2\right)^{-1/2} \\ &= \frac{1}{r_1}\left[1 + \left(-\frac{2\mathbf{r}_1 \cdot \mathbf{r}_2}{r_1^2} + \frac{r_2^2}{r_1^2}\right)\right]^{-1/2}, \quad \text{for } r_1 > r_2 \\ &= \frac{1}{r_1}\left[1 + \frac{\mathbf{r}_1 \cdot \mathbf{r}_2}{r_1^2} - \frac{1}{2}\frac{r_2^2}{r_1^2} + \frac{3}{2}\frac{(\mathbf{r}_1 \cdot \mathbf{r}_2)^2}{r_1^4} + \mathcal{O}\left(\frac{r_2}{r_1}\right)^3\right]. \end{aligned} \tag{11.22b}$$

For $r_1 = 1, r_2 = t$, and $\mathbf{r}_1 \cdot \mathbf{r}_2 = xt$, Eq. (11.22b) reduces to the generating function, Eq. (11.4).

The first term in the square bracket, 1, yields a potential

$$\varphi_0(\mathbf{r}_1) = \frac{1}{4\pi\varepsilon_0}\frac{1}{r_1} \int \rho(\mathbf{r}_2) d\tau_2. \tag{11.22c}$$

The integral contains the total charge. This part of the total potential is an electric **monopole**.

The second term yields

$$\varphi_1(\mathbf{r}_1) = \frac{1}{4\pi\varepsilon_0}\frac{\mathbf{r}_1 \cdot}{r_1^3} \int \mathbf{r}_2 \rho(\mathbf{r}_2) d\tau_2, \tag{11.22d}$$

where the integral is the dipole moment whose charge density $\rho(\mathbf{r}_2)$ is weighted by a moment arm $\mathbf{r}_2$. We have an electric dipole potential. For atomic or nuclear states of definite parity, $\rho(\mathbf{r}_2)$ is an even function and the dipole integral

is identically zero. However, in the presence of an applied electric field a superposition of odd/even parity states may develop so that the resulting induced dipole moment is no longer zero. The last two terms, both of order $(r_2/r_1)^2$, may be handled by using Cartesian coordinates

$$(\mathbf{r}_1 \cdot \mathbf{r}_2)^2 = \sum_{i=1}^{3} x_{1i}x_{2i} \sum_{j=1}^{3} x_{1j}x_{2j}.$$

Rearranging variables to keep the x_2 inside the integral yields

$$\varphi_2(\mathbf{r}_1) = \frac{1}{4\pi\varepsilon_0}\frac{1}{2r_1^5}\sum_{i,j=1}^{3} x_{1i}x_{1j}\int \left[3x_{2i}x_{2j} - \delta_{ij}r_2^2\right]\rho(\mathbf{r}_2)d\tau_2. \tag{11.22e}$$

This is the electric **quadrupole** term. Note that the square bracket in the integrand forms a symmetric tensor of zero trace.

A general electrostatic **multipole expansion** can also be developed by using Eq. (11.22a) for the potential $\varphi(r_1)$ and replacing $1/(4\pi|\mathbf{r}_1 - \mathbf{r}_2|)$ by a (double) series of the angular solutions of the Poisson equation (which are the same as those of the Laplace equation of Section 8.9).

Before leaving multipole fields, we emphasize three points:

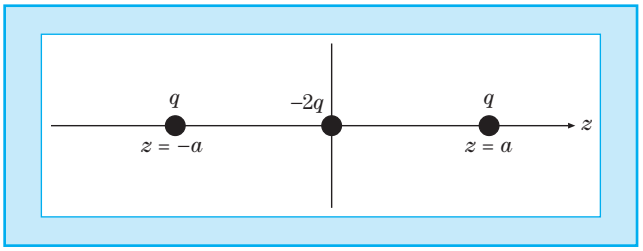
- First, an electric (or magnetic) multipole has a value independent of the origin (reference point) only if all lower order terms vanish. For instance, the potential of one charge q at $z = a$ was expanded in a series of Legendre polynomials. Although we refer to the $P_1(\cos\theta)$ term in this expansion as a dipole term, it should be remembered that this term exists only because of our choice of coordinates. We actually have a monopole, $P_0(\cos\theta)$, the term of leading magnitude.
- Second, in physical systems we rarely encounter pure multipoles. For example, the potential of the finite dipole (q at $z = a$, $-q$ at $z = -a$) contained a $P_3(\cos\theta)$ term. These higher order terms may be eliminated by shrinking the multipole to a point multipole, in this case keeping the product qa constant ($a \to 0$, $q \to \infty$) to maintain the same dipole moment.
- Third, the multipole expansion is not restricted to electrical phenomena. Planetary configurations are described in terms of mass multipoles.

It might also be noted that a multipole expansion is actually a decomposition into the irreducible representations of the rotation group (Section 4.2). The lth multipole involves the eigenfunctions of orbital angular momentum, $|lm\rangle$, one for each component m of the multipole l (see Chapter 4). These $2l + 1$ components of the multipole form an irreducible representation because the lowering operator L_- applied repeatedly to the eigenfunction $|ll\rangle$ generates all other eigenfunctions $|lm\rangle$, down to $m = -l$. The raising and lowering operators $L_\pm$ are generators of the rotation group along with L_z, whose eigenvalue is m.

EXERCISES

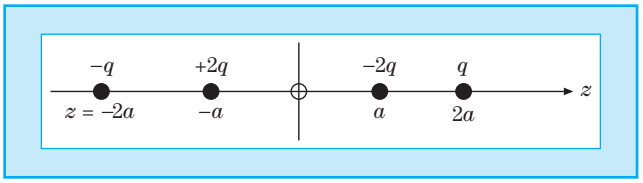
11.1.1 Develop the electrostatic potential for the array of charges shown. This is a linear electric quadrupole (Fig. 11.4).

Figure 11.4
Linear Electric Quadrupole



11.1.2 Calculate the electrostatic potential of the array of charges shown in Fig. 11.5. This is an example of two equal but oppositely directed dipoles. The dipole contributions cancel, but the octupole terms do not cancel.

Figure 11.5
Linear Electric Octupole



11.1.3 Show that the electrostatic potential produced by a charge q at $z = a$ for $r < a$ is

$$\varphi(\mathbf{r}) = \frac{q}{4\pi\varepsilon_0 a}\sum_{n=0}^{\infty}\left(\frac{r}{a}\right)^n P_n(\cos\theta).$$

11.1.4 Using $\mathbf{E} = -\nabla\varphi$, determine the components of the electric field corresponding to the (pure) electric dipole potential

$$\varphi(\mathbf{r}) = \frac{2aqP_1(\cos\theta)}{4\pi\varepsilon_0 r^2}.$$

Here, it is assumed that $r \gg a$.

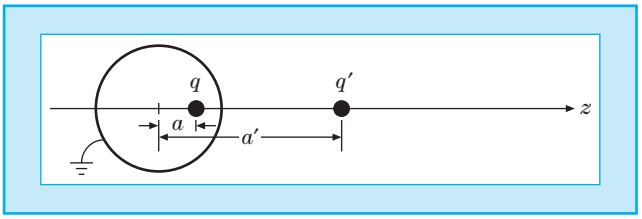
$$ANS. \quad E_r = +\frac{4aq\cos\theta}{4\pi\varepsilon_0 r^3}, \qquad E_\theta = +\frac{2aq\sin\theta}{4\pi\varepsilon_0 r^3}, \quad E_\varphi = 0.$$

11.1.5 A point electric dipole of strength $p^{(1)}$ is placed at $z = a$; a second point electric dipole of equal but opposite strength is at the origin. Keeping the product $p^{(1)}a$ constant, let $a \to 0$. Show that this results in a point electric quadrupole.

11.1.6 A point charge q is in the interior of a hollow conducting sphere of radius r_0. The charge q is displaced a distance a from the center of the sphere. If the conducting sphere is grounded, show that the potential in the interior produced by q and the distributed induced charge is the same as that produced by q and its image charge q'. The image charge is at a distance $a' = r_0^2/a$ from the center, collinear with q and the origin (Fig. 11.6).

Figure 11.6

Image Charge q'



Hint. Calculate the electrostatic potential for $a < r_0 < a'$. Show that the potential vanishes for $r = r_0$ if we take $q' = -qr_0/a$.

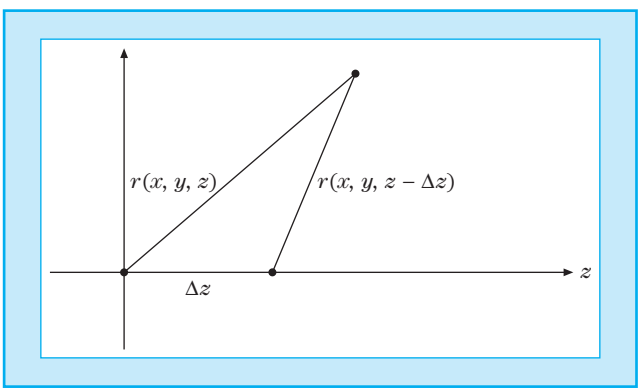
11.1.7 Prove that

$$P_n(\cos\theta) = (-1)^n \frac{r^{n+1}}{n!} \frac{\partial^n}{\partial z^n} \left(\frac{1}{r}\right).$$

Hint. Compare the Legendre polynomial expansion of the generating function ($a \to \Delta z$; Fig. 11.1) with a Taylor series expansion of $1/r$, where z dependence of r changes from z to $z - \Delta z$ (Fig. 11.7).

Figure 11.7

Geometry for $z \to z - \Delta z$



11.1.8 By differentiation and direct substitution of the series form, Eq. (11.18), show that $P_n(x)$ satisfies Legendre's ODE. Note that we may have any x, $-\infty < x < \infty$ and indeed any z in the entire finite complex plane.

11.2 Recurrence Relations and Special Properties

Recurrence Relations

The Legendre polynomial generating function provides a convenient way of deriving the recurrence relations[6] and some special properties. If our generating function [Eq. (11.4)] is differentiated with respect to t, we obtain

$$\frac{\partial g(t,x)}{\partial t} = \frac{x-t}{(1-2xt+t^2)^{3/2}} = \sum_{n=0}^{\infty} nP_n(x)t^{n-1}. \tag{11.23}$$

By substituting Eq. (11.4) into this and rearranging terms, we have

$$(1-2xt+t^2)\sum_{n=0}^{\infty} nP_n(x)t^{n-1} + (t-x)\sum_{n=0}^{\infty} P_n(x)t^n = 0. \tag{11.24}$$

The left-hand side is a power series in t. Since this power series vanishes for all values of t, the coefficient of each power of t is equal to zero; that is, our power series is unique (Section 5.7). These coefficients are found by separating the individual summations and using appropriate summation indices as follows:

$$\sum_{m=0}^{\infty} mP_m(x)t^{m-1} - \sum_{n=0}^{\infty} 2nxP_n(x)t^n + \sum_{s=0}^{\infty} sP_s(x)t^{s+1} + \sum_{s=0}^{\infty} P_s(x)t^{s+1} - \sum_{n=0}^{\infty} xP_n(x)t^n = 0. \tag{11.25}$$

Now letting $m = n+1$, $s = n-1$, we find

$$(2n+1)xP_n(x) = (n+1)P_{n+1}(x) + nP_{n-1}(x), \quad n = 1, 2, 3, \ldots. \tag{11.26}$$

With this three-term recurrence relation we may easily construct the higher Legendre polynomials. If we take $n = 1$ and insert the values of $P_0(x)$ and $P_1(x)$ [Exercise 11.1.7 or Eq. (11.18)], we obtain

$$3xP_1(x) = 2P_2(x) + P_0(x), \quad \text{or } P_2(x) = \frac{1}{2}(3x^2-1).$$

This process may be continued indefinitely; the first few Legendre polynomials are listed in Table 11.1.

Cumbersome as it may appear at first, this technique is actually more efficient for a computer than is direct evaluation of the series [Eq. (11.18)]. For greater stability (to avoid undue accumulation and magnification of round off error), Eq. (11.26) is rewritten as

$$P_{n+1}(x) = 2xP_n(x) - P_{n-1}(x) - [xP_n(x) - P_{n-1}(x)]/(n+1). \tag{11.26a}$$

[6] We can also apply the explicit series form [Eq. (11.18)] directly.

One starts with $P_0(x) = 1$, $P_1(x) = x$, and computes the **numerical** values of all the $P_n(x)$ for a given value of x, up to the desired $P_N(x)$. The values of $P_n(x)$, $0 \le n < N$ are available as a fringe benefit.

To practice, let us derive another recursion relation from the generating function.

EXAMPLE 11.2.1 **Recursion Formula** Consider the product

$$\begin{aligned} g(t, x)g(t, -x) &= (1 - 2xt + t^2)^{-1/2}(1 + 2xt + t^2)^{-1/2} \\ &= [(1 + t^2)^2 - 4x^2t^2]^{-1/2} = [t^4 + 2t^2(1 - 2x^2) + 1]^{-1/2} \end{aligned}$$

and recognize the generating function, upon replacing $t^2 \to t$, $2x^2 - 1 \to x$. Using Eq. (11.4) and comparing coefficients of the power series in t we therefore have derived

$$g(t, x)g(t, -x) = \sum_{m,n} P_m(x)P_n(-x)t^{m+n} = \sum_N P_N(2x^2 - 1)t^{2N},$$

or, for $m + n = 2N$ and $m + n = 2N - 1$, respectively,

$$P_N(2x^2 - 1) = \sum_{n=0}^{2N} P_{2N-n}(x)P_n(-x), \tag{11.27a}$$

$$\sum_{n=0}^{2N-1} P_{2N-n-1}(x)P_n(-x) = 0. \tag{11.27b}$$

For $N = 1$ we check first that

$$\sum_{n=0}^{1} P_{1-n}(x)P_n(-x) = x \cdot 1 - 1 \cdot x = 0$$

and second that

$$P_1(2x^2 - 1) = \sum_{n=0}^{2} P_{2-n}(x)P_n(-x) = x - x - x^2 + 2\left(\frac{3}{2}x^2 - \frac{1}{2}\right) = 2x^2 - 1. \quad \blacksquare$$

Differential Equations

More information about the behavior of the Legendre polynomials can be obtained if we now differentiate Eq. (11.4) with respect to x. This gives

$$\frac{\partial g(t, x)}{\partial x} = \frac{t}{(1 - 2xt + t^2)^{3/2}} = \sum_{n=0}^{\infty} P_n'(x)t^n \tag{11.28}$$

or

$$(1 - 2xt + t^2)\sum_{n=0}^{\infty} P_n'(x)t^n - t\sum_{n=0}^{\infty} P_n(x)t^n = 0. \tag{11.29}$$

As before, the coefficient of each power of t is set equal to zero and we obtain

$$P_{n+1}'(x) + P_{n-1}'(x) = 2xP_n'(x) + P_n(x). \tag{11.30}$$

A more useful relation may be found by differentiating Eq. (11.26) with respect to x and multiplying by 2. To this we add $(2n+1)$ times Eq. (11.30), canceling the P_n' term. The result is

$$P_{n+1}'(x) - P_{n-1}'(x) = (2n+1)P_n(x). \tag{11.31}$$

From Eqs. (11.30) and (11.31) numerous additional equations may be developed,[7] including

$$P_{n+1}'(x) = (n+1)P_n(x) + xP_n'(x), \tag{11.32}$$

$$P_{n-1}'(x) = -nP_n(x) + xP_n'(x), \tag{11.33}$$

$$(1-x^2)P_n'(x) = nP_{n-1}(x) - nxP_n(x), \tag{11.34}$$

$$(1-x^2)P_n'(x) = (n+1)xP_n(x) - (n+1)P_{n+1}(x). \tag{11.35}$$

By differentiating Eq. (11.34) and using Eq. (11.33) to eliminate $P_{n-1}'(x)$, we find that $P_n(x)$ satisfies the linear, second-order ODE

$$(1-x^2)P_n''(x) - 2xP_n'(x) + n(n+1)P_n(x) = 0$$

or

$$\frac{d}{dx}\left[(1-x^2)\frac{dP_n(x)}{dx}\right] + n(n+1)P_n(x) = 0. \tag{11.36}$$

In the second form the ODE is self-adjoint. The previous equations, Eqs. (11.30)–(11.35), are all first-order ODEs but with polynomials of two different indices. The price for having all indices alike is a second-order differential equation. Equation (11.36) is **Legendre's** ODE. We now see that the polynomials $P_n(x)$ generated by the power series for $(1-2xt+t^2)^{-1/2}$ satisfy Legendre's equation, which, of course, is why they are called Legendre polynomials.

In Eq. (11.36) differentiation is with respect to x $(= \cos\theta)$. Frequently, we encounter Legendre's equation expressed in terms of differentiation with respect to θ:

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{dP_n(\cos\theta)}{d\theta}\right) + n(n+1)P_n(\cos\theta) = 0. \tag{11.37}$$

[7] Using the equation number in parentheses to denote the left-hand side of the equation, we may write the derivatives as

$$\begin{aligned}
2\cdot\tfrac{d}{dx}(11.26) + (2n+1)\cdot(11.30) &\Rightarrow (11.31)\\
\tfrac{1}{2}\{(11.30)+(11.31)\} &\Rightarrow (11.32)\\
\tfrac{1}{2}\{(11.30)-(11.31)\} &\Rightarrow (11.33)\\
(11.32)_{n\to n-1} + x\cdot(11.33) &\Rightarrow (11.34)\\
\tfrac{d}{dx}(11.34) + n\cdot(11.33) &\Rightarrow (11.36).
\end{aligned}$$

Upper and Lower Bounds for $P_n(\cos\theta)$

Finally, in addition to these results, our generating function enables us to set an upper limit on $|P_n(\cos\theta)|$. We have

$$\begin{aligned}(1-2t\cos\theta+t^2)^{-1/2} &= (1-te^{i\theta})^{-1/2}(1-te^{-i\theta})^{-1/2}\\ &= \left(1+\tfrac{1}{2}te^{i\theta}+\tfrac{3}{8}t^2e^{2i\theta}+\cdots\right)\\ &\quad\cdot\left(1+\tfrac{1}{2}te^{-i\theta}+\tfrac{3}{8}t^2e^{-2i\theta}+\cdots\right),\end{aligned}\tag{11.38}$$

with all coefficients **positive**. Our Legendre polynomial, $P_n(\cos\theta)$, still the coefficient of t^n, may now be written as a sum of terms of the form

$$\tfrac{1}{2}a_m(e^{im\theta}+e^{-im\theta}) = a_m\cos m\theta \tag{11.39a}$$

with all the a_m **positive**. Then

$$P_n(\cos\theta) = \sum_{m=0 \text{ or } 1}^{n} a_m\cos m\theta. \tag{11.39b}$$

This series, Eq. (11.39b), is clearly a maximum when $\theta = 0$ and all $\cos m\theta = 1$ are maximal. However, for $x = \cos\theta = 1$, Eq. (11.6) shows that $P_n(1) = 1$. Therefore,

$$|P_n(\cos\theta)| \le P_n(1) = 1. \tag{11.39c}$$

A fringe benefit of Eq. (11.39b) is that it shows that **our Legendre polynomial is a linear combination of** $\cos m\theta$. This means that the **Legendre polynomials form a complete set for any functions that may be expanded in series of** $\cos m\theta$ **over the interval** $[0, \pi]$.

SUMMARY

In this section, various useful properties of the Legendre polynomials are derived from the generating function, Eq. (11.4). The explicit series representation, Eq. (11.18), offers an alternate and sometimes superior approach.

EXERCISES

11.2.1 Given the series

$$\alpha_0+\alpha_2\cos^2\theta+\alpha_4\cos^4\theta+\alpha_6\cos^6\theta = a_0P_0+a_2P_2+a_4P_4+a_6P_6,$$

express the coefficients α_i as a column vector $\boldsymbol{\alpha}$ and the coefficients a_i as a column vector $\mathbf{a}$ and determine the matrices A and B such that

$$\mathsf{A}\boldsymbol{\alpha} = \mathbf{a} \qquad \text{and} \qquad \mathsf{B}\mathbf{a} = \boldsymbol{\alpha}.$$

Check your computation by showing that $\mathsf{AB} = 1$ (unit matrix). Repeat for the odd case

$$\alpha_1\cos\theta+\alpha_3\cos^3\theta+\alpha_5\cos^5\theta+\alpha_7\cos^7\theta = a_1P_1+a_3P_3+a_5P_5+a_7P_7.$$

Note. $P_n(\cos\theta)$ and $\cos^n\theta$ are tabulated in terms of each other in AMS-55.

11.2.2 By differentiating the generating function, $g(t, x)$, with respect to t, multiplying by $2t$, and then adding $g(t, x)$, show that

$$\frac{1-t^2}{(1-2tx+t^2)^{3/2}} = \sum_{n=0}^{\infty}(2n+1)P_n(x)t^n.$$

This result is useful in calculating the charge induced on a grounded metal sphere by a point charge q.

11.2.3 (a) Derive Eq. (11.35)

$$(1-x^2)P_n'(x) = (n+1)xP_n(x) - (n+1)P_{n+1}(x).$$

(b) Write out the relation of Eq. (11.35) to preceding equations in symbolic form analogous to the symbolic forms for Eqs. (11.31)–(11.34).

11.2.4 A point electric octupole may be constructed by placing a point electric quadrupole (pole strength $p^{(2)}$ in the z-direction) at $z = a$ and an equal but opposite point electric quadrupole at $z = 0$ and then letting $a \to 0$, subject to $p^{(2)}a =$ constant. Find the electrostatic potential corresponding to a point electric octupole. Show from the construction of the point electric octupole that the corresponding potential may be obtained by differentiating the point quadrupole potential.

11.2.5 Operating in **spherical polar coordinates**, show that

$$\frac{\partial}{\partial z}\left[\frac{P_n(\cos\theta)}{r^{n+1}}\right] = -(n+1)\frac{P_{n+1}(\cos\theta)}{r^{n+2}}.$$

This is the key step in the mathematical argument that the derivative of one multipole leads to the next higher multipole.
Hint. Compare Exercise 2.5.12.

11.2.6 From

$$P_L(\cos\theta) = \frac{1}{L!}\frac{\partial^L}{\partial t^L}(1-2t\cos\theta+t^2)^{-1/2}\Big|_{t=0}$$

show that

$$P_L(1) = 1, \quad P_L(-1) = (-1)^L.$$

11.2.7 Prove that

$$P_n'(1) = \frac{d}{dx}P_n(x)\Big|_{x=1} = \frac{1}{2}n(n+1).$$

11.2.8 Show that $P_n(\cos\theta) = (-1)^nP_n(-\cos\theta)$ by use of the recurrence relation relating P_n, P_{n+1}, and P_{n-1} and your knowledge of P_0 and P_1.

11.2.9 From Eq. (11.38) write out the coefficient of t^2 in terms of $\cos n\theta$, $n \le 2$. This coefficient is $P_2(\cos\theta)$.

11.3 Orthogonality

Legendre's ODE [Eq. (11.36)] may be written in the form (Section 9.1)

$$\frac{d}{dx}[(1-x^2)P_n'(x)] + n(n+1)P_n(x) = 0, \tag{11.40}$$

showing clearly that it is self-adjoint. Subject to satisfying certain boundary conditions, then, we know that the eigenfunction solutions $P_n(x)$ are orthogonal. Upon comparing Eq. (11.40) with Eqs. (9.6) and (9.8) we see that the weight function $w(x) = 1$, $\mathcal{L} = (d/dx)(1-x^2)(d/dx)$, $p(x) = 1-x^2$ and the eigenvalue $\lambda = n(n+1)$. The integration limits on x are ± 1, where $p(\pm 1) = 0$. Then for $m \neq n$, Eq. (9.34) becomes

$$\int_{-1}^{1} P_n(x)P_m(x)\,dx = 0,^{8} \tag{11.41}$$

$$\int_{0}^{\pi} P_n(\cos\theta)P_m(\cos\theta)\sin\theta\,d\theta = 0, \tag{11.42}$$

showing that $P_n(x)$ and $P_m(x)$ are orthogonal for the interval $[-1, 1]$.

We need to evaluate the integral [Eq. (11.41)] when $n = m$. Certainly, it is no longer zero. From our generating function

$$(1-2tx+t^2)^{-1} = \left[\sum_{n=0}^{\infty} P_n(x)t^n\right]^2. \tag{11.43}$$

Integrating from $x = -1$ to $x = +1$, we have

$$\int_{-1}^{1} \frac{dx}{1-2tx+t^2} = \sum_{n=0}^{\infty} t^{2n} \int_{-1}^{1} [P_n(x)]^2\,dx. \tag{11.44}$$

The cross terms in the series vanish by means of Eq. (11.41). Using $y = 1 - 2tx + t^2$, we obtain

$$\int_{-1}^{1} \frac{dx}{1-2tx+t^2} = \frac{1}{2t}\int_{(1-t)^2}^{(1+t)^2} \frac{dy}{y} = \frac{1}{t}\ln\left(\frac{1+t}{1-t}\right). \tag{11.45}$$

Expanding this in a power series (Exercise 5.4.1) gives us

$$\frac{1}{t}\ln\left(\frac{1+t}{1-t}\right) = 2\sum_{n=0}^{\infty} \frac{t^{2n}}{2n+1}. \tag{11.46}$$

---

[8] In Section 9.4 such integrals are intepreted as inner products in a linear vector (function) space. Alternate notations are

$$\int_{-1}^{1} P_n(x)P_m(x)\,dx \equiv \langle P_n(x)|P_m(x)\rangle \equiv (P_n(x), P_m(x)).$$

The $\langle\,\rangle$ form, popularized by Dirac, is common in physics literature. The form $(\,,\,)$ is more common in mathematics literature.

Comparing power series coefficients of Eqs. (11.44) and (11.46), we must have

$$\int_{-1}^{1} [P_n(x)]^2\, dx = \frac{2}{2n+1}. \tag{11.47}$$

Combining Eq. (11.41) with Eq. (11.47) we have the orthonormality condition

$$\int_{-1}^{1} P_m(x)P_n(x)\, dx = \frac{2\delta_{mn}}{2n+1}. \tag{11.48}$$

Therefore, P_n **are not normalized to unity**. We return to this normalization in Section 11.5, when we construct the orthonormal spherical harmonics.

Expansion of Functions, Legendre Series

In addition to orthogonality, the Sturm–Liouville theory shows that the Legendre polynomials form a complete set. Let us assume, then, that the series

$$\sum_{n=0}^{\infty} a_n P_n(x) = f(x), \qquad \text{or} \quad |f\rangle = \sum_n a_n |P_n\rangle, \tag{11.49}$$

defines $f(x)$ in the sense of convergence in the mean (Section 9.4) in the interval $[-1, 1]$. This demands that $f(x)$ and $f'(x)$ be at least sectionally continuous in this interval. The coefficients a_n are found by multiplying the series by $P_m(x)$ and integrating term by term. Using the orthogonality property expressed in Eqs. (11.42) and (11.48), we obtain

$$\frac{2}{2m+1}a_m = \int_{-1}^{1} P_m(x)f(x)\, dx = \langle P_m|f\rangle = \sum_n a_n \langle P_m|P_n\rangle. \tag{11.50}$$

We replace the variable of integration x by t and the index m by n. Then, substituting into Eq. (11.49), we have

$$f(x) = \sum_{n=0}^{\infty} \frac{2n+1}{2} \left(\int_{-1}^{1} f(t)P_n(t)\, dt \right) P_n(x). \tag{11.51}$$

This expansion in a series of Legendre polynomials is usually referred to as a Legendre series.[9] Its properties are quite similar to the more familiar Fourier series (Chapter 14). In particular, we can use the orthogonality property [Eq. (11.48)] to show that the series is unique.

On a more abstract (and more powerful) level, Eq. (11.51) gives the representation of $f(x)$ in the linear vector space of Legendre polynomials (a Hilbert space; Section 9.4).

Equation (11.51) may also be interpreted in terms of the **projection operators** of quantum theory. We may define a projection operator

$$\mathcal{P}_m \equiv P_m(x)\frac{2m+1}{2}\int_{-1}^{1} P_m(t)[\ ]dt$$

[9] Note that Eq. (11.50) gives a_m as a **definite** integral, that is, a number for a given $f(x)$.

as an (integral) operator, ready to operate on $f(t)$. [The $f(t)$ would go in the square bracket as a factor in the integrand.] Then, from Eq. (11.50)

$$\mathcal{P}_m f = a_m P_m(x).^{10}$$

The operator $\mathcal{P}_m$ projects out the mth component of the function f.

EXAMPLE 11.3.1 **Legendre Expansion** Expand $f(x) = x(x+1)(x-1)$ in the interval $-1 \le x \le 1$.

Because $f(x)$ is odd under parity and is a third-order polynomial, we expect only $P_1,\ P_3$. However, we check all coefficients:

$$2a_0 = \int_{-1}^{1} (x^3 - x)\,dx = \left[\frac{1}{4}x^4 - \frac{1}{2}x^2\right]\Big|_{-1}^{1} = 0, \quad \text{also by parity,}$$

$$\frac{2}{3}a_1 = \int_{-1}^{1} (x^4 - x^2)\,dx = \left[\frac{1}{5}x^5 - \frac{1}{3}x^3\right]\Big|_{-1}^{1} = \frac{2}{5} - \frac{2}{3} = -\frac{4}{15},$$

$$\frac{2}{5}a_2 = \frac{1}{2}\int_{-1}^{1} (x^3 - x)(3x^2 - 1)\,dx = 0, \quad \text{by parity;}$$

$$\frac{2}{7}a_3 = \frac{1}{2}\int_{-1}^{1} (x^3 - x)(5x^3 - 3x)\,dx = \frac{1}{2}\int_{-1}^{1} (5x^6 - 8x^4 + 3x^2)\,dx$$

$$= \frac{1}{2}\left[\frac{5}{7}x^7 - \frac{8}{5}x^5 + x^3\right]\Big|_{-1}^{1} = \frac{5}{7} - \frac{8}{5} + 1 = \frac{4}{35}.$$

Finally, using $a_1,\ a_3$, we verify that $-\frac{2}{5}x + \frac{1}{5}(5x^3 - 3x) = x(x^2 - 1)$. ■

Equation (11.3), which leads directly to the generating function definition of Legendre polynomials, is a Legendre expansion of $1/r_1$. Going beyond a simple Coulomb field, the $1/r_{12}$ is often replaced by a potential $V(|\mathbf{r}_1 - \mathbf{r}_2|)$ and the solution of the problem is again effected by a Legendre expansion.

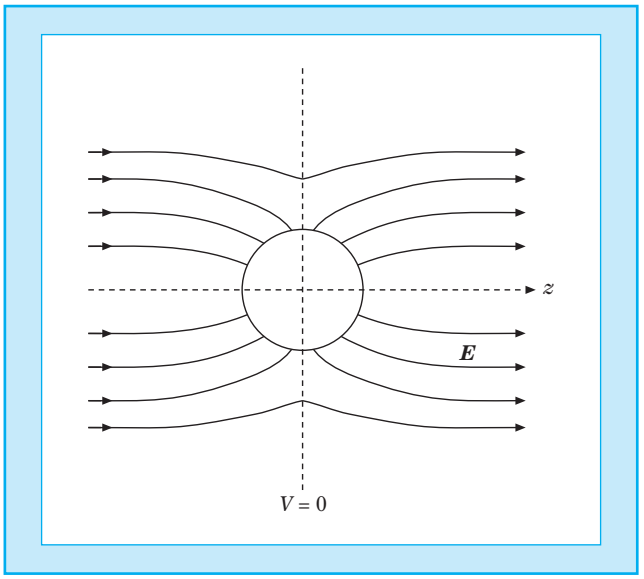
The Legendre series, Eq. (11.49), has been treated as a **known** function $f(x)$ that we arbitrarily chose to expand in a series of Legendre polynomials. Sometimes the origin and nature of the Legendre series are different. In the next examples we consider **unknown** functions we know can be represented by a Legendre series because of the differential equation the unknown functions satisfy. As before, the problem is to determine the unknown coefficients in the series expansion. Here, however, the coefficients are not found by Eq. (11.50). Rather, they are determined by demanding that the Legendre series match a known solution at a boundary. These are boundary value problems.

EXAMPLE 11.3.2 **Sphere in a Uniform Field** Another illustration of the use of Legendre polynomials is provided by the problem of a neutral conducting sphere (radius r_0) placed in a (previously) uniform electric field (Fig. 11.8). The problem is to

[10] The dependent variables are arbitrary. Here, x came from the x in $\mathcal{P}_m$.

Figure 11.8

Conducting Sphere in a Uniform Field



find the new, perturbed, electrostatic potential. The electrostatic potential[11] V satisfies

$$\nabla^2 V = 0, \tag{11.52}$$

Laplace's equation. We select spherical polar coordinates because of the spherical shape of the conductor. (This will simplify the application of the boundary condition at the surface of the conductor.) We can write the unknown potential $V(r, \theta)$ in the region outside the sphere as a linear combination of solutions of the Laplace equation, called harmonic polynomials (check by applying the Laplacian in spherical polar coordinates from Chapter 2):

$$V(r, \theta) = \sum_{n=0}^{\infty} a_n r^n P_n(\cos\theta) + \sum_{n=0}^{\infty} b_n \frac{P_n(\cos\theta)}{r^{n+1}}. \tag{11.53}$$

No φ dependence appears because of the **axial (azimuthal) symmetry** of our problem. (The center of the conducting sphere is taken as the origin and the z-axis is oriented parallel to the original uniform field.)

It might be noted here that n is an integer because only for integral n is the θ dependence well behaved at $\cos\theta = \pm 1$. For nonintegral n, the solutions of Legendre's equation diverge at the ends of the interval $[-1, 1]$, the poles $\theta = 0, \pi$ of the sphere (compare Exercises 5.2.11 and 8.5.5). It is for this same reason that the irregular solution of Legendre's equation is also excluded.

[11] It should be emphasized that this is not a presentation of a Legendre series expansion of a known $V(\cos\theta)$. Here, we deal with a **boundary value** problem of a partial differential equation (see Section 8.9).

Now we turn to our (Dirichlet) boundary conditions to determine the unknown a_n and b_n of our series solution, Eq. (11.53). If the original unperturbed electrostatic field is $E_0 = |\mathbf{E}_0|$, we require, as one boundary condition,

$$V(r \to \infty) = -E_0 z = -E_0 r\cos\theta = -E_0 r P_1(\cos\theta). \tag{11.54}$$

Since our Legendre series is unique, we may equate coefficients of $P_n(\cos\theta)$ in Eq. (11.53) ($r \to \infty$) and Eq. (11.54) to obtain

$$a_n = 0, \quad n > 1 \quad \text{and} \quad n = 0, \qquad a_1 = -E_0. \tag{11.55}$$

If $a_n \neq 0$ for $n > 1$, these terms would dominate at large r and the boundary condition [Eq. (11.54)] could not be satisfied.

As a second boundary condition, we may choose the conducting sphere and the plane $\theta = \pi/2$ to be at zero potential, which means that Eq. (11.53) now becomes

$$V(r = r_0) = \frac{b_0}{r_0} + \left(\frac{b_1}{r_0^2} - E_0 r_0\right) P_1(\cos\theta) + \sum_{n=2}^{\infty} b_n \frac{P_n(\cos\theta)}{r_0^{n+1}} = 0. \tag{11.56}$$

In order that this may hold for all values of θ, each coefficient of $P_n(\cos\theta)$ must vanish.[12] Hence,

$$b_0 = 0,^{13} \qquad b_n = 0, \quad n \geq 2, \tag{11.57}$$

whereas

$$b_1 = E_0 r_0^3. \tag{11.58}$$

The electrostatic potential (outside the sphere) is then

$$V = -E_0 r P_1(\cos\theta) + \frac{E_0 r_0^3}{r^2} P_1(\cos\theta) = -E_0 r P_1(\cos\theta)\left(1 - \frac{r_0^3}{r^3}\right). \tag{11.59}$$

It can be shown that a solution of Laplace's equation that satisfies the boundary conditions over the entire boundary is unique. The electrostatic potential V, as given by Eq. (11.59), is a solution of Laplace's equation. It satisfies our boundary conditions and therefore is the solution of Laplace's equation for this problem.

It may further be shown (Exercise 11.3.13) that there is an induced surface charge density

$$\sigma = -\varepsilon_0 \left.\frac{\partial V}{\partial r}\right|_{r=r_0} = 3\varepsilon_0 E_0 \cos\theta \tag{11.60}$$

[12] Again, this is equivalent to saying that a series expansion in Legendre polynomials (or any complete orthogonal set) is unique.

[13] The coefficient of P_0 is b_0/r_0. We set $b_0 = 0$ since there is no net charge on the sphere. If there is a net charge q, then $b_0 \neq 0$.

on the surface of the sphere and an induced electric dipole moment

$$P = 4\pi r_0^3 \varepsilon_0 E_0. \tag{11.61}$$

■

EXAMPLE 11.3.3

Electrostatic Potential of a Ring of Charge As a further example, consider the electrostatic potential produced by a conducting ring carrying a total electric charge q (Fig. 11.9). From electrostatics (and Section 1.14) the potential ψ satisfies Laplace's equation. Separating variables in spherical polar coordinates, we obtain

$$\psi(r, \theta) = \sum_{n=0}^{\infty} c_n \frac{a^n}{r^{n+1}} P_n(\cos\theta), \quad r > a, \tag{11.62a}$$

where a is the radius of the ring that is assumed to be in the $\theta = \pi/2$ plane. There is no φ (azimuthal) dependence because of the cylindrical symmetry of the system. The terms with positive exponent in the radial dependence have been rejected since the potential must have an asymptotic behavior

$$\psi \sim \frac{q}{4\pi\varepsilon_0} \cdot \frac{1}{r}, \quad r \gg a. \tag{11.62b}$$

The problem is to determine the coefficients c_n in Eq. (11.62a). This may be done by evaluating $\psi(r, \theta)$ at $\theta = 0$, $r = z$, and comparing with an independent

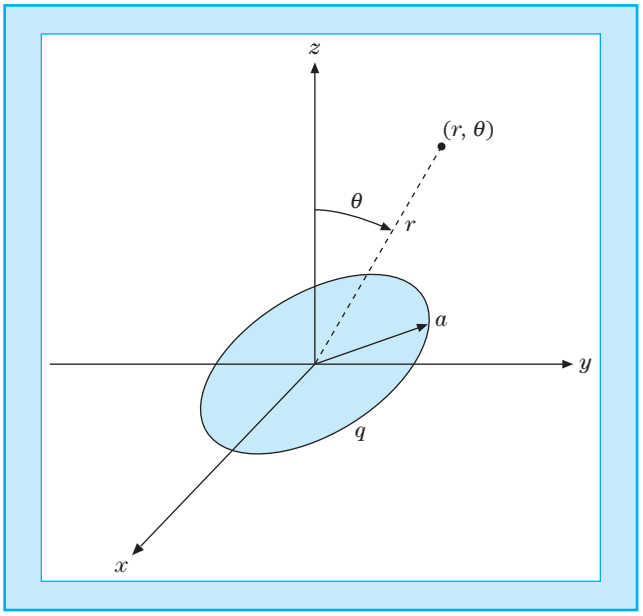


Figure 11.9

Charged, Conducting Ring

calculation of the potential from Coulomb's law. In effect, we are using a boundary condition along the z-axis. From Coulomb's law (with all charge equidistant),

$$\psi(r,\theta) = \frac{q}{4\pi\varepsilon_0}\cdot\frac{1}{(z^2+a^2)^{1/2}}, \qquad \begin{cases}\theta = 0\\ r = z,\end{cases}$$

$$= \frac{q}{4\pi\varepsilon_0 z}\sum_{s=0}^{\infty}(-1)^s\frac{(2s)!}{2^{2s}(s!)^2}\left(\frac{a}{z}\right)^{2s}, \quad z > a. \tag{11.62c}$$

The last step uses the result of Exercise 10.1.15. Now, Eq. (11.62a) evaluated at $\theta = 0$, $r = z$ [with $P_n(1) = 1$], yields

$$\psi(r,\theta) = \sum_{n=0}^{\infty} c_n\frac{a^n}{z^{n+1}}, \quad r = z. \tag{11.62d}$$

Comparing Eqs. (11.62c) and (11.62d), we get $c_n = 0$ for n odd. Setting $n = 2s$, we have

$$c_{2s} = \frac{q}{4\pi\varepsilon_0}(-1)^s\frac{(2s)!}{2^{2s}(s!)^2}, \tag{11.62e}$$

and our electrostatic potential $\psi(r,\theta)$ is given by

$$\psi(r,\theta) = \frac{q}{4\pi\varepsilon_0 r}\sum_{s=0}^{\infty}(-1)^s\frac{(2s)!}{2^{2s}(s!)^2}\left(\frac{a}{r}\right)^{2s}P_{2s}(\cos\theta), \quad r > a. \tag{11.62f}$$

■

EXERCISES

11.3.1 You have constructed a set of orthogonal functions by the Gram–Schmidt process (Section 9.3), taking $u_m(x) = x^n$, $n = 0, 1, 2, \ldots$, in increasing order with $w(x) = 1$ and an interval $-1 \le x \le 1$. Prove that the nth such function constructed is proportional to $P_n(x)$.
Hint. Use mathematical induction.

11.3.2 Expand the Dirac delta function in a series of Legendre polynomials using the interval $-1 \le x \le 1$.

11.3.3 Verify the Dirac delta function expansions

$$\delta(1-x) = \sum_{n=0}^{\infty}\frac{2n+1}{2}P_n(x),$$

$$\delta(1+x) = \sum_{n=0}^{\infty}(-1)^n\frac{2n+1}{2}P_n(x).$$

These expressions appear in a resolution of the Rayleigh plane wave expansion (Exercise 11.4.7) into incoming and outgoing spherical waves.

Note. Assume that the **entire** Dirac delta function is covered when integrating over $[-1, 1]$.

11.3.4 Neutrons (mass 1) are being scattered by a nucleus of mass $A (A > 1)$. In the center of the mass system the scattering is isotropic. Then, in the lab system the average of the cosine of the angle of deflection of the neutron is

$$\langle \cos\psi \rangle = \frac{1}{2}\int_0^\pi \frac{A\cos\theta + 1}{(A^2 + 2A\cos\theta + 1)^{1/2}} \sin\theta \, d\theta.$$

Show, by expansion of the denominator, that $\langle \cos\psi \rangle = 2/3A$.

11.3.5 A particular function $f(x)$ defined over the interval $[-1, 1]$ is expanded in a Legendre series over this same interval. Show that the expansion is unique.

11.3.6 A function $f(x)$ is expanded in a Legendre series $f(x) = \sum_{n=0}^{\infty} a_n P_n(x)$. Show that

$$\int_{-1}^{1} [f(x)]^2 \, dx = \sum_{n=0}^{\infty} \frac{2a_n^2}{2n+1}.$$

This is the Legendre form of the Fourier series Parseval identity (Exercise 14.4.2). It also illustrates Bessel's inequality [Eq. (9.73)] becoming an equality for a complete set.

11.3.7 Derive the recurrence relation

$$(1 - x^2)P_n'(x) = nP_{n-1}(x) - nxP_n(x)$$

from the Legendre polynomial generating function.

11.3.8 Evaluate $\int_0^1 P_n(x)\,dx$.

ANS. $n = 2s$; 1 for $s = 0$, 0 for $s > 0$,
$n = 2s + 1$; $P_{2s}(0)/(2s + 2) = (-1)^s(2s - 1)!!/1(2s + 2)!!$

Hint. Use a recurrence relation to replace $P_n(x)$ by derivatives and then integrate by inspection. Alternatively, you can integrate the generating function.

11.3.9 (a) For

$$f(x) = \begin{cases} +1, & 0 < x < 1 \\ -1, & -1 < x < 0, \end{cases}$$

show that

$$\int_{-1}^{1} [f(x)]^2 \, dx = 2\sum_{n=0}^{\infty} (4n+3)\left[\frac{(2n-1)!!}{(2n+2)!!}\right]^2.$$

(b) By testing the series, prove that the series is convergent.

11.3.10 Prove that

$$\begin{aligned}\int_{-1}^{1} x(1-x^2)P_n'P_m'\,dx &= 0, \quad \text{unless } m = n \pm 1,\\ &= \frac{2n(n^2-1)}{4n^2-1}\delta_{m,n-1}, \qquad \text{if } m < n.\\ &= \frac{2n(n+2)(n+1)}{(2n+1)(2n+3)}\delta_{m,n+1}, \quad \text{if } m > n.\end{aligned}$$

11.3.11 The amplitude of a scattered wave is given by

$$f(\theta) = \frac{1}{k}\sum_{l=0}^{\infty}(2l+1)\exp[i\delta_l]\sin\delta_l P_l(\cos\theta),$$

where θ is the angle of scattering, l is the angular momentum, $\hbar k$ is the incident momentum, and δ_l is the phase shift produced by the central potential that is doing the scattering. The total cross section is $\sigma_{\text{tot}} = \int |f(\theta)|^2 d\Omega$. Show that

$$\sigma_{\text{tot}} = \frac{4\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\sin^2\delta_l.$$

11.3.12 The coincidence counting rate, $W(\theta)$, in a gamma–gamma angular correlation experiment has the form

$$W(\theta) = \sum_{n=0}^{\infty} a_{2n}P_{2n}(\cos\theta).$$

Show that data in the range $\pi/2 \le \theta \le \pi$ can, in principle, define the function $W(\theta)$ (and permit a determination of the coefficients a_{2n}). This means that although data in the range $0 \le \theta < \pi/2$ may be useful as a check, they are not essential.

11.3.13 A conducting sphere of radius r_0 is placed in an initially uniform electric field, $\mathbf{E}_0$. Show the following:

(a) The induced surface charge density is

$$\sigma = 3\varepsilon_0 E_0\cos\theta.$$

(b) The induced electric dipole moment is

$$P = 4\pi r_0^3\varepsilon_0 E_0.$$

The induced electric dipole moment can be calculated either from the surface charge [part (a)] or by noting that the final electric field $\mathbf{E}$ is the result of superimposing a dipole field on the original uniform field.

11.3.14 A charge q is displaced a distance a along the z-axis from the center of a spherical cavity of radius R.

(a) Show that the electric field averaged over the volume $a \le r \le R$ is zero.

(b) Show that the electric field averaged over the volume $0 \le r \le a$ is

$$\mathbf{E} = \hat{\mathbf{z}} E_z = -\hat{\mathbf{z}} \frac{q}{4\pi\varepsilon_0 a^2} \quad \text{(SI units)} = -\hat{\mathbf{z}} \frac{nqa}{3\varepsilon_0},$$

where n is the number of such displaced charges per unit volume. This is a basic calculation in the polarization of a dielectric.
Hint. $\mathbf{E} = -\nabla\varphi$.

11.3.15 Determine the electrostatic potential (Legendre expansion) of a circular ring of electric charge for $r < a$.

11.3.16 Calculate the electric field produced by the charged conducting ring of Exercise 11.3.15 for
(a) $r > a$, (b) $r < a$.

11.3.17 Find the potential $\psi(r, \theta)$ produced by a charged conducting disk (Fig. 11.10) for $r > a$, the radius of the disk. The charge density σ (on each side of the disk) is

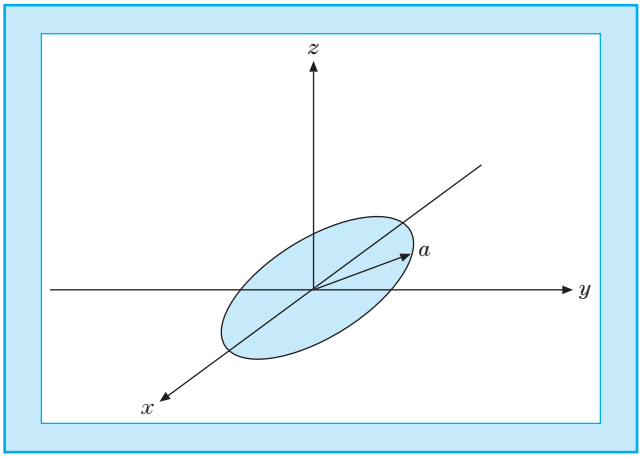
$$\sigma(\rho) = \frac{q}{4\pi a(a^2 - \rho^2)^{1/2}}, \quad \rho^2 = x^2 + y^2.$$

Hint. The definite integral you get can be evaluated as a beta function. For more details, see Section 5.03 of Smythe in Additional Reading.

$$\textit{ANS.} \quad \psi(r, \theta) = \frac{q}{4\pi\varepsilon_0 r} \sum_{l=0}^{\infty} (-1)^l \frac{1}{2l+1} \left(\frac{a}{r}\right)^{2l} P_{2l}(\cos\theta).$$

Figure 11.10

Charged, Conducting Disk



11.3.18 From the result of Exercise 11.3.17 calculate the potential of the disk. Since you are violating the condition $r > a$, justify your calculation carefully.
Hint. You may run into the hypogeometric series given in Exercise 5.2.9.

11.3.19 The hemisphere defined by $r = a$, $0 \le \theta < \pi/2$ has an electrostatic potential $+V_0$. The hemisphere $r = a$, $\pi/2 < \theta \le \pi$ has an electrostatic

potential $-V_0$. Show that the potential at interior points is

$$V = V_0 \sum_{n=0}^{\infty} \frac{4n+3}{2n+2} \left(\frac{r}{a}\right)^{2n+1} P_{2n}(0) P_{2n+1}(\cos\theta)$$

$$= V_0 \sum_{n=0}^{\infty} (-1)^n \frac{(4n+3)(2n-1)!!}{(2n+2)!!} \left(\frac{r}{a}\right)^{2n+1} P_{2n+1}(\cos\theta).$$

Hint. You need Exercise 11.3.8.

11.3.20 A conducting sphere of radius a is divided into two electrically separate hemispheres by a thin insulating barrier at its equator. The top hemisphere is maintained at a potential V_0 and the bottom hemisphere at $-V_0$.

(a) Show that the electrostatic potential **exterior** to the two hemispheres is

$$V(r,\theta) = V_0 \sum_{s=0}^{\infty} (-1)^s (4s+3) \frac{(2s-1)!!}{(2s+2)!!} \left(\frac{a}{r}\right)^{2s+2} P_{2s+1}(\cos\theta).$$

(b) Calculate the electric charge density σ on the outside surface. Note that your series diverges at $\cos\theta = \pm 1$ as you expect from the infinite capacitance of this system (zero thickness for the insulating barrier).

$$ANS. \quad \sigma = \varepsilon_0 E_n = -\varepsilon_0 \left.\frac{\partial V}{\partial r}\right|_{r=a}$$

$$= \varepsilon_0 V_0 \sum_{s=0}^{\infty} (-1)^s (4s+3) \frac{(2s-1)!!}{(2s)!!} P_{2s+1}(\cos\theta).$$

11.3.21 In the notation of Section 9.4 $\langle x|\varphi_s\rangle = \sqrt{(2s+1)/2}\,P_s(x)$, a Legendre polynomial is renormalized to unity. Explain how $|\varphi_s\rangle\langle\varphi_s|$ acts as a projection operator. In particular, show that if $|f\rangle = \sum_n a'_n |\varphi_n\rangle$, then

$$|\varphi_s\rangle\langle\varphi_s|f\rangle = a'_s|\varphi_s\rangle.$$

11.3.22 Expand x^8 as a Legendre series. Determine the Legendre coefficients from Eq. (11.50),

$$a_m = \frac{2m+1}{2} \int_{-1}^{1} x^8 P_m(x)\,dx.$$

Check your values against AMS-55, Table 22.9. This illustrates the expansion of a simple function. Actually, if $f(x)$ is expressed as a power series, the recursion Eq. (11.26) is both faster and more accurate.
Hint. Gaussian quadrature can be used to evaluate the integral.

11.3.23 Expand $\arcsin x$ in Legendre polynomials.

11.3.24 Expand the polynomials $2+5x$, $1+x+x^3$ in a Legendre series and plot your results and the polynomials for the larger interval $-2 \le x \le 2$.

11.4 Alternate Definitions of Legendre Polynomials

Rodrigues's Formula

The series form of the Legendre polynomials [Eq. (11.18)] of Section 11.1 may be transformed as follows. From Eq. (11.18)

$$P_n(x) = \sum_{r=0}^{[n/2]} (-1)^r \frac{(2n-2r)!}{2^n r!(n-2r)!} x^{n-2r}. \tag{11.63}$$

For n an integer

$$\begin{aligned} P_n(x) &= \sum_{r=0}^{[n/2]} (-1)^r \frac{1}{2^n r!(n-r)!} \left(\frac{d}{dx}\right)^n x^{2n-2r} \\ &= \frac{1}{2^n n!} \left(\frac{d}{dx}\right)^n \sum_{r=0}^{n} \frac{(-1)^r n!}{r!(n-r)!} x^{2n-2r}. \end{aligned} \tag{11.64}$$

Note the extension of the upper limit. The reader is asked to show in Exercise 11.4.1 that the additional terms $[n/2]+1$ to n in the summation contribute nothing. However, the effect of these extra terms is to permit the replacement of the new summation by $(x^2-1)^n$ (binomial theorem once again) to obtain

$$P_n(x) = \frac{1}{2^n n!} \left(\frac{d}{dx}\right)^n (x^2-1)^n. \tag{11.65}$$

This is Rodrigues's formula. It is useful in proving many of the properties of the Legendre polynomials, such as orthogonality. A related application is seen in Exercise 11.4.3. The Rodrigues definition can be extended to define the associated Legendre functions.

EXAMPLE 11.4.1 **Lowest Legendre Polynomials** For $n=0$, $P_0=1$ follows right away from Eq. (11.65), as well as $P_1(x) = \frac{2x}{2} = x$. For $n=2$ we obtain

$$P_2(x) = \frac{1}{8}\frac{d^2}{dx^2}(x^4-2x^2+1) = \frac{1}{8}(12x^2-4) = \frac{3}{2}x^2 - \frac{1}{2},$$

and for $n=3$

$$P_3(x) = \frac{1}{48}\frac{d^3}{dx^3}(x^6-3x^4+3x^2-1) = \frac{1}{48}(120x^3-72x) = \frac{5}{2}x^3 - \frac{3}{2}x,$$

in agreement with Table 11.1. ■

EXERCISES

11.4.1 Show that **each** term in the summation

$$\sum_{r=[n/2]+1}^{n} \left(\frac{d}{dx}\right)^n \frac{(-1)^r n!}{r!(n-r)!} x^{2n-2r}$$

vanishes (r and n integral).

11.4.2 Using Rodrigues's formula, show that the $P_n(x)$ are orthogonal and that

$$\int_{-1}^{1} [P_n(x)]^2 \, dx = \frac{2}{2n+1}.$$

Hint. Use Rodrigues's formula and integrate by parts.

11.4.3 Show that $\int_{-1}^{1} x^m P_n(x) dx = 0$ when $m < n$.
Hint. Use Rodrigues's formula or expand x^m in Legendre polynomials.

11.4.4 Show that

$$\int_{-1}^{1} x^n P_n(x) dx = \frac{2^{n+1} n! n!}{(2n+1)!}.$$

Note. You are expected to use Rodrigues's formula and integrate by parts, but also see if you can get the result from Eq. (11.18) by inspection.

11.4.5 Show that

$$\int_{-1}^{1} x^{2r} P_{2n}(x) dx = \frac{2^{2n+1}(2r)!(r+n!)}{(2r+2n+1)!(r-n)!}, \quad r \geq n.$$

11.4.6 As a generalization of Exercises 11.4.4 and 11.4.5, show that the Legendre expansions of x^s are

(a) $$x^{2r} = \sum_{n=0}^{r} \frac{2^{2n}(4n+1)(2r)!(r+n)!}{(2r+2n+1)!(r-n)!} P_{2n}(x), \quad s = 2r,$$

(b) $$x^{2r+1} = \sum_{n=0}^{r} \frac{2^{2n+1}(4n+3)(2r+1)!(r+n+1)!}{(2r+2n+3)!(r-n)!} P_{2n+1}(x),$$

$s = 2r + 1$.

11.4.7 A plane wave may be expanded in a series of spherical waves by the Rayleigh equation

$$e^{ikr\cos\gamma} = \sum_{n=0}^{\infty} a_n j_n(kr) P_n(\cos\gamma).$$

Show that $a_n = i^n(2n+1)$.
Hint.

1. Use the orthogonality of the P_n to solve for $a_n j_n(kr)$.
2. Differentiate n times with respect to (kr) and set $r = 0$ to eliminate the r dependence.
3. Evaluate the remaining integral by Exercise 11.4.4.

Note. This problem may also be treated by noting that both sides of the equation satisfy the Helmholtz equation. The equality can be established by showing that the solutions have the same behavior at the origin and also behave alike at large distances.

11.4.8 Verify the Rayleigh equation of Exercise 11.4.7 by starting with the following steps:

(a) Differentiate with respect to (kr) to establish

$$\sum_n a_n j_n'(kr) P_n(\cos\gamma) = i \sum_n a_n j_n(kr) \cos\gamma\, P_n(\cos\gamma).$$

(b) Use a recurrence relation to replace $\cos\gamma\, P_n(\cos\gamma)$ by a linear combination of P_{n-1} and P_{n+1}.

(c) Use a recurrence relation to replace j_n' by a linear combination of j_{n-1} and j_{n+1}. See Chapter 12 for Bessel functions.

11.4.9 In numerical work (Gauss–Legendre quadrature) it is useful to establish that $P_n(x)$ has n real zeros in the interior of $[-1, 1]$. Show that this is so.

Hint. Rolle's theorem shows that the first derivative of $(x^2 - 1)^{2n}$ has one zero in the interior of $[-1, 1]$. Extend this argument to the second, third, and ultimately to the nth derivative.

11.5 Associated Legendre Functions

When Laplace's equation is separated in spherical polar coordinates (Section 8.9), one of the separated ODEs is the associated Legendre equation

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{dP_n^m(\cos\theta)}{d\theta}\right) + \left[n(n+1) - \frac{m^2}{\sin^2\theta}\right] P_n^m(\cos\theta) = 0. \quad (11.66)$$

With $x = \cos\theta$, this becomes

$$(1-x^2)\frac{d^2}{dx^2}P_n^m(x) - 2x\frac{d}{dx}P_n^m(x) + \left[n(n+1) - \frac{m^2}{1-x^2}\right] P_n^m(x) = 0. \quad (11.67)$$

If the azimuthal separation constant $m^2 = 0$ we have Legendre's equation, Eq. (11.36). The regular solutions (with m not necessarily zero), relabeled $P_n^m(x)$, are

$$P_n^m(x) = (1 - x^2)^{m/2}\frac{d^m}{dx^m}P_n(x). \quad (11.68)$$

These are the associated Legendre functions.[14] Since the highest power of x in $P_n(x)$ is x^n, we must have $m \le n$ (or the m-fold differentiation will drive our function to zero). In quantum mechanics the requirement that $m \le n$ has

[14] One finds (as in AMS-55) the associated Legendre functions defined with an additional factor of $(-1)^m$. This phase $(-1)^m$ seems an unnecessary complication at this point. It will be included in the definition of the spherical harmonics $Y_n^m(\theta, \varphi)$. Note also that **the upper index m is not an exponent**.

the physical interpretation that the expectation value of the square of the z-component of the angular momentum is less than or equal to the expectation value of the square of the angular momentum vector $\mathbf{L}$ (Section 4.3),

$$\langle L_z^2 \rangle \leq \langle L^2 \rangle \equiv \int \psi_{nm}^* \mathbf{L}^2 \psi_{nm} d^3r,$$

where m is the eigenvalue of L_z, and $n(n+1)$ is the eigenvalue of $\mathbf{L}^2$. From the form of Eq. (11.68), we might expect m to be nonnegative. However, if $P_n(x)$ is expressed by Rodrigues's formula, this limitation on m is relaxed and we may have $-n \leq m \leq n$, with negative as well as positive values of m being permitted. Using Leibniz's differentiation formula once again, the reader may show that $P_n^m(x)$ and $P_n^{-m}(x)$ are related by

$$P_n^{-m}(x) = (-1)^m \frac{(n-m)!}{(n+m)!} P_n^m(x). \tag{11.69}$$

From our definition of the associated Legendre functions, $P_n^m(x)$,

$$P_n^0(x) = P_n(x). \tag{11.70}$$

As with the Legendre polynomials, a generating function for the associated Legendre functions is obtained via Eq. (11.67) from that of ordinary Legendre polynomials:

$$\frac{(2m)!(1-x^2)^{m/2}}{2^m m!(1-2tx+t^2)^{m+1/2}} = \sum_{s=0}^{\infty} P_{s+m}^m(x) t^s. \tag{11.71}$$

If we drop the factor $(1-x^2)^{m/2} = \sin^m\theta$ from this formula and define the **polynomials** $\mathcal{P}_{s+m}^m(x) = P_{s+m}^m(x)(1-x^2)^{-m/2}$, then we obtain a practical form of the generating function

$$g_m(x,t) \equiv \frac{(2m)!}{2^m m!(1-2tx+t^2)^{m+1/2}} = \sum_{s=0}^{\infty} \mathcal{P}_{s+m}^m(x) t^s. \tag{11.72}$$

We can derive a recursion relation for associated Legendre polynomials that is analogous to Eqs. (11.23) and (11.26) by differentiation as follows:

$$(1-2tx+t^2)\frac{\partial g_m}{\partial t} = (2m+1)(x-t)g_m(x,t).$$

Substituting the defining expansions for associated Legendre polynomials we get

$$(1-2tx+t^2)\sum_s s\mathcal{P}_{s+m}^m(x)t^{s-1} = (2m+1)\sum_s \left[x\mathcal{P}_{s+m}^m t^s - \mathcal{P}_{s+m}^m t^{s+1}\right].$$

Comparing coefficients of powers of t in these power series, we obtain the recurrence relation

$$(s+1)\mathcal{P}_{s+m+1}^m - (2m+1+2s)x\mathcal{P}_{s+m}^m + (s+2m)\mathcal{P}_{s+m-1}^m = 0. \tag{11.73}$$

For $m=0$ and $s=n$ this relation is Eq. (11.26).

Before we can use this relation we need to initialize it, that is, relate the associated Legendre polynomials with $m = 1$ to ordinary Legendre polynomials. We observe that

$$(1 - 2xt + t^2)g_1(x, t) = (1 - 2xt + t^2)^{-1/2} = \sum_s P_s(x)t^s \tag{11.74}$$

so that upon inserting Eq. (11.72) we get the recursion

$$\mathcal{P}^1_{s+1} - 2x\mathcal{P}^1_s + \mathcal{P}^1_{s-1} = P_s(x). \tag{11.75}$$

More generally, we also have the identity

$$(1 - 2xt + t^2)g_{m+1}(x, t) = (2m + 1)g_m(x, t), \tag{11.76}$$

from which we extract the recursion

$$\mathcal{P}^{m+1}_{s+m+1} - 2x\mathcal{P}^{m+1}_{s+m} + \mathcal{P}^{m+1}_{s+m-1} = (2m + 1)\mathcal{P}^m_{s+m}(x), \tag{11.77}$$

which relates the associated Legendre polynomials with superindex $m + 1$ to those with m. For $m = 0$ we recover the initial recursion Eq. (11.75).

EXAMPLE 11.5.1

Lowest Associated Legendre Polynomials Now we are ready to derive the entries of Table 11.2. For $m = 1$ and $s = 0$ Eq. (11.75) yields $\mathcal{P}^1_1 = 1$ because $\mathcal{P}^1_0 = 0 = \mathcal{P}^1_{-1}$ do not occur in the definition, Eq. (11.72), of the associated Legendre polynomials. Multiplying by $(1-x^2)^{1/2} = \sin\theta$ we get the first line of Table 11.2. For $s = 1$ we find from Eq. (11.75),

$$\mathcal{P}^1_2(x) = P_1 + 2x\mathcal{P}^1_1 = x + 2x = 3x,$$

from which the second line of Table 11.2, $3\cos\theta\sin\theta$, follows upon multiplying by $\sin\theta$. For $s = 2$ we get

$$\mathcal{P}^1_3(x) = P_2 + 2x\mathcal{P}^1_2 - \mathcal{P}^1_1 = \frac{1}{2}(3x^2 - 1) + 6x^2 - 1 = \frac{15}{2}x^2 - \frac{3}{2},$$

Table 11.2

Associated Legendre Functions

$P^1_1(x) = (1 - x^2)^{1/2} = \sin\theta$

$P^1_2(x) = 3x(1 - x^2)^{1/2} = 3\cos\theta\sin\theta$

$P^2_2(x) = 3(1 - x^2) = 3\sin^2\theta$

$P^1_3(x) = \frac{3}{2}(5x^2 - 1)(1 - x^2)^{1/2} = \frac{3}{2}(5\cos^2\theta - 1)\sin\theta$

$P^2_3(x) = 15x(1 - x^2) = 15\cos\theta\sin^2\theta$

$P^3_3(x) = 15(1 - x^2)^{3/2} = 15\sin^3\theta$

$P^1_4(x) = \frac{5}{2}(7x^3 - 3x)(1 - x^2)^{1/2} = \frac{5}{2}(7\cos^3\theta - 3\cos\theta)\sin\theta$

$P^2_4(x) = \frac{15}{2}(7x^2 - 1)(1 - x^2) = \frac{15}{2}(7\cos^2\theta - 1)\sin^2\theta$

$P^3_4(x) = 105x(1 - x^2)^{3/2} = 105\cos\theta\sin^3\theta$

$P^4_4(x) = 105(1 - x^2)^2 = 105\sin^4\theta$

in agreement with line 4 of Table 11.2. To get line 3 we use Eq. (11.76). For $m = 1,\ s = 0$, this gives $\mathcal{P}_2^2(x) = 3\mathcal{P}_1^1(x) = 3$, and multiplying by $1-x^2 = \sin^2\theta$ reproduces line 3 of Table 11.2. For lines 5, 8, and 9, Eq. (11.72) may be used, which we leave as an exercise. ■

EXAMPLE 11.5.2

Special Values For $x = 1$ we use

$$(1 - 2t + t^2)^{-m-1/2} = (1-t)^{-2m-1} = \sum_{s=0}^{\infty} \binom{-2m-1}{s} t^s$$

in Eq. (11.72) and find

$$\mathcal{P}_{s+m}^m(1) = \frac{(2m)!}{2^m m!} \binom{-2m-1}{s}. \tag{11.78}$$

For $m = 1,\ s = 0$ we have $\mathcal{P}_1^1(1) = \binom{-3}{0} = 1$; for $s = 1,\ \mathcal{P}_2^1(1) = -\binom{-3}{1} = 3$; and for $s = 2$, $\mathcal{P}_3^1(1) = \binom{-3}{2} = \frac{(-3)(-4)}{2} = 6 = \frac{3}{2}(5-1)$. These all agree with Table 11.2.

For $x = 0$ we can also use the binomial expansion, which we leave as an exercise. ■

EXAMPLE 11.5.3

Parity From the identity $g_m(-x, -t) = g_m(x, t)$ we obtain the parity relation

$$\mathcal{P}_{s+m}^m(-x) = (-1)^s \mathcal{P}_{s+m}^m(x). \tag{11.79}$$

■

We have the **orthogonality integral**

$$\int_{-1}^{1} P_p^m(x) P_q^m(x)\, dx = \frac{2}{2q+1} \cdot \frac{(q+m)!}{(q-m)!} \delta_{pq} \tag{11.80}$$

or, in spherical polar coordinates,

$$\int_0^{\pi} P_p^m(\cos\theta) P_q^m(\cos\theta) \sin\theta\, d\theta = \frac{2}{2q+1} \cdot \frac{(q+m)!}{(q-m)!} \delta_{pq}. \tag{11.81}$$

The orthogonality of the Legendre polynomials is a special case of this result, obtained by setting m equal to zero; that is, for $m = 0$, Eq. (11.80) reduces to Eqs. (11.47) and (11.48). In both Eqs. (11.80) and (11.81) our Sturm–Liouville theory of Chapter 9 could provide the Kronecker delta. A special calculation is required for the normalization constant.

Spherical Harmonics

The functions $\Phi_m(\varphi) = e^{im\varphi}$ are orthogonal when integrated over the azimuthal angle φ, whereas the functions $P_n^m(\cos\theta)$ are orthogonal upon integrating over the polar angle θ. We take the product of the two and define

$$Y_n^m(\theta, \varphi) \equiv (-1)^m \sqrt{\frac{2n+1}{4\pi} \frac{(n-m)!}{(n+m)!}} P_n^m(\cos\theta) e^{im\varphi} \tag{11.82}$$

Table 11.3

Spherical Harmonics (Condon-Shortley Phase)

$$Y_0^0(\theta,\varphi) = \frac{1}{\sqrt{4\pi}}$$

$$Y_1^1(\theta,\varphi) = -\sqrt{\frac{3}{8\pi}}\sin\theta e^{i\varphi}$$

$$Y_1^0(\theta,\varphi) = \sqrt{\frac{3}{4\pi}}\cos\theta$$

$$Y_1^{-1}(\theta,\varphi) = +\sqrt{\frac{3}{8\pi}}\sin\theta e^{-i\varphi}$$

$$Y_2^2(\theta,\varphi) = \sqrt{\frac{5}{96\pi}}3\sin^2\theta e^{2i\varphi}$$

$$Y_2^1(\theta,\varphi) = -\sqrt{\frac{5}{24\pi}}3\sin\theta\cos\theta e^{i\varphi}$$

$$Y_2^0(\theta,\varphi) = \sqrt{\frac{5}{4\pi}}\left(\frac{3}{2}\cos^2\theta - \frac{1}{2}\right)$$

$$Y_2^{-1}(\theta,\varphi) = +\sqrt{\frac{5}{24\pi}}3\sin\theta\cos\theta e^{-i\varphi}$$

$$Y_2^{-2}(\theta,\varphi) = \sqrt{\frac{5}{96\pi}}3\sin^2\theta e^{-2i\varphi}$$

to obtain functions of two angles (and two indices) that are orthonormal over the spherical surface. These $Y_n^m(\theta,\varphi)$ are spherical harmonics. The complete orthogonality integral becomes

$$\int_{\varphi=0}^{2\pi}\int_{\theta=0}^{\pi} Y_{n_1}^{m_1*}(\theta,\varphi)Y_{n_2}^{m_2}(\theta,\varphi)\sin\theta\, d\theta\, d\varphi = \delta_{n_1n_2}\delta_{m_1m_2} \tag{11.83}$$

and explains the presence of the complicated normalization constant in Eq. (11.82).

The extra $(-1)^m$ included in the defining equation of $Y_n^m(\theta,\varphi)$ with $-n \le m \le n$ deserves some comment. It is clearly legitimate since Eq. (11.68) is linear and homogeneous. It is not necessary, but in moving on to certain quantum mechanical calculations, particularly in the quantum theory of angular momentum, it is most convenient. The factor $(-1)^m$ is a phase factor often called the Condon–Shortley phase after the authors of a classic text on atomic spectroscopy. The effect of this $(-1)^m$ [Eq. (11.82)] and the $(-1)^m$ of Eq. (11.69) for $P_n^{-m}(\cos\theta)$ is to introduce an alternation of sign among the positive m spherical harmonics. This is shown in Table 11.3.

The functions $Y_n^m(\theta,\varphi)$ acquired the name spherical harmonics because they are defined over the surface of a sphere with θ the polar angle and φ the azimuth. The "harmonic" was included because solutions of Laplace's equation were called harmonic functions and $Y_n^m(\cos,\varphi)$ is the angular part of such a solution.

EXAMPLE 11.5.4

Lowest Spherical Harmonics For $n = 0$ we have $m = 0$ and $Y_0^0 = \frac{1}{\sqrt{4\pi}}$ from Eq. (11.82). For $n = 1$ we have $m = \pm1, 0$ and $Y_1^0 = \sqrt{\frac{3}{4\pi}}\cos\theta$, whereas for $m = \pm1$ we see from Table 11.2 that $\cos\theta$ is replaced by $\sin\theta$ and we have the additional factor $(\mp1)\frac{e^{\pm i\varphi}}{\sqrt{2}}$, which checks with Table 11.3. ■

In the framework of quantum mechanics Eq. (11.67) becomes an orbital angular momentum equation and the solution $Y_L^M(\theta, \varphi)$ (n replaced by L and m by M) is an angular momentum eigenfunction, with L being the angular momentum quantum number and M the z-axis projection of L. These relationships are developed in more detail in Section 4.3.

EXAMPLE 11.5.5

Spherical Symmetry of Probability Density of Atomic States What is the angular dependence of the probability density of the degenerate atomic states with principal quantum number $n = 2$?

Here we have to sum the absolute square of the wave functions for $n = 2$ and orbital angular momentum $l = 0,\ m = 0;\ l = 1,\ m = -1, 0, +1$; that is, s and three p states. We ignore the radial dependence. The s state has orbital angular momentum $l = 0$ and $m = 0$ and is independent of angles. For the p states with $l = 1$ and $m = \pm 1, 0$

$$\psi_{200} \sim Y_0^0 = \frac{1}{\sqrt{4\pi}}, \qquad \psi_{21m} \sim Y_1^m,$$

we have to evaluate the sum

$$\sum_{m=-1}^{1} |Y_1^m|^2 = \frac{3}{4\pi}\left[2\left(\frac{1}{\sqrt{2}}\sin\theta\right)^2 + \cos^2\theta\right] = 1$$

upon substituting the spherical harmonics from Table 11.3. This result is spherically symmetric, as is the density for the s state alone or the sum of the three p states. These results can be generalized to higher orbital angular momentum l. ■

SUMMARY

Legendre polynomials are naturally defined by their generating function in a multipole expansion of the Coulomb potential. They appear in physical systems with azimuthal symmetry. They also arise in the separation of partial differential equations with spherical or cylindrical symmetry or as orthogonal eigenfunctions of the Sturm–Liouville theory of their second-order differential equation. Associated Legendre polynomials appear as ingredients of the spherical harmonics in situations that lack in azimuthal symmetry.

EXERCISES

11.5.1 Show that the parity of $Y_L^M(\theta, \varphi)$ is $(-1)^L$. Note the disappearance of any M dependence.
Hint. For the parity operation in spherical polar coordinates, see Section 2.5 and Section 11.2.

11.5.2 Prove that

$$Y_L^M(0, \varphi) = \left(\frac{2L+1}{4\pi}\right)^{1/2} \delta_{M0}.$$

11.5.3 In the theory of Coulomb excitation of nuclei we encounter $Y_L^M(\pi/2, 0)$. Show that

$$Y_L^M\left(\frac{\pi}{2}, 0\right) = \left(\frac{2L+1}{4\pi}\right)^{1/2} \frac{[(L-M)!(L+M)!]^{1/2}}{(L-M)!!(L+M)!!}(-1)^{(L+M)/2}$$
$$\text{for } L+M \text{ even},$$
$$= 0 \quad \text{for } L+M \text{ odd}.$$

Here,

$$(2n)!! = 2n(2n-2)\cdots 6\cdot 4\cdot 2,$$
$$(2n+1)!! = (2n+1)(2n-1)\cdots 5\cdot 3\cdot 1.$$

11.5.4 (a) Express the elements of the quadrupole moment tensor $x_i x_j$ as a linear combination of the spherical harmonics Y_2^m (and Y_0^0).
Note. The tensor $x_i x_j$ is reducible. The Y_0^0 indicates the presence of a scalar component.

(b) The quadrupole moment tensor is usually defined as

$$Q_{ij} = \int (3x_i x_j - r^2\delta_{ij})\rho(\mathbf{r})\, d\tau,$$

with $\rho(\mathbf{r})$ the charge density. Express the components of $(3x_i x_j - r^2\delta_{ij})$ in terms of $r^2 Y_2^M$.

(c) What is the significance of the $-r^2\delta_{ij}$ term?
Hint. Contract the indices i, j.

11.5.5 The orthogonal azimuthal functions yield a useful representation of the Dirac delta function. Show that

$$\delta(\varphi_1 - \varphi_2) = \frac{1}{2\pi}\sum_{m=-\infty}^{\infty} \exp[im(\varphi_1 - \varphi_2)].$$

11.5.6 Derive the spherical harmonic closure relation

$$\sum_{l=0}^{\infty}\sum_{m=-l}^{+l} Y_l^m(\theta_1, \varphi_1)Y_l^{m*}(\theta_2, \varphi_2) = \frac{1}{\sin\theta_1}\delta(\theta_1 - \theta_2)\delta(\varphi_1 - \varphi_2)$$
$$= \delta(\cos\theta_1 - \cos\theta_2)\delta(\varphi_1 - \varphi_2).$$

11.5.7 The quantum mechanical angular momentum operators $L_x \pm iL_y$ are given by

$$L_x + iL_y = e^{i\varphi}\left(\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\varphi}\right),$$
$$L_x - iL_y = -e^{-i\varphi}\left(\frac{\partial}{\partial\theta} - i\cot\theta\frac{\partial}{\partial\varphi}\right).$$

Show that

(a) $(L_x + iL_y)Y_L^M(\theta, \varphi), = \sqrt{(L-M)(L+M+1)}\,Y_L^{M+1}(\theta, \varphi)$,

(b) $(L_x - iL_y)Y_L^M(\theta, \varphi), = \sqrt{(L-M)(L-M+1)}\,Y_L^{M-1}(\theta, \varphi)$.

11.5.8 With $L_\pm$ given by

$$L_\pm = L_x \pm iL_y = \pm e^{\pm i\varphi}\left[\frac{\partial}{\partial\theta} \pm i\cot\theta\frac{\partial}{\partial\varphi}\right],$$

show that

(a) $Y_l^m = \sqrt{\dfrac{(l+m)!}{(2l)!(l-m)!}}(L_-)^{l-m}Y_l^l$,

(b) $Y_l^m = \sqrt{\dfrac{(l-m)!}{(2l)!(l+m)!}}(L_+)^{l+m}Y_l^{-l}$.

11.5.9 In some circumstances it is desirable to replace the imaginary exponential of our spherical harmonic by sine or cosine. Morse and Feshbach define

$$Y_{mn}^e = P_n^m(\cos\theta)\cos m\varphi,$$
$$Y_{mn}^o = P_n^m(\cos\theta)\sin m\varphi,$$

where

$$\int_0^{2\pi}\int_0^{\pi}[Y_{mn}^{e \text{ or } o}(\theta,\varphi)]^2\sin\theta\, d\theta\, d\varphi = \frac{4\pi}{2(2n+1)}\frac{(n+m)!}{(n-m)!}, \quad n = 1, 2, \ldots$$
$$= 4\pi \quad \text{for} \quad n = 0 \ (Y_{00}^o \text{ is undefined}).$$

These spherical harmonics are often named according to the patterns of their positive and negative regions on the surface of a sphere zonal harmonics for $m = 0$, sectoral harmonics for $m = n$, and tesseral harmonics for $0 < m < n$. For Y_{mn}^e, $n = 4$, $m = 0, 2, 4$, indicate on a diagram of a hemisphere (one diagram for each spherical harmonic) the regions in which the spherical harmonic is positive.

11.5.10 A function $f(r, \theta, \varphi)$ may be expressed as a Laplace series

$$f(r,\theta,\varphi) = \sum_{l,m} a_{lm}r^l Y_l^m(\theta,\varphi).$$

With $\langle\rangle_{\text{sphere}}$ used to mean the average over a sphere (centered on the origin), show that

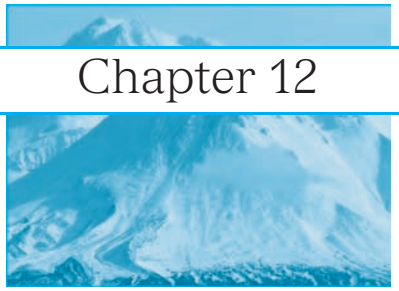
$$\langle f(r,\theta,\varphi)\rangle_{\text{sphere}} = f(0,0,0).$$

Additional Reading

Hobson, E. W. (1955). *The Theory of Spherical and Ellipsoidal Harmonics*. Chelsea, New York. This is a very complete reference, which is the classic text on Legendre polynomials and all related functions.

Smythe, W. R. (1989). *Static and Dynamic Electricity*, 3rd ed. McGraw-Hill, New York.

See also the references listed in Section 4.4 and at the end of Chapter 13.



Chapter 12

Bessel Functions

12.1 Bessel Functions of the First Kind, $J_\nu(x)$

Bessel functions appear in a wide variety of physical problems. When one analyzes the sound vibrations of a drum, the partial differential wave equation (PDE) is solved in cylindrical coordinates. By separating the radial and angular variables, $R(r)e^{in\varphi}$, one is led to the Bessel ordinary differential equation (ODE) for $R(r)$ involving the integer n as a parameter (see Example 12.1.4). The Wentzel-Kramers-Brioullin (WKB) approximation in quantum mechanics involves Bessel functions. A spherically symmetric square well potential in quantum mechanics is solved by spherical Bessel functions. Also, the extraction of phase shifts from atomic and nuclear scattering data requires spherical Bessel functions. In Sections 8.5 and 8.6 series solutions to Bessel's equation were developed. In Section 8.9 we have seen that the Laplace equation in cylindrical coordinates also leads to a form of Bessel's equation. Bessel functions also appear in integral form—integral representations. This may result from integral transforms (Chapter 15).

Bessel functions and closely related functions form a rich area of mathematical analysis with many representations, many interesting and useful properties, and many interrelations. Some of the major interrelations are developed in Section 12.1 and in succeeding sections. Note that Bessel functions are not restricted to Chapter 12. The asymptotic forms are developed in Section 7.3 as well as in Section 12.3, and the series solutions are discussed in Sections 8.5 and 8.6.

Biographical Data

Bessel, Friedrich Wilhelm. Bessel, a German astronomer, was born in Minden, Prussia, in 1784 and died in Königsberg, Prussia (now Russia) in 1846. At the age of 20, he recalculated the orbit of Halley's comet, impressing the well-known astronomer Olbers sufficiently to support him in 1806 for a post at an observatory. There he developed the functions named after him in refinements of astronomical calculations. The first parallax measurement of a star, 61 Cygni about 6 light-years away from Earth, due to him in 1838, proved definitively that Earth was moving in accord with Copernican theory. His calculations of irregularities in the orbit of Uranus paved the way for the later discovery of Neptune by Leverrier and J. C. Adams, a triumph of Newton's theory of gravity.

Generating Function for Integral Order

Although Bessel functions $J_\nu(x)$ are of interest primarily as solutions of Bessel's differential equation, Eq. (8.62),

$$x^2\frac{d^2J_\nu}{dx^2}+x\frac{dJ_\nu}{dx}+(x^2-\nu^2)J_\nu=0,$$

it is instructive and convenient to develop them from a generating function, just as for Legendre polynomials in Chapter 11.[1] This approach has the advantages of finding recurrence relations, special values, and normalization integrals and focusing on the functions themselves rather than on the differential equation they satisfy. Since there is no physical application that provides the generating function in closed form, such as the electrostatic potential for Legendre polynomials in Chapter 11, we have to find it from a suitable differential equation.

We therefore start by deriving from Bessel's series [Eq. (8.70)] for integer index $\nu=n$,

$$J_n(x)=\sum_{s=0}^{\infty}\frac{(-1)^s}{s!(s+n)!}\left(\frac{x}{2}\right)^{2s+n},$$

that converges absolutely for all x, the recursion relation

$$\frac{d}{dx}(x^{-n}J_n(x))=-x^{-n}J_{n+1}(x). \tag{12.1}$$

This can also be written as

$$\frac{n}{x}J_n(x)-J_{n+1}(x)=J_n'(x). \tag{12.2}$$

To show this, we replace the summation index $s\to s-1$ in the Bessel function series [Eq. (8.70)] for $J_{n+1}(x)$,

$$J_{n+1}(x)=\sum_{s=0}^{\infty}\frac{(-1)^s}{s!(s+n+1)!}\left(\frac{x}{2}\right)^{2s+n+1}, \tag{12.3}$$

[1] Generating functions were also used in Chapter 5. In Section 5.6, the generating function $(1+x)^n$ defines the binomial coefficients; $x/(e^x-1)$ generates the Bernoulli numbers in the same sense.

in order to change the denominator $(s+n+1)!$ to $(s+n)!$. Thus, we obtain the series

$$J_{n+1}(x) = -\frac{1}{x}\sum_{s=0}^{\infty}\frac{(-1)^s 2s}{s!(s+n)!}\left(\frac{x}{2}\right)^{n+2s}, \tag{12.4}$$

which is almost the series for $J_n(x)$, except for the factor s. If we divide by x^n and differentiate, this factor s is produced so that we get from Eq. (12.4)

$$x^{-n}J_{n+1}(x) = -\frac{d}{dx}\sum_{n}\frac{(-1)^s}{s!(s+n)!}\left(\frac{x}{2}\right)^{2s}2^{-n} = -\frac{d}{dx}[x^{-n}J_n(x)], \tag{12.5}$$

that is, Eq. (12.1).

A similar argument for J_{n-1}, with summation index s replaced first by $s-n$ and then by $s \to s+1$, yields

$$\frac{d}{dx}(x^n J_n(x)) = x^n J_{n-1}(x), \tag{12.6}$$

which can be written as

$$J_{n-1}(x) - \frac{n}{x}J_n(x) = J_n'(x). \tag{12.7}$$

Eliminating J_n' from Eqs. (12.2) and (12.7), we obtain the recurrence

$$J_{n-1}(x) + J_{n+1}(x) = \frac{2n}{x}J_n(x), \tag{12.8}$$

which we substitute into the **generating series**

$$g(x,t) = \sum_{n=-\infty}^{\infty} J_n(x)t^n. \tag{12.9}$$

This gives the ODE in t (with x a parameter)

$$\sum_{n=-\infty}^{\infty} t^n\,(J_{n-1}(x) + J_{n+1}(x)) = \left(t + \frac{1}{t}\right)g(x,t) = \frac{2t}{x}\frac{\partial g}{\partial t}. \tag{12.10}$$

Writing it as

$$\frac{1}{g}\frac{\partial g}{\partial t} = \frac{x}{2}\left(1 + \frac{1}{t^2}\right), \tag{12.11}$$

and integrating we get

$$\ln g = \frac{x}{2}\left(t - \frac{1}{t}\right) + \ln c,$$

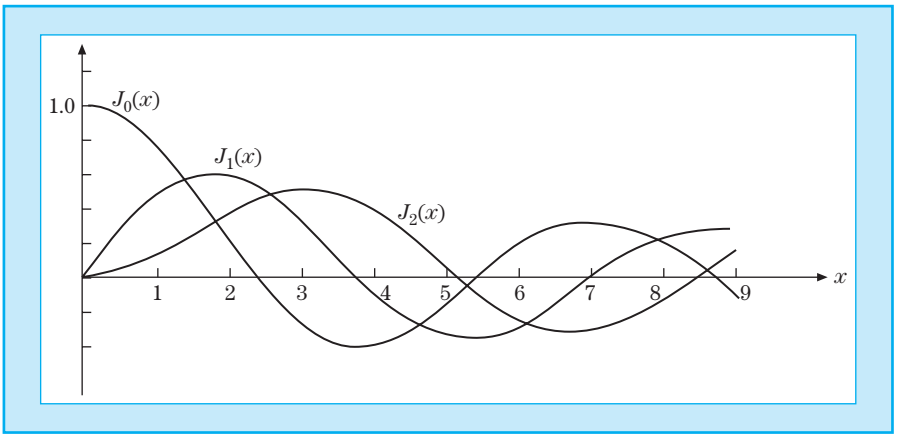
which, when exponentiated, leads to

$$g(x,t) = e^{(x/2)(t-1/t)}c(x), \tag{12.12}$$

where c is the integration constant that may depend on the parameter x. Now taking $x = 0$ and using $J_n(0) = \delta_{n0}$ (from Example 12.1.1) in Eq. (12.9) gives $g(0,t) = 1$ and $c(0) = 1$. To determine $c(x)$ for **all** x, we expand the

Figure 12.1

Bessel Functions, $J_0(x)$, $J_1(x)$, and $J_2(x)$



exponential in Eq. (12.12). The $1/t$ term leads to a Laurent series (see Section 6.5). Incidentally, we understand why the summation in Eq. (12.9) has to run over negative integers as well. So we have a product of Maclaurin series in $xt/2$ and $-x/2t$,

$$e^{xt/2} \cdot e^{-x/2t} = \sum_{r=0}^{\infty} \left(\frac{x}{2}\right)^r \frac{t^r}{r!} \sum_{s=0}^{\infty} (-1)^s \left(\frac{x}{2}\right)^s \frac{t^{-s}}{s!}. \tag{12.13}$$

For a given s we get $t^n (n \geq 0)$ from $r = n + s$

$$\left(\frac{x}{2}\right)^{n+s} \frac{t^{n+s}}{(n+s)!} (-1)^s \left(\frac{x}{2}\right)^s \frac{t^{-s}}{s!}. \tag{12.14}$$

The coefficient of t^n is then[2]

$$J_n(x) = \sum_{s=0}^{\infty} \frac{(-1)^s}{s!(n+s)!} \left(\frac{x}{2}\right)^{n+2s} = \frac{x^n}{2^n n!} - \frac{x^{n+2}}{2^{n+2}(n+1)!} + \cdots \tag{12.15}$$

so that $c(x) \equiv 1$ for all x in Eq. (12.12) by comparing the coefficient of t^0, $J_0(x)$, with Eq. (12.3) for $n = -1$. Thus, the generating function is

$$g(x, t) = e^{(x/2)(t-1/t)} = \sum_{n=-\infty}^{\infty} J_n(x) t^n. \tag{12.16}$$

This series form, Eq. (12.15), exhibits the behavior of the Bessel function $J_n(x)$ for all x, converging everywhere, and permits numerical evaluation of $J_n(x)$. The results for J_0, J_1, and J_2 are shown in Fig. 12.1. From Section 5.3, the error in using only a finite number of terms in numerical evaluation is less than the first term omitted. For instance, if we want $J_n(x)$ to $\pm 1\%$ accuracy, the first term alone of Eq. (12.15) will suffice, provided the ratio of the second term to the first is less than 1% (in magnitude) or $x < 0.2(n+1)^{1/2}$. The Bessel

[2]From the steps leading to this series and from its absolute convergence properties it should be clear that this series converges absolutely, with x replaced by z and with z any point in the finite complex plane.

functions oscillate but are **not periodic**; however, in the limit as $x \to \infty$ the zeros become equidistant (Section 12.3). The amplitude of $J_n(x)$ is not constant but decreases asymptotically as $x^{-1/2}$. [See Eq. (12.106) for this envelope.]

Equation (12.15) actually holds for $n < 0$, also giving

$$J_{-n}(x) = \sum_{s=0}^{\infty} \frac{(-1)^s}{s!(s-n)!}\left(\frac{x}{2}\right)^{2s-n}, \tag{12.17}$$

which amounts to replacing n by $-n$ in Eq. (12.15). Since n is an integer (here), $(s-n)! \to \infty$ for $s = 0, \ldots, (n-1)$. Hence, the series may be considered to start with $s = n$. Replacing s by $s+n$, we obtain

$$J_{-n}(x) = \sum_{s=0}^{\infty} \frac{(-1)^{s+n}}{s!(s+n)!}\left(\frac{x}{2}\right)^{n+2s},$$

showing that $J_n(x)$ and $J_{-n}(x)$ are not independent but are related by

$$J_{-n}(x) = (-1)^n J_n(x) \qquad \text{(integral } n\text{)}. \tag{12.18}$$

These series expressions [Eqs. (12.15) and (12.17)] may be used with n replaced by ν to **define** $J_\nu(x)$ and $J_{-\nu}(x)$ for nonintegral ν (compare Exercise 12.1.11).

EXAMPLE 12.1.1 **Special Values** Setting $x = 0$ in Eq. (12.12), using the series [Eq. (12.9)] yields

$$1 = \sum_{n=-\infty}^{\infty} J_n(0)t^n,$$

from which we infer (uniqueness of Laurent expansion)

$$J_0(0) = 1, \qquad J_n(0) = 0 = J_{-n}(0), \quad n \geq 1.$$

From $t = 1$ we find the identity

$$1 = \sum_{n=-\infty}^{\infty} J_n(x) = J_0(x) + 2\sum_{n=1}^{\infty} J_n(x)$$

using the symmetry relation [Eq. (12.18)].

Finally, the identity $g(-x, t) = g(x, -t)$ implies

$$\sum_{n=-\infty}^{\infty} J_n(-x)t^n = \sum_{n=-\infty}^{\infty} J_n(x)(-t)^n,$$

and again the parity relations $J_n(-x) = (-1)^n J_n(x)$. These results can also be extracted from the identity $g(-x, 1/t) = g(x, t)$. ■

Applications of Recurrence Relations

We have already derived the basic recurrence relations Eqs. (12.1), (12.2), (12.6), and (12.7) that led us to the generating function. Many more can be derived as follows.

EXAMPLE 12.1.2 **Addition Theorem** The linearity of the generating function in the exponent x suggests the identity

$$g(u+v,\,t) = e^{(u+v)/2(t-1/t)} = e^{(u/2)(t-1/t)}e^{(v/2)(t-1/t)} = g(u,\,t)g(v,\,t),$$

which implies the Bessel expansions

$$\sum_{n=-\infty}^{\infty} J_n(u+v)t^n = \sum_{l=-\infty}^{\infty} J_l(u)t^l \cdot \sum_{k=-\infty}^{\infty} J_k(v)t^k = \sum_{k,l=-\infty}^{\infty} J_l(u)J_k(v)t^{l+k}$$

$$= \sum_{m=-\infty}^{\infty} t^m \sum_{l=-\infty}^{\infty} J_l(u)J_{m-l}(v)$$

denoting $m = k + l$. Comparing coefficients yields the **addition theorem**

$$J_m(u+v) = \sum_{l=-\infty}^{\infty} J_l(u)J_{m-l}(v). \tag{12.19}$$

■

Differentiating Eq. (12.16) partially with respect to x, we have

$$\frac{\partial}{\partial x}g(x,\,t) = \frac{1}{2}\left(t - \frac{1}{t}\right)e^{(x/2)(t-1/t)} = \sum_{n=-\infty}^{\infty} J_n'(x)t^n. \tag{12.20}$$

Again, substituting in Eq. (12.16) and equating the coefficients of like powers of t, we obtain

$$J_{n-1}(x) - J_{n+1}(x) = 2J_n'(x), \tag{12.21}$$

which can also be obtained by adding Eqs. (12.2) and (12.7). As a special case of this recurrence relation,

$$J_0'(x) = -J_1(x). \tag{12.22}$$

Bessel's Differential Equation

Suppose we consider a set of functions $Z_\nu(x)$ that satisfies the basic recurrence relations [Eqs. (12.8) and (12.21)], but with ν not necessarily an integer and Z_ν not necessarily given by the series [Eq. (12.15)]. Equation (12.7) may be rewritten ($n \to \nu$) as

$$xZ_\nu'(x) = xZ_{\nu-1}(x) - \nu Z_\nu(x). \tag{12.23}$$

On differentiating with respect to x, we have

$$xZ_\nu''(x) + (\nu+1)Z_\nu' - xZ_{\nu-1}' - Z_{\nu-1} = 0. \tag{12.24}$$

Multiplying by x and then subtracting Eq. (12.23) multiplied by ν gives us

$$x^2Z_\nu'' + xZ_\nu' - \nu^2Z_\nu + (\nu-1)xZ_{\nu-1} - x^2Z_{\nu-1}' = 0. \tag{12.25}$$

Now we rewrite Eq. (12.2) and replace n by $\nu - 1$:

$$xZ'_{\nu-1} = (\nu - 1)Z_{\nu-1} - xZ_\nu. \tag{12.26}$$

Using Eq. (12.26) to eliminate $Z_{\nu-1}$ and $Z'_{\nu-1}$ from Eq. (12.25), we finally get

$$x^2 Z''_\nu + xZ'_\nu + (x^2 - \nu^2)Z_\nu = 0. \tag{12.27}$$

This is **Bessel's ODE.** Hence, any functions, $Z_\nu(x)$, that satisfy the recurrence relations [Eqs. (12.2) and (12.7), (12.8) and (12.21), or (12.1) and (12.6)] satisfy Bessel's equation; that is, the unknown Z_ν are Bessel functions. In particular, we have shown that the functions $J_n(x)$, defined by our generating function, satisfy Bessel's ODE. Under the parity transformation, $x \to -x$, Bessel's ODE stays invariant, thereby relating $Z_\nu(-x)$ to $Z_\nu(x)$, up to a phase factor. If the argument is $k\rho$ rather than x, which is the case in many physics problems, then Eq. (12.27) becomes

$$\rho^2 \frac{d^2}{d\rho^2} Z_\nu(k\rho) + \rho \frac{d}{d\rho} Z_\nu(k\rho) + (k^2\rho^2 - \nu^2)Z_\nu(k\rho) = 0. \tag{12.28}$$

Integral Representations

A particularly useful and powerful way of treating Bessel functions employs integral representations. If we return to the generating function [Eq. (12.16)] and substitute $t = e^{i\theta}$, we get

$$\begin{aligned} e^{ix\sin\theta} &= J_0(x) + 2[J_2(x)\cos 2\theta + J_4(x)\cos 4\theta + \cdots] \\ &\quad + 2i[J_1(x)\sin\theta + J_3(x)\sin 3\theta + \cdots], \end{aligned} \tag{12.29}$$

in which we have used the relations

$$\begin{aligned} J_1(x)e^{i\theta} + J_{-1}(x)e^{-i\theta} &= J_1(x)(e^{i\theta} - e^{-i\theta}) \\ &= 2iJ_1(x)\sin\theta, \\ J_2(x)e^{2i\theta} + J_{-2}(x)e^{-2i\theta} &= 2J_2(x)\cos 2\theta, \end{aligned} \tag{12.30}$$

and so on. In summation notation, equating real and imaginary parts of Eq. (12.29), we have

$$\begin{aligned} \cos(x\sin\theta) &= J_0(x) + 2\sum_{n=1}^{\infty} J_{2n}(x)\cos(2n\theta), \\ \sin(x\sin\theta) &= 2\sum_{n=1}^{\infty} J_{2n-1}(x)\sin[(2n-1)\theta]. \end{aligned} \tag{12.31}$$

It might be noted that angle θ (in radians) has no dimensions, just as x. Likewise, $\sin\theta$ has no dimensions and the function $\cos(x\sin\theta)$ is perfectly proper from a dimensional standpoint.

If n and m are **positive** integers (zero is excluded),[3] we recall the orthogonality properties of cosine and sine:[4]

$$\int_0^\pi \cos n\theta \cos m\theta \, d\theta = \frac{\pi}{2}\delta_{nm}, \tag{12.32}$$

$$\int_0^\pi \sin n\theta \sin m\theta \, d\theta = \frac{\pi}{2}\delta_{nm}. \tag{12.33}$$

Multiplying Eq. (12.31) by $\cos n\theta$ and $\sin n\theta$, respectively, and integrating we obtain

$$\frac{1}{\pi}\int_0^\pi \cos(x\sin\theta)\cos n\theta \, d\theta = \begin{cases} J_n(x) & n \text{ even}, \\ 0, & n \text{ odd}, \end{cases} \tag{12.34}$$

$$\frac{1}{\pi}\int_0^\pi \sin(x\sin\theta)\sin n\theta \, d\theta = \begin{cases} 0, & n \text{ even}, \\ J_n(x), & n \text{ odd}, \end{cases} \tag{12.35}$$

upon employing the orthogonality relations Eqs. (12.32) and (12.33). If Eqs. (12.34) and (12.35) are added together, we obtain

$$\begin{aligned} J_n(x) &= \frac{1}{\pi}\int_0^\pi [\cos(x\sin\theta)\cos n\theta + \sin(x\sin\theta)\sin n\theta]d\theta \\ &= \frac{1}{\pi}\int_0^\pi \cos(n\theta - x\sin\theta)d\theta, \quad n = 0, 1, 2, 3, \ldots. \end{aligned} \tag{12.36}$$

As a special case,

$$J_0(x) = \frac{1}{\pi}\int_0^\pi \cos(x\sin\theta)d\theta. \tag{12.37}$$

Noting that $\cos(x\sin\theta)$ repeats itself in all four quadrants ($\theta_1 = \theta, \theta_2 = \pi - \theta, \theta_3 = \pi + \theta, \theta_4 = -\theta$), $\cos(x\sin\theta_2) = \cos(x\sin\theta)$, etc., we may write Eq. (12.37) as

$$J_0(x) = \frac{1}{2\pi}\int_0^{2\pi} \cos(x\sin\theta)d\theta. \tag{12.38}$$

On the other hand, $\sin(x\sin\theta)$ reverses its sign in the third and fourth quadrants so that

$$\frac{1}{2\pi}\int_0^{2\pi} \sin(x\sin\theta)d\theta = 0. \tag{12.39}$$

Adding Eq. (12.38) and i times Eq. (12.39), we obtain the complex exponential representation

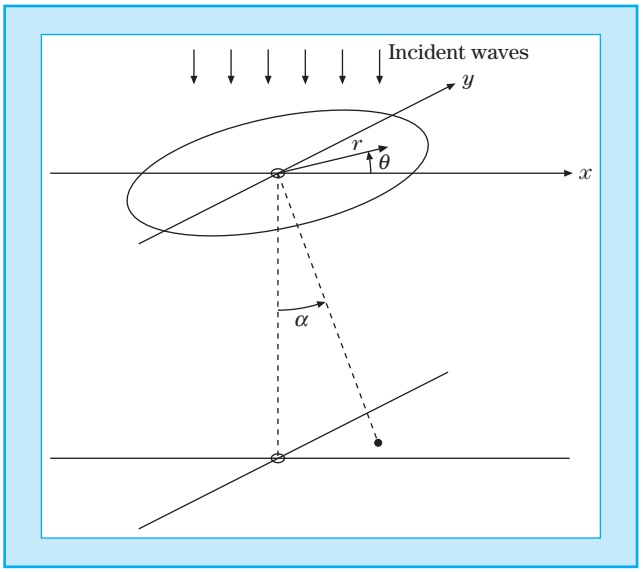
$$J_0(x) = \frac{1}{2\pi}\int_0^{2\pi} e^{ix\sin\theta}d\theta = \frac{1}{2\pi}\int_0^{2\pi} e^{ix\cos\theta}d\theta. \tag{12.40}$$

[3]Equations (12.32) and (12.33) hold for either m or $n = 0$. If both m and $n = 0$, the constant in Eq. (12.32) becomes π; the constant in Eq. (12.33) becomes 0.

[4]They are eigenfunctions of a self-adjoint equation (oscillator ODE of classical mechanics) and satisfy appropriate boundary conditions (compare Section 9.2).

Figure 12.2

Fraunhofer Diffraction-Circular Aperture



This integral representation [Eq. (12.40)] may be obtained more directly by employing contour integration.[5] Many other integral representations exist.

EXAMPLE 12.1.3

Fraunhofer Diffraction, Circular Aperture In the theory of diffraction through a circular aperture we encounter the integral

$$\Phi \sim \int_0^a \int_0^{2\pi} e^{ibr\cos\theta}\, d\theta r\, dr \tag{12.41}$$

for Φ, the amplitude of the diffracted wave. Here, the parameter b is defined as

$$b = \frac{2\pi}{\lambda}\sin\alpha, \tag{12.42}$$

where λ is the wavelength of the incident wave, α is the angle defined by a point on a screen below the circular aperture relative to the normal through the center point,[6] and θ is an azimuth angle in the plane of the circular aperture of radius a. The other symbols are defined in Fig. 12.2. From Eq. (12.40) we get

$$\Phi \sim 2\pi \int_0^a J_0(br) r\, dr. \tag{12.43}$$

[5] For $n = 0$ a simple integration over θ from 0 to 2π will convert Eq. (12.29) into Eq. (12.40).

[6] The exponent $ibr\cos\theta$ gives the phase of the wave on the distant screen at angle α relative to the phase of the wave incident on the aperture at the point (r, θ). The imaginary exponential form of this integrand means that the integral is technically a Fourier transform (Chapter 15). In general, the Fraunhofer diffraction pattern is given by the Fourier transform of the aperture.

Table 12.1

Zeros of the Bessel Functions and Their First Derivatives

Number of Zeros	$J_0(x)$	$J_1(x)$	$J_2(x)$	$J_3(x)$	$J_4(x)$	$J_5(x)$
1	2.4048	3.8317	5.1356	6.3802	7.5883	8.7715
2	5.5201	7.0156	8.4172	9.7610	11.0647	12.3386
3	8.6537	10.1735	11.6198	13.0152	14.3725	15.7002
4	11.7915	13.3237	14.7960	16.2235	17.6160	18.9801
5	14.9309	16.4706	17.9598	19.4094	20.8269	22.2178
	$J_0'(x)$[a]	$J_1'(x)$	$J_2'(x)$	$J_3'(x)$		
1	3.8317	1.8412	3.0542	4.2012		
2	7.0156	5.3314	6.7061	8.0152		
3	10.1735	8.5363	9.9695	11.3459		

[a] $J_0'(x) = -J_1(x)$.

Equation (12.6) enables us to integrate Eq. (12.43) immediately to obtain

$$\Phi \sim \frac{2\pi ab}{b^2} J_1(ab) \sim \frac{\lambda a}{\sin\alpha} J_1\left(\frac{2\pi a}{\lambda}\sin\alpha\right). \tag{12.44}$$

The intensity of the light in the diffraction pattern is proportional to Φ^2 and

$$\Phi^2 \sim \left\{\frac{J_1[(2\pi a/\lambda)\sin\alpha]}{\sin\alpha}\right\}^2. \tag{12.45}$$

From Table 12.1, which lists some zeros of the Bessel functions and their first derivatives,[7] Eq. (12.45) will have its smallest zero at

$$\frac{2\pi a}{\lambda}\sin\alpha = 3.8317\ldots \tag{12.46}$$

or

$$\sin\alpha = \frac{3.8317\lambda}{2\pi a}. \tag{12.47}$$

For green light $\lambda = 5.5 \times 10^{-7}$ m. Hence, if $a = 0.5$ cm,

$$\alpha \approx \sin\alpha = 6.7 \times 10^{-5}(\text{radian}) \approx 14 \text{ sec of arc}, \tag{12.48}$$

which shows that the bending or spreading of the light ray is extremely small, because most of the intensity of light is in the principal maximum. If this analysis had been known in the 17th century, the arguments against the wave theory of light would have collapsed. In the mid-20th century this same diffraction pattern appears in the scattering of nuclear particles by atomic nuclei—a striking demonstration of the wave properties of the nuclear particles. ■

[7] Additional roots of the Bessel functions and their first derivatives may be found in C. L. Beattie, Table of first 700 zeros of Bessel functions. *Bell Syst. Tech. J.* **37**, 689 (1958), and *Bell Monogr.* **3055**.

Orthogonality

If Bessel's equation [Eq. (12.28)] is divided by ρ, we see that it becomes self-adjoint, and therefore by the Sturm–Liouville theory of Section 9.2 the solutions are expected to be orthogonal—if we can arrange to have appropriate boundary conditions satisfied. To take care of the boundary conditions, for a finite interval $[0, a]$, we introduce parameters a and $\alpha_{\nu m}$ into the argument of J_ν to get $J_\nu(\alpha_{\nu m}\rho/a)$. Here, a is the upper limit of the cylindrical radial coordinate ρ. From Eq. (12.28),

$$\rho\frac{d^2}{d\rho^2}J_\nu\left(\alpha_{\nu m}\frac{\rho}{a}\right)+\frac{d}{d\rho}J_\nu\left(\alpha_{\nu m}\frac{\rho}{a}\right)+\left(\frac{\alpha_{\nu m}^2\rho}{a^2}-\frac{\nu^2}{\rho}\right)J_\nu\left(\alpha_{\nu m}\frac{\rho}{a}\right)=0. \quad (12.49)$$

Changing the parameter $\alpha_{\nu m}$ to $\alpha_{\nu n}$, we find that $J_\nu(\alpha_{\nu n}\rho/a)$ satisfies

$$\rho\frac{d^2}{d\rho^2}J_\nu\left(\alpha_{\nu n}\frac{\rho}{a}\right)+\frac{d}{d\rho}J_\nu\left(\alpha_{\nu n}\frac{\rho}{a}\right)+\left(\frac{\alpha_{\nu n}^2\rho}{a^2}-\frac{\nu^2}{\rho}\right)J_\nu\left(\alpha_{\nu n}\frac{\rho}{a}\right)=0. \quad (12.50)$$

Proceeding as in Section 9.2, we multiply Eq. (12.49) by $J_\nu(\alpha_{\nu n}\rho/a)$ and Eq. (12.50) by $J_\nu(\alpha_{\nu m}\rho/a)$ and subtract, obtaining

$$\begin{aligned}&J_\nu\left(\alpha_{\nu n}\frac{\rho}{a}\right)\frac{d}{d\rho}\left[\rho\frac{d}{d\rho}J_\nu\left(\alpha_{\nu m}\frac{\rho}{a}\right)\right]-J_\nu\left(\alpha_{\nu m}\frac{\rho}{d\rho}\right)\frac{d}{d\rho}\left[\rho\frac{d}{d\rho}J_\nu\left(\alpha_{\nu n}\frac{\rho}{a}\right)\right]\\&\quad=\frac{\alpha_{\nu n}^2-\alpha_{\nu m}^2}{a^2}\rho J_\nu\left(\alpha_{\nu m}\frac{\rho}{a}\right)J_\nu\left(\alpha_{\nu n}\frac{\rho}{a}\right). \quad (12.51)\end{aligned}$$

Integrating from $\rho=0$ to $\rho=a$, we obtain

$$\begin{aligned}&\int_0^a J_\nu\left(\alpha_{\nu n}\frac{\rho}{a}\right)\frac{d}{d\rho}\left[\rho\frac{d}{d\rho}J_\nu\left(\alpha_{\nu m}\frac{\rho}{a}\right)\right]d\rho\\&\quad-\int_0^a J_\nu\left(\alpha_{\nu m}\frac{\rho}{a}\right)\frac{d}{d\rho}\left[\rho\frac{d}{d\rho}J_\nu\left(\alpha_{\nu n}\frac{\rho}{a}\right)\right]d\rho\\&\quad=\frac{\alpha_{\nu n}^2-\alpha_{\nu m}^2}{a^2}\int_0^a J_\nu\left(\alpha_{\nu m}\frac{\rho}{a}\right)J_\nu\left(\alpha_{\nu n}\frac{\rho}{a}\right)\rho\,d\rho. \quad (12.52)\end{aligned}$$

Upon integrating by parts, the left-hand side of Eq. (12.52) becomes

$$\rho J_\nu\left(\alpha_{\nu n}\frac{\rho}{a}\right)\frac{d}{d\rho}J_\nu\left(\alpha_{\nu m}\frac{\rho}{a}\right)\Bigg|_0^a-\rho J_\nu\left(\alpha_{\nu m}\frac{\rho}{a}\right)\frac{d}{d\rho}J_\nu\left(\alpha_{\nu n}\frac{\rho}{a}\right)\Bigg|_0^a. \quad (12.53)$$

For $\nu\geq 0$ the factor ρ guarantees a zero at the lower limit, $\rho=0$. Actually, the lower limit on the index ν may be extended down to $\nu>-1$.[8] At $\rho=a$, each expression vanishes if we choose the parameters $\alpha_{\nu n}$ and $\alpha_{\nu m}$ to be zeros or

[8] The case $\nu=-1$ reverts to $\nu=+1$, Eq. (12.18).

roots of J_ν; that is, $J_\nu(\alpha_{\nu m}) = 0$. The subscripts now become meaningful: $\alpha_{\nu m}$ is the mth zero of J_ν.

With this choice of parameters, the left-hand side vanishes (the Sturm–Liouville boundary conditions are satisfied) and for $m \neq n$

$$\int_0^a J_\nu\left(\alpha_{\nu m}\frac{\rho}{a}\right) J_\nu\left(\alpha_{\nu n}\frac{\rho}{a}\right)\rho\, d\rho = 0. \tag{12.54}$$

This gives us orthogonality over the interval $[0, a]$.

Normalization

The normalization integral may be developed by returning to Eq. (12.53), setting $\alpha_{\nu n} = \alpha_{\nu m} + \varepsilon$, and taking the limit $\varepsilon \to 0$. With the aid of the recurrence relation, Eq. (12.2), the result may be written as

$$\int_0^a \left[J_\nu\left(\alpha_{\nu m}\frac{\rho}{a}\right)\right]^2 \rho\, d\rho = \frac{a^2}{2}[J_{\nu+1}(\alpha_{\nu m})]^2. \tag{12.55}$$

Bessel Series

If we assume that the set of Bessel functions $J_\nu(\alpha_{\nu m}\rho/a)$($\nu$ fixed, $m = 1, 2, 3, \ldots$) is complete, then any well-behaved, but otherwise arbitrary, function $f(\rho)$ may be expanded in a Bessel series (Bessel–Fourier or Fourier–Bessel)

$$f(\rho) = \sum_{m=1}^{\infty} c_{\nu m} J_\nu\left(\alpha_{\nu m}\frac{\rho}{a}\right), \qquad 0 \le \rho \le a, \quad \nu > -1. \tag{12.56}$$

The coefficients $c_{\nu m}$ are determined by using Eq. (12.55),

$$c_{\nu m} = \frac{2}{a^2[J_{\nu+1}(\alpha_{\nu m})]^2}\int_0^a f(\rho) J_\nu\left(\alpha_{\nu m}\frac{\rho}{a}\right)\rho\, d\rho. \tag{12.57}$$

An application of the use of Bessel functions and their roots is provided by drumhead vibrations in Example 12.1.4 and the electromagnetic resonant cavity, Example 12.1.5, and the exercises of Section 12.1.

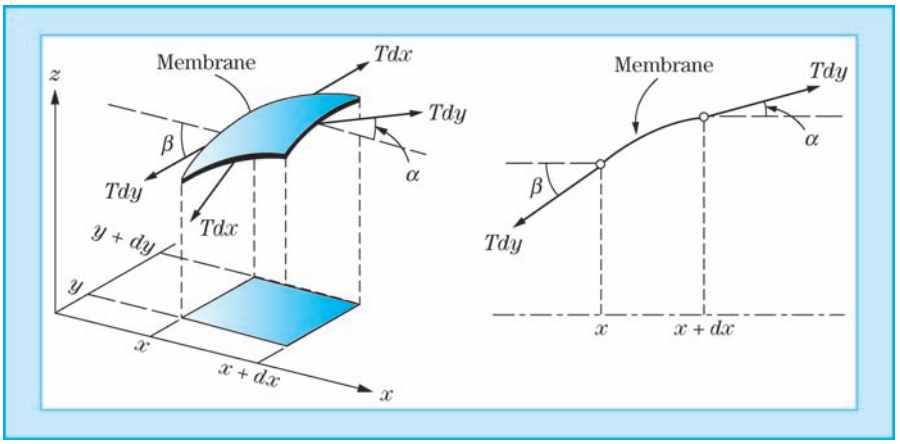
EXAMPLE 12.1.4

Vibrations of a Plane Circular Membrane Vibrating membranes are of great practical importance because they occur not only in drums but also in telephones, microphones, pumps, and other devices. We will show that their vibrations are governed by the two-dimensional wave equation and then solve this PDE in terms of Bessel functions by separating variables.

We assume that the membrane is made of elastic material of constant mass per unit area, ρ, without resistance to (slight) bending. It is stretched along all of its boundary in the xy-plane generating **constant tension** T per unit length in all relevant directions, which does not change while the membrane vibrates. The deflected membrane surface is denoted by $z = z(x, y, t)$, and $|z|$, $|\partial z/\partial x|$, $|\partial z/\partial y|$ are small compared to a, the **radius of the drumhead** for all times t. For small transverse (to the membrane surface) vibrations of a **thin elastic membrane** these assumptions are valid and lead to an accurate description of a drumhead.

Figure 12.3

Rectangular Patch of a Vibrating Membrane



To derive the PDE we analyze a small rectangular patch of lengths dx, dy and area $dx\,dy$. The forces on the sides of the patch are $T\,dx$ and $T\,dy$ acting tangentially while the membrane is deflected slightly from its horizontal equilibrium position (Fig. 12.3). The angles α, β at opposite ends of the deflected membrane patch are small so that $\cos\alpha \sim \cos\beta \sim 1$, upon keeping only terms linear in α. Hence, the horizontal force components, $T\cos\alpha$, $T\cos\beta \sim T$ are practically equal so that **horizontal movements are negligible**.

The z components of the forces are $T\,dy\sin\alpha$ and $-T\,dy\sin\beta$ at opposite sides in the y-direction, up (positive) at $x+dx$ and down (negative) at x. Their sum is

$$T\,dy(\sin\alpha - \sin\beta) \sim T\,dy(\tan\alpha - \tan\beta)$$
$$= T\,dy\left[\frac{\partial z(x+dx,\,y,\,t)}{\partial x} - \frac{\partial z(x,\,y,\,t)}{\partial x}\right]$$

because $\tan\alpha$, $\tan\beta$ are the slopes of the deflected membrane in the x-direction at $x+dx$ and x, respectively. Similarly, the sum of the forces at opposite sides in the other direction is

$$T\,dx\left[\frac{\partial z(x,\,y+dy,\,t)}{\partial y} - \frac{\partial z(x,\,y,\,t)}{\partial y}\right].$$

According to Newton's force law the sum of these forces is equal to the mass of the undeflected membrane area, $\rho\,dx\,dy$, times the acceleration; that is,

$$\rho\,dx\,dy\frac{\partial^2 z}{\partial t^2} = T\,dx\left[\frac{\partial z(x,\,y+dy,\,t)}{\partial y} - \frac{\partial z(x,\,y,\,t)}{\partial y}\right]$$
$$+ T\,dy\left[\frac{\partial z(x+dx,\,y,\,t)}{\partial x} - \frac{\partial z(x,\,y,\,t)}{\partial x}\right].$$

Dividing by the patch area $dx\,dy$ we obtain the second-order PDE

$$\frac{\rho}{T}\frac{\partial^2 z}{\partial t^2} = \frac{\frac{\partial z(x,y+dy,t)}{\partial y} - \frac{\partial z(x,y,t)}{\partial y}}{dy} + \frac{\frac{\partial z(x+dx,y,t)}{\partial x} - \frac{\partial z(x,y,t)}{\partial x}}{dx},$$

or, with the constant $c^2 = T/\rho$ and in the limit $dx, dy \to 0$

$$\frac{1}{c^2}\frac{\partial^2 z}{\partial t^2} = \frac{\partial^2 z}{\partial x^2} + \frac{\partial^2 z}{\partial y^2}, \tag{12.58}$$

which is called the **two-dimensional wave equation**.

Because there are no mixed derivatives, such as $\frac{\partial^2 z}{\partial t \partial x}$, we can separate the time dependence in a **product form of the solution** $z = v(t)w(x, y)$. Substituting this z and its derivatives into our wave equation and dividing by $v(t)w(x, y)$ yields

$$\frac{1}{c^2 v(t)}\frac{\partial^2 v}{\partial t^2} = \frac{1}{w(x, y)}\left(\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2}\right).$$

Here, the left-hand side depends on the variable t only, whereas the right-hand side contains the spatial variables only. This implies that both sides must be equal to a constant, $-k^2$, leading to the harmonic oscillator ODE in t and the two-dimensional Helmholtz equation in x and y:

$$\frac{d^2 v}{dt^2} + k^2 c^2 v(t) = 0, \quad \frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} + k^2 w(x, y) = 0. \tag{12.59}$$

Further steps will depend on our boundary conditions and their symmetry. We have chosen the negative sign for the **separation constant** $-k^2$ because this sign will correspond to oscillatory solutions,

$$v(t) = A\cos(kct) + B\sin(kct),$$

in time rather than exponentially damped ones we would get for a positive separation constant. Note that, in our derivation of the wave equation, we have tacitly assumed **no damping** of the membrane (which could lead to a more complicated PDE). Besides the dynamics, this choice is also dictated by the **boundary conditions** that we have in mind and will discuss in more detail next.

The circular shape of the membrane suggests using cylindrical coordinates so that $z = z(t, \rho, \varphi)$. Invariance under rotations about the z-axis suggests no dependence of the deflected membrane on the azimuthal angle φ. Therefore, $z = z(t, \rho)$, provided the **initial** deflection (dent) and its velocity at time $t = 0$ (needed because our PDE is second order in time)

$$z(0, \rho) = f(\rho), \quad \frac{\partial z}{\partial t}(0, \rho) = g(\rho)$$

also have no angular dependence. Moreover, the **membrane is fixed at the circular boundary** $\rho = a$ **at all times**, $z(t, a) \equiv 0$.

In cylindrical coordinates, using Eq. (2.21) for the two-dimensional Laplacian, the wave equation becomes

$$\frac{1}{c^2}\frac{\partial^2 z}{\partial t^2} = \frac{\partial^2 z}{\partial \rho^2} + \frac{1}{\rho}\frac{\partial z}{\partial \rho} + \frac{1}{\rho^2}\frac{\partial^2 z}{\partial \varphi^2}, \tag{12.60}$$

where we delete the angular dependence, reducing the wave equation to

$$\frac{1}{c^2}\frac{\partial^2 z}{\partial t^2} = \frac{\partial^2 z}{\partial \rho^2} + \frac{1}{\rho}\frac{\partial z}{\partial \rho}.$$

Now we separate variables again seeking a solution of the product form $z = v(t)w(\rho)$. Substituting this z and its derivatives into our wave equation [Eq. (12.60)] and dividing by $v(t)w(\rho)$ yields the same harmonic oscillator ODE for $v(t)$ and

$$\frac{d^2 w}{d\rho^2} + \frac{1}{\rho}\frac{dw}{d\rho} + k^2 w(\rho) = 0$$

instead of Eq. (12.59). Dimensional arguments suggest rescaling $\rho \to r = k\rho$ and dividing by k^2, yielding

$$\frac{d^2 w}{dr^2} + \frac{1}{r}\frac{dw}{dr} + w(r) = 0,$$

which is Bessel's ODE for $\nu = 0$.

We adopt the solution $J_0(r)$ because it is finite everywhere, whereas the second independent solution is singular at the origin, which is ruled out by our initial and boundary conditions.

The boundary condition $w(a) = 0$ requires $J_0(ka) = 0$ so that

$$k = k_n = \gamma_n/a, \quad \text{with} \quad J_0(\gamma_n) = 0,\ n = 1, 2, \ldots.$$

The zeros $\gamma_1 = 2.4048, \ldots$ are listed in Table 12.1. The general solution

$$z(t, \rho) = \sum_{n=1}^{\infty} [A_n \cos(\gamma_n ct/a) + B_n \sin(\gamma_n ct/a)] J_0(\gamma_n \rho/a) \tag{12.61}$$

follows from the superposition principle. The initial conditions at $t = 0$ require expanding

$$f(\rho) = \sum_{n=1}^{\infty} A_n J_0(\gamma_n \rho/a), \quad g(\rho) = \sum_{n=1}^{\infty} \frac{\gamma_n c}{a} B_n J_0(\gamma_n \rho/a), \tag{12.62}$$

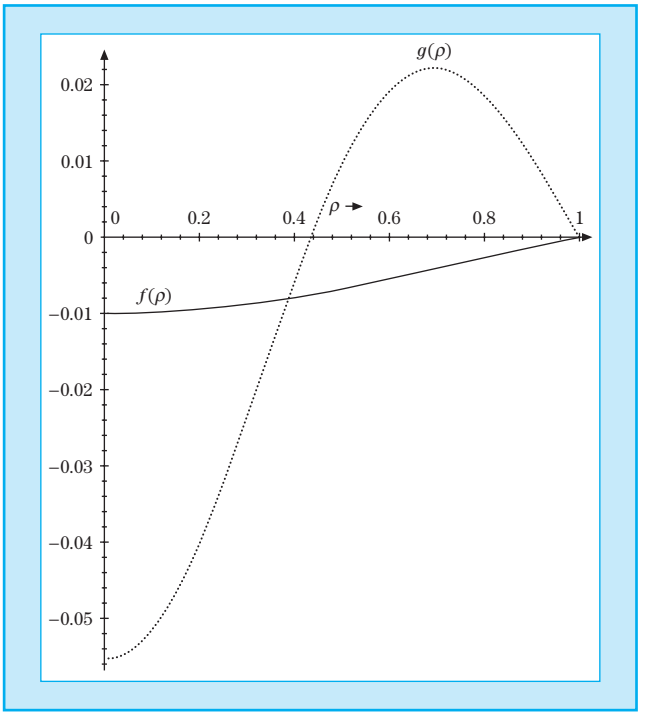
where the coefficients A_n, B_n may be obtained by projection from these Bessel series expansions of the given functions $f(\rho)$, $g(\rho)$ using orthogonality properties of the Bessel functions [see Eq. (12.57)] in the general case

$$A_n = \frac{2}{a^2 [J_1(\gamma_n)]^2} \int_0^a f(\rho) J_0(\gamma_n \rho/a) \rho \, d\rho. \tag{12.63}$$

A similar relation holds for the B_n involving $g(\rho)$.

Figure 12.4

Initial Central Bang on Drumhead



To illustrate a simpler case, let us assume initial conditions

$$f(\rho) = -0.01aJ_0(\gamma_1\rho/a), \quad g(\rho) = -0.1\frac{\gamma_2 c}{a}J_0(\gamma_2\rho/a),$$

corresponding to an initial central bang on the drumhead (Fig. 12.4) at $t = 0$. Then our complete solution (with $c^2 = T/\rho$)

$$z(t, \rho) = -0.01aJ_0\left(2.4048\frac{\rho}{a}\right)\cos\frac{2.4048ct}{a} - 0.1J_0\left(5.5201\frac{\rho}{a}\right)\sin\frac{5.5201ct}{a}$$

contains only the $n = 1$ and $n = 2$ terms as dictated by the initial conditions (Fig. 12.5). ■

EXAMPLE 12.1.5

Cylindrical Resonant Cavity The propagation of electromagnetic waves in hollow metallic cylinders is important in many practical devices. If the cylinder has end surfaces, it is called a cavity. Resonant cavities play a crucial role in many particle accelerators.

We take the z-axis along the center of the cavity with end surfaces at $z = 0$ and $z = l$ and use cylindrical coordinates suggested by the geometry. Its walls are perfect conductors so that the tangential electric field vanishes on them (as in Fig. 12.6):

$$E_z = 0 \quad \text{for} \quad \rho = a, \quad E_\rho = 0 = E_\varphi \quad \text{for} \quad z = 0, l. \tag{12.64}$$

Figure 12.5

Drumhead Solution, $a = 1, c = 0.1$

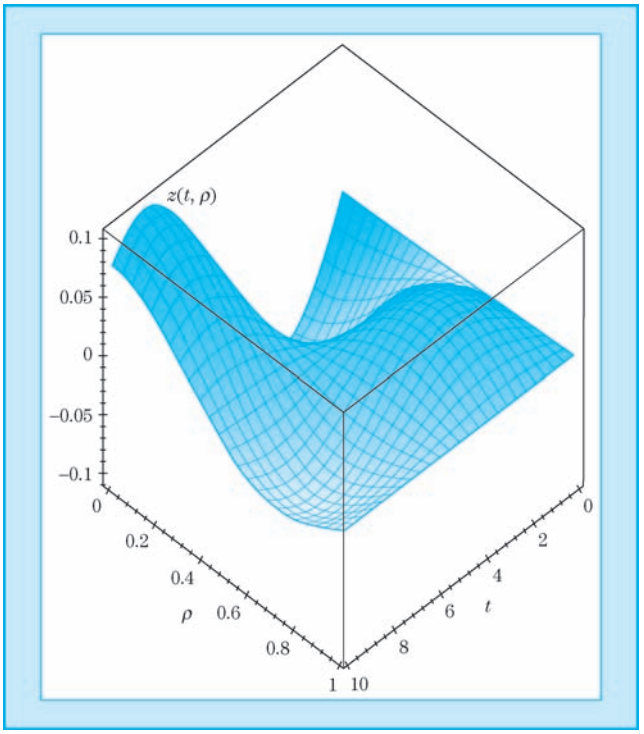
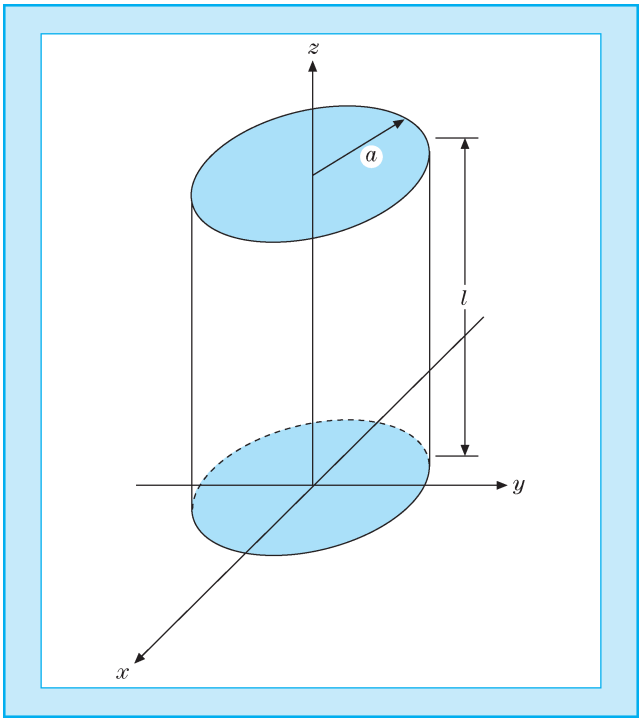


Figure 12.6

Cylindrical Resonant Cavity



Inside the cavity we have a vacuum so that $\varepsilon_0\mu_0 = 1/c^2$. In the interior of a resonant cavity electromagnetic waves oscillate with harmonic time dependence $e^{-i\omega t}$, which follows from separating the time from the spatial variables in Maxwell's equations (Section 1.8) so that

$$\boldsymbol{\nabla}\times\boldsymbol{\nabla}\times\mathbf{E} = -\frac{1}{c^2}\frac{\partial^2\mathbf{E}}{\partial t^2} = k_0^2\mathbf{E}, \quad k_0^2 = \omega^2/c^2.$$

With $\boldsymbol{\nabla}\cdot\mathbf{E} = 0$ (vacuum, no charges) and Eq. (1.96), we obtain for the space part of the electric field

$$\boldsymbol{\nabla}^2\mathbf{E} + k_0^2\mathbf{E} = 0,$$

which is called the vector Helmholtz PDE. The z component (E_z, space part only) satisfies the scalar Helmholtz equation [three-dimensional generalization of Eq. (12.59) in Example 12.1.4]

$$\boldsymbol{\nabla}^2 E_z + k_0^2 E_z = 0. \tag{12.65}$$

The transverse electric field components $\mathbf{E}_\perp = (E_\rho, E_\varphi)$ obey the same PDE but different boundary conditions given previously.

As in Example 12.1.4, we can separate the z variable from ρ and φ because there are no mixed derivatives $\frac{\partial^2 E_z}{\partial z\partial\rho}$, etc. The product solution $E_z = v(\rho, \varphi)w(z)$ is substituted into Eq. (12.65) using Eq. (2.21) for $\boldsymbol{\nabla}^2$ in cylindrical coordinates; then we divide by vw, yielding

$$-\frac{1}{w(z)}\frac{d^2w}{dz^2} = \frac{1}{v(\rho,\varphi)}\left(\frac{\partial^2 v}{\partial\rho^2} + \frac{1}{\rho}\frac{\partial v}{\partial\rho} + \frac{1}{\rho^2}\frac{\partial^2 v}{\partial\varphi^2} + k_0^2 v\right) = k^2,$$

where k^2 is the separation constant because the left- and right-hand sides depend on different variables. For $w(z)$ we find the harmonic oscillator ODE with standing wave solution

$$w(z) = A\sin kz + B\cos kz,$$

with A, B constants. For $v(\rho, \varphi)$ we obtain

$$\frac{\partial^2 v}{\partial\rho^2} + \frac{1}{\rho}\frac{\partial v}{\partial\rho} + \frac{1}{\rho^2}\frac{\partial^2 v}{\partial\varphi^2} + \gamma^2 v = 0, \quad \gamma^2 = k_0^2 - k^2.$$

In this PDE we can separate the ρ and φ variables because there is no mixed term $\frac{\partial^2 v}{\partial\rho\partial\varphi}$. The product form $v = u(\rho)\Phi(\varphi)$ yields

$$\frac{\rho^2}{u(\rho)}\left(\frac{d^2u}{d\rho^2} + \frac{1}{\rho}\frac{du}{d\rho} + \gamma^2 u\right) = -\frac{1}{\Phi(\varphi)}\frac{d^2\Phi}{d\varphi^2} = m^2,$$

where the **separation constant** m^2 **must be an integer** because the angular solution, $\Phi = e^{im\varphi}$ of the ODE

$$\frac{d^2\Phi}{d\varphi^2} + m^2\Phi = 0,$$

must be periodic in the azimuthal angle.

This leaves us with the radial ODE

$$\frac{d^2u}{d\rho^2} + \frac{1}{\rho}\frac{du}{d\rho} + \left(\gamma^2 - \frac{m^2}{\rho^2}\right)^u = 0.$$

Dimensional arguments suggest rescaling $\rho \to r = \gamma\rho$ and dividing by γ^2, which yields

$$\frac{d^2u}{dr^2} + \frac{1}{r}\frac{du}{dr} + \left(1 - \frac{m^2}{r^2}\right)^u = 0.$$

This is Bessel's ODE for $\nu = m$.

We use the regular solution $J_m(\gamma\rho)$ because the (irregular) second independent solution is singular at the origin, which is unacceptable. The complete solution is

$$E_z = J_m(\gamma\rho)e^{im\varphi}(A\sin kz + B\cos kz), \tag{12.66}$$

where the constant γ is determined from the **boundary condition** $E_z = 0$ on the cavity surface $\rho = a$ (i.e., that γa be a root of the Bessel function J_m) (Table 12.1). This gives a discrete set of values $\gamma = \gamma_{mn}$, where n designates the nth root of J_m (Table 12.1).

For the transverse magnetic (TM) mode of oscillation with $H_z = 0$, Maxwell's equations imply (see "Resonant Cavities" in J. D. Jackson's *Electrodynamics*)

$$\mathbf{E}_\perp \sim \boldsymbol{\nabla}_\perp \frac{\partial E_z}{\partial z}, \quad \boldsymbol{\nabla}_\perp = \left(\frac{\partial}{\partial\rho}, \frac{1}{\rho}\frac{\partial}{\partial\varphi}\right).$$

The form of this result suggests $E_z \sim \cos kz$, that is, setting $A = 0$, so that $\mathbf{E}_\perp \sim \sin kz = 0$ at $z = 0, l$ can be satisfied by

$$k = \frac{p\pi}{l}, \quad p = 0, 1, 2, \ldots. \tag{12.67}$$

Thus, the **tangential** electric fields E_ρ and E_φ vanish at $z = 0$ and l. In other words, $A = 0$ corresponds to $dE_z/dz = 0$ at $z = 0$ and $z = a$ for the TM mode. Altogether then, we have

$$\gamma^2 = \frac{\omega^2}{c^2} - k^2 = \frac{\omega^2}{c^2} - \frac{p^2\pi^2}{l^2}, \tag{12.68}$$

with

$$\gamma = \gamma_{mn} = \frac{\alpha_{mn}}{a}, \tag{12.69}$$

where α_{mn} is the nth zero of J_m. The general solution

$$E_z = \sum_{m,n,p} J_m(\gamma_{mn}\rho)e^{\pm im\varphi} B_{mnp} \cos\frac{p\pi z}{l}, \tag{12.70}$$

with constants B_{mnp}, now follows from the superposition principle.

The consequence of the two boundary conditions and the separation constant m^2 is that the angular frequency of our oscillation depends on three discrete parameters:

$$\omega_{mnp} = c\sqrt{\frac{\alpha_{mn}^2}{a^2} + \frac{p^2\pi^2}{l^2}}, \qquad \begin{cases} m = 0, 1, 2, \ldots \\ n = 1, 2, 3, \ldots \\ p = 0, 1, 2, \ldots \end{cases} \tag{12.71}$$

These are the allowed resonant frequencies for the TM mode. Feynman *et al.*[9] develops Bessel functions from cavity resonators. ■

Bessel Functions of Nonintegral Order

The generating function approach is very convenient for deriving two recurrence relations, Bessel's differential equation, integral representations, addition theorems (Example 12.1.2), and upper and lower bounds (Exercise 12.1.1). However, the generating function defines only Bessel functions of integral order J_0, J_1, J_2, and so on. This is a limitation of the generating function approach that can be avoided by using a contour integral (Section 12.3) instead. However, the Bessel function of the first kind, $J_\nu(x)$, may easily be defined for nonintegral ν by using the series [Eq. (12.15)] as a new definition.

We have verified the recurrence relations by substituting in the series form of $J_\nu(x)$. From these relations Bessel's equation follows. In fact, if ν is not an integer, there is actually an important simplification. It is found that J_ν and $J_{-\nu}$ are independent because no relation of the form of Eq. (12.18) exists. On the other hand, for $\nu = n$, an integer, we need another solution. The development of this second solution and an investigation of its properties are the subject of Section 12.2.

EXERCISES

12.1.1 From the product of the generating functions $g(x, t) \cdot g(x, -t)$ show that

$$1 = [J_0(x)]^2 + 2[J_1(x)]^2 + 2[J_2(x)]^2 + \cdots$$

and therefore that $|J_0(x)| \le 1$ and $|J_n(x)| \le 1/\sqrt{2}$, $n = 1, 2, 3, \ldots$.
Hint. Use uniqueness of power series (Section 5.7).

[9] Feynman, R. P., Leighton, R. B., and Sands, M. (1964). *The Feynman Lectures on Physics*, Vol. 2, Chap. 23. Addison-Wesley, Reading, MA.

12.1.2 Derive the Jacobi–Anger expansion

$$e^{iz\cos\theta} = \sum_{m=-\infty}^{\infty} i^m J_m(z) e^{im\theta}.$$

This is an expansion of a plane wave in a series of cylindrical waves.

12.1.3 Show that

(a) $\cos x = J_0(x) + 2\sum_{n=1}^{\infty}(-1)^n J_{2n}(x)$,

(b) $\sin x = 2\sum_{n=1}^{\infty}(-1)^{n+1} J_{2n+1}(x)$.

12.1.4 Prove that

$$\frac{\sin x}{x} = \int_0^{\pi/2} J_0(x\cos\theta)\cos\theta\, d\theta, \qquad \frac{1-\cos x}{x} = \int_0^{\pi/2} J_1(x\cos\theta)\, d\theta.$$

Hint. The definite integral

$$\int_0^{\pi/2} \cos^{2s+1}\theta\, d\theta = \frac{2\cdot 4\cdot 6\cdots(2s)}{1\cdot 3\cdot 5\cdots(2s+1)}$$

may be useful.

12.1.5 Show that

$$J_0(x) = \frac{2}{\pi}\int_0^1 \frac{\cos xt}{\sqrt{1-t^2}}\, dt.$$

This integral is a Fourier cosine transform (compare Section 15.4). The corresponding Fourier sine transform,

$$J_0(x) = \frac{2}{\pi}\int_1^\infty \frac{\sin xt}{\sqrt{t^2-1}}\, dt,$$

is established using a Hankel function integral representation.

12.1.6 Derive

$$J_n(x) = (-1)^n x^n \left(\frac{1}{x}\frac{d}{dx}\right)^n J_0(x).$$

Hint. Rewrite the recursion so that it serves to step from n to $n+1$ in a proof by mathematical induction.

12.1.7 Show that between any two consecutive zeros of $J_n(x)$ there is one and only one zero of $J_{n+1}(x)$.
Hint. Equations (12.1) and (12.6) may be useful.

12.1.8 An analysis of antenna radiation patterns for a system with a circular aperture involves the equation

$$g(u) = \int_0^1 f(r) J_0(ur) r\, dr.$$

If $f(r) = 1 - r^2$, show that

$$g(u) = \frac{2}{u^2} J_2(u).$$

12.1.9 The differential cross section in a nuclear scattering experiment is given by $d\sigma/d\Omega = |f(\theta)|^2$. An approximate treatment leads to

$$f(\theta) = \frac{-ik}{2\pi}\int_0^{2\pi}\int_0^R \exp[ik\rho\sin\theta\sin\varphi]\rho\, d\rho\, d\varphi,$$

where θ is an angle through which the scattered particle is scattered, and R is the nuclear radius. Show that

$$\frac{d\sigma}{d\Omega} = (\pi R^2)\frac{1}{\pi}\left[\frac{J_1(kR\sin\theta)}{\sin\theta}\right]^2.$$

12.1.10 A set of functions $C_n(x)$ satisfies the recurrence relations

$$C_{n-1}(x) - C_{n+1}(x) = \frac{2n}{x}C_n(x),$$
$$C_{n-1}(x) + C_{n+1}(x) = 2C_n'(x).$$

(a) What linear second-order ODE does the $C_n(x)$ satisfy?
(b) By a change of variable, transform your ODE into Bessel's equation. This suggests that $C_n(x)$ may be expressed in terms of Bessel functions of transformed argument.

12.1.11 (a) From

$$J_\nu(x) = \frac{1}{2\pi i}\left(\frac{x}{2}\right)^\nu \int t^{-\nu-1}e^{t-x^2/4t}dt$$

with a suitably defined contour, derive the recurrence relation

$$J_\nu'(x) = \frac{\nu}{x}J_\nu(x) - J_{\nu+1}(x).$$

(b) From

$$J_\nu(x) = \frac{1}{2\pi i}\int t^{-\nu-1}e^{(x/2)(t-1/t)}\,dt$$

with the same contour, derive the recurrence relation

$$J_\nu'(x) = \frac{1}{2}[J_{\nu-1}(x) - J_{\nu+1}(x)].$$

12.1.12 Show that the recurrence relation

$$J_n'(x) = \frac{1}{2}[J_{n-1}(x) - J_{n+1}(x)]$$

follows directly from differentiation of

$$J_n(x) = \frac{1}{\pi}\int_0^\pi \cos(n\theta - x\sin\theta)\,d\theta.$$

12.1.13 Evaluate

$$\int_0^\infty e^{-ax}J_0(bx)\,dx, \quad a, b > 0.$$

Actually the results hold for $a \geq 0$, $-\infty < b < \infty$. This is a Laplace transform of J_0.

Hint. Either an integral representation of J_0 or a series expansion or a Laplace transformation of Bessel's ODE will be helpful.

12.1.14 Using trigonometric forms [Eq. (12.29)], verify that

$$J_0(br) = \frac{1}{2\pi}\int_0^{2\pi} e^{ibr\sin\theta}\,d\theta.$$

12.1.15 The fraction of light incident on a circular aperture (normal incidence) that is transmitted is given by

$$T = \int_0^{2ka} J_2(x)\left(\frac{2}{x} - \frac{1}{2ka}\right)dx,$$

where a is the radius of the aperture, and k is the wave number, $2\pi/\lambda$. Show that

(a) $T = 1 - \dfrac{1}{ka}\displaystyle\sum_{n=0}^{\infty} J_{2n+1}(2ka)$, (b) $T = 1 - \dfrac{1}{2ka}\displaystyle\int_0^{2ka} J_0(x)\,dx$.

12.1.16 Show that, defining

$$I_{m,n}(a) \equiv \int_0^a x^m J_n(x)\,dx, \qquad m \geq n \geq 0,$$

(a) $I_{3,0}(x) = \displaystyle\int_0^x t^3 J_0(t)\,dt = x^3 J_1(x) - 2x^2 J_2(x)$;

(b) is integrable in terms of Bessel functions and powers of x [such as $a^p J_q(a)$] for $m+n$ odd;

(c) may be reduced to integrated terms plus $\int_0^a J_0(x)\,dx$ for $m+n$ even.

12.1.17 Solve the ODE $x^2y''(x) + axy'(x) + (1 + b^2x^2)y(x) = 0$, where a, b are real parameters, using the substitution $y(x) = x^{-n}v(x)$. Adjust n and a so that the ODE for v becomes Bessel's ODE for J_0. Find the general solution $y(x)$ for this value of a.

12.2 Neumann Functions, Bessel Functions of the Second Kind

From the theory of ODEs it is known that Bessel's second-order ODE has two independent solutions. Indeed, for nonintegral order ν we have already found two solutions and labeled them $J_\nu(x)$ and $J_{-\nu}(x)$ using the infinite series [Eq. (12.15)]. The trouble is that when ν is integral, Eq. (12.18) holds and we have but one independent solution. A second solution may be developed by the methods of Section 8.6. This yields a perfectly good second solution of Bessel's equation but is not the standard form.

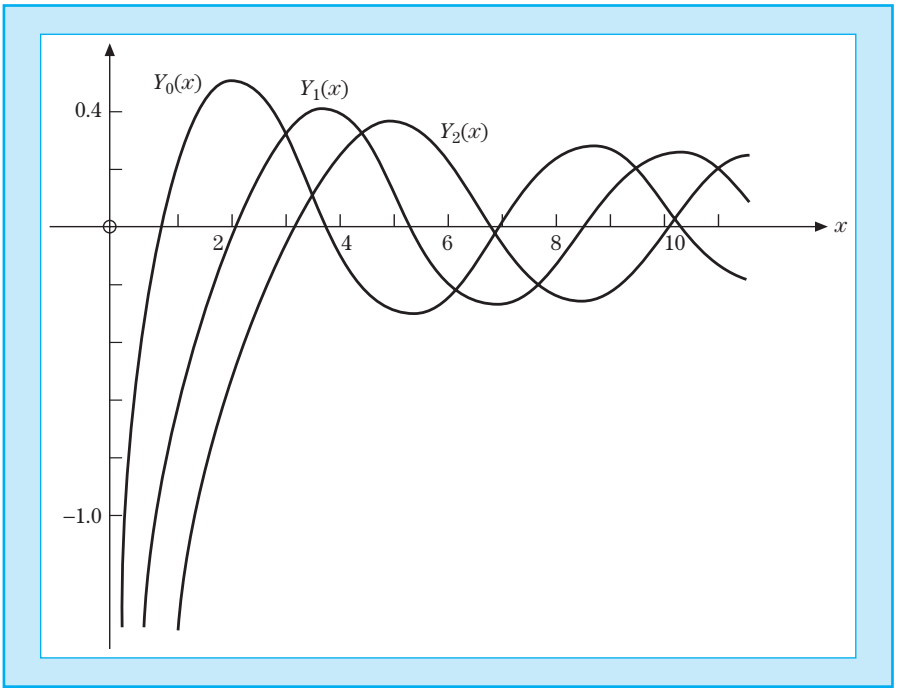
Definition and Series Form

As an alternate approach, we take the particular linear combination of $J_\nu(x)$ and $J_{-\nu}(x)$

$$Y_\nu(x) = \frac{\cos(\nu\pi)J_\nu(x) - J_{-\nu}(x)}{\sin\nu\pi}. \tag{12.72}$$

Figure 12.7

Neumann Functions $Y_0(x)$, $Y_1(x)$, and $Y_2(x)$



This is the Neumann function (Fig. 12.7).[10] For nonintegral ν, $Y_\nu(x)$ clearly satisfies Bessel's equation because it is a linear combination of known solutions, $J_\nu(x)$ and $J_{-\nu}(x)$. Substituting the power series [Eq. (12.15)] for $n \to \nu$ yields

$$Y_\nu(x) = -\frac{(\nu-1)!}{\pi}\left(\frac{2}{x}\right)^\nu + \cdots \tag{12.73}$$

for $\nu > 0$. However, for integral ν, Eq. (12.18) applies and Eq. (12.58)[11] becomes indeterminate. The definition of $Y_\nu(x)$ was chosen deliberately for this indeterminate property. Again substituting the power series and evaluating $Y_\nu(x)$ for $\nu \to 0$ by l'Hôpital's rule for indeterminate forms, we obtain the limiting value

$$Y_0(x) = \frac{2}{\pi}(\ln x + \gamma - \ln 2) + \mathcal{O}(x^2) \tag{12.74}$$

for $n = 0$ and $x \to 0$, using

$$\nu!(-\nu)! = \frac{\pi\nu}{\sin \pi\nu} \tag{12.75}$$

from Eq. (10.32). The first and third terms in Eq. (12.74) come from using $(d/d\nu)(x/2)^\nu = (x/2)^\nu \ln(x/2)$, whereas γ comes from $(d/d\nu)\nu!$ for $\nu \to 0$

[10] We use the notation in AMS-55 and in most mathematics tables.
[11] Note that this limiting form applies to both integral and nonintegral values of the index ν.

using Eqs. (10.38) and (10.40). For $n > 0$ we obtain similarly

$$Y_n(x) = -\frac{(n-1)!}{\pi}\left(\frac{2}{x}\right)^n + \cdots + \frac{2}{\pi}\left(\frac{x}{2}\right)^n \frac{1}{n!}\ln\left(\frac{x}{2}\right) + \cdots. \tag{12.76}$$

Equations (12.74) and (12.76) exhibit the logarithmic dependence that was to be expected. This, of course, verifies the independence of J_n and Y_n.

Other Forms

As with all the other Bessel functions, $Y_\nu(x)$ has integral representations. For $Y_0(x)$ we have

$$Y_0(x) = -\frac{2}{\pi}\int_0^\infty \cos(x\cosh t)\,dt = -\frac{2}{\pi}\int_1^\infty \frac{\cos(xt)}{(t^2-1)^{1/2}}\,dt, \quad x > 0.$$

These forms can be derived as the imaginary part of the Hankel representations of Section 12.3. The latter form is a Fourier cosine transform.

The most general solution of Bessel's ODE for any ν can be written as

$$y(x) = AJ_\nu(x) + BY_\nu(x). \tag{12.77}$$

It is seen from Eqs. (12.74) and (12.76) that Y_n diverges at least logarithmically. Some boundary condition that requires the solution of a problem with Bessel function solutions to be finite at the origin automatically excludes $Y_n(x)$. Conversely, in the absence of such a requirement $Y_n(x)$ must be considered.

Biographical Data

Neumann, Karl. Neumann, a German mathematician and physicist, was born in 1832 and died in 1925. He was appointed a professor of mathematics at the University of Leipzig in 1868. His main contributions were to potential theory and partial differential and integral equations.

Recurrence Relations

Substituting Eq. (12.72) for $Y_\nu(x)$ (nonintegral ν) or Eq. (12.76) (integral ν) into the recurrence relations [Eqs. (12.8) and (12.21)] for $J_n(x)$, we see immediately that $Y_\nu(x)$ satisfies these same recurrence relations. This actually constitutes another proof that Y_ν is a solution. Note that the converse is not necessarily true. All solutions need not satisfy the same recurrence relations because Y_ν for nonintegral ν also involves $J_{-\nu} \neq J_\nu$ obeying recursions with $\nu \to -\nu$.

Wronskian Formulas

From Section 8.6 and Exercise 9.1.3 we have the Wronskian formula[12] for solutions of the Bessel equation

$$u_\nu(x)v'_\nu(x) - u'_\nu(x)v_\nu(x) = \frac{A_\nu}{x}, \tag{12.78}$$

[12]This result depends on $P(x)$ of Section 8.5 being equal to $p'(x)/p(x)$, the corresponding coefficient of the self-adjoint form of Section 9.1.

in which A_ν is a parameter that depends on the particular Bessel functions $u_\nu(x)$ and $v_\nu(x)$ being considered. It is a constant in the sense that it is independent of x. Consider the special case

$$u_\nu(x) = J_\nu(x), \quad v_\nu(x) = J_{-\nu}(x), \tag{12.79}$$

$$J_\nu J'_{-\nu} - J'_\nu J_{-\nu} = \frac{A_\nu}{x}. \tag{12.80}$$

Since A_ν is a constant, it may be identified using the leading terms in the power series expansions [Eqs. (12.15) and (12.17)]. All other powers of x cancel. We obtain

$$\begin{aligned} J_\nu &\to x^\nu/(2^\nu \nu!), & J_{-\nu} &\to 2^\nu x^{-\nu}/(-\nu)!, \\ J'_\nu &\to \nu x^{\nu-1}/(2^\nu \nu!), & J'_{-\nu} &\to -\nu 2^\nu x^{-\nu-1}/(-\nu)!. \end{aligned} \tag{12.81}$$

Substitution into Eq. (12.80) yields

$$J_\nu(x)J'_{-\nu}(x) - J'_\nu(x)J_{-\nu}(x) = \frac{-2\nu}{x\nu!(-\nu)!} = -\frac{2\sin\nu\pi}{\pi x}. \tag{12.82}$$

Note that A_ν vanishes for integral ν, as it must since the nonvanishing of the Wronskian is a test of the independence of the two solutions. By Eq. (12.18), J_n and J_{-n} are clearly linearly dependent.

Using our recurrence relations, we may readily develop a large number of alternate forms, among which are

$$J_\nu J_{-\nu+1} + J_{-\nu}J_{\nu-1} = \frac{2\sin\nu\pi}{\pi x}, \tag{12.83}$$

$$J_\nu J_{-\nu-1} + J_{-\nu}J_{\nu+1} = -\frac{2\sin\nu\pi}{\pi x}, \tag{12.84}$$

$$J_\nu Y'_\nu - J'_\nu Y_\nu = \frac{2}{\pi x}, \tag{12.85}$$

$$J_\nu Y_{\nu+1} - J_{\nu+1}Y_\nu = -\frac{2}{\pi x}. \tag{12.86}$$

Many more can be found in Additional Reading.

The reader will recall that in Chapter 8 Wronskians were of great value in two respects: (i) in establishing the linear independence or linear dependence of solutions of differential equations and (ii) in developing an integral form of a second solution. Here, the specific forms of the Wronskians and Wronskian-derived combinations of Bessel functions are useful primarily to illustrate the general behavior of the various Bessel functions. Wronskians are of great use in checking tables of Bessel functions numerically.

EXAMPLE 12.2.1

Coaxial Waveguides We are interested in an electromagnetic wave confined between the concentric, conducting cylindrical surfaces $\rho = a$ and $\rho = b$. Most of the mathematics is worked out in Example 12.1.5. That is, we work in cylindrical coordinates and separate the time dependence as before, which is that of a traveling wave $e^{i(kz-\omega t)}$ now instead of standing waves in Example 12.1.5.

To implement this, we let $A = iB$ in the solution $w(z) = A\sin kz + B\cos kz$ and obtain

$$E_z = \sum_{m,n} b_{mn} J_m(\gamma\rho) e^{\pm im\varphi} e^{i(kz-\omega t)}. \tag{12.87}$$

For the coaxial waveguide both the Bessel and Neumann functions contribute because the origin $\rho = 0$ can no longer be used to exclude the Neumann functions because it is not part of the physical region ($0 < a \le \rho \le b$). It is consistent that there are now two boundary conditions, at $\rho = a$ and $\rho = b$. With the Neumann function $Y_m(\gamma\rho)$, $E_z(\rho, \varphi, z, t)$ becomes

$$E_z = \sum_{m,n} [b_{mn} J_m(\gamma_{mn}\rho) + c_{mn} Y_m(\gamma_{mn}\rho)] e^{\pm im\varphi} e^{i(kz-\omega t)}, \tag{12.88}$$

where γ_{mn} will be determined from boundary conditions. With the transverse magnetic field condition

$$H_z = 0 \tag{12.89}$$

everywhere, we have the basic equations for a TM wave.

The (tangential) electric field must vanish at the conducting surfaces (Dirichlet boundary condition), or

$$b_{mn} J_m(\gamma_{mn} a) + c_{mn} Y_m(\gamma_{mn} a) = 0, \tag{12.90}$$

$$b_{mn} J_m(\gamma_{mn} b) + c_{mn} Y_m(\gamma_{mn} b) = 0. \tag{12.91}$$

For a nontrivial solution b_{mn}, c_{mn} of these homogeneous linear equations to exist, their determinant must be zero. The resulting transcendental equation, $J_m(\gamma_{mn}a)Y_m(\gamma_{mn}b) = J_m(\gamma_{mn}b)Y_m(\gamma_{mn}a)$, may be solved for γ_{mn}, and then the ratio c_{mn}/b_{mn} can be determined. From Example 12.1.5,

$$k^2 = \omega^2 \mu_0 \varepsilon_0 - \gamma_{mn}^2 = \frac{\omega^2}{c^2} - \gamma_{mn}^2, \tag{12.92}$$

where c is the velocity of light. Since k^2 must be positive for an oscillatory solution, the minimum frequency that will be propagated (in this TM mode) is

$$\omega = \gamma_{mn} c, \tag{12.93}$$

with γ_{mn} fixed by the boundary conditions, Eqs. (12.90) and (12.91). This is the cutoff frequency of the waveguide. In general, at any given frequency only a finite number of modes can propagate. The dimensions ($a < b$) of the cylindrical guide are often chosen so that, at given frequency, only the lowest mode k can propagate.

There is also a transverse electric mode with $E_z = 0$ and H_z given by Eq. (12.88). ■

SUMMARY

To conclude this discussion of Neumann functions, we introduce the Neumann function, $Y_\nu(x)$, for the following reasons:

1. It is a second, independent solution of Bessel's equation, which completes the general solution.
2. It is required for specific physical problems, such as electromagnetic waves in coaxial cables and quantum mechanical scattering theory.
3. It leads directly to the two Hankel functions (Section 12.3).

EXERCISES

12.2.1 Prove that the Neumann functions Y_n (with n an integer) satisfy the recurrence relations

$$Y_{n-1}(x) + Y_{n+1}(x) = \frac{2n}{x} Y_n(x)$$

$$Y_{n-1}(x) - Y_{n+1}(x) = 2Y_n'(x).$$

Hint. These relations may be proved by differentiating the recurrence relations for J_ν or by using the limit form of Y_ν but **not** dividing everything by zero.

12.2.2 Show that

$$Y_{-n}(x) = (-1)^n Y_n(x).$$

12.2.3 Show that

$$Y_0'(x) = -Y_1(x).$$

12.2.4 If Y and Z are any two solutions of Bessel's equation, show that

$$Y_\nu(x)Z_\nu'(x) - Y_\nu'(x)Z_\nu(x) = \frac{A_\nu}{x},$$

in which A_ν may depend on ν but is independent of x. This is a special case of Exercise 9.1.3.

12.2.5 Verify the Wronskian formulas

$$J_\nu(x)J_{-\nu+1}(x) + J_{-\nu}(x)J_{\nu-1}(x) = \frac{2\sin\nu\pi}{\pi x},$$

$$J_\nu(x)Y_\nu'(x) - J_\nu'(x)Y_\nu(x) = \frac{2}{\pi x}.$$

12.2.6 As an alternative to letting x approach zero in the evaluation of the Wronskian constant, we may invoke uniqueness of power series (Section 5.7). The coefficient of x^{-1} in the series expansion of $u_\nu(x)v_\nu'(x) - u_\nu'(x)v_\nu(x)$ is then A_ν. Show by series expansion that the coefficients of x^0 and x^1 of $J_\nu(x)J_{-\nu}'(x) - J_\nu'(x)J_{-\nu}(x)$ are each zero.

12.2.7 (a) By differentiating and substituting into Bessel's ODE, show that

$$\int_0^\infty \cos(x\cosh t)\,dt$$

is a solution.
Hint. You can rearrange the final integral as

$$\int_0^\infty \frac{d}{dt}\{x\sin(x\cosh t)\sinh t\}\,dt.$$

(b) Show that

$$Y_0(x) = -\frac{2}{\pi}\int_0^\infty \cos(x\cosh t)\,dt$$

is linearly independent of $J_0(x)$.

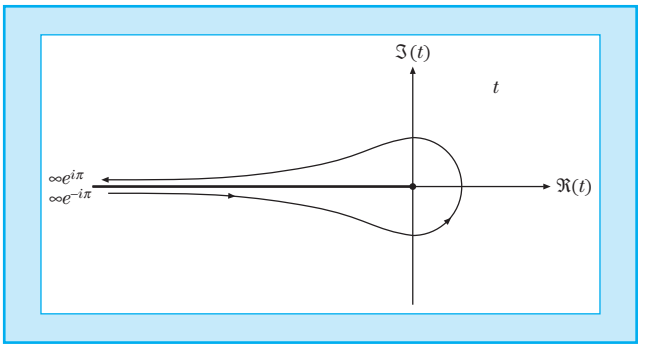
12.3 Asymptotic Expansions

Frequently, in physical problems there is a need to know how a given Bessel function behaves for large values of the argument, that is, the asymptotic behavior. This is one occasion when computers are not very helpful, except in matching numerical solutions to known asymptotic forms or checking an asymptotic guess numerically. One possible approach is to develop a power series solution of the differential equation, as in Section 8.5, but now using negative powers. This is Stokes's method. The limitation is that starting from some positive value of the argument (for convergence of the series), we do not know what mixture of solutions or multiple of a given solution we have. The problem is to relate the asymptotic series (useful for large values of the variable) to the power series or related definition (useful for small values of the variable). This relationship can be established by introducing a suitable **integral representation** and then using either the method of steepest descent (Section 7.3) or the direct expansion as developed in this section.

Integral representations have appeared before: Eq. (10.35) for $\Gamma(z)$ and various representations of $J_\nu(z)$ in Section 12.1. With these integral representations of the Bessel (and Hankel) functions, it is perhaps appropriate to ask why we are interested in integral representations. There are at least four reasons. The first is simply aesthetic appeal. Second, the integral representations help to distinguish between two linearly independent solutions (Section 7.3). Third, the integral representations facilitate manipulations, analysis, and the development of relations among the various special functions. Fourth, and probably most important, the integral representations are extremely useful in developing asymptotic expansions. One approach, the method of steepest descents, appears in Section 7.3 and is used here.

Figure 12.8

Bessel Function Contour



Hankel functions are introduced here for the following reasons:

- As Bessel function analogs of $e^{\pm ix}$ they are useful for describing traveling waves.
- They offer an alternate (contour integral) and an elegant definition of Bessel functions.

Expansion of an Integral Representation

As a direct approach, consider the integral representation (Schlaefli integral)

$$J_\nu(z) = \frac{1}{2\pi i}\int_C e^{(z/2)(t-1/t)}t^{-\nu-1}dt, \tag{12.94}$$

with the contour C around the origin in the positive mathematical sense displayed in Fig. 12.8. This formula follows from Cauchy's theorem, applied to the defining Eq. (12.9) of the generating function given by Eq. (12.16) as the exponential in the integral. This proves Eq. (12.94) for $-\pi < \arg z < 2\pi$, but only for $\nu =$ integer. If ν is not an integer, the integrand is not single-valued and a cut line is needed in our complex t plane. Choosing the negative real axis as the cut line and using the contour shown in Fig. 12.8, we can extend Eq. (12.94) to nonintegral ν. For this case, we still need to verify Bessel's ODE by substituting the integral representation [Eq. (12.94)],

$$\begin{aligned} &z^2J''(z)_\nu + zJ'_\nu(z) + (z^2-\nu^2)J_\nu(z) \\ &\quad = \frac{1}{2\pi i}\int_C e^{(z/2)(t-1/t)}t^{-\nu-1}\left[\frac{z^2}{4}\left(t+\frac{1}{t}\right)^2 + \frac{z}{2}\left(t-\frac{1}{t}\right) - \nu^2\right]dt, \end{aligned} \tag{12.95}$$

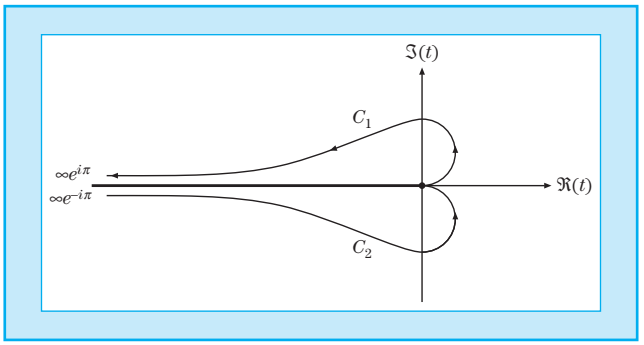
where the integrand can be verified to be the following exact derivative that vanishes as $t \to \infty e^{\pm i\pi}$:

$$\frac{d}{dt}\left\{\exp\left[\frac{z}{2}\left(t-\frac{1}{t}\right)\right]t^{-\nu}\left[\nu + \frac{z}{2}\left(t+\frac{1}{t}\right)\right]\right\}. \tag{12.96}$$

Hence, the integral in Eq. (12.95) vanishes and Bessel's ODE is satisfied.

Figure 12.9

Hankel Function Contours



We now deform the contour so that it approaches the origin along the positive real axis, as shown in Fig. 12.9. This particular approach guarantees that the exact derivative in Eq. (12.96) will vanish as $t \to 0$ because of the $e^{-z/2t}$ factor. Hence, each of the separate portions corresponding to $\infty e^{-i\pi}$ to 0 and 0 to $\infty e^{i\pi}$ is a solution of Bessel's ODE. We define

$$H_\nu^{(1)}(z) = \frac{1}{\pi i}\int_0^{\infty e^{i\pi}} e^{(z/2)(t-1/t)}\frac{dt}{t^{\nu+1}}, \tag{12.97}$$

$$H_\nu^{(2)}(z) = \frac{1}{\pi i}\int_{\infty e^{-i\pi}}^{0} e^{(z/2)(t-1/t)}\frac{dt}{t^{\nu+1}} \tag{12.98}$$

so that

$$J_\nu(z) = \frac{1}{2}\left[H_\nu^{(1)}(z) + H_\nu^{(2)}(z)\right]. \tag{12.99}$$

These expressions are particularly convenient because they may be handled by the method of steepest descents (Section 7.3). $H_\nu^{(1)}(z)$ has a saddle point at $t = +i$, whereas $H_\nu^{(2)}(z)$ has a saddle point at $t = -i$. To leading order Eq. (7.84) yields

$$H_\nu^{(1)}(z) \sim \sqrt{\frac{2}{\pi z}}\exp\left(i\left[z - \left(\nu + \frac{1}{2}\right)\frac{\pi}{2}\right]\right) \tag{12.100}$$

for large $|z|$ in the region $-\pi < \arg z < 2\pi$. The second Hankel function is just the complex conjugate of the first (for real argument z) so that

$$H_\nu^{(2)}(z) = \sqrt{\frac{2}{\pi z}}\exp\left(-i\left[z - \left(\nu + \frac{1}{2}\right)\frac{\pi}{2}\right]\right) \tag{12.101}$$

for large $|z|$ with $-2\pi < \arg z < \pi$.

In addition to Eq. (12.99) we can also show that

$$Y_\nu(z) = \frac{1}{2i}\left[H_\nu^{(1)}(z) - H_\nu^{(2)}(z)\right]. \tag{12.102}$$

This may be accomplished by the following steps:

1. With the substitutions $t = e^{i\pi}/s$ for $H_\nu^{(1)}$ in Eq. (12.97) and $t = e^{-i\pi}/s$ for $H_\nu^{(2)}$ in Eq. (12.98), we obtain

$$H_\nu^{(1)}(z) = e^{-i\nu\pi} H_{-\nu}^{(1)}(z), \tag{12.103}$$

$$H_\nu^{(2)}(z) = e^{i\nu\pi} H_{-\nu}^{(2)}(z). \tag{12.104}$$

2. From Eqs. (12.99) ($\nu \to -\nu$), (12.103), and (12.104), we get

$$J_{-\nu}(z) = \frac{1}{2}\left[e^{i\nu\pi} H_\nu^{(1)}(z) + e^{-i\nu\pi} H_\nu^{(2)}(z)\right]. \tag{12.105}$$

3. Finally, substitute J_ν [Eq. (12.99)] and $J_{-\nu}$ [Eq. (12.105)] into the defining equation for Y_ν, Eq. (12.72). This leads to Eq. (12.102) and establishes the contour integrals [Eqs. (12.97) and (12.98)] as the standard Hankel functions.

Since $J_\nu(z)$ is the real part of $H_\nu^{(1)}(z)$ for real z,

$$J_\nu(z) \sim \sqrt{\frac{2}{\pi z}} \cos\left[z - \left(\nu + \frac{1}{2}\right)\frac{\pi}{2}\right] \tag{12.106}$$

for large $|z|$ with $-\pi < \arg z < \pi$. The Neumann function is the imaginary part of $H_\nu^{(1)}(z)$ or

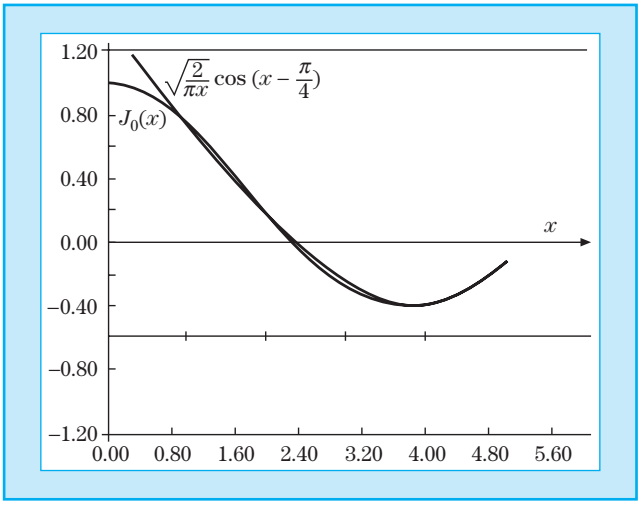
$$Y_\nu(z) \sim \sqrt{\frac{2}{\pi z}} \sin\left[z - \left(\nu + \frac{1}{2}\right)\frac{\pi}{2}\right] \tag{12.107}$$

for large $|z|$ with $-\pi < \arg z < \pi$.

It is of interest to consider the accuracy of the asymptotic forms, taking only the first term [Eq. (12.106)], for example (Fig. 12.10). Clearly, the condition for the validity of Eq. (12.106) is that the next (a nonleading sine) term in Eq. (12.106) be negligible; estimating this leads to $8x \gg 4n^2 - 1$.

Figure 12.10

Asymptotic Approximation of $J_0(x)$



To a certain extent the definition of the Neumann function $Y_n(x)$ is arbitrary. Equations (12.72) and (12.76) contain terms of the form $a_n J_n(x)$. Clearly, any finite value of the constant a_n would still give us a second solution of Bessel's equation. Why should a_n have the particular value implicit in Eqs. (12.72) and (12.76)? The answer is given by the asymptotic dependence developed here. If J_n corresponds to a cosine wave asymptotically [Eq. (12.106)], then Y_n corresponds to a sine wave [Eq. (12.107)]. This simple and convenient asymptotic phase relationship is a consequence of the particular admixture of J_n in Y_n.

This completes our determination of the asymptotic expansions. However, it is worth noting the primary characteristics. Apart from the ubiquitous $z^{-1/2}$, $J_\nu(z)$, and $Y_\nu(z)$ behave as cosine and sine, respectively. The zeros are **almost** evenly spaced at intervals of π; the spacing becomes exactly π in the limit as $z \to \infty$. The Hankel functions have been defined to behave like the imaginary exponentials. This asymptotic behavior may be sufficient to eliminate immediately one of these functions as a solution for a physical problem. This is illustrated in the next example.

EXAMPLE 12.3.1

Cylindrical Traveling Waves As an illustration of the use of Hankel functions, consider a two-dimensional wave problem similar to the vibrating circular membrane of Example 12.1.4. Now imagine that the waves are generated at $\rho = 0$ and move outward to infinity. We replace our standing waves by traveling ones. The differential equation remains the same, but the boundary conditions change. We now demand that for large ρ the solution behaves like

$$U \to e^{i(k\rho - \omega t)} \tag{12.108}$$

to describe an outgoing wave. As before, k is the wave number. This assumes, for simplicity, that there is no azimuthal dependence, that is, no angular momentum, or $m = 0$. In Sections 7.4 and 12.3, $H_0^{(1)}(k\rho)$ is shown to have the asymptotic behavior (for $\rho \to \infty$)

$$H_0^{(1)}(k\rho) \to e^{ik\rho}. \tag{12.109}$$

This boundary condition at infinity then determines our wave solution as

$$U(\rho, t) = H_0^{(1)}(k\rho)e^{-i\omega t}. \tag{12.110}$$

This solution diverges as $\rho \to 0$, which is just the behavior to be expected with a source at the origin representing a singularity reflected by singular behavior of the solution. ■

The choice of a two-dimensional wave problem to illustrate the Hankel function $H_0^{(1)}(z)$ is not accidental. Bessel functions may appear in a variety of ways, such as in the separation in conical coordinates. However, they enter most commonly from the radial equations from the separation of variables in the Helmholtz equation in cylindrical and in spherical polar coordinates. We have used a degenerate form of cylindrical coordinates for this illustration.

Had we used spherical polar coordinates (spherical waves), we should have encountered index $\nu = n + \frac{1}{2}$, n an integer. These special values yield the spherical Bessel functions discussed in Section 12.4.

Finally, as pointed out in Section 12.2, the asymptotic forms may be used to evaluate the various Wronskian formulas (compare Exercise 12.3.2).

Numerical Evaluation

When a computer program calls for one of the Bessel or modified Bessel functions, the programmer has two alternatives: to store all the Bessel functions and tell the computer how to locate the required value or to instruct the computer to simply calculate the needed value. The first alternative would be fairly slow and would place unreasonable demands on storage capacity. Thus, our programmer adopts the "compute it yourself" alternative.

Let us discuss the computation of $J_n(x)$ using the recurrence relation [Eq. (12.8)]. Given J_0 and J_1, for example, J_2 (and any other integral order J_n) may be computed from Eq. (12.8). With the opportunities offered by computers, Eq. (12.8) has acquired an interesting new application. In computing a numerical value of $J_N(x_0)$ for a given x_0, one could use the series form of Eq. (12.15) for small x or the asymptotic form [Eq. (12.106)] for large x. A better way, in terms of accuracy and machine utilization, is to use the recurrence relation [Eq. (12.8)] and work **down**.[13] With $n \gg N$ and $n \gg x_0$, assume

$$J_{n+1}(x_0) = 0 \quad \text{and} \quad J_n(x_0) = \alpha,$$

where α is some small number. Then Eq. (12.8) leads to $J_{n-1}(x_0)$, $J_{n-2}(x_0)$, and so on, and finally to $J_0(x_0)$. Since α is arbitrary, the J_n are all off by a common factor. This factor is determined by the condition

$$J_0(x_0) + 2\sum_{m=1}^{\infty} J_{2m}(x_0) = 1.$$

(See Example 12.1.1.) The accuracy of this calculation is checked by trying again at $n' = n + 3$. This technique yields the desired $J_N(x_0)$ and all the lower integral index J_n down to J_0, and it avoids the fatal **accumulation of rounding errors in a recursion relation that works up**. High-precision numerical computation is more or less an art. Modifications and refinements of this and other numerical techniques are proposed every year. For information on the current "state of the art," the student will have to consult the literature, such as *Numerical Recipes* in Additional Reading of Chapter 8, *Atlas for Computing Mathematical Functions* in Additional Reading of Chapter 13, or the journal *Mathematics of Computation*.

[13] Stegun, I.A., and Abramowitz, M. (1957). Generation of Bessel functions on computers. *Math. Tables Aids Comput.* **11**, 255–257.

Table 12.2

Equations for the Computation of Neumann Functions

Note: In practice, it is convenient to limit the series (power or asymptotic) computation of $Y_n(x)$ to $n = 0, 1$. Then $Y_n(x)$, $n \geq 2$ is computed using the recurrence relation, Eq. (12.8).

	Power Series	Asymptotic Series
$Y_n(x)$	Eq. (12.76), $x \leq 4$	Eq. (12.107), $x > 4$

For Y_n, the preferred methods are the series if x is small and the asymptotic forms (with many terms in the series of negative powers) if x is large. The criteria of large and small may vary as shown in Table 12.2.

EXERCISES

12.3.1 In checking the normalization of the integral representation of $J_\nu(z)$ [Eq. (12.94)], we assumed that $Y_\nu(z)$ was not present. How do we know that the integral representation [Eq. (12.94)] does not yield $J_\nu(z) + \varepsilon Y_\nu(z)$ with $\varepsilon \neq 0$ albeit small?

12.3.2 Use the asymptotic expansions to verify the following Wronskian formulas:

(a) $J_\nu(x)J_{-\nu-1}(x) + J_{-\nu}(x)J_{\nu+1}(x) = -2\sin \nu\pi/\pi x$,
(b) $J_\nu(x)Y_{\nu+1}(x) - J_{\nu+1}(x)Y_\nu(x) = -2/\pi x$,
(c) $J_\nu(x)H_\nu^{(2)}(x) - J_{\nu-1}(x)H_\nu^{(2)}(x) = 2/i\pi x$.

12.3.3 Stokes's method.

(a) Replace the Bessel function in Bessel's equation by $x^{-1/2}y(x)$ and show that $y(x)$ satisfies

$$y''(x) + \left(1 - \frac{\nu^2 - \frac{1}{4}}{x^2}\right) y(x) = 0.$$

(b) Develop a power series solution with negative powers of x starting with the assumed form

$$y(x) = e^{ix} \sum_{n=0}^{\infty} a_n x^{-n}.$$

Determine the recurrence relation giving a_{n+1} in terms of a_n. Check your result against the asymptotic formula, Eq. (12.106).

(c) From the results of Section 7.3, determine the initial coefficient, a_0.

12.3.4 (a) Write a subroutine that will generate Bessel functions $J_n(x)$, that is, will generate the numerical value of $J_n(x)$ given x and n.

(b) Check your subroutine by using symbolic software, such as Maple and Mathematica. If possible, compare the machine time needed for this check for several n and x with the time required for your subroutine.

12.4 Spherical Bessel Functions

When the Helmholtz equation is separated in spherical coordinates the radial equation has the form

$$r^2\frac{d^2R}{dr^2}+2r\frac{dR}{dr}+[k^2r^2-n(n+1)]R=0. \tag{12.111}$$

This is Eq. (8.62) of Section 8.5, as we now show. The parameter k enters from the original Helmholtz equation, whereas $n(n+1)$ is a separation constant. From the behavior of the polar angle function (Legendre's equation; Sections 4.3, 8.9, and 11.2), the separation constant must have this form, with n a nonnegative integer. Equation (12.111) has the virtue of being self-adjoint, but clearly it is not Bessel's ODE. However, if we substitute

$$R(kr)=\frac{Z(kr)}{(kr)^{1/2}},$$

Equation (12.111) becomes

$$r^2\frac{d^2Z}{dr^2}+r\frac{dZ}{dr}+\left[k^2r^2-\left(n+\frac{1}{2}\right)^2\right]Z=0, \tag{12.112}$$

which **is Bessel's equation**. Z is a Bessel function of order $n+\frac{1}{2}$ (n an integer). Because of the importance of spherical coordinates, this combination,

$$\frac{Z_{n+1/2}(kr)}{(kr)^{1/2}},$$

occurs often in physics problems.

Definitions

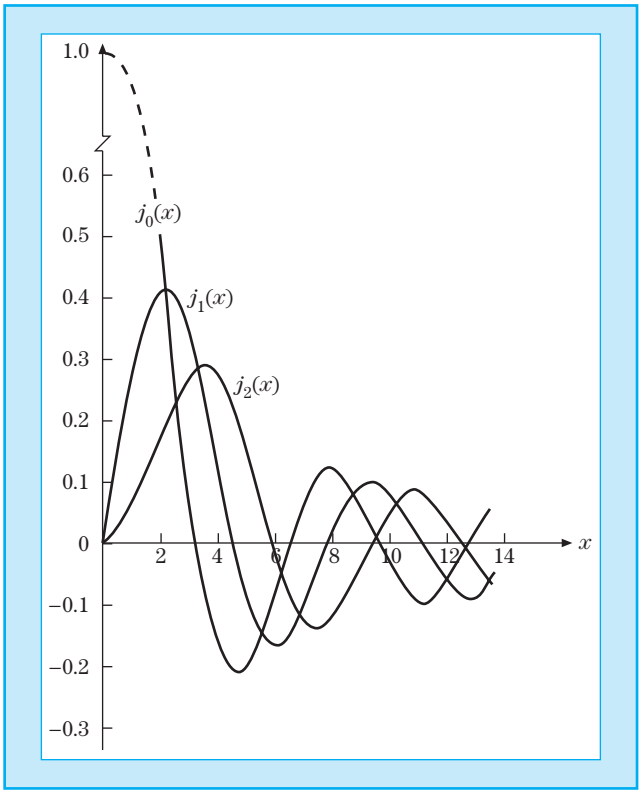
It is convenient to label these functions spherical Bessel functions, with the following defining equations:

$$\begin{aligned}
j_n(x)&=\sqrt{\frac{\pi}{2x}}J_{n+1/2}(x),\\
y_n(x)&=\sqrt{\frac{\pi}{2x}}Y_{n+1/2}(x)=(-1)^{n+1}\sqrt{\frac{\pi}{2x}}J_{-n-1/2}(x),\text{[14]}\\
h_n^{(1)}(x)&=\sqrt{\frac{\pi}{2x}}H_{n+1/2}^{(1)}(x)=j_n(x)+iy_n(x),\\
h_n^{(2)}(x)&=\sqrt{\frac{\pi}{2x}}H_{n+1/2}^{(2)}(x)=j_n(x)-iy_n(x).
\end{aligned} \tag{12.113}$$

[14] This is possible because $\cos(n+\frac{1}{2})\pi=0$ for n an integer.

Figure 12.11

Spherical Bessel Functions



These spherical Bessel functions (Figs. 12.11 and 12.12) can be expressed in series form by using the series [Eq. (12.15)] for J_n, replacing n with $n + \frac{1}{2}$:

$$J_{n+1/2}(x) = \sum_{s=0}^{\infty} \frac{(-1)^s}{s!(s+n+\frac{1}{2})!}\left(\frac{x}{2}\right)^{2s+n+1/2}. \tag{12.114}$$

Using the Legendre duplication formula (Section 10.1),

$$z!\left(z+\frac{1}{2}\right)! = 2^{-2z-1}\pi^{1/2}(2z+1)!, \tag{12.115}$$

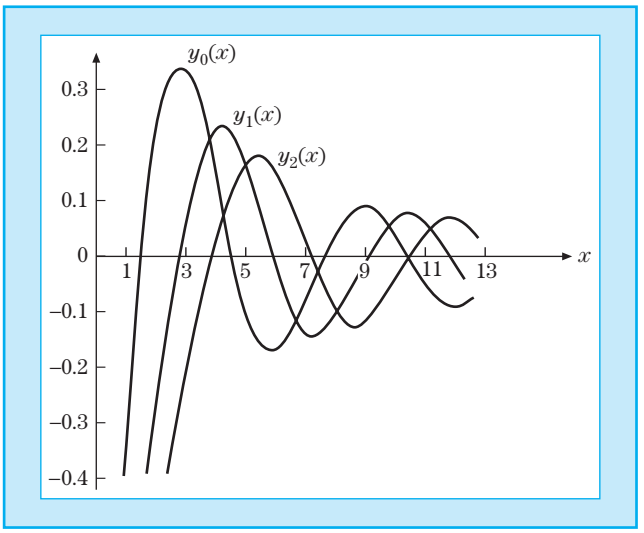
we have

$$j_n(x) = \sqrt{\frac{\pi}{2x}} \sum_{s=0}^{\infty} \frac{(-1)^s 2^{2s+2n+1}(s+n)!}{\pi^{1/2}(2s+2n+1)!s!}\left(\frac{x}{2}\right)^{2s+n+1/2}$$

$$= 2^n x^n \sum_{s=0}^{\infty} \frac{(-1)^s (s+n)!}{s!(2s+2n+1)!} x^{2s}. \tag{12.116}$$

Figure 12.12

Spherical Neumann Functions



Now

$$Y_{n+1/2}(x) = (-1)^{n+1} J_{-n-1/2}(x) = (-1)^{n+1} j_{-n-1}(x)\sqrt{\frac{2x}{\pi}} \tag{12.117}$$

from Eq. (12.72), and from Eq. (12.15) we find that

$$J_{-n-1/2}(x) = \sum_{s=0}^{\infty} \frac{(-1)^s}{s!\left(s-n-\frac{1}{2}\right)!}\left(\frac{x}{2}\right)^{2s-n-1/2}. \tag{12.118}$$

This yields

$$y_n(x) = (-1)^{n+1}\frac{2^n \pi^{1/2}}{x^{n+1}} \sum_{s=0}^{\infty} \frac{(-1)^s}{s!\left(s-n-\frac{1}{2}\right)!}\left(\frac{x}{2}\right)^{2s}. \tag{12.119}$$

We can also use Eq. (12.117), replacing $n \to -n-1$ in Eq. (12.116) to give

$$y_n(x) = \frac{(-1)^{n+1}}{2^n x^{n+1}} \sum_{s=0}^{\infty} \frac{(-1)^s (s-n)!}{s!(2s-2n)!} x^{2s}. \tag{12.120}$$

These series forms, Eqs. (12.116) and (12.120), are useful in two ways:

- limiting values as $x \to 0$,
- closed form representations for $n = 0$.

For the special case $n = 0$ we find from Eq. (12.116)

$$j_0(x) = \sum_{s=0}^{\infty} \frac{(-1)^s}{(2s+1)!} x^{2s} = \frac{\sin x}{x}, \tag{12.121}$$

whereas for y_0, Eq. (12.120) yields

$$y_0(x) = -\frac{\cos x}{x}. \tag{12.122}$$

From the definition of the spherical Hankel functions [Eq. (12.113)],

$$h_0^{(1)}(x) = \frac{1}{x}(\sin x - i\cos x) = -\frac{i}{x}e^{ix}$$
$$h_0^{(2)}(x) = \frac{1}{x}(\sin x + i\cos x) = \frac{i}{x}e^{-ix}. \tag{12.123}$$

Equations (12.121) and (12.122) suggest expressing all spherical Bessel functions as combinations of sine, cosine, and inverse powers of x. The appropriate combinations can be developed from the power series solutions, Eqs. (12.116) and (12.120), but this approach is awkward. We will use recursion relations instead.

Limiting Values

For $x \ll 1$,[15] Eqs. (12.116) and (12.120) yield

$$j_n(x) \approx \frac{2^n n!}{(2n+1)!}x^n = \frac{x^n}{(2n+1)!!} \tag{12.124}$$

$$y_n(x) \approx \frac{(-1)^{n+1}}{2^n}\cdot\frac{(-n)!}{(-2n)!}x^{-n-1}$$
$$= -\frac{(2n)!}{2^n n!}x^{-n-1} = -(2n-1)!!x^{-n-1}. \tag{12.125}$$

The transformation of factorials in the expressions for $y_n(x)$ employs Exercise 10.1.3. The limiting values of the spherical Hankel functions go as $\pm iy_n(x)$.

The asymptotic values of j_n, y_n, $h_n^{(2)}$, and $h_n^{(1)}$ may be obtained from the Bessel asymptotic forms (Section 12.3). We find

$$j_n(x) \sim \frac{1}{x}\sin\left(x - \frac{n\pi}{2}\right), \tag{12.126}$$

$$y_n(x) \sim -\frac{1}{x}\cos\left(x - \frac{n\pi}{2}\right), \tag{12.127}$$

$$h_n^{(1)}(x) \sim (-i)^{n+1}\frac{e^{ix}}{x} = -i\frac{e^{i(x-n\pi/2)}}{x}, \tag{12.128a}$$

$$h_n^{(2)}(x) \sim i^{n+1}\frac{e^{-ix}}{x} = i\frac{e^{-i(x-n\pi/2)}}{x}. \tag{12.128b}$$

The condition for these spherical Bessel forms is that $x \gg n(n+1)/2$. From these asymptotic values we see that $j_n(x)$ and $y_n(x)$ are appropriate for a description of **standing spherical waves**; $h_n^{(1)}(x)$ and $h_n^{(2)}(x)$ correspond to **traveling spherical waves**. If the time dependence for the traveling waves is taken to be $e^{-i\omega t}$, then $h_n^{(1)}(x)$ yields an outgoing traveling spherical wave and

[15] The condition that the second term in the series be negligible compared to the first is actually $x \ll 2[(2n+2)(2n+3)/(n+1)]^{1/2}$ for $j_n(x)$.

$h_n^{(2)}(x)$ an incoming wave. Radiation theory in electromagnetism and scattering theory in quantum mechanics provide many applications.

EXAMPLE 12.4.1

Particle in a Sphere An illustration of the use of the spherical Bessel functions is provided by the problem of a quantum mechanical particle in a sphere of radius a. Quantum theory requires that the wave function ψ, describing our particle, satisfy

$$-\frac{\hbar^2}{2m}\nabla^2\psi = E\psi, \tag{12.129}$$

and the boundary conditions (i) $\psi(r \le a)$ remains finite, (ii) $\psi(a) = 0$. This corresponds to a square well potential $V = 0, r \le a$, and $V = \infty, r > a$. Here, $\hbar$ is Planck's constant divided by 2π, m is the mass of our particle, and E is its energy. Let us determine the **minimum** value of the energy for which our wave equation has an acceptable solution. Equation (12.129) is Helmholtz's equation with a radial part (compare Example 12.1.4):

$$\frac{d^2R}{dr^2} + \frac{2}{r}\frac{dR}{dr} + \left[k^2 - \frac{n(n+1)}{r^2}\right]R = 0, \tag{12.130}$$

with $k^2 = 2mE/\hbar^2$. Hence, by Eq. (12.111), with $n = 0$,

$$R = Aj_0(kr) + By_0(kr).$$

We choose the orbital angular momentum index $n = 0$. Any angular dependence would raise the energy because of the repulsive angular momentum barrier [involving $n(n+1) > 0$]. The spherical Neumann function is rejected because of its divergent behavior at the origin. To satisfy the second boundary condition (for all angles), we require

$$ka = \frac{\sqrt{2mE}}{\hbar}a = \alpha, \tag{12.131}$$

where α is a root of j_0; that is, $j_0(\alpha) = 0$. This has the effect of limiting the allowable energies to a certain discrete set; in other words, application of boundary condition (ii) quantizes the energy E. The smallest α is the first zero of j_0,

$$\alpha = \pi$$

and

$$E_{\min} = \frac{\pi^2\hbar^2}{2ma^2} = \frac{h^2}{8ma^2}, \tag{12.132}$$

which means that for any finite sphere the particle energy will have a positive minimum or zero point energy. Compare this energy with $E = \frac{h^2}{8m}(\frac{1}{a^2} + \frac{1}{b^2} + \frac{1}{c^2})$ of an infinite rectangular square well of lengths $a,\ b,\ c$. This example is an illustration of the Heisenberg uncertainty principle for $\Delta p \sim \hbar\pi/a$ from de Broglie's relation and $\Delta r \sim a$ so that $\Delta p \Delta r \sim h/2$. ■

Recurrence Relations

The recurrence relations to which we now turn provide a convenient way of developing the higher order spherical Bessel functions. These recurrence relations may be derived from the series, but as with the modified Bessel functions, it is easier to substitute into the known recurrence relations [Eqs. (12.8) and (12.21)]. This gives

$$f_{n-1}(x) + f_{n+1}(x) = \frac{2n+1}{x} f_n(x), \tag{12.133}$$

$$nf_{n-1}(x) - (n+1)f_{n+1}(x) = (2n+1)f_n'(x). \tag{12.134}$$

Rearranging these relations [or substituting into Eqs. (12.1) and (12.6)], we obtain

$$\frac{d}{dx}[x^{n+1} f_n(x)] = x^{n+1} f_{n-1}(x) \tag{12.135}$$

$$\frac{d}{dx}[x^{-n} f_n(x)] = -x^{-n} f_{n+1}(x), \tag{12.136}$$

where f_n may represent j_n, y_n, $h_n^{(1)}$, or $h_n^{(2)}$.

Specific forms may also be readily obtained from Eqs. (12.133) and (12.134):

$$h_1^{(1)}(x) = e^{ix}\left(-\frac{1}{x} - \frac{i}{x^2}\right), \tag{12.137a}$$

$$h_2^{(1)}(x) = e^{ix}\left(\frac{i}{x} - \frac{3}{x^2} - \frac{3i}{x^3}\right), \tag{12.137b}$$

$$\begin{aligned} j_1(x) &= \frac{\sin x}{x^2} - \frac{\cos x}{x}, \\ j_2(x) &= \left(\frac{3}{x^3} - \frac{1}{x}\right)\sin x - \frac{3}{x^2}\cos x, \end{aligned} \tag{12.138}$$

$$\begin{aligned} y_1(x) &= -\frac{\cos x}{x^2} - \frac{\sin x}{x}, \\ y_2(x) &= -\left(\frac{3}{x^3} - \frac{1}{x}\right)\cos x - \frac{3}{x^2}\sin x, \end{aligned} \tag{12.139}$$

and so on.

By mathematical induction one may establish the Rayleigh formulas

$$j_n(x) = (-1)^n x^n \left(\frac{1}{x}\frac{d}{dx}\right)^n \left(\frac{\sin x}{x}\right), \tag{12.140}$$

$$y_n(x) = -(-1)^n x^n \left(\frac{1}{x}\frac{d}{dx}\right)^n \left(\frac{\cos x}{x}\right), \tag{12.141}$$

$$\begin{aligned} h_n^{(1)}(x) &= -i(-1)^n x^n \left(\frac{1}{x}\frac{d}{dx}\right)^n \left(\frac{e^{ix}}{x}\right), \\ h_n^{(2)}(x) &= i(-1)^n x^n \left(\frac{1}{x}\frac{d}{dx}\right)^n \left(\frac{e^{-ix}}{x}\right). \end{aligned} \tag{12.142}$$

Numerical Computation

The spherical Bessel functions are computed using the same techniques described in Sections 12.1 and 12.3 for evaluating the Bessel functions. For $j_n(x)$ it is convenient to use Eq. (12.133) and work **downward**, as is done for $J_n(x)$. Normalization is accomplished by comparing with the known forms of $j_0(x)$, Eqs. (12.121) and Exercise 12.4.11. For $y_n(x)$, Eq. (12.120) is used again, but this time working upward, starting with the known forms of $y_0(x)$, $y_1(x)$ [Eqs. (12.122) and (12.139)].

EXAMPLE 12.4.2

Phase Shifts Here we show that spherical Bessel functions are needed to define phase shifts for scattering from a spherically symmetric potential $V(r)$. The radial wave function $R_l(r) = u(r)/r$ of the Schrödinger equation satisfies the ODE

$$\left[-\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right) + \frac{l(l+1)}{r^2} + \frac{2m}{\hbar^2}V(r) - k^2\right]R_l(r) = 0, \tag{12.143}$$

where m is the reduced mass, $E = \hbar^2k^2/2m$ the energy eigenvalue, and the scattering potential V goes to zero (exponentially) for $r \to \infty$. At large values of r, where V is negligible, this ODE is identical to Eqs. (12.111), with the general solution a linear combination of the regular and irregular solutions; that is,

$$R_l(r) = A_l j_l(kr) + B_l y_l(kr), \quad r \to \infty. \tag{12.144}$$

Using the asymptotic expansions Eqs. (12.126) and (12.127) we have

$$R_l(r) \sim A_l\frac{\sin(kr - l\pi/2)}{kr} - B_l\frac{\cos(kr - l\pi/2)}{kr}, \quad r \to \infty. \tag{12.145}$$

If there is no scattering, that is, $V(r) = 0$, then the incident plane wave is our solution and $B_l = 0$ because it has no y_l contribution, being finite everywhere. Therefore, $B_l/A_l \equiv -\tan\delta_l(k)$ is a measure for the amount of scattering at momentum $\hbar k$.

Because we can rewrite Eq. (12.145) as

$$R_l(r) \sim C_l\frac{\sin(kr - l\pi/2 + \delta_l)}{kr}, \quad C_l = \frac{A_l}{\cos\delta_l}, \tag{12.146}$$

δ_l is called the phase shift; it depends on the incident energy.

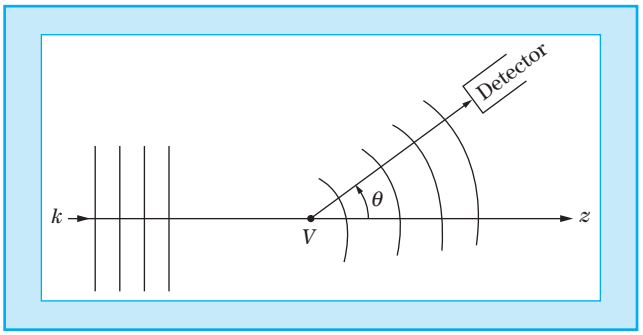
We expand the scattering wave function ψ in Legendre polynomials $P_l(\cos\theta)$ with the scattering angle θ defined by the position $\mathbf{r}$ of the detector (Fig. 12.13). Then we compare with the asymptotic expression of the wave function

$$\psi(\mathbf{r}) \sim e^{ikz} + f(\theta)\frac{e^{ikr}}{r}$$

by substituting the Rayleigh expansion (Exercise 12.4.21) for the incident plane wave and replacing the spherical Bessel functions in this expansion by their asymptotic form. For further details, see Griffiths, *Introduction to Quantum Mechanics*, Section 11.2. Prentice-Hall, New York (1994). As a result, one finds

Figure 12.13

Incident Plane Wave Is Scattered by a Potential V into an Outgoing Radial Wave



the partial wave expansion of the scattering amplitude as the coefficient of the outgoing radial wave,

$$f(\theta) = \frac{1}{k}\sum_{l=0}^{\infty}(2l+1)e^{i\delta_l(k)}\sin\delta_l P_l(\cos\theta). \tag{12.147}$$

Upon integrating $|f(\theta)|^2$ over the scattering angle using the orthogonality of Legendre polynomials we obtain the total scattering cross section

$$\sigma = \int |f(\theta|^2\, d\Omega = \frac{4\pi}{k}\sum_{l=0}^{\infty}(2l+1)\sin^2\delta_l. \tag{12.148}$$

SUMMARY

Bessel functions of integer order are defined by a power series expansion of their generating function

$$e^{(x/2)(t-1/t)} = \sum_{n=-\infty}^{\infty} J_n(x)t^n.$$

Bessel and Neumann functions are the regular and irregular solutions of Bessel's ODE, which arises in the separation of variables in prominent PDEs, such as Laplace's equation with spherical or cylindrical symmetry and the heat and Helmholtz equations. Many of the properties of Bessel functions are consequences of the Sturm–Liouville theory of their differential equation.

EXERCISES

12.4.1 Show that if

$$y_n(x) = \sqrt{\frac{\pi}{2x}}Y_{n+1/2}(x),$$

it automatically equals

$$(-1)^{n+1}\sqrt{\frac{\pi}{2x}}J_{-n-1/2}(x).$$

12.4.2 Derive the trigonometric–polynomial forms of $j_n(z)$ and $y_n(z)$:[16]

$$j_n(z) = \frac{1}{z}\sin\left(z - \frac{n\pi}{2}\right)\sum_{s=0}^{[n/2]}\frac{(-1)^s(n+2s)!}{(2s)!(2z)^{2s}(n-2s)!} + \frac{1}{z}\cos\left(z - \frac{n\pi}{2}\right)\sum_{s=0}^{[(n-1)/2]}\frac{(-1)^s(n+2s+1)!}{(2s+1)!(2z)^{2s}(n-2s-1)!}$$

$$y_n(z) = \frac{(-1)^{n+1}}{z}\cos\left(z + \frac{n\pi}{2}\right)\sum_{s=0}^{[n/2]}\frac{(-1)^s(n+2s)!}{(2s)!(2z)^{2s}(n-2s)!} + \frac{(-1)^{n+1}}{z}\sin\left(z + \frac{n\pi}{2}\right)\sum_{s=0}^{[(n-1)/2]}\frac{(-1)^s(n+2s+1)!}{(2s+1)!(2z)^{2s+1}(n-2s-1)!}.$$

12.4.3 Use the integral representation of $J_\nu(x)$,

$$J_\nu(x) = \frac{1}{\pi^{1/2}(\nu - \frac{1}{2})!}\left(\frac{x}{2}\right)^\nu \int_{-1}^{1} e^{\pm ixp}(1-p^2)^{\nu-1/2}\,dp,$$

to show that the spherical Bessel functions $j_n(x)$ are expressible in terms of trigonometric functions; that is, for example,

$$j_0(x) = \frac{\sin x}{x}, \qquad j_1(x) = \frac{\sin x}{x^2} - \frac{\cos x}{x}.$$

12.4.4 (a) Derive the recurrence relations

$$f_{n-1}(x) + f_{n+1}(x) = \frac{2n+1}{x}f_n(x),$$

$$n f_{n-1}(x) - (n+1)f_{n+1}(x) = (2n+1)f_n'(x),$$

satisfied by the spherical Bessel functions $j_n(x)$, $y_n(x)$, $h_n^{(1)}(x)$, and $h_n^{(2)}(x)$.

(b) Show from these two recurrence relations that the spherical Bessel function $f_n(x)$ satisfies the differential equation

$$x^2 f_n''(x) + 2x f_n'(x) + [x^2 - n(n+1)]f_n(x) = 0.$$

12.4.5 Prove by mathematical induction that

$$j_n(x) = (-1)^n x^n \left(\frac{1}{x}\frac{d}{dx}\right)^n \left(\frac{\sin x}{x}\right)$$

for n an arbitrary nonnegative integer.

12.4.6 From the discussion of orthogonality of the spherical Bessel functions, show that a Wronskian relation for $j_n(x)$ and $y_n(x)$ is

$$j_n(x)y_n'(x) - j_n'(x)\,y_n(x) = \frac{1}{x^2}.$$

[16]The upper limit on the summation $[n/2]$ means the largest **integer** that does not exceed $n/2$.

12.4.7 Verify

$$h_n^{(1)}(x)h_n^{(2)'}(x) - h_n^{(1)'}(x)h_n^{(2)}(x) = -\frac{2i}{x^2}.$$

12.4.8 Verify Poisson's integral representation of the spherical Bessel function,

$$j_n(z) = \frac{z^n}{2^{n+1}n!}\int_0^\pi \cos(z\cos\theta)\sin^{2n+1}\theta\, d\theta.$$

12.4.9 Show that

$$\int_0^\infty J_\mu(x)J_\nu(x)\frac{dx}{x} = \frac{2}{\pi}\frac{\sin[(\mu-\nu)\pi/2]}{\mu^2-\nu^2}, \qquad \mu+\nu>0.$$

12.4.10 Derive

$$\int_{-\infty}^{\infty} j_m(x)j_n(x)\,dx = 0, \qquad \begin{matrix} m\neq n \\ m,\, n\geq 0. \end{matrix}$$

12.4.11 Derive

$$\int_{-\infty}^{\infty}[j_n(x)]^2\,dx = \frac{\pi}{2n+1}.$$

12.4.12 Set up the orthogonality integral for $j_l(kr)$ in a sphere of radius R with the boundary condition

$$j_l(kR) = 0.$$

The result is used in classifying electromagnetic radiation according to its angular momentum l.

12.4.13 The Fresnel integrals (Fig. 12.14) occurring in diffraction theory are given by

$$x(t) = \int_0^t \cos(v^2)\,dv, \qquad y(t) = \int_0^t \sin(v^2)\,dv.$$

Show that these integrals may be expanded in series of spherical Bessel functions

$$x(s) = \frac{1}{2}\int_0^s j_{-1}(u)u^{1/2}\,du = s^{1/2}\sum_{n=0}^{\infty} j_{2n}(s),$$

$$y(s) = \frac{1}{2}\int_0^s j_0(u)u^{1/2}\,du = s^{1/2}\sum_{n=0}^{\infty} j_{2n+1}(s).$$

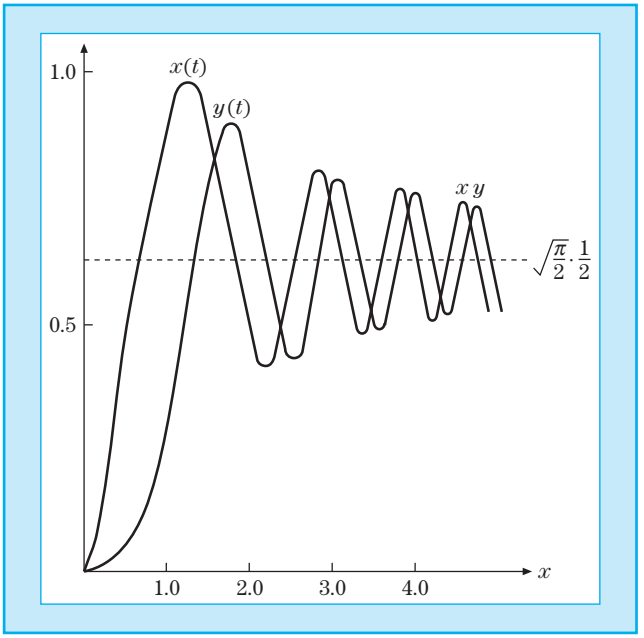
Hint. To establish the equality of the integral and the sum, you may wish to work with their derivatives. The spherical Bessel analogs of Eqs. (12.7) and (12.21) are helpful.

12.4.14 A hollow sphere of radius a (Helmholtz resonator) contains standing sound waves. Find the minimum frequency of oscillation in terms of the radius a and the velocity of sound v. The sound waves satisfy the wave equation

$$\nabla^2\psi = \frac{1}{v^2}\frac{\partial^2\psi}{\partial t^2}$$

Figure 12.14

Fresnel Integrals



and the boundary condition

$$\frac{\partial \psi}{\partial r} = 0, \quad r = a.$$

This is a Neumann boundary condition. Example 12.4.1 has the same PDE but with a Dirichlet boundary condition.

ANS. $\nu_{\min} = 0.3313v/a, \quad \lambda_{\max} = 3.018a.$

12.4.15 A quantum particle is trapped in a spherically symmetric well of radius a. The Schrödinger equation potential is

$$V(r) = \begin{cases} -V_0, & 0 \le r < a \\ 0, & r > a. \end{cases}$$

The particle's energy E is negative (an eigenvalue).

(a) Show that the radial part of the wave function is given by $j_l(k_1 r)$ for $0 \le r < a$ and $j_l^{\text{out}}(k_2 r)$ for $r > a$. [We require that $\psi(0)$ and $\psi(\infty)$ be finite.] Here, $k_1^2 = 2M(E + V_0)/\hbar^2$, $k_2^2 = -2ME/\hbar^2$, and l is the angular momentum [n in Eq. (12.111)].

(b) The boundary condition at $r = a$ is that the wave function $\psi(r)$ and its first derivative be continuous. Show that this means

$$\left.\frac{(d/dr) j_l(k_1 r)}{j_l(k_1 r)}\right|_{r=a} = \left.\frac{(d/dr) j_l^{\text{out}}(k_2 r)}{j_l^{\text{out}}(k_2 r)}\right|_{r=a}.$$

This equation determines the energy eigenvalues.

Note. This is a generalization of the deuteron Example 9.1.3.

12.4.16 The quantum mechanical radial wave function for a scattered wave is given by

$$\psi_k = \frac{\sin(kr + \delta_0)}{kr},$$

where k is the wave number, $k = \sqrt{2mE/\hbar}$, and δ_0 is the scattering phase shift. Show that the normalization integral is

$$\int_0^\infty \psi_k(r)\psi_{k'}(r)r^2\,dr = \frac{\pi}{2k}\delta(k - k').$$

Hint. You can use a sine representation of the Dirac delta function.

12.4.17 Derive the spherical Bessel function closure relation

$$\frac{2a^2}{\pi}\int_0^\infty j_n(ar)j_n(br)r^2\,dr = \delta(a - b).$$

Note. An interesting derivation involving Fourier transforms, the Rayleigh plane wave expansion, and spherical harmonics has been given by P. Ugincius, *Am. J. Phys.* **40**, 1690 (1972).

12.4.18 The wave function of a particle in a sphere (Example 12.4.2) with angular momentum l is $\psi(r, \theta, \varphi) = Aj_l((\sqrt{2ME})r/\hbar)Y_l^m(\theta, \varphi)$. The $Y_l^m(\theta, \varphi)$ is a spherical harmonic, described in Section 11.5. From the boundary condition $\psi(a, \theta, \varphi) = 0$ or $j_l((\sqrt{2ME})a/\hbar) = 0$, calculate the 10 lowest energy states. Disregard the m degeneracy ($2l+1$ values of m for each choice of l). Check your results against Maple, Mathematica, etc.

Check values. $j_l(\alpha_{ls}) = 0$

$$\alpha_{01} = 3.1416$$
$$\alpha_{11} = 4.4934$$
$$\alpha_{21} = 5.7635$$
$$\alpha_{02} = 6.2832.$$

12.4.19 Let Example 12.4.1 be modified so that the potential is a finite V_0 outside ($r > a$). Use symbolic software (Mathematica, Maple, etc.).
(a) For $E < V_0$ show that

$$\psi_{\text{out}}(r, \theta, \varphi) \sim j_l^{\text{out}}\left(\frac{r}{\hbar}\sqrt{2M(V_0 - E)}\right).$$

(b) The new boundary conditions to be satisfied at $r = a$ are

$$\psi_{\text{in}}(a, \theta, \varphi) = \psi_{\text{out}}(a, \theta, \varphi)$$
$$\frac{\partial}{\partial r}\psi_{\text{in}}(a, \theta, \varphi) = \frac{\partial}{\partial r}\psi_{\text{out}}(a, \theta, \varphi)$$

or

$$\frac{1}{\psi_{\text{in}}}\frac{\partial\psi_{\text{in}}}{\partial r}\bigg|_{r=a} = \frac{1}{\psi_{\text{out}}}\frac{\partial\psi_{\text{out}}}{\partial r}\bigg|_{r=a}.$$

For $l = 0$ show that the boundary condition at $r = a$ leads to

$$f(E) = k\left\{\cot ka - \frac{1}{ka}\right\} + k'\left\{1 + \frac{1}{k'a}\right\} = 0,$$

where $k = \sqrt{2ME}/\hbar$ and $k' = \sqrt{2M(V_0 - E)}/\hbar$.

(c) With $a = \hbar^2/Me^2$ (Bohr radius) and $V_0 = 4Me^4/2\hbar^2$, compute the possible bound states ($0 < E < V_0$).
Hint. Call a root-finding subroutine after you know the approximate location of the roots of

$$f(E) = 0, \quad (0 \le E \le V_0).$$

(d) Show that when $a = \hbar^2/Me^2$ the minimum value of V_0 for which a bound state exists is $V_0 = 2.4674Me^4/2\hbar^2$.

12.4.20 In some nuclear stripping reactions the differential cross section is proportional to $j_l(x)^2$, where l is the angular momentum. The location of the maximum on the curve of experimental data permits a determination of l if the location of the (first) maximum of $j_l(x)$ is known. Compute the location of the first maximum of $j_1(x)$, $j_2(x)$, and $j_3(x)$.
Note. For better accuracy, look for the first zero of $j_l'(x)$. Why is this more accurate than direct location of the maximum?

12.4.21 A plane wave may be expanded in a series of spherical waves by the Rayleigh equation

$$e^{ikr\cos\gamma} = \sum_{n=0}^{\infty} a_n j_n(kr) P_n(\cos\gamma).$$

Show that $a_n = i^n(2n + 1)$.
Hint.

- Use the orthogonality of the P_n to solve for $a_n j_n(kr)$.
- Differentiate n times with respect to kr and set $r = 0$ to eliminate the r dependence.
- Evaluate the remaining integral by Exercise 11.4.4.

12.4.22 Verify the Rayleigh expansion of Exercise 12.4.21 by starting with the following steps:

- Differentiate with respect to kr to establish

$$\sum_n j_n'(kr) P_n(\cos\gamma) = i\sum_n a_n j_n(kr)\cos\gamma\, P_n(\cos\gamma).$$

- Use a recurrence relation to replace $\cos\gamma\, P_n(\cos\gamma)$ by a linear combination of P_{n-1} and P_{n+1}.
- Use a recurrence relation to replace j_n' by a linear combination of j_{n-1} and j_{n+1}.

12.4.23 The Legendre polynomials and the spherical Bessel functions are related by

$$j_n(z) = \frac{1}{2}(-1)^n \int_0^{\pi} e^{iz\cos\theta} P_n(\cos\theta)\sin\theta\, d\theta, \quad n = 0, 1, 2 \ldots.$$

Verify this relation by transforming the right-hand side into

$$\frac{z^n}{2^{n+1}n!}\int_0^\pi \cos(z\cos\theta)\sin^{2n+1}\theta\,d\theta$$

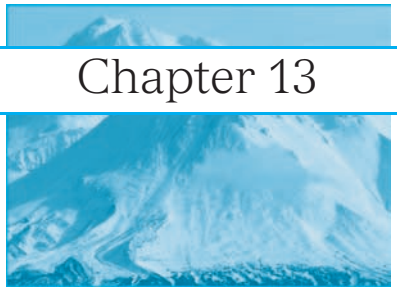
using Exercise 12.4.21.

Additional Reading

McBride, E. B. (1971). *Obtaining Generating Functions*. Springer-Verlag, New York. An introduction to methods of obtaining generating functions.

Watson, G. N. (1922). *A Treatise on the Theory of Bessel Functions*. Cambridge Univ. Press, Cambridge, UK.

Watson, G. N. (1952). *A Treatise on the Theory of Bessel Functions*, 2nd ed. Cambridge Univ. Press, Cambridge, UK. This is the definitive text on Bessel functions and their properties. Although difficult reading, it is invaluable as the ultimate reference.



Chapter 13

Hermite and Laguerre Polynomials

In this chapter we study two sets of orthogonal polynomials, Hermite and Laguerre polynomials. These sets are less common in mathematical physics than the Legendre and Bessel functions of Chapters 11 and 12, but Hermite polynomials occur in solutions of the simple harmonic oscillator of quantum mechanics and Laguerre polynomials in wave functions of the hydrogen atom.

Because the general mathematical techniques are similar to those of the preceding two chapters, the development of these functions is only outlined. Some detailed proofs, along the lines of Chapters 11 and 12, are left to the reader. We start with Hermite polynomials.

13.1 Hermite Polynomials

Quantum Mechanical Simple Harmonic Oscillator

For the physicist, Hermite polynomials are synonymous with the one-dimensional (i.e., simple) harmonic oscillator of quantum mechanics. For a potential energy

$$V = \frac{1}{2}Kz^2 = \frac{1}{2}m\omega^2 z^2, \quad \text{force} \quad F_z = -\partial V/\partial z = -Kz,$$

the Schrödinger equation of the quantum mechanical system is

$$-\frac{\hbar^2}{2m}\frac{d^2}{dz^2}\Psi(z) + \frac{1}{2}Kz^2\Psi(z) = E\Psi(z). \tag{13.1}$$

Our oscillating particle has mass m and total energy E. From quantum mechanics, we recall that for bound states the boundary conditions

$$\lim_{z\to\pm\infty} \Psi(z) = 0 \tag{13.2}$$

restrict the energy eigenvalue E to a discrete set $E_n = \lambda_n \hbar\omega$, where ω is the angular frequency of the corresponding classical oscillator. It is introduced by rescaling the coordinate z in favor of the dimensionless variable x and transforming the parameters as follows:

$$x = \alpha z \quad \text{with} \quad \alpha^4 \equiv \frac{mK}{\hbar^2} \equiv \frac{m^2\omega^2}{\hbar^2}, \tag{13.3}$$
$$2\lambda_n \equiv \frac{2E_n}{\hbar}\left(\frac{m}{K}\right)^{1/2} = \frac{2E_n}{\hbar\omega}.$$

Eq.(13.1) becomes [with $\Psi(z) = \Psi(x/\alpha) = \psi(x)$] the ordinary differential equation (ODE)

$$\frac{d^2\psi_n(x)}{dx^2} + (2\lambda_n - x^2)\psi_n(x) = 0. \tag{13.4}$$

If we substitute $\psi_n(x) = e^{-x^2/2}H_n(x)$ into Eq. (13.4), we obtain the ODE

$$H_n'' - 2xH_n' + (2\lambda_n - 1)H_n = 0 \tag{13.5}$$

of Exercise 8.5.6. A power series solution of Eq. (13.5) shows that $H_n(x)$ will behave as e^{x^2} for large x, unless $\lambda_n = n + 1/2$, $n = 0, 1, 2, \ldots$. Thus, $\psi_n(x)$ and $\Psi_n(z)$ will blow up at infinity, and it will be impossible for the wave function $\Psi(z)$ to satisfy the boundary conditions [Eq. (13.2)] unless

$$E_n = \lambda_n\hbar\omega = \left(n + \frac{1}{2}\right)\hbar\omega, \quad n = 0, 1, 2\ldots \tag{13.6}$$

This is the key property of the harmonic oscillator spectrum. We see that the energy is quantized and that there is a minimum or zero point energy

$$E_{\min} = E_0 = \frac{1}{2}\hbar\omega.$$

This zero point energy is an aspect of the uncertainty principle, a genuine quantum phenomenon. Also, with $2\lambda_n - 1 = 2n$, Eq. (13.5) becomes Hermite's ODE and $H_n(x)$ are the Hermite polynomials. The solutions ψ_n (Fig. 13.1) of Eq. (13.4) are proportional to the Hermite polynomials[1] $H_n(x)$.

This is the differential equations approach, a standard quantum mechanical treatment. However, we shall prove these statements next employing the method of ladder operators.

Raising and Lowering Operators

The following development is analogous to the use of the raising and lowering operators for angular momentum operators presented in Section 4.3. The key aspect of Eq. (13.4) is that its Hamiltonian

$$-2\mathcal{H} \equiv \frac{d^2}{dx^2} - x^2 = \left(\frac{d}{dx} - x\right)\left(\frac{d}{dx} + x\right) + \left[x, \frac{d}{dx}\right] \tag{13.7}$$

[1]Note the absence of a superscript, which distinguishes Hermite polynomials from the unrelated Hankel functions in Chapter 12.

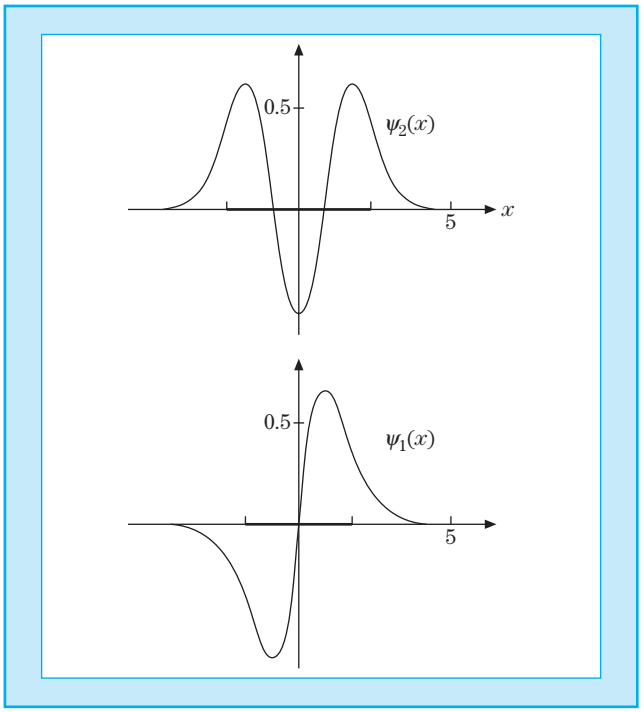


Figure 13.1

Quantum Mechanical Oscillator Wave Functions. The Heavy Bar on the x-Axis Indicates the Allowed Range of the Classical Oscillator with the Same Total Energy

almost factorizes. Using naively $a^2 - b^2 = (a-b)(a+b)$, the basic commutator $[p_x, x] = \hbar/i$ of quantum mechanics [with momentum $p_x = (\hbar/i)d/dx$] enters as a correction in Eq. (13.7). [Because p_x is Hermitian, d/dx is anti-Hermitian, $(d/dx)^\dagger = -d/dx$.] This commutator can be evaluated as follows. Imagine the differential operator d/dx acts on a wave function $\psi(x)$ to the right, as in Eq. (13.4), so that

$$\frac{d}{dx}(x\psi) = x\frac{d}{dx}\psi + \psi \tag{13.8}$$

by the product rule. Dropping the wave function ψ from Eq. (13.8), we rewrite Eq. (13.8) as

$$\frac{d}{dx}x - x\frac{d}{dx} \equiv \left[\frac{d}{dx}, x\right] = 1, \tag{13.9}$$

a constant, and then verify Eq. (13.7) directly by expanding the product. The product form of Eq. (13.7), up to the constant commutator, suggests introducing the non-Hermitian operators

$$\hat{a}^\dagger \equiv \frac{1}{\sqrt{2}}\left(x - \frac{d}{dx}\right), \qquad \hat{a} \equiv \frac{1}{\sqrt{2}}\left(x + \frac{d}{dx}\right), \tag{13.10}$$

with $(\hat{a})^\dagger = \hat{a}^\dagger$. They obey the commutation relations

$$[\hat{a}, \hat{a}^\dagger] = \left[\frac{d}{dx}, x\right] = 1, \qquad [\hat{a}, \hat{a}] = 0 = [\hat{a}^\dagger, \hat{a}^\dagger], \tag{13.11}$$

which are characteristic of these operators and straightforward to derive from Eq. (13.9) and

$$[d/dx, d/dx] = 0 = [x, x] \quad \text{and} \quad [x, d/dx] = -[d/dx, x].$$

Returning to Eq. (13.7) and using Eq. (13.10), we rewrite the Hamiltonian as

$$\mathcal{H} = \hat{a}^\dagger \hat{a} + \frac{1}{2} = \hat{a}^\dagger \hat{a} + \frac{1}{2}[\hat{a}, \hat{a}^\dagger] = \frac{1}{2}(\hat{a}^\dagger \hat{a} + \hat{a}\hat{a}^\dagger) \tag{13.12}$$

and introduce the Hermitian **number operator** $N = \hat{a}^\dagger \hat{a}$ so that $\mathcal{H} = N + 1/2$. We also use the simpler notation $\psi_n = |n\rangle$ so that Eq. (13.4) becomes

$$\mathcal{H}|n\rangle = \lambda_n |n\rangle.$$

Now we prove the key property that N has nonnegative integer eigenvalues

$$N|n\rangle = \left(\lambda_n - \frac{1}{2}\right)|n\rangle = n|n\rangle, \quad n = 0, 1, 2, \ldots, \tag{13.13}$$

that is, $\lambda_n = n + 1/2$. From

$$|\hat{a}|n\rangle|^2 = \langle n|\hat{a}^\dagger \hat{a}|n\rangle = \left(\lambda_n - \frac{1}{2}\right) \geq 0, \tag{13.14}$$

we see that N has nonnegative eigenvalues.

We now show that the commutation relations

$$[N, \hat{a}^\dagger] = \hat{a}^\dagger, \qquad [N, \hat{a}] = -\hat{a}, \tag{13.15}$$

which follow from Eq. (13.11), characterize N as the number operator that counts the oscillator quanta in the eigenstate $|n\rangle$. To this end, we determine the eigenvalue of N for the states $\hat{a}^\dagger|n\rangle$ and $\hat{a}|n\rangle$. Using $\hat{a}\hat{a}^\dagger = N + 1$, we see that

$$N(\hat{a}^\dagger|n\rangle) = \hat{a}^\dagger(N+1)|n\rangle = \left(\lambda_n + \frac{1}{2}\right)\hat{a}^\dagger|n\rangle = (n+1)\hat{a}^\dagger|n\rangle, \tag{13.16}$$

$$N(\hat{a}|n\rangle) = (\hat{a}\hat{a}^\dagger - 1)\hat{a}|n\rangle = \hat{a}(N-1)|n\rangle = \left(\lambda_n - \frac{1}{2}\right)\hat{a}|n\rangle$$
$$= (n-1)\hat{a}|n\rangle.$$

In other words, N acting on $\hat{a}^\dagger|n\rangle$ shows that $\hat{a}^\dagger$ has raised the eigenvalue n of $|n\rangle$ by one unit; hence its name **raising or creation operator**. Applying $\hat{a}^\dagger$ repeatedly, we can reach all higher excitations. There is no upper limit to the sequence of eigenvalues. Similarly, $\hat{a}$ lowers the eigenvalue n by one unit; hence, it is a **lowering or annihilation operator**. Therefore,

$$\hat{a}^\dagger|n\rangle \sim |n+1\rangle, \qquad \hat{a}|n\rangle \sim |n-1\rangle. \tag{13.17}$$

Applying $\hat{a}$ repeatedly, we can reach the lowest or ground state $|0\rangle$ with eigenvalue λ_0. We cannot step lower because $\lambda_0 \geq 1/2$. Therefore, $\hat{a}|0\rangle \equiv 0$,

suggesting we construct $\psi_0 = |0\rangle$ from the (factored) **first-order** ODE

$$\sqrt{2}\hat{a}\psi_0 = \left(\frac{d}{dx} + x\right)\psi_0 = 0. \tag{13.18}$$

Integrating

$$\frac{\psi_0'}{\psi_0} = -x, \tag{13.19}$$

we obtain

$$\ln \psi_0 = -\frac{1}{2}x^2 + \ln c_0, \tag{13.20}$$

where c_0 is an integration constant. The solution

$$\psi_0(x) = c_0 e^{-x^2/2} \tag{13.21}$$

can be normalized, with $c_0 = \pi^{-1/4}$ using the error integral. Substituting ψ_0 into Eq. (13.4) we find

$$\mathcal{H}|0\rangle = \left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)|0\rangle = \frac{1}{2}|0\rangle \tag{13.22}$$

so that its energy eigenvalue is $\lambda_0 = 1/2$ and its number eigenvalue is $n = 0$, confirming the notation $|0\rangle$. Applying $\hat{a}^\dagger$ repeatedly to $\psi_0 = |0\rangle$, all other eigenvalues are confirmed to be $\lambda_n = n + 1/2$, proving Eq. (13.13). The normalizations in Eq. (13.17) follow from Eqs. (13.14), (13.16), and

$$|\hat{a}^\dagger|n\rangle|^2 = \langle n|\hat{a}\hat{a}^\dagger|n\rangle = \langle n|\hat{a}^\dagger\hat{a} + 1|n\rangle = n + 1, \tag{13.23}$$

showing

$$\sqrt{n+1}|n+1\rangle = \hat{a}^\dagger|n\rangle, \qquad \sqrt{n}|n-1\rangle = \hat{a}|n\rangle. \tag{13.24}$$

Thus, the excited-state wave functions, ψ_1, ψ_2, and so on, are generated by the raising operator

$$|1\rangle = \hat{a}^\dagger|0\rangle = \frac{1}{\sqrt{2}}\left(x - \frac{d}{dx}\right)\psi_0(x) = \frac{x\sqrt{2}}{\pi^{1/4}}e^{-x^2/2}, \tag{13.25}$$

yielding [and leading to Eq. (13.5)]

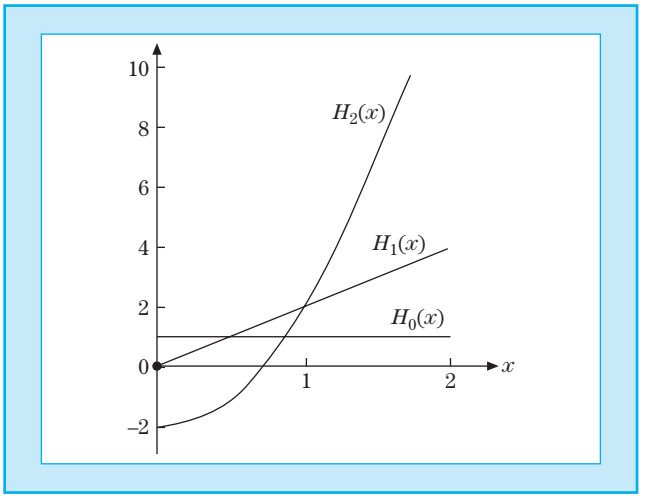
$$\psi_n(x) = N_n H_n(x) e^{-x^2/2}, \qquad N_n = \pi^{-1/4}(2^n n!)^{-1/2}, \tag{13.26}$$

where H_n are the Hermite polynomials (Fig. 13.2).

Biographical Data

Hermite, Charles. Hermite, a French mathematician, was born in Dieuze in 1822 and died in Paris in 1902. His most famous result is the first proof that e is a transcendental number; that is, e is not the root of any polynomial with integer coefficients. He also contributed to elliptic and modular functions. Having been recognized slowly, he became a professor at the Sorbonne in 1870.

Figure 13.2
Hermite Polynomials



Recurrence Relations and Generating Function

Now we can establish the recurrence relations

$$2xH_n(x) - H_n'(x) = H_{n+1}(x), \qquad H_n'(x) = 2nH_{n-1}(x), \tag{13.27}$$

from which

$$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x) \tag{13.28}$$

follows by adding them. To prove Eq. (13.27), we apply

$$x - \frac{d}{dx} = -e^{x^2/2}\frac{d}{dx}e^{-x^2/2} \tag{13.29}$$

to $\psi_n(x)$ of Eq. (13.26) and recall Eq. (13.24) to find

$$N_{n+1}H_{n+1}e^{-x^2/2} = -\frac{N_n}{\sqrt{2(n+1)}}e^{-x^2/2}(-2xH_n + H_n'), \tag{13.30}$$

that is, the first part of Eq. (13.27). Using $x + d/dx$ instead, we get the second half of Eq. (13.27).

EXAMPLE 13.1.1

The First Few Hermite Polynomials We expect the first Hermite polynomial to be a constant, $H_0(x) = 1$, being normalized. Then $n = 0$ in the recursion relation [Eq. (13.28)] yields $H_1 = 2xH_0 = 2x$; $n = 1$ implies $H_2 = 2xH_1 - 2H_0 = 4x^2 - 2$, and $n = 2$ implies

$$H_3(x) = 2xH_2(x) - 4H_1(x) = 2x(4x^2 - 2) - 8x = 8x^3 - 12x.$$

Comparing with Eq. (13.27) for $n = 0, 1, 2$, we verify that our results are consistent: $2xH_0 - H_0' = H_1 = 2x \cdot 1 - 0$, etc. For convenient reference, the first several Hermite polynomials are listed in Table 13.1. ■

Table 13.1

Hermite Polynomials

$H_0(x) = 1$
$H_1(x) = 2x$
$H_2(x) = 4x^2 - 2$
$H_3(x) = 8x^3 - 12x$
$H_4(x) = 16x^4 - 48x^2 + 12$
$H_5(x) = 32x^5 - 160x^3 + 120x$
$H_6(x) = 64x^6 - 480x^4 + 720x^2 - 120$

The Hermite polynomials $H_n(x)$ may be summed to yield the **generating function**

$$g(x, t) = e^{-t^2+2tx} = \sum_{n=0}^{\infty} H_n(x)\frac{t^n}{n!}, \tag{13.31}$$

which we derive next from the recursion relation [Eq. (13.28)]:

$$0 \equiv \sum_{n=1}^{\infty} \frac{t^n}{n!}(H_{n+1} - 2xH_n + 2nH_{n-1}) = \frac{\partial g}{\partial t} - 2xg + 2tg. \tag{13.32}$$

Integrating this ODE in t by separating the variables t and g, we get

$$\frac{1}{g}\frac{\partial g}{\partial t} = 2(x - t), \tag{13.33}$$

which yields

$$\ln g = 2xt - t^2 + \ln c, \qquad g(x, t) = e^{-t^2+2xt}c(x), \tag{13.34}$$

where c is an integration constant that may depend on the parameter x. Direct expansion of the exponential in Eq. (13.34) gives $H_0(x) = 1$ and $H_1(x) = 2x$ along with $c(x) \equiv 1$.

EXAMPLE 13.1.2

Special Values Special values of the Hermite polynomials follow from the generating function for $x = 0$; that is,

$$g(x = 0, t) = e^{-t^2} = \sum_{n=0}^{\infty} H_n(0)\frac{t^n}{n!} = \sum_{n=0}^{\infty}(-1)^n\frac{t^{2n}}{n!}.$$

A comparison of coefficients of these power series yields

$$H_{2n}(0) = (-1)^n\frac{(2n)!}{n!}, \qquad H_{2n+1}(0) = 0. \tag{13.35}$$

■

EXAMPLE 13.1.3

Parity Similarly, we obtain from the generating function identity

$$g(-x, t) = e^{-t^2-2tx} = g(x, -t) \tag{13.36}$$

the power series identity

$$\sum_{n=0}^{\infty} H_n(-x)\frac{t^n}{n!} = \sum_{n=0}^{\infty} H_n(x)\frac{(-t)^n}{n!},$$

which implies the important **parity relation**

$$H_n(x) = (-1)^n H_n(-x). \tag{13.37}$$

In quantum mechanical problems, particularly in molecular spectrosopy, a number of integrals of the form

$$\int_{-\infty}^{\infty} x^r e^{-x^2} H_n(x) H_m(x) dx$$

are needed. Examples for $r = 1$ and $r = 2$ (with $n = m$) are included in the exercises at the end of this section. Many other examples are contained in Wilson *et al.*[2] The oscillator potential has also been employed extensively in calculations of nuclear structure (nuclear shell model) and quark models of hadrons.

There is a second independent solution to Eq. (13.4). This Hermite function is an infinite series (Sections 8.5 and 8.6) and of no physical interest yet.

Alternate Representations

Differentiation of the generating function[3] n times with respect to t and then setting t equal to zero yields

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2}. \tag{13.38}$$

This gives us a Rodrigues representation of $H_n(x)$. A second representation may be obtained by using the calculus of residues (Chapter 7). If we multiply Eq. (13.31) by t^{-m-1} and integrate around the origin, only the term with $H_m(x)$ will survive:

$$H_m(x) = \frac{m!}{2\pi i} \oint t^{-m-1} e^{-t^2+2tx} dt. \tag{13.39}$$

Also, from Eq. (13.31) we may write our Hermite polynomial $H_n(x)$ in series form:

$$\begin{aligned} H_n(x) &= (2x)^n - \frac{2n!}{(n-2)!2!}(2x)^{n-2} + \frac{4n!}{(n-4)!4!}(2x)^{n-4} 1 \cdot 3 \cdots \\ &= \sum_{s=0}^{[n/2]} (-2)^s (2x)^{n-2s} \binom{n}{2s} 1 \cdot 3 \cdot 5 \cdots (2s-1) \\ &= \sum_{s=0}^{[n/2]} (-1)^s (2x)^{n-2s} \frac{n!}{(n-2s)!s!}. \end{aligned} \tag{13.40}$$

This series terminates for integral n and yields our Hermite polynomial.

[2] Wilson, E. B., Jr., Decius, J. C., and Cross, P. C. (1955). *Molecular Vibrations*. McGraw-Hill, New York. Reprinted, Dover, New York (1980).

[3] Rewrite the generating function as $g(x, t) = e^{x^2} e^{-(t-x)^2}$. Note that

$$\frac{\partial}{\partial t} e^{-(t-x)^2} = -\frac{\partial}{\partial x} e^{-(t-x)^2}.$$

EXAMPLE 13.1.4

The Lowest Hermite Polynomials For $n = 0$, we find from the series, Eq. (13.40), $H_0(x) = (-1)^0(2x)^0\frac{0!}{0!0!} = 1$; for $n = 1$, $H_1(x) = (-1)^0(2x)^1\frac{1!}{1!0!} = 2x$; and for $n = 2$, the $s = 0$ and $s = 1$ terms in Eq. (13.40) give

$$H_2(x) = (-1)^0(2x)^2\frac{2!}{2!0!} - (2x)^0\frac{2!}{0!1!} = 4x^2 - 2,$$

etc. ■

Orthogonality

The recurrence relations [Eqs. (13.27) and (13.28)] lead to the second-order ODE

$$H_n''(x) - 2xH_n'(x) + 2nH_n(x) = 0, \tag{13.41}$$

which is clearly **not** self-adjoint.

To put Eq. (13.41) in self-adjoint form, we multiply by $\exp(-x^2)$ (Exercise 9.1.2). This leads to the orthogonality integral

$$\int_{-\infty}^{\infty} H_m(x)H_n(x)e^{-x^2}dx = 0, \quad m \neq n, \tag{13.42}$$

with the weighting function $\exp(-x^2)$ a consequence of putting the differential equation into self-adjoint form. The interval $(-\infty, \infty)$ is dictated by the boundary conditions of the harmonic oscillator, which are consistent with the Hermitian operator boundary conditions (Section 9.1). It is sometimes convenient to absorb the weighting function into the Hermite polynomials. We may define

$$\varphi_n(x) = e^{-x^2/2}H_n(x), \tag{13.43}$$

with $\varphi_n(x)$ no longer a polynomial.

Substituting $H_n = e^{x^2/2}\varphi_n$ into Eq. (13.41) yields the quantum mechanical harmonic oscillator ODE [Eq. (13.4)] for $\varphi_n(x)$:

$$\varphi_n''(x) + (2n + 1 - x^2)\varphi_n(x) = 0, \tag{13.44}$$

which is self-adjoint. Thus, its solutions $\varphi_n(x)$ are orthogonal for the interval $(-\infty < x < \infty)$ with a unit weighting function. The problem of normalizing these functions remains. Proceeding as in Section 11.3, we multiply Eq. (13.31) by itself and then by e^{-x^2}. This yields

$$e^{-x^2}e^{-s^2+2sx}e^{-t^2+2tx} = \sum_{m,n=0}^{\infty} e^{-x^2}H_m(x)H_n(x)\frac{s^m t^n}{m!n!}. \tag{13.45}$$

When we integrate over x from $-\infty$ to $+\infty$ the cross terms of the double sum drop out because of the orthogonality property[4]

$$\sum_{n=0}^{\infty} \frac{(st)^n}{n!n!} \int_{-\infty}^{\infty} e^{-x^2} [H_n(x)]^2 dx = \int_{-\infty}^{\infty} e^{-x^2-s^2+2sx-t^2+2tx}\, dx$$

$$= \int_{-\infty}^{\infty} e^{-(x-s-t)^2} e^{2st}\, dx = \pi^{1/2} e^{2st} = \pi^{1/2} \sum_{n=0}^{\infty} \frac{2^n (st)^n}{n!}. \tag{13.46}$$

By equating coefficients of like powers of st, we obtain

$$\int_{-\infty}^{\infty} e^{-x^2} [H_n(x)]^2\, dx = 2^n \pi^{1/2} n! \tag{13.47}$$

which yields the normalization N_n in Eq. (13.26).

SUMMARY

Hermite polynomials are solutions of the simple harmonic oscillator of quantum mechanics. Their properties directly follow from writing their ODE as a product of creation and annihilation operators and the Sturm–Liouville theory of their ODE.

EXERCISES

13.1.1 In developing the properties of the Hermite polynomials, start at a number of different points, such as

(1) Hermite's ODE, Eqs. (13.5) and (13.44);
(2) Rodrigues's formula, Eq. (13.38);
(3) Integral representation, Eq. (13.39);
(4) Generating function, Eq. (13.31); and
(5) Gram–Schmidt construction of a complete set of orthogonal polynomials over $(-\infty, \infty)$ with a weighting factor of $\exp(-x^2)$, Section 9.3.

Outline how you can go from any one of these starting points to all the other points.

13.1.2 From the generating function, show that

$$H_n(x) = \sum_{s=0}^{[n/2]} (-1)^s \frac{n!}{(n-2s)!s!} (2x)^{n-2s}.$$

13.1.3 From the generating function, derive the recurrence relations

$$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x),$$

$$H_n'(x) = 2nH_{n-1}(x).$$

[4]The cross terms ($m \neq n$) may be left in, if desired. Then, when the coefficients of $s^\alpha t^\beta$ are equated, the orthogonality will be apparent.

13.1.4 Prove that

$$\left(2x - \frac{d}{dx}\right)^n 1 = H_n(x).$$

Hint. Check out the first couple of examples and then use mathematical induction.

13.1.5 Prove that

$$|H_n(x)| \le |H_n(ix)|.$$

13.1.6 Rewrite the series form of $H_n(x)$ [Eq. (13.40)] as an **ascending** power series.

ANS.
$$H_{2n}(x) = (-1)^n \sum_{s=0}^{n} (-1)^{2s} (2x)^{2s} \frac{(2n)!}{(2s)!(n-s)!},$$
$$H_{2n+1}(x) = (-1)^n \sum_{s=0}^{n} (-1)^{s} (2x)^{2s+1} \frac{(2n+1)!}{(2s+1)!(n-s)!}.$$

13.1.7 (a) Expand x^{2r} in a series of even-order Hermite polynomials.
(b) Expand x^{2r+1} in a series of odd-order Hermite polynomials.

ANS. (a) $x^{2r} = \dfrac{(2r)!}{2^{2r}} \displaystyle\sum_{n=0}^{r} \frac{H_{2n}(x)}{(2n)!(r-n)!}$,

(b) $x^{2r+1} = \dfrac{(2r+1)!}{2^{2r+1}} \displaystyle\sum_{n=0}^{r} \frac{H_{2n+1}(x)}{(2n+1)!(r-n)!}$, $\quad r = 0, 1, 2, \ldots$.

Hint. Use a Rodrigues representation of $H_{2n}(x)$ and integrate by parts.

13.1.8 Show that

(a) $$\int_{-\infty}^{\infty} H_n(x) \exp[-x^2/2] dx \begin{cases} 2\pi n!/(n/2)!, & n \text{ even} \\ 0, & n \text{ odd.} \end{cases}$$

(b) $$\int_{-\infty}^{\infty} x H_n(x) \exp[-x^2/2] dx \begin{cases} 0, & n \text{ even} \\ 2\pi \dfrac{(n+1)!}{((n+1)/2)!}, & n \text{ odd.} \end{cases}$$

13.1.9 Show that

$$\int_{-\infty}^{\infty} x^m e^{-x^2} H_n(x)\, dx = 0 \quad \text{for } m \text{ an integer}, \quad 0 \le m \le n-1.$$

13.1.10 The transition probability between two oscillator states, m and n, depends on

$$\int_{-\infty}^{\infty} x e^{-x^2} H_n(x) H_m(x) dx.$$

Show that this integral equals $\pi^{1/2}2^{n-1}n!\delta_{m,n-1}+\pi^{1/2}2^n(n+1)!\delta_{m,n+1}$. This result shows that such transitions can occur only between states of adjacent energy levels, $m=n\pm1$.
Hint. Multiply the generating function [Eq. (13.31)] by itself using two different sets of variables (x, s) and (x, t). Alternatively, the factor x may be eliminated by a recurrence relation in Eq. (13.27).

13.1.11 Show that

$$\int_{-\infty}^{\infty} x^2 e^{-x^2} H_n(x)H_n(x)dx = \pi^{1/2}2^n n!\left(n+\frac{1}{2}\right).$$

This integral occurs in the calculation of the mean square displacement of our quantum oscillator.
Hint. Use a recurrence relation Eq. (13.27) and the orthogonality integral.

13.1.12 Evaluate

$$\int_{-\infty}^{\infty} x^2 e^{-x^2} H_n(x)H_m(x)dx$$

in terms of n and m and appropriate Kronecker delta functions.

ANS. $2^{n-1}\pi^{1/2}(2n+1)n!\delta_{n,m}+2^n\pi^{1/2}(n+2)!\delta_{n+2,m}+2^{n-2}\pi^{1/2}n!\delta_{n-2,m}$.

13.1.13 Show that

$$\int_{-\infty}^{\infty} x^r e^{-x^2} H_n(x)H_{n+p}(x)dx = \begin{cases} 0, & p>r \\ 2^n\pi^{1/2}(n+r)!, & p=r. \end{cases}$$

n, p, and r are nonnegative integers.
Hint. Use a recurrence relation, Eq. (13.27), p times.

13.1.14 (a) Using the Cauchy integral formula, develop an integral representation of $H_n(x)$ based on Eq. (13.31) with the contour enclosing the point $z=-x$.

$$\textit{ANS.}\quad H_n(x)=\frac{n!}{2\pi i}e^{x^2}\oint\frac{e^{-z^2}}{(z+x)^{n+1}}\,dz.$$

(b) Show by direct substitution that this result satisfies the Hermite equation.

13.1.15 (a) Verify the operator identity

$$x-\frac{d}{dx}=-\exp[x^2/2]\frac{d}{dx}\exp[-x^2/2].$$

(b) The normalized simple harmonic oscillator wave function is

$$\psi_n(x)=(\pi^{1/2}2^n n!)^{-1/2}\exp[-x^2/2]H_n(x).$$

Show that this may be written as

$$\psi_n(x) = (\pi^{1/2}2^n n!)^{-1/2}\left(x - \frac{d}{dx}\right)^n \exp[-x^2/2].$$

Note. This corresponds to an n-fold application of the raising operator.

13.1.16 Write a program that will generate the coefficients a_s in the polynomial form of the Hermite polynomial, $H_n(x) = \sum_{s=0}^{n} a_s x^s$.

13.1.17 A function $f(x)$ is expanded in a Hermite series:

$$f(x) = \sum_{n=0}^{\infty} a_n H_n(x).$$

From the orthogonality and normalization of the Hermite polynomials the coefficient a_n is given by

$$a_n = \frac{1}{2^n \pi^{1/2} n!} \int_{-\infty}^{\infty} f(x) H_n(x) e^{-x^2}\, dx.$$

For $f(x) = x^8$, determine the Hermite coefficients a_n by the Gauss–Hermite quadrature. Check your coefficients against AMS-55, Table 22.12.

13.1.18 Calculate and tabulate the normalized linear oscillator wave functions

$$\psi_n(x) = 2^{-n/2}\pi^{-1/4}(n!)^{-1/2} H_n(x) \exp(-x^2/2) \quad \text{for } x = 0.0 \text{ to } 5.0$$

in steps of 0.1 and $n = 0, 1, \ldots, 5$. Plot your results.

13.1.19 Consider two harmonic oscillators that are interacting through a potential $V = cx_1x_2$, $|c| < m\omega^2$, where x_1 and x_2 are the oscillator variables, m is the common mass, and ω's the common oscillator frequency. Find the exact energy levels. If $c > m\omega^2$, sketch the potential surface $V(x_1, x_2)$ and explain why there is no ground state in this case.

13.2 Laguerre Functions

Differential Equation—Laguerre Polynomials

If we start with the appropriate generating function, it is possible to develop the Laguerre polynomials in analogy with the Hermite polynomials. Alternatively, a series solution may be developed by the methods of Section 8.5. Instead, to illustrate a different technique, let us start with Laguerre's ODE and obtain a solution in the form of a contour integral. From this integral representation a generating function will be derived. We want to use Laguerre's ODE

$$xy''(x) + (1 - x)y'(x) + ny(x) = 0 \tag{13.48}$$

over the interval $0 < x < \infty$ and for integer $n \geq 0$, which is motivated by the radial ODE of Schrödinger's partial differential equation for the hydrogen atom.

We shall attempt to represent y, or rather y_n since y will depend on n, by the contour integral

$$y_n(x) = \frac{1}{2\pi i}\oint \frac{e^{-xz/(1-z)}}{(1-z)z^{n+1}}dz, \tag{13.49}$$

and demonstrate that it satisfies Laguerre's ODE. The contour includes the origin but does not enclose the point $z = 1$. By differentiating the exponential in Eq. (13.49), we obtain

$$y_n'(x) = -\frac{1}{2\pi i}\oint \frac{e^{-xz/(1-z)}}{(1-z)^2 z^n}dz, \tag{13.50}$$

$$y_n''(x) = \frac{1}{2\pi i}\oint \frac{e^{-xz/(1-z)}}{(1-z)^3 z^{n-1}}dz. \tag{13.51}$$

Substituting into the left-hand side of Eq (13.48), we obtain

$$\frac{1}{2\pi i}\oint \left[\frac{x}{(1-z)^3 z^{n-1}} - \frac{1-x}{(1-z)^2 z^n} + \frac{n}{(1-z)z^{n+1}}\right] e^{-xz/(1-z)}dz,$$

which is equal to

$$-\frac{1}{2\pi i}\oint \frac{d}{dz}\left[\frac{e^{-xz/(1-z)}}{(1-z)z^n}\right]dz. \tag{13.52}$$

If we integrate our perfect differential around a contour chosen so that the final value equals the initial value (Fig. 13.3), the integral will vanish, thus verifying that $y_n(x)$ [Eq. (13.49)] is a solution of Laguerre's equation. We also see how the coefficients of Laguerre's ODE [Eq. (13.48)] determine the exponent of the

Figure 13.3

Laguerre Function Contour

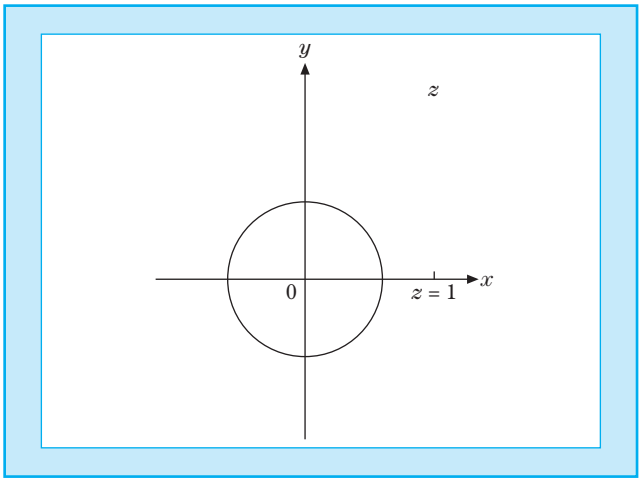
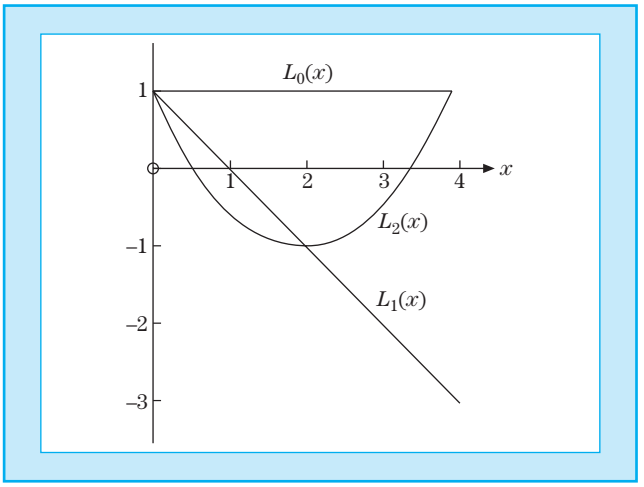


Figure 13.4

Laguerre Polynomials



generating function by comparing with Eq. (13.52), thus making Eq. (13.49) perhaps a bit less of a lucky guess.

It has become customary to define $L_n(x)$, the Laguerre polynomial (Fig. 13.4), by[5]

$$L_n(x) = \frac{1}{2\pi i}\oint \frac{e^{-xz/(1-z)}}{(1-z)z^{n+1}}dz. \tag{13.53}$$

This is exactly what we would obtain from the series

$$g(x,z) = \frac{e^{-xz/(1-z)}}{1-z} = \sum_{n=0}^{\infty} L_n(x)z^n, \quad |z| < 1 \tag{13.54}$$

if we multiplied it by z^{-n-1} and integrated around the origin. Applying the residue theorem (Section 7.2), only the z^{-1} term in the series survives. On this basis we identify $g(x, z)$ as the **generating function** for the Laguerre polynomials.

With the transformation

$$\frac{xz}{1-z} = s - x \quad \text{or} \quad z = \frac{s-x}{s}, \tag{13.55}$$

$$L_n(x) = \frac{e^x}{2\pi i}\oint \frac{s^n e^{-s}}{(s-x)^{n+1}}\,ds, \tag{13.56}$$

the new contour enclosing the point $s = x$ in the s-plane. By Cauchy's integral formula (for derivatives)

$$L_n(x) = \frac{e^x}{n!}\frac{d^n}{dx^n}(x^n e^{-x}) \quad (\text{integral } n), \tag{13.57}$$

[5]Other notations of $L_n(x)$ are in use. Here, the definitions of the Laguerre polynomial $L_n(x)$ and the associated Laguerre polynomial $L_n^k(x)$ agree with AMS-55 (Chapter 22).

giving Rodrigues's formula for Laguerre polynomials. From these representations of $L_n(x)$ we find the series form (for integral n),

$$L_n(x) = \frac{(-1)^n}{n!}\left[x^n - \frac{n^2}{1!}x^{n-1} + \frac{n^2(n-1)^2}{2!}x^{n-2} - \cdots + (-1)^n n!\right]$$
$$= \sum_{m=0}^{n} \frac{(-1)^m n! x^m}{(n-m)!m!m!} = \sum_{s=0}^{n} \frac{(-1)^{n-s} n! x^{n-s}}{(n-s)!(n-s)!s!}. \tag{13.58}$$

EXAMPLE 13.2.1 **Lowest Laguerre Polynomials** For $n = 0$, Eq. (13.57) yields $L_0 = \frac{e^x}{0!}(x^0 e^{-x}) = 1$; for $n = 1$, we get $L_1 = e^x \frac{d}{dx}(xe^{-x}) = e^x(e^{-x} - xe^{-x}) = 1 - x$; and for $n = 2$,

$$L_2 = \frac{1}{2}e^x \frac{d^2}{dx^2}(x^2 e^{-x}) = \frac{1}{2}e^x \frac{d}{dx}(2xe^{-x} - x^2 e^{-x})$$
$$= \frac{1}{2}e^x(2 - 2x - 2x + x^2)e^{-x} = 1 - 2x + \frac{1}{2}x^2,$$

etc., the specific polynomials listed in Table 13.2 (Exercise 13.2.1). ■

Table 13.2
Laguerre Polynomials

$L_0(x) = 1$
$L_1(x) = -x + 1$
$2!L_2(x) = x^2 - 4x + 2$
$3!L_3(x) = -x^3 + 9x^2 - 18x + 6$
$4!L_4(x) = x^4 - 16x^3 + 72x^2 - 96x + 24$
$5!L_5(x) = -x^5 + 25x^4 - 200x^3 + 600x^2 - 600x + 120$
$6!L_6(x) = x^6 - 36x^5 + 450x^4 - 2400x^3 + 5400x^2 - 4320x + 720$

EXAMPLE 13.2.2 **Recursion Relation** Carrying out the innermost differentiation in Eq. (13.57), we find

$$L_n(x) = \frac{e^x}{n!}\frac{d^{n-1}}{dx^{n-1}}(nx^{n-1} - x^n)e^{-x} = L_{n-1}(x) - \frac{e^x}{n!}\frac{d^{n-1}}{dx^{n-1}}x^n e^{-x},$$

a formula from which we can derive the recursion $L_n' = L_{n-1}' - L_{n-1}$. To generate L_n from the last term in the previous equation, we multiply it by e^{-x} and differentiate it, getting

$$\frac{d}{dx}(e^{-x}L_n(x)) = \frac{d}{dx}(e^{-x}L_{n-1}(x)) - \frac{1}{n!}\frac{d^n}{dx^n}(x^n e^{-x}),$$

which can also be written as

$$e^{-x}(-L_n + L_n' + L_{n-1} - L_{n-1}') = -\frac{1}{n!}\frac{d^n}{dx^n}(x^n e^{-x}).$$

Multiplying this result by e^x and using the definition [Eq. (13.57)] yields

$$L_n'(x) = L_{n-1}'(x) - L_{n-1}(x). \tag{13.59}$$

■

By differentiating the generating function in Eq. (13.54) with respect to x we can rederive this recursion relation as follows:

$$(1-z)\frac{\partial g}{\partial x} = -\frac{z}{1-z}e^{-xz/(1-z)} = -zg(x,z).$$

Expanding this result according to the definition of the generating function, Eq. (13.54), yields

$$\sum_n L_n'(z^n - z^{n+1}) = \sum_{n=0}^{\infty}(L_n' - L_{n-1}')z^n = -\sum_{n=1}^{\infty} L_{n-1}z^n,$$

which implies the recursion relation [Eq. (13.59)].

By differentiating the generating function in Eq. (13.54) with respect to x and z, we obtain other recurrence relations

$$\begin{aligned}(n+1)L_{n+1}(x) &= (2n+1-x)L_n(x) - nL_{n-1}(x),\\ xL_n'(x) &= nL_n(x) - nL_{n-1}(x).\end{aligned} \tag{13.60}$$

Equation (13.60), modified to read

$$\begin{aligned}L_{n+1}(x) &= 2L_n(x) - L_{n-1}(x)\\ &\quad - [(1+x)L_n(x) - L_{n-1}(x)]/(n+1)\end{aligned} \tag{13.61}$$

for reasons of economy and numerical stability, is used for computation of numerical values of $L_n(x)$. The computer starts with known numerical values of $L_0(x)$ and $L_1(x)$ (Table 13.2) and works up step by step. This is the same technique discussed for computing Legendre polynomials in Section 11.2.

EXAMPLE 13.2.3

Special Values From Eq. (13.54) for $x = 0$ and arbitrary z, we find

$$g(0,z) = \frac{1}{1-z} = \sum_{n=0}^{\infty} z^n = \sum_{n=0}^{\infty} L_n(0)z^n,$$

and, therefore, the special values

$$L_n(0) = 1, \tag{13.62}$$

by comparing coefficients of both power series. ■

As is seen from the form of the generating function, the form of Laguerre's ODE, or from Table 13.2, the Laguerre polynomials have neither odd nor even symmetry (parity).

The Laguerre ODE is not self-adjoint and the Laguerre polynomials, $L_n(x)$, do not by themselves form an orthogonal set. However, following the method of Section 9.1, if we multiply Eq. (13.48) by e^{-x} (Exercise 9.1.1) we obtain

$$\int_0^{\infty} e^{-x}L_m(x)L_n(x)dx = \delta_{mn}. \tag{13.63}$$

This orthogonality is a consequence of the Sturm–Liouville theory (Section 9.1). The normalization follows from the generating function. It is sometimes

convenient to define orthogonal Laguerre functions (with unit weighting function) by

$$\varphi_n(x) = e^{-x/2}L_n(x). \tag{13.64}$$

EXAMPLE 13.2.4 **Special Integrals** Setting $z = 1/2$ in the generating function, Eq. (13.54), gives the relation

$$g\left(x, \frac{1}{2}\right) = 2e^{-x} = \sum_{n=0}^{\infty} L_n(x)2^{-n}.$$

Multiplying by $e^{-x}L_m(x)$, integrating, and using orthogonality yields

$$2\int_0^{\infty} e^{-2x}L_m(x)dx = 2^{-m}.$$

Setting $z = -1/2,\ \pm 1/3$, etc., we can derive numerous other special integrals. ■

Our new orthonormal function $\varphi_n(x)$ satisfies the ODE

$$x\varphi_n''(x) + \varphi_n'(x) + \left(n + \frac{1}{2} - \frac{x}{4}\right)\varphi_n(x) = 0, \tag{13.65}$$

which is seen to have the (self-adjoint) Sturm–Liouville form. Note that it is the boundary conditions in the Sturm–Liouville theory that fix our interval as $(0 \le x < \infty)$.

Biographical Data
Laguerre, Edmond Nicolas. Laguerre, a French mathematician, was born in 1834 and died in Bar-le-Duc in 1886. He contributed to continued fractions and the theory of algebraic equations, and he was one of the founders of modern axiomatic geometry.

Associated Laguerre Polynomials

In many applications, particularly the hydrogen atom wave functions in quantum theory, we also need the associated Laguerre polynomials as in Example 13.2.5 defined by[6]

$$L_n^k(x) = (-1)^k \frac{d^k}{dx^k} L_{n+k}(x). \tag{13.66}$$

From the series form of $L_n(x)$,

$$\begin{aligned} L_0^k(x) &= 1 \\ L_1^k(x) &= -x + k + 1 \\ L_2^k(x) &= \frac{x^2}{2} - (k+2)x + \frac{(k+2)(k+1)}{2}. \end{aligned} \tag{13.67}$$

[6]Some authors use $\mathcal{L}_{n+k}^k(x) = (d^k/dx^k)[L_{n+k}(x)]$. Hence our $L_n^k(x) = (-1)^k\mathcal{L}_{n+k}^k(x)$.

In general,

$$L_n^k(x) = \sum_{m=0}^{n} (-1)^m \frac{(n+k)!}{(n-m)!(k+m)!m!} x^m, \quad k > -1. \tag{13.68}$$

A generating function may be developed by differentiating the Laguerre generating function k times. Adjusting the index to L_{n+k}, we obtain

$$\frac{e^{-xz/(1-z)}}{(1-z)^{k+1}} = \sum_{n=0}^{\infty} L_n^k(x) z^n, \quad |z| < 1. \tag{13.69}$$

From this, for $x = 0$, the binomial expansion yields

$$L_n^k(0) = \frac{(n+k)!}{n!k!}. \tag{13.70}$$

Recurrence relations can easily be derived from the generating function or by differentiating the Laguerre polynomial recurrence relations. Among the numerous possibilities are

$$(n+1)L_{n+1}^k(x) = (2n+k+1-x)L_n^k(x) - (n+k)L_{n-1}^k(x), \tag{13.71}$$

$$x\frac{dL_n^k(x)}{dx} = nL_n^k(x) - (n+k)L_{n-1}^k(x). \tag{13.72}$$

From these or from differentiating Laguerre's ODE k times, we have the associated Laguerre ODE

$$x\frac{d^2L_n^k(x)}{dx^2} + (k+1-x)\frac{dL_n^k(x)}{dx} + nL_n^k(x) = 0. \tag{13.73}$$

When associated Laguerre polynomials appear in a physical problem, it is usually because that physical problem involves the ODE [Eq. (13.73)].

A Rodrigues representation of the associated Laguerre polynomial is

$$L_n^k(x) = \frac{e^x x^{-k}}{n!}\frac{d^n}{dx^n}(e^{-x}x^{n+k}). \tag{13.74}$$

Note that all these formulas for $g(x)$ reduce to the corresponding expressions for $L_n(x)$, when $k = 0$.

The associated Laguerre equation [Eq. (13.73)] is not self-adjoint, but it can be put in self-adjoint form by multiplying by $e^{-x}x^k$, which becomes the weighting function (Section 9.1). We obtain

$$\int_0^{\infty} e^{-x}x^k L_n^k(x)L_m^k(x)dx = \frac{(n+k)!}{n!}\delta_{mn}, \tag{13.75}$$

which shows the same orthogonality interval $[0, \infty)$ as that for the Laguerre polynomials. However, with a new weighting function, we have a new set of orthogonal polynomials, the associated Laguerre polynomials.

By letting $\psi_n^k(x) = e^{x/2}x^{k/2}L_n^k(x)$, $\psi_n^k(x)$ satisfies the self-adjoint equation

$$x\frac{d^2\psi_n^k(x)}{dx^2} + \frac{d\psi_n^k(x)}{dx} + \left(-\frac{x}{4} + \frac{2n+k+1}{2} - \frac{k^2}{4x}\right)\psi_n^k(x) = 0. \tag{13.76}$$

The $\psi_n^k(x)$ are sometimes called **Laguerre functions**. Equation (13.65) is the special case $k = 0$.

A further useful form is given by defining[7]

$$\Phi_n^k(x) = e^{-x/2}x^{(k+1)/2}L_n^k(x). \tag{13.77}$$

Substitution into the associated Laguerre equation yields

$$\frac{d^2\Phi_n^k(x)}{dx^2} + \left(-\frac{1}{4} + \frac{2n+k+1}{2x} - \frac{k^2-1}{4x^2}\right)\Phi_n^k(x) = 0. \tag{13.78}$$

The corresponding normalization integral is

$$\int_0^\infty e^{-x}x^{k+1}\left[L_n^k(x)\right]^2\,dx = \frac{(n+k)!}{n!}(2n+k+1). \tag{13.79}$$

Notice that the $\Phi_n^k(x)$ do **not** form an orthogonal set (except with x^{-1} as a weighting function) because of the x^{-1} in the term $(2n+k+1)/2x$.

EXAMPLE 13.2.5

The Hydrogen Atom The most important application of the Laguerre polynomials is in the solution of the Schrödinger equation for the hydrogen atom. This equation is

$$-\frac{\hbar^2}{2m}\nabla^2\psi - \frac{Ze^2}{4\pi\epsilon_0 r}\psi = E\psi, \tag{13.80}$$

where $Z = 1$ for hydrogen, 2 for singly ionized helium, and so on. Separating variables, we find that the angular dependence of ψ is on the spherical harmonics $Y_L^M(\theta, \varphi)$ (see Section 11.5). The radial part, $R(r)$, satisfies the equation

$$-\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) - \frac{Ze^2}{4\pi\epsilon_0 r}R + \frac{\hbar^2}{2m}\frac{L(L+1)}{r^2}R = ER. \tag{13.81}$$

For bound states $R \to 0$ as $r \to \infty$, and R is finite at the origin, $r = 0$. These are the boundary conditions. We ignore the continuum states with positive energy. Only when the latter are included do the hydrogen wave functions form a complete set. By use of the abbreviations (resulting from rescaling r to the dimensionless radial variable ρ)

$$\rho = \beta r \quad \text{with} \quad \beta^2 = -\frac{8mE}{\hbar^2}, \quad E < 0, \qquad \lambda = \frac{mZe^2}{2\pi\epsilon_0\beta\hbar^2}, \tag{13.82}$$

[7]This corresponds to modifying the function ψ in Eq. (13.76) to eliminate the first derivative (compare Exercise 8.6.3).

Eq. (13.81) becomes

$$\frac{1}{\rho^2}\frac{d}{d\rho}\left(\rho^2\frac{d\chi(\rho)}{d\rho}\right)+\left(\frac{\lambda}{\rho}-\frac{1}{4}-\frac{L(L+1)}{\rho^2}\right)\chi(\rho)=0, \tag{13.83}$$

where $\chi(\rho) = R(\rho/\beta)$. A comparison with Eq. (13.78) for $\Phi_n^k(x)$ shows that Eq. (13.83) is satisfied by

$$\chi(\rho)=e^{-\rho/2}\rho^L L_{\lambda-L-1}^{2L+1}(\rho), \tag{13.84}$$

in which k is replaced by $2L+1$ and n by $\lambda - L - 1$.

We must restrict the parameter λ by requiring it to be an integer n, $n = 1, 2, 3, \ldots$.[8] This is necessary because the Laguerre function of nonintegral n would diverge as $\rho^n e^\rho$, which is unacceptable for our physical problem with the boundary condition

$$\lim_{r\to\infty} R(r)=0.$$

This restriction on λ, imposed by our boundary condition, has the effect of quantizing the energy

$$E_n=-\frac{Z^2m}{2n^2\hbar^2}\left(\frac{e^2}{4\pi\epsilon_0}\right)^2. \tag{13.85}$$

The negative sign indicates that we are dealing here with bound states, as $E = 0$ corresponds to an electron that is just able to escape to infinity, where the Coulomb potential goes to zero. Using this result for E_n, we have

$$\beta=\frac{me^2}{2\pi\epsilon_0\hbar^2}\cdot\frac{Z}{n}=\frac{2Z}{na_0},\qquad \rho=\frac{2Z}{na_0}r \tag{13.86}$$

with

$$a_0=\frac{4\pi\epsilon_0\hbar^2}{me^2},\qquad \text{the Bohr radius.}$$

Thus, the final normalized hydrogen wave function is written as

$$\psi_{nLM}(r,\theta,\varphi)=\left[\left(\frac{2Z}{na_0}\right)^3\frac{(n-L-1)!}{2n(n+L)!}\right]^{1/2}e^{-\beta r/2}(\beta r)^L L_{n-L-1}^{2L+1}(\beta r)Y_L^M(\theta,\varphi). \tag{13.87}$$

■

SUMMARY

Laguerre polynomials arise as solutions of the Coulomb potential in quantum mechanics. Separating the Schrödinger equation in spherical polar coordinates defines their radial ODE. The Sturm–Liouville theory of this ODE implies their properties.

[8] This is the conventional notation for λ. It is not the same n as the index n in $\Phi_n^k(x)$.

EXERCISES

13.2.1 Show with the aid of the Leibniz formula that the series expansion of $L_n(x)$ [Eq. (13.58)] follows from the Rodrigues representation [Eq. (13.57)].

13.2.2 (a) Using the explicit series form [Eq. (13.58)], show that

$$L_n'(0) = -n$$
$$L_n''(0) = \frac{1}{2}n(n-1).$$

(b) Repeat without using the explicit series form of $L_n(x)$.

13.2.3 From the generating function derive the Rodrigues representation

$$L_n^k(x) = \frac{e^x x^{-k}}{n!}\frac{d^n}{dx^n}(e^{-x}x^{n+k}).$$

13.2.4 Derive the normalization relation [Eq. (13.75)] for the associated Laguerre polynomials.

13.2.5 Expand x^r in a series of associated Laguerre polynomials $L_n^k(x)$, k fixed and n ranging from 0 to r (or to ∞ if r is not an integer).
Hint. The Rodrigues form of $L_n^k(x)$ will be useful.

$$ANS.\quad x^r = (r+k)!r!\sum_{n=0}^{r}\frac{(-1)^n L_n^k(x)}{(n+k)!(r-n)!},\qquad 0 \le x \le \infty.$$

13.2.6 Expand e^{-ax} in a series of associated Laguerre polynomials $L_n^k(x)$, k fixed and n ranging from 0 to ∞. Plot partial sums as a function of the upper limit $N = 1, 2, \ldots, 10$ to check the convergence.
(a) Evaluate directly the coefficients in your assumed expansion.
(b) Develop the desired expansion from the generating function.

$$ANS.\quad e^{-ax} = \frac{1}{(1+a)^{1+k}}\sum_{n=0}^{\infty}\left(\frac{a}{1+a}\right)^n L_n^k(x),\qquad 0 \le x \le \infty.$$

13.2.7 Show that

$$\int_0^\infty e^{-x}x^{k+1}L_n^k(x)L_n^k(x)\,dx = \frac{(n+k)!}{n!}(2n+k+1).$$

Hint. Note that

$$xL_n^k = (2n+k+1)L_n^k - (n+k)L_{n-1}^k - (n+1)L_{n+1}^k.$$

13.2.8 Assume that a particular problem in quantum mechanics has led to the ODE

$$\frac{d^2y}{dx^2} - \left[\frac{k^2-1}{4x^2} - \frac{2n+k+1}{2x} + \frac{1}{4}\right]y = 0.$$

Write $y(x)$ as

$$y(x) = A(x)B(x)C(x)$$

with the requirements that

(a) $A(x)$ be a **negative** exponential giving the required asymptotic behavior of $y(x)$; and

(b) $B(x)$ be a **positive** power of x giving the behavior of $y(x)$ for $0 \le x \ll 1$.

Determine $A(x)$ and $B(x)$. Find the relation between $C(x)$ and the associated Laguerre polynomial.

$$ANS. \quad A(x) = e^{-x/2}, \qquad B(x) = x^{(k+1)/2}, \qquad C(x) = L_n^k(x).$$

13.2.9 From Eq. (13.87) the normalized radial part of the hydrogenic wave function is

$$R_{nL}(r) = \left[\beta^3 \frac{(n-L-1)!}{2n(n+L)!}\right]^{1/2} e^{-\beta r}(\beta r)^L L_{n-L-1}^{2L+1}(\beta r),$$

where $\beta = 2Z/na_0 = Zme^2/(2\pi\epsilon_0\hbar^2)$. Evaluate

(a) $\langle r\rangle = \displaystyle\int_0^\infty r R_{nL}(\beta r) R_{nL}(\beta r) r^2\, dr,$

(b) $\langle r^{-1}\rangle = \displaystyle\int_0^\infty r^{-1} R_{nL}(\beta r) R_{nL}(\beta r) r^2\, dr.$

The quantity $\langle r\rangle$ is the average displacement of the electron from the nucleus, whereas $\langle r^{-1}\rangle$ is the average of the reciprocal displacement.

$$ANS. \quad \langle r\rangle = \frac{a_0}{2}[3n^2 - L(L+1)] \qquad \langle r^{-1}\rangle = \frac{1}{n^2 a_0}.$$

13.2.10 Derive the recurrence relation for the hydrogen wave function expectation values:

$$\frac{s+2}{n^2}\langle r^{s+1}\rangle - (2s+3)a_0\langle r^s\rangle + \frac{s+1}{4}[(2L+1)^2 - (s+1)^2]a_0^2\langle r^{s-1}\rangle = 0,$$

with $s \ge -2L-1$ and $\langle r^s\rangle$ defined as in Exercise 13.2.9(a).

Hint. Transform Eq. (13.83) into a form analogous to Eq. (13.78). Multiply by $\rho^{s+2}u' - c\rho^{s+1}u$. Here, $u = \rho\Phi$. Adjust c to cancel terms that do not yield expectation values.

13.2.11 The hydrogen wave functions, Eq. (13.87), are mutually orthogonal, as they should be since they are eigenfunctions of the self-adjoint Schrödinger equation

$$\int \psi^*_{n_1L_1M_1}\psi_{n_2L_2M_2} r^2 dr d\Omega = \delta_{n_1n_2}\delta_{L_1L_2}\delta_{M_1M_2}.$$

However, the radial integral has the (misleading) form

$$\int_0^\infty e^{-\beta r/2}(\beta r)^L L_{n_1-L-1}^{2L+1}(\beta r)e^{-\beta r/2}(\beta r)^L L_{n_2-L-1}^{2L+1}(\beta r)r^2 dr,$$

which **appears** to match Eq. (13.79) and not the associated Laguerre orthogonality relation [Eq. (13.75)]. How do you resolve this paradox?

ANS. The parameter β is dependent on n. The first three β previously shown are $2Z/n_1a_0$. The last three are $2Z/n_2a_0$. For $n_1 = n_2$, Eq. (13.79) applies. For $n_1 \neq n_2$, neither Eq. (13.75) nor Eq. (13.79) is applicable.

13.2.12 A quantum mechanical analysis of the Stark effect (in parabolic coordinates) leads to the ODE

$$\frac{d}{d\xi}\left(\xi\frac{du}{d\xi}\right) + \left(\frac{1}{2}E\xi + L - \frac{m^2}{4\xi} - \frac{1}{4}F\xi^2\right)u = 0,$$

where F is a measure of the perturbation energy introduced by an external electric field. Find the unperturbed wave functions ($F = 0$) in terms of associated Laguerre polynomials.

ANS. $u(\xi) = e^{-\varepsilon\xi/2}\xi^{m/2}L_p^m(\varepsilon\xi)$, with $\varepsilon = \sqrt{-2E} > 0$, $p = \alpha/\varepsilon - (m+1)/2$, a nonnegative integer.

13.2.13 The wave equation for the three-dimensional harmonic oscillator is

$$-\frac{\hbar^2}{2M}\nabla^2\psi + \frac{1}{2}M\omega^2 r^2\psi = E\psi,$$

where ω is the angular frequency of the corresponding classical oscillator. Show that the radial part of ψ (in spherical polar coordinates) may be written in terms of associated Laguerre functions of argument (βr^2), where $\beta = M\omega/\hbar$.
Hint. As in Exercise 13.2.8, split off radial factors of r^l and $e^{-\beta r^2/2}$. The associated Laguerre function will have the form $L_{(n-l-1)/2}^{l+1/2}(\beta r^2)$.

13.2.14 Write a program (in Basic or Fortran or use symbolic software) that will generate the coefficients a_s in the polynomial form of the Laguerre polynomial, $L_n(x) = \sum_{s=0}^n a_s x^s$.

13.2.15 Write a subroutine that will transform a finite power series $\sum_{n=0}^N a_n x^n$ into a Laguerre series $\sum_{n=0}^N b_n L_n(x)$. Use the recurrence relation Eq. (13.60).

13.2.16 Tabulate $L_{10}(x)$ for $x = 0.0$ to 30.0 in steps of 0.1. This will include the 10 roots of L_{10}. Beyond $x = 30.0$, $L_{10}(x)$ is monotonically increasing. Plot your results.

Check value. Eighth root = 16.279.

Additional Reading

Abramowitz, M., and Stegun, I. A. (Eds.) (1964). *Handbook of Mathematical Functions*, Applied Mathematics Series-55 (AMS-55). National Bureau of Standards, Washington, DC. Paperback edition, Dover, New York (1974). Chapter 22 is a detailed summary of the properties and representations of orthogonal polynomials. Other chapters summarize properties of Bessel, Legendre, hypergeometric, and confluent hypergeometric functions and much more.

Erdelyi, A., Magnus, W., Oberhettinger, F., and Tricomi, F. G. (1953). *Higher Transcendental Functions*. McGraw-Hill, New York. Reprinted, Krieger, Melbourne, FL (1981). A detailed, almost exhaustive listing of the properties of the special functions of mathematical physics.

Lebedev, N. N. (1965). *Special Functions and Their Applications* (R. A. Silverman, Trans.). Prentice-Hall, Englewood Cliffs, NJ. Paperback, Dover, New York (1972).

Luke, Y. L. (1969). *The Special Functions and Their Approximations*. Academic Press, New York. Volume 1 is a thorough theoretical treatment of gamma functions, hypergeometric functions, confluent hypergeometric functions, and related functions. Volume 2 develops approximations and other techniques for numerical work.

Luke, Y. L. (1975). *Mathematical Functions and Their Approximations*. Academic Press, New York. This is an updated supplement to *Handbook of Mathematical Functions with Formulas, Graphs and Mathematical Tables* (AMS-55).

Magnus, W., Oberhettinger, F., and Soni, R. P. (1966). *Formulas and Theorems for the Special Functions of Mathematical Physics*. Springer, New York. An excellent summary of just what the title says, including the topics of Chapters 10–13.

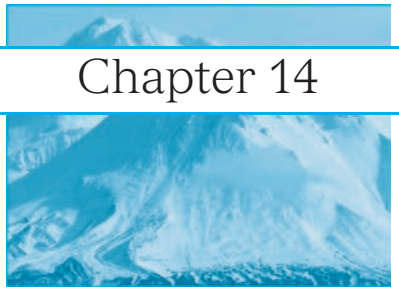
Rainville, E. D. (1960). *Special Functions*. Macmillan, New York. Reprinted, Chelsea, New York (1971). This book is a coherent, comprehensive account of almost all the special functions of mathematical physics that the reader is likely to encounter.

Sansone, G. (1959). *Orthogonal Functions* (A. H. Diamond, Trans.). Interscience, New York. Reprinted, Dover, New York (1991).

Sneddon, I. N. (1980). *Special Functions of Mathematical Physics and Chemistry*, 3rd ed. Longman, New York.

Thompson, W. J. (1997). *Atlas for Computing Mathematical Functions: An Illustrated Guidebook for Practitioners with Programs in Fortran 90 and Mathematica*. Wiley, New York.

Whittaker, E. T., and Watson, G. N. (1997). *A Course of Modern Analysis* (reprint). Cambridge Univ. Press, Cambridge, UK. The classic text on special functions and real and complex analysis.



Chapter 14

Fourier Series

14.1 General Properties

Periodic phenomena involving waves [$\sim \sin(2\pi x/\lambda)$ as a crude approximation to water waves, for example], motors, rotating machines (harmonic motion), or some repetitive pattern of a driving force are described by periodic functions. Fourier series are a basic tool for solving ordinary differential equations (ODEs) and partial differential equations (PDEs) with periodic boundary conditions. Fourier integrals for nonperiodic phenomena are developed in Chapter 15. The common name for the whole field is **Fourier analysis**.

A Fourier series is defined as an expansion of a function or representation of a function in a series of sines and cosines, such as

$$f(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty} a_n \cos nx + \sum_{n=1}^{\infty} b_n \sin nx. \tag{14.1}$$

The coefficients a_0, a_n, and b_n are related to the periodic function $f(x)$ by definite integrals:

$$a_n = \frac{1}{\pi} \int_0^{2\pi} f(x) \cos nx\, dx, \tag{14.2}$$

$$b_n = \frac{1}{\pi} \int_0^{2\pi} f(x) \sin nx\, dx, \quad n = 0, 1, 2, \ldots. \tag{14.3}$$

This result, of course, is subject to the requirement that the integrals exist. They do if $f(x)$ is piecewise continuous (or square integrable). Notice that a_0 is singled out for special treatment by the inclusion of the factor $\frac{1}{2}$. This is done so that Eq. (14.2) will apply to all a_n, $n = 0$ as well as $n > 0$.

The Sturm–Liouville theory of the harmonic oscillator in Example 9.1.4 guarantees the validity of Eqs. (14.2) and (14.3) and, by use of the orthogonality relations (Example 9.2.1), allows us to compute the expansion coefficients.

Another way of describing what we are doing here is to say that $f(x)$ is part of an infinite-dimensional Hilbert space, with the orthogonal $\cos nx$ and $\sin nx$ as the basis. The statement that $\cos nx$ and $\sin nx\,(n = 0, 1, 2, \ldots)$ span this Hilbert space is equivalent to saying that they form a complete set. Finally, the **expansion coefficients** a_n and b_n **correspond to the projections** of $f(x)$, with the integral inner products [Eqs. (14.2) and (14.3)] playing the role of the dot product of Section 1.2. These points are outlined in Section 9.4.

The conditions imposed on $f(x)$ to make Eq. (14.1) valid, and the series convergent, are that $f(x)$ has only a finite number of finite discontinuities and only a finite number of extreme values, maxima, and minima in the interval $[0, 2\pi]$.[1] Functions satisfying these conditions are called **piecewise regular**. The conditions are known as the **Dirichlet conditions**. Although there are some functions that do not obey these Dirichlet conditions, they may well be labeled pathological for purposes of Fourier expansions. In the vast majority of physical problems involving a Fourier series, these conditions will be satisfied. In most physical problems we shall be interested in functions that are square integrable, for which the sines and cosines form a complete orthogonal set. This in turn means that Eq. (14.1) is valid in the sense of convergence in the mean (see Eq. 9.63).

Completeness

The Fourier expansion and the completeness property may be expected because the functions $\sin nx$, $\cos nx$, e^{inx} are all eigenfunctions of a self-adjoint linear ODE,

$$y'' + n^2 y = 0. \tag{14.4}$$

We obtain orthogonal eigenfunctions for different values of the eigenvalue n for the interval $[0, 2\pi]$ to satisfy the boundary conditions in the Sturm–Liouville theory (Chapter 9). The different eigenfunctions for the same eigenvalue n are orthogonal. We have

$$\int_0^{2\pi} \sin mx \sin nx\,dx = \begin{cases} \pi\delta_{mn}, & m \neq 0, \\ 0, & m = 0, \end{cases} \tag{14.5}$$

$$\int_0^{2\pi} \cos mx \cos nx\,dx = \begin{cases} \pi\delta_{mn}, & m \neq 0, \\ 2\pi, & m = n = 0, \end{cases} \tag{14.6}$$

$$\int_0^{2\pi} \sin mx \cos nx\,dx = 0, \quad \text{for all integral } m \text{ and } n. \tag{14.7}$$

Note that any interval $x_0 \leq x \leq x_0 + 2\pi$ will be equally satisfactory. Frequently, we use $x_0 = -\pi$ to obtain the interval $-\pi \leq x \leq \pi$. For the complex eigenfunctions $e^{\pm inx}$, orthogonality is usually **defined** in terms of the complex

[1] These conditions are **sufficient** but not **necessary**.

conjugate of one of the two factors,

$$\int_0^{2\pi} (e^{imx})^* e^{inx} dx = 2\pi \delta_{mn}. \tag{14.8}$$

This agrees with the treatment of the spherical harmonics (Section 11.5).

EXAMPLE 14.1.1

Sawtooth Wave Let us apply Eqs. (14.2) and (14.3) to the sawtooth shape shown in Fig. 14.1 to derive its Fourier series. Our sawtooth function can also be expressed as

$$f(x) = \begin{cases} x, & 0 \le x < \pi, \\ x - 2\pi, & \pi \le x \le 2\pi, \end{cases}$$

which is an odd function of the variable x. Hence, we expect a pure sine expansion. Integrating by parts, we indeed find

$$a_n = \frac{1}{\pi}\int_{-\pi}^{\pi} x\cos nx\,dx = \frac{x}{n\pi}\sin nx\Big|_{-\pi}^{\pi} - \frac{1}{n\pi}\int_{-\pi}^{\pi}\sin nx\,dx$$
$$= \frac{1}{n^2\pi}\cos nx\Big|_{-\pi}^{\pi} = \frac{1}{n^2\pi}[(-1)^n - (-1)^n] = 0,$$

while

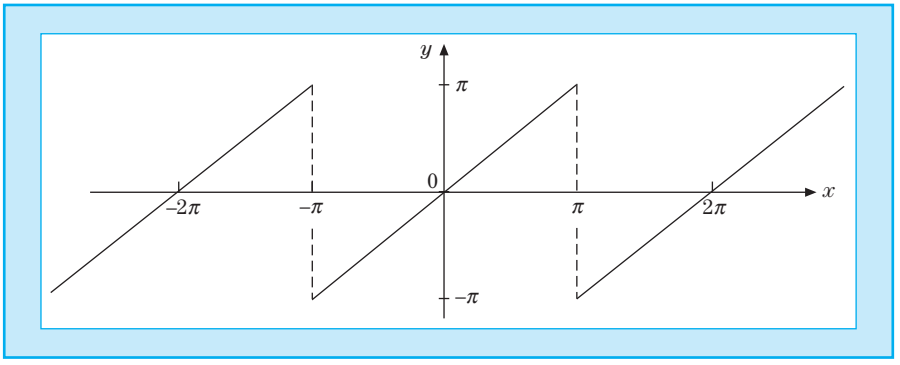
$$b_n = \frac{1}{\pi}\int_{-\pi}^{\pi} x\sin nx\,dx = -\frac{x}{n\pi}\cos nx\Big|_{-\pi}^{\pi} + \frac{1}{n\pi}\int_{-\pi}^{\pi}\sin nx\,dx$$
$$= -\frac{2}{n}(-1)^n - \frac{1}{n^2\pi}\cos nx\Big|_{-\pi}^{\pi} = -\frac{2}{n}(-1)^n.$$

This establishes the Fourier expansion

$$f(x) = 2\left[\sin x - \frac{\sin 2x}{2} + \frac{\sin 3x}{3} - \cdots + (-1)^{n+1}\frac{\sin nx}{n} + \cdots\right]$$
$$= 2\sum_{n=1}^{\infty}(-1)^{n+1}\frac{\sin nx}{n} = x, \quad -\pi < x < \pi, \tag{14.9}$$

Figure 14.1

Sawtooth Wave



which converges only conditionally, not absolutely, because of the discontinuity of $f(x)$ at $x = \pm\pi$. It makes no difference whether a discontinuity is in the interior of the expansion interval or at its ends: It will give rise to conditional convergence of the Fourier series. In terms of physical applications with $x = \omega$ a frequency, conditional convergence means that our square wave is dominated by **high-frequency components**. ■

Behavior of Discontinuities

The behavior at $x = n\pi$ is an example of a general rule that at a finite discontinuity the series converges to the arithmetic mean. For a discontinuity at $x = x_0$ the series yields

$$f(x_0) = \frac{1}{2}[f(x_0 + 0) + f(x_0 - 0)], \tag{14.10}$$

where the arithmetic mean of the right and left approaches to $x = x_0$. A general proof using partial sums is given by Jeffreys and by Carslaw (see Additional Reading).

An idea of the convergence of a Fourier series and the error in using only a finite number of terms in the series may be obtained by considering the expansion of the sawtooth shape of Fig. 14.1. Figure 14.2 shows $f(x)$ for $0 \leq x < \pi$ for the sum of 4, 6, and 10 terms of the series. Three features deserve comment:

1. There is a steady increase in the accuracy of the representation as the number of terms included is increased.
2. All the curves pass through the midpoint $f(x) = 0$ at $x = \pi$.
3. In the vicinity of $x = \pi$ there is an overshoot that persists and shows no sign of diminishing. This **overshoot (and undershoot)** is called the **Gibbs phenomenon** and is a typical feature of Fourier series. The inclusion of more terms does nothing to remove the overshoot (undershoot) but merely moves it closer to the point of discontinuity. The Gibbs phenomenon is not

Figure 14.2

Fourier Representation of Sawtooth Wave

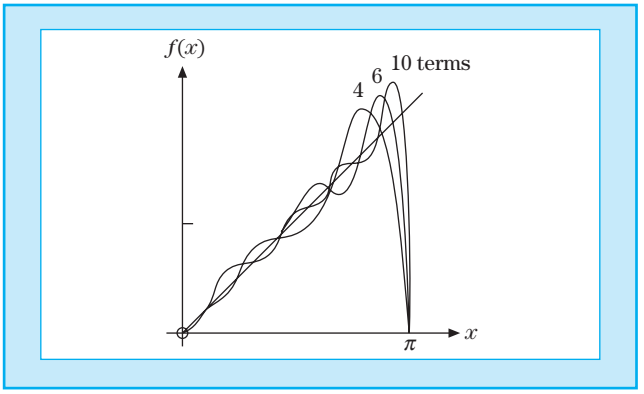
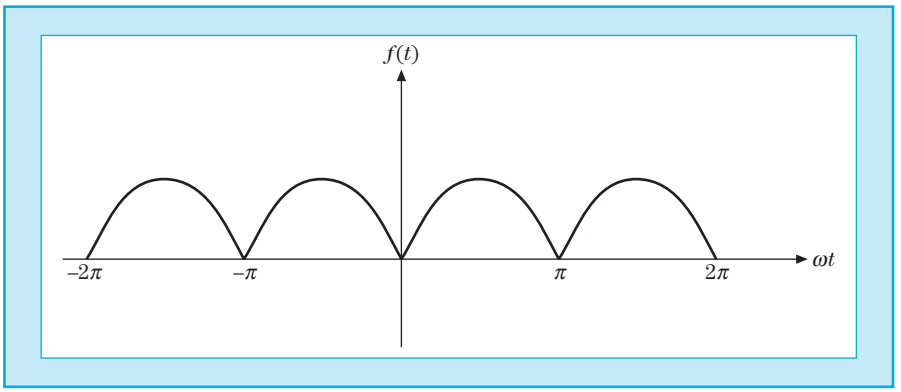


Figure 14.3

Full Wave Rectifier



limited to Fourier series. It occurs with other eigenfunction expansions. For more details, see W. J. Thomson, Fourier series and the Gibbs phenomenon, *Am. J. Phys.* **60**, 425 (1992).

One of the advantages of a Fourier representation over some other representation, such as a Taylor series, is that it can represent a discontinuous function. An example is the sawtooth wave in the preceding section and Example 14.1.3. Other examples are considered in the exercises.

EXAMPLE 14.1.2

Full-Wave Rectifier Consider the case of an absolutely convergent Fourier series representing a continuous periodic function, displayed in Fig. 14.3. Let us ask how well the output of a full-wave rectifier approaches pure direct current. Our rectifier may be thought of as having passed the positive peaks of an incoming sine wave and inverting the negative peaks. This yields

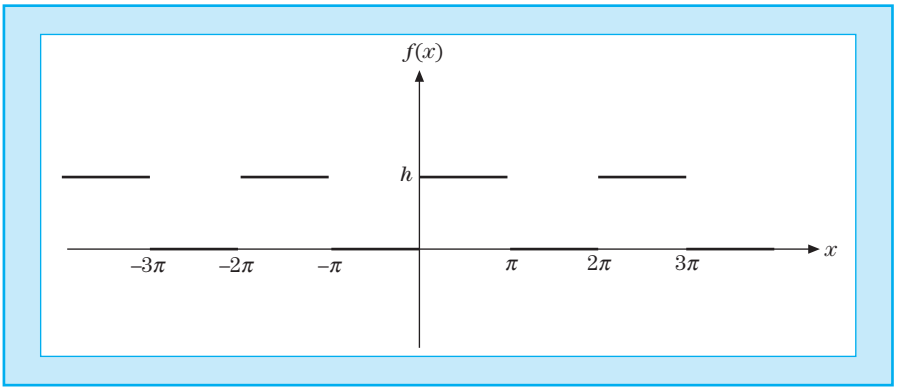
$$\begin{aligned} f(t) &= \sin \omega t, \qquad 0 < \omega t < \pi, \\ f(t) &= -\sin \omega t, \quad -\pi < \omega t < 0. \end{aligned} \tag{14.11}$$

Since $f(t)$ defined here is even, no terms of the form $\sin n\omega t$ will appear. Again, from Eqs. (14.2) and (14.3), we have

$$\begin{aligned} a_0 &= -\frac{1}{\pi}\int_{-\pi}^{0} \sin \omega t \, d(\omega t) + \frac{1}{\pi}\int_{0}^{\pi} \sin \omega t \, d(\omega t) \\ &= \frac{2}{\pi}\int_{0}^{\pi} \sin \omega t \, d(\omega t) = \frac{4}{\pi}, \end{aligned} \tag{14.12}$$

$$\begin{aligned} a_n &= \frac{2}{\pi}\int_{0}^{\pi} \sin \omega t \cos n\omega t \, d(\omega t) \\ &= -\frac{2}{\pi}\frac{2}{n^2-1}, \quad n \text{ even}, \\ &= 0, \quad n \text{ odd}. \end{aligned} \tag{14.13}$$

Figure 14.4
Square Wave



Note that $(0, \pi)$ is not an orthogonality interval for both sines and cosines together and we do not get zero for even n. The resulting series is

$$f(t) = \frac{2}{\pi} - \frac{4}{\pi} \sum_{n=2,4,6,\ldots}^{\infty} \frac{\cos n\omega t}{n^2 - 1}. \tag{14.14}$$

The original frequency ω has been eliminated. The lowest frequency oscillation is 2ω. The high-frequency components fall off as n^{-2}, showing that the full-wave rectifier does a fairly good job of approximating direct current. Whether this good approximation is adequate depends on the particular application. If the remaining ac components are objectionable, they may be further suppressed by appropriate filter circuits. These two examples highlight two features characteristic of Fourier expansions:[2]

- If $f(x)$ has discontinuities (as in the sawtooth wave in Example 14.1.1), we can expect the nth coefficient to be decreasing as $\mathcal{O}(1/n)$. Convergence is conditional only.[3]
- If $f(x)$ is continuous (although possibly with discontinuous derivatives as in the full-wave rectifier of Example 14.1.2), we can expect the nth coefficient to be decreasing as $1/n^2$, that is, absolute convergence. ■

EXAMPLE 14.1.3

Square Wave–High Frequencies One application of Fourier series, the analysis of a "square" wave (Fig. 14.4) in terms of its Fourier components, occurs in electronic circuits designed to handle sharply rising pulses. This example explains the physical meaning of conditional convergence. Suppose that our wave is defined by

$$\begin{aligned} f(x) &= 0, \quad -\pi < x < 0, \\ f(x) &= h, \quad 0 < x < \pi. \end{aligned} \tag{14.15}$$

[2] Raisbeek, G. (1955). Order of magnitude of Fourier coefficients. *Am. Math. Mon.* **62**, 149–155.
[3] A technique for improving the rate of convergence is developed in the exercises of Section 5.9.

From Eqs. (14.2) and (14.3) we find

$$a_0 = \frac{1}{\pi}\int_0^{\pi} h\,dt = h, \tag{14.16}$$

$$a_n = \frac{1}{\pi}\int_0^{\pi} h\cos nt\,dt = 0, \quad n = 1, 2, 3, \ldots, \tag{14.17}$$

$$b_n = \frac{1}{\pi}\int_0^{\pi} h\sin nt\,dt = \frac{h}{n\pi}(1 - \cos n\pi); \tag{14.18}$$

$$b_n = \frac{2h}{n\pi}, \quad n \text{ odd}, \tag{14.19}$$

$$b_n = 0, \quad n \text{ even}. \tag{14.20}$$

The resulting series is

$$f(x) = \frac{h}{2} + \frac{2h}{\pi}\left(\frac{\sin x}{1} + \frac{\sin 3x}{3} + \frac{\sin 5x}{5} + \cdots\right). \tag{14.21}$$

Except for the first term, which represents an average of $f(x)$ over the interval $[-\pi, \pi]$, all the cosine terms have vanished. Since $f(x) - h/2$ is odd, we have a Fourier sine series. Although only the odd terms in the sine series occur, they fall only as n^{-1}. This **conditional convergence** is like that of the harmonic series. Physically, this means that our square wave contains a lot of **high-frequency components**. If the electronic apparatus will not pass these components, our square wave input will emerge more or less rounded off, perhaps as an amorphous blob. ■

Biographical Data

Fourier, Jean Baptiste Joseph, Baron. Fourier, a French mathematician, was born in 1768 in Auxerre, France, and died in Paris in 1830. After his graduation from a military school in Paris, he became a professor at the school in 1795. In 1808, after his great mathematical discoveries involving the series and integrals named after him, he was made a baron by Napoleon. Earlier, he had survived Robespierre and the French Revolution. When Napoleon returned to France in 1815 after his abdication and first exile to Elba, Fourier rejoined him and, after Waterloo, fell out of favor for a while. In 1822, his book on the *Analytic Theory of Heat* appeared and inspired Ohm to new thoughts on the flow of electricity.

SUMMARY

Fourier series are finite or infinite sums of sines and cosines that describe periodic functions that can have discontinuities and thus represent a wider class of functions than we have considered so far. Because $\sin nx$, $\cos nx$ are eigenfunctions of a self-adjoint ODE, the classical harmonic oscillator equation, the Hilbert space properties of Fourier series are consequences of the Sturm–Liouville theory.

EXERCISES

14.1.1 A function $f(x)$ (quadratically integrable) is to be represented by a **finite** Fourier series. A convenient measure of the accuracy of the series is given by the integrated square of the deviation

$$\Delta_p = \int_0^{2\pi} \left[f(x) - \frac{a_0}{2} - \sum_{n=1}^{p} (a_n \cos nx + b_n \sin nx) \right]^2 dx.$$

Show that the requirement that Δ_p be minimized, that is,

$$\frac{\partial \Delta_p}{\partial a_n} = 0, \quad \frac{\partial \Delta_p}{\partial b_n} = 0,$$

for all n, leads to choosing a_n and b_n, as given in Eqs. (14.2) and (14.3). *Note.* Your coefficients a_n and b_n are independent of p. This independence is a consequence of orthogonality and would not hold for powers of x, fitting a curve with polynomials.

14.1.2 In the analysis of a complex waveform (ocean tides, earthquakes, musical tones, etc.) it might be more convenient to have the Fourier series written as

$$f(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty} \alpha_n \cos(nx - \theta_n).$$

Show that this is equivalent to Eq. (14.1) with

$$a_n = \alpha_n \cos\theta, \quad \alpha_n^2 = a_n^2 + b_n^2,$$
$$b_n = \alpha_n \sin\theta, \quad \tan\theta_n = b_n/a_n.$$

Note. The coefficients α_n^2 as a function of n define what is called the **power spectrum**. The importance of α_n^2 lies in its invariance under a shift in the phase θ_n.

14.1.3 Assuming that $\int_{-\pi}^{\pi} [f(x)]^2 dx$ is finite, show that

$$\lim_{m\to\infty} a_m = 0, \quad \lim_{m\to\infty} b_m = 0.$$

Hint. Integrate $[f(x) - s_n(x)]^2$, where $s_n(x)$ is the nth partial sum, and use Bessel's inequality (Section 9.4). For our finite interval the assumption that $f(x)$ is square integrable ($\int_{-\pi}^{\pi} |f(x)|^2\, dx$ is finite) implies that $\int_{-\pi}^{\pi} |f(x)|\, dx$ is also finite. The converse does not hold.

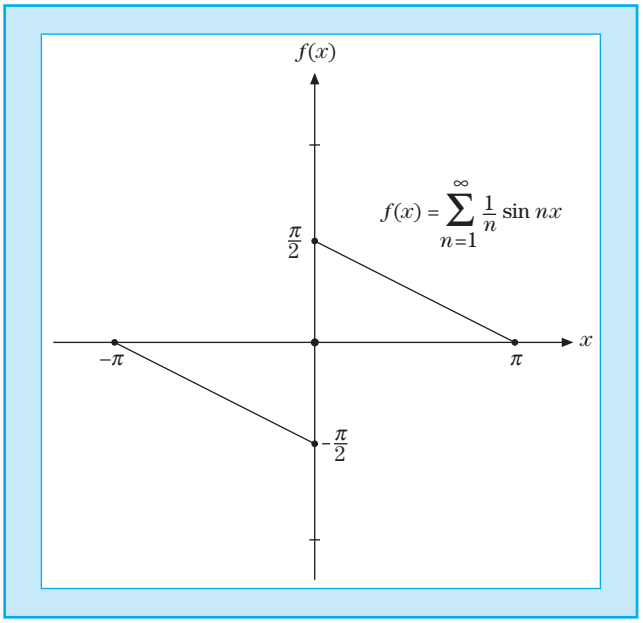
14.1.4 Apply the summation technique of this section to show that

$$\sum_{n=1}^{\infty} \frac{\sin nx}{n} = \begin{cases} \frac{1}{2}(\pi - x), & 0 < x \le \pi \\ -\frac{1}{2}(\pi + x), & -\pi \le x < 0 \end{cases}$$

(Fig. 14.5).

Figure 14.5

Reverse Sawtooth Wave



14.1.5 Sum the trigonometric series

$$\sum_{n=0}^{\infty} \frac{\sin(2n+1)x}{2n+1},$$

and show that it equals

$$\begin{cases} \pi/4, & 0 < x < \pi \\ -\pi/4, & -\pi < x < 0. \end{cases}$$

14.2 Advantages and Uses of Fourier Series

Periodic Functions

Related to the advantage of describing discontinuous functions is the usefulness of a Fourier series in representing a periodic function. If $f(x)$ has a period of 2π, perhaps it is only natural that we expand it in a series of functions with period 2π, $2\pi/2$, $2\pi/3$, ... This guarantees that if our periodic $f(x)$ is represented over one interval $[0, 2\pi]$ or $[-\pi, \pi]$, the representation holds for all finite x.

At this point, we may conveniently consider the properties of **symmetry**. Using the interval $[-\pi, \pi]$, $\sin x$ is odd and $\cos x$ is an even function of x. Hence, by Eqs. (14.2) and (14.3),[4] if $f(x)$ is odd, all $a_n = 0$, and if $f(x)$ is even,

[4] With the range of integration $-\pi \le x \le \pi$.

all $b_n = 0$. In other words,

$$f(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty} a_n \cos nx, \quad f(x) \text{ even}, \tag{14.22}$$

$$f(x) = \sum_{n=1}^{\infty} b_n \sin nx, \quad f(x) \text{ odd}. \tag{14.23}$$

Frequently, these properties are helpful in expanding a given function.

We have noted that the Fourier series is periodic. This is important in considering whether Eq. (14.1) holds outside the initial interval. Suppose we are given only that

$$f(x) = x, \quad 0 \le x < \pi \tag{14.24}$$

and are asked to represent $f(x)$ by a series expansion. Let us take three of the infinite number of possible expansions:

1. If we assume a Taylor expansion, we have

$$f(x) = x, \tag{14.25}$$

   a one-term series. This (one-term) series is defined for all finite x.
2. Using the Fourier cosine series [Eq. (14.22)], we predict that

$$\begin{aligned} f(x) &= -x, \qquad -\pi < x \le 0, \\ f(x) &= 2\pi - x, \quad \pi < x \le 2\pi. \end{aligned} \tag{14.26}$$

3. Finally, from the Fourier sine series [Eq. (14.23)], we have

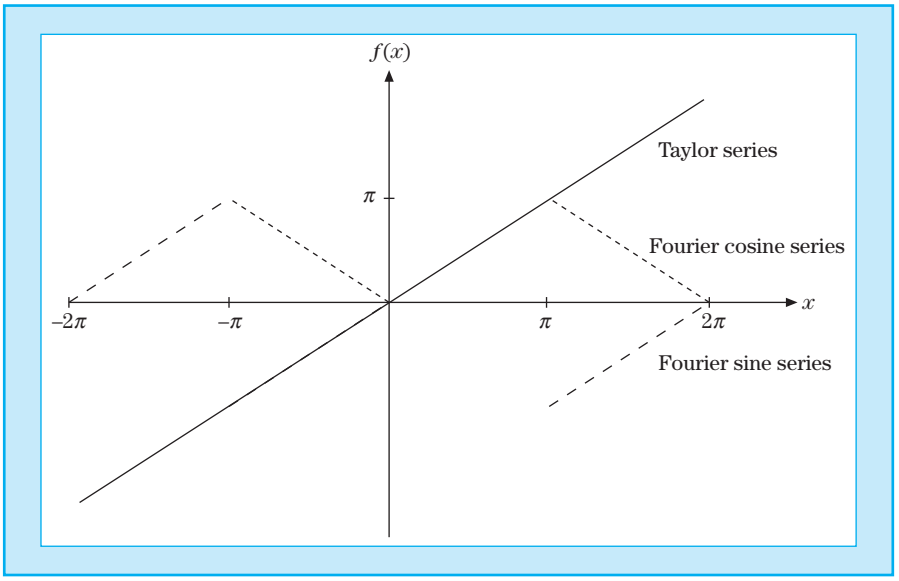
$$\begin{aligned} f(x) &= x, \qquad -\pi < x \le 0, \\ f(x) &= x - 2\pi, \quad \pi < x \le 2\pi. \end{aligned} \tag{14.27}$$

These three possibilities—Taylor series, Fourier cosine series, and Fourier sine series—are each perfectly valid in the original interval $[0, \pi]$. Outside, however, their behavior is strikingly different (compare Fig. 14.6). Which of the three, then, is correct? This question has no answer, unless we are given more information about $f(x)$. It may be any of the three or none of them. Our Fourier expansions are valid over the basic interval. Unless the function $f(x)$ is known to be periodic, with a period equal to our basic interval, or $(1/n)$th of our basic interval, there is no assurance whatever that the representation [Eq. (14.1)] will have any meaning outside the basic interval. Clearly, the interval of length 2π, which defines the expansion, makes a real difference for a nonperiodic function because the Fourier series repeats the pattern of the basic interval in adjacent intervals. This also follows from Fig. 14.6.

In addition to the advantages of representing discontinuous and periodic functions, there is a third very real advantage in using a Fourier series. Suppose that we are solving the equation of motion of an oscillating particle, subject to

Figure 14.6

Comparison of Fourier Cosine Series, Fourier Sine Series, and Taylor Series



a periodic driving force. The Fourier expansion of the driving force then gives us the fundamental term and a series of harmonics. The (linear) ODE may be solved for each of these harmonics individually, a process that may be much easier than dealing with the original driving force. Then, as long as the ODE is linear, all the solutions may be added together to obtain the final solution.[5] This is more than just a clever mathematical trick.

- It corresponds to finding the response of the system to the fundamental frequency and to each of the harmonic frequencies, called Fourier analysis.

The following question is sometimes raised: Were the harmonics there all along, or were they created by our Fourier analysis? One answer compares the functional resolution into harmonics with the resolution of a vector into rectangular components. The components may have been present in the sense that they may be isolated and observed, but the resolution is certainly not unique. Hence, many authorities prefer to say that the harmonics were created by our choice of expansion. Other expansions in other sets of orthogonal functions would give different results. For further discussion, we refer to a series of notes and letters in the *American Journal of Physics*.[6]

[5] One of the nastier features of nonlinear differential equations is that this principle of superposition is not valid.

[6] Robinson, B. L. (1953). Concerning frequencies resulting from distortion. *Am. J. Phys.* **21**, 391; Van Name, F. W., Jr. (1954). Concerning frequencies resulting from distortion. *Am. J. Phys.* **22**, 94.

Change of Interval

So far, attention has been restricted to an interval of length 2π. This restriction may easily be relaxed. If $f(x)$ is periodic with a period $2L$, we may write

$$f(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty} \left[a_n \cos \frac{n\pi x}{L} + b_n \sin \frac{n\pi x}{L} \right], \tag{14.28}$$

with

$$a_n = \frac{1}{L} \int_{-L}^{L} f(t) \cos \frac{n\pi t}{L}\, dt, \quad n = 0, 1, 2, 3, \ldots, \tag{14.29}$$

$$b_n = \frac{1}{L} \int_{-L}^{L} f(t) \sin \frac{n\pi t}{L}\, dt, \quad n = 1, 2, 3, \ldots, \tag{14.30}$$

replacing x in Eq. (14.1) with $\pi x/L$ and t in Eqs. (14.2) and (14.3) with $\pi t/L$. [For convenience, the interval in Eqs. (14.2) and (14.3) is shifted to $-\pi \le t \le \pi$.] The choice of the symmetric interval $[-L, L]$ is **not** essential. For $f(x)$ periodic with a period of $2L$, any interval $(x_0, x_0 + 2L)$ will do. The choice is a matter of convenience or literally personal preference.

If our function $f(-x) = f(x)$ is even in x, then it has a pure cosine series because, by substituting $t \to -t$,

$$\int_{-L}^{0} f(t) \cos \frac{n\pi t}{L} dt = \int_{0}^{L} f(t) \cos \frac{n\pi t}{L} dt,$$
$$\int_{-L}^{0} f(t) \sin \frac{n\pi t}{L} dt = -\int_{0}^{L} f(t) \sin \frac{n\pi t}{L} dt$$

so that all $b_n = 0$ and

$$a_n = \frac{2}{L} \int_{0}^{L} f(t) \cos \frac{n\pi t}{L} dt.$$

Similarly, if $f(-x) = -f(x)$ is odd in x, then $f(x)$ has a pure sine series with coefficients

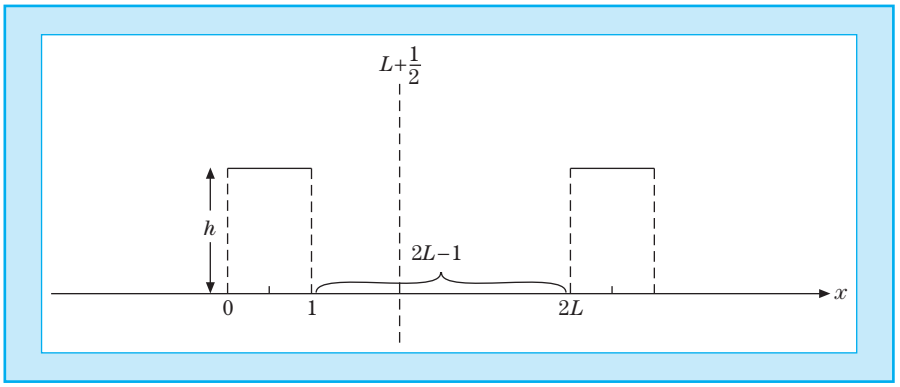
$$b_n = \frac{2}{L} \int_{0}^{L} f(t) \sin \frac{n\pi t}{L} dt.$$

EXAMPLE 14.2.1 **Asymmetric Square Wave** Let us derive the Fourier expansion for the square wave in Fig. 14.7:

$$f(x) = h, \quad 0 < x < 1,$$
$$f(x) = 0, \quad 1 < x < 2L$$

for $L \ge 1$ and $h > 0$. The expansion interval is $[-L, L]$.

Figure 14.7
Asymmetric Square Wave



The geometry of the square pulse implies that its Fourier coefficients are given by Eqs. (14.29) and (14.30) as

$$a_n = \frac{h}{L}\int_0^1 \cos\frac{n\pi x}{L}dx = \frac{h}{n\pi}\sin\frac{n\pi x}{L}\bigg|_0^1 = \frac{h}{n\pi}\sin\frac{n\pi}{L}, \quad n = 0, 1, \ldots,$$

$$b_n = \frac{h}{L}\int_0^1 \sin\frac{n\pi x}{L}dx = -\frac{h}{n\pi}\cos\frac{n\pi x}{L}\bigg|_0^1 = \frac{h}{n\pi}\left(1-\cos\frac{n\pi}{L}\right), \quad n = 1, 2, \ldots.$$

The resulting Fourier series

$$f(x) = \frac{h}{\pi}\sum_{n=1}^{\infty}\frac{1}{n}\left[\sin\frac{n\pi}{L}\cos\frac{n\pi x}{L} + \left(1-\cos\frac{n\pi}{L}\right)\sin\frac{n\pi x}{L}\right]$$

for $L = 1$ agrees with the square wave series of Example 14.1.3 because $\sin n\pi = 0$ and $\cos n\pi = (-1)^n$.

Because f is symmetric about $x = \frac{2L+1}{2}$ (dashed vertical line in Fig. 14.7), we shift the origin of our coordinates from $x = 0$ to this new origin, calling $\xi = x - \frac{2L+1}{2}$ the new variable. We expect a pure cosine series with coefficients

$$\begin{aligned} A_n &= \frac{h}{L}\int_{L-1/2}^{L+1/2}\cos\frac{n\pi\xi}{L}d\xi = \frac{h}{n\pi}\sin\frac{n\pi\xi}{L}\bigg|_{L-1/2}^{L+1/2} \\ &= \frac{h}{n\pi}\left(\sin\frac{n\pi(2L+1)}{2L} - \sin\frac{n\pi(2L-1)}{2L}\right) = (-1)^n\frac{2h}{n\pi}\sin\frac{n\pi}{2L}, \end{aligned}$$

and $B_n = 0$. The Fourier series

$$f(x) = \frac{2h}{\pi}\sum_{n=1}^{\infty}\frac{(-1)^n}{n}\sin\frac{n\pi}{2L}\cos\frac{n\pi(x-L-1/2)}{L}$$

can be seen to be equivalent to our first result using the addition formulas for trigonometric functions

$$\cos\frac{n\pi(x-L-1/2)}{L}=(-1)^n\left[\cos\frac{n\pi}{2L}\cos\frac{n\pi x}{L}+\sin\frac{n\pi}{2L}\sin\frac{n\pi x}{L}\right]. \quad \blacksquare$$

EXERCISES

14.2.1 The boundary conditions [such as $\psi(0)=\psi(l)=0$] may suggest solutions of the form $\sin(n\pi x/l)$ and eliminate the corresponding cosines.

(a) Verify that the boundary conditions used in the Sturm–Liouville theory are satisfied for the interval $(0, l)$. Note that this is only half the usual Fourier interval.

(b) Show that the set of functions $\varphi_n(x)=\sin(n\pi x/l)$, $n=1,2,3,\ldots$ satisfies an orthogonality relation

$$\int_0^l \varphi_m(x)\varphi_n(x)dx=\frac{l}{2}\delta_{mn}, \quad n>0.$$

14.2.2 (a) Expand $f(x)=x$ in the interval $[0, 2L]$. Sketch the series you have found (right-hand side of Answer) over $[-2L, 2L]$.

$$ANS. \quad x=L-\frac{2L}{\pi}\sum_{n=1}^{\infty}\frac{1}{n}\sin\left(\frac{n\pi x}{L}\right).$$

(b) Expand $f(x)=x$ as a sine series in the **half** interval $(0, L)$. Sketch the series you have found (right-hand side of Answer) over $[-2L, 2L]$.

$$ANS. \quad x=\frac{4}{\pi}\sum_{n=0}^{\infty}\frac{1}{2n+1}\sin\frac{(2n+1)\pi x}{L}.$$

14.2.3 In some problems it is convenient to approximate $\sin\pi x$ over the interval $[0, 1]$ by a parabola $ax(1-x)$, where a is a constant. To get a feeling for the accuracy of this approximation, expand $4x(1-x)$ in a Fourier sine series:

$$f(x)=\left\{\begin{array}{ll}4x(1-x), & 0\le x\le 1\\ 4x(1+x), & -1\le x\le 0\end{array}\right\}=\sum_{n=1}^{\infty}b_n\sin n\pi x.$$

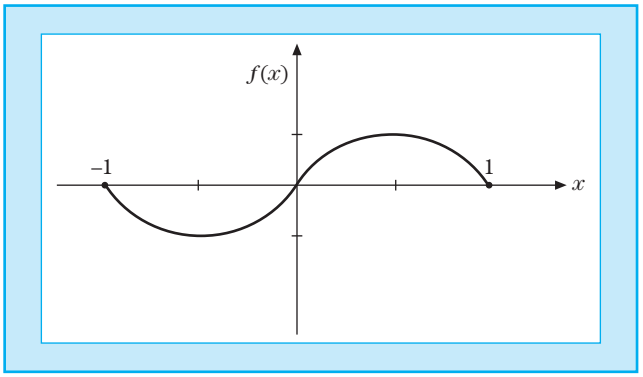
$$ANS. \quad b_n=\frac{32}{\pi^3}\cdot\frac{1}{n^3}, \quad n \text{ odd}$$

$$b_n=0, \quad n \text{ even}$$

(Fig. 14.8).

14.2.4 Take $-\pi\le x\le\pi$ as the basic interval for the function $f(x)=x$ and repeat the arguments leading to Eqs. (14.25)–(14.27). Compare your results with those in Fig. 14.6 and plot them.

Figure 14.8
Parabolic Sine Wave



14.3 Complex Fourier Series

One way of summing a trigonometric Fourier series is to transform it into exponential form and compare it with a Laurent series (see Section 6.5). If we expand $f(z)$ in a Laurent series [assuming $f(z)$ is analytic],

$$f(z) = \sum_{n=-\infty}^{\infty} c_n z^n, \tag{14.31}$$

then on the unit circle $z = e^{i\theta} = \cos\theta + i\sin\theta$ by Euler's identity so that

$$f(z) = f(e^{i\theta}) = \sum_{n=-\infty}^{\infty} c_n e^{in\theta}. \tag{14.32}$$

Expressing $\cos nx$ and $\sin nx$ in exponential form and setting $x = \theta$,

$$\cos nx = \frac{1}{2}(e^{inx} + e^{-inx}), \qquad \sin nx = \frac{1}{2i}(e^{inx} - e^{-inx}),$$

we may rewrite the general Fourier series [Eq. (14.1)] as

$$\begin{aligned} f(x) &= \frac{a_0}{2} + \sum_{n=1}^{\infty}\left[a_n\frac{1}{2}(e^{inx} + e^{-inx}) + b_n\frac{1}{2i}(e^{inx} - e^{-inx})\right] \\ &= \sum_{n=-\infty}^{\infty} c_n e^{inx}, \end{aligned} \tag{14.33}$$

in which

$$c_n = \frac{1}{2}(a_n - ib_n), \quad c_{-n} = \frac{1}{2}(a_n + ib_n), \quad n > 0, \quad c_0 = \frac{1}{2}a_0. \tag{14.34}$$

The Laurent expansion on the unit circle [Eq. (14.32)] has the same form as the complex Fourier series [Eq. (14.33)], which shows the equivalence between the two expansions.

When the function $f(z)$ is known, the complex Fourier coefficients may be directly derived by projection from it:

$$c_n = \frac{1}{2\pi}\int_0^{2\pi} e^{-inx} f(x)dx, \quad -\infty < n < \infty,$$

based on the orthogonality relation [Eq. (14.8)].

Abel's Theorem

Consider a function $f(z)$ represented by a convergent power series

$$f(z) = \sum_{n=0}^{\infty} c_n z^n = \sum_{n=0}^{\infty} c_n r^n e^{in\theta}. \tag{14.35}$$

This is our Fourier exponential series [Eq. (14.32)]. Separating real and imaginary parts

$$u(r,\theta) = \sum_{n=0}^{\infty} c_n r^n \cos n\theta, \qquad v(r,\theta) = \sum_{n=1}^{\infty} c_n r^n \sin n\theta, \tag{14.36}$$

the Fourier cosine and sine series. Abel's theorem asserts that if $u(1,\theta)$ and $v(1,\theta)$ are convergent for a given θ, then

$$u(1,\theta) + iv(1,\theta) = \lim_{r\to 1} f(re^{i\theta}). \tag{14.37}$$

An application of this theorem appears as Exercise 14.3.11, and it is used in the next example.

EXAMPLE 14.3.1

Summation of a Complex Fourier Series Consider the series $\sum_{n=1}^{\infty}(1/n)\cos nx$, $x \in (0, 2\pi)$. Since this series is only conditionally convergent (see Example 5.3.1) and diverges at $x = 0$ so that Dirichlet's conditions are violated, we take

$$\sum_{n=1}^{\infty} \frac{\cos nx}{n} = \lim_{r\to 1} \sum_{n=1}^{\infty} \frac{r^n \cos nx}{n} \tag{14.38}$$

absolutely convergent for $|r| < 1$. Our procedure is again to try forming a power series by transforming the trigonometric functions into exponential form:

$$\sum_{n=1}^{\infty} \frac{r^n \cos nx}{n} = \frac{1}{2}\sum_{n=1}^{\infty} \frac{r^n e^{inx}}{n} + \frac{1}{2}\sum_{n=1}^{\infty} \frac{r^n e^{-inx}}{n}. \tag{14.39}$$

Now these power series may be identified as Maclaurin expansions of $-\ln(1-z)$, $z = re^{ix}, re^{-ix}$ [Eq. (5.65)], and

$$\begin{aligned}\sum_{n=1}^{\infty} \frac{r^n \cos nx}{n} &= -\frac{1}{2}[\ln(1-re^{ix}) + \ln(1-re^{-ix})] \\ &= -\ln[(1+r^2) - 2r\cos x]^{1/2}.\end{aligned} \tag{14.40}$$

Table 14.1

	Fourier Series	Reference
1.	$\displaystyle\sum_{n=1}^{\infty}\frac{1}{n}\sin nx=\begin{cases}-\frac{1}{2}(\pi+x), & -\pi\le x<0\\ \frac{1}{2}(\pi-x), & 0\le x<\pi\end{cases}$	Exercise 14.1.4 Exercise 14.3.3
2.	$\displaystyle\sum_{n=1}^{\infty}(-1)^{n+1}\frac{1}{n}\sin nx=\frac{1}{2}x, \quad -\pi<x<\pi$	Example 14.1.1 Exercise 14.3.2
3.	$\displaystyle\sum_{n=0}^{\infty}\frac{1}{2n+1}\sin(2n+1)x=\begin{cases}-\pi/4, & -\pi<x<0\\ +\pi/4, & 0<x<\pi\end{cases}$	Exercise 14.1.5 Eq. (14.52)
4.	$\displaystyle\sum_{n=1}^{\infty}\frac{\cos nx}{n}=-\ln\left[2\sin\left(\frac{\lvert x\rvert}{2}\right)\right], \quad -\pi<x<\pi$	Eq. (14.38)
5.	$\displaystyle\sum_{n=1}^{\infty}(-1)^n\frac{1}{n}\cos nx=-\ln\left[2\cos\left(\frac{x}{2}\right)\right], \quad -\pi<x<\pi$	Exercise 14.3.11
6.	$\displaystyle\sum_{n=0}^{\infty}\frac{1}{2n+1}\cos(2n+1)x=\frac{1}{2}\ln\left[\cot\frac{\lvert x\rvert}{2}\right], \quad -\pi<x<\pi$	(Item 5 − Item 4)
7.	$\displaystyle\sum_{n=1}^{\infty}(-1)^n\frac{\cos nx}{n^2}=\frac{x^2}{4}-\frac{\pi^2}{12}, \quad -\pi<x<\pi$	Example 14.4.2
8.	$\displaystyle\sum_{n=0}^{\infty}\frac{\cos(2n+1)x}{(2n+1)^2}=\frac{\pi}{4}\left(\frac{\pi}{2}-\lvert x\rvert\right), \quad -\pi<x<\pi$	Exercise 14.3.4

Letting $r = 1$ based on Abel's theorem, we obtain item 4 of Table 14.1

$$\sum_{n=1}^{\infty}\frac{\cos nx}{n}=-\ln(2-2\cos x)^{1/2}$$

$$=-\ln\left(2\sin\frac{x}{2}\right), \quad x\in(0,2\pi).^{7} \tag{14.41}$$

Both sides of this expression diverge as $x\to 0$ and 2π. ■

EXERCISES

14.3.1 Develop the Fourier series representation of

$$f(t)=\begin{cases}0, & -\pi\le\omega t\le 0,\\ \sin\omega t, & 0\le\omega t\le\pi.\end{cases}$$

This is the output of a simple half-wave rectifier. It is also an approximation of the solar thermal effect that produces "tides" in the atmosphere.

ANS. $\displaystyle f(t)=\frac{1}{\pi}+\frac{1}{2}\sin\omega t-\frac{2}{\pi}\sum_{n=2,4,6,\ldots}^{\infty}\frac{\cos n\omega t}{n^2-1}.$

[7] The limits may be shifted to $(-\pi,\pi)$ (and $x\neq 0$) using $|x|$ on the right-hand side.

14.3.2 A sawtooth wave is given by

$$f(x) = x, \quad -\pi < x < \pi.$$

Show that

$$f(x) = 2\sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n} \sin nx.$$

14.3.3 A different sawtooth wave is described by

$$f(x) = \begin{cases} -\frac{1}{2}(\pi + x), & -\pi \le x < 0 \\ +\frac{1}{2}(\pi - x), & 0 < x \le \pi. \end{cases}$$

Show that $f(x) = \sum_{n=1}^{\infty} (\sin nx/n)$.

14.3.4 A triangular wave (Fig. 14.9) is represented by

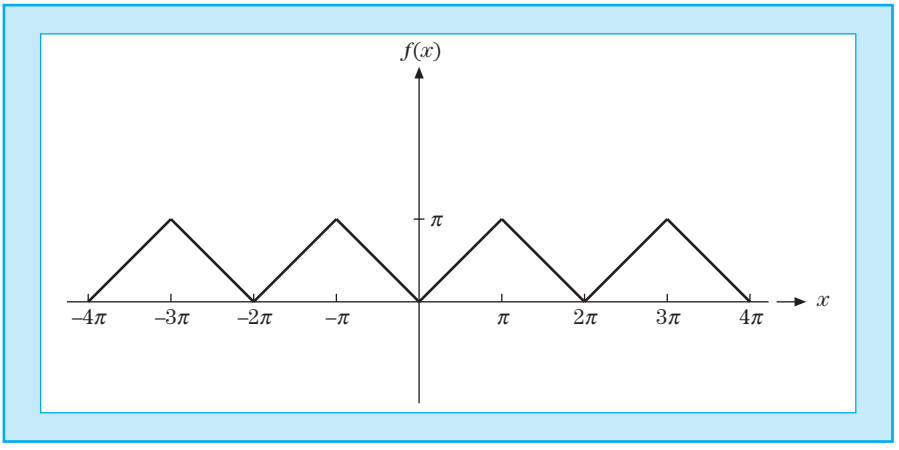
$$f(x) = \begin{cases} x, & 0 \le x \le \pi \\ -x, & -\pi \le x \le 0. \end{cases}$$

Represent $f(x)$ by a Fourier series.

ANS. $f(x) = \dfrac{\pi}{2} - \dfrac{4}{\pi} \sum_{n=1,3,5,\ldots} \dfrac{\cos nx}{n^2}.$

Figure 14.9

Triangular Wave



14.3.5 Expand

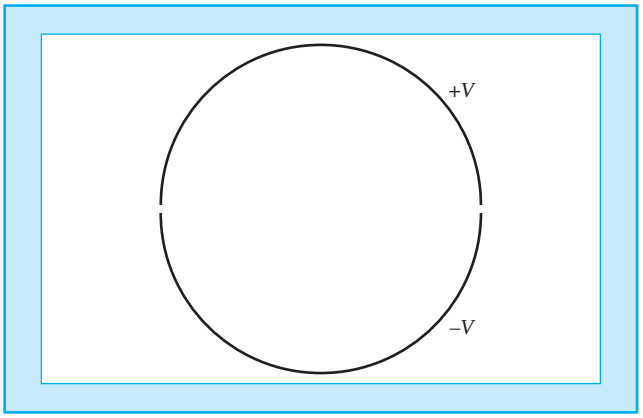
$$f(x) = \begin{cases} 1, & x^2 < x_0^2 \\ 0, & x^2 > x_0^2 \end{cases}$$

in the interval $[-\pi, \pi]$.

Note. This variable-width square wave is important in electronic music.

Figure 14.10

Cross Section of Split Tube



14.3.6 A metal cylindrical tube of radius a is split lengthwise into two nontouching halves. The top half is maintained at a potential $+V$ and the bottom half at a potential $-V$ (Fig. 14.10). Separate the variables in Laplace's equation and solve for the electrostatic potential for $r \leq a$. Observe the resemblance between your solution for $r = a$ and the Fourier series for a square wave.

14.3.7 A metal cylinder is placed in a (previously) uniform electric field, E_0, with the axis of the cylinder perpendicular to that of the original field.
(a) Find the perturbed electrostatic potential.
(b) Find the induced surface charge on the cylinder as a function of angular position.

14.3.8 Expand $\delta(x-t)$ in a Fourier series.

$$\textit{ANS.} \quad \delta(x-t) = \frac{1}{2\pi} + \frac{1}{\pi}\sum_{n=1}^{\infty}(\cos nx\cos nt + \sin nx\sin nt)$$
$$= \frac{1}{2\pi} + \frac{1}{\pi}\sum_{n=1}^{\infty}\cos n(x-t).$$

14.3.9 Verify that

$$\delta(\varphi_1-\varphi_2) = \frac{1}{2\pi}\sum_{m=-\infty}^{\infty} e^{im(\varphi_1-\varphi_2)}$$

is a Dirac delta function by showing that it satisfies the definition of a Dirac delta function:

$$\int_{-\pi}^{\pi} f(\varphi_2)\frac{1}{2\pi}\sum_{m=-\infty}^{\infty} e^{im(\varphi_1-\varphi_2)}d\varphi_2 = f(\varphi_1).$$

Hint. Represent $f(\varphi_2)$ by an exponential Fourier series.

Note. The continuum analog of this expression is developed in Section 15.2.

14.3.10 (a) Find the Fourier series representation of

$$f(x) = \begin{cases} 0, & -\pi < x \le 0 \\ x, & 0 \le x < \pi. \end{cases}$$

(b) From the Fourier expansion show that

$$\frac{\pi^2}{8} = 1 + \frac{1}{3^2} + \frac{1}{5^2} + \cdots.$$

14.3.11 Let $f(z) = \ln(1+z) = \sum_{n=1}^{\infty}(-1)^{n+1}z^n/n$. (This series converges to $\ln(1+z)$ for $|z| \le 1$, except at the point $z = -1$.)

(a) From the imaginary parts (item 5 of Table 14.1) show that

$$\ln\left(2\cos\frac{\theta}{2}\right) = \sum_{n=1}^{\infty}(-1)^{n+1}\frac{\cos n\theta}{n}, \quad -\pi < \theta < \pi.$$

(b) Using a change of variable, transform part (a) into

$$-\ln\left(2\sin\frac{\theta}{2}\right) = \sum_{n=1}^{\infty}(-1)^{n+1}\frac{\cos n\theta}{n}, \quad 0 < \theta < 2\pi.$$

14.3.12 A symmetric triangular pulse of adjustable height and width is described by

$$f(x) = \begin{cases} a(1 - x/b), & 0 \le |x| \le b \\ 0, & b \le |x| \le \pi. \end{cases}$$

(a) Show that the Fourier coefficients are

$$a_0 = \frac{ab}{\pi}, \quad a_n = \frac{2ab}{\pi}(1 - \cos nb)/(nb)^2.$$

Sum the finite Fourier series through $n = 10$ and through $n = 100$ for $x/\pi = 0(l/9)1$. Take $a = 1$ and $b = \pi/2$.

(b) Call a Fourier analysis subroutine (if available) to calculate the Fourier coefficients of $f(x)$, a_0 through a_{10}.

14.3.13 (a) Using a Fourier analysis subroutine, calculate the Fourier cosine coefficients a_0 through a_{10} of

$$f(x) = [1 - (x/\pi)^2]^{1/2}, \quad x \in [-\pi, \pi].$$

(b) Spot check by calculating some of the preceding coefficients by direct numerical quadrature.

Check values. $a_0 = 0.785$, $a_2 = 0.284$.

14.3.14 A function $f(x)$ is expanded in an exponential Fourier series

$$f(x) = \sum_{n=-\infty}^{\infty} c_n e^{inx}.$$

If $f(x)$ is real, $f(x) = f^*(x)$, what restriction is imposed on the coefficients c_n?

14.4 Properties of Fourier Series

Convergence

Note that our Fourier series should not be expected to be uniformly convergent if it represents a discontinuous function. A uniformly convergent series of continuous functions ($\sin nx$, $\cos nx$) always yields a continuous function $f(x)$ (compare Section 5.5). If, however, (i) $f(x)$ is continuous, $-\pi \le x \le \pi$, (ii) $f(-\pi) = f(+\pi)$, and (iii) $f'(x)$ is sectionally continuous, the Fourier series for $f(x)$ will converge uniformly. These restrictions do not demand that $f(x)$ be periodic, but they will be satisfied by continuous, differentiable, periodic functions (period of 2π). For a proof of uniform convergence we refer to the literature.[8] With or without a discontinuity in $f(x)$, the Fourier series will yield convergence in the mean (Section 9.4).

If a function is square integrable, then Sturm–Liouville theory implies the validity of the Bessel inequality [Eq. (9.73)]

$$2a_0^2 + \sum_{n=1}^{\infty} (a_n^2 + b_n^2) \le \frac{1}{\pi} \int_{-\pi}^{\pi} f^2(x)dx \tag{14.42}$$

so that at least the sum of squares of its Fourier coefficients converges.

EXAMPLE 14.4.1

Absolutely Convergent Fourier Series If the periodic function $f(x)$ has a bounded second derivative $f''(x)$, then its Fourier series converges absolutely. Note that the converse is not valid, as the full-wave rectifier (Example 14.1.2) demonstrates.

To show this, let us integrate by parts the Fourier coefficients

$$a_n = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \cos nx\, dx = \frac{f(x) \sin nx}{n\pi} \bigg|_{-\pi}^{\pi} - \frac{1}{n\pi} \int_{-\pi}^{\pi} f'(x) \sin nx\, dx,$$

where the integrated term vanishes. Because the first derivative $f'(x)$ is bounded a fortiori, $|a_n| = \mathcal{O}(\frac{1}{n})$, and similarly $b_n \to 0$ for $n \to \infty$, at least as fast as $1/n$, which is not sufficient for absolute convergence. However, another integration by parts can be done, yielding

$$a_n = \frac{f'(x) \cos nx}{n^2\pi} \bigg|_{-\pi}^{\pi} - \frac{1}{n^2\pi} \int_{-\pi}^{\pi} f''(x) \cos nx\, dx, \tag{14.43}$$

[8] See, for instance, Churchill, R. V. (1993). *Fourier Series and Boundary Value Problems*, 5th ed., Section 38. McGraw-Hill, New York.

where the integrated terms cancel each other because f' is continuous and periodic; that is, $f'(\pi) = f'(-\pi)$. Since $|f''(x)| \le M$, we find the upper bound

$$|a_n| \le \frac{M}{n^2\pi} \int_{-\pi}^{\pi} dx = \frac{2M}{n^2}, \tag{14.44}$$

which implies absolute convergence (by the integral test of Chapter 5), and the same applies to b_n. ■

If the $|a_n|$, $|b_n| \le n^{-\alpha}$ with $0 < \alpha \le 1$, then we have at least conditional convergence, and the function $f(x)$ may have discontinuities. If $\alpha > 1$, then there is absolute convergence by the integral test of Chapter 5.

Integration

Term-by-term integration of the series

$$f(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty} a_n \cos nx + \sum_{n=1}^{\infty} b_n \sin nx \tag{14.45}$$

yields

$$\int_{x_0}^{x} f(x)dx = \frac{a_0 x}{2}\bigg|_{x_0}^{x} + \sum_{n=1}^{\infty} \frac{a_n}{n} \sin nx\bigg|_{x_0}^{x} - \sum_{n=1}^{\infty} \frac{b_n}{n} \cos nx\bigg|_{x_0}^{x}. \tag{14.46}$$

Clearly, the effect of integration is to place an additional power of n in the denominator of each coefficient. This results in more rapid convergence than before. Consequently, a convergent Fourier series may always be integrated term by term, with the resulting series converging uniformly to the integral of the original function. Indeed, term-by-term integration may be valid even if the original series [Eq. (14.45)] is not convergent. The function $f(x)$ need only be integrable. A discussion will be found in Jeffreys and Jeffreys, Section 14.06 (see Additional Reading).

Strictly speaking, Eq. (14.46) may not be a Fourier series; that is, if $a_0 \ne 0$, there will be a term $\frac{1}{2}a_0 x$. However,

$$\int_{x_0}^{x} f(x)dx - \frac{1}{2}a_0 x \tag{14.47}$$

will still be a Fourier series.

EXAMPLE 14.4.2 **Integration of Fourier Series** Consider the sawtooth series for

$$f(x) = x, \quad -\pi < x < \pi. \tag{14.48}$$

Comparing with Exercise 14.1.1, the Fourier series is

$$x = 2\sum_{n=1}^{\infty} (-1)^{n+1} \frac{\sin nx}{n}, \quad -\pi < x < \pi,$$

which converges conditionally, but not absolutely, because the harmonic series diverges. Now we integrate it and obtain item 7 of Table 14.1

$$\begin{aligned} 2\int_0^x \sum_{n=1}^{\infty}(-1)^{n-1}\frac{\sin nx}{n}dx &= 2\sum_{n=1}^{\infty}\frac{(-1)^{n-1}}{n}\int_0^x \sin nx\,dx \\ &= 2\sum_{n=1}^{\infty}\frac{(-1)^{n-1}}{n^2}(1-\cos nx) \\ &= \frac{\pi^2}{6}+2\sum_{n=1}^{\infty}(-1)^n\frac{\cos nx}{n^2} = \frac{x^2}{2} \end{aligned}$$

using Exercise 14.4.1. Because $|\cos nx| \le 1$ is bounded and the series $\sum_n 1/n^2$ converges, our integrated Fourier series converges absolutely to the limit $\int_0^x x\,dx = x^2/2$. ■

Differentiation

The situation regarding differentiation is quite different from that of integration. Here the word is caution.

EXAMPLE 14.4.3 **Differentiation of Fourier Series** Consider again the series of Example 14.4.2. Differentiating term by term, we obtain

$$1 = 2\sum_{n=1}^{\infty}(-1)^{n+1}\cos nx, \tag{14.49}$$

which is not convergent for any value of x. **Warning:** Check the convergence of your derivative.

For a triangular wave (Exercise 14.3.4), in which the convergence is more rapid (and uniform),

$$f(x) = \frac{\pi}{2} - \frac{4}{\pi}\sum_{n=1,\text{odd}}^{\infty}\frac{\cos nx}{n^2}. \tag{14.50}$$

Differentiating term by term,

$$f'(x) = \frac{4}{\pi}\sum_{n=1,\text{odd}}^{\infty}\frac{\sin nx}{n}, \tag{14.51}$$

which is the Fourier expansion of a square wave

$$f'(x) = \begin{cases} 1, & 0 < x < \pi, \\ -1, & -\pi < x < 0. \end{cases} \tag{14.52}$$

Inspection of Fig. 14.4 verifies that this is indeed the derivative of our triangular wave. ■

- As the inverse of integration, the operation of differentiation has placed an additional factor n in the numerator of each term. This reduces the rate of convergence and may, as in the first case mentioned, render the differentiated series divergent.
- In general, term-by-term differentiation is permissible under the same conditions listed for uniform convergence in Chapter 5.

From the expansion of x and expansions of other powers of x, numerous other infinite series can be evaluated. A few are included in the subsequent exercises.

EXERCISES

14.4.1 Show that integration of the Fourier expansion of $f(x) = x$, $-\pi < x < \pi$, leads to

$$\frac{\pi^2}{12} = \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n^2} = 1 - \frac{1}{4} + \frac{1}{9} - \frac{1}{16} + \cdots.$$

14.4.2 Parseval's identity.

(a) Assuming that the Fourier expansion of $f(x)$ is uniformly convergent, show that

$$\frac{1}{\pi}\int_{-\pi}^{\pi} [f(x)]^2\, dx = \frac{a_0^2}{2} + \sum_{n=1}^{\infty} \left(a_n^2 + b_n^2\right).$$

This is Parseval's identity. It is actually a special case of the completeness relation [Eq. (9.73)].

(b) Given

$$x^2 = \frac{\pi^2}{3} + 4\sum_{n=1}^{\infty} \frac{(-1)^n \cos nx}{n^2}, \quad -\pi \le x \le \pi,$$

apply Parseval's identity to obtain $\zeta(4)$ in closed form.

(c) The condition of uniform convergence is not necessary. Show this by applying the Parseval identity to the square wave

$$f(x) = \begin{cases} -1, & -\pi < x < 0 \\ 1, & 0 < x < \pi \end{cases}$$

$$= \frac{4}{\pi}\sum_{n=1}^{\infty} \frac{\sin(2n-1)x}{2n-1}.$$

14.4.3 Show that integrating the Fourier expansion of the Dirac delta function (Exercise 14.3.8) leads to the Fourier representation of the square wave [Eq. (14.21)], with $h = 1$.

Note. Integrating the constant term $(1/2\pi)$ leads to a term $x/2\pi$. What are you going to do with this?

14.4.4 Integrate the Fourier expansion of the unit step function

$$f(x) = \begin{cases} 0, & -\pi < x < 0 \\ x, & 0 \le x < \pi. \end{cases}$$

Show that your integrated series agrees with Exercise 14.3.12.

14.4.5 In the interval $[-\pi, \pi]$,

$$\delta_n(x) = n, \quad \text{for } |x| < 1/(2n),$$
$$0, \quad \text{for } |x| > 1/(2n)$$

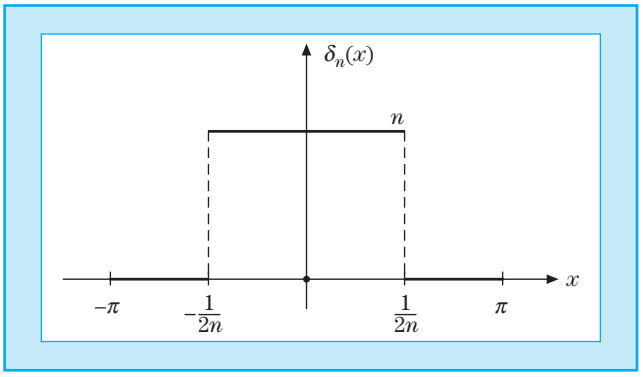
(Fig. 14.11).

(a) Expand $\delta_n(x)$ as a Fourier cosine series.

(b) Show that your Fourier series agrees with a Fourier expansion of $\delta(x)$ in the limit as $n \to \infty$.

Figure 14.11

Rectangular Pulse



14.4.6 Confirm the delta function nature of your Fourier series of Exercise 14.4.5 by showing that for any $f(x)$ that is finite in the interval $[-\pi, \pi]$ and continuous at $x = 0$,

$$\int_{-\pi}^{\pi} f(x)[\text{Fourier expansion of } \delta_\infty(x)]\, dx = f(0).$$

14.4.7 Find the charge distribution over the interior surfaces of the semicircles of Exercise 14.3.6.

Note. You obtain a divergent series and this Fourier approach fails. Using conformal mapping techniques, we may show the charge density to be proportional to $\csc\theta$. Does $\csc\theta$ have a Fourier expansion?

14.4.8 Given

$$\varphi_1(x) = \sum_{n=1}^{\infty} \frac{\sin nx}{n} = \begin{cases} -(\pi + x)/2, & -\pi \le x < 0 \\ (\pi - x)/2 & 0 < x \le \pi, \end{cases}$$

show by integrating that

$$\varphi_2(x) \equiv \sum_{n=1}^{\infty} \frac{\cos nx}{n^2} = \begin{cases} (\pi + x)^2/4 - \pi^2/(12), & -\pi \le x \le 0 \\ (\pi - x)^2/4 - \pi^2/(12), & 0 \le x \le \pi. \end{cases}$$

Additional Reading

Carslaw, H. S. (1921). *Introduction to the Theory of Fourier's Series and Integrals*, 2nd ed. Macmillan, London. Paperback, 3rd ed., Dover, New York (1952). This is a detailed and classic work.

Hamming, R. W. (1973). *Numerical Methods for Scientists and Engineers*, 2nd ed. McGraw-Hill, New York. Reprinted, Dover, New York (1987).

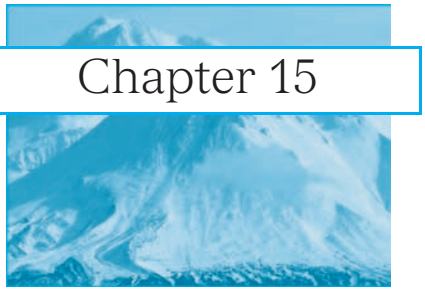
Jeffreys, H., and Jeffreys, B. S. (1972). *Methods of Mathematical Physics*, 3rd ed. Cambridge Univ. Press, Cambridge, UK.

Kufner, A., and Kadlec, J. (1971). *Fourier Series*. Iliffe, London. This book is a clear account of Fourier series in the context of Hilbert space.

Lanczos, C. (1956). *Applied Analysis*. Prentice-Hall, Englewood Cliffs, NJ. Reprinted, Dover, New York (1988). The book gives a well-written presentation of the Lanczos convergence technique (which suppresses the Gibbs phenomenon oscillations). This and several other topics are presented from the point of view of a mathematician who wants useful numerical results and not just abstract existence theorems.

Oberhettinger, F. (1973). *Fourier Expansions, A Collection of Formulas*. Academic Press, New York.

Zygmund, A. (1988). *Trigonometric Series*. Cambridge Univ. Press, Cambridge, UK. The volume contains an extremely complete exposition, including relatively recent results in the realm of pure mathematics.



Chapter 15

Integral Transforms

15.1 Introduction and Definitions

Frequently in physics we encounter pairs of functions related by an integral of the form

$$F(\alpha) = \int_a^b f(t)K(\alpha, t)dt. \tag{15.1}$$

The function $F(\alpha)$ is called the (integral) transform of $f(t)$ by the kernel $K(\alpha, t)$. The operation may also be described as mapping a function $f(t)$ in t-space into another function $F(\alpha)$ in α-space. This interpretation takes on physical significance in the time–frequency relation of Fourier transforms, such as Example 15.4.4.

Linearity

These integral transforms are linear operators; that is,

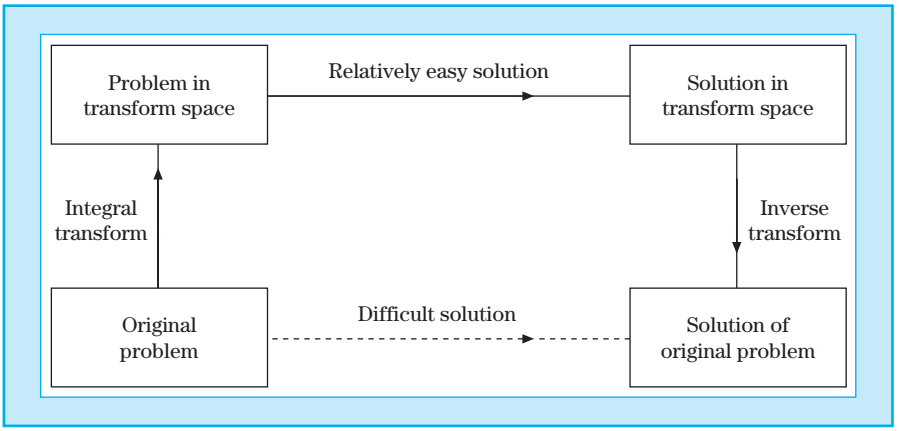
$$\begin{aligned}\int_a^b [c_1 f_1(t) + c_2 f_2(t)]K(\alpha, t)dt \\ &= c_1 \int_a^b f_1(t)K(\alpha, t)dt + c_2 \int_a^b f_2(t)K(\alpha, t)dt, \\ &= c_1 F_1(\alpha) + c_2 F_2(\alpha),\end{aligned} \tag{15.2}$$

$$\int_a^b cf(t)K(\alpha, t)dt = c\int_a^b f(t)K(\alpha, t)dt, \tag{15.3}$$

where c_1, c_2, c are constants, and $f_1(t)$, $f_2(t)$ are functions for which the integral transform is well defined.

Figure 15.1

Schematic Integral Transforms



Representing our linear integral transform by the operator $\mathcal{L}$, we obtain

$$F = \mathcal{L}f. \tag{15.4}$$

We expect an inverse operator $\mathcal{L}^{-1}$ exists, such that[1]

$$f = \mathcal{L}^{-1}F. \tag{15.5}$$

For our three Fourier transforms $\mathcal{L}^{-1}$ is given in Section 15.4. In general, the evaluation of the inverse transform is the main problem in using integral transforms. The inverse Laplace transform is discussed in Section 15.12.

Integral transforms have many special physical applications and interpretations that are noted in the remainder of this chapter. The most common application is outlined in Fig. 15.1. Perhaps an original problem can be solved only with difficulty, if at all, in the original coordinates (space). It often happens that the transform of the problem can be solved relatively easily. Then, the inverse transform returns the solution from the transform coordinates to the original system. Examples 15.5.2 and 15.5.4 illustrate this technique.

15.2 Fourier Transform

One of the most useful of the infinite number of possible transforms is the Fourier transform, given by

$$F(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(t)e^{i\omega t}dt. \tag{15.6}$$

[1]Expectation is not proof, and here proof of existence is complicated because we are actually in an **infinite**-dimensional space. We shall prove existence in the special cases of interest by actual construction.

Two modifications of this form, developed in Section 15.4, are the Fourier cosine and Fourier sine transforms:

$$F_c(\omega) = \sqrt{\frac{2}{\pi}} \int_0^\infty f(t) \cos \omega t \, dt, \tag{15.7}$$

$$F_s(\omega) = \sqrt{\frac{2}{\pi}} \int_0^\infty f(t) \sin \omega t \, dt. \tag{15.8}$$

All these integrals exist if $\int_{-\infty}^{\infty} |f(t)|dt < \infty$, a condition denoted $f \in L(-\infty, \infty)$ in the mathematical literature and meaning that the function f belongs to the space of absolutely integrable functions. Moreover, then Riemann's lemma holds

$$\int_{-\infty}^{\infty} f(t) \cos \omega t \, dt \to 0, \qquad \int_{-\infty}^{\infty} f(t) \sin \omega t \, dt \to 0, \quad \text{as } \omega \to \infty.$$

The Fourier transform is based on the kernel $e^{i\omega t}$ and its real and imaginary parts taken separately, $\cos \omega t$ and $\sin \omega t$. Because these kernels are the functions used to describe waves, due to their periodicity, Fourier transforms appear frequently in studies of waves and the extraction of information from waves, particularly when phase information is involved. The output of a stellar interferometer, for instance, involves a Fourier transform of the brightness across a stellar disk. The electron charge distribution in an atom may be obtained from a Fourier transform of the amplitude of scattered X-rays. In quantum mechanics the physical origin of the Fourier relations of Section 15.7 is the wave nature of matter and our description of matter in terms of waves.

If we differentiate the Fourier transform

$$\frac{dF(\omega)}{d\omega} = \frac{i}{\sqrt{2\pi}} \int_{-\infty}^{\infty} t f(t) e^{i\omega t} dt,$$

we see that the original function $f(t)$ is multiplied by it. This is one way of generating new Fourier transforms.

If we differentiate a cosine transform with respect to ω, we are led to a sine transform and vice versa. Many examples are given by Titchmarsh (see Additional Reading).

EXAMPLE 15.2.1

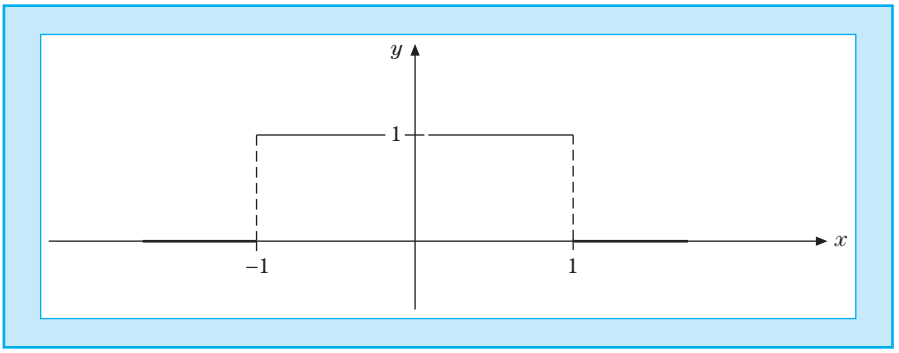
Square Pulse Let us find the Fourier transform for the shape in Fig. 15.2:

$$f(t) = \begin{cases} 1, & |t| < 1, \\ 0, & |t| > 1, \end{cases}$$

which is an even function of t. This is the single slit diffraction problem of physical optics. The slit is described by $f(t)$. The diffraction pattern **amplitude**

Figure 15.2

Square Pulse



is given by the Fourier transform $F(\omega)$. Starting from Eq.(15.6),

$$F(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(t) e^{i\omega t} dt = \frac{1}{\sqrt{2\pi}} \int_{-1}^{1} e^{i\omega t} dt = \frac{1}{\sqrt{2\pi}} \frac{e^{i\omega t}}{i\omega} \Big|_{-1}^{1}$$
$$= \frac{e^{i\omega} - e^{-i\omega}}{i\omega\sqrt{2\pi}} = \sqrt{\frac{2}{\pi}} \frac{\sin\omega}{\omega},$$

which is an even function of ω. ■

EXAMPLE 15.2.2 **Fourier Transform of Gaussian** The Fourier transform of a Gaussian,

$$F(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-a^2 t^2} e^{i\omega t} dt, \tag{15.9}$$

can be done analytically by completing the square in the exponent,

$$-a^2 t^2 + i\omega t = -a^2 \left(t - \frac{i\omega}{2a^2} \right)^2 - \frac{\omega^2}{4a^2},$$

which we check by evaluating the square. Substituting this identity we obtain

$$F(\omega) = \frac{1}{\sqrt{2\pi}} e^{-\omega^2/4a^2} \int_{-\infty}^{\infty} e^{-a^2 t^2} dt$$

upon shifting the integration variable $t \to t + \frac{i\omega}{2a^2}$. This is justified by an application of Cauchy's theorem to the rectangle with vertices $-T$, T, $T + \frac{i\omega}{2a^2}$, $-T + \frac{i\omega}{2a^2}$ for $T \to \infty$, noting that the integrand has no singularities in this region and the integrals over the sides from $\pm T$ to $\pm T + \frac{i\omega}{2a^2}$ become negligible for $T \to \infty$. Finally, we rescale the integration variable as $\xi = at$ in the integral

$$\int_{-\infty}^{\infty} e^{-a^2 t^2} dt = \frac{1}{a} \int_{-\infty}^{\infty} e^{-\xi^2} d\xi = \frac{\sqrt{\pi}}{a}.$$

Substituting these results we find

$$F(\omega) = \frac{1}{a\sqrt{2}} \exp\left(-\frac{\omega^2}{4a^2}\right), \tag{15.10}$$

again a Gaussian, but in ω-space. The smaller a is (i.e., the wider the original Gaussian $e^{-a^2t^2}$ is), the narrower is its Fourier transform $\sim e^{-\omega^2/4a^2}$. Differentiating $F(\omega)$, the Fourier transform of $i\omega e^{-\omega^2/4a^2}$ is $\sim te^{-a^2t^2}$, etc. ■

Laplace Transform

The equally important Laplace transform is related to a Fourier transform by replacing the frequency ω with an imaginary variable and changing the integration interval, that is, $\exp(i\omega x) \to \exp(-sx)$, which will be developed in Sections 15.8–15.12. The Laplace transform

$$F(s) = \int_0^\infty f(t)e^{-st}dt \tag{15.11}$$

has the kernel e^{-st}. Clearly, the possible types of integral transforms are unlimited. The Laplace transform has been useful in mathematical analysis as well as in physics and engineering applications. The Laplace and Fourier transforms are by far the most used. For Mellin, Hankel, Bessel, and other transforms, see Additional Reading.

If the integrand of a Fourier integral is analytic, then the integral may be evaluated using the residue theorem according to Eq. (7.30). See Example 7.2.3 and Exercises 7.2.4 and 7.2.15. The same method applies to Laplace transforms.

EXAMPLE 15.2.3 **Euler Integral as Laplace Transform** If we generalize the Euler integral [Eq. (10.5)] to

$$\int_0^\infty e^{-st}t^z\,dt = \frac{1}{s^{z+1}}\int_0^\infty e^{-st}(st)^z\,d(st) = \frac{\Gamma(z+1)}{s^{z+1}},$$

where z is a complex parameter with $\Re(z) > -1$, the Laplace transform of the power t^z is the inverse power s^{-z-1} up to the normalization factor $\Gamma(z+1)$. ■

Laplace transforms will be treated in detail starting in Section 15.8.

EXERCISES

15.2.1 (a) Show that $F(-\omega) = F^*(\omega)$ is a necessary and sufficient condition for the Fourier transform $f(t)$ to be real.

(b) Show that $F(-\omega) = -F^*(\omega)$ is a necessary and sufficient condition for $f(t)$ to be pure imaginary.

15.2.2 Let $F(\omega)$ be the Fourier (exponential) transform of $f(t)$ and $G(\omega)$ the Fourier transform of $g(t) = f(t+a)$. Show that

$$G(\omega) = e^{-ia\omega}F(\omega).$$

15.2.3 Prove the identities involved in Exercise 6.5.15.

15.2.4 Find the Fourier sine and cosine transforms of $e^{-a|t|}$.

15.2.5 Find the Fourier exponential, sine, and cosine transforms of $e^{-a|t|}\cos bt$ and $e^{-a|t|}\sin bt$.

15.2.6 Find the Fourier exponential, sine, and cosine transforms of $1/(a^2+t^2)^n$ for $n = 2, 3$.

15.3 Development of the Inverse Fourier Transform

Fourier series, such as $\sum_n a_n \cos(n\pi t/L)$, that we studied in the previous chapter are sums of terms each involving a multiple $n\Delta\omega$ of a basic frequency $\omega = n\pi/L$. If we let the periodicity interval of length $L \to \infty$, then $n\Delta\omega$ becomes a continuous frequency variable ω, and the Fourier series goes over into a Fourier integral $A(t) = \int_{-\infty}^{\infty} a(\omega)\cos\omega t\, d\omega$ for a nonperiodic function $A(t)$. This transition from Fourier series to integral is now described in more detail.

In Chapter 14, it was shown that Fourier series are useful in representing certain functions over a limited range $[0, 2\pi]$, $[-L, L]$, and so on, if the function is periodic. We now turn our attention to the problem of representing a **nonperiodic function** over the infinite range, letting $L \to \infty$. Physically, this sometimes means resolving a single pulse or wave packet into sinusoidal waves or a temperature distribution that decays at $\pm\infty$ into wave components.

We have seen (Section 14.2) that for the interval $[-L, L]$ the coefficients a_n and b_n could be written as

$$a_n = \frac{1}{L}\int_{-L}^{L} f(t)\cos\frac{n\pi t}{L}dt, \tag{15.12}$$

$$b_n = \frac{1}{L}\int_{-L}^{L} f(t)\sin\frac{n\pi t}{L}dt. \tag{15.13}$$

The resulting Fourier series

$$f(x) = \frac{1}{2L}\int_{-L}^{L} f(t)dt + \frac{1}{L}\sum_{n=1}^{\infty}\cos\frac{n\pi x}{L}\int_{-L}^{L} f(t)\cos\frac{n\pi t}{L}dt + \frac{1}{L}\sum_{n=1}^{\infty}\sin\frac{n\pi x}{L}\int_{-L}^{L} f(t)\sin\frac{n\pi t}{L}dt \tag{15.14}$$

or

$$f(x) = \frac{1}{2L}\int_{-L}^{L} f(t)dt + \frac{1}{L}\sum_{n=1}^{\infty}\int_{-L}^{L} f(t)\cos\frac{n\pi}{L}(t-x)dt \tag{15.15}$$

is Eq. (14.28). However, we now let the parameter L approach infinity, transforming the finite interval $[-L, L]$ into the infinite interval $(-\infty, \infty)$. We set

$$\frac{n\pi}{L} = \omega, \qquad \frac{\pi}{L} = \Delta\omega, \quad \text{with } L \to \infty.$$

Then we have

$$f(x) \to \frac{1}{\pi} \sum_{n=1}^{\infty} \Delta\omega \int_{-\infty}^{\infty} f(t) \cos \omega(t - x) dt \tag{15.16}$$

or

$$f(x) = \frac{1}{\pi} \int_{0}^{\infty} d\omega \int_{-\infty}^{\infty} f(t) \cos \omega(t - x) dt, \tag{15.17}$$

replacing the infinite sum by the integral over ω. The first term (corresponding to a_0) has been absorbed at $\omega = 0$, assuming that $\int_{-\infty}^{\infty} f(t)dt$ exists. This **Fourier cosine formula** is valid if f is continuous at x. If f is only piecewise continuous, then $f(x)$ must be replaced by $\frac{1}{2}[f(x+0) + f(x-0)]$, which is the average of the limiting values of f to the left and right of the point x. Also, integrals $\int_{-\infty}^{\infty} f(t)dt$, etc., are always understood as the limit $\lim_{T\to\infty} \int_{-T}^{T} f(t)dt$.

It must be emphasized that this Fourier integral representation of $f(x)$ [Eq. (15.17)] is purely formal. It is not intended as a rigorous derivation, but it can be made rigorous (compare I. N. Sneddon, *Fourier Transforms*, Section 3.2; see Additional Reading). It is subject to the conditions that $f(x)$ is

- piecewise continuous;
- differentiable almost everywhere (of bounded variation); and
- absolutely integrable; that is, $\int_{-\infty}^{\infty} |f(x)|dx$ is finite.

Inverse Fourier Transform—Exponential Form

Our Fourier integral [Eq. (15.17)] may be put into exponential form by noting that because $\cos \omega(t - x)$ is an even function of ω and $\sin \omega(t - x)$ is an odd function of ω,

$$f(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \int_{-\infty}^{\infty} f(t) \cos \omega(t - x) dt, \tag{15.18}$$

whereas

$$\frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \int_{-\infty}^{\infty} f(t) \sin \omega(t - x) dt = 0. \tag{15.19}$$

Adding Eqs. (15.18) and (15.19) (with a factor i), we obtain

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-i\omega x} d\omega \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(t) e^{i\omega t} dt \tag{15.20}$$

or, in terms of the Fourier transform $F(\omega)$ of $f(t)$,

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F(\omega) e^{-i\omega x} d\omega, \qquad F(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(t) e^{i\omega t} dt. \tag{15.21}$$

The variable ω introduced here is an arbitrary mathematical variable. In many physical problems, however, t and x are time variables and then ω corresponds to a frequency. We may then interpret Eq. (15.18) or Eq. (15.20) as a representation of $f(x)$ in terms of a distribution of infinitely long sinusoidal wave trains of angular frequency ω in which this frequency is a **continuous** variable.

EXAMPLE 15.3.1 **Inversion of Square Pulse** Using the Fourier transform in Example 15.2.1, the square pulse can now be inverted as follows:

$$f(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \sqrt{\frac{2}{\pi}} \frac{\sin\omega}{\omega} e^{-i\omega t} d\omega = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{\sin\omega}{\omega} e^{-i\omega t} d\omega.$$

Splitting the integral into one over $(-\infty, 0)$ and another over $(0, \infty)$ gives

$$f(t) = \frac{1}{\pi} \int_{0}^{\infty} \frac{\sin\omega}{\omega} (e^{-i\omega t} + e^{i\omega t}) d\omega = \frac{2}{\pi} \int_{0}^{\infty} \frac{\sin\omega}{\omega} \cos\omega t \, d\omega,$$

an inverse cosine transform.

Alternatively, we can differentiate the Heaviside unit step function expression [using $\frac{du(x)}{dx} = \delta(x)$]

$$f(t) = u(t+1) - u(-1+t) \quad \text{giving} \quad \frac{df(t)}{dt} = \delta(t+1) - \delta(-1+t).$$

This yields

$$\begin{aligned} \frac{df(t)}{dt} &= \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-i\omega t} d\omega \int_{-\infty}^{\infty} [\delta(t'+1) - \delta(t'-1)] e^{-i\omega t'} dt' \\ &= \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-i\omega t} (e^{i\omega} - e^{-i\omega}) d\omega = \frac{i}{\pi} \int_{-\infty}^{\infty} e^{-i\omega t} \sin\omega \, d\omega, \end{aligned}$$

and by integrating the result $f(t) = \frac{1}{\pi} \int_{-\infty}^{\infty} e^{-i\omega t} \frac{\sin\omega}{\omega} d\omega$, as above. As a final check, Exercise 7.2.15 gives us

$$f(t) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{\sin\omega}{\omega} e^{-i\omega t} d\omega = \begin{cases} 0, & |t| > 1, \\ 1, & |t| < 1. \end{cases}$$ ■

Dirac Delta Function Derivation

If the order of integration of Eq. (15.20) is reversed, we may rewrite it as

$$f(x) = \int_{-\infty}^{\infty} f(t) \left\{ \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\omega(t-x)} d\omega \right\} dt. \tag{15.22}$$

Apparently, the quantity in curly brackets behaves as a delta function $\delta(t-x)$. We might take Eq. (15.22) as presenting us with a Fourier integral representation of the Dirac delta function. Alternatively, we take it as a clue to a new derivation of the Fourier integral theorem.

From Eq. (1.160) (shifting the singularity from $t = 0$ to $t = x$),

$$f(x) = \lim_{n\to\infty} \int_{-\infty}^{\infty} f(t) \delta_n(t-x) dt, \tag{15.23}$$

where $\delta_n(t-x)$ is a sequence defining the distribution $\delta(t-x)$. Note that Eq. (15.23) assumes that $f(t)$ is continuous at $t = x$. We take $\delta_n(t-x)$ to be

$$\delta_n(t-x) = \frac{\sin n(t-x)}{\pi(t-x)} = \frac{1}{2\pi} \int_{-n}^{n} e^{i\omega(t-x)} d\omega, \tag{15.24}$$

using Eq. (1.156). Substituting Eq. (15.24) into Eq. (15.23), we have

$$f(x) = \lim_{n\to\infty} \frac{1}{2\pi} \int_{-\infty}^{\infty} f(t) \int_{-n}^{n} e^{i\omega(t-x)} d\omega\, dt. \tag{15.25}$$

Interchanging the order of integration and then taking the limit, as $n \to \infty$, we have Eq. (15.20), the Fourier integral theorem.

With the understanding that it belongs under an integral sign as in Eq. (15.22), the identification

$$\delta(t-x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\omega(t-x)} d\omega \tag{15.26}$$

provides a very useful **Fourier integral representation of the delta function**. It is used to great advantage in Sections 15.6 and 15.7.

EXERCISES

15.3.1 Prove that

$$\frac{\hbar}{2\pi i} \int_{-\infty}^{\infty} \frac{e^{-i\omega t} d\omega}{E_0 - i\Gamma/2 - \hbar\omega} = \begin{cases} \exp(-\Gamma t/2\hbar)\exp(-iE_0 t/\hbar), & t > 0, \\ 0, & t < 0. \end{cases}$$

This Fourier integral appears in a variety of problems in quantum mechanics: Wentzel, Kramers, Brillouin (WKB) barrier penetration, scattering, time-dependent perturbation theory, and so on.
Hint. Try contour integration.

15.3.2 Find the Fourier transform of the triangular pulse (Fig. 15.3)

$$f(t) = \begin{cases} h(1 - a|t|), & |t| < 1/a, \\ 0, & |t| > 1/a. \end{cases}$$

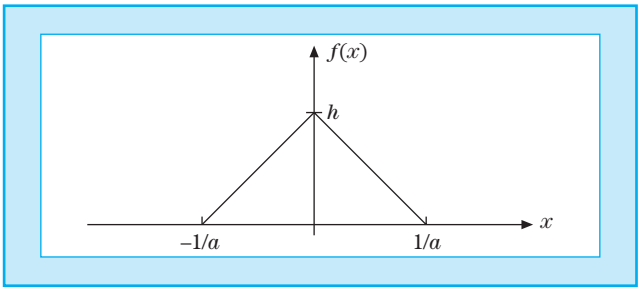
Note. This function provides another delta sequence with $h = a$ and $a \to \infty$.

15.3.3 Prove

$$\int_0^{\infty} \frac{\cos \omega t\, d\omega}{a^2 + \omega^2} = \frac{\pi}{2a} e^{-a|t|}$$

by choosing a suitable contour and applying the residue theorem.

Figure 15.3
Triangular Pulse



15.3.4 Find the Fourier cosine, sine, and complex transforms of $e^{-a^2x^2}$.

15.3.5 Define a sequence

$$\delta_n(x) = \begin{cases} n, & |x| < 1/2n, \\ 0, & |x| > 1/2n. \end{cases}$$

[This is Eq.(1.153).] Express $\delta_n(x)$ as a Fourier integral and show that we may write

$$\delta(x) = \lim_{n\to\infty} \delta_n(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-ikx}dk.$$

15.3.6 Using the sequence

$$\delta_n(x) = \frac{n}{\sqrt{\pi}}\exp(-n^2x^2),$$

show that

$$\delta(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-ikx}dk.$$

Note. Remember that $\delta(x)$ is defined in terms of its behavior as part of an integrand [Section 1.14, especially Eqs. (1.151) and (1.152)].

15.4 Fourier Transforms—Inversion Theorem

Let us **define** $F(\omega)$, the Fourier transform of the function $f(t)$, by

$$F(\omega) \equiv \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} f(t)e^{i\omega t}dt. \tag{15.27}$$

Exponential Transform

Then from Eq. (15.20) we have the inverse relation

$$f(t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} F(\omega)e^{-i\omega t}d\omega. \tag{15.28}$$

Note that Eqs. (15.27) and (15.28) are almost but not quite symmetrical, differing only in the sign of i.

Here two points deserve comment. First, the $1/\sqrt{2\pi}$ symmetry is a matter of choice, not of necessity. Many authors attach the entire $1/(2\pi)$ factor of Eq. (15.20) to either Eq. (15.27) or Eq. (15.28). Second, although the Fourier integral [Eq. (15.20)] has received much attention in the mathematics literature, we shall be primarily interested in the Fourier transform and its inverse. They are the equations with physical significance.

When we move the Fourier transform pair to three-dimensional space, it becomes

$$F(\mathbf{k}) = \frac{1}{(2\pi)^{3/2}} \int f(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}} d^3r, \tag{15.29}$$

$$f(\mathbf{r}) = \frac{1}{(2\pi)^{3/2}} \int F(\mathbf{k}) e^{-i\mathbf{k}\cdot\mathbf{r}} d^3k. \tag{15.30}$$

The integrals are over all space. Verification, if desired, follows immediately by substituting the left-hand side of one equation into the integrand of the other equation and using the three-dimensional delta function.[2] Equation (15.30) may be interpreted as an expansion of a function $f(\mathbf{r})$ in a continuum of plane wave eigenfunctions; $F(\mathbf{k})$ then becomes the amplitude of the wave $\exp(-i\mathbf{k}\cdot\mathbf{r})$.

Cosine Transform

If $f(x)$ is odd or even, these transforms may be expressed in a different form. Consider, first, $f_c(x) = f_c(-x)$, even. Writing the exponential of Eq. (15.27) in trigonometric form, we have

$$\begin{aligned} F_c(\omega) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f_c(t)(\cos\omega t + i\sin\omega t)\,dt \\ &= \sqrt{\frac{2}{\pi}} \int_0^{\infty} f_c(t)\cos\omega t\,dt, \end{aligned} \tag{15.31}$$

the $\sin\omega t$ dependence vanishing on integration over the symmetric interval $(-\infty, \infty)$. Similarly, since $\cos\omega t$ is even, Eq. (15.27) transforms to

$$f_c(t) = \sqrt{\frac{2}{\pi}} \int_0^{\infty} F_c(\omega)\cos\omega t\,d\omega. \tag{15.32}$$

Equations (15.31) and (15.32) are known as Fourier cosine transforms.

EXAMPLE 15.4.1

Evaluation of Fourier Cosine Transform Evaluate the Fourier cosine integral of e^{-ax} with a a positive constant. Integrating by parts twice, we obtain

$$\begin{aligned} \int_0^{\infty} e^{-ax}\cos\omega x\,dx &= -\frac{1}{a}e^{-ax}\cos\omega x\Big|_0^{\infty} - \frac{\omega}{a}\int_0^{\infty} e^{-ax}\sin\omega x\,dx \\ &= \frac{1}{a} - \frac{\omega}{a}\left[-\frac{1}{a}e^{-ax}\sin\omega x\Big|_0^{\infty} + \frac{\omega}{a}\int_0^{\infty} e^{-ax}\cos\omega x\,dx\right]. \end{aligned}$$

Now we combine the integral on the right-hand side with that on the left, giving

$$\left(1 + \frac{\omega^2}{a^2}\right)\int_0^{\infty} e^{-ax}\cos\omega x\,dx = \frac{1}{a}$$

[2] $\delta(\mathbf{r}_1 - \mathbf{r}_2) = \delta(x_1 - x_2)\delta(y_1 - y_2)\delta(z_1 - z_2)$ with Fourier integral $\delta(x_1 - x_2) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \exp[ik_1(x_1 - x_2)]dk_1$, etc.

or

$$\int_0^\infty e^{-ax}\cos\omega x\,dx = \frac{a}{a^2+\omega^2}. \quad \blacksquare$$

Sine Transform

The corresponding pair of Fourier sine transforms is obtained by assuming that $f_s(x) = -f_s(-x)$, odd, and applying the same symmetry arguments. The equations are

$$F_s(\omega) = \sqrt{\frac{2}{\pi}}\int_0^\infty f_s(t)\sin\omega t\,dt,^3 \tag{15.33}$$

$$f_s(t) = \sqrt{\frac{2}{\pi}}\int_0^\infty F_s(\omega)\sin\omega t\,d\omega. \tag{15.34}$$

From the last equation we may develop the physical interpretation that $f(t)$ is being described by a continuum of sine waves. The amplitude of $\sin\omega t$ is given by $\sqrt{2/\pi}F_s(\omega)$, in which $F_s(\omega)$ is the Fourier sine transform of $f(t)$. It will be seen that Eq. (15.34) is the integral analog of the summation [Eq. (14.23)]. Similar interpretations hold for the cosine and exponential cases.

EXAMPLE 15.4.2

Evaluation of Fourier Sine Transform Evaluate the Fourier sine integral of $\frac{\omega}{a^2+\omega^2}$ with a a positive constant. The denominator has the poles $\omega = \pm ia$, suggesting contour integration in the complex ω-plane. With this in mind, we replace $\omega \to -\omega$ and show that

$$-\int_0^\infty \frac{\omega e^{-i\omega t}d\omega}{a^2+\omega^2} = \int_{-\infty}^0 \frac{\omega e^{i\omega t}d\omega}{a^2+\omega^2}$$

so that our Fourier sine integral becomes

$$\int_0^\infty \frac{\omega\sin\omega t\,d\omega}{a^2+\omega^2} = \frac{1}{2i}\int_0^\infty \frac{\omega(e^{i\omega t}-e^{-i\omega x})}{a^2+\omega^2} = \frac{1}{2i}\int_{-\infty}^\infty \frac{\omega e^{i\omega t}}{a^2+\omega^2}.$$

For $t > 0$, we close the contour in the upper ω-plane by a large half-circle, which does not contribute to the integral as its radius goes to ∞. We pick up the residue $iae^{-at}/2ia$ at the pole $\omega = ia$ and find

$$\int_0^\infty \frac{\omega\sin\omega t\,d\omega}{a^2+\omega^2} = \frac{\pi}{2}e^{-at}. \quad \blacksquare$$

If we take Eqs. (15.27), (15.31), and (15.33) as the direct integral transforms, described by $\mathcal{L}$ in Eq. (15.4) (Section 15.1), the corresponding inverse transforms, $\mathcal{L}^{-1}$ of Eq. (15.5), are given by Eqs. (15.28), (15.32), and (15.34).

[3] Note that a factor $-i$ has been absorbed into this $F_s(\omega)$.

EXAMPLE 15.4.3

Proton Charge Form Factor The charge form factor

$$G_E(\mathbf{q}^2) = \int \rho(\mathbf{r}) e^{i\mathbf{q}\cdot\mathbf{r}} d^3r$$

of a particle is defined as the Fourier transform of its charge density ρ, except for the factor $(2\pi)^{-3/2}$; G_E can be measured by elastically scattering electrons from a target of particles (H atoms for the proton) because the (so-called Mott) cross section of a pointlike particle is modified by the charge form factor squared for a particle with finite size, if magnetic scattering is neglected. This is a good approximation at small scattering angle θ. The momentum transfer $\mathbf{q} = \mathbf{p}' - \mathbf{p}$ is taken in units of $\hbar$, where $\mathbf{p}$ is the incident electron momentum and $\mathbf{p}'$ the scattered electron momentum in the laboratory frame (rest frame of the proton). For elastic scattering $p = |\mathbf{p}| = |\mathbf{p}'| = p'$, if recoil is neglected at low momentum p. Figure 15.4 shows that $q = |\mathbf{q}| = 2p \sin\theta/2$.

For a **pointlike particle** of charge Q, $\rho(\mathbf{r}) = Q\delta(\mathbf{r})$ so that the charge form factor

$$G_E(\mathbf{q}^2) = Q \int \delta(\mathbf{r}) e^{i\mathbf{q}\cdot\mathbf{r}} = Q$$

is constant.

At $q = 0$, $G_E(0) = \int \rho d^3r = Q$ is the total charge Q in units of the elementary charge $|e|$; for the proton $Q = 1$.

In case of spherical symmetry, we use polar coordinates r, θ, φ in which the charge form factor takes the form

$$G_E(q^2) = \int_0^\infty \rho(r) r^2 dr \int_{-1}^{1} e^{iqr\cos\theta} d\cos\theta \int_0^{2\pi} d\varphi \tag{15.35}$$

$$= \frac{2\pi}{iq} \int_0^\infty \rho(r) r dr e^{iqr\cos\theta}\Big|_{\cos\theta=-1}^{1} = \frac{4\pi}{q} \int_0^\infty \rho(r) \sin(qr) r\, dr.$$

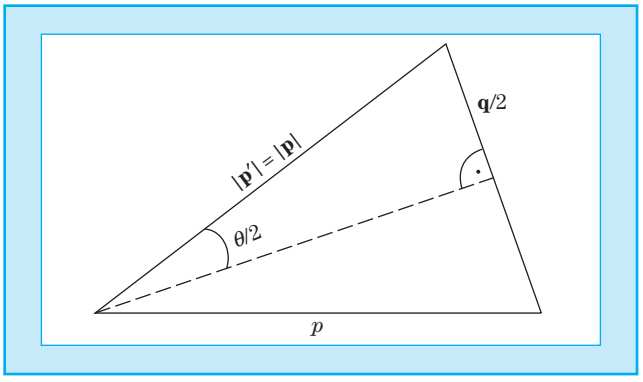


Figure 15.4

Proton Charge Form Factor

Inverting this sine transform, one can extract the charge density from the measured charge form factor $G_E(q^2)$. This is how the proton, nuclear radii, and sizes of atoms and molecules are measured by electron scattering.

At small q compared to the inverse radius of the proton, we can use the power series for $\sin qr$ and obtain

$$G_E(q^2) = 4\pi \int_0^\infty \rho(r) r^2\, dr - \frac{q^2}{6} \int_0^\infty \rho(r) r^4\, dr + \cdots = 1 - \frac{q^2}{6}\langle r^2\rangle + \cdots,$$

where the first term is the charge $Q = 1$ and the integral in the second term is the mean square radius $\langle r^2\rangle$ of the proton, because the density $\rho = |\psi|^2$ is given by the quark wave function ψ, quarks being the constituents of the proton. Thus, the proton size can be extracted from the measured slope of the proton charge form factor,

$$\langle r^2\rangle = -6 \frac{dG_E(q^2)}{dq^2}\bigg|_{q=0}.$$

Since the proton has a finite radius of approximately 1 fm $= 10^{-13}$ cm, we consider a spherically symmetric model (Fig. 15.5A)

$$\rho(r) = \frac{N}{r}[e^{-r/R_1} - e^{-r/R}],$$

where $R \ll R_1$ are finite size parameters yet to be determined. The normalization N follows from the charge 1 of the proton, in units of the elementary charge e; that is, $G_E(0) = 1$. The same model applies to the charge density of the ^{3}He nucleus, except for the charge $G_E(0) = 2$ and its larger radius, because it is made up of two protons and one neutron instead of three quarks for the proton.

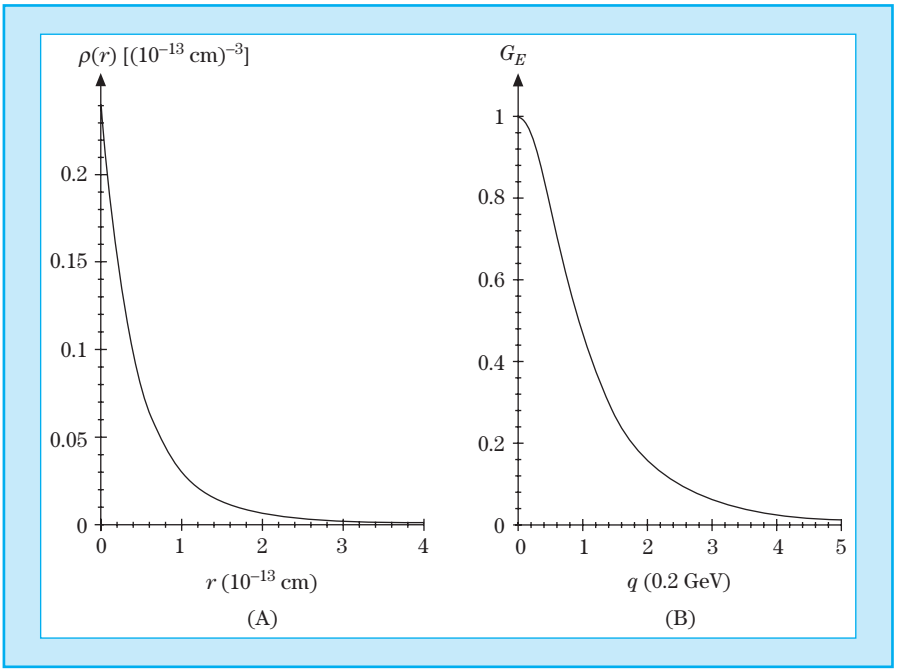


Figure 15.5

Charge Density (A) and Form Factor (B) of the Proton

Let us start by determining N from $G_E(0) = 1$ by integrating by parts as follows:

$$\begin{aligned} 1 &= 4\pi \int_0^\infty \rho(r) r^2\, dr = 4\pi N \int_0^\infty [e^{-r/R_1} - e^{-r/R}] r\, dr \\ &= 4\pi N[-rR_1 e^{-r/R_1} + rRe^{-r/R}]\Big|_0^\infty + 4\pi N \int_0^\infty [R_1 e^{-r/R_1} - Re^{-r/R}] dr \\ &= 4\pi N\big(R_1^2 - R^2\big), \quad N = \frac{1}{4\pi\big(R_1^2 - R^2\big)}. \end{aligned}$$

A look at the sine transform for $G_E(q)$ [Eq. (15.35)] tells us that we also need to calculate the integral

$$\begin{aligned} \int_0^\infty e^{-r/R} \sin qr\, dr &= -Re^{-r/R} \sin qr\Big|_0^\infty + qR \int_0^\infty e^{-r/R} \cos qr\, dr \\ &= qR\left[-Re^{-r/R} \cos qr\Big|_0^\infty - qR \int_0^\infty e^{-r/R} \sin qr\, dr\right], \end{aligned}$$

which we do by integrating by parts twice. This yields the same integral on the right-hand side, which we combine with that on the left-hand side, so that

$$\int_0^\infty e^{-r/R} \sin qr\, dr = \frac{qR^2}{1 + q^2R^2}.$$

Substituting this result into the G_E sine transform formula [Eq. (15.35)] yields

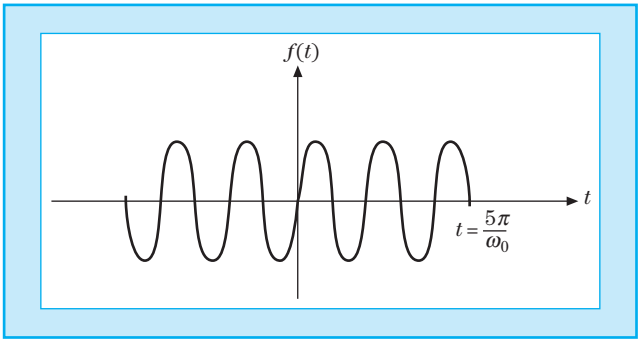
$$\begin{aligned} G_E(q^2) &= \frac{4\pi N}{q} \int_0^\infty [e^{-r/R_1} - e^{-r/R}] \sin qr\, dr \\ &= \frac{1}{R_1^2 - R^2}\left(\frac{R_1^2}{1 + q^2R_1^2} - \frac{R^2}{1 + q^2R^2}\right). \end{aligned}$$

Note that at $q = 0$ this charge form factor is properly normalized to unity, whereas at large q it falls like q^{-4}. This falloff is called quark counting and predicted by quantum chromodynamics, the quantum field theory of the strong interaction that binds quarks in the proton. Our nonrelativistic model simulates this behavior. Now we choose $R_1 = 1$ fm, approximately the size of the proton, and $R = 1/4$ fm; this is shown in Fig. 15.5. ■

Note that the Fourier cosine transforms and the Fourier sine transforms each involve only positive values (and zero) of the arguments. We use the parity of $f(t)$ to establish the transforms, but once the transforms are established, the behavior of the functions f and g for negative argument is irrelevant. In effect, the transform equations impose a **definite parity: even for the Fourier cosine** transform and **odd for the Fourier sine** transform.

Figure 15.6

Finite Wave Train



EXAMPLE 15.4.4

Finite Wave Train An important application of the Fourier transform is the resolution of a finite pulse into sinusoidal waves. Imagine that an infinite wave train $\sin \omega_0 t$ is clipped by Kerr cell or saturable dye cell shutters so that

$$f(t) = \begin{cases} \sin \omega_0 t, & |t| < \frac{N\pi}{\omega_0}, \\ 0, & |t| > \frac{N\pi}{\omega_0}. \end{cases} \tag{15.36}$$

This corresponds to N cycles of our original wave train (Fig. 15.6). Since $f(t)$ is odd, we may use the Fourier sine transform [Eq. (15.33)] to obtain

$$F_s(\omega) = \sqrt{\frac{2}{\pi}} \int_0^{N\pi/\omega_0} \sin \omega_0 t \sin \omega t \, dt. \tag{15.37}$$

Integrating, we find our amplitude function

$$F_s(\omega) = \sqrt{\frac{2}{\pi}} \left[\frac{\sin[(\omega_0 - \omega)(N\pi/\omega_0)]}{2(\omega_0 - \omega)} - \frac{\sin[(\omega_0 + \omega)(N\pi/\omega_0)]}{2(\omega_0 + \omega)} \right]. \tag{15.38}$$

It is of considerable interest to see how $F_s(\omega)$ depends on frequency. For large ω_0 and $\omega \approx \omega_0$, only the first term will be of any importance because of the denominators. It is plotted in Fig. 15.7. This is the amplitude curve for the single slit diffraction pattern.

There are zeros at

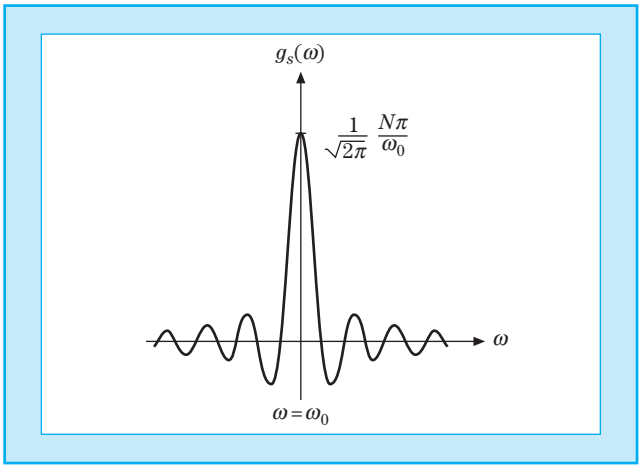
$$\frac{\omega_0 - \omega}{\omega_0} = \frac{\Delta\omega}{\omega_0} = \pm\frac{1}{N}, \pm\frac{2}{N}, \quad \text{and so on.} \tag{15.39}$$

For large N, $F_s(\omega)$ may also be interpreted as a Dirac delta distribution, as in Section 1.14. Since the contributions outside the central maximum are small in this case, we may take

$$\Delta\omega = \frac{\omega_0}{N} \tag{15.40}$$

Figure 15.7

Fourier Transform of Finite Wave Train



as a good measure of the spread in frequency of our wave pulse. Clearly, if N is large (a long pulse), the frequency spread will be small. On the other hand, if our pulse is clipped short (N is small), the frequency distribution will be wider and the secondary maxima are more important. ■

EXERCISES

15.4.1 The function

$$f(t) = \begin{cases} 1, & |t| < 1 \\ 0, & |t| > 1 \end{cases}$$

is a symmetrical finite step function.

(a) Find the $F_c(\omega)$, Fourier cosine transform of $f(t)$.

(b) Taking the inverse cosine transform, show that

$$f(t) = \frac{2}{\pi}\int_0^\infty \frac{\sin\omega\cos\omega t}{\omega}d\omega.$$

(c) From part (b) show that

$$\int_0^\infty \frac{\sin\omega\cos\omega t}{\omega}d\omega = \begin{cases} 0, & |t| > 1, \\ \frac{\pi}{4}, & |t| = 1, \\ \frac{\pi}{2}, & |t| < 1. \end{cases}$$

15.4.2 Derive sine and cosine representations of $\delta(t-x)$ that are comparable to the exponential representation [Eq. (15.26)].

ANS. $\frac{2}{\pi}\int_0^\infty \sin\omega t\sin\omega x\,d\omega$, $\frac{2}{\pi}\int_0^\infty \cos\omega t\cos\omega x\,d\omega$.

15.4.3 In a resonant cavity, an electromagnetic oscillation of frequency ω_0 dies out as

$$A(t) = A_0 e^{-\omega_0 t/2Q} e^{-i\omega_0 t}, \quad t > 0.$$

(Take $A(t) = 0$ for $t < 0$.)
The parameter Q is a measure of the ratio of stored energy to energy loss per cycle. Calculate the frequency distribution of the oscillation, $a^*(\omega)a(\omega)$, where $a(\omega)$ is the Fourier transform of $A(t)$.
Note. The larger Q is, the sharper your resonance line will be.

$$\textit{ANS.} \quad a^*(\omega)a(\omega) = \frac{A_0^2}{2\pi} \frac{1}{(\omega - \omega_0)^2 + (\omega_0/2Q)^2}.$$

15.4.4 (a) Calculate the Fourier exponential transform of $f(t) = t^n e^{-a|t|}$ for $n = 1, 2, 3$.
(b) Calculate the inverse transform by employing the calculus of residues (Section 7.2).

15.5 Fourier Transform of Derivatives

Figure 15.1 outlines the overall technique of using Fourier transforms and inverse transforms to solve a problem. Here, we take an initial step in **solving a differential equation**—obtaining the Fourier transform of a derivative.

Using the exponential form, we determine that the Fourier transform of $f(t)$ is

$$F(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(t) e^{i\omega t} dt, \tag{15.41}$$

and for $df(t)/dt$

$$F_1(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \frac{df(t)}{dt} e^{i\omega t} dt. \tag{15.42}$$

Integrating Eq. (15.42) by parts, we obtain

$$F_1(\omega) = \frac{e^{i\omega t}}{\sqrt{2\pi}} f(t)\Big|_{-\infty}^{\infty} - \frac{i\omega}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(t) e^{i\omega t} dt. \tag{15.43}$$

If $f(t)$ vanishes[4] as $t \to \pm\infty$, we have

$$F_1(\omega) = -i\omega F(\omega); \tag{15.44}$$

that is, the transform of the derivative is $(-i\omega)$ times the transform of the original function. This may readily be generalized to the nth derivative to yield

$$F_n(\omega) = (-i\omega)^n F(\omega), \tag{15.45}$$

[4]Apart from cases such as Exercises 15.3.5 and 15.3.6, $f(t)$ must vanish as $t \to \pm\infty$ in order for the Fourier transform of $f(t)$ to exist.

provided all the integrated parts of Eq. (15.43) vanish as $t \to \pm\infty$. This is the power of the Fourier transform, the main reason it is so useful in solving (partial) differential equations. The operation of **differentiation in coordinate space has been replaced by a multiplication in ω space**. Such properties of the kernel are the key in applications of integral transforms to solving ordinary differential equations (ODEs) and partial differential equations (PDEs), developed next.

EXAMPLE 15.5.1

Driven Harmonic Oscillator If we substitute the Fourier integral $y(t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} Y(\omega)e^{i\omega t}dt$ into the harmonic oscillator ODE $\frac{d^2y}{dt^2} + \Omega^2 y = A\cos(\omega_0 t)$, where t is the time now, we obtain an **algebraic** equation for $Y(\omega)$ called the Fourier transform of our solution $y(t)$,

$$\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} Y(\omega)(\Omega^2 - \omega^2)e^{i\omega t}d\omega = \frac{A}{2}\int_{-\infty}^{\infty} e^{i\omega t}[\delta(\omega-\omega_0)+\delta(\omega+\omega_0)]d\omega,$$

because differentiating twice corresponds to multiplying $Y(\omega)$ by $(i\omega)^2$, and we represent the driving term as a Fourier integral with the only frequencies $\pm\omega_0$. Upon comparing integrands, valid because the integrals are over the same interval in the same variable ω (or, more rigorously, using the inverse Fourier transform), we find

$$Y(\omega) = \sqrt{\frac{\pi}{2}}\frac{A}{\Omega^2-\omega^2}[\delta(\omega-\omega_0)+\delta(\omega+\omega_0)].$$

The resulting integral,

$$y(t) = \frac{A}{2}\int_{-\infty}^{\infty}\frac{e^{i\omega t}}{\Omega^2-\omega^2}[\delta(\omega-\omega_0)+\delta(\omega+\omega_0)]d\omega = \frac{A}{\Omega^2-\omega_0^2}\cos(\omega_0 t),$$

is the steady-state and particular solution of our inhomogeneous ODE. Note that **the assumption that the end points in the partially integrated term** in Eq. (15.43) **do not contribute eliminates solutions of the homogeneous harmonic oscillator ODE (called transients in physics**; undamped $\sin\Omega t$, $\cos\Omega t$ solutions in our case).

Alternatively, we Fourier transform the ODE as follows:

$$\begin{aligned}\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\left(\frac{d^2y}{dt^2}+\Omega^2 y\right)e^{i\omega t}dt &= \frac{A}{2\sqrt{2\pi}}\int_{-\infty}^{\infty}(e^{i\omega_0 t}+e^{-i\omega_0 t})e^{i\omega t}dt \\ &= A\sqrt{\pi}2[\delta(\omega-\omega_0)+\delta(\omega+\omega_0)].\end{aligned}$$

We integrate by parts twice,

$$\begin{aligned}\int_{-\infty}^{\infty}\frac{d^2y}{dt^2}e^{i\omega t}dt &= \frac{dy}{dt}e^{i\omega t}\Big|_{-\infty}^{\infty} - i\omega\int_{-\infty}^{\infty}\frac{dy}{dt}e^{i\omega t}dt \\ &= -i\omega\left[ye^{i\omega t}\Big|_{-\infty}^{\infty} - i\omega\int_{-\infty}^{\infty}ye^{i\omega t}dt\right] = -\omega^2\int_{-\infty}^{\infty}ye^{i\omega t}dt,\end{aligned}$$

assuming that $y(t) \to 0$ and $\frac{dy(t)}{dt} \to 0$ sufficiently fast, as $t \to \pm\infty$. The result of comparing integrands (using the inverse Fourier transform) is the same as before:

$$(\Omega^2 - \omega^2)Y(\omega) = \sqrt{\frac{\pi}{2}} A[\delta(\omega - \omega_0) + \delta(\omega + \omega_0)]. \quad \blacksquare$$

Similarly, a PDE might become an ODE, such as the heat flow PDE considered next.

EXAMPLE 15.5.2

Heat Flow PDE To illustrate the transformation of a PDE into an ODE, let us Fourier transform the heat flow partial differential equation

$$\frac{\partial \psi}{\partial t} = a^2 \frac{\partial^2 \psi}{\partial x^2},$$

where the solution $\psi(x, t)$ is the temperature in space as a function of time. By substituting the Fourier integral solution

$$\psi(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(\omega, t) e^{-i\omega x}\, d\omega,$$

this yields an ODE for the Fourier transform Ψ of ψ,

$$\frac{\partial \Psi}{\partial t} = -a^2\omega^2 \Psi(\omega, t),$$

in the time variable t. Alternatively and equivalently, apply the inverse Fourier transform to each side of the heat PDE. Integrating, we obtain

$$\ln \Psi = -a^2\omega^2 t + \ln C, \quad \text{or} \quad \Psi = Ce^{-a^2\omega^2 t},$$

where the integration constant C may still depend on ω and, in general, is determined by initial conditions. Putting this solution back into our inverse Fourier transform,

$$\psi(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} C(\omega) e^{-i\omega x} e^{-a^2\omega^2 t} d\omega,$$

yields a separation of the x and t variables. For simplicity, we here take C ω-independent (assuming appropriate initial conditions) and integrate by completing the square in ω, as in Example 15.2.2, making appropriate changes of variables and parameters ($a^2 \to a^2 t$, $\omega \to x, t \to -\omega$). This yields the particular solution of the heat flow PDE,

$$\psi(x, t) = \frac{C}{a\sqrt{2t}} \exp\left(-\frac{x^2}{4a^2 t}\right),$$

that appears as a clever guess in Section 16.2. In effect, we have shown that ψ is the inverse Fourier transform of $C \exp(-a^2\omega^2 t)$. $\blacksquare$

EXAMPLE 15.5.3

Inversion of PDE Derive a Fourier integral for the Green's function G_0 of Poisson's PDE, which is a solution of

$$\nabla^2 G_0(\mathbf{r}, \mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}').$$

Once G_0 is known, the general solution of Poisson's PDE

$$\nabla^2\Phi = -4\pi\rho(\mathbf{r})$$

of electrostatics is given as

$$\Phi(\mathbf{r}) = \int G_0(\mathbf{r}, \mathbf{r}')4\pi\rho(\mathbf{r}')d^3r'.$$

Applying ∇^2 to Φ and using the PDE the Green's function satisfies, we check that

$$\nabla^2\Phi(\mathbf{r}) = \int \nabla^2 G_0(\mathbf{r}, \mathbf{r}')4\pi\rho(\mathbf{r}')d^3r' = \int \delta(\mathbf{r}-\mathbf{r}')4\pi\rho(\mathbf{r}')d^3r' = 4\pi\rho(\mathbf{r}).$$

Now we use Fourier transforms of the δ function and G_0, writing

$$\nabla^2 \int g_0(\mathbf{p}) e^{i\mathbf{p}\cdot(\mathbf{r}-\mathbf{r}')}\frac{d^3p}{(2\pi)^3} = \int e^{i\mathbf{p}\cdot(\mathbf{r}-\mathbf{r}')}\frac{d^3p}{(2\pi)^3}.$$

Because the integrands of equal Fourier integrals must be the same (almost) everywhere, which follows from the inverse Fourier transform, and with

$$\nabla e^{i\mathbf{p}\cdot(\mathbf{r}-\mathbf{r}')} = i\mathbf{p}e^{i\mathbf{p}\cdot(\mathbf{r}-\mathbf{r}')},$$

this yields $-\mathbf{p}^2 g_0(\mathbf{p}) = 1$. Substituting this solution into the inverse Fourier transform for G_0 gives

$$G_0(\mathbf{r}, \mathbf{r}') = -\int e^{i\mathbf{p}\cdot(\mathbf{r}-\mathbf{r}')}\frac{d^3p}{(2\pi)^3\mathbf{p}^2} = -\frac{1}{4\pi|\mathbf{r}-\mathbf{r}'|}.$$

We can verify the last part of this result by applying ∇^2 to G_0 again and recalling from Chapter 1 that $\nabla^2\frac{1}{|\mathbf{r}-\mathbf{r}'|} = -4\pi\delta(\mathbf{r}-\mathbf{r}')$.

The inverse Fourier transform can be evaluated using polar coordinates exploiting the spherical symmetry of $\mathbf{p}^2$, similar to the charge form factor in Example 15.4.3 for a spherically symmetric charge density. For simplicity, we write $\mathbf{R} = \mathbf{r} - \mathbf{r}'$ and call θ the angle between $\mathbf{R}$ and $\mathbf{p}$ so that

$$\begin{aligned}\int e^{i\mathbf{p}\cdot\mathbf{R}}\frac{d^3p}{p^2} &= \int_0^\infty dp \int_{-1}^1 e^{ipR\cos\theta} d\cos\theta \int_0^{2\pi} d\varphi \\ &= \frac{2\pi}{iR}\int_0^\infty \frac{dp}{p} e^{ipR\cos\theta}\Big|_{\cos\theta=-1}^1 = \frac{4\pi}{R}\int_0^\infty \frac{\sin pR}{p}dp \\ &= \frac{4\pi}{R}\int_0^\infty \frac{\sin pR}{pR}d(pR) = \frac{2\pi^2}{R},\end{aligned}$$

where θ and φ are the angles of $\mathbf{p}$, and $\int_0^\infty \frac{\sin x}{x}dx = \frac{\pi}{2}$ from Example 7.2.4. Dividing by $-(2\pi)^3$, we obtain $G_0(R) = -1/(4\pi R)$, as claimed. An evaluation of this Fourier transform by contour integration is given in Example 16.3.2. ■

EXAMPLE 15.5.4

Wave Equation The Fourier transform technique may be used to advantage in handling PDEs with constant coefficients. To illustrate the technique further, let us derive a familiar expression of elementary physics. An infinitely long

string is vibrating freely. The amplitude y of the (small) vibrations satisfies the wave equation

$$\frac{\partial^2 y}{\partial x^2} = \frac{1}{v^2}\frac{\partial^2 y}{\partial t^2}. \tag{15.46}$$

We shall assume an initial condition

$$y(x, 0) = f(x), \tag{15.47}$$

where f is localized, that is, approaches zero at large x.

Applying our Fourier transform to both sides of our PDE [Eq. (15.46)] means multiplying by $e^{i\alpha x}/\sqrt{2\pi}$ and integrating over x according to

$$Y(\alpha, t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} y(x, t)e^{i\alpha x}dx \tag{15.48}$$

and using Eq. (15.43) for the second derivative. Note that the integrated part of $\frac{\partial Y}{\partial x}$ and $\frac{\partial^2 Y}{\partial x^2}$ vanishes: The wave has not yet gone to $\pm\infty$, as it is propagating forward in time, and there is no source at infinity [$f(\pm\infty) = 0$]. We obtain

$$\int_{-\infty}^{\infty} \frac{\partial^2 y(x, t)}{\partial x^2}e^{i\alpha x}dx = \frac{1}{v^2}\int_{-\infty}^{\infty} \frac{\partial^2 y(x, t)}{\partial t^2}e^{i\alpha x}dx \tag{15.49}$$

or

$$(-i\alpha)^2 Y(\alpha, t) = \frac{1}{v^2}\frac{\partial^2 Y(\alpha, t)}{\partial t^2}. \tag{15.50}$$

Since no derivatives with respect to α appear, Eq. (15.50) is actually an ODE—in fact, it is the linear oscillator equation. This transformation, from a PDE to an ODE, is a significant simplification. We solve Eq. (15.50) subject to the appropriate initial conditions. At $t = 0$, applying Eq. (15.47), Eq. (15.48) reduces to

$$Y(\alpha, 0) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} f(x)e^{i\alpha x}dx = F(\alpha), \tag{15.51}$$

where $F(\alpha)$ is the Fourier transform of the initial condition $f(x)$. The general solution of Eq. (15.50) in exponential form is

$$Y(\alpha, t) = F(\alpha)e^{\pm iv\alpha t}. \tag{15.52}$$

Using the inversion formula [Eq. (15.28)], we have

$$y(x, t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} Y(\alpha, t)e^{-i\alpha x}d\alpha, \tag{15.53}$$

and, by Eq. (15.52),

$$y(x, t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} F(\alpha)e^{-i\alpha(x\mp vt)}d\alpha. \tag{15.54}$$

Since $f(x)$ is the Fourier inverse transform of $F(\alpha)$,

$$y(x, t) = f(x \mp vt), \tag{15.55}$$

corresponding to waves advancing in the $+x$- and $-x$-directions, respectively.

The boundary condition of Eq. (15.47) is built into these particular linear combinations of waves. ■

The accomplishment of the Fourier transform here deserves special emphasis.

- The Fourier transform converts a PDE into an ODE, where the "degree of transcendence" of the problem is reduced.

In Section 15.10, Laplace transforms are used to convert ODEs (with constant coefficients) into algebraic equations. Again, the degree of transcendence is reduced. The problem is simplified, as outlined in Fig. 15.1.

EXERCISES

15.5.1 Equation (15.45) yields

$$F_2(\omega) = -\omega^2 F(\omega)$$

for the Fourier transform of the second derivative of $f(x)$. The condition $f(x) \to 0$ for $x \to \pm\infty$ may be relaxed slightly. Find the least restrictive condition for the preceding equation for $F_2(\omega)$ to hold.

ANS. $$\left[\frac{df(x)}{dx} - i\omega f(x)\right] e^{i\omega x}\Big|_{-\infty}^{\infty} = 0.$$

15.5.2 (a) Given that $F(\mathbf{k})$ is the three-dimensional Fourier transform of $f(\mathbf{r})$ and $F_1(\mathbf{k})$ is the three-dimensional Fourier transform of $\nabla f(\mathbf{r})$, show that

$$F_1(\mathbf{k}) = (-i\mathbf{k})F(\mathbf{k}).$$

This is a three-dimensional generalization of Eq. (15.45) for $n = 1$.

(b) Show that the three-dimensional Fourier transform of $\nabla \cdot \nabla f(\mathbf{r})$ is

$$F_2(\mathbf{k}) = (-i\mathbf{k})^2 F(\mathbf{k}).$$

Note. Vector $\mathbf{k}$ is in the transform space. In Section 15.7, we shall have $\hbar\mathbf{k} = \mathbf{p}$, linear momentum.

15.5.3 Show

$$\int e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')} \frac{d^3k}{(2\pi)^3\mathbf{k}^2} = \frac{1}{4\pi|\mathbf{r}-\mathbf{r}'|}$$

by contour integration in conjunction with the residue theorem.

Hint. Use spherical polar coordinates in k-space.

15.5.4 Solve the PDE

$$\frac{\partial y}{\partial t} = \frac{\partial^2 y}{\partial x^2} - a^2 y$$

by Fourier transform, where $y(x, t = 0) = 0,\ x > 0,\ y(x = 0, t) = f(t),\ t > 0$, and a is a constant.

15.5.5 Show that the three-dimensional Fourier exponential transform of a radially symmetric function may be rewritten as a Fourier sine transform:

$$\frac{1}{(2\pi)^{3/2}} \int_{-\infty}^{\infty} f(r) e^{i\mathbf{k}\cdot\mathbf{r}}\, d^3x = \frac{1}{k}\sqrt{\frac{2}{\pi}} \int_{-\infty}^{\infty} [rf(r)] \sin kr\, dr.$$

15.6 Convolution Theorem

We employ convolutions to solve differential equations and to normalize momentum wave functions.

Let us consider two functions $f(x)$ and $g(x)$ with Fourier transforms $F(\omega)$ and $G(\omega)$, respectively. We define the operation

$$f * g \equiv \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} g(y) f(x - y)\, dy \tag{15.56}$$

as the **convolution** of the two functions f and g over the interval $(-\infty, \infty)$. This form of an integral appears in probability theory in the determination of the probability density of two random, independent variables. Our solution of Poisson's equation (i.e., the Coulomb potential) may be interpreted as a convolution of a charge distribution, $\rho(\mathbf{r}_2)$, and a weighting function, $(4\pi\varepsilon_0|\mathbf{r}_1 - \mathbf{r}_2|)^{-1}$. In other works this is sometimes referred to as the **Faltung**, the German term for "folding."[5] We now transform the integral in Eq. (15.56) by introducing the Fourier transforms, interchanging the order of integration, and transforming $g(y)$:

$$\begin{aligned}
\int_{-\infty}^{\infty} g(y) f(x - y)\, dy &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} g(y) \int_{-\infty}^{\infty} F(\omega) e^{-i\omega(x-y)}\, d\omega\, dy \\
&= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F(\omega) \left[\int_{-\infty}^{\infty} g(y) e^{i\omega y}\, dy \right] e^{-i\omega x}\, d\omega \\
&= \int_{-\infty}^{\infty} F(\omega) G(\omega) e^{-i\omega x} d\omega.
\end{aligned} \tag{15.57}$$

Comparing with Eq. (15.56), this shows that

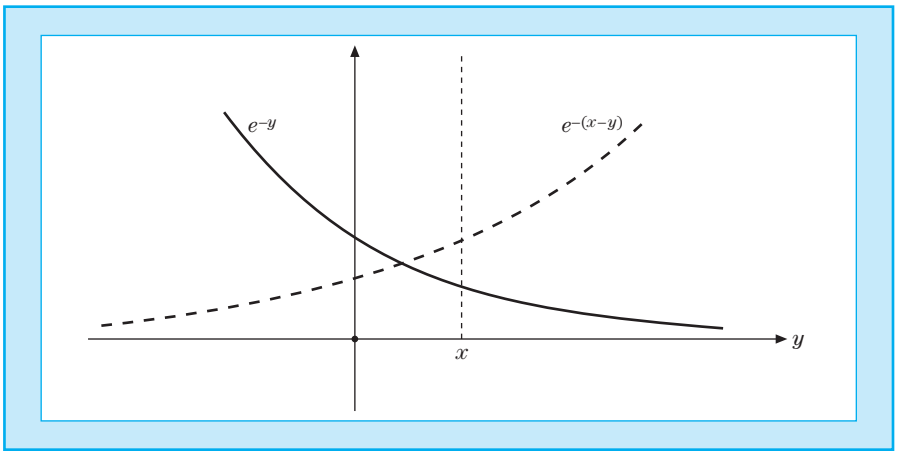
$$f * g = \mathcal{L}^{-1}(FG).$$

In other words, the Fourier inverse transform of a **product** of Fourier transforms is the convolution of the original functions, $f * g$.

[5] For $f(y) = e^{-y}$, $f(y)$ and $f(x - y)$ are plotted in Fig. 15.8. Clearly, $f(y)$ and $f(x - y)$ are mirror images of each other in relation to the vertical line $y = x/2$; that is, we could generate $f(x - y)$ by folding over $f(y)$ on the line $y = x/2$.

Figure 15.8

Convolution–Faltung



EXAMPLE 15.6.1

Convolution Integral Let us apply the convolution Eq. (15.57) with f, F from Example 15.2.2 and g, G from Example 15.4.1 so that

$$f(x) = e^{-a^2x^2}, \qquad F(\omega) = \frac{1}{a\sqrt{2}} \exp\left(-\frac{\omega^2}{4a^2}\right);$$
$$g(y) = \sqrt{\frac{\pi}{2b^2}} e^{-b|y|}, \qquad G(\omega) = \frac{1}{b^2+\omega^2}.$$

From Example 15.4.1, recall that

$$\int_{-\infty}^{\infty} \frac{e^{i\omega y}\,dt}{b^2+\omega^2} = 2\int_0^{\infty} \frac{\cos\omega y\,d\omega}{b^2+\omega^2} = \frac{\pi}{b} e^{-by}, \qquad y > 0,$$

using the Euler identity $e^{i\omega y} = \cos\omega y + i\sin\omega y$ and noticing that the sine integral vanishes because its integrand is odd under reversal of sign of t, whereas the cosine integrand is even.

Now we apply the convolution formula [Eq. (15.57)]

$$\frac{\mathcal{I}}{b}\sqrt{\frac{\pi}{2}} \equiv \int_{-\infty}^{\infty} \sqrt{\frac{\pi}{2}}\frac{1}{b} e^{-b|y|} \exp(-a^2(x-y)^2)\,dy = \frac{1}{a\sqrt{2}} \int_{-\infty}^{\infty} \frac{e^{-i\omega x}}{b^2+\omega^2} e^{-\omega^2/4a^2}\,d\omega.$$

The integral $\mathcal{I}$ can be manipulated into the error integral erfc (Section 10.4) by splitting the interval and substituting $y \to -y$ in the $(-\infty, 0)$ part, giving

$$\mathcal{I} = \int_{-\infty}^{\infty} e^{-b|y|} \exp(-a^2(x-y)^2)\,dy$$
$$= \int_0^{\infty} e^{-by} \exp(-a^2(x-y)^2)\,dy + \int_0^{\infty} e^{-by} \exp(-a^2(x+y)^2)\,dy.$$

Now we substitute $\xi = y - x$ in the first integral and $\xi = y + x$ in the second, yielding

$$\mathcal{I} = e^{-bx}\int_{-x}^{\infty} e^{-b\xi - a^2\xi^2}d\xi + e^{bx}\int_{x}^{\infty} e^{-b\xi - a^2\xi^2}d\xi.$$

Completing the square in the exponent as in Example 15.2.2 using

$$a^2\xi^2 + b\xi = a^2\left(\xi + \frac{b}{2a^2}\right)^2 - \frac{b^2}{4a^2},$$

we obtain, with the substitution $a\eta = \xi + b/2a^2$,

$$\mathcal{I} = \frac{1}{a}e^{-bx+b^2/4a^2}\int_{-ax+b/2a}^{\infty} e^{-\eta^2}d\eta + \frac{1}{a}e^{bx+b^2/4a^2}\int_{ax+b/2a}^{\infty} e^{-\eta^2}d\eta$$

so that finally

$$\sqrt{\frac{\pi}{2b^2}}\mathcal{I} = \frac{\pi}{2ab\sqrt{2}}e^{b^2/4a^2}\left[e^{-bx}\,\mathrm{erfc}\left(\frac{b}{2a} - ax\right) + e^{bx}\mathrm{erfc}\left(\frac{b}{2a} + ax\right)\right]. \tag{15.58}$$

Another example is provided by changing $g(y)$ in the previous example to the square pulse $g(y) = 1$, for $|y| < 1$ and zero elsewhere. Its Fourier transform is given in Example 15.2.1 as

$$G(\omega) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} g(y)e^{i\omega y}\,dy = \sqrt{\frac{2}{\pi}}\frac{\sin\omega}{\omega}.$$

The convolution with $f(x)$ takes the interesting form

$$\int_{-1}^{1}\exp(-a^2(x-y)^2)dy = \frac{1}{a\sqrt{\pi}}\int_{-\infty}^{\infty} e^{-\omega^2/4a^2}\frac{\sin\omega}{\omega}e^{-i\omega x}d\omega,$$

where the left-hand side can again be converted to a difference of error integrals

$$\int_{-1}^{1}\exp(-a^2(x-y)^2)dy = \frac{\sqrt{\pi}}{2a}[\mathrm{erfc}(-a(1+x)) - \mathrm{erfc}(a(1-x))]. \quad \blacksquare$$

EXAMPLE 15.6.2

Coulomb Potential by Convolution The Coulomb potential for an extended charge distribution ρ of a composite system,

$$V(\mathbf{r}) = \int \frac{\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}d^3r',$$

appears to be a three-dimensional case of a convolution integral. If we recall the charge form factor G_E as the Fourier transform of the charge density from Example 15.4.3,

$$\frac{1}{(2\pi)^{3/2}}\int \rho(\mathbf{r})e^{i\mathbf{p}\cdot\mathbf{r}}d^3r = \frac{G_E(\mathbf{p}^2)}{(2\pi)^{3/2}},$$

and $1/\mathbf{p}^2$ as the Fourier transform of $1/|\mathbf{r}-\mathbf{r}'|$ from Example 15.5.3,

$$\frac{(2\pi)^{3/2}}{4\pi|\mathbf{r}-\mathbf{r}'|}=\int\frac{e^{i\mathbf{p}\cdot(\mathbf{r}-\mathbf{r}')}}{(2\pi)^{3/2}\mathbf{p}^2}d^3p,$$

being careful to include all normalizations, then we can apply the convolution theorem to obtain

$$V(\mathbf{r})=\int\rho(\mathbf{r}')\frac{d^3r'}{|\mathbf{r}-\mathbf{r}'|}=4\pi\int\frac{G_E(\mathbf{p}^2)}{\mathbf{p}^2}e^{-i\mathbf{p}\cdot\mathbf{r}}\frac{d^3p}{(2\pi)^3}. \tag{15.59}$$

Let us now evaluate this result for the proton Example 15.4.3. This gives

$$\begin{aligned}V(\mathbf{r})&=\frac{4\pi}{R_1^2-R^2}\int\left(\frac{R_1^2}{1+p^2R_1^2}-\frac{R^2}{1+p^2R^2}\right)\frac{e^{-i\mathbf{p}\cdot\mathbf{r}}}{\mathbf{p}^2}\frac{d^3p}{(2\pi)^3}\\&=\frac{4\pi}{R_1^2-R^2}\int\left[\left(-\frac{R_1^2}{1+p^2R_1^2}+\frac{1}{p^2}\right)R_1^2-R^2\left(\frac{1}{p^2}-\frac{R^2}{1+p^2R^2}\right)\right]\\&\quad\times e^{-i\mathbf{p}\cdot\mathbf{r}}\frac{d^3p}{(2\pi)^3}\\&=\frac{R_1^2}{R_1^2-R^2}\left(\frac{1}{r}-\frac{e^{-r/R_1}}{r}\right)-\frac{R^2}{R_1^2-R^2}\left(\frac{1}{r}-\frac{e^{-r/R}}{r}\right)\\&=\frac{1}{r}\left[1-\frac{1}{R_1^2-R^2}\left(R_1^2e^{-r/R_1}-R^2e^{-r/R}\right)\right]\end{aligned}$$

for the electrostatic potential, a pointlike Coulomb potential combined with a Yukawa shape which remains finite as $r\to 0$. ■

Parseval's Relation

Results analogous to Eq. (15.57) may be derived for the Fourier sine and cosine transforms (Exercises 15.6.1 and 15.6.2).

For the special case $x=0$ in Eq. (15.57), we have

$$\int_{-\infty}^{\infty}F(\omega)G(\omega)d\omega=\int_{-\infty}^{\infty}f(-y)g(y)dy. \tag{15.60}$$

Equation (15.60) and the corresponding sine and cosine convolutions are often called Parseval's relations by analogy with Parseval's theorem for Fourier series (Chapter 14, Exercise 14.4.2). However, the minus sign in $-y$ suggests that modifications be tried. We now do this with g^* instead of g using a different technique.

The Parseval relation[6,7]

$$\int_{-\infty}^{\infty}F(\omega)G^*(\omega)d\omega=\int_{-\infty}^{\infty}f(t)g^*(t)dt \tag{15.61}$$

[6]Note that all arguments are positive, in contrast to Eq. (15.60).

[7]Some authors prefer to restrict Parseval's name to series and refer to Eq. (15.61) as Rayleigh's theorem.

may be derived elegantly using the Dirac delta function representation [Eq. (15.26)]. We have

$$\int_{-\infty}^{\infty} f(t)g^*(t)dt = \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F(\omega)e^{-i\omega t}d\omega \cdot \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} G^*(x)e^{ixt}dx\,dt, \tag{15.62}$$

with attention to the complex conjugation in the $G^*(x)$ to $g^*(t)$ transform. Integrating over t first and using Eq. (15.26), we obtain

$$\begin{aligned}\int_{-\infty}^{\infty} f(t)g^*(t)\,dt &= \int_{-\infty}^{\infty} F(\omega) \int_{-\infty}^{\infty} G^*(x)\delta(x-\omega)dx\,d\omega \\ &= \int_{-\infty}^{\infty} F(\omega)G^*(\omega)d\omega,\end{aligned} \tag{15.63}$$

our desired Parseval relation. (The $*$ of complex conjugation can also be applied to f and F instead.) If $f(t) = g(t)$, then the integrals in the Parseval relation are normalization integrals (Section 9.4). Equation (15.63) guarantees that if a function $f(t)$ is normalized to unity, its transform $F(\omega)$ is likewise normalized to unity. This is extremely important in quantum mechanics, as discussed in the next section.

It may be shown that the Fourier transform is a unitary operation (in the Hilbert space L^2 of square integrable functions). The Parseval relation is a reflection of this unitary property—analogous to Exercise 3.4.14 for matrices.

In Fraunhofer diffraction optics, the diffraction pattern (amplitude) appears as the transform of the function describing the aperture (compare Example 15.2.1). With intensity proportional to the square of the amplitude, the Parseval relation implies that the energy passing through the aperture seems to be somewhere in the diffraction pattern—a statement of the conservation of energy.

Parseval's relations may be developed independently of the inverse Fourier transform and then used rigorously to derive the inverse transform. Details are given by Morse and Feshbach,[8] Section 4.8 (see also Exercise 15.6.3).

EXAMPLE 15.6.3

Integral by Parseval's Relation Evaluate the integral $\int_{-\infty}^{\infty} \frac{d\omega}{(a^2+\omega^2)^2}$. We start by recalling from Example 15.4.1 that

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \frac{e^{i\omega x}d\omega}{a^2+\omega^2} = \frac{2}{\sqrt{\pi}} \int_0^{\infty} \frac{\cos\omega x\,d\omega}{a^2+\omega^2} = \sqrt{\frac{\pi}{2a^2}}e^{-ax}, \quad x > 0.$$

Next we apply Parseval's relation to

$$\begin{aligned}\int_{-\infty}^{\infty} \frac{d\omega}{(a^2+\omega^2)^2} &= \frac{\pi}{2a^2} \int_{-\infty}^{\infty} e^{-2a|x|}dx = \frac{\pi}{a^2} \int_0^{\infty} e^{-2ax}dx \\ &= -\frac{\pi}{2a^3}e^{-2ax}\Big|_0^{\infty} = \frac{\pi}{2a^3}.\end{aligned}$$

■

[8] Morse, P. M., and Feshbach, H. (1953). *Methods of Theoretical Physics*. McGraw-Hill, New York.

EXERCISES

15.6.1 Work out the convolution equation corresponding to Eq. (15.57) for
(a) Fourier sine transforms

$$\frac{1}{2}\int_0^\infty g(y)[f(y+x)+f(y-x)]dy = \int_0^\infty F_s(t)G_s(t)\cos tx\,dt,$$

where f and g are odd functions.
(b) Fourier cosine transforms

$$\frac{1}{2}\int_0^\infty g(y)[f(y+x)+f(|x-y|)]dy = \int_0^\infty F_c(t)G_c(t)\cos tx\,dt,$$

where f and g are even functions.

15.6.2 Show that for both Fourier sine and Fourier cosine transforms Parseval's relation has the form

$$\int_0^\infty F(t)G(t)dt = \int_0^\infty f(y)g(y)dy.$$

15.6.3 Starting from Parseval's relation [Eq. (15.61)], let $g(y) = 1$, $0 \le y \le \alpha$, and zero elsewhere. From this derive the Fourier inverse transform [Eq. (15.28)].
Hint. Differentiate with respect to α.

15.6.4 Solve Poisson's equation $\nabla^2\psi(\mathbf{r}) = -\rho(\mathbf{r})/\varepsilon_0$ by the following sequence of operations:
(a) Take the Fourier transform of both sides of this equation. Solve for the Fourier transform of $\psi(\mathbf{r})$.
(b) Carry out the Fourier inverse transform by using a three-dimensional analog of the convolution theorem [Eq. (15.57)].

15.6.5 With $F(\omega)$ and $G(\omega)$ the Fourier transforms of $f(t)$ and $g(t)$, respectively, show that

$$\int_{-\infty}^\infty |f(t)-g(t)|^2\,dt = \int_{-\infty}^\infty |F(\omega)-G(\omega)|^2\,d\omega.$$

If $g(t)$ is an approximation to $f(t)$, the preceding relation indicates that the mean square deviation in ω-space is equal to the mean square deviation in t-space.

15.6.6 Use the Parseval relation to evaluate $\int_{-\infty}^\infty \frac{\omega^2 d\omega}{(\omega^2+a^2)^2}$.
Hint. Compare Example 15.4.2.

ANS. $\dfrac{\pi}{2a}$.

15.7 Momentum Representation

In advanced mechanics and in quantum mechanics, linear momentum and spatial position occur on an equal footing. In this section, we start with the usual space distribution and derive the corresponding momentum distribution. For the one-dimensional case, our wave function $\psi(x)$, a solution of the Schrödinger wave equation, has the following properties:

1. $\psi^*(x)\psi(x)dx$ is the probability of finding the quantum particle between x and $x + dx$ and

2. $$\int_{-\infty}^{\infty} \psi^*(x)\psi(x)dx = 1, \tag{15.64}$$

   corresponding to **one** particle (along the x-axis).
   In addition, we have

3. $$\langle x\rangle = \int_{-\infty}^{\infty} \psi^*(x)x\psi(x)dx \tag{15.65}$$

   for the **average** position of the particle along the x-axis. This is often called an expectation value.

We want a function $g(p)$ that will give the same information about the momentum.

1. $g^*(p)g(p)dp$ is the probability that our quantum particle has a momentum between p and $p + dp$.

2. $$\int_{-\infty}^{\infty} g^*(p)g(p)\,dp = 1. \tag{15.66}$$

3. $$\langle p\rangle = \int_{-\infty}^{\infty} g^*(p)p\,g(p)dp. \tag{15.67}$$

As subsequently shown, such a function is given by the Fourier transform of our space function $\psi(x)$. Specifically,[9]

$$g(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \psi(x)e^{-ipx/\hbar}dx \tag{15.68}$$

$$g^*(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \psi^*(x)e^{ipx/\hbar}dx. \tag{15.69}$$

The corresponding three-dimensional momentum function is

$$g(\mathbf{p}) = \frac{1}{(2\pi\hbar)^{3/2}} \iiint_{-\infty}^{\infty} \psi(\mathbf{r})e^{-i\mathbf{r}\cdot\mathbf{p}/\hbar}d^3r.$$

To verify Eqs. (15.68) and (15.69), let us check properties 2 and 3.

[9] The $\hbar$ may be avoided by using the wave number k, $p = k\hbar$ (and $\mathbf{p} = \mathbf{k}\hbar$) so that

$$\varphi(k) = \frac{1}{(2\pi)^{1/2}} \int \psi(x)e^{-ikx}dx.$$

Property 2, the normalization, is automatically satisfied as a Parseval relation [Eq. (15.61)]. If the space function $\psi(x)$ is normalized to unity, the momentum function $g(p)$ is also normalized to unity.

To check property 3, we must show that

$$\langle p\rangle = \int_{-\infty}^{\infty} g^*(p)pg(p)dp = \int_{-\infty}^{\infty} \psi^*(x)\frac{\hbar}{i}\frac{d}{dx}\psi(x)dx, \tag{15.70}$$

where $(\hbar/i)(d/dx)$ is the momentum operator in the space representation. We replace the momentum functions by Fourier transformed space functions, and the first integral becomes

$$\frac{1}{2\pi\hbar}\iiint_{-\infty}^{\infty} pe^{-ip(x-x')/\hbar}\psi^*(x')\psi(x)dp\,dx'\,dx. \tag{15.71}$$

Now

$$pe^{-ip(x-x')/\hbar} = \frac{d}{dx}\left[-\frac{\hbar}{i}e^{-ip(x-x')/\hbar}\right]. \tag{15.72}$$

Substituting into Eq. (15.71) and integrating by parts, holding x' and p constant, we obtain

$$\langle p\rangle = \iint_{-\infty}^{\infty}\left[\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} e^{-ip(x-x')/\hbar}dp\right]\cdot\psi^*(x')\frac{\hbar}{i}\frac{d}{dx}\psi(x)dx'\,dx. \tag{15.73}$$

Here, we assume $\psi(x)$ vanishes as $x \to \pm\infty$, eliminating the integrated part. Again using the Dirac delta function [Eq. (15.23)], Eq. (15.73) reduces to Eq. (15.70) to verify our momentum representation. Note that technically we have employed the inverse Fourier transform in Eq. (15.68). This was chosen deliberately to yield the proper sign in Eq. (15.73).

EXAMPLE 15.7.1

Hydrogen Atom The hydrogen atom ground state[10] may be described by the spatial wave function

$$\psi(\mathbf{r}) = \left(\frac{1}{\pi a_0^3}\right)^{1/2} e^{-r/a_0}, \tag{15.74}$$

with a_0 being the Bohr radius, $\hbar^2/me^2$. We now have a three-dimensional wave function. The transform corresponding to Eq. (15.68) is

$$g(\mathbf{p}) = \frac{1}{(2\pi\hbar)^{3/2}}\int \psi(\mathbf{r})e^{-i\mathbf{p}\cdot\mathbf{r}/\hbar}d^3r. \tag{15.75}$$

Substituting Eq. (15.74) into Eq. (15.75) and using

$$\int e^{-ar+i\mathbf{b}\cdot\mathbf{r}}d^3r = \frac{8\pi a}{(a^2+b^2)^2}, \tag{15.76}$$

[10]For a momentum representation treatment of the hydrogen atom, $l = 0$ states, see Ivash, E. V. (1972). A momentum representation treatment of the hydrogen atom problem. *Am. J. Phys.* **40**, 1095.

we obtain the hydrogenic momentum wave function

$$g(\mathbf{p}) = \frac{2^{3/2}}{\pi} \frac{a_0^{3/2}\hbar^{5/2}}{\left(a_0^2 p^2 + \hbar^2\right)^2}. \tag{15.77}$$

Such momentum functions have been found useful in problems such as Compton scattering from atomic electrons, the wavelength distribution of the scattered radiation, depending on the momentum distribution of the target electrons.

The relation between the ordinary space representation and the momentum representation may be clarified by considering the basic commutation relations of quantum mechanics. We go from a classical Hamiltonian to the Schrödinger equation by requiring that momentum p and position x **not** commute. Instead, we require that

$$[p, x] \equiv px - xp = -i\hbar. \tag{15.78}$$

For the multidimensional case, Eq. (15.78) is replaced by

$$[p_k, x_j] = -i\hbar\delta_{kj}. \tag{15.79}$$

The Schrödinger (space) representation is obtained by using

$$(x): \qquad p_k \to -i\hbar\frac{\partial}{\partial x_k},$$

replacing the momentum by a partial space derivative. We see that

$$[p, x]\psi(x) = -i\hbar\psi(x). \tag{15.80}$$

However, Eq. (15.78) can equally well be satisfied by using

$$(p): \qquad x_j \to i\hbar\frac{\partial}{\partial p_j}.$$

This is the momentum representation. Then

$$[p, x]g(p) = -i\hbar g(p). \tag{15.81}$$

Hence, the representation (x) is not unique; (p) is an alternate possibility.

In general, the Schrödinger representation (x) leading to the Schrödinger equation is more convenient because the potential energy V is generally given as a function of position $V(x, y, z)$. The momentum representation (p) usually leads to an integral equation. For an exception, consider the harmonic oscillator.

EXAMPLE 15.7.2

Simple Harmonic Oscillator The classical Hamiltonian (kinetic energy + potential energy = total energy) is

$$H(p, x) = \frac{p^2}{2m} + \frac{1}{2}kx^2 = E, \tag{15.82}$$

where k is Hooke's law constant.

In the Schrödinger representation we obtain

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}+\frac{1}{2}kx^2\psi(x)=E\psi(x). \tag{15.83}$$

For total energy E equal to $\sqrt{(k/m)}\hbar/2$, there is a solution (Section 13.1)

$$\psi(x)=e^{-(\sqrt{mk}/(2\hbar))x^2}. \tag{15.84}$$

The momentum representation leads to

$$\frac{p^2}{2m}g(p)-\frac{\hbar^2 k}{2}\frac{d^2g(p)}{dp^2}=Eg(p). \tag{15.85}$$

Again, for

$$E=\sqrt{\frac{k}{m}}\frac{\hbar}{2} \tag{15.86}$$

the momentum wave equation (15.85) is satisfied by

$$g(p)=e^{-p^2/(2\hbar\sqrt{mk})}. \tag{15.87}$$

Either representation, space or momentum (and an infinite number of other possibilities), may be used, depending on which is more convenient for the particular problem under consideration.

The demonstration that $g(p)$ is the momentum wave function corresponding to Eq. (15.83)—that it is the Fourier inverse transform of Eq. (15.83)—is left as Exercise 15.7.3. ■

SUMMARY

Fourier integrals derive their importance from the momentum space representation in quantum mechanics. Fourier transformation of an ODE with constant coefficients leads to a polynomial, and that of a PDE with constant coefficients converts the PDE to an ODE.

EXERCISES

15.7.1 A linear quantum oscillator in its ground state has a wave function

$$\psi(x)=a^{-1/2}\pi^{-1/4}e^{-x^2/2a^2}.$$

Show that the corresponding momentum function is

$$g(p)=a^{1/2}\pi^{-1/4}\hbar^{-1/2}e^{-a^2p^2/2\hbar^2}.$$

15.7.2 The nth excited state of the linear quantum oscillator is described by

$$\psi_n(x)=a^{-1/2}2^{-n/2}\pi^{-1/4}(n!)^{-1/2}e^{-x^2/2a^2}H_n(x/a),$$

where $H_n(x/a)$ is the nth Hermite polynomial (Section 13.1). As an extension of Exercise 15.7.1, find the momentum function corresponding to $\psi_n(x)$.

Hint. $\psi_n(x)$ may be represented by $\mathcal{L}_+^n \psi_0(x)$, where $\mathcal{L}_+$ is the raising operator.

15.7.3 A free particle in quantum mechanics is described by a plane wave

$$\psi_k(x, t) = e^{i[kx - (\hbar k^2/2m)t]}.$$

Combining waves of adjacent momentum with an amplitude weighting factor $\varphi(k)$, we form a wave packet

$$\Psi(x, t) = \int_{-\infty}^{\infty} \varphi(k) e^{i[kx - (\hbar k^2/2m)t]} dk.$$

(a) Solve for $\varphi(k)$ given that

$$\Psi(x, 0) = e^{-x^2/2a^2}.$$

(b) Using the known value of $\varphi(k)$, integrate to get the explicit form of $\Psi(x, t)$. Note that this wave packet diffuses or spreads out with time.

$$ANS. \quad \Psi(x, t) = \frac{e^{-\{x^2/2[a^2 + (i\hbar/m)t]\}}}{[1 + (i\hbar t/ma^2)]^{1/2}}.$$

Note. An interesting discussion of this problem from the evolution operator point of view is given by S. M. Blinder, Evolution of a Gaussian wave-packet. *Am. J. Phys.* **36**, 525 (1968).

15.7.4 Find the time-dependent momentum wave function $g(k, t)$ corresponding to $\Psi(x, t)$ of Exercise 15.7.3. Show that the momentum wave packet $g^*(k, t)g(k, t)$ is **independent** of time.

15.7.5 The deuteron (Example 9.1.2) may be described reasonably well with a Hulthén wave function

$$\psi(\mathbf{r}) = A[e^{-\alpha r} - e^{-\beta r}]/r,$$

with A, α, and β constants. Find $g(\mathbf{p})$, the corresponding momentum wave function.
Note. The Fourier transform may be rewritten as Fourier sine and cosine transforms or as a Laplace transform (Section 15.8).

15.7.6 The nuclear form factor $F(k)$ and the charge distribution $\rho(r)$ are three-dimensional Fourier transforms of each other:

$$F(k) = \frac{1}{(2\pi)^{3/2}} \int \rho(r) e^{i\mathbf{k}\cdot\mathbf{r}} d^3r.$$

If the measured form factor is

$$F(k) = (2\pi)^{-3/2} \left(1 + \frac{k^2}{a^2}\right)^{-1},$$

find the corresponding charge distribution.

$$ANS. \quad \rho(r) = \frac{a^2}{4\pi} \frac{e^{-ar}}{r}.$$

15.7.7 Check the normalization of the hydrogen momentum wave function

$$g(\mathbf{p}) = \frac{2^{3/2}}{\pi} \frac{a_0^{3/2}\hbar^{5/2}}{\left(a_0^2 p^2 + \hbar^2\right)^2}$$

by direct evaluation of the integral

$$\int g^*(\mathbf{p}) g(\mathbf{p}) d^3p.$$

15.7.8 With $\psi(\mathbf{r})$ a wave function in ordinary space and $\varphi(\mathbf{p})$ the corresponding momentum function, show that

(a) $$\frac{1}{(2\pi\hbar)^{3/2}} \int \mathbf{r}\psi(\mathbf{r}) e^{-i\mathbf{r}\cdot\mathbf{p}/\hbar} d^3r = i\hbar \nabla_p \varphi(\mathbf{p}),$$

(b) $$\frac{1}{(2\pi\hbar)^{3/2}} \int \mathbf{r}^2\psi(\mathbf{r}) e^{-i\mathbf{r}\cdot\mathbf{p}/\hbar} d^3r = (i\hbar \nabla_p)^2 \varphi(\mathbf{p}).$$

Note. ∇_p is the gradient in momentum space:

$$\hat{\mathbf{x}}\frac{\partial}{\partial p_x} + \hat{\mathbf{y}}\frac{\partial}{\partial p_y} + \hat{\mathbf{z}}\frac{\partial}{\partial p_z}.$$

These results may be extended to any positive integer power of r and therefore to any (analytic) function that may be expanded as a Maclaurin series in r.

15.7.9 The ordinary space wave function $\psi(\mathbf{r}, t)$ satisfies the time-dependent Schrödinger equation

$$i\hbar \frac{\partial \psi(\mathbf{r}, t)}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + V(\mathbf{r})\psi.$$

Show that the corresponding time-dependent momentum wave function satisfies the analogous equation

$$i\hbar \frac{\partial \varphi(\mathbf{p}, t)}{\partial t} = \frac{p^2}{2m}\varphi + V(i\hbar\nabla_p)\varphi.$$

Note. Assume that $V(\mathbf{r})$ may be expressed by a Maclaurin series and use Exercise 15.7.10. $V(i\hbar\nabla_p)$ is the same function of the variable $i\hbar\nabla_p$ as $V(\mathbf{r})$ is of the variable $\mathbf{r}$.

15.7.10 The one-dimensional, time-independent Schrödinger equation is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x).$$

For the special case of $V(x)$ an analytic function of x, show that the corresponding momentum wave equation is

$$V\left(i\hbar\frac{d}{dp}\right) g(p) + \frac{p^2}{2m} g(p) = E g(p).$$

Derive this momentum wave equation from the Fourier transform [Eq. (15.68)] and its inverse. Do not use the substitution $x \to i\hbar(d/dp)$ directly.

15.8 Laplace Transforms

Definition

The Laplace transform $f(s)$ or $\mathcal{L}$ of a function $F(t)$ is defined by[11]

$$f(s) = \mathcal{L}\{F(t)\} = \lim_{a\to\infty} \int_0^a e^{-st} F(t)dt = \int_0^\infty e^{-st} F(t)dt. \tag{15.88}$$

A few comments on the existence of the integral are in order. The infinite integral of $F(t)$,

$$\int_0^\infty F(t)dt,$$

need not exist. For instance, $F(t)$ may diverge exponentially for large t. However, if there is some constant such that

$$|e^{-s_0 t} F(t)| \le M, \tag{15.89}$$

a positive constant for sufficiently large t, $t > t_0$, the Laplace transform [Eq. (15.88)] will exist for $s > s_0$; $F(t)$ is said to be of exponential order. As a counterexample, $F(t) = e^{t^2}$ does not satisfy the condition given by Eq. (15.89) and is **not** of exponential order. $\mathcal{L}\{e^{t^2}\}$ does **not** exist.

The Laplace transform may also fail to exist because of a sufficiently strong singularity in the function $F(t)$ as $t \to 0$; that is,

$$\int_0^\infty e^{-st} t^n \, dt$$

diverges at the origin for $n \le -1$. The Laplace transform $\mathcal{L}\{t^n\}$ does not exist for $n \le -1$.

Since for two functions $F(t)$ and $G(t)$, for which the integrals exist,

$$\mathcal{L}\{aF(t) + bG(t)\} = a\mathcal{L}\{F(t)\} + b\mathcal{L}\{G(t)\}, \tag{15.90}$$

the operation denoted by $\mathcal{L}$ is **linear**.

EXAMPLE 15.8.1

Elementary Functions To illustrate the Laplace transform, let us apply the operation to some of the elementary functions. If

$$F(t) = 1, \quad t > 0,$$

then

$$\mathcal{L}\{1\} = \int_0^\infty e^{-st} dt = \frac{1}{s}, \quad \text{for} \quad s > 0. \tag{15.91}$$

[11] This is sometimes called a one-sided Laplace transform; the integral from $-\infty$ to $+\infty$ is referred to as a two-sided Laplace transform. Some authors introduce an additional factor of s. This extra s appears to have little advantage and continually gets in the way (see Additional Reading, Jeffreys and Jeffreys, Section 14.13). Generally, we take s to be real and positive. It is possible to have s complex, provided $\Re(s) > 0$.

Again, let

$$F(t) = e^{kt}, \quad t > 0.$$

The Laplace transform becomes

$$\mathcal{L}\{e^{kt}\} = \int_0^\infty e^{-st} e^{kt} dt = \frac{1}{s-k}, \quad \text{for } s > k, \tag{15.92}$$

where the integral is finite. Using this relation, we obtain the Laplace transform of certain other functions. Since

$$\cosh kt = \frac{1}{2}(e^{kt} + e^{-kt}), \qquad \sinh kt = \frac{1}{2}(e^{kt} - e^{-kt}), \tag{15.93}$$

we have

$$\begin{aligned} \mathcal{L}\{\cosh kt\} &= \frac{1}{2}\left(\frac{1}{s-k} + \frac{1}{s+k}\right) = \frac{s}{s^2-k^2}, \\ \mathcal{L}\{\sinh kt\} &= \frac{1}{2}\left(\frac{1}{s-k} - \frac{1}{s+k}\right) = \frac{k}{s^2-k^2}, \end{aligned} \tag{15.94}$$

both valid for $s > k$, where the integrals are finite. Because the results are analytic functions of s, they may be continued analytically over the complex s-plane. This will prove useful for the inverse Laplace transform in Section 15.12. We use the relations

$$\cos kt = \cosh ikt, \qquad \sin kt = -i \sinh ikt$$

in Eq. (15.94), with k replaced by ik, to find that the Laplace transforms

$$\begin{aligned} \mathcal{L}\{\cos kt\} &= \frac{s}{s^2+k^2}, \\ \mathcal{L}\{\sin kt\} &= \frac{k}{s^2+k^2}, \end{aligned} \tag{15.95}$$

both valid for $s > 0$, where the integrals are finite. Another derivation of this last transform is given in the next section. Note that $\lim_{s\to 0} \mathcal{L}\{\sin kt\} = 1/k$. This suggests we assign a value of $1/k$ to the Laplace transform $\lim_{s\to 0} \int_0^\infty e^{-st} \sin kt\, dt$.

Finally, for $F(t) = t^n$, we have

$$\mathcal{L}\{t^n\} = \int_0^\infty e^{-st} t^n\, dt,$$

which is the factorial function. Hence,

$$\mathcal{L}\{t^n\} = \frac{n!}{s^{n+1}}, \quad s > 0, n > -1. \tag{15.96}$$

Note that in all these transforms we have the variable s in the denominator-negative powers of s. In particular, $\lim_{s\to\infty} f(s) = 0$. The significance of this point is that if $f(s)$ involves positive powers of s, then $\lim_{s\to\infty} f(s) \to \infty$ and no inverse transform exists. ■

Inverse Transform

There is little importance to these operations, unless we can carry out the inverse transform as in Fourier transforms. That is, with

$$\mathcal{L}\{F(t)\} = f(s),$$

then

$$\mathcal{L}^{-1}\{f(s)\} = F(t).$$

Taken literally, this inverse transform is **not** unique. However, to the physicist and engineer the inverse operation may almost always be taken as unique in practical problems.

The inverse transform can be determined in various ways. A table of transforms can be built up and used to carry out the inverse transformation exactly as a table of logarithms can be used to look them up. The preceding transforms constitute the beginnings of such a table. For a more complete set of Laplace transforms, see AMS-55, Chapter 29. Employing partial fraction expansions and various operational theorems, which are considered in succeeding sections, facilitates use of the tables. There is some justification for suspecting that these tables are probably of more value in solving textbook exercises than in solving real-world problems.

A general technique for $\mathcal{L}^{-1}$ will be developed in Section 15.12 by using the calculus of residues. The difficulties and the possibilities of a numerical approach—numerical inversion—are considered at the end of this section.

Partial Fraction Expansion

Utilization of a table of transforms (or inverse transforms) is facilitated by expanding $f(s)$ in **partial fractions**.

Frequently, $f(s)$, our transform, occurs in the form $g(s)/h(s)$, where $g(s)$ and $h(s)$ are polynomials with no common factors, $g(s)$ being of lower degree than $h(s)$. If the factors of $h(s)$ are all linear and distinct, then by the theory of partial fractions, we may write

$$f(s) = \frac{c_1}{s-a_1} + \frac{c_2}{s-a_2} + \cdots + \frac{c_n}{s-a_n}, \tag{15.97}$$

where the c_i are independent of s. The a_i are the roots of $h(s)$. If any one of the roots (e.g., a_1) is multiple (occurring m times), then $f(s)$ has the form

$$f(s) = \frac{c_{1,m}}{(s-a_1)^m} + \frac{c_{1,m-1}}{(s-a_1)^{m-1}} + \cdots + \frac{c_{1,1}}{s-a_1} + \sum_{i=2}^{n} \frac{c_i}{s-a_i}. \tag{15.98}$$

Finally, if one of the factors is quadratic, $(s^2 + ps + q)$, the numerator, instead of being a simple constant, will have the form

$$\frac{as+b}{s^2+ps+q}.$$

There are various ways of determining the constants introduced. For instance, in Eq. (15.97) we may multiply through by $(s - a_i)$ and obtain

$$c_i = \lim_{s \to a_i} (s - a_i) f(s). \tag{15.99}$$

In elementary cases a direct solution is often the easiest.

EXAMPLE 15.8.2

Partial Fraction Expansion Let

$$f(s) = \frac{k^2}{s(s^2 + k^2)}. \tag{15.100}$$

We want to bring $f(s)$ to the form

$$f(s) = \frac{c}{s} + \frac{as + b}{s^2 + k^2}.$$

Putting the right side of this equation over a common denominator and equating like powers of s in the numerator, we obtain

$$\frac{k^2}{s(s^2 + k^2)} = \frac{c(s^2 + k^2) + s(as + b)}{s(s^2 + k^2)}, \tag{15.101}$$

$$c + a = 0, \quad s^2; \qquad b = 0, \quad s^1; \qquad ck^2 = k^2, \quad s^0.$$

Solving these $(s \neq 0)$, we have

$$c = 1, \quad b = 0, \quad a = -1,$$

giving

$$f(s) = \frac{1}{s} - \frac{s}{s^2 + k^2} \tag{15.102}$$

and

$$\mathcal{L}^{-1}\{f(s)\} = 1 - \cos kt \tag{15.103}$$

by Eqs. (15.91) and (15.95). ■

EXAMPLE 15.8.3

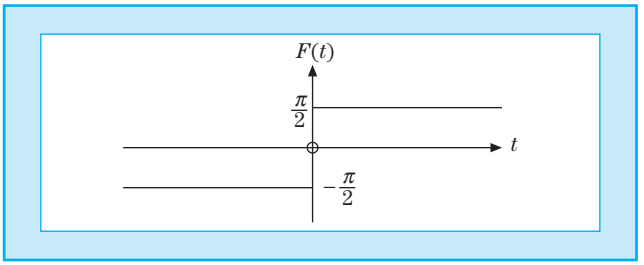
A Step Function As one application of Laplace transforms, consider the evaluation of

$$F(t) = \int_0^\infty \frac{\sin tx}{x} dx. \tag{15.104}$$

Suppose we take the Laplace transform of this definite integral, which is finite by virtue of the sign changes of the sine:

$$\mathcal{L}\left\{\int_0^\infty \frac{\sin tx}{x} dx\right\} = \int_0^\infty e^{-st} \int_0^\infty \frac{\sin tx}{x} dx\, dt. \tag{15.105}$$

Figure 15.9
$F(t) = \int_0^\infty \frac{\sin tx}{x} dx$, a Step Function



Now interchanging the order of integration (which is justified),[12] we get

$$\int_0^\infty \frac{1}{x}\left[\int_0^\infty e^{-st}\sin tx\,dt\right]dx = \int_0^\infty \frac{dx}{s^2+x^2} \tag{15.106}$$

by integrating by parts as in Example 15.4.1. The factor in square brackets is the Laplace transform of $\sin tx$ from Eq. (15.95). Hence,

$$\int_0^\infty \frac{dx}{s^2+x^2} = \frac{1}{s}\tan^{-1}\left(\frac{x}{s}\right)\Big|_0^\infty = \frac{\pi}{2s} = f(s). \tag{15.107}$$

By Eq. (15.91) we carry out the inverse transformation to obtain

$$F(t) = \frac{\pi}{2}, \quad t > 0, \tag{15.108}$$

in agreement with an evaluation by the calculus of residues (Section 7.2). It has been assumed that $t > 0$ in $F(t)$. For $F(-t)$ we need note only that $\sin(-tx) = -\sin tx$, giving $F(-t) = -F(t)$. Finally, if $t = 0$, $F(0)$ is clearly zero. Therefore,

$$\int_0^\infty \frac{\sin tx}{x}dx = \frac{\pi}{2}[2u(t)-1] = \begin{cases} \frac{\pi}{2}, & t > 0 \\ 0, & t = 0 \\ -\frac{\pi}{2}, & t < 0, \end{cases} \tag{15.109}$$

where $u(t)$ is the Heaviside unit step function of Example 15.3.1. Note that $\int_0^\infty (\sin tx/x)dx$, taken as a function of t, describes a step function (Fig. 15.9), a step of height π at $t = 0$. ■

The technique in the preceding example was to

- introduce a second integration—the Laplace transform;
- reverse the order of integration and integrate; and
- take the inverse Laplace transform.

There are many opportunities in which this technique of reversing the order of integration can be applied and proved very useful. Exercise 15.8.6 is a variation of this.

[12] See Jeffreys and Jeffreys (1966), Chapter 1 (uniform convergence of integrals).

Numerical Inversion

As an integration, the Laplace transform is a highly stable operation—stable in the sense that small fluctuations (or errors) in $F(t)$ are averaged out in the determination of the area under a curve. Also, the weighting factor, e^{-st}, means that the behavior of $F(t)$ at large t is effectively ignored—unless s is small. As a result of these two effects, a large change in $F(t)$ at large t indicates a very small, perhaps insignificant, change in $f(s)$. In contrast to the Laplace transform operation, going from $f(s)$ to $F(t)$ is highly unstable. A minor change in $f(s)$ may result in a wild variation of $F(t)$. All significant figures may disappear. In a matrix formulation, the matrix is ill conditioned with respect to inversion.

There is no general, completely satisfactory numerical method for inverting Laplace transforms. However, if we are willing to restrict attention to relatively smooth functions, various possibilities open up. Bellman, Kalaba, and Lockett[13] convert the Laplace transform to a Mellin transform ($x = e^{-t}$) and use numerical quadrature based on shifted Legendre polynomials, $P_n^*(x) = P_n(1-2x)$. The key step is analytic inversion of the resulting matrix. Krylov and Skoblya[14] focus on the evaluation of the Bromwich integral (Section 15.12). As one technique, they replace the integrand with an interpolating polynomial of negative powers and integrate analytically.

EXERCISES

15.8.1 Prove that

$$\lim_{s\to\infty} sf(s) = \lim_{t\to+0} F(t).$$

Hint. Assume that $F(t)$ can be expressed as $F(t) = \sum_{n=0}^{\infty} a_n t^n$.

15.8.2 Show that

$$\frac{1}{\pi}\lim_{s\to 0}\mathcal{L}\{\cos xt\} = \delta(x).$$

15.8.3 Verify that

$$\mathcal{L}\left\{\frac{\cos at - \cos bt}{b^2 - a^2}\right\} = \frac{s}{(s^2+a^2)(s^2+b^2)}, \quad a^2 \neq b^2.$$

15.8.4 Using partial fraction expansions, show that

(a) $$\mathcal{L}^{-1}\left\{\frac{1}{(s+a)(s+b)}\right\} = \frac{e^{-at}-e^{-bt}}{b-a}, \quad a \neq b.$$

(b) $$\mathcal{L}^{-1}\left\{\frac{s}{(s+a)(s+b)}\right\} = \frac{ae^{-at}-be^{-bt}}{a-b}, \quad a \neq b.$$

[13] Bellman, R., Kalaba, R. E., and Lockett, J. A. (1966). *Numerical Inversion of the Laplace Transforms*. Elsevier, New York.

[14] Krylov, V. I., and Skoblya, N. S. (1969). *Handbook of Numerical Inversion of Laplace Transforms* (D. Louvish, Trans.). Israel Program for Scientific Translations, Jerusalem.

15.8.5 Using partial fraction expansions, show that for $a^2 \neq b^2$,

(a) $$\mathcal{L}^{-1}\left\{\frac{1}{(s^2+a^2)(s^2+b^2)}\right\} = -\frac{1}{a^2-b^2}\left\{\frac{\sin at}{a} - \frac{\sin bt}{b}\right\},$$

(b) $$\mathcal{L}^{-1}\left\{\frac{s^2}{(s^2+a^2)(s^2+b^2)}\right\} = \frac{1}{a^2-b^2}\{a\sin at - b\sin bt\}.$$

15.8.6 The electrostatic potential of a charged conducting disk is known to have the general form (circular cylindrical coordinates)

$$\Phi(\rho, z) = \int_0^\infty e^{-k|z|} J_0(k\rho) f(k)\, dk,$$

with $f(k)$ unknown. At large distances ($z \to \infty$) the potential must approach the Coulomb potential $Q/4\pi\varepsilon_0 z$. Show that

$$\lim_{k\to 0} f(k) = \frac{q}{4\pi\varepsilon_0}.$$

Hint. You may set $\rho = 0$ and assume a Maclaurin expansion of $f(k)$ or, using e^{-kz}, construct a delta sequence.

15.8.7 A function $F(t)$ can be expanded in a power series (Maclaurin); that is,

$$F(t) = \sum_{n=0}^{\infty} a_n t^n.$$

Then

$$\mathcal{L}\{F(t)\} = \int_0^\infty e^{-st} \sum_{n=0}^{\infty} a_n t^n\, dt = \sum_{n=0}^{\infty} a_n \int_0^\infty e^{-st} t^n\, dt.$$

Show that $f(s)$, the Laplace transform of $F(t)$, contains no powers of s greater than s^{-1}. Check your result by calculating $\mathcal{L}\{\delta(t)\}$ and comment on this fiasco.

15.9 Laplace Transform of Derivatives

Perhaps the main application of Laplace transforms is in converting differential equations into simpler forms that may be solved more easily. It will be seen, for instance, that **coupled differential equations with constant coefficients transform to simultaneous linear algebraic equations**.

Let us transform the first derivative of $F(t)$:

$$\mathcal{L}\{F'(t)\} = \int_0^\infty e^{-st} \frac{dF(t)}{dt} dt.$$

Integrating by parts, we obtain

$$\begin{aligned}\mathcal{L}\{F'(t)\} &= e^{-st}F(t)\Big|_0^\infty + s\int_0^\infty e^{-st}F(t)dt \\ &= s\mathcal{L}\{F(t)\} - F(0).\end{aligned} \tag{15.110}$$

Strictly speaking, $F(0) = F(+0)$,[15] and dF/dt is required to be at least piecewise continuous for $0 \le t < \infty$. Naturally, both $F(t)$ and its derivative must be such that the integrals do not diverge. Incidentally, Eq. (15.110) provides another proof of Exercise 15.8.7. An extension gives

$$\mathcal{L}\{F^{(2)}(t)\} = s^2\mathcal{L}\{F(t)\} - sF(+0) - F'(+0), \tag{15.111}$$

$$\mathcal{L}\{F^{(n)}(t)\} = s^n\mathcal{L}\{F(t)\} - s^{n-1}F(+0) - \cdots - F^{(n-1)}(+0). \tag{15.112}$$

The Laplace transform, like the Fourier transform, replaces differentiation with multiplication. In the following examples, ODEs become algebraic equations. Here is the power and the utility of the Laplace transform. When the coefficients of the derivatives are not constant, Laplace transforms do not simplify the ODE, as a rule.

Note how the initial conditions, $F(+0)$, $F'(+0)$, and so on, are incorporated into the transform. Equation (15.111) may be used to derive $\mathcal{L}\{\sin kt\}$. We use the identity

$$-k^2 \sin kt = \frac{d^2}{dt^2}\sin kt. \tag{15.113}$$

Then, applying the Laplace transform operation, we have

$$\begin{aligned} -k^2\mathcal{L}\{\sin kt\} &= \mathcal{L}\left\{\frac{d^2}{dt^2}\sin kt\right\} \\ &= s^2\mathcal{L}\{\sin kt\} - s\sin(0) - \frac{d}{dt}\sin kt|_{t=0}. \end{aligned} \tag{15.114}$$

Since $\sin(0) = 0$ and $d/dt \sin kt|_{t=0} = k$,

$$\mathcal{L}\{\sin kt\} = \frac{k}{s^2 + k^2}, \tag{15.115}$$

verifying Eq. (15.95).

EXAMPLE 15.9.1

Classical Harmonic Oscillator As a physical example, consider a mass m oscillating under the influence of an ideal spring, spring constant k. Friction is neglected. Then Newton's second law becomes

$$m\frac{d^2X(t)}{dt^2} + kX(t) = 0. \tag{15.116}$$

The initial conditions are taken to be

$$X(0) = X_0, \qquad X'(0) = 0.$$

Applying the Laplace transform, we obtain

$$m\mathcal{L}\left\{\frac{d^2X}{dt^2}\right\} + k\mathcal{L}\{X(t)\} = 0, \tag{15.117}$$

[15] Zero is approached from the positive side.

and by use of Eq. (15.111) this becomes

$$ms^2x(s) - msX_0 + kx(s) = 0, \tag{15.118}$$

$$x(s) = X_0\frac{s}{s^2+\omega_0^2}, \quad \text{with } \omega_0^2 \equiv \frac{k}{m}. \tag{15.119}$$

From Eq. (15.95) this is seen to be the transform of $\cos\omega_0 t$, which gives

$$X(t) = X_0\cos\omega_0 t, \tag{15.120}$$

as expected. ■

Dirac Delta Function

For use with differential equations, one further transform is helpful—the Dirac delta function:[16]

$$\mathcal{L}\{\delta(t-t_0)\} = \int_0^\infty e^{-st}\delta(t-t_0)dt = e^{-st_0}, \quad \text{for } t_0 \geq 0, \tag{15.121}$$

and for $t_0 = 0$,

$$\mathcal{L}\{\delta(t)\} = 1, \tag{15.122}$$

where, for Laplace transforms, $\delta(0)$ is interpreted as

$$\delta(0) = \lim_{t_0\to 0^+}\delta(t-t_0). \tag{15.123}$$

As an alternate method, $\delta(t)$ may be considered the limit as $\varepsilon \to 0$ of $F(t)$, where

$$F(t) = \begin{cases} 0, & t < 0, \\ \varepsilon^{-1}, & 0 < t < \varepsilon, \\ 0, & t > \varepsilon. \end{cases} \tag{15.124}$$

By direct calculation,

$$\mathcal{L}\{F(t)\} = \frac{1-e^{-\varepsilon s}}{\varepsilon s}. \tag{15.125}$$

Taking the limit of the integral (instead of the integral of the limit), we have

$$\lim_{\varepsilon\to 0}\mathcal{L}\{F(t)\} = 1$$

or Eq. (15.122)

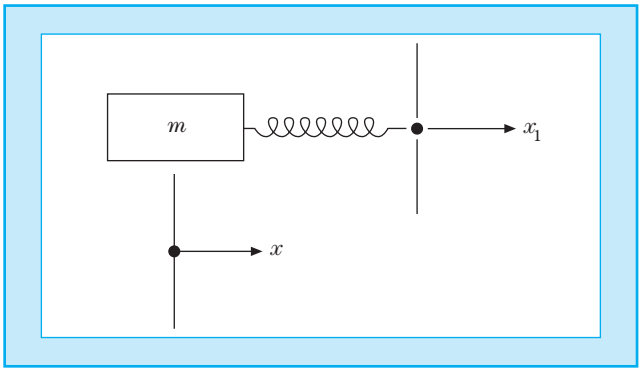
$$\mathcal{L}\{\delta(t)\} = 1.$$

This delta function is frequently called the impulse function because it is so useful in describing impulsive forces, that is, forces lasting only a short time.

[16]Strictly speaking, the Dirac delta function is undefined. However, the integral over it is well defined. This approach is developed in Section 1.14 using delta sequences.

Figure 15.10

Spring



EXAMPLE 15.9.2

Impulsive Force Newton's second law for impulsive force acting on a particle of mass m becomes

$$m\frac{d^2X}{dt^2} = P\delta(t), \tag{15.126}$$

where P is a constant. Transforming, we obtain

$$ms^2x(s) - msX(0) - mX'(0) = P. \tag{15.127}$$

For a particle starting from rest, $X'(0) = 0$.[17] We shall also take $X(0) = 0$. Then

$$x(s) = \frac{P}{ms^2}, \tag{15.128}$$

and

$$X(t) = \frac{P}{m}t, \tag{15.129}$$

$$\frac{dX(t)}{dt} = \frac{P}{m}, \quad \text{a constant.} \tag{15.130}$$

The effect of the impulse $P\delta(t)$ is to transfer (instantaneously) P units of linear momentum to the particle. ■

EXERCISES

15.9.1 Use the expression for the transform of a second derivative to obtain the transform of $\cos kt$.

15.9.2 A mass m is attached to one end of an unstretched spring, spring constant k (Fig. 15.10). At time $t = 0$ the free end of the spring experiences a constant acceleration, a, away from the mass. Using Laplace transforms,

[17] This really should be $X'(+0)$. To include the effect of the impulse, consider that the impulse will occur at $t = \varepsilon$ and let $\varepsilon \to 0$.

(a) find the position x of m as a function of time; and
(b) determine the limiting form of $x(t)$ for small t.

$$\textit{ANS.} \quad (a)\ x = \frac{1}{2}at^2 - \frac{a}{\omega^2}(1 - \cos\omega t), \quad \omega^2 = \frac{k}{m},$$
$$(b)\ x = \frac{a\omega^2}{4!}t^4, \quad \omega t \ll 1.$$

15.10 Other Properties

Substitution

If we replace the parameter s by $s-a$ in the definition of the Laplace transform [Eq. (15.88)], we have

$$f(s-a) = \int_0^\infty e^{-(s-a)t}F(t)dt = \int_0^\infty e^{-st}e^{at}F(t)dt$$
$$= \mathcal{L}\{e^{at}F(t)\}. \tag{15.131}$$

Hence, the replacement of s with $s-a$ corresponds to multiplying $F(t)$ by e^{at} and conversely. This result can be used to good advantage in extending our table of transforms. From Eq. (15.95) we find immediately that

$$\mathcal{L}\{e^{at}\sin kt\} = \frac{k}{(s-a)^2 + k^2}; \tag{15.132}$$

also,

$$\mathcal{L}\{e^{at}\cos kt\} = \frac{s-a}{(s-a)^2 + k^2}, \quad s > a. \tag{15.133}$$

EXAMPLE 15.10.1

Damped Oscillator These expressions are useful when we consider an oscillating mass with damping proportional to the velocity. Equation (15.116), with such damping added, becomes

$$mX''(t) + bX'(t) + kX(t) = 0, \tag{15.134}$$

where b is a proportionality constant. Let us assume that the particle starts from rest at $X(0) = X_0$, $X'(0) = 0$. The transformed equation is

$$m[s^2x(s) - sX_0] + b[sx(s) - X_0] + kx(s) = 0 \tag{15.135}$$

so that

$$x(s) = X_0\frac{ms + b}{ms^2 + bs + k}. \tag{15.136}$$

This may be handled by completing the square of the denominator,

$$s^2 + \frac{b}{m}s + \frac{k}{m} = \left(s + \frac{b}{2m}\right)^2 + \left(\frac{k}{m} - \frac{b^2}{4m^2}\right). \tag{15.137}$$

If the damping is small, $b^2 < 4km$, the last term is positive and will be denoted by ω_1^2. Splitting the numerator of $x(s)$ into $(s + b/2m) + b/2m$ gives

$$x(s) = X_0 \frac{s + b/m}{(s + b/2m)^2 + \omega_1^2}$$
$$= X_0 \frac{s + b/2m}{(s + b/2m)^2 + \omega_1^2} + X_0 \frac{(b/2m\omega_1)\omega_1}{(s + b/2m)^2 + \omega_1^2}. \tag{15.138}$$

By Eqs. (15.132) and (15.133),

$$X(t) = X_0 e^{-(b/2m)t}\left(\cos \omega_1 t + \frac{b}{2m\omega_1} \sin \omega_1 t\right)$$
$$= X_0 \frac{\omega_0}{\omega_1} e^{-(b/2m)t} \cos(\omega_1 t - \varphi), \tag{15.139}$$

where

$$\tan \varphi = \frac{b}{2m\omega_1}, \qquad \omega_0^2 = \frac{k}{m}. \tag{15.140}$$

Of course, as $b \to 0$, this solution goes over to the undamped solution (Section 15.9). ■

RLC Analog

It is worth noting the similarity between this damped simple harmonic oscillation of a mass on a spring and a resistance, inductance, and capacitance (RLC) circuit (Fig. 15.11). At any instant the sum of the potential differences around the loop must be zero (Kirchhoff's law, conservation of energy). This gives

$$L\frac{dI}{dt} + RI + \frac{1}{C}\int_0^t I\, dt = 0. \tag{15.141}$$

Differentiating the current I with respect to time (to eliminate the integral), we have

$$L\frac{d^2I}{dt^2} + R\frac{dI}{dt} + \frac{1}{C}I = 0. \tag{15.142}$$

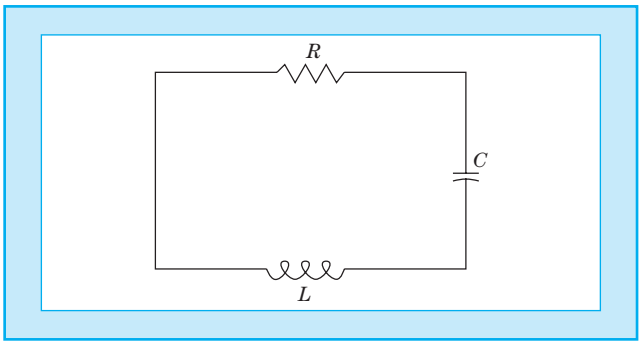
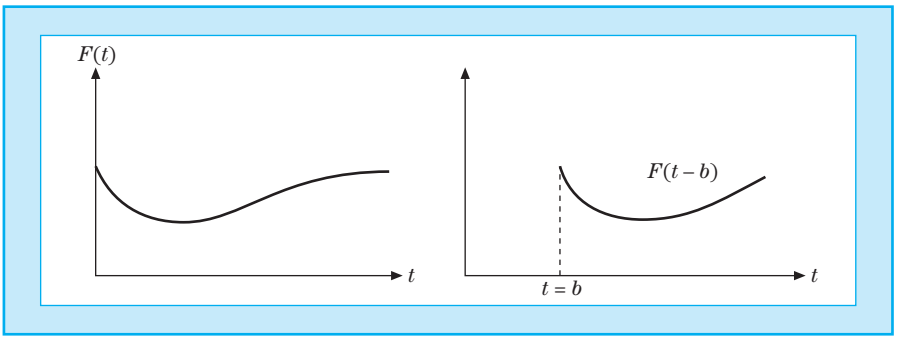


Figure 15.11
RLC Circuit

Figure 15.12
Translation



If we replace $I(t)$ with $X(t)$, L with m, R with b, and C^{-1} with k, Eq. (15.142) is identical to the mechanical problem. It is but one example of the unification of diverse branches of physics by mathematics. A more complete discussion is provided by Olson.[18]

Translation

This time, let $f(s)$ be multiplied by e^{-bs}, $b > 0$:

$$e^{-bs}f(s) = e^{-bs}\int_0^\infty e^{-st}F(t)dt$$
$$= \int_0^\infty e^{-s(t+b)}F(t)dt. \tag{15.143}$$

Now let $t + b = \tau$; then Eq. (15.143) becomes

$$e^{-bs}f(s) = \int_b^\infty e^{-s\tau}F(\tau - b)d\tau$$
$$= \int_0^\infty e^{-s\tau}F(\tau - b)d\tau, \tag{15.144}$$

if we assume that $F(t) = 0$ for $t < 0$, so that $F(\tau - b) = 0$ for $0 \le \tau < b$. In that case, we can extend the lower limit to zero without changing the value of the integral. This relation is often called the Heaviside shifting theorem (Fig. 15.12). We obtain

$$e^{-bs}f(s) = \mathcal{L}\{F(t-b)\}, \quad F(t) = 0, \ t < 0. \tag{15.145}$$

EXAMPLE 15.10.2

Electromagnetic Waves The electromagnetic wave equation with $E = E_y$ or E_z, a transverse wave propagating along the x-axis, is

$$\frac{\partial^2 E(x,t)}{\partial x^2} - \frac{1}{v^2}\frac{\partial^2 E(x,t)}{\partial t^2} = 0. \tag{15.146}$$

[18] Olson, H. F. (1943). *Dynamical Analogies*. Van Nostrand, New York.

Transforming this equation with respect to t, we get

$$\frac{\partial^2}{\partial x^2}\mathcal{L}\{E(x,t)\} - \frac{s^2}{v^2}\mathcal{L}\{E(x,t)\} + \frac{s}{v^2}E(x,0) + \frac{1}{v^2}\frac{\partial E(x,t)}{\partial t}\bigg|_{t=0} = 0. \quad (15.147)$$

If we have the initial conditions $E(x,0) = 0$ and

$$\frac{\partial E(x,t)}{\partial t}\bigg|_{t=0} = 0,$$

then

$$\frac{\partial^2}{\partial x^2}\mathcal{L}\{E(x,t)\} = \frac{s^2}{v^2}\mathcal{L}\{E(x,t)\}. \quad (15.148)$$

The solution (of this **ODE**) is

$$\mathcal{L}\{E(x,t)\} = c_1 e^{-(s/v)x} + c_2 e^{+(s/v)x}. \quad (15.149)$$

The "constants" c_1 and c_2 are obtained by additional boundary conditions. They are constant with respect to x but may depend on s. If our wave remains finite as $x \to \infty$, $\mathcal{L}\{E(x,t)\}$ will also remain finite. Hence, $c_2 = 0$.

If $E(0,t)$ is denoted by $F(t)$, then $c_1 = f(s)$ and

$$\mathcal{L}\{E(x,t)\} = e^{-(s/v)x} f(s). \quad (15.150)$$

From the translation property [Eq. (15.144)] we find immediately that

$$E(x,t) = \begin{cases} F\left(t - \frac{x}{v}\right), & t \geq \frac{x}{v}, \\ 0, & t < \frac{x}{v}, \end{cases} \quad (15.151)$$

which is consistent with our initial condition. Differentiation and substitution into Eq. (15.146) verifies Eq. (15.151). Our solution represents a wave (or pulse) moving in the positive x-direction with velocity v. Note that for $x > vt$ the region remains undisturbed; the pulse has not had time to get there. The other independent solution has $c_1 = 0$ and corresponds to a signal propagated along the negative x-axis. ■

Derivative of a Transform

When $F(t)$, which is at least piecewise continuous, and s are chosen so that $e^{-st}F(t)$ converges exponentially for large s, the integral

$$f(s) = \int_0^\infty e^{-st}F(t)dt$$

is uniformly convergent and may be differentiated (under the integral sign) with respect to s. Then

$$f'(s) = \int_0^\infty (-t)e^{-st}F(t)dt = \mathcal{L}\{-tF(t)\}. \quad (15.152)$$

Continuing this process, we obtain

$$f^{(n)}(s) = \mathcal{L}\{(-t)^n F(t)\}. \tag{15.153}$$

All the integrals so obtained will be uniformly convergent because of the decreasing exponential behavior of $e^{-st}F(t)$.

This same technique may be applied to generate more transforms. For example,

$$\mathcal{L}\{e^{kt}\} = \int_0^\infty e^{-st}e^{kt}dt = \frac{1}{s-k}, \quad s > k. \tag{15.154}$$

Differentiating with respect to s (or with respect to k), we obtain

$$\mathcal{L}\{te^{kt}\} = \frac{1}{(s-k)^2}, \quad s > k. \tag{15.155}$$

Integration of Transforms

Again, with $F(t)$ at least piecewise continuous and x large enough, so that $e^{-xt}F(t)$ decreases exponentially (as $x \to \infty$), the integral

$$f(x) = \int_0^\infty e^{-xt}F(t)dt \tag{15.156}$$

is uniformly convergent with respect to x. This justifies reversing the order of integration in the following equation:

$$\begin{aligned}\int_s^b f(x)dx &= \int_s^b \int_0^\infty e^{-xt}F(t)dt\,dx \\ &= \int_0^\infty \frac{F(t)}{t}(e^{-st} - e^{-bt})dt,\end{aligned} \tag{15.157}$$

on integrating with respect to x. The lower limit s is chosen large enough so that $f(s)$ is within the region of uniform convergence. Now letting $b \to \infty$, we have

$$\int_s^\infty f(x)dx = \int_0^\infty \frac{F(t)}{t}e^{-st}dt = \mathcal{L}\left\{\frac{F(t)}{t}\right\}, \tag{15.158}$$

provided that $F(t)/t$ is finite at $t = 0$ or diverges less strongly than t^{-1} [so that $\mathcal{L}\{F(t)/t\}$ will exist].

Limits of Integration—Unit Step Function

The actual limits of integration for the Laplace transform may be specified with the (Heaviside) unit step function

$$u(t-k) = \begin{cases} 0, & t < k \\ 1, & t \geq k. \end{cases}$$

For instance,

$$\mathcal{L}\{u(t-k)\} = \int_k^\infty e^{-st}dt = \frac{1}{s}e^{-ks}.$$

A rectangular pulse of width k and unit height is described by $F(t) = u(t) - u(t-k)$. Taking the Laplace transform, we obtain

$$\mathcal{L}\{u(t) - u(t-k)\} = \int_0^k e^{-st}\,dt = \frac{1}{s}(1 - e^{-ks}).$$

The unit step function is implicit in Eq. (15.144) and could also be invoked in Exercise 15.10.13.

EXERCISES

15.10.1 Solve Eq. (15.134), which describes a damped simple harmonic oscillator for $X(0) = X_0$, $X'(0) = 0$, and
(a) $b^2 = 4\,k\,m$ (critically damped),
(b) $b^2 > 4\,k\,m$ (overdamped).

ANS. (a) $X(t) = X_0 e^{-(b/2m)t}\left(1 + \dfrac{b}{2m}t\right)$.

15.10.2 Solve Eq. (15.134), which describes a damped simple harmonic oscillator for $X(0) = 0$, $X'(0) = v_0$, and
(a) $b^2 < 4\,k\,m$ (underdamped),
(b) $b^2 = 4\,k\,m$ (critically damped),

ANS. (a) $X(t) = \dfrac{v_0}{\omega_1}e^{-(b/2m)t}\sin\omega_1 t$,
(b) $X(t) = v_0 t e^{-(b/2m)t}$.

(c) $b^2 > 4\,k\,m$ (overdamped).

15.10.3 The motion of a body falling in a resisting medium may be described by

$$m\frac{d^2X(t)}{dt^2} = mg - b\frac{dX(t)}{dt}$$

when the retarding force is proportional to the velocity. Find $X(t)$ and $dX(t)/dt$ for the initial conditions

$$X(0) = \left.\frac{dX}{dt}\right|_{t=0} = 0.$$

15.10.4 With $J_0(t)$ expressed as a contour integral, apply the Laplace transform operation, reverse the order of integration, and thus show that

$$\mathcal{L}\{J_0(t)\} = (s^2+1)^{-1/2}, \quad \text{for } s > 0.$$

15.10.5 Develop the Laplace transform of $J_n(t)$ from $\mathcal{L}\{J_0(t)\}$ by using the Bessel function recurrence relations.
Hint. Here is a chance to use mathematical induction.

15.10.6 A calculation of the magnetic field of a circular current loop in circular cylindrical coordinates leads to the integral

$$\int_0^\infty e^{-kz} k J_1(ka) dk, \quad \Re(z) \geq 0.$$

Show that this integral is equal to $a/(z^2 + a^2)^{3/2}$.

15.10.7 Verify the following Laplace transforms:

(a) $\mathcal{L}\{j_0(at)\} = \mathcal{L}\left\{\dfrac{\sin at}{at}\right\} = \dfrac{1}{a}\cot^{-1}\left(\dfrac{s}{a}\right)$,

(b) $\mathcal{L}\{y_0(at)\}$ does not exist.

15.10.8 Develop a Laplace transform solution of Laguerre's ODE

$$tF''(t) + (1 - t)F'(t) + nF(t) = 0.$$

Note that you need a derivative of a transform and a transform of derivatives. Go as far as you can with n; then (and only then) set $n = 0$.

15.10.9 Show that the Laplace transform of the Laguerre polynomial $L_n(at)$ is given by

$$\mathcal{L}\{L_n(at)\} = \frac{(s - a)^n}{s^{n+1}}, \quad s > 0.$$

15.10.10 Show that

$$\mathcal{L}\{E_1(t)\} = \frac{1}{s}\ln(s + 1), \quad s > 0,$$

where

$$E_1(t) = \int_t^\infty \frac{e^{-\tau}}{\tau} d\tau = \int_1^\infty \frac{e^{-xt}}{x} dx.$$

$E_1(t)$ is the exponential–integral function.

15.10.11 (a) From Eq. (15.158) show that

$$\int_0^\infty f(x)dx = \int_0^\infty \frac{F(t)}{t} dt,$$

provided the integrals exist.

(b) From the preceding result show that

$$\int_0^\infty \frac{\sin t}{t} dt = \frac{\pi}{2},$$

in agreement with Eqs. (15.109) and (7.41).

15.10.12 (a) Show that

$$\mathcal{L}\left\{\frac{\sin kt}{t}\right\} = \cot^{-1}\left(\frac{s}{k}\right).$$

(b) Using this result (with $k = 1$), prove that

$$\mathcal{L}\{\text{si}(t)\} = -\frac{1}{s}\tan^{-1} s,$$

where

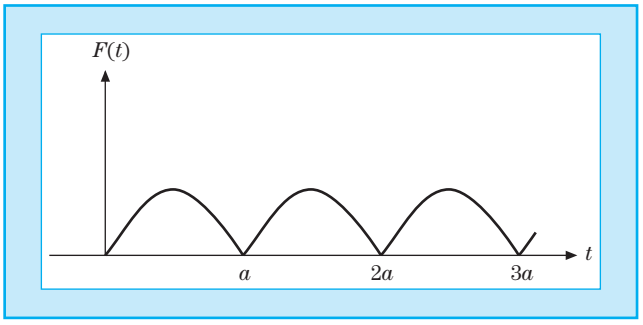
$$\text{si}(t) = -\int_t^\infty \frac{\sin x}{x}dx, \quad \text{the sine integral.}$$

15.10.13 If $F(t)$ is periodic (Fig. 15.13) with a period a so that $F(t+a) = F(t)$ for all $t \geq 0$, show that

$$\mathcal{L}\{F(t)\} = \frac{\int_0^a e^{-st}F(t)\,dt}{1 - e^{-as}},$$

with the integration now over only the **first period** of $F(t)$.

Figure 15.13
Periodic Function



15.10.14 Find the Laplace transform of the square wave (period a) defined by

$$F(t) = \begin{cases} 1, & 0 < t < a/2 \\ 0, & a/2 < t < a. \end{cases}$$

ANS. $f(s) = \dfrac{1}{s} \cdot \dfrac{1 - e^{-as/2}}{1 - e^{-as}}.$

15.10.15 Show that

(a) $\mathcal{L}\{\cosh at \cos at\} = \dfrac{s^3}{s^4 + 4a^4}$, (c) $\mathcal{L}\{\sinh at \cos at\} = \dfrac{as^2 - 2a^3}{s^4 + 4a^4}$,

(b) $\mathcal{L}\{\cosh at \sin at\} = \dfrac{as^2 + 2a^3}{s^4 + 4a^4}$, (d) $\mathcal{L}\{\sinh at \sin at\} = \dfrac{2a^2 s}{s^4 + 4a^4}$.

15.10.16 Show that

(a) $\mathcal{L}^{-1}\{(s^2 + a^2)^{-2}\} = \dfrac{1}{2a^3}\sin at - \dfrac{1}{2a^2}t\cos at,$

(b) $\mathcal{L}^{-1}\{s(s^2 + a^2)^{-2}\} = \dfrac{1}{2a}t\sin at,$

(c) $\mathcal{L}^{-1}\{s^2(s^2 + a^2)^{-2}\} = \dfrac{1}{2a}\sin at + \dfrac{1}{2}t\cos at,$

(d) $\mathcal{L}^{-1}\{s^3(s^2 + a^2)^{-2}\} = \cos at - \dfrac{a}{2}t\sin at.$

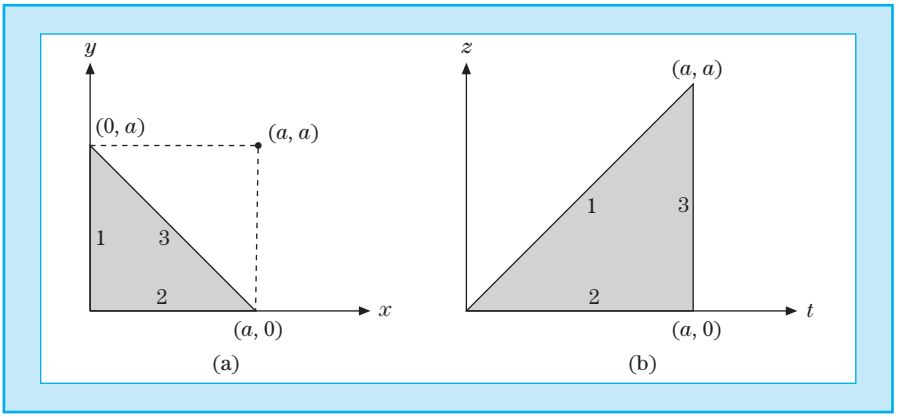


Figure 15.14

Change of Variables: (a) xy-Plane and (b) zt-Plane

15.11 Convolution or Faltungs Theorem

One of the most important properties of the Laplace transform is that given by the convolution or Faltungs theorem.[19] We take two transforms

$$f_1(s) = \mathcal{L}\{F_1(t)\} \quad \text{and} \quad f_2(s) = \mathcal{L}\{F_2(t)\} \tag{15.159}$$

and multiply them together. To avoid complications, when changing variables, we hold the upper limits finite:

$$f_1(s) \cdot f_2(s) = \lim_{a\to\infty} \int_0^a e^{-sx} F_1(x)\,dx \int_0^{a-x} e^{-sy} F_2(y)\,dy. \tag{15.160}$$

The upper limits are chosen so that the area of integration, shown in Fig. 15.14a, is the shaded triangle, not the square. Substituting $x = t - z$, $y = z$, the region of integration is mapped into the triangle, shown in Fig. 15.14b. If we integrate over a square in the xy-plane, we have a parallelogram in the tz-plane, which simply adds complications. This modification is permissible because the two integrands are assumed to decrease exponentially. In the limit $a \to \infty$, the integral over the unshaded triangle will give zero contribution. To verify the mapping, map the vertices: $t = x + y$, $z = y$. Using Jacobians to transform the element of area (Chapter 2), we have

$$dx\,dy = \begin{vmatrix} \dfrac{\partial x}{\partial t} & \dfrac{\partial y}{\partial t} \\ \dfrac{\partial x}{\partial z} & \dfrac{\partial y}{\partial z} \end{vmatrix} dt\,dz = \begin{vmatrix} 1 & 0 \\ -1 & 1 \end{vmatrix} dt\,dz \tag{15.161}$$

[19] An alternate derivation employs the Bromwich integral (Section 15.12). This is Exercise 15.12.3.

or $dx\,dy = dt\,dz$. With this substitution, Eq. (15.160) becomes

$$f_1(s)\cdot f_2(s) = \lim_{a\to\infty}\int_0^a e^{-st}\int_0^t F_1(t-z)F_2(z)dz\,dt$$
$$= \mathcal{L}\left\{\int_0^t F_1(t-z)F_2(z)dz\right\}. \tag{15.162}$$

For convenience this integral is represented by the symbol

$$\int_0^t F_1(t-z)F_2(z)dz \equiv F_1 * F_2, \tag{15.163}$$

and referred to as the **convolution**, closely analogous to the Fourier convolution (Section 15.6). If we interchange $f_1 \to f_2$ and $F_1 \to F_2$ (or replace $z \to t - z$), we find

$$F_1 * F_2 = F_2 * F_1, \tag{15.164}$$

showing that the relation is symmetric.

Carrying out the inverse transform, we also find

$$\mathcal{L}^{-1}\{f_1(s)\cdot f_2(s)\} = \int_0^t F_1(t-z)F_2(z)dz. \tag{15.165}$$

This can be useful in the development of new transforms or as an alternative to a partial fraction expansion. One immediate application is in the solution of integral equations. Since the upper limit t is variable, this Laplace convolution is useful in treating Volterra integral equations. The Fourier convolution with fixed (infinite) limits would apply to Fredholm integral equations.

EXAMPLE 15.11.1

Driven Oscillator with Damping As an illustration of the use of the convolution theorem, let us return to the mass m on a spring, with damping and a driving force $F(t)$. The equation of motion [Eq. (15.134)] now becomes

$$mX''(t) + bX'(t) + kX(t) = F(t). \tag{15.166}$$

Initial conditions $X(0) = 0$, $X'(0) = 0$ are used to simplify this illustration, and the transformed equation is

$$ms^2x(s) + bs\,x(s) + kx(s) = f(s) \tag{15.167}$$

or

$$x(s) = \frac{f(s)}{m}\cdot\frac{1}{(s+b/2m)^2+\omega_1^2}, \tag{15.168}$$

where $\omega_1^2 \equiv k/m - b^2/4m^2$, as before.

By the convolution theorem [Eq. (15.160) or Eq. (15.165)], and noting that

$$\frac{\omega_1}{(s+b/2m)^2+\omega_1^2} = \mathcal{L}(e^{-bt/2m}\sin\omega_1 t),$$

we have

$$X(t) = \frac{1}{m\omega_1}\int_0^t F(t-z)e^{-(b/2m)z}\sin\omega_1 z\,dz. \tag{15.169}$$

If the force is impulsive, $F(t) = P\delta(t)$,[20]

$$X(t) = \frac{P}{m\omega_1}e^{-(b/2m)t}\sin\omega_1 t. \tag{15.170}$$

P represents the momentum transferred by the impulse, and the constant P/m takes the place of an initial velocity $X'(0)$.

If $F(t) = F_0\sin\omega t$, Eq. (15.168) may be used, but a partial fraction expansion is perhaps more convenient. With

$$f(s) = \frac{F_0\omega}{s^2+\omega^2},$$

Eq. (15.168) becomes

$$\begin{aligned} x(s) &= \frac{F_0\omega}{m}\cdot\frac{1}{s^2+\omega^2}\cdot\frac{1}{(s+b/2m)^2+\omega_1^2} \\ &= \frac{F_0\omega}{m}\left[\frac{a's+b'}{s^2+\omega^2}+\frac{c's+d'}{(s+b/2m)^2+\omega_1^2}\right]. \end{aligned} \tag{15.171}$$

The coefficients a', b', c', and d' are independent of s. Direct calculation shows

$$\begin{aligned} -\frac{1}{a'} &= \frac{b}{m}\omega^2+\frac{m}{b}\left(\omega_0^2-\omega^2\right)^2, \\ -\frac{1}{b'} &= -\frac{m}{b}\left(\omega_0^2-\omega^2\right)\left[\frac{b}{m}\omega^2+\frac{m}{b}\left(\omega_0^2-\omega^2\right)^2\right]. \end{aligned}$$

Since the $c's+d'$ term will lead to exponentially decreasing terms (transients, as shown above the denominator is the Laplace transform of $e^{-bt/2m}\sin\omega_1 t$), they will be discarded here. Carrying out the inverse operation, we find for the steady-state solution

$$X(t) = \frac{F_0}{\left[b^2\omega^2+m^2\left(\omega_0^2-\omega^2\right)^2\right]^{1/2}}\sin(\omega t-\varphi), \tag{15.172}$$

where

$$\tan\varphi = \frac{b\omega}{m\left(\omega_0^2-\omega^2\right)}.$$

Differentiating the denominator, we find that the amplitude has a maximum when

$$\omega^2 = \omega_0^2-\frac{b^2}{2m^2} = \omega_1^2-\frac{b^2}{4m^2}. \tag{15.173}$$

[20]Note that $\delta(t)$ lies **inside** the interval $[0, t]$.

This is the resonance condition.[21] At resonance the amplitude becomes $F_0/b\omega_1$, showing that the mass m goes into infinite oscillation at resonance if damping is neglected ($b = 0$). It is worth noting that we have had three different characteristic frequencies: resonance for forced oscillations, with damping,

$$\omega_2^2 = \omega_0^2 - \frac{b^2}{2m^2};$$

free oscillation frequency, with damping,

$$\omega_1^2 = \omega_0^2 - \frac{b^2}{4m^2};$$

and free oscillation frequency, no damping,

$$\omega_0^2 = \frac{k}{m}.$$

They coincide only if the damping is zero ($b = 0$).

Returning to Eqs. (15.166) and (15.167), Eq. (15.167) is our ODE for the response of a dynamical system to an arbitrary driving force. The final response clearly depends on both the driving force and the characteristics of our system. This dual dependence is separated in the transform space. In Eq. (15.168) the transform of the response (output) appears as the product of two factors, one describing the driving force (input) and the other describing the dynamical system. This latter part, which modifies the input and yields the output, is often called a **transfer function**. Specifically, $[(s + b/2m)^2 + \omega_1^2]^{-1}$ is the transfer function corresponding to this damped oscillator. The concept of a transfer function is of great use in the field of servomechanisms. Often, the characteristics of a particular servomechanism are described by giving its transfer function. The convolution theorem then yields the output signal for a particular input signal. ■

EXERCISES

15.11.1 From the convolution theorem, show that

$$\frac{1}{s}f(s) = \mathcal{L}\left\{\int_0^t F(x)dx\right\},$$

where $f(s) = \mathcal{L}\{F(t)\}$.

15.11.2 Using the convolution integral, calculate

$$\mathcal{L}^{-1}\left\{\frac{s}{(s^2 + a^2)(s^2 + b^2)}\right\}, \quad a^2 \neq b^2.$$

15.11.3 An undamped oscillator is driven by a force $F_0 \sin \omega t$. Find the displacement as a function of time. Notice that it is a linear combination of two simple harmonic motions, one with the frequency of the driving

[21] The amplitude (squared) has the typical resonance denominator, the Lorentz line shape.

force and one with the frequency ω_0 of the free oscillator. (Assume $X(0) = X'(0) = 0$.)

$$ANS. \quad X(t) = \frac{F_0/m}{\omega^2 - \omega_0^2}\left(\frac{\omega}{\omega_0}\sin\omega_0 t - \sin\omega t\right).$$

15.12 Inverse Laplace Transform

Bromwich Integral

We now develop an expression for the inverse Laplace transform, $\mathcal{L}^{-1}$, appearing in the equation

$$F(t) = \mathcal{L}^{-1}\{f(s)\}. \tag{15.174}$$

One approach lies in the Fourier transform for which we know the inverse relation. There is a difficulty, however. Our Fourier transformable function had to satisfy the Dirichlet conditions. In particular, we required that

$$\lim_{\omega\to\infty} G(\omega) = 0 \tag{15.175}$$

so that the infinite integral would be well defined.[22] Now we wish to treat functions, $F(t)$, that may diverge exponentially. To surmount this difficulty, we extract an exponential factor, $e^{\gamma t}$, from our (possibly) divergent Laplace function and write

$$F(t) = e^{\gamma t}G(t). \tag{15.176}$$

If $F(t)$ diverges as $e^{\alpha t}$, we require γ to be greater than α so **that $G(t)$ will be convergent**. Now, with $G(t) = 0$ for $t < 0$ and otherwise suitably restricted so that it may be represented by a Fourier transform [Eq. (15.20)],

$$G(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{iut}du\int_0^{\infty} G(v)e^{-iuv}dv. \tag{15.177}$$

Using Eq. (15.177), we may rewrite Eq. (15.176) as

$$F(t) = \frac{e^{\gamma t}}{2\pi}\int_{-\infty}^{\infty} e^{iut}du\int_0^{\infty} F(v)e^{-\gamma v}e^{-iuv}dv. \tag{15.178}$$

Now with the change of variable,

$$s = \gamma + iu, \tag{15.179}$$

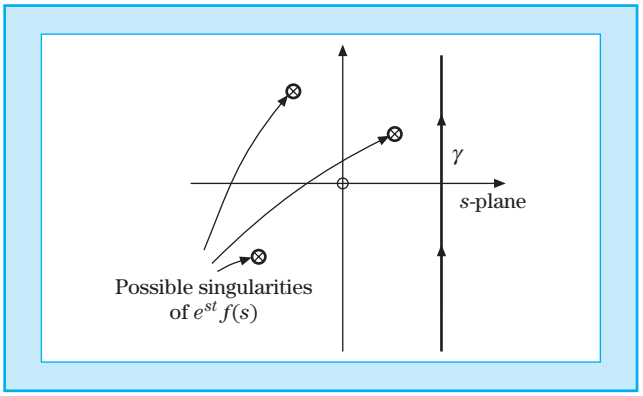
the integral over v is cast into the form of a Laplace transform

$$\int_0^{\infty} F(v)e^{-sv}dv = f(s); \tag{15.180}$$

[22] If delta functions are included, $G(\omega)$ may be a cosine. Although this does not satisfy Eq. (15.175), $G(\omega)$ is still bounded.

Figure 15.15

Singularities of $e^{st}f(s)$



s is now a complex variable and $\Re(s) \geq \gamma$ to guarantee convergence. Notice that the Laplace transform has mapped a function specified on the positive real axis onto the complex plane, $\Re(s) \geq \gamma$. [23]

Because γ is a constant, $ds = idu$. Substituting Eq. (15.180) into Eq. (15.178), we obtain

$$F(t) = \frac{1}{2\pi i}\int_{\gamma-i\infty}^{\gamma+i\infty} e^{st}f(s)ds. \tag{15.181}$$

Here is our **inverse transform**. We have rotated the line of integration through 90° (by using $ds = idu$). The path has become an infinite vertical line in the complex plane, the constant γ having been chosen so that all the singularities of $f(s)$ are to the left of the line $\gamma + is$ (Fig. 15.15).

Equation (15.181), our inverse transformation, is usually known as the Bromwich integral, although sometimes it is referred to as the Fourier–Mellin theorem or Fourier–Mellin integral. This integral may now be evaluated by the regular methods of contour integration (Chapter 7), if there are no branch cuts—that is, f is a single-valued analytic function. If $t > 0$, the contour may be closed by an infinite semicircle in the left half-plane, provided the integral over this semicircle is negligible. Then, by the residue theorem (Section 7.2),

$$F(t) = \Sigma(\text{residues included for } \Re(s) < \gamma). \tag{15.182}$$

Possibly, this means of evaluation, with $\Re(s)$ ranging through negative values, seems paradoxical in view of our previous requirement that $\Re(s) \geq \gamma$. The paradox disappears when we recall that the requirement $\Re(s) \geq \gamma$ was imposed to guarantee convergence of the Laplace transform integral that defined $f(s)$. Once $f(s)$ is obtained, we may proceed to exploit its properties as

[23] For a derivation of the inverse Laplace transform using only real variables, see C. L. Bohn and R. W. Flynn, Real variable inversion of Laplace transforms: An application in plasma physics. *Am. J. Phys.* **46**, 1250 (1978).

an analytical function in the complex plane wherever we choose.[24] In effect, we are employing analytic continuation to get $\mathcal{L}\{F(t)\}$ in the left half-plane exactly as the recurrence relation for the factorial function was used to extend the Euler integral definition [Eq. (10.5)] to the left half-plane.

Perhaps two examples may clarify the evaluation of Eq. (15.182).

EXAMPLE 15.12.1 **Inversion via Calculus of Residues** If $f(s) = a/(s^2 - a^2)$, then

$$e^{st} f(s) = \frac{ae^{st}}{s^2 - a^2} = \frac{ae^{st}}{(s + a)(s - a)}. \tag{15.183}$$

The residues may be found by using Exercise 7.1.1 or various other means. The first step is to identify the singularities, the poles. Here, we have one simple pole at $s = a$ and another simple pole at $s = -a$. By Exercise 7.1.1, the residue at $s = a$ is $(\frac{1}{2})e^{at}$ and the residue at $s = -a$ is $(-\frac{1}{2})e^{-at}$. Then

$$\text{Residues} = \left(\frac{1}{2}\right)(e^{at} - e^{-at}) = \sinh at = F(t), \tag{15.184}$$

in agreement with Eq. (15.94). ■

EXAMPLE 15.12.2 **Another Inversion** If

$$f(s) = \frac{1 - e^{-as}}{s}, \quad a > 0,$$

then $e^{s(t-a)}$ grows exponentially for $t < a$ on the semicircle in the left-hand s-plane so that contour integration and the residue theorem are not applicable. However, we can evaluate the integral explicitly as follows. We let $\gamma \to 0$ and substitute $s = iy$ so that

$$F(t) = \frac{1}{2\pi i}\int_{\gamma - i\infty}^{\gamma + i\infty} e^{st} f(s) = \frac{1}{2\pi}\int_{-\infty}^{\infty} [e^{iyt} - e^{it(t-a)}]\frac{dy}{y}. \tag{15.185}$$

Using the Euler identity, only the sines survive that are odd in y, and we obtain

$$F(t) = \frac{1}{\pi}\int_{-\infty}^{\infty}\left[\frac{\sin ty}{y} - \frac{\sin(t - a)y}{y}\right]. \tag{15.186}$$

If $k > 0$, $\int_0^\infty \frac{\sin ky}{y} dy$ gives $\pi/2$ and $-\pi/2$ if $k < 0$. As a consequence, $F(t) = 0$ if $t > a > 0$ and if $t < 0$. If $0 < t < a$, then $F(t) = 1$. This can be written compactly in terms of the Heaviside unit step function $u(t)$ as follows:

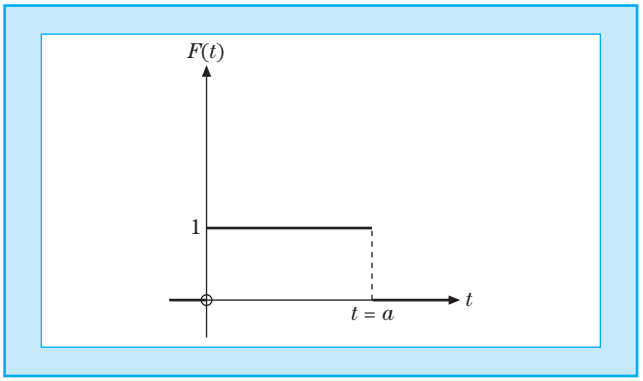
$$F(t) = u(t) - u(t - a) = \begin{cases} 0, & t < 0, \\ 1, & 0 < t < a, \\ 0, & t > a. \end{cases} \tag{15.187}$$

Thus, $F(t)$ is a step function of unit height and length a (Fig. 15.16). ■

[24] In numerical work, $f(s)$ may well be available only for discrete real, positive values of s. Then numerical procedures are indicated. See Section 15.8 and the Krylov and Skoblya reference in Additional Reading.

Figure 15.16

Finite-Length Step Function $u(t) - u(t-a)$



Two general comments are in order. First, these two examples hardly begin to show the usefulness and power of the Bromwich integral. It is always available for inverting a complicated transform, when the tables prove inadequate.

Second, this derivation is not presented as a rigorous one. Rather, it is given more as a plausibility argument, although it can be made rigorous. The determination of the inverse transform is similar to the solution of a differential equation. It makes little difference how you get the solution. Guess at it if you want. The solution can always be checked by substitution back into the original differential equation. Similarly, $F(t)$ can (and, to check for careless errors, should) be checked by determining whether by Eq. (15.88)

$$\mathcal{L}\{F(t)\} = f(s).$$

Two alternate derivations of the Bromwich integral are the subjects of Exercises 15.12.1 and 15.12.2.

As a final illustration of the use of the Laplace inverse transform, we discuss some results from the work of Brillouin and Sommerfeld (1914) in electromagnetic theory.

EXAMPLE 15.12.3

Velocity of Electromagnetic Waves in a Dispersive Medium The **group velocity** u of traveling waves is related to the phase velocity v by the equation

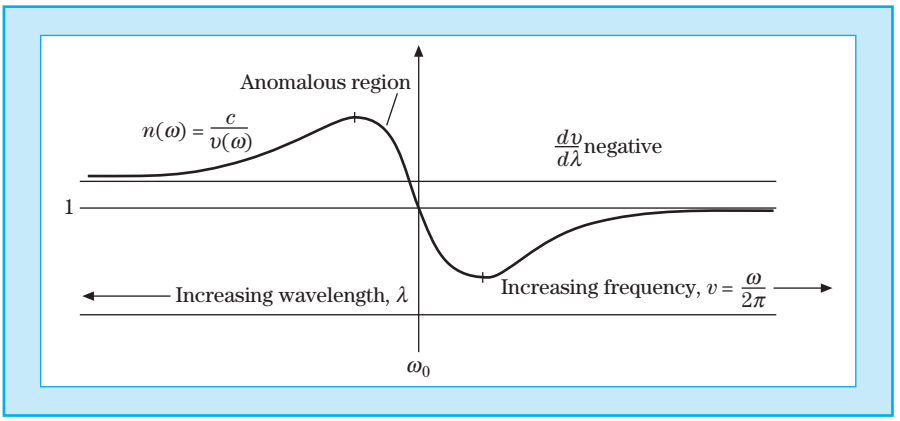
$$u = v - \lambda \frac{dv}{d\lambda}, \tag{15.188}$$

where λ is the wavelength. In the vicinity of an absorption line (resonance) $dv/d\lambda$ may be sufficiently negative so that $u > c$ (Fig. 15.17). The question immediately arises whether a signal can be transmitted faster than c, the velocity of light in vacuum. This question, which assumes that such a group velocity is meaningful, is of fundamental importance to the theory of special relativity. We need a solution to the wave equation

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{1}{v^2} \frac{\partial^2 \psi}{\partial t^2}, \tag{15.189}$$

Figure 15.17

Optical Dispersion



corresponding to a harmonic vibration starting at the origin at time zero. Our medium is **dispersive**, meaning that v is a function of the angular frequency. Imagine, for instance, a plane wave, angular frequency ω, incident on a shutter at the origin. At $t = 0$ the shutter is (instantaneously) opened, and the wave is permitted to advance along the positive x-axis.

Let us then build up a solution starting at $x = 0$. It is convenient to use the Cauchy integral formula [Eq. (6.37)],

$$\psi(0, t) = \frac{1}{2\pi i} \oint \frac{e^{-izt}}{z - z_0} dz = e^{-iz_0 t}$$

(for a contour encircling $z = z_0$ in the positive sense). Using $s = -iz$ and $z_0 = \omega$, we obtain

$$\psi(0, t) = \frac{1}{2\pi i} \int_{\gamma - i\infty}^{\gamma + i\infty} \frac{e^{st}}{s + i\omega} ds = \begin{cases} 0, & t < 0, \\ e^{-i\omega t}, & t > 0. \end{cases} \tag{15.190}$$

To be complete, the loop integral is along the vertical line $\Re(s) = \gamma$ **and** an infinite semicircle as shown in Fig. 15.18. The location of the infinite semicircle is chosen so that the integral over it vanishes. This means a semicircle in the left half-plane for $t > 0$ and the residue is enclosed. For $t < 0$ we choose the right half-plane and no singularity is enclosed. The fact that this is the Bromwich integral may be verified by noting that

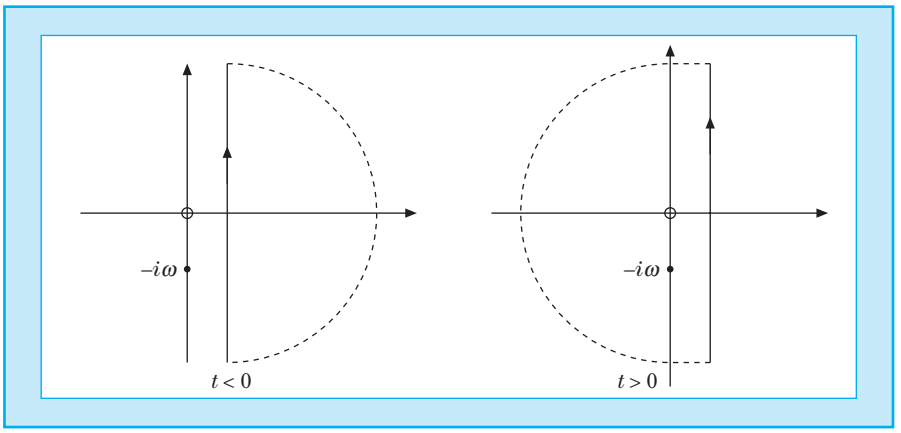
$$F(t) = \begin{cases} 0, & t < 0, \\ e^{-i\omega t}, & t > 0 \end{cases} \tag{15.191}$$

and applying the Laplace transform. The transformed function $f(s)$ becomes

$$f(s) = \frac{1}{s + i\omega}. \tag{15.192}$$

Figure 15.18

Possible Closed Contours



Our Cauchy–Bromwich integral provides us with the time dependence of a signal leaving the origin at $t = 0$. To include the space dependence, we note that

$$e^{s(t-x/v)}$$

satisfies the wave equation. With this as a clue, we replace t by $t - x/v$ and write a solution

$$\psi(x, t) = \frac{1}{2\pi i} \int_{\gamma-i\infty}^{\gamma+i\infty} \frac{e^{s(t-x/v)}}{s + i\omega} ds. \tag{15.193}$$

It was seen in the derivation of the Bromwich integral that our variable s replaces the ω of the Fourier transformation. Hence, the wave velocity v becomes a function of s, that is, $v(s)$. Its particular form need not concern us here. We need only the property

$$\lim_{|s|\to\infty} v(s) = c, \text{ constant.} \tag{15.194}$$

This is suggested by the asymptotic behavior of the curve on the right side of Fig. 15.17.[25]

Evaluating Eq. (15.193) by the calculus of residues, we may close the path of integration by a semicircle in the right half-plane, provided

$$t - \frac{x}{c} < 0.$$

Hence,

$$\psi(x, t) = 0, \qquad t - \frac{x}{c} < 0, \tag{15.195}$$

[25]Equation (15.193) follows rigorously from the theory of anomalous dispersion and the Kronig–Kramers optical dispersion relations.

Table 15.1 Laplace Transform Operations

	Operations	Equation No.
Laplace transform	$f(s) = \mathcal{L}\{F(t)\} = \int_0^\infty e^{-st} F(t)\, dt$	(15.88)
Transform of derivative	$sf(s) - F(+0) = \mathcal{L}\{F'(t)\}$	(15.110)
	$s^2 f(s) - sF(+0) - F'(+0) = \mathcal{L}\{F''(t)\}$	(15.111)
Transform of integral	$\frac{1}{s} f(s) = \mathcal{L}\left\{ \int_0^t F(x)dx \right\}$	Exercise 15.11.1
Substitution	$f(s-a) = \mathcal{L}\{e^{at} F(t)\}$	(15.131)
Translation	$e^{-bs} f(s) = \mathcal{L}\{F(t-b)u(t-b)\}$	(15.145)
Derivative of transform	$f^{(n)}(s) = \mathcal{L}\{(-t)^n F(t)\}$	(15.153)
Integral of transform	$\int_s^\infty f(x)\, dx = \mathcal{L}\left\{ \frac{F(t)}{t} \right\}$	(15.158)
Convolution	$f_1(s) f_2(s) = \mathcal{L}\left\{ \int_0^t F_1(t-z) F_2(z)\, dz \right\}$	(15.162)
Inverse transform, Bromwich integral	$\frac{1}{2\pi i} \int_{\gamma - i\infty}^{\gamma + i\infty} e^{st} f(s)\, ds = F(t)$	(15.181)

which means that the velocity of our signal cannot exceed the velocity of light in vacuum c. This simple but very significant result was extended by Sommerfeld and Brillouin to show just how the wave advanced in the dispersive medium. ■

Summary: Inversion of Laplace Transform

- Direct use of tables and references; use of partial fractions (Section 15.8) and the operational theorems of Table 15.1.
- Bromwich integral [Eq. (15.181)] and the calculus of residues.
- Numerical inversion (Section 15.8) and references.

EXERCISES

15.12.1 Derive the Bromwich integral from Cauchy's integral formula.
Hint. Apply the inverse transform $\mathcal{L}^{-1}$ to

$$f(s) = \frac{1}{2\pi i} \lim_{\alpha \to \infty} \int_{\gamma - i\alpha}^{\gamma + i\alpha} \frac{f(z)}{s - z} dz,$$

where $f(z)$ is analytic for $\Re(z) \geq \gamma$.

15.12.2 Starting with

$$\frac{1}{2\pi i} \int_{\gamma - i\infty}^{\gamma + i\infty} e^{st} f(s) ds,$$

show that by introducing

$$f(s) = \int_0^\infty e^{-sz} F(z) dz,$$

we can convert one integral into the Fourier representation of a Dirac delta function. From this, derive the inverse Laplace transform.

15.12.3 Derive the Laplace transformation convolution theorem by use of the Bromwich integral.

15.12.4 Find

$$\mathcal{L}^{-1}\left\{\frac{s}{s^2-k^2}\right\}$$

(a) by a partial fraction expansion,
(b) repeat using the Bromwich integral.

15.12.5 Find

$$\mathcal{L}^{-1}\left\{\frac{k^2}{s(s^2+k^2)}\right\}$$

(a) by using a partial fraction expansion,
(b) repeat using the convolution theorem,
(c) repeat using the Bromwich integral.

ANS. $F(t) = 1 - \cos kt$.

15.12.6 Use the Bromwich integral to find the function whose transform is $f(s) = s^{-1/2}$. Note that $f(s)$ has a branch point at $s = 0$. The negative x-axis may be taken as a cut line.

ANS. $F(t) = (\pi t)^{-1/2}$.

15.12.7 Evaluate the inverse Laplace transform

$$\mathcal{L}^{-1}\left\{(s^2-a^2)^{-1/2}\right\}$$

by each of the following methods:
(a) Expansion in a series and term-by-term inversion.
(b) Direct evaluation of the Bromwich integral.
(c) Change of variable in the Bromwich integral: $s = (a/2)(z + z^{-1})$.

15.12.8 Show that

$$\mathcal{L}^{-1}\left\{\frac{\ln s}{s}\right\} = -\ln t - \gamma,$$

where $\gamma = 0.5772\ldots$, the Euler–Mascheroni constant.

15.12.9 Evaluate the Bromwich integral for

$$f(s) = \frac{s}{(s^2+a^2)^2}.$$

15.12.10 Heaviside expansion theorem. If the transform $f(s)$ may be written as a ratio

$$f(s) = \frac{g(s)}{h(s)},$$

where $g(s)$ and $h(s)$ are analytic functions, with $h(s)$ having simple, isolated zeros at $s = s_i$, show that

$$F(t) = \mathcal{L}^{-1}\left\{\frac{g(s)}{h(s)}\right\} = \sum_i \frac{g(s_i)}{h'(s_i)} e^{s_i t}.$$

Hint. See Exercise 7.1.2.

15.12.11 Using the Bromwich integral, invert $f(s) = s^{-2}e^{-ks}$. Express $F(t) = \mathcal{L}^{-1}\{f(s)\}$ in terms of the (shifted) unit step function $u(t-k)$.

ANS. $F(t) = (t-k)u(t-k)$.

15.12.12 You have the following Laplace transform:

$$f(s) = \frac{1}{(s+a)(s+b)}, \quad a \neq b.$$

Invert this transform by each of three methods:
(a) partial fractions and use of tables;
(b) convolution theorem; and
(c) Bromwich integral.

ANS. $F(t) = \dfrac{e^{-bt} - e^{-at}}{a-b}, \quad a \neq b.$

Additional Reading

Champeney, D. C. (1973). *Fourier Transforms and Their Physical Applications.* Academic Press, New York. Fourier transforms are developed in a careful, easy to follow manner. Approximately 60% of the book is devoted to applications of interest in physics and engineering.

Erdelyi, A., Magnus, W., Oberhettinger, F., and Tricomi, F. G. (1954). *Tables of Integral Transforms.* McGraw-Hill, New York. This text contains extensive tables of Fourier sine, cosine, and exponential transforms, Laplace and inverse Laplace transforms, Mellin and inverse Mellin transforms, Hankel transforms, and other more specialized integral transforms.

Hanna, J. R. (1990). *Fourier Series and Integrals of Boundary Value Problems.* Wiley, Somerset, NJ. This book is a broad treatment of the Fourier solution of boundary value problems. The concepts of convergence and completeness are given careful attention.

Jeffreys, H., and Jeffreys, B. S. (1972). *Methods of Mathematical Physics*, 3rd ed. Cambridge Univ. Press, Cambridge, UK.

Krylov, V. I., and Skoblya, N. S. (1969). *Handbook of Numerical Inversion of Laplace Transform.* Israel Program for Scientific Translations, Jerusalem.

Lepage, W. R. (1961). *Complex Variables and the Laplace Transform for Engineers.* McGraw-Hill, New York. Reprinted, Dover, New York (1980). A complex variable analysis which is carefully developed and then applied to Fourier and Laplace transforms. It is written to be read by students, but it is intended for the serious student.

McCollum, P. A., and Brown, B. F. (1965). *Laplace Transform Tables and Theorems.* Holt, Rinehart and Winston, New York.

Miles, J. W. (1971). *Integral Transforms in Applied Mathematics*. Cambridge Univ. Press, Cambridge, UK. This is a brief but interesting and useful treatment for the advanced undergraduate. It emphasizes applications rather than abstract mathematical theory.

Papoulis, A. (1962). *The Fourier Integral and Its Applications*. McGraw-Hill, New York. This is a rigorous development of Fourier and Laplace transforms and has extensive applications in science and engineering.

Roberts, G. E., and Kaufman, H. (1966). *Table of Laplace Transforms*. Saunders, Philadelphia.

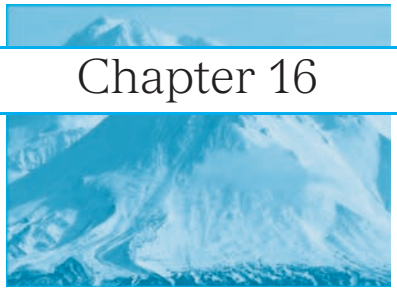
Sneddon, I. N. (1951). *Fourier Transforms*. McGraw-Hill, New York. Reprinted, Dover, New York (1995). A detailed comprehensive treatment, this book is loaded with applications to a wide variety of fields of modern and classical physics.

Sneddon, I. H. (1972). *The Use of Integral Transforms*. McGraw-Hill, New York. Written for students in science and engineering in terms they can understand, this book covers all the integral transforms mentioned in this chapter as well as in several others. Many applications are included.

Van der Pol, B., and Bremmer, H. (1987). *Operational Calculus Based on the Two-Sided Laplace Integral*, 3rd ed. Cambridge Univ. Press, Cambridge, UK. Here is a development based on the integral range $-\infty$ to $+\infty$, rather than the useful 0 to ∞. Chapter 5 contains a detailed study of the Dirac delta function (impulse function).

Wolf, K. B. (1979). *Integral Transforms in Science and Engineering*. Plenum, New York. This book is a very comprehensive treatment of integral transforms and their applications.

Titchmarsh, E. C. (1937). *Introduction to the Theory of Fourier Integrals*, 2nd ed. Oxford Univ. Press, New York.



Chapter 16

Partial Differential Equations

16.1 Examples of Partial Differential Equations and Boundary Conditions

Let us continue our discussion of partial differential equations (PDEs) by mentioning examples of PDEs in physics. Among the most frequently encountered PDEs are the following:

1. Laplace's equation, $\nabla^2\psi(\mathbf{r}) = 0$.
   This very common and very important equation occurs in studies of
   a. electromagnetic phenomena, including electrostatics in regions containing no electric charges, dielectrics, steady currents, and magnetostatics;
   b. hydrodynamics (irrotational flow of perfect fluids and surface waves);
   c. heat flow and diffusion; and
   d. gravitation in regions containing no masses.
2. Poisson's equation, $\nabla^2\psi(\mathbf{r}) = -\rho/\varepsilon_0$.
   In contrast to the homogeneous Laplace equation, Poisson's equation is nonhomogeneous, with a source term $-\rho(\mathbf{r})/\varepsilon_0$ in electrostatics and (with $\epsilon_0 \to 1$) in Newtonian gravity.
3. The wave (Helmholtz) and time-independent diffusion equations, $\nabla^2\psi(\mathbf{r}) \pm k^2\psi = 0$.
   These equations also appear in such diverse phenomena as
   a. elastic waves in solids, including vibrating strings, bars, and membranes;
   b. sound or acoustics;
   c. electromagnetic waves; and
   d. nuclear reactors.

4. The diffusion or heat flow equation
$$\nabla^2\psi(t,\mathbf{r}) = \frac{1}{a^2}\frac{\partial\psi}{\partial t}.$$
5. The corresponding four-dimensional form in the time-dependent wave equation of electrodynamics involving the d'Alembertian, a four-dimensional analog of the Laplacian in Minkowski space (Chapters 2 and 4),
$$\partial^\mu\partial_\mu\varphi(x) = \partial^2\varphi = \left[\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \nabla^2\right]\varphi = 0.$$
6. The time-dependent scalar potential equation, $\partial^2\psi(x) = \rho/\varepsilon_0$.
Like Poisson's equation, this equation occurs in electrodynamics and is nonhomogeneous with a source term ρ/ε_0.
7. The Klein–Gordon equation, $\partial^2\psi(x) = -\mu^2\psi(x)$ for mass μ, and the corresponding vector equations in which the scalar function ψ is replaced by a vector field. Other more complicated forms are common.
8. The Schrödinger wave equation,
$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = i\hbar\frac{\partial\psi}{\partial t}$$
and, for the time-independent case,
$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi.$$
9. The equations for elastic waves and viscous fluids and the telegraphy equation containing the operators ∇^2, $\partial^2/\partial t^2$, and $\partial/\partial t$.
10. Maxwell's coupled partial differential equations for electric and magnetic fields and Dirac's equation for relativistic electron wave functions. For Maxwell's equations, see Section 1.8.

Some general techniques for solving second-order PDEs were discussed in Chapter 8 and are further discussed in this chapter:

1. Separation of variables (Section 8.9), where the PDE is split into ordinary differential equations (ODEs) that are related by common constants that appear as eigenvalues of linear operators, $\mathcal{L}\psi = l\psi$, usually in one variable. This method is closely related to **symmetries of the PDE and a group of transformations** (see Section 4.2). The Helmholtz equation, given as example 3 above, has this form, where the constant k^2 may arise by separation of the time t from the spatial variables. Likewise, in example 8, the energy E is an eigenvalue that arises in the separation of t from $\mathbf{r}$ in the Schrödinger equation. The resulting separated ODEs are discussed in Chapter 9 in greater detail.
2. Conversion of a PDE into an integral equation using **Green's functions** applies to **inhomogeneous** PDEs, such as examples 2 and 7 given previously. An introduction to the Green's function technique is given in Section 16.3.

3. Other analytical methods, such as the use of integral transforms, are developed and applied in Chapter 15.
4. Numerical calculations: The development of computers has opened up a wealth of possibilities based on the calculus of finite differences.[1]

Occasionally, we encounter equations of higher order. In both the theory of the slow motion of a viscous fluid and the theory of an elastic body, we find the equation

$$(\nabla^2)^2\psi = 0.$$

These higher order differential equations are rare and so are not discussed here.

Although not frequently encountered, and perhaps not as important as second-order ODEs, first-order ODEs do appear in theoretical physics and are sometimes intermediate steps for second-order ODEs. The solutions of some more important types of first-order ODEs are developed in Section 8.2. First-order PDEs can always be reduced to ODEs. This is a straightforward but lengthy process.

Boundary Conditions

Usually, when we know the state of a physical system at some time and the law governing its evolution, then we are able to predict its outcome. Such initial conditions are the most common boundary conditions associated with ODEs and PDEs. Problems in which one is finding solutions that match given points, curves, or surfaces are referred to as boundary value problems. Eigenfunctions are usually required to satisfy most boundary conditions. These boundary conditions may take three forms:

- Cauchy boundary conditions: The value of a function and its normal derivative are specified on the boundary. In electrostatics, this would mean φ, the potential, and E_n, the normal component of the electric field.
- Dirichlet boundary conditions: The value of a function is specified on the boundary.
- Neumann boundary conditions: The normal derivative (normal gradient) of a function is specified on the boundary. In the electrostatic case, this would be E_n, and therefore σ, the surface charge density.

A summary of the relation of these three types of boundary conditions to the three types of two-dimensional PDEs is given in Table 16.1. For extended discussions of these PDEs, consult Sommerfeld (Chapter 2) or Morse and Feshbach (Chapter 6) and R. Courant and D. Hilbert, *Methods of Mathematical Physics* (Interscience, New York, 1989) (see also Additional Reading).

Parts of Table 16.1 are simply a matter of maintaining internal consistency or common sense. For instance, for Poisson's equation with a closed surface,

[1]For further details of numerical computation, see R. W. Hamming's *Numerical Methods for Scientists and Engineers* (McGraw-Hill, New York, 1973) and proceed to specialized references.

Table 16.1

Boundary condition	TYPE OF PDE Elliptic	Hyperbolic	Parabolic
	Laplace, Poisson in (x, y)	Wave equation in (x, t)	Diffusion equation in (x, t)
Cauchy			
Open surface	Unphysical results (instability)	**Unique, stable solution**	Too restrictive
Closed surface	Too restrictive	Too restrictive	Too restrictive
Dirichlet			
Open surface	Insufficient	Insufficient	**Unique, stable solution**
Closed surface	**Unique, stable solution**	Solution not unique	Too restrictive
Neumann			
Open surface	Insufficient	Insufficient	**Unique, stable solution**
Closed surface	**Unique, stable solution**	Solution not unique	Too restrictive

Table 16.2

Solutions in Spherical Polar Coordinates[a]

$$\psi = \sum_{l,\,m} a_{lm}\psi_{lm}$$

$$\nabla^2\psi = 0 \quad \psi_{lm} = \begin{Bmatrix} r^l \\ r^{-l-1} \end{Bmatrix} \begin{Bmatrix} P_l^m(\cos\theta) \\ Q_l^m(\cos\theta) \end{Bmatrix} \begin{Bmatrix} \cos m\varphi \\ \sin m\varphi \end{Bmatrix}^b$$

$$\nabla^2\psi + k^2\psi = 0 \quad \psi_{lm} = \begin{Bmatrix} j_l(kr) \\ y_l(kr) \end{Bmatrix} \begin{Bmatrix} P_l^m(\cos\theta) \\ Q_l^m(\cos\theta) \end{Bmatrix} \begin{Bmatrix} \cos m\varphi \\ \sin m\varphi \end{Bmatrix}^b$$

$$\nabla^2\psi - k^2\psi = 0 \quad \psi_{lm} = \begin{Bmatrix} i_l(kr) \\ k_l(kr) \end{Bmatrix} \begin{Bmatrix} P_l^m(\cos\theta) \\ Q_l^m(\cos\theta) \end{Bmatrix} \begin{Bmatrix} \cos m\varphi \\ \sin m\varphi \end{Bmatrix}^b$$

[a] References for some of the functions are $P_l^m(\cos\theta)$, $m = 0$, Section 11.1; $m \neq 0$, Section 11.5; $Q_l^m(\cos\theta)$, irregular Legendre solution; $j_l(kr)$, $y_l(kr)$, $i_l(kr) \equiv i^{-l} j_l(ix)$, and $k_l(kr) \equiv -i^l h_l^{(1)}(ix)$.
[b] $\cos m\varphi$ and $\sin m\varphi$ may be replaced by $e^{\pm i m\varphi}$.

Dirichlet conditions lead to a unique, stable solution. Neumann conditions likewise lead to a unique, stable solution independent of the Dirichlet solution. Therefore, Cauchy boundary conditions (meaning Dirichlet plus Neumann) could lead to an inconsistency.

The term boundary conditions includes the concept of initial conditions. For instance, specifying the initial position x_0 and the initial velocity v_0 in some dynamical problem would correspond to the Cauchy boundary conditions. The only difference in the present usage of boundary conditions in these one-dimensional problems is that we are going to apply the conditions on **both** ends of the allowed range of the variable.

For convenient reference, the forms of the solutions of Laplace's equation, Helmholtz's equation, and the diffusion equation for spherical polar coordinates are shown in Table 16.2. The solutions of Laplace's equation in circular cylindrical coordinates are presented in Table 16.3.

Table 16.3

Solutions in Circular Cylindrical Coordinates[a]

$$\psi = \sum_{m,\alpha} a_{m\alpha}\psi_{m\alpha}, \qquad \nabla^2\psi = 0$$

$$\psi_{m\alpha} = \left\{\begin{matrix} J_m(\alpha\rho) \\ Y_m(\alpha\rho)\end{matrix}\right\}\left\{\begin{matrix}\cos m\varphi \\ \sin m\varphi\end{matrix}\right\}\left\{\begin{matrix} e^{-\alpha z} \\ e^{\alpha z}\end{matrix}\right\}$$

$$\psi_{m\alpha} = \left\{\begin{matrix} I_m(\alpha\rho) \\ K_m(\alpha\rho)\end{matrix}\right\}\left\{\begin{matrix}\cos m\varphi \\ \sin m\varphi\end{matrix}\right\}\left\{\begin{matrix}\cos \alpha z \\ \sin \alpha z\end{matrix}\right\}$$

If $\alpha = 0$ (no z-dependence) $\psi_m = \left\{\begin{matrix} \rho^m \\ \rho^{-m}\end{matrix}\right\}\left\{\begin{matrix}\cos m\varphi \\ \sin m\varphi\end{matrix}\right\}$

[a] References for the radial functions are $J_m(\alpha\rho)$, Section 12.1; $Y_m(\alpha\rho)$, Section 12.2; $I_m(\alpha\rho) \equiv i^{-m}J_m(ix)$ and $K_m(\alpha\rho) \equiv \pi/2i^{m+1}H_m^{(1)}(ix)$.

For the Helmholtz and the diffusion equation (see Section 16.2) the constant $\pm k^2$ is added to the separation constant $\pm\alpha^2$ to define a new parameter γ^2 or $-\gamma^2$. For the choice $+\gamma^2$ (with $\gamma^2 > 0$), we get Bessel functions $J_m(\gamma\rho)$ and $Y_m(\gamma\rho)$. For the choice $-\gamma^2$ (with $\gamma^2 > 0$), we get modified Bessel functions $I_m(\gamma\rho)$ and $K_m(\gamma\rho)$.

These ODEs and two generalizations of them will be examined and systematized in the following sections. General properties following from the form of the differential equations are discussed in Chapter 9. The individual solutions are developed and applied in Chapters 11–13.

The practicing physicist will probably meet other second-order ODEs, some of which may possibly be transformed into the examples studied here. Some of these ODEs may be solved by the techniques of Sections 8.5 and 8.6. Others may require a computer for a numerical solution.

16.2 Heat Flow or Diffusion PDE

Here, we address the full time-dependent diffusion PDE for an isotropic medium. Assuming isotropy is actually not much of a restriction because, in case we have different (constant) rates of diffusion in different directions (e.g., in wood), our heat flow PDE takes the form

$$\frac{\partial\psi}{\partial t} = a^2\frac{\partial^2\psi}{\partial x^2} + b^2\frac{\partial^2\psi}{\partial y^2} + c^2\frac{\partial^2\psi}{\partial z^2} \tag{16.1}$$

if we put the coordinate axes along the principal directions of anisotropy. Now we simply rescale the coordinates using the substitutions $x = a\xi$, $y = b\eta$, $z = c\zeta$ to get back the original isotropic form of Eq. (16.1),

$$\frac{\partial\Phi}{\partial t} = \frac{\partial^2\Phi}{\partial\xi^2} + \frac{\partial^2\Phi}{\partial\eta^2} + \frac{\partial^2\Phi}{\partial\zeta^2} \tag{16.2}$$

for the temperature distribution function $\Phi(\xi, \eta, \zeta, t) = \psi(\frac{x}{a}, \frac{y}{b}, \frac{z}{c}, t)$.

For simplicity, we first solve the time-dependent PDE for a homogeneous one-dimensional medium, for example, a long metal rod in the x-direction:

$$\frac{\partial \psi}{\partial t} = a^2 \frac{\partial^2 \psi}{\partial x^2}, \tag{16.3}$$

where the constant a measures the diffusivity or heat conductivity of the medium. We attempt to solve this linear PDE with constant coefficients with the relevant **exponential product ansatz** $\psi = e^{\alpha x} \cdot e^{\beta t}$, which, when substituted into Eq. (16.3), solves the PDE with the constraint $\beta = a^2\alpha^2$ for the parameters. We seek exponentially decaying solutions for large times, that is, solutions with negative β values, and therefore set $\alpha = i\omega$, $\alpha^2 = -\omega^2$ for real ω and have

$$\psi = e^{i\omega x} e^{-\omega^2 a^2 t} = (\cos \omega x + i \sin \omega x) e^{-\omega^2 a^2 t}.$$

Forming real linear combinations, we obtain the solution

$$\psi(\mathbf{x}, t) = (A \cos \omega x + B \sin \omega x) e^{-\omega^2 a^2 t}$$

for any choice of A, B, ω, which are introduced to satisfy boundary conditions. Upon summing over multiples $n\omega$ of the basic frequency for periodic boundary conditions or **integrating over the parameter** ω for general (nonperiodic boundary conditions), we find a solution

$$\psi(x, t) = \int [A(\omega) \cos \omega x + B(\omega) \sin \omega x] e^{-a^2 \omega^2 t} d\omega, \tag{16.4}$$

that is general enough to be adapted to boundary conditions at $t = 0$, for example. When the boundary condition gives a nonzero temperature ψ_0, as for our rod, then the summation method applies (Fourier expansion of the boundary condition). If the space is unrestricted (as for an infinitely extended rod) the Fourier integral applies.

- This summation or integration over parameters is one of the standard methods for generalizing specific PDE solutions in order to adapt them to boundary conditions.

EXAMPLE 16.2.1

A Specific Boundary Condition Let us solve a one-dimensional case explicitly, where the temperature at time $t = 0$ is $\psi_0(x) = 1 = \text{const.}$ in the interval between $x = +1$ and $x = -1$ and zero for $x > 1$ and $x < 1$. At the ends, $x = \pm 1$, the temperature is always held at zero.

For a finite interval we choose the $\cos(l\pi x/2)$ spatial solutions of Eq. (16.3) for integer l because they vanish at $x = \pm 1$. Thus, at $t = 0$ our solution is a Fourier series (see Example 8.9.1),

$$\psi(x, 0) = \sum_{l=1}^{\infty} a_l \cos(\pi l x/2) = 1, \quad -1 < x < 1,$$

with coefficients (see Section 14.1)

$$a_l = \int_{-1}^{1} 1 \cdot \cos\frac{\pi l x}{2} = \frac{2}{l\pi}\sin\frac{\pi l x}{2}\bigg|_{x=-1}^{1}$$
$$= \frac{4}{\pi l}\sin\frac{l\pi}{2} = \frac{4(-1)^m}{(2m+1)\pi}, \quad l = 2m+1;$$
$$a_l = 0, \quad l = 2m.$$

Including its time dependence, the full solution is given by the series

$$\psi(x,t) = \frac{4}{\pi}\sum_{m=0}^{\infty}\frac{(-1)^m}{2m+1}\cos\left[(2m+1)\frac{\pi x}{2}\right]e^{-t((2m+1)\pi a/2)^2}, \tag{16.5}$$

which converges absolutely for $t > 0$, but only conditionally at $t = 0$, as a result of the discontinuity at $x = \pm 1$.

Without the restriction to zero temperature at the end points of the previous finite interval, the Fourier series is replaced by a Fourier integral. The general solution is then given by Eq. (16.4). At $t = 0$, the given temperature distribution $\psi_0 = 1$ gives the coefficients as (see Section 15.2)

$$A(\omega) = \frac{1}{\pi}\int_{-1}^{1}\cos\omega x\,dx = \frac{1}{\pi}\frac{\sin\omega x}{\omega}\bigg|_{x=-1}^{1} = \frac{2\sin\omega}{\pi\omega}, \quad B(\omega) = 0.$$

Therefore,

$$\psi(x,t) = \frac{2}{\pi}\int_0^{\infty}\frac{\sin\omega}{\omega}\cos(\omega x)e^{-a^2\omega^2 t}d\omega. \tag{16.6}$$

■

In **three dimensions** the corresponding exponential ansatz $\psi = e^{i\mathbf{k}\cdot\mathbf{r}/a+\beta t}$ leads to a solution with the relation $\beta = -\mathbf{k}^2 = -k^2$ for its parameter, and the three-dimensional form of Eq. (16.3) becomes

$$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2} + k^2\psi = 0, \tag{16.7}$$

which is called the **Helmholtz** equation and may be solved by the separation method just like the previously discussed Laplace equation in Cartesian, cylindrical, or spherical coordinates.

In Cartesian coordinates, with the product ansatz of Eq. (8.114) the separated x and y ODEs from Eq. (16.3) are the same as Eqs. (8.117) and (8.120), whereas the z ODE [Eq. (8.121)] generalizes to

$$\frac{1}{Z}\frac{d^2Z}{dz^2} = -k^2 + l^2 + m^2 = n^2 > 0, \tag{16.8}$$

where we introduce another separation constant n^2, constrained by

$$k^2 = l^2 + m^2 - n^2 \tag{16.9}$$

to produce a symmetric set of equations. Now our solution of Helmholtz's Eq. (16.7) is labeled according to the choice of all three separation constants l, m, n subject to the constraint Eq. (16.9). As before, the z ODE [Eq. (16.8)] yields exponentially decaying solutions $\sim e^{-nz}$. The boundary condition at $z = 0$ fixes the expansion coefficients a_{lm} by the same Eq. (8.123).

In cylindrical coordinates, we now use the separation constant l^2 for the z ODE with an exponentially decaying solution in mind,

$$\frac{d^2Z}{dz^2} = l^2 Z > 0, \tag{16.10}$$

so that $Z \sim e^{-lz}$ because the temperature goes to zero at large z. Setting $k^2 + l^2 = n^2$, Eqs. (8.131)–(8.132) stay the same so that we end up with the same Fourier–Bessel expansion [Eq.(8.137)], as before.

In spherical coordinates, the separation method leads to the same angular ODEs in Eqs. (8.142) and (8.145), whereas the radial ODE now becomes

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + k^2 R - \frac{QR}{r^2} = 0, \quad Q = l(l+1) \tag{16.11}$$

instead of Eq. (8.146), whose solutions are the spherical Bessel functions of Section 12.4. They are listed in Table 16.2.

The restriction that k^2 be a constant is unnecessarily severe. The separation process will still work with Helmholtz's PDE for k^2 as general as

$$k^2 = f(r) + \frac{1}{r^2}g(\theta) + \frac{1}{r^2\sin^2\theta}h(\varphi) + k'^2. \tag{16.12}$$

In the hydrogen atom we have $k^2 = f(r)$ in the Schrödinger wave equation, and this leads to a closed-form solution involving Laguerre polynomials.

Biographical Data

Helmholtz, Hermann Ludwig Ferdinand von. Helmholtz, a German physiologist and physicist, was born in 1821 in Potsdam near Berlin and died in 1894 in Charlottenburg, now Berlin. He studied medicine in Berlin, graduating in 1842. In 1849, with Humboldt's support, he was appointed professor of physiology at the University of Königsberg in Prussia, now Russia. He studied the function of the human eye and ear, defining the quality of a tone in terms of overtones (more rapid vibrations than the basic one). However, he is best known for his contributions to physics and energy conservation in particular. He showed that the earth's age would be less than 25 million years if the sun's energy came from gravitational contraction. He suggested to his student Heinrich Hertz that he should prove that the electromagnetic spectrum extends well beyond the visible light.

Alternate Solutions

In a new approach to the heat flow PDE suggested by experiments, we now return to the one-dimensional PDE [Eq. (16.3)], seeking solutions of a new functional form $\psi(x, t) = u(x/\sqrt{t})$, which is suggested by Example 15.2.2.

Substituting $u(\xi)$, $\xi = x/\sqrt{t}$, into Eq. (16.3) using

$$\frac{\partial\psi}{\partial x} = \frac{u'}{\sqrt{t}}, \quad \frac{\partial^2\psi}{\partial x^2} = \frac{u''}{t}, \quad \frac{\partial\psi}{\partial t} = -\frac{x}{2\sqrt{t^3}}u' \tag{16.13}$$

with the notation $u'(\xi) \equiv \frac{du}{d\xi}$, the PDE is reduced to the ODE

$$2a^2u''(\xi) + \xi u'(\xi) = 0. \tag{16.14}$$

Writing this ODE as

$$\frac{u''}{u'} = -\frac{\xi}{2a^2},$$

we can integrate it once to get $\ln u' = -\frac{\xi^2}{4a^2} + \ln C_1$ with an integration constant C_1. Exponentiating and integrating again, we find the solution

$$u(\xi) = C_1 \int_0^\xi e^{-\frac{\xi^2}{4a^2}} d\xi + C_2, \tag{16.15}$$

involving two integration constants C_i. Normalizing this solution at time $t = 0$ to temperature $+1$ for $x > 0$ and -1 for $x < 0$, our boundary conditions, fixes the constants C_i so that

$$\psi = \frac{1}{a\sqrt{\pi}} \int_0^{\frac{x}{\sqrt{t}}} e^{-\frac{\xi^2}{4a^2}} d\xi = \frac{2}{\sqrt{\pi}} \int_0^{\frac{x}{2a\sqrt{t}}} e^{-v^2} dv = \Phi\left(\frac{x}{2a\sqrt{t}}\right), \tag{16.16}$$

where Φ denotes Gauss's error function (see Exercise 5.10.4). See Example 15.2.2 for a derivation using a Fourier transform. We need to generalize this specific solution to adapt it to boundary conditions.

To this end, we now generate **new solutions of the PDE with constant coefficients by differentiating a special solution** [Eq. (16.16)]. In other words, if $\psi(x, t)$ solves the PDE in Eq. (16.3), so do $\frac{\partial\psi}{\partial t}$ and $\frac{\partial\psi}{\partial x}$ because these derivatives and the differentiations of the PDE commute; that is, the order in which they are carried out does not matter. Note that this method no longer works if any coefficient of the PDE depends on t or x explicitly. However, PDEs with constant coefficients dominate in physics. Examples are Newton's equations of motion (ODEs) in classical mechanics, the wave equations of electrodynamics, and Poisson's and Laplace's equations in electrostatics and gravity. Even Einstein's nonlinear field equations of general relativity take on this special form in local geodesic coordinates.

Therefore, by differentiating Eq. (16.16) with respect to x, we find the simpler, more basic solution

$$\psi_1(x, t) = \frac{1}{a\sqrt{t\pi}} e^{-\frac{x^2}{4a^2t}}, \tag{16.17}$$

and, repeating the process, another basic solution

$$\psi_2(x, t) = \frac{x}{2a^3\sqrt{t^3\pi}} e^{-\frac{x^2}{4a^2t}}. \tag{16.18}$$

Again, these solutions have to be generalized to adapt them to boundary conditions. Also, there is another method of generating new solutions of a PDE with constant coefficients: We can **translate** a given solution, for example, $\psi_1(x, t) \to \psi_1(x - \alpha, t)$, and then **integrate over the translation parameter** α. Therefore,

$$\psi(x, t) = \frac{1}{2a\sqrt{t\pi}} \int_{-\infty}^{\infty} C(\alpha) e^{-\frac{(x-\alpha)^2}{4a^2 t}} d\alpha \tag{16.19}$$

is again a solution, which we rewrite using the substitution

$$\xi = \frac{x - \alpha}{2a\sqrt{t}}, \quad \alpha = x - 2a\xi\sqrt{t}, \quad d\alpha = -2ad\xi\sqrt{t}. \tag{16.20}$$

Thus, we find that

$$\psi(x, t) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} C(x - 2a\xi\sqrt{t}) e^{-\xi^2} d\xi \tag{16.21}$$

is a solution of our PDE. In this form we recognize the significance of the weight function $C(x)$ from the translation method because, at $t = 0$, $\psi(x, 0) = C(x) = \psi_0(x)$ is determined by the boundary condition, and $\int_{-\infty}^{\infty} e^{-\xi^2} d\xi = \sqrt{\pi}$. Therefore, we can write the solution as

$$\psi(x, t) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} \psi_0(x - 2a\xi\sqrt{t}) e^{-\xi^2} d\xi, \tag{16.22}$$

displaying the role of the boundary condition explicitly. From Eq. (16.22) we see that the initial temperature distribution $\psi_0(x)$ spreads out over time and is damped by the Gaussian weight function.

EXAMPLE 16.2.2

Special Boundary Condition Again Let us express the solution of Example 16.2.1 in terms of the error function solution of Eq. (16.16). The boundary condition at $t = 0$ is $\psi_0(x) = 1$ for $-1 < x < 1$ and zero for $|x| > 1$. From Eq. (16.22) we find the limits on the integration variable ξ by setting $x - 2a\xi\sqrt{t} = \pm 1$. This yields the integration end points $\xi = (\pm 1 + x)/2a\sqrt{t}$. Therefore, our solution becomes

$$\psi(x, t) = \frac{1}{\sqrt{\pi}} \int_{\frac{x-1}{2a\sqrt{t}}}^{\frac{x+1}{2a\sqrt{t}}} e^{-\xi^2} d\xi.$$

Using the error function defined in Eq. (16.16) we can also write this solution as follows:

$$\psi(x, t) = \frac{1}{2}\left[\Phi\left(\frac{x+1}{2a\sqrt{t}}\right) - \Phi\left(\frac{x-1}{2a\sqrt{t}}\right)\right]. \tag{16.23}$$

Comparing this form of our solution with that from Example 16.2.1, we see that we can express Eq. (16.23) as the Fourier integral of Example 16.2.1, an identity that gives the Fourier integral [Eq. (16.6)], in closed form of the tabulated error function. ■

Finally, we consider the heat flow case for an extended **spherically symmetric** medium centered at the origin, which prescribes polar coordinates r, θ, φ. We expect a solution of the form $\psi(\mathbf{r}, t) = u(r, t)$. Using Eq. (2.77) we find the PDE

$$\frac{\partial u}{\partial t} = a^2 \left(\frac{\partial^2 u}{\partial r^2} + \frac{2}{r} \frac{\partial u}{\partial r} \right), \tag{16.24}$$

which we transform to the one-dimensional heat flow PDE by the substitution

$$u = \frac{v(r, t)}{r}, \quad \frac{\partial u}{\partial r} = \frac{1}{r} \frac{\partial v}{\partial r} - \frac{v}{r^2}, \quad \frac{\partial u}{\partial t} = \frac{1}{r} \frac{\partial v}{\partial t},$$
$$\frac{\partial^2 u}{\partial r^2} = \frac{1}{r} \frac{\partial^2 v}{\partial r^2} - \frac{2}{r^2} \frac{\partial v}{\partial r} + \frac{2v}{r^3}. \tag{16.25}$$

This yields the PDE

$$\frac{\partial v}{\partial t} = a^2 \frac{\partial^2 v}{\partial r^2}. \tag{16.26}$$

EXAMPLE 16.2.3

Spherically Symmetric Heat Flow Let us apply the one-dimensional heat flow PDE with the solution Eq. (16.16) to a spherically symmetric heat flow under fairly common boundary conditions, where x is replaced by the radial variable. Initially, we have zero temperature everywhere. Then, at time $t = 0$, a finite amount of heat energy Q is released at the origin, spreading evenly in all directions. What is the resulting spatial and temporal temperature distribution?

Inspecting our special solution in Eq. (16.18), we see that, for $t \to 0$, the temperature

$$\frac{v(r, t)}{r} = \frac{C}{\sqrt{t^3}} e^{-\frac{r^2}{4a^2 t}} \tag{16.27}$$

goes to zero for all $r \neq 0$ so that zero initial temperature is guaranteed. As $t \to \infty$, the temperature $v/r \to 0$ for all r, including the origin, which is implicit in our boundary conditions. The constant C can be determined from energy conservation, which gives the constraint

$$Q = \sigma\rho \int \frac{v}{r} d^3 r = \frac{4\pi\sigma\rho C}{\sqrt{t^3}} \int_0^\infty r^2 e^{-\frac{r^2}{4a^2 t}} dr = 8\sqrt{\pi^3}\sigma\rho a^3 C, \tag{16.28}$$

where ρ is the constant density of the medium and σ its specific heat. Here, we have rescaled the integration variable and integrated by parts to get

$$\int_0^\infty e^{-\frac{r^2}{4a^2 t}} r^2 \, dr = (2a\sqrt{t})^3 \int_0^\infty e^{-\xi^2} \xi^2 \, d\xi,$$
$$\int_0^\infty e^{-\xi^2} \xi^2 d\xi = -\frac{\xi}{2} e^{-\xi^2} \Big|_0^\infty + \frac{1}{2} \int_0^\infty e^{-\xi^2} d\xi = \frac{\sqrt{\pi}}{4}.$$

The temperature, as given by Eq. (16.27) at any moment, that is at fixed t is a Gaussian distribution that flattens out as time increases because its width is proportional to $\sqrt{t}$. As a function of time, the temperature is proportional to $t^{-3/2}e^{-T/t}$, with $T \equiv r^2/4a^2$, which rises from zero to a maximum and then falls to zero again for large times. To find the maximum, we set

$$\frac{d}{dt}(t^{-3/2}e^{-T/t}) = t^{-5/2}e^{-T/t}\left(\frac{T}{t} - \frac{3}{2}\right) = 0, \tag{16.29}$$

from which we find $t = 2T/3$. ■

In the case of **cylindrical symmetry** (in the plane $z = 0$ in plane polar coordinates $\rho = \sqrt{x^2 + y^2}, \varphi$) we search for a temperature $\psi = u(\rho, t)$ that then satisfies the ODE [using Eq. (2.21) in the diffusion equation]

$$\frac{\partial u}{\partial t} = a^2\left(\frac{\partial^2 u}{\partial \rho^2} + \frac{1}{\rho}\frac{\partial u}{\partial \rho}\right), \tag{16.30}$$

which is the planar analog of Eq. (16.26). This ODE also has solutions with the functional dependence $\rho/\sqrt{t} \equiv r$. Upon substituting

$$u = v\left(\frac{\rho}{\sqrt{t}}\right), \quad \frac{\partial u}{\partial t} = -\frac{\rho v'}{2t^{3/2}}, \quad \frac{\partial u}{\partial \rho} = \frac{v'}{\sqrt{t}}, \quad \frac{\partial^2 u}{\partial \rho^2} = \frac{v'}{t} \tag{16.31}$$

into Eq. (16.30) with the notation $v' \equiv \frac{dv}{dr}$, we find the ODE

$$a^2 v'' + \left(\frac{a^2}{r} + \frac{r}{2}\right)v' = 0. \tag{16.32}$$

This is a first-order ODE for v', which we can integrate when we separate the variables v and r as

$$\frac{v''}{v'} = -\left(\frac{1}{r} + \frac{r}{2a^2}\right). \tag{16.33}$$

This yields

$$v(r) = \frac{C}{r}e^{-\frac{r^2}{4a^2}} = C\frac{\sqrt{t}}{\rho}e^{-\frac{\rho^2}{4a^2 t}}. \tag{16.34}$$

This special solution for cylindrical symmetry can be similarly generalized and adapted to boundary conditions as for the spherical case. Finally, the z-dependence can be factored in, as z separates from the plane polar radial variable ρ.

SUMMARY

PDEs can be solved with initial conditions, just like ODEs, or with boundary conditions prescribing the value of the solution or its derivative on boundary surfaces, curves, or points. When the solution is prescribed on the boundary, the PDE is called a **Dirichlet** problem; if the normal derivative of the solution is prescribed on the boundary, the PDE is called a **Neumann** problem.

When the initial temperature is prescribed for the one-dimensional or three-dimensional heat equation (with spherical or cylindrical symmetry), it becomes a weight function of the solution in terms of an integral over the generic Gaussian solution. The three-dimensional heat equation, with spherical or cylindrical boundary conditions, is solved by separation of the variables leading to eigenfunctions in each separated variable and eigenvalues as separation constants. For finite boundary intervals in each spatial coordinate, the sum over separation constants leads to a Fourier series solution, whereas infinite boundary conditions lead to a Fourier integral solution. The separation of variables method attempts to solve a PDE by writing the solution as a product of functions of one variable each. General conditions for the separation method to work are provided by the symmetry properties of the PDE to which continuous group theory applies.

EXERCISES

16.2.1 By letting the operator $\nabla^2 + k^2$ act on the general form $a_1\psi_1(x, y, z) + a_2\psi_2(x, y, z)$, show that it is linear; that is, $(\nabla^2 + k^2)(a_1\psi_1 + a_2\psi_2) = a_1(\nabla^2 + k^2)\psi_1 + a_2(\nabla^2 + k^2)\psi_2$.

16.2.2 Show that the Helmholtz equation

$$\nabla^2\psi + k^2\psi = 0$$

is separable in circular cylindrical coordinates if k^2 is generalized to $k^2 + f(\rho) + (1/\rho^2)g(\varphi) + h(z)$.

16.2.3 Separate variables in the Helmholtz equation in spherical polar coordinates, splitting off the radial dependence **first**. Show that your separated equations have the same form as Eqs. (8.142) and (8.145), whereas Eq. (8.146) is modified. Describe in your own words what this exercise tells you.

16.2.4 Verify that

$$\nabla^2\psi(r, \theta, \varphi) + \left[k^2 + f(r) + \frac{1}{r^2}g(\theta) + \frac{1}{r^2\sin^2\theta}h(\varphi)\right]\psi(r, \theta, \varphi) = 0$$

is separable (in spherical polar coordinates). The functions f, g, and h are functions only of the variables indicated; k^2 is a constant.

16.2.5 For a homogeneous spherical solid with constant thermal diffusivity, K, and no heat sources, the equation of heat conduction becomes

$$\frac{\partial T(r, t)}{\partial t} = K\nabla^2 T(r, t).$$

Assume a solution of the form

$$T = R(r)T(t)$$

and separate variables. Show that the radial equation may take on the standard form

$$r^2\frac{d^2R}{dr^2}+2r\frac{dR}{dr}+[\alpha^2r^2-n(n+1)]R=0;\quad n=\text{integer}.$$

The solutions of this equation are called spherical Bessel functions.

16.2.6 Separate variables in the thermal diffusion equation of Eq. (8.112) in circular cylindrical coordinates. Assume that you can neglect end effects and take $\psi = T(\rho, t)$.

16.3 Inhomogeneous PDE—Green's Function

The series substitution of Section 8.5 and the Wronskian double integral of Section 8.6 provide the most general solution of the **homogeneous**, linear, second-order ODE. The specific solution, y_p, is linearly dependent on the source term [$F(x)$ of Eq. (8.44)] and may be cranked out by the variation of parameters method. In this section, we discuss a different method of solution for PDEs—Green's functions.

For a brief introduction to the Green's function method as applied to the solution of a nonhomogeneous PDE, it is helpful to use the electrostatic analog. In the presence of charges, the electrostatic potential ψ satisfies Poisson's nonhomogeneous equation (compare Section 1.13)

$$\nabla^2\psi=-\frac{\rho}{\varepsilon_0}\quad\text{(mks units)}\tag{16.35}$$

and Laplace's homogeneous equation,

$$\nabla^2\psi=0,\tag{16.36}$$

in the absence of electric charge ($\rho = 0$). If the charges are point charges q_i located at $\mathbf{r}_i$, we know that the solution is

$$\psi(\mathbf{r})=\frac{1}{4\pi\varepsilon_0}\sum_i\frac{q_i}{|\mathbf{r}-\mathbf{r}_i|},\tag{16.37}$$

a superposition of single-point charge solutions obtained from Coulomb's law for the force between two point charges q_1 and q_2 a distance r apart,

$$\mathbf{F}=\frac{q_1q_2\hat{\mathbf{r}}}{4\pi\varepsilon_0r^2}.\tag{16.38}$$

By replacement of the discrete point charges with a smeared out distributed charge, charge density ρ [Eq. (16.37)] becomes

$$\psi(r=0)=\frac{1}{4\pi\varepsilon_0}\int\frac{\rho(\mathbf{r})}{r}d\tau\tag{16.39}$$

or, for the potential at $\mathbf{r}$ away from the origin and the charge at $\mathbf{r}_2$,

$$\psi(\mathbf{r})=\frac{1}{4\pi\varepsilon_0}\int\frac{\rho(\mathbf{r}_2)}{|\mathbf{r}-\mathbf{r}_2|}d\tau_2.\tag{16.40}$$

We use ψ as the potential corresponding to the given distribution of charge and therefore satisfying Poisson's equation [Eq. (16.35)], whereas a function G, which we label Green's function, is required to satisfy Poisson's equation with a point source at the point defined by $\mathbf{r}_2$:

$$\nabla_1^2 G = -\delta(\mathbf{r}_1 - \mathbf{r}_2). \tag{16.41}$$

Physically, then, G is the potential at $\mathbf{r}_1$ corresponding to a unit source at $\mathbf{r}_2$. By Green's theorem (Section 1.10),

$$\int (\psi \nabla^2 G - G\nabla^2 \psi) d\tau_2 = \int (\psi \nabla G - G\nabla\psi) \cdot d\boldsymbol{\sigma}_2. \tag{16.42}$$

Assuming that the integrand falls off faster than r^{-2}, we may simplify our problem by taking the volume so large that the surface integral vanishes, leaving

$$\int \psi \nabla^2 G d\tau_2 = \int G\nabla^2 \psi d\tau_2, \tag{16.43}$$

or by substituting in Eqs. (16.35) and (16.41), we have

$$-\int \psi(\mathbf{r}_2)\delta(\mathbf{r}_1 - \mathbf{r}_2) d\tau_2 = -\int \frac{G(\mathbf{r}_1, \mathbf{r}_2)\rho(\mathbf{r}_2)}{\varepsilon_0} d\tau_2. \tag{16.44}$$

Integration by employing the defining property of the Dirac delta function [Eq. (1.151)] produces

$$\psi(\mathbf{r}) = \frac{1}{\varepsilon_0} \int G(\mathbf{r}, \mathbf{r}_2)\rho(\mathbf{r}_2) d\tau_2. \tag{16.45}$$

Note that we have used Eq. (16.41) to eliminate $\nabla^2 G$, but that the function G is still unknown. In Section 1.14, Gauss's law, we found that

$$\int \nabla^2 \left(\frac{1}{r}\right) d\tau = \begin{cases} 0, \\ -4\pi, \end{cases} \tag{16.46}$$

0 if the volume did not include the origin and -4π if the origin was included. This result from Section 1.14 may be rewritten as in Eq. (1.148), or

$$\nabla^2 \left(\frac{1}{4\pi r}\right) = -\delta(\mathbf{r}) \quad \text{or} \quad \nabla^2 \left(\frac{1}{4\pi r_{12}}\right) = -\delta(\mathbf{r}_1 - \mathbf{r}_2), \tag{16.47}$$

corresponding to a shift of the electrostatic charge from the origin to the position $\mathbf{r} = \mathbf{r}_2$. Here, $r_{12} = |\mathbf{r}_1 - \mathbf{r}_2|$, and the Dirac delta function $\delta(\mathbf{r}_1 - \mathbf{r}_2)$ vanishes unless $\mathbf{r}_1 = \mathbf{r}_2$. Therefore, in a comparison of Eqs. (16.47) and (16.41), the function G (Green's function) is given by

$$G(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{4\pi|\mathbf{r}_1 - \mathbf{r}_2|}. \tag{16.48}$$

The solution of our differential equation (Poisson's equation) is

$$\psi(\mathbf{r}_1) = \frac{1}{4\pi\varepsilon_0} \int \frac{\rho(\mathbf{r}_2)}{|\mathbf{r}_1 - \mathbf{r}_2|} d\tau_2, \tag{16.49}$$

in complete agreement with Eq. (16.40). Actually, $\psi(\mathbf{r})$ [Eq. (16.49)] is the particular solution of Poisson's equation. We may add solutions of Laplace's equation [compare Eq. (8.113)]. Such solutions could describe an external field.

These results can be generalized to the second-order linear but inhomogeneous, differential equation

$$\mathcal{L}y(\mathbf{r}_1) = -f(\mathbf{r}_1), \tag{16.50}$$

where $\mathcal{L}$ is a linear differential operator. The Green's function is taken to be a solution of

$$\mathcal{L}G(\mathbf{r}_1, \mathbf{r}_2) = -\delta(\mathbf{r}_1 - \mathbf{r}_2) \tag{16.51}$$

[analogous to Eq. (16.41)]. Then the particular solution $y(\mathbf{r}_1)$ becomes

$$y(\mathbf{r}_1) = \int G(\mathbf{r}_1, \mathbf{r}_2) f(\mathbf{r}_2) d\tau_2, \tag{16.52}$$

which can be verified by applying $\mathcal{L}$ to $y(\mathbf{r})$. (There may also be an integral over a bounding surface depending on the conditions specified.)

SUMMARY

In summary, the Green's function, often written $G(\mathbf{r}_1, \mathbf{r}_2)$ as a reminder of the name, is a solution of Eq. (16.41) or Eq. (16.51) more generally. It enters in an integral solution of our differential equation, as in Eq. (16.45). For the simple, but important, electrostatic case, we obtain Green's function $G(\mathbf{r}_1, \mathbf{r}_2)$ by Gauss's law, comparing Eqs. (16.41) and (16.47). Finally, from the final solution [Eq. (16.49)] it is possible to develop a physical interpretation of Green's function. It occurs as a weighting function or propagator function that enhances or reduces the effect of the charge element $\rho(\mathbf{r}_2)d\tau_2$ according to its distance from the field point $\mathbf{r}_1$. The Green's function, $G(\mathbf{r}_1, \mathbf{r}_2)$, gives the effect of a unit point source at $\mathbf{r}_2$ in producing a potential at $\mathbf{r}_1$. This is how it was introduced in Eq. (16.41); this is how it appears in Eq. (16.49).

EXAMPLE 16.3.1

Quantum Mechanical Scattering—Neumann Series Solution The quantum theory of scattering provides a good illustration of integral equation techniques and an application of a Green's function. Our physical picture of scattering is as follows. A beam of particles moves along the negative z-axis toward the origin. A small fraction of the particles are scattered by the potential $V(\mathbf{r})$ and go off as an outgoing spherical wave, as shown schematically in Fig. 16.1. Our wave function $\psi(\mathbf{r})$ must satisfy the time-independent Schrödinger equation

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r}) + V(\mathbf{r})\psi(\mathbf{r}) = E\psi(\mathbf{r}) \tag{16.53a}$$

or

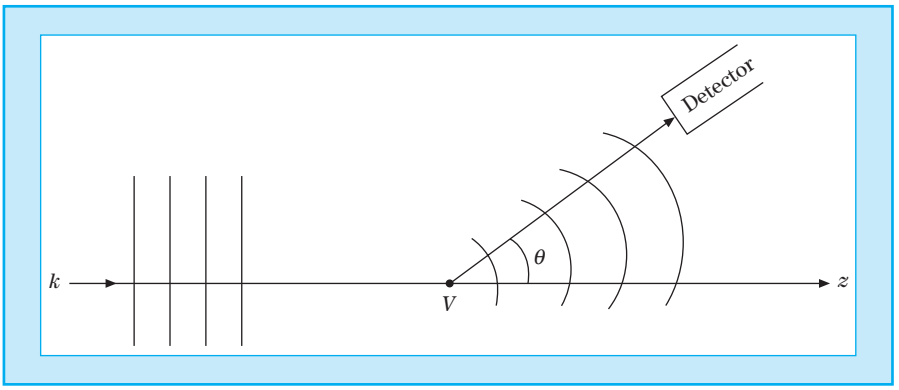
$$\nabla^2\psi(\mathbf{r}) + k^2\psi(\mathbf{r}) = -\left[-\frac{2m}{\hbar^2}V(\mathbf{r})\psi(\mathbf{r})\right], \qquad k^2 = \frac{2mE}{\hbar^2}. \tag{16.53b}$$

From the physical picture just presented, we search for a solution having an **asymptotic** form

$$\psi(\mathbf{r}) \sim e^{i\mathbf{k}_0\cdot\mathbf{r}} + f_k(\theta, \varphi)\frac{e^{ikr}}{r}, \tag{16.54}$$

Figure 16.1

Incident Plane Wave Scattered by a Potential V into an Outgoing Spherical Wave



which we shall derive from the integral equation following from the Schrödinger equation. Here, $e^{i\mathbf{k}_0\cdot\mathbf{r}}$ is the incident plane wave,[2] with $\mathbf{k}_0$ the propagation vector carrying the subscript 0 to indicate that it is in the $\theta = 0$ (z-axis) direction. The magnitudes k_0 and k are equal (for elastic scattering ignoring recoil of the target), and e^{ikr}/r is the outgoing spherical wave with an angular (and energy)-dependent amplitude factor $f_k(\theta, \varphi)$.[3] In quantum mechanics texts, it is shown that the differential probability of scattering, $d\sigma/d\Omega$, the scattering cross section per unit solid angle, is given by $|f_k(\theta, \varphi)|^2$.

Identifying $[-(2m/\hbar^2)V(\mathbf{r})\psi(\mathbf{r})]$ with $f(\mathbf{r})$ of Eq. (16.50), we have

$$\psi(\mathbf{r}) = -\frac{2m}{\hbar^2}\int V(\mathbf{r}_2)\psi(\mathbf{r}_2)G(\mathbf{r}, \mathbf{r}_2)d^3r_2 \tag{16.55}$$

by Eq. (16.52). This does not have the desired asymptotic form of Eq. (16.54), but we may add $e^{i\mathbf{k}_0\cdot\mathbf{r}}$ to Eq. (16.55), a solution of the homogeneous equation, and put $\psi(\mathbf{r})$ into the desired form:

$$\psi(\mathbf{r}) = e^{i\mathbf{k}_0\cdot\mathbf{r}} - \frac{2m}{\hbar^2}\int V(\mathbf{r}_2)\psi(\mathbf{r}_2)G(\mathbf{r}, \mathbf{r}_2)d^3r_2. \tag{16.56}$$

Our Green's function is the inverse of the operator $\mathcal{L} = \nabla^2 + k^2$ [Eq. (16.53)] satisfying the boundary condition that it describe an outgoing wave. Then, from Example 16.3.2,

$$G(\mathbf{r}_1, \mathbf{r}_2) = \frac{\exp(ik|\mathbf{r}_1 - \mathbf{r}_2|)}{4\pi|\mathbf{r}_1 - \mathbf{r}_2|},$$

and

$$\psi(\mathbf{r}) = e^{i\mathbf{k}_0\cdot\mathbf{r}} - \frac{2m}{4\pi\hbar^2}\int V(\mathbf{r}_2)\psi(\mathbf{r}_2)\frac{e^{ik|\mathbf{r}-\mathbf{r}_2|}}{|\mathbf{r} - \mathbf{r}_2|}d^3r_2. \tag{16.57}$$

[2]For simplicity, we assume a continuous incident beam. In a more sophisticated and more realistic treatment, Eq. (16.54) would be one component of a Fourier wave packet.

[3]If $V(\mathbf{r})$ represents a central force, f_k will be a function of θ only, independent of azimuth.

This integral equation analog of the original Schrödinger wave equation is **exact**.

Now to prove the asymptotic relation [Eq. (16.54)], we let $r \to \infty$, while the integration variable r_2 in Eq. (16.57) is restricted to the small target volume. We approximate the denominator by $|\mathbf{r} - \mathbf{r}_2| \sim r$, but in the oscillatory numerator of absolute value unity we have to be more precise. Here, we expand

$$|\mathbf{r} - \mathbf{r}_2|^2 = (\mathbf{r} - \mathbf{r}_2)^2 = \mathbf{r}^2 - 2\mathbf{r} \cdot \mathbf{r}_2 + \mathbf{r}_2^2 \sim r^2 \left(1 - \frac{2}{r}\hat{\mathbf{r}} \cdot \mathbf{r}_2\right)$$

so that

$$|\mathbf{r} - \mathbf{r}_2| \sim r - \hat{\mathbf{r}} \cdot \mathbf{r}_2, \quad r \to \infty.$$

Substituting these asymptotic expressions into Eq. (16.57) yields

$$\psi(\mathbf{r}) \sim e^{i\mathbf{k}_0 \cdot \mathbf{r}} - \frac{2m}{4\pi\hbar^2} \frac{e^{ikr}}{r} \int V(\mathbf{r}_2)\psi(\mathbf{r}_2)e^{-ik\hat{\mathbf{r}} \cdot \mathbf{r}_2} d^3r_2, \tag{16.58}$$

which is the asymptotic relation [Eq. (16.54)] with

$$f_k(\theta, \varphi) = -\frac{2m}{4\pi\hbar^2} \int V(\mathbf{r}_2)\psi(\mathbf{r}_2)e^{-ik\hat{\mathbf{r}} \cdot \mathbf{r}_2} d^3r_2, \tag{16.59}$$

where $\mathbf{r} = (r, \theta, \varphi)$ for large r is the location of the detector that measures the scattered wave so that θ is the scattering angle.

Employing an iterative (Neumann) series technique (remember that the scattering probability is very small), we have

$$\psi_0(\mathbf{r}) = e^{i\mathbf{k}_0 \cdot \mathbf{r}}, \tag{16.60a}$$

which has the physical interpretation of no scattering.

Substituting $\psi_0(\mathbf{r}_2) = e^{i\mathbf{k}_0 \cdot \mathbf{r}_2}$ into the integral, we obtain the first correction term

$$\psi_1(\mathbf{r}) = e^{i\mathbf{k}_0 \cdot \mathbf{r}} - \frac{2m}{4\pi\hbar^2} \int V(\mathbf{r}_2) \frac{e^{ik|\mathbf{r} - \mathbf{r}_2|}}{|\mathbf{r} - \mathbf{r}_2|} e^{i\mathbf{k}_0 \cdot \mathbf{r}_2} d^3r_2. \tag{16.60b}$$

This is the famous **Born approximation**. It is expected to be most accurate for weak potentials and high incident energy. If a more accurate approximation is desired, the perturbation series may be continued.[4] Substituting the incident plane wave into the scattering amplitude, Eq. (16.59) yields the first-order Born approximation

$$f_k(\theta, \varphi) = -\frac{m}{2\pi\hbar^2} \int V(\mathbf{r}_2)e^{i(\mathbf{k}_0 - \mathbf{k}) \cdot \mathbf{r}_2} d^3r_2, \tag{16.61}$$

[4]This assumes the iteration (Neumann) series is convergent. In some physical situations, it is not convergent and then other techniques are needed.

where $\mathbf{k} \equiv k\hat{\mathbf{r}}$ is the scattered wave vector, and $\mathbf{q} = \mathbf{k}_0 - \mathbf{k}$ is the momentum transfer. In other words, the elastic scattering amplitude in first-order Born approximation is proportional to the Fourier transform of the potential at $\mathbf{q}$. ■

EXAMPLE 16.3.2

Quantum Mechanical Scattering—Green's Function Again, we consider the Schrödinger wave equation [Eq. (16.53b)] for the scattering problem. This time we use Fourier transform techniques and we derive the desired form of the Green's function by contour integration.

We solve the PDE for the Green's function corresponding to Eq. (16.53b)

$$(\nabla^2 + k^2)G(\mathbf{r}, \mathbf{r}_2) = -\delta(\mathbf{r} - \mathbf{r}_2) = -\int \frac{d^3p}{(2\pi)^3} e^{i\mathbf{p}\cdot(\mathbf{r}-\mathbf{r}_2)} \tag{16.62}$$

in terms of a Fourier integral

$$G(\mathbf{r}, \mathbf{r}_2) = \int \frac{d^3p}{(2\pi)^3} g_0(\mathbf{p}) e^{i\mathbf{p}\cdot(\mathbf{r}-\mathbf{r}_2)} \tag{16.63}$$

of the same type as the delta function driving term. Substituting the Fourier integral into the PDE, we see that

$$\nabla e^{i\mathbf{p}\cdot(\mathbf{r}-\mathbf{r}_2)} = i\mathbf{p}e^{i\mathbf{p}\cdot(\mathbf{r}-\mathbf{r}_2)}$$

so that the PDE becomes the trivial algebraic equation $(k^2 - \mathbf{p}^2)g_0(\mathbf{p}) = -1$ for the Fourier transform g_0 of G. To find G, we need to evaluate the Fourier integral

$$\int d^3p \frac{e^{ip\rho\cos\theta}}{\mathbf{p}^2 - k^2}, \tag{16.64}$$

where $p^2/(p^2 - k^2)$ is part of the radial integral, and $d^3p = p^2 dp \sin\theta d\theta d\varphi$. Here, $p\rho\cos\theta$ has replaced $\mathbf{p}\cdot(\mathbf{r} - \mathbf{r}_2)$ for simplicity. With the substitution $x = \cos\theta$, $dx = -\sin\theta d\theta$, the angular part in polar coordinates in momentum space is elementary. Integrating over φ by inspection, we pick up a 2π. The θ integration then leads to

$$\int_0^{2\pi} d\varphi \int_{\theta=0}^{\pi} e^{ip\rho\cos\theta} \sin\theta d\theta = 2\pi \int_{-1}^{1} e^{ip\rho x} dx = \frac{2\pi}{ip\rho}(e^{ip\rho} - e^{-ip\rho}). \tag{16.65}$$

The remaining radial integral is given by

$$G(\mathbf{r}, \mathbf{r}_2) = \frac{1}{4\pi^2\rho i} \int_0^{\infty} \frac{e^{ip\rho} - e^{-ip\rho}}{p^2 - k^2} p dp, \tag{16.66}$$

and since the integrand is an even function of p, we may set

$$G(\mathbf{r}, \mathbf{r}_2) = \frac{1}{8\pi^2\rho i} \int_{-\infty}^{\infty} \frac{(e^{i\kappa} - e^{-i\kappa})}{\kappa^2 - \sigma^2} \kappa d\kappa. \tag{16.67}$$

The latter step is taken in anticipation of the evaluation of $G_k(\mathbf{r}, \mathbf{r}_2)$ as a contour integral. The symbols κ and $\sigma(\sigma > 0)$ represent $p\rho$ and $k\rho$, respectively.

If the integral in Eq. (16.67) is interpreted as a Riemann integral, the integral does not exist. This implies that $\mathcal{L}^{-1}$ does not exist, and in a literal sense it does not. $\mathcal{L} = \nabla^2 + k^2$ is singular since there exist nontrivial solutions ψ for which the homogeneous equation $\mathcal{L}\psi = 0$. We avoid this problem by introducing a parameter γ, defining a different operator $\mathcal{L}_\gamma^{-1}$, and taking the limit as $\gamma \to 0$.

Splitting the integral into two parts so each part may be written as a suitable contour integral gives us

$$G(\mathbf{r}, \mathbf{r}_2) = \frac{1}{8\pi^2\rho i}\oint_{C_1}\frac{\kappa e^{i\kappa}\,d\kappa}{\kappa^2-\sigma^2} + \frac{1}{8\pi^2\rho i}\oint_{C_2}\frac{\kappa e^{-i\kappa}\,d\kappa}{\kappa^2-\sigma^2}. \tag{16.68}$$

Contour C_1 is closed by a semicircle in the upper half-plane, and C_2 is closed by a semicircle in the lower half-plane. These integrals were evaluated in Chapter 7 by using appropriately chosen infinitesimal semicircles to go around the singular points $\kappa = \pm\sigma$. As an alternative procedure, let us first displace the singular points from the real axis by replacing σ by $\sigma + i\gamma$ and then, after evaluation, taking the limit as $\gamma \to 0$ (Fig. 16.2).

For γ positive, contour C_1 encloses the singular point $\kappa = \sigma + i\gamma$ and the first integral contributes

$$2\pi i \cdot \frac{1}{2} e^{i(\sigma+i\gamma)}.$$

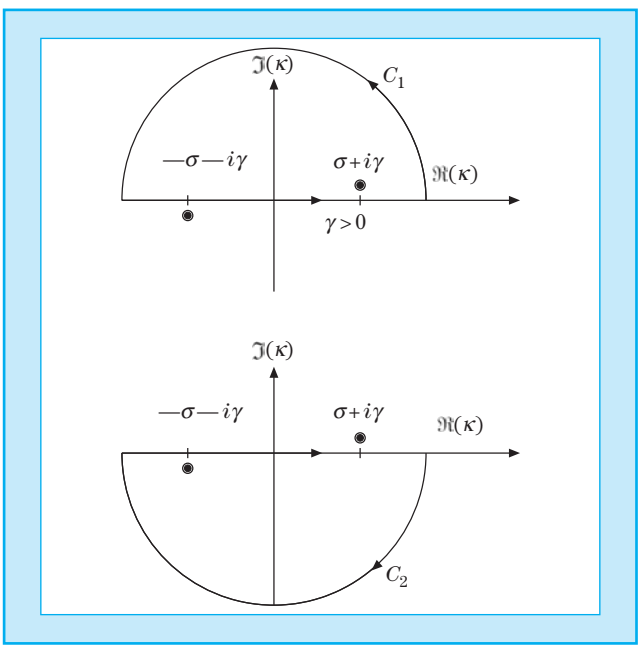


Figure 16.2

Possible Green's Function Contours of Integration

From the second integral we also obtain

$$2\pi i \cdot \frac{1}{2} e^{i(\sigma + i\gamma)},$$

the enclosed singularity being $\kappa = -(\sigma + i\gamma)$. Returning to Eq. (16.68) and letting $\gamma \to 0$, we have the retarded Green's function that propagates forward in time,

$$G(\mathbf{r}, \mathbf{r}_2) = \frac{1}{4\pi\rho} e^{i\sigma} = \frac{e^{ik|\mathbf{r}-\mathbf{r}_2|}}{4\pi|\mathbf{r}-\mathbf{r}_2|}, \tag{16.69}$$

in full agreement with Exercise 16.3.15. This solution of Helmholtz's PDE for a point source depends on starting with γ positive. Had we chosen γ negative, our Green's function would have included $e^{i\sigma}$, which corresponds to an **incoming** wave. The choice of positive γ is dictated by the boundary conditions we wish to satisfy.

Equations (16.57) and (16.69) reproduce the scattered wave in Eq. (16.53b) and constitute an exact solution of the approximate Eq. (16.53b). Exercises 16.3.17, 16.3.18, and 16.3.19 extend these results. ■

EXERCISES

16.3.1 Verify Eq. (16.42):

$$\int (v\mathcal{L}_2 u - u\mathcal{L}_2 v) d\tau_2 = \int p(\nabla_2 u - u\nabla_2 v) \cdot d\sigma_2.$$

16.3.2 Show that the terms $+k^2$ in the Helmholtz operator and $-k^2$ in the modified Helmholtz operator do not affect the behavior of $G(\mathbf{r}_1, \mathbf{r}_2)$ in the immediate vicinity of the singular point $\mathbf{r}_1 = \mathbf{r}_2$. Specifically, show that

$$\lim_{|\mathbf{r}_1 - \mathbf{r}_2| \to 0} \int k^2 G(\mathbf{r}_1, \mathbf{r}_2) d\tau_2 = 0.$$

16.3.3 Show that

$$\frac{\exp(ik|\mathbf{r}_1 - \mathbf{r}_2|)}{4\pi|\mathbf{r}_1 - \mathbf{r}_2|}$$

satisfies the two appropriate criteria and therefore is a Green's function for the Helmholtz equation.

16.3.4 (a) Find the Green's function for the three-dimensional Helmholtz equation, Exercise 16.3.3, when the wave is a standing wave.
(b) How is this Green's function related to the spherical Bessel functions?

16.3.5 The homogeneous Helmholtz equation

$$\nabla^2 \varphi + \lambda^2 \varphi = 0$$

has eigenvalues λ_i^2 and eigenfunctions φ_i. Show that the corresponding Green's function that satisfies

$$\nabla^2 G(\mathbf{r}_1, \mathbf{r}_2) + \lambda^2 G(\mathbf{r}_1, \mathbf{r}_2) = -\delta(\mathbf{r}_1 - \mathbf{r}_2)$$

may be written as

$$G(\mathbf{r}_1, \mathbf{r}_2) = \sum_{i=1}^{\infty} \frac{\varphi_i(\mathbf{r}_1)\varphi_i(\mathbf{r}_2)}{\lambda_i^2 - \lambda^2}.$$

An expansion of this form is called a bilinear expansion. If the Green's function is available in **closed** form, this provides a means of generating functions (e.g., see Chapter 11).

16.3.6 An electrostatic potential (mks units) is

$$\varphi(\mathbf{r}) = \frac{Z}{4\pi\varepsilon_0} \cdot \frac{e^{-ar}}{r}.$$

Reconstruct the electrical charge distribution that will produce this potential. Note that $\varphi(r)$ vanishes exponentially for large r, showing that the net charge is zero.

$$ANS. \quad \rho(r) = Z\delta(r) - \frac{Za^2}{4\pi}\frac{e^{-ar}}{r}.$$

16.3.7 Transform the ODE

$$\frac{d^2y(r)}{dr^2} - k^2 y(r) + V_0 \frac{e^{-r}}{r} y(r) = 0$$

and the boundary conditions $y(0) = y(\infty) = 0$ into a Fredholm integral equation of the form

$$y(r) = \lambda \int_0^{\infty} G(r, t) \frac{e^{-t}}{t} y(t) dt.$$

The quantities $V_0 = \lambda$ and k^2 are constants. The ODE is derived from the Schrödinger wave equation with a mesonic potential.

$$G(r, t) = \begin{cases} \frac{1}{k} e^{-kt} \sinh kr, & 0 \le r < t, \\ \frac{1}{k} e^{-kr} \sinh kt, & t < r < \infty. \end{cases}$$

16.3.8 A charged conducting ring of radius a (Example 11.3.3) may be described by

$$\rho(\mathbf{r}) = \frac{q}{2\pi a^2} \delta(r - a)\delta(\cos\theta).$$

Using the known Green's function for this system, find the electrostatic potential.
Hint. Exercise 11.3.3 will be helpful.

16.3.9 Changing a separation constant from k^2 to $-k^2$ and putting the discontinuity of the first derivative into the z-dependence, show that

$$\frac{1}{4\pi|\mathbf{r}_1-\mathbf{r}_2|}=\frac{1}{4\pi}\sum_{m=-\infty}^{\infty}\int_0^\infty e^{im(\varphi_1-\varphi_2)}J_m(k\rho_1)J_m(k\rho_2)e^{-k|z_1-z_2|}dk.$$

Hint. Develop $\delta(\rho_1-\rho_2)$ from Exercise 15.5.3.

16.3.10 Derive the expansion

$$\frac{\exp[ik|\mathbf{r}_1-\mathbf{r}_2|]}{4\pi|\mathbf{r}_1-\mathbf{r}_2|}=ik\sum_{l=0}^{\infty}\left\{\begin{array}{ll} j_l(kr_1)h_l^{(1)}(kr_2), & r_1<r_2\\ j_l(kr_2)h_l^{(1)}(kr_1), & r_1>r_2\end{array}\right\}\cdot\times\sum_{m=-l}^{l}Y_l^m(\theta_1\varphi_1)Y_l^{m*}(\theta_2,\varphi_2).$$

Hint. The left side is a known Green's function. Assume a spherical harmonic expansion and work on the remaining radial dependence. The spherical harmonic closure relation covers the angular dependence.

16.3.11 Show that the modified Helmholtz operator Green's function

$$\frac{\exp(-k|\mathbf{r}_1-\mathbf{r}_2|)}{4\pi|\mathbf{r}_1-\mathbf{r}_2|}$$

has the spherical polar coordinate expansion

$$\frac{\exp(-k|\mathbf{r}_1-\mathbf{r}_2|)}{4\pi|\mathbf{r}_1-\mathbf{r}_2|}=ik\sum_{l=0}^{\infty}i_l(kr_<)k_l(kr_>)\sum_{m=-l}^{l}Y_l^m(\theta_1,\varphi_1)Y_l^{m*}(\theta_2,\varphi_2).$$

Note. The modified spherical Bessel functions $i_l(kr)$ and $k_l(kr)$ are defined in Table 16.2.

16.3.12 A pointlike particle of mass m generates a Yukawa potential $V=-Ge^{-r/\lambda}/(mr)$. Obtain the potential outside a spherical distribution of such particles of total mass M and radius R.

16.3.13 From the spherical Green's function of Exercise 16.3.10, derive the plane wave expansion

$$e^{i\mathbf{k}\cdot\mathbf{r}}=\sum_{l=0}^{\infty}i^l(2l+1)j_l(kr)P_l(\cos\gamma),$$

where γ is the angle included between $\mathbf{k}$ and $\mathbf{r}$. This is the Rayleigh equation of Exercise 11.4.7.
Hint. Take $\mathbf{r}_2\gg\mathbf{r}_1$ so that

$$|\mathbf{r}_1-\mathbf{r}_2|\to r_2-\mathbf{r}_{20}\cdot\mathbf{r}_1=r_2-\frac{\mathbf{k}\cdot\mathbf{r}_1}{k}.$$

Let $r_2\to\infty$ and cancel a factor of e_2^{ikr}/r_2.

16.3.14 From the results of Exercises 16.3.10 and 16.3.13, show that

$$e^{ix} = \sum_{l=0}^{\infty} i^l (2l+1) j_l(x).$$

16.3.15 Noting that

$$\psi_k(\mathbf{r}) = \frac{1}{(2\pi)^{3/2}} e^{i\mathbf{k}\cdot\mathbf{r}}$$

is an eigenfunction of

$$(\nabla^2 + k^2)\psi_k(\mathbf{r}) = 0,$$

show that the Green's function of $\mathcal{L} = \nabla^2$ may be expanded as

$$\frac{1}{4\pi|\mathbf{r}_1 - \mathbf{r}_2|} = \frac{1}{(2\pi)^3} \int e^{i\mathbf{k}\cdot(\mathbf{r}_1 - \mathbf{r}_2)} \frac{d^3k}{k^2}.$$

16.3.16 Using Fourier transforms, show that the Green's function satisfying the nonhomogeneous Helmholtz equation

$$\left(\nabla^2 + k_0^2\right) G(\mathbf{r}_1, \mathbf{r}_2) = -\delta(\mathbf{r}_1 - \mathbf{r}_2)$$

is

$$G(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{(2\pi)^3} \int \frac{e^{i\mathbf{k}\cdot(\mathbf{r}_1 - \mathbf{r}_2)}}{k^2 - k_0^2} d^3k.$$

16.3.17 The basic equation of the scalar Kirchhoff diffraction theory is

$$\psi(\mathbf{r}_1) = \frac{1}{4\pi} \int_{S_2} \left[\frac{e^{ikr}}{r} \nabla\psi(\mathbf{r}_2) - \psi(\mathbf{r}_2) \nabla\left(\frac{e^{ikr}}{r}\right) \right] \cdot d\sigma_2,$$

where ψ satisfies the homogeneous Helmholtz equation and $r = |\mathbf{r}_1 - \mathbf{r}_2|$. Derive this equation. Assume that $\mathbf{r}_1$ is interior to the closed surface S_2.
Hint. Use Green's theorem.

16.3.18 The Born approximation for the scattered wave is given by Eq. (16.54) [and Eq. (16.61)]. From the asymptotic form [Eq. (16.58)],

$$f_k(\theta, \varphi) \frac{e^{ikr}}{r} = -\frac{2m}{\hbar^2} \int V(\mathbf{r}_2) \frac{e^{ik|\mathbf{r} - \mathbf{r}_2|}}{4\pi|\mathbf{r} - \mathbf{r}_2|} e^{i\mathbf{k}_0\cdot\mathbf{r}_2} d^3r_2.$$

For a scattering potential $V(\mathbf{r}_2)$ that is independent of angles and for $r \gg r_2$, show that

$$f_k(\theta, \varphi) = -\frac{2m}{\hbar^2} \int_0^{\infty} r_2 V(\mathbf{r}_2) \frac{\sin(|\mathbf{k}_0 - \mathbf{k}|r_2)}{|\mathbf{k}_0 - \mathbf{k}|} dr_2.$$

Here, $\mathbf{k}_0$ is in the $\theta = 0$ (original z-axis) direction, whereas $\mathbf{k}$ is in the (θ, φ) direction. The magnitudes are equal: $|\mathbf{k}_0| = |\mathbf{k}|$; m is the reduced mass.

Hint. You have Exercise 16.3.13 to simplify the exponential and Example 15.5.3 to transform the three-dimensional Fourier exponential transform into a one-dimensional Fourier sine transform.

16.3.19 Calculate the scattering amplitude $f_k(\theta, \varphi)$ for a mesonic potential $\mathbf{V}(r) = V_0(e^{-\alpha r}/\alpha r)$, V_0 a constant.
Hint. This particular potential permits the Born integral, Exercise 16.3.18, to be evaluated as a Laplace transform.

$$ANS. \quad f_k(\theta, \varphi) = -\frac{2mV_0}{\hbar^2\alpha}\frac{1}{\alpha^2 + (\mathbf{k}_0 - \mathbf{k})^2}.$$

16.3.20 The mesonic potential $V(r) = V_0(e^{-\alpha r}/\alpha r)$ may be used to describe the Coulomb scattering of two charges q_1 and q_2. We let $\alpha \to 0$ and $V_0 \to 0$ but take the ratio V_0/α to be $q_1q_2/4\pi\varepsilon_0$. (For Gaussian units, omit the $4\pi\varepsilon_0$.) Show that the differential scattering cross section $d\sigma/d\Omega = |f_k(\theta, \varphi|^2$ is given by

$$\frac{d\sigma}{d\Omega} = \left(\frac{q_1q_2}{4\pi\varepsilon_0}\right)^2 \frac{1}{16E^2\sin^4(\theta/2)}, \qquad E = \frac{p^2}{2m} = \frac{\hbar^2k^2}{2m}.$$

It happens (coincidentally) that this Born approximation is in exact agreement with both the exact quantum mechanical calculations and the classical Rutherford calculation.

Additional Reading

Bateman, H. (1944). *Partial Differential Equations of Mathematical Physics*. Dover, New York. A wealth of applications of various PDEs in classical physics. Excellent examples of the use of different coordinate systems—ellipsoidal, paraboloidal, toroidal coordinates, and so on.

Cohen, H. (1992). *Mathematics for Scientists and Engineers*. Prentice-Hall, Englewood Cliffs, NJ.

Courant, R., and Hilbert, D. (1953). *Methods of Mathematical Physics*, Vol. 1 (English edition). Interscience, New York. Reprinted, Wiley, New York (1989). This is one of the classic works of mathematical physics. Originally published in German in 1924, the revised English edition is an excellent reference for a rigorous treatment of Green's functions and a wide variety of other topics on mathematical physics.

Davis, P. J., and Rabinowitz, P. (1967). *Numerical Integration*. Blaisdell, Waltham, MA. This book covers a great deal of material in a relatively easy-to-read form. Appendix 1 (On the Practical Evaluation of Integrals by M. Abramowitz) is excellent as an overall view.

Garcia, A. L. (1994). *Numerical Methods for Physics*. Prentice-Hall, Englewood Cliffs, NJ.

Hamming, R.W. (1973). *Numerical Methods for Scientists and Engineers*, 2nd ed. McGraw-Hill, New York. Reprinted, Dover, New York (1987). This well-written text discusses a wide variety of numerical methods from zeros of functions to the fast Fourier transform. All topics are selected and developed with a modern high-speed computer in mind.

Hubbard, J., and West, B. H. (1995). *Differential Equations*. Springer, Berlin.

Margenau, H., and Murphy, G. M. (1956). *The Mathematics of Physics and Chemistry*, 2nd ed. Van Nostrand, Princeton, NJ. Chapter 5 covers curvilinear coordinates and 13 specific coordinate systems.

Morse, P. M., and Feshbach, H. (1953). *Methods of Theoretical Physics*. McGraw-Hill, New York. Chapter 5 includes a description of several different coordinate systems. Note that Morse and Feshbach are not above using left-handed coordinate systems even for Cartesian coordinates. Elsewhere in this excellent (and difficult) book there are many examples of the use of the various coordinate systems in solving physical problems. Eleven additional fascinating but seldom encountered orthogonal coordinate systems are discussed in the second edition of *Mathematical Methods for Physicists* (1970). Chapter 7 is a particularly detailed, complete discussion of Green's functions from the point of view of mathematical physics. Note, however, that Morse and Feshbach frequently choose a source of $4\pi\delta(\mathbf{r}-\mathbf{r}')$ in place of our $\delta(\mathbf{r}-\mathbf{r}')$. Considerable attention is devoted to bounded regions.

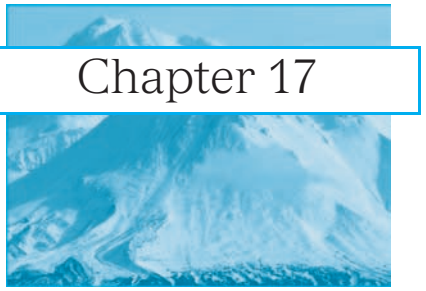
Press, W. H., Flannery, B. P., Teukolsky, S. A., and Vetterling, W. T. (1992). *Numerical Recipes*, 2nd ed. Cambridge Univ. Press, Cambridge, UK.

Ralston, A., and Wilf, H. (Eds.) (1960). *Mathematical Methods for Digital Computers*. Wiley, New York.

Ritger, P. D., and Rose, N. J. (1968). *Differential Equations with Applications*. McGraw-Hill, New York.

Stakgold, I. (1997). *Green's Functions and Boundary Value Problems*, 2nd ed. Wiley, New York.

Stoer, J., and Burlirsch, R. (1992). *Introduction to Numerical Analysis*. Springer-Verlag, New York.



Chapter 17

Probability

Probabilities arise in many problems dealing with random events or large numbers of particles defining random variables. An event is called **random** if it is practically impossible to predict from the initial state. This includes those cases in which we have merely incomplete information about initial states and/or the dynamics, as in statistical mechanics, in which we may know the energy of the system that corresponds to very many possible microscopic configurations, preventing us from predicting individual outcomes. Often, the average properties of many similar events are predictable, as in quantum theory. This is why probability theory can be and has been developed.

Random variables are involved when data depend on chance, such as weather reports or stock prices. The theory of probability describes mathematical models of chance processes in terms of probability distributions of random variables that describe how some "random events" are more likely than others. In this sense, probability is a measure of our ignorance, giving quantitative meaning to qualitative statements such as "It will probably rain tomorrow" or "I'm unlikely to draw the heart queen." Probabilities are of fundamental importance in quantum mechanics and statistical mechanics and are applied in meteorology, economics, games, and many other areas of daily life.

To a mathematician, probabilities are based on axioms, but we discuss here practical ways of calculating probabilities for random events. Because experiments in the sciences are always subject to errors, theories of errors and their propagation involve probabilities. In statistics we deal with the applications of probability theory to experimental data.

17.1 Definitions, Simple Properties

All possible **mutually exclusive**[1] outcomes of an experiment that is subject to chance represent the events or points of the **sample space** S. For example,

[1]This means that given that one particular event did occur, the others could not have occurred.

each time we toss a coin we give the trial a number $i = 1, 2, \ldots$, and observe the outcomes x_i. Here, the sample consists of two events, heads or tails, and the x_i represent a discrete random variable that takes on two values, heads or tails. When two coins are tossed, the sample contains the events two heads, one head and one tail, and two tails; the number of heads is a good value to assign to the random variable, so the possible values are 2, 1, and 0. There are four equally probable outcomes, of which one has value 2, two have value 1, and one has value 0. So the probabilities of the three values of the random variable are 1/4 for two heads (value 2), 1/4 for no heads (value 0), and 1/2 for value 1. In other words, we define the theoretical probability P of an event denoted by the point x_i of the sample as

$$P(x_i) \equiv \frac{\text{number of outcomes of event } x_i}{\text{total number of all events}}. \tag{17.1}$$

An experimental definition applies when the total number of events is not well defined (or difficult to obtain) or equally likely outcomes do not always occur. Then

$$P(x_i) \equiv \frac{\text{number of times event } x_i \text{ occurs}}{\text{total number of trials}} \tag{17.2}$$

is more appropriate. A large, thoroughly mixed pile of black and white sand grains of the same size and in equal proportions is a relevant example because it is impractical to count them all. However, we can count the grains in a small sample volume that we pick. This way, we can check that white and black grains turn up with approximately equal probability 1/2, provided we put back each sample and mix the pile again. It is found that the larger the sample volume, the smaller the spread about 1/2 will be. The more trials we run, the closer to 1/2 the average probability of all trial counts will be to 1/2. We could even pick single grains and check if the probability 1/4 of picking two black grains in a row equals that of two white grains, etc. There are many statistics questions we can pursue. Therefore, piles of colored sand provide for instructive experiments.

The following axioms are self-evident:

- Probabilities satisfy $0 \leq P \leq 1$. Probability 1 means certainty and probability 0 means impossibility.
- The entire sample has probability 1. For example, drawing an arbitrary card has probability 1.
- The probability for mutually exclusive events add. The probability for getting one head in two coin tosses is $1/2 = 1/4 + 1/4$ because it is 1/4 for head first and then tail, plus 1/4 for tail first and then head.

EXAMPLE 17.1.1

Probability for *A* or *B* What is the probability for drawing[2] a club or a jack from a shuffled deck of cards if one draws very often? Because there are

[2]These are examples of non-mutually exclusive events.

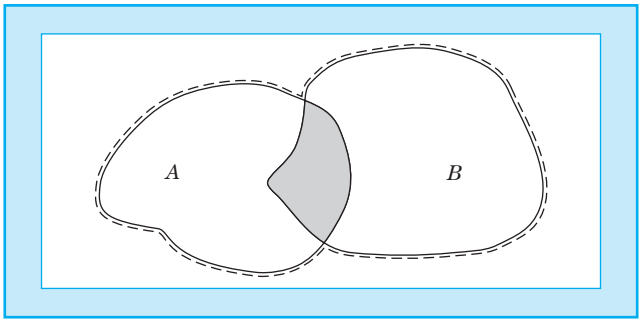


Figure 17.1

The Shaded Area Gives the Intersection $A \cap B$ Corresponding to the A and B Events, and the Dashed Line Encloses $A \cup B$ Corresponding to A or B Events

52 cards in a deck, each being equally likely, 13 cards for each suit and 4 jacks, there are 13 clubs, including the club jack and 3 other jacks; that is, there are 16 possible cards out of 52, giving the probability $(13 + 3)/52 = 16/52 = 4/13$. ■

If we represent the sample space by a set, S, of points, then events are subsets A, $B, \ldots$ of S denoted as $A \subset S$, etc. Two sets A, B are equal if A is contained in B, $A \subset B$, and B is contained in A, $B \subset A$. The **union** $A \cup B$ consists of all points (events) that are in A or B or both (Fig. 17.1). The **intersection** $A \cap B$ consists of all points that are in both A and B. If A and B have no common points, their intersection is the **empty set**, $A \cap B = \emptyset$, which has no elements (events). The set of points in A that are not in the intersection of A and B is denoted by $A - A \cap B$, **defining a subtraction of sets**. If we take the club suit in Example 17.1.1 as set A, while the four jacks are set B, then their union comprises all clubs and jacks, whereas their intersection is the club jack only.

Each subset A has its probability $P(A) \geq 0$. In terms of these set theory concepts and notations, the probability laws we just discussed become

$$0 \leq P(A) \leq 1.$$

The entire sample space has $P(S) = 1$. The probability of the union $A \cup B$ of mutually exclusive events is the sum

$$P(A \cup B) = P(A) + P(B), \quad A \cap B = \emptyset.$$

The **addition rule** for probabilities of arbitrary sets is given by the theorem

$$P(A \cup B) = P(A) + P(B) - P(A \cap B). \tag{17.3}$$

To prove this, we decompose the union into two mutually exclusive sets $A \cup B = A \cup (B - B \cap A)$, subtracting the intersection of A and B from B before joining them. Their probabilities are $P(A)$, $P(B) - P(B \cap A)$, which we add. We could also have decomposed $A \cup B = (A - A \cap B) \cup B$, from which our theorem follows similarly by adding these probabilities $P(A \cup B) = [P(A) - P(A \cap B)] + P(B)$. Note that $A \cap B = B \cap A$ (Fig. 17.1).

Sometimes the rules and definitions of probabilities that we have discussed so far are not sufficient, however.

EXAMPLE 17.1.2

Conditional Probability A simple example consists of a box of 10 identical red and 20 identical blue pens arranged in random order from which we remove pens successively, that is, without putting them back. Suppose we draw a red pen first, event A. That will happen with probability $P(A) = 10/30 = 1/3$ if the pens are thoroughly mixed up. The probability of drawing a blue pen in the next round, event B, however, will depend on the fact that we drew a red pen in the first round. It is given by $P(B|A) = 20/29$. There are $10 \cdot 20$ possible sample points in two rounds, and the sample has $30 \cdot 29$ events, so the combined probability is $P(A \cap B) = \frac{10}{30}\frac{20}{29} = \frac{10 \cdot 20}{30 \cdot 29} = \frac{20}{87}$. ■

In general, the probability $P(A \cap B)$ that A and B happen is given by the product of the probability that A happens, $P(A)$, and the probability that B happens if A does, $P(B|A)$:

$$P(A \cap B) = P(A)P(B|A). \tag{17.4}$$

In other words, the **conditional probability** $P(B|A)$ is given by the ratio

$$P(B|A) = \frac{P(A \cap B)}{P(A)}. \tag{17.5}$$

If the conditional probability $P(B|A) = P(B)$ is independent of A, then the events A and B are called **independent**, and the combined probability

$$P(A \cap B) = P(A)P(B) \tag{17.6}$$

is simply the **product of both probabilities**.

EXAMPLE 17.1.3

SAT Tests Colleges and universities rely on the verbal and mathematics SAT test scores, among others, as predictors of a student's success in passing courses and graduating. A research university is known to admit mostly students with a combined verbal and mathematics score of more than 1400 points. The graduation rate is 95%; that is, 5% drop out or transfer elsewhere. Of those who graduate, 97% have an SAT score of more than 1400 points, whereas 80% of those who drop out have an SAT score below 1400. Suppose a student has an SAT score below 1400; what is his/her probability of graduating?

Let A be the cases having an SAT test score below 1400, B represent those with scores above 1400, mutually exclusive events with $P(A) + P(B) = 1$, and C those students who graduate. That is, we want to know the conditional probabilities $P(C|A)$ and $P(C|B)$. To apply Eq. (17.5) we need $P(A)$ and $P(B)$. There are 3% of students with scores below 1400 among those who graduate

(95%) and 80% of the 5% who do not graduate, so

$$P(A) = 0.03 \cdot 0.95 + \frac{4}{5}0.05 = 0.0685, \quad P(B) = 0.97 \cdot 0.95 + 0.05/5 = 0.9315,$$

and also

$$P(C \cap A) = 0.03 \cdot 0.95 = 0.0285 \quad \text{and} \quad P(C \cap B) = 0.97 \cdot 0.95 = 0.9215.$$

Therefore,

$$P(C|A) = \frac{P(C \cap A)}{P(A)} = \frac{0.0285}{0.0685} \sim 41.6\%,$$
$$P(C|B) = \frac{P(C \cap B)}{P(B)} = \frac{0.9215}{0.9315} \sim 98.9\%,$$

that is, slightly less than 42% is the probability for a student with a score below 1400 to graduate at this particular university. ■

As a corollary to the definition [Eq. (17.5)] of a conditional probability, we compare $P(A|B) = P(A \cap B)/P(B)$ and $P(B|A) = P(A \cap B)/P(B)$, which leads to Bayes theorem

$$P(A|B) = \frac{P(A)}{P(B)}P(B|A). \tag{17.7}$$

This can be generalized to the theorem: If the random events A_i with probabilities $P(A_i) > 0$ are mutually exclusive and their union represents the entire sample S, then an arbitrary random event $B \subset S$ has the probability

$$P(B) = \sum_{i=1}^{n} P(A_i)P(B|A_i). \tag{17.8}$$

This decomposition law resembles the expansion of a vector into a basis of unit vectors defining the components of the vector. This relation follows from the obvious decomposition $B = \cup_i (B \cap A_i)$ (Fig. 17.2), which implies $P(B) = \sum_i P(B \cap A_i)$ for the probabilities because the components $B \cap A_i$ are mutually exclusive. For each i we know from Eq. (17.5) that $P(B \cap A_i) = P(A_i)P(B|A_i)$, which proves the theorem.

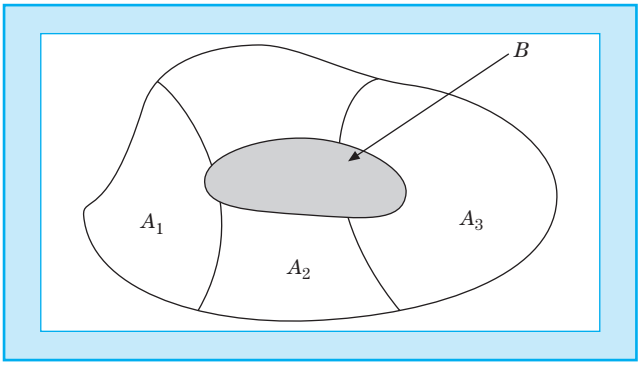


Figure 17.2

The Shaded Area *B* Is Composed of Mutually Exclusive Subsets of *B* Belonging also to A_1, A_2, A_3, where A_i Are Mutually Exclusive

Counting of Permutations and Combinations

Counting particles in samples can help us find probabilities, as in statistical mechanics.

If we have n different molecules, let us ask in how many ways we can arrange them in a row, that is, permute them. This number is defined as the number of their **permutations**. Thus, by definition, the **order matters in permutations**. There are n choices of picking the first molecule, $n-1$ for the second, etc. Altogether, there are $n!$ permutations of n **different** molecules or objects.

Generalizing this, suppose there are n people but only $k < n$ chairs to seat them. In how many ways can we seat k people in the chairs? Counting as before, we get

$$n(n-1)\cdots(n-k+1) = \frac{n!}{(n-k)!}$$

for the number of permutations of n different objects, k at a time.

We now consider the number of **combinations** of objects when their **order is irrelevant** by definition. For example, three letters a, b, c can be combined, two letters at a time, in $3 = \frac{3!}{2!}$ ways: ab, ac, bc. If letters can be repeated, then we add the pairs aa, bb, cc, and have six combinations. Thus, a **combination** of different particles differs from a permutation in that their **order does not matter**. Combinations occur with repetition (the mathematician's way of treating indistinguishable objects) and without, where no two sets contain the same particles.

The number of different combinations of n particles, k at a time and without repetitions, is given by the binomial coefficient

$$\frac{n(n-1)\cdots(n-k+1)}{k!} = \binom{n}{k}.$$

If repetition is allowed, then the number is

$$\binom{n+k-1}{k}.$$

In the number $n!/(n-k)!$ of permutations of n particles, k at a time, we have to divide out the number $k!$ of permutations of the groups of k particles because their order does not matter in a combination. This proves the first claim. The second one is shown by mathematical induction.

In statistical mechanics, we ask in how many ways we can put n particles in k boxes so that there will be n_i (alike) particles in the ith box, without regard to order in each box, with $\sum_{i=1}^{k} n_i = n$. Counting as before, there are n choices for selecting the first particle, $n-1$ for picking the second, etc., but the $n_1!$ permutations within the first box are discounted, and $n_2!$ disregarded permutations within the second box, etc. Therefore, the number of combinations is

$$\frac{n!}{n_1!n_2!\cdots n_k!}, \qquad n_1 + n_2 + \cdots + n_k = n.$$

In statistical mechanics, particles that obey

- Maxwell–Boltzmann (MB) statistics are distinguishable without restriction on their number in each state;
- Bose–Einstein (BE) statistics are indistinguishable with no restriction on the number of particles in each quantum state; and
- Fermi–Dirac (FD) statistics are indistinguishable with at most one particle per state.

For example, putting three particles in four boxes, there are 4^3 equally likely arrangements for the MB case because each particle can be put into any box in four ways, giving a total of 4^3 choices. For BE statistics, the number of combinations with repetitions is $\binom{3+4-1}{3} = \binom{6}{3}$. For FD statistics, it is $\binom{3+1}{3} = \binom{4}{3}$. More generally for MB statistics, the number of distinct arrangements of n particles among k states (boxes) is k^n, for BE statistics it is $\binom{n+k-1}{n}$ with $k > n$, and for FD statistics it is $\binom{k}{n}$.

EXERCISES

17.1.1 A card is drawn from a shuffled deck. (a) What is the probability that it is black, (b) a red nine, (c) or a queen of spades?

17.1.2 Find the probability of drawing two kings from a shuffled deck of cards (a) if the first card is put back before the second is drawn, and (b) if the first card is not put back after being drawn.

17.1.3 When two fair dice are thrown, what is the probability of (a) observing a number less than 4 or (b) a number greater than or equal to 4, but less than 6?

17.1.4 Rolling three fair dice, what is the probability of obtaining six points?

17.1.5 Determine the probability $P(A \cap B \cap C)$ in terms of $P(A)$, $P(B)$, $P(C)$, etc.

17.1.6 Determine directly or by mathematical induction the probability of a distribution of N (Maxwell–Boltzmann) particles in k boxes with N_1 in box 1, N_2 in box 2, $\ldots$, N_k in the kth box for any numbers $N_j \geq 1$ with $N_1 + N_2 + \cdots + N_k = N,\ k < N$. Repeat this for Fermi–Dirac and Bose–Einstein particles.

17.1.7 Show that $P(A \cup B \cup C) = P(A) + P(B) + P(C) - P(A \cap B) - P(A \cap C) - P(B \cap C) + P(A \cap B \cap C)$.

17.1.8 Determine the probability that a positive integer $n \leq 100$ is divisible by a prime number $p \leq 100$. Verify your result for $p = 3, 5, 7$.

17.1.9 Put two particles obeying Maxwell–Boltzmann (Fermi–Dirac, or Bose–Einstein) statistics in three boxes. How many ways are there in each case?

17.2 Random Variables

Each time we toss a die, we give the trial a number $i = 1, 2, \ldots$ and observe the point $x_i = 1$ or 2, 3, 4, 5, 6 with probability 1/6. If i denotes the trial number, then x_i is a discrete random variable that takes the discrete values from 1 to 6 with a definite probability $P(x_i) = 1/6$ over many trials.

EXAMPLE 17.2.1

Discrete Random Variable If we toss two dice and record the sum of the points shown in each trial, then this sum is also a discrete random variable that takes on the value 2 when both dice show 1 with probability $(1/6)^2$; the value 3 when one die has 1 and the other 2 hence with probability $(1/6)^2 + (1/6)^2 = 1/18$; the value 4 when both dice have 2 or one has 1 and the other 3, hence with probability $(1/6)^2 + (1/6)^2 + (1/6)^2 = 1/12$; the value 5 with probability $4(1/6)^2 = 1/9$; the value 6 with probability 5/36; the value 7 with the maximum probability $6(1/6)^2 = 1/6$; up to the value 12 when both dice show 6 points with probability $(1/6)^2$. This probability distribution is symmetric about 7. This symmetry is obvious from Fig. 17.3 and becomes visible algebraically when we write the rising and falling linear parts as

$$P(x) = \frac{x-1}{36} = \frac{6-(7-x)}{36}, \quad x = 2, 3, \ldots, 7,$$
$$P(x) = \frac{13-x}{36} = \frac{6+(7-x)}{36}, \quad x = 7, 8, \ldots, 12. \blacksquare$$

SUMMARY

In summary, the different values x_i that a random variable X assumes denote and distinguish the events in the sample space of an experiment; each event occurs by chance with a probability $P(X = x_i) = p_i \geq 0$ that is a function of the random variable X. A random variable $X(e_i) = x_i$ is defined on the sample space, that is, for the events $e_i \in S$.

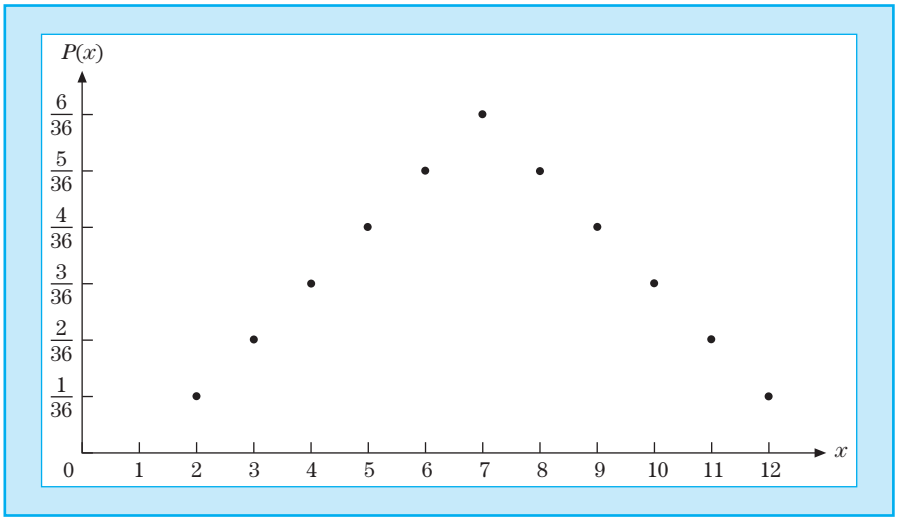


Figure 17.3

Probability Distribution $P(x)$ of the Sum of Points when Two Dice Are Tossed

We define the probability density $f(x)$ of a **continuous random variable** X as

$$P(x \le X \le x + dx) = f(x)dx, \tag{17.9}$$

that is, $f(x)dx$ is the probability that X lies in the interval $x \le X \le x+dx$. For $f(x)$ to be a probability density, it has to satisfy $f(x) \ge 0$ and $\int f(x)dx = 1$. The generalization to probability distributions depending on several random variables is straightforward. Quantum physics abounds in examples.

EXAMPLE 17.2.2

Continuous Random Variable: Hydrogen Atom Quantum mechanics gives the probability $|\psi|^2\, d^3r$ of finding a $1s$ electron in a hydrogen atom in volume[3] d^3r, where $\psi = Ne^{-r/a}$ is the wave function that is normalized to

$$1 = \int |\psi|^2\, dV = 4\pi N^2 \int_0^\infty e^{-2r/a} r^2\, dr = \pi a^3 N^2, \quad dV = r^2\, dr d\cos\theta\, d\varphi$$

being the volume element and a the Bohr radius. The radial integral is found by repeated integration by parts or by rescaling it to the gamma function

$$\int_0^\infty e^{-2r/a} r^2\, dr = \left(\frac{a}{2}\right)^3 \int_0^\infty e^{-x} x^2\, dx = a^3\Gamma(3)/8 = a^3/4.$$

Here, all points in space constitute the sample and represent three random variables, but the probability density $|\psi|^2$ in this case depends only on the radial variable because of the spherical symmetry of the $1s$ state.

A measure for the size of the hydrogen atom is given by the average radial distance of the electron from the proton at the center, which is called the expectation value

$$\langle 1s|r|1s\rangle = \int r|\psi|^2 dV = 4\pi N^2 \int_0^\infty r e^{-2r/a} r^2\, dr = \frac{3}{2}a$$

in quantum mechanics. We shall define this concept for arbitrary probability distributions later. ■

- A random variable that takes only discrete values $x_1, x_2, \ldots, x_n$ with probabilities $p_1, p_2, \ldots, p_n$, respectively, is called a discrete random variable so that $\sum_i p_i = 1$. If an "experiment" or trial is performed, some outcome must occur, with unit probability.
- If the values comprise a continuous range of values $a \le x \le b$, then we deal with a continuous random variable whose probability distribution may or may not be a continuous function as well.

[3]Note that $|\psi|^2 4\pi r^2 dr$ gives the probability for the electron to be found between r and $r + dr$, at any angle.

When we measure a quantity x n times, obtaining the values x_j, we define the **average value**

$$\bar{x} \equiv \frac{1}{n}\sum_{j=1}^{n} x_j \tag{17.10}$$

of the trials, also called the **mean or expectation value**, where this formula assumes that every observed value x_i is equally likely and occurs with probability $1/n$. This connection is the key link of experimental data with probability theory. This observation and practical experience suggest defining the **mean value for a discrete random variable** X as

$$\langle X\rangle \equiv \sum_i x_i p_i \tag{17.11}$$

and for a **continuous random variable** as

$$\langle X\rangle \equiv \int x f(x) dx. \tag{17.12}$$

These are linear averages. Other notations in the literature are $\bar{X}$ or $E(X)$.

The use of the arithmetic mean $\bar{x}$ of n measurements as the average value is suggested by simplicity and plain experience, assuming equal probability for each x_i again. Why do we not consider the geometric mean

$$x_g = (x_1 \cdot x_2 \cdots x_n)^{1/n} \tag{17.13}$$

or the harmonic mean x_h determined by the relation

$$\frac{1}{x_h} = \frac{1}{n}\left(\frac{1}{x_1} + \frac{1}{x_1} + \cdots + \frac{1}{x_n}\right) \tag{17.14}$$

or that value $\tilde{x}$ which minimizes the sum of absolute deviations $|x_i - \tilde{x}|$? Here, the x_i are taken to increase monotonically. When we plot $O(x) = \sum_{i=1}^{2n+1} |x_i - x|$ as in Fig. 17.4(a) for an odd number of points, we realize that it has a minimum

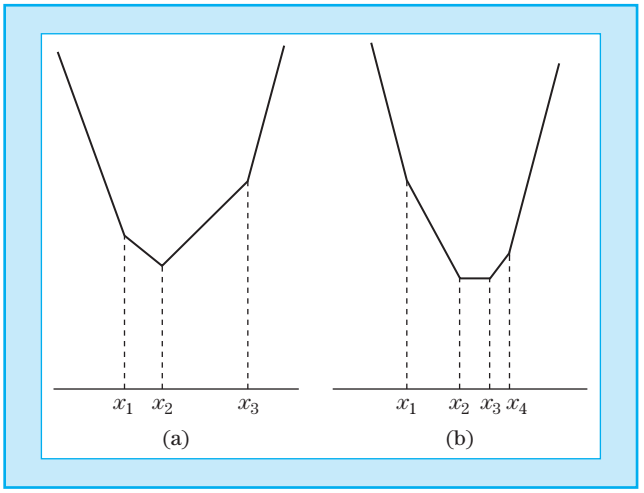


Figure 17.4

(a) $\sum_{i=1}^{3} |x_i - x|$ for an Odd Number of Points; (b) $\sum_{i=1}^{4} |x_i - x|$ for an Even Number of Points

at its central value $i = n$, whereas for an even number of points $E(x) = \sum_{i=1}^{2n} |x_i - x|$ is flat in its central region, as shown in Fig. 17.4(b). These properties make these functions unacceptable for determining average values. Instead, when we minimize the sum of quadratic deviations

$$\sum_{i=1}^{n} (x - x_i)^2 = \text{ minimum}, \tag{17.15}$$

setting the derivative equal to zero, yields $2\sum_i (x - x_i) = 0$ or

$$x = \frac{1}{n} \sum_i x_i = \bar{x};$$

that is, the arithmetic mean. It has another important property: If we denote the deviations by $v_i = x_i - \bar{x}$, then $\sum_i v_i = 0$; that is, the sum of positive deviations equals the sum of negative deviations. This principle of minimizing the quadratic sum of deviations is called the **method of least squares** and is due to C. F. Gauss, among others.

How close a fit of the mean value is to a set of data points depends on the spread of the individual measurements from this mean. Again, we reject the average sum of deviations $\sum_{i=1}^{n} |x_i - \bar{x}|/n$ as a measure of the spread because it selects the central measurement as the best value for no good reason. A more appropriate definition of the spread is the average of the deviations from the mean, squared, or **standard deviation**

$$\sigma = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (x_i - \bar{x})^2},$$

where the square root is motivated by dimensional analysis.

EXAMPLE 17.2.3

Standard Deviation of Measurements From the measurements $x_1 = 7$, $x_2 = 9, x_3 = 10, x_4 = 11, x_5 = 13$, we extract $\bar{x} = 10$ for the mean value and $\sigma = \sqrt{(9 + 1 + 1 + 9)/4} = 2.2361$ for the standard deviation or spread, using the experimental formula [Eq. (17.2)] because the probabilities are not known. ■

There is another interpretation of the variance in terms of the sum of squares of measurement differences

$$\begin{aligned} \sum_{i<k} (x_i - x_k)^2 &= \frac{1}{2} \sum_{i=1}^{n} \sum_{k=1}^{n} \left(x_i^2 + x_k^2 - 2x_i x_k\right) \\ &= \frac{1}{2} (2n^2 \langle x^2 \rangle - 2n^2 \langle x \rangle^2) = n^2 \sigma^2, \end{aligned} \tag{17.16}$$

because by multiplying out the square in the definition of σ^2, we obtain

$$\sigma^2 = \frac{1}{n}\sum_i (x_i - \langle x\rangle)^2 = \frac{1}{n}\sum_i x_i^2 - \frac{2\langle x\rangle}{n}\sum_i x_i + \langle x\rangle^2$$
$$= \frac{1}{n}\sum_i x_i^2 - \langle x\rangle^2 = \langle x^2\rangle - \langle x\rangle^2. \tag{17.17}$$

This formula is often used and widely applied for σ^2.

Now we are ready to generalize the spread in a set of n measurements with equal probability $1/n$ to the **variance** of an arbitrary probability distribution. For a discrete random variable X with probabilities p_i at $X = x_i$ we define the **variance**

$$\sigma^2 = \sum_j (x_j - \langle X\rangle)^2 p_j, \tag{17.18}$$

and similarly for a continuous probability distribution

$$\sigma^2 = \int_{-\infty}^{\infty} (x - \langle X\rangle)^2 f(x)dx. \tag{17.19}$$

These definitions imply the following theorem: If a random variable $Y = aX + b$ is linearly related to X, then we can immediately derive the mean value $\langle Y\rangle = a\langle X\rangle + b$ and variance $\sigma^2(Y) = a^2\sigma^2(X)$ from these definitions.

We prove this theorem only for a continuous distribution and leave the case of a discrete random variable as an exercise for the reader. For the infinitesimal probability we know that $f(x)dx = g(y)dy$, with $y = ax+b$, because the linear transformation has to preserve probability, so

$$\langle Y\rangle = \int_{-\infty}^{\infty} yg(y)dy = \int_{-\infty}^{\infty} (ax + b)f(x)dx = a\langle X\rangle + b$$

since $\int f(x)dx = 1$. For the variance we similarly obtain

$$\sigma^2(Y) = \int_{-\infty}^{\infty} (y - \langle Y\rangle)^2 g(y)dy = \int_{-\infty}^{\infty} (ax + b - a\langle X\rangle - b)^2 f(x)dx$$
$$= a^2\sigma^2(X)$$

after substituting our result for the mean value $\langle Y\rangle$.

Finally, we prove the general **Chebyshev inequality**

$$P(|x - \langle X\rangle| \geq k\sigma) \leq \frac{1}{k^2}, \tag{17.20}$$

which demonstrates why the standard deviation serves as a measure of the spread of an arbitrary probability distribution from its mean value $\langle X\rangle$ and shows why experimental or other data are often characterized according to their spread in numbers of standard deviations. We first show the simpler inequality

$$P(Y \geq K) \leq \frac{\langle Y\rangle}{K}$$

for a continuous random variable Y whose values $y \geq 0$. (The proof for a discrete random variable follows along similar lines.) This inequality follows from

$$\langle Y\rangle = \int_0^\infty yf(y)dy = \int_0^K yf(y)dy + \int_K^\infty yf(y)dy$$
$$\geq \int_K^\infty yf(y)dy \geq K\int_K^\infty f(y)dy = KP(Y \geq K).$$

Next, we apply the same method to the positive variance integral

$$\sigma^2 = \int (x - \langle X\rangle)^2 f(x)dx \geq \int_{|x-\langle X\rangle|\geq k\sigma} (x - \langle X\rangle)^2 f(x)dx$$
$$\geq k^2\sigma^2 \int_{|x-\langle X\rangle|\geq k\sigma} f(x)dx = k^2\sigma^2 P(|x - \langle X\rangle| \geq k\sigma),$$

decreasing the right-hand side first by omitting the part of the positive integral with $|x-\langle X\rangle| \leq k\sigma$, then again by replacing $(x-\langle X\rangle)^2$ in the remaining integral by its lowest limit $k^2\sigma^2$. This proves the Chebyshev inequality. For $k = 3$ we have the conventional three standard deviation estimate

$$P(|x - \langle X\rangle| \geq 3\sigma) \leq \frac{1}{9}. \tag{17.21}$$

It is straightforward to generalize the mean value to higher moments of probability distributions relative to the mean value $\langle X\rangle$:

$$\langle (X - \langle X\rangle)^k\rangle = \sum_j (x_j - \langle X\rangle)^k p_j, \quad \text{discrete distribution,} \tag{17.22}$$

$$\langle (X - \langle X\rangle)^k\rangle = \int_{-\infty}^\infty (x - \langle X\rangle)^k f(x)dx, \quad \text{continuous distribution.}$$

The **moment generating function**

$$\langle e^{tX}\rangle = \int e^{tx} f(x)dx = 1 + t\langle X\rangle + \frac{t^2}{2!}\langle X^2\rangle + \cdots \tag{17.23}$$

is a weighted sum of the moments of the continuous random variable X upon substituting the Taylor expansion of the exponential function. Therefore, $\langle X\rangle = \frac{d\langle e^{tX}\rangle}{dt}|_{t=0}$. Notice that the moments here are not relative to the expectation value; they are called central moments. The nth central moment $\langle X^n\rangle = \frac{d^n\langle e^{tX}\rangle}{dt^n}|_{t=0}$ is given by the nth derivative of the moment generating function at $t = 0$. By a change of the parameter $t \to it$, the moment generating function is related to the **characteristic function** $\langle e^{itX}\rangle$, which is the often used Fourier transform of the probability density $f(x)$.

Moreover, mean values, moments, and variance can be defined similarly for probability distributions that depend on several random variables. For simplicity, let us restrict our attention to two continuous random variables

$X,\ Y$ and list the corresponding quantities

$$\langle X\rangle = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} xf(x,\,y)\,dx\,dy,$$

$$\langle Y\rangle = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} yf(x,\,y)\,dx\,dy, \tag{17.24}$$

$$\sigma^2(X) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} (x-\langle X\rangle)^2 f(x,\,y)\,dx\,dy,$$

$$\sigma^2(Y) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} (y-\langle Y\rangle)^2 f(x,\,y)\,dx\,dy. \tag{17.25}$$

Two random variables are said to be **independent if the probability density** $f(x,\,y)$ **factorizes** into a product $f(x)g(y)$ of probability distributions of one random variable each.

The covariance defined as

$$\operatorname{cov}(X,\,Y) = \langle (X-\langle X\rangle)(Y-\langle Y\rangle)\rangle \tag{17.26}$$

is a measure of how much the random variables $X,\ Y$ are correlated (or related): It is zero for independent random variables because

$$\begin{aligned}\operatorname{cov}(X,\,Y) &= \int (x-\langle X\rangle)(y-\langle Y\rangle)f(x,\,y)\,dx\,dy\\ &= \int (x-\langle X\rangle)f(x)\,dx\int (y-\langle Y\rangle)g(y)\,dy\\ &= (\langle X\rangle-\langle X\rangle)(\langle Y\rangle-\langle Y\rangle) = 0.\end{aligned}$$

The normalized covariance $\frac{\operatorname{cov}(X,Y)}{\sigma(X)\sigma(Y)}$ that has values between -1 and $+1$ is often called **correlation**.

In order to demonstrate that the correlation is bounded by

$$-1 \le \frac{\operatorname{cov}(X,\,Y)}{\sigma(X)\sigma(Y)} \le 1,$$

we analyze the positive mean value

$$\begin{aligned}Q &= \langle [u(X-\langle X\rangle)+v(Y-\langle Y\rangle)]^2\rangle\\ &= u^2\langle [X-\langle X\rangle]^2\rangle + 2uv\langle [X-\langle X\rangle][Y-\langle Y\rangle]\rangle + v^2\langle [Y-\langle Y\rangle]^2\rangle\\ &= u^2\sigma(X)^2 + 2uv\,\operatorname{cov}(X,\,Y) + v^2\sigma(Y)^2 \ge 0,\end{aligned} \tag{17.27}$$

where $u,\,v$ are numbers, not functions. For this quadratic form to be non-negative, its discriminant must obey $\operatorname{cov}(X,\,Y)^2 - \sigma(X)^2\sigma(Y)^2 \le 0$, which proves the desired inequality.

The usefulness of the correlation as a quantitative measure is emphasized by the following theorem: $P(Y = aX + b) = 1$ is valid if, and only if, the correlation is equal to ± 1. This theorem states that a $\pm 100\%$ correlation between

X, Y implies not only some functional relation between both random variables but also a **linear relation** between them. We denote by $\langle B|A\rangle$ the expectation value of the conditional probability distribution $P(B|A)$.

To prove this strong correlation property, we apply Bayes's decomposition law [Eq. (17.8)] to the mean value and variance of the random variable Y, assuming first $P(Y = aX + b) = 1$, so that $P(Y \neq aX + b) = 0$. This yields

$$\begin{aligned}\langle Y\rangle &= P(Y = aX + b)\langle Y|Y = aX + b\rangle \\ &\quad + P(Y \neq aX + b)\langle Y|Y \neq aX + b\rangle \\ &= \langle aX + b\rangle = a\langle X\rangle + b,\end{aligned}$$

$$\begin{aligned}\sigma(Y)^2 &= P(Y = aX + b)\langle [Y - \langle Y\rangle]^2|Y = aX + b\rangle \\ &\quad + P(Y \neq aX + b)\langle [Y - \langle Y\rangle]^2|Y \neq aX + b\rangle \\ &= \langle [aX + b - \langle Y\rangle]^2\rangle = \langle a^2[X - \langle X\rangle]^2\rangle = a^2\sigma(X)^2,\end{aligned}$$

substituting $\langle Y\rangle = a\langle X\rangle + b$. Similarly, we obtain $\text{cov}(X, Y) = a^2\sigma(X)^2$. These results show that the correlation is ± 1.

Conversely, we start from $\text{cov}(X, Y)^2 = \sigma(X)^2\sigma(Y)^2$. Hence, the quadratic form in Eq. (17.27) must be zero for (practically) all x for some $(u_0, v_0) \neq (0, 0)$

$$\langle [u_0(X - \langle X\rangle) + v_0(Y - \langle Y\rangle)]^2\rangle = 0.$$

Because the argument of this mean value is positive definite, this relationship is satisfied only if $P(u_0(X - \langle X\rangle) + v_0(Y - \langle Y\rangle) = 0) = 1$, which means that Y and X are linearly related.

When we integrate out one random variable we are left with the probability distribution of the other random variable

$$F(x) = \int f(x, y)\,dy, \quad \text{or} \quad G(y) = \int f(x, y)\,dx \tag{17.28}$$

and analogously for discrete probability distributions. When one or more random variables are integrated out, the remaining probability distribution is called **marginal,** motivated by the geometric aspects of projection. It is straightforward to show that these marginal distributions satisfy all the requirements of properly normalized probability distributions.

If we are interested in the distribution of the random variable X for a definite value $y = y_0$ of the other random variable, then we deal with a **conditional probability distribution** $P(X = x|Y = y_0)$. The corresponding continuous probability density is $f(x, y_0)$.

EXAMPLE 17.2.4

Repeated Draws of Cards When we draw cards repeatedly, we shuffle the deck often because we want to make sure these events stay independent. So we draw the first card at random from a bridge deck containing 52 cards and then place it back at a random place. Now we repeat the process for a second card. Then the deck is reshuffled, etc. We now define the random variables

- $X =$ number of so-called honors; that is, 10s, jacks, queens, kings, or aces;
- $Y =$ number of 2s or 3s.

In a single draw the probability of a 10 to ace is $a = 5 \cdot 4/52 = 5/13$, and $b = 2 \cdot 4/52 = 2/13$ for 2 or 3 to be drawn and $c = (13 - 5 - 2)/13 = 6/13$ for anything else with $a + b + c = 1$.

In two drawings X and Y can be $x = 0 = y$, when no 10 to ace show up nor 2 or 3. This case has probability c^2. In general, X, Y can be any combination of 0, 1, or 2 so that $0 \le x + y \le 2$ because we will hold two cards at the end. The probability function of $(X = x, Y = y)$ is given by the product of the probabilities of the three possibilities a^x, b^y, c^{2-x-y} times the number of distributions (or permutations) of two cards over the three cases with probabilities a, b, c, which is $2!/[x!y!(2 - x - y)!]$. This number is the coefficient of the power $a^x b^y c^{2-x-y}$ in the generalized binomial expansion of all possibilities in two drawings with probability 1:

$$1 = (a + b + c)^2 = \sum_{0 \le x+y \le 2} \frac{2!}{x!y!(2 - x - y)!} a^x b^y c^{2-x-y} \tag{17.29}$$

$$= a^2 + b^2 + c^2 + 2(ab + ac + bc).$$

Hence, the probability distribution of our discrete random variables is given by

$$f(X = x, Y = y) = \frac{2!}{x!y!(2 - x - y)!} \left(\frac{5}{13}\right)^x \left(\frac{2}{13}\right)^y \left(\frac{6}{13}\right)^{2-x-y},$$
$$x, y = 0, 1, 2; 0 \le x + y \le 2 \tag{17.30}$$

or more explicitly as

$$f(0, 0) = \left(\frac{6}{13}\right)^2, \quad f(1, 0) = 2 \cdot \frac{5}{13} \cdot \frac{6}{13} = \frac{60}{13^2},$$
$$f(2, 0) = \left(\frac{5}{13}\right)^2, \quad f(0, 1) = 2 \cdot \frac{2}{13} \cdot \frac{6}{13} = \frac{24}{13^2},$$
$$f(0, 2) = \left(\frac{2}{13}\right)^2, \quad f(1, 1) = 2 \cdot \frac{5}{13} \cdot \frac{2}{13} = \frac{20}{13^2}.$$

The probability distribution is properly normalized according to Eq. (17.29). Its expectation values are given by

$$\langle X \rangle = \sum_{0 \le x+y \le 2} x f(x, y) = f(1, 0) + f(1, 1) + 2f(2, 0)$$
$$= \frac{60}{13^2} + \frac{20}{13^2} + 2\left(\frac{5}{13}\right)^2 = \frac{130}{13^2} = \frac{10}{13} = 2a$$

and

$$\langle Y\rangle = \sum_{0\le x+y\le 2} y f(x,y) = f(0,1) + f(1,1) + 2f(0,2)$$
$$= \frac{24}{13^2} + \frac{20}{13^2} + 2\left(\frac{2}{13}\right)^2 = \frac{52}{13^2} = \frac{4}{13} = 2b,$$

as expected because we are drawing a card two times. The variances are

$$\sigma^2(X) = \sum_{0\le x+y\le 2} \left(x - \frac{10}{13}\right)^2 f(x,y)$$
$$= \left(\frac{10}{13}\right)^2 [f(0,0) + f(0,1) + f(0,2)]$$
$$+ \left(\frac{3}{13}\right)^2 [f(1,0) + f(1,1)] + \left(\frac{16}{13}\right)^2 f(2,0)$$
$$= \frac{10^2\cdot 64 + 3^2\cdot 80 + 16^2\cdot 5^2}{13^4} = \frac{4^2\cdot 5\cdot 169}{13^4} = \frac{80}{13^2},$$

$$\sigma^2(Y) = \sum_{0\le x+y\le 2} \left(y - \frac{4}{13}\right)^2 f(x,y)$$
$$= \left(\frac{4}{13}\right)^2 [f(0,0) + f(1,0) + f(2,0)]$$
$$+ \left(\frac{9}{13}\right)^2 [f(0,1) + f(1,1)] + \left(\frac{22}{13}\right)^2 f(0,2)$$
$$= \frac{4^2\cdot 11^2 + 9^2\cdot 44 + 22^2\cdot 2^2}{13^4} = \frac{11\cdot 4\cdot 169}{13^4} = \frac{44}{13^2}.$$

It is reasonable that $\sigma^2(Y) < \sigma^2(X)$ because Y takes only two values 2, 3, whereas X varies over the five honors. The covariance is given by

$$\operatorname{cov}(X,Y) = \sum_{0\le x+y\le 2} \left(x - \frac{10}{13}\right)\left(y - \frac{4}{13}\right) f(x,y)$$
$$= \frac{10\cdot 4}{13^2}\cdot\frac{6^2}{13^2} - \frac{10\cdot 9}{13^2}\cdot\frac{24}{13^2} - \frac{10\cdot 22}{13^2}\cdot\frac{4}{13^2} - \frac{3\cdot 4}{13^2}\cdot\frac{60}{13^2}$$
$$+ \frac{3\cdot 9}{13^2}\cdot\frac{20}{13^2} - \frac{16\cdot 4}{13^2}\cdot\frac{5^2}{13^2} = -\frac{20\cdot 169}{13^4} = -\frac{20}{13^2}.$$

Therefore, the correlation of the random variables X, Y is given by

$$\frac{\operatorname{cov}(X,Y)}{\sigma(X)\sigma(Y)} = -\frac{20}{8\sqrt{5\cdot 11}} = -\frac{1}{2}\sqrt{\frac{5}{11}} = -0.3371,$$

which means that there is a small (negative) correlation between these random variables because if a card is an honor it cannot be a 2 or 3 and vice versa.

Finally, let us determine the marginal distribution

$$F(X = x) = \sum_{y=0}^{2} f(x, y) \tag{17.31}$$

or explicitly

$$F(0) = f(0, 0) + f(0, 1) + f(0, 2) = \left(\frac{6}{13}\right)^2 + \frac{24}{13^2} + \left(\frac{2}{13}\right)^2 = \left(\frac{8}{13}\right)^2,$$
$$F(1) = f(1, 0) + f(1, 1) = \frac{60}{13^2} + \frac{20}{13^2} = \frac{80}{13^2},$$
$$F(2) = f(2, 0) = \left(\frac{5}{13}\right)^2,$$

which is properly normalized because

$$F(0) + F(1) + F(2) = \frac{64 + 80 + 25}{13^2} = \frac{169}{13^2} = 1.$$

Its mean value is given by

$$\langle X\rangle_F = \sum_{x=0}^{2} xF(x) = F(1) + 2F(2) = \frac{80 + 2 \cdot 25}{13^2} = \frac{130}{13^2} = \frac{10}{13} = \langle X\rangle,$$

and its variance

$$\sigma_F^2 = \sum_{x=0}^{2} \left(x - \frac{10}{13}\right)^2 F(x) = \left(\frac{10}{13}\right)^2 \cdot \left(\frac{8}{13}\right)^2 + \left(\frac{3}{13}\right)^2 \frac{80}{13^2} + \left(\frac{16}{13}\right)^2 \cdot \left(\frac{5}{13}\right)^2$$
$$= \frac{80 \cdot 169}{13^4} = \frac{80}{13^2} = \sigma^2(X).$$

From the definitions, it follows that these results hold generally. ■

Finally, we address the transformation of two random variables X, Y into $U(X, Y)$, $V(X, Y)$. We treat the continuous case, leaving the discrete case as an exercise. If

$$u = u(x, y), \quad v = v(x, y); \quad x = x(u, v), \quad y = y(u, v), \tag{17.32}$$

describe the transformation and its inverse; then the probability stays invariant and the integral of the density transforms according to the rules of Chapter 2 so that the transformed probability density becomes

$$g(u, v) = f(x(u, v), y(u, v))|J|, \tag{17.33}$$

with the Jacobian

$$J = \frac{\partial(x, y)}{\partial(u, v)} = \begin{vmatrix} \frac{\partial x}{\partial u} & \frac{\partial x}{\partial v} \\ \frac{\partial y}{\partial u} & \frac{\partial y}{\partial v} \end{vmatrix}. \tag{17.34}$$

EXAMPLE 17.2.5

Sum, Product, and Ratio of Random Variables Let us consider three examples. **First, the sum** $Z = X + Y$, where the transformation may be taken to be

$$x = x, \quad z = x + y, \quad J = \begin{vmatrix} 1 & 1 \\ 0 & 1 \end{vmatrix},$$

using

$$\frac{\partial x}{\partial x} = 1, \quad \frac{\partial(z - y)}{\partial z} = 1, \quad \frac{\partial y}{\partial x} = 0, \quad \frac{\partial(z - x)}{\partial z} = 1,$$

so that the probability is given by

$$F(Z) = \int_{-\infty}^{Z} \int_{-\infty}^{\infty} f(x, z - x)\, dx\, dz. \tag{17.35}$$

If the random variables X, Y are independent with densities f_1, f_2, then

$$F(Z) = \int_{-\infty}^{Z} \int_{-\infty}^{\infty} f_1(x) f_2(z - x)\, dx\, dz. \tag{17.36}$$

Second, the product $Z = XY$ taking X, Z as the new variables leads to the Jacobian

$$J = \begin{vmatrix} 1 & \frac{1}{y} \\ 0 & \frac{1}{x} \end{vmatrix} = \frac{1}{x},$$

using

$$\frac{\partial x}{\partial x} = 1, \quad \frac{\partial\left(\frac{z}{y}\right)}{\partial z} = \frac{1}{y}, \quad \frac{\partial y}{\partial x} = 0, \quad \frac{\partial\left(\frac{z}{x}\right)}{\partial z} = \frac{1}{x},$$

so that the probability is given by

$$F(Z) = \int_{-\infty}^{Z} \int_{-\infty}^{\infty} f\left(x, \frac{z}{x}\right) \frac{dx}{|x|} dz. \tag{17.37}$$

If the random variables X, Y are independent with densities f_1, f_2, then

$$F(Z) = \int_{-\infty}^{Z} \int_{-\infty}^{\infty} f_1(x) f_2\left(\frac{z}{x}\right) \frac{dx}{|x|} dz. \tag{17.38}$$

Third, the ratio $Z = \frac{X}{Y}$ taking Y, Z as the new variables has the Jacobian

$$J = \begin{vmatrix} z & y \\ 1 & 0 \end{vmatrix} = -y,$$

using

$$\frac{\partial(yz)}{\partial y} = z, \quad \frac{\partial(yz)}{\partial z} = y, \quad \frac{\partial y}{\partial y} = 1, \quad \frac{\partial y}{\partial z} = 0,$$

so that the probability is given by

$$F(Z) = \int_{-\infty}^{Z} \int_{-\infty}^{\infty} f(yz, y)|y| dy\, dz. \tag{17.39}$$

If the random variables X, Y are independent with densities f_1, f_2, then

$$F(Z) = \int_{-\infty}^{Z} \int_{-\infty}^{\infty} f_1(yz) f_2(y)|y| dy\, dz. \tag{17.40}$$

EXERCISES

17.2.1 Show that adding a constant c to a random variable X changes the expectation value $\langle X \rangle$ by that same constant but not the variance. Show also that multiplying a random variable by a constant multiplies both the mean and variance by that constant. Show that the random variable $X - \langle X \rangle$ has mean value zero.

17.2.2 If $\langle X \rangle$, $\langle Y \rangle$ are the average values of two independent random variables X, Y, what is the expectation value of the product $X \cdot Y$?

17.2.3 A velocity $v_j = x_j/t_j$ is measured by recording the distances x_j at the corresponding times t_j. Show that $\bar{x}/\bar{t}$ is a good approximation for the average velocity v provided all the errors $|x_j - \bar{x}| \ll |\bar{x}|$ and $|t_j - \bar{t}| \ll |\bar{t}|$ are small.

17.2.4 Define the random variable Y in Example 17.2.4 as the number of 4, or 5, or 6, or 7, or 8, or 9. Then determine the correlation of the X and Y random variables.

17.2.5 If X and Y are two independent random variables with different probability densities and the function $f(x, y)$ has derivatives of any order, express $\langle f(X, Y) \rangle$ in terms of $\langle X \rangle$ and $\langle Y \rangle$. Develop similarly the covariance and correlation.

17.2.6 Let $f(x, y)$ be the joint probability density of two random variables X, Y. Find the variance $\sigma^2(aX + bY)$, where a, b are constants. What happens when X, Y are independent?

17.2.7 The probablility that a particle of an ideal gas travels a small distance dx between collisions is $\sim e^{-x/f} dx$, where f is the constant mean free path. Verify that f is the average distance between collisions and determine the probability of a free path of length $l \geq 3f$.

17.2.8 Determine the probability density for a particle in simple harmonic motion in the interval $-A \leq x \leq A$.

Hint. The probability of the particle being between x and $x + dx$ is proportional to the time it takes to travel across the interval.

17.3 Binomial Distribution

EXAMPLE 17.3.1

Repeated Tosses of Dice What is the probability of three 6s in four tosses, all trials being independent? Getting one 6 in a single toss of a fair die has probability $a = 1/6$, and anything else has probability $b = 5/6$ with $a + b = 1$. Let the random variable $X = x$ be the number of 6s. In four tosses, $0 \le x \le 4$. The probability distribution $f(X)$ is given by the product of the two possibilities, a^x and b^{4-x}, times the number of combinations of four tosses over the two cases with probabilities a, b. This number is the coefficient of the power $a^x b^{4-x}$ in the binomial expansion of all possibilities in four tosses with probability 1:

$$\begin{aligned} 1 = (a+b)^4 &= \sum_{x=0}^{4} \frac{4!}{x!(4-x)!} a^x b^{4-x} \\ &= a^4 + b^4 + 4a^3 b + 4ab^3 + 6a^2 b^2. \end{aligned} \tag{17.41}$$

Hence, the probability distribution of our discrete random variable is given by

$$f(X = x) = \frac{4!}{x!(4-x)!} a^x b^{4-x}, \quad 0 \le x \le 4$$

or more explicitly

$$f(0) = b^4, \ f(1) = 4ab^3, \ f(2) = 6a^2 b^2, \ f(3) = 4a^3 b, \ f(4) = a^4.$$

The probability distribution is properly normalized according to Eq. (17.41). The probability of three 6s in four tosses is $4a^3 b = 4\frac{5/6}{6^3} = \frac{5}{4 \cdot 3^4}$, which is fairly small. ■

This case dealt with repeated independent trials, each with two possible outcomes of constant probability p for a hit and $q = 1 - p$ for a miss, and is typical of many applications, such as defective products, hits or misses of a target, and decays of radioactive atoms. The generalization to $X = x$ successes in n trials is given by the **binomial probability distribution**

$$f(X = x) = \frac{n!}{x!(n-x)!} p^x q^{n-x} = \binom{n}{x} p^x q^{n-x} \tag{17.42}$$

using the binomial coefficients (see Chapter 5). This distribution is normalized to the probability 1 of all possibilities in n trials, as can be seen from the binomial expansion

$$1 = (p+q)^n = p^n + np^{n-1}q + \cdots + npq^{n-1} + q^n. \tag{17.43}$$

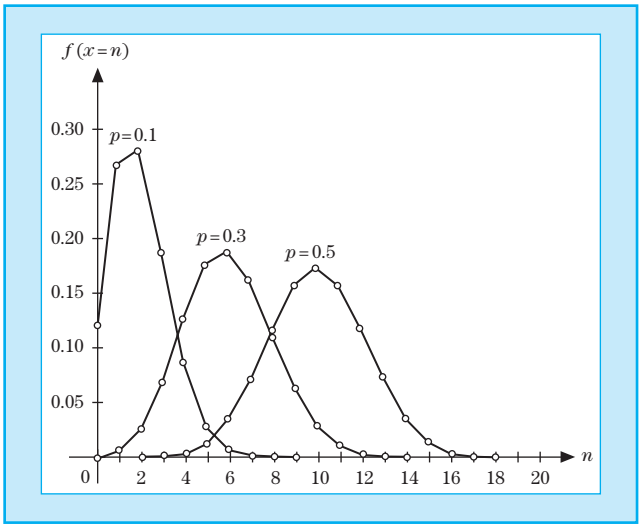


Figure 17.5

Binomial Probability Distributions for $n = 20$ and $p = 0.1, 0.3,$ and 0.5

Figure 17.5 shows typical histograms. The random variable X takes the values $0, 1, 2, \ldots, n$ in discrete steps and can also be viewed as a composition $\sum_i X_i$ of n-independent random variables X_i, one for each trial, that have the value 0 for a miss and 1 for a hit. This observation allows us to employ the moment generating functions

$$\langle e^{tX_i}\rangle = P(X_i = 0) + e^t P(X_i = 1) = q + pe^t \tag{17.44}$$

and

$$\langle e^{tX}\rangle = \prod_i \langle e^{tX_i}\rangle = (pe^t + q)^n, \tag{17.45}$$

from which the mean values and higher moments can be read off upon differentiating and setting $t = 0$. Using

$$\frac{\partial\langle e^{tX}\rangle}{\partial t} = npe^t(pe^t + q)^{n-1},$$

$$\left.\frac{\partial\langle e^{tX}\rangle}{\partial t}\right|_{t=0} = \langle X\rangle = \sum_i x_i f(x_i) = np,$$

$$\frac{\partial^2\langle e^{tX}\rangle}{\partial t^2} = npe^t(pe^t + q)^{n-1} + n(n-1)p^2e^{2t}(pe^t + q)^{n-2},$$

$$\langle X^2\rangle = \left.\frac{\partial^2\langle e^{tX}\rangle}{\partial t^2}\right|_{t=0} = \sum_i x_i^2 f(x_i) = np + n(n-1)p^2,$$

we obtain, with Eq. (17.17),

$$\begin{aligned}\sigma^2(X) &= \langle X^2\rangle - \langle X\rangle^2 = np + n(n-1)p^2 - n^2p^2 \\ &= np(1-p) = npq.\end{aligned} \tag{17.46}$$

Figure 17.5 illustrates these results with peaks at $\langle X\rangle = np = 2, 6, 10$, which widen with increasing p.

EXERCISES

17.3.1 Show that the variable $X = x$ number of heads in n coin tosses is a random variable and determine its probability distribution. Describe the sample space. What are its mean value, the variance, and standard deviation? Plot the probability function $f(x) = n!/[x!(n-x)!2^n]$ for $n = 10, 20, 30$ using graphical software.

17.3.2 Plot the binomial probability function for the probabilities $p = 1/6$, $q = 5/6$, and $n = 6$ throws of a die.

17.3.3 A hardware company knows that mass producing nails includes a small probability, $p = 0.03$, of defective nails (without a sharp tip usually). What is the probability of finding more than 2 defective nails in its commercial box of 100 nails?

17.3.4 Four cards are drawn from a shuffled bridge deck. What is the probability that they are all red? That they are all hearts? That they are honors? Compare the probabilities when the cards are put back at random places, or not.

17.3.5 Show that for the binomial distribution of Eq. (17.42), the most probable value of x is np.

17.4 Poisson Distribution

The Poisson distribution typically occurs in situations involving an event repeated at a constant rate of probability. The decay of a radioactive sample is a case in point. If the observation time dt is small enough so that the emission of two or more particles is negligible, then the probability that one particle (He^4 in α decay or an electron in β decay) is emitted is $\mu\, dt$ with constant μ and $\mu\, dt \ll 1$. We can set up a recursion relation for the probability $P_n(t)$ of observing n counts during a time interval t. For $n > 0$ the probability $P_n(t+dt)$ is composed of two mutually exclusive events that (i) n particles are emitted in the time t, none in dt, and (ii) $n-1$ particles in time t, one in dt. Therefore,

$$P_n(t+dt) = P_n(t)P_0(dt) + P_{n-1}(t)P_1(dt).$$

Here, we substitute the probability of observing one particle $P_1(dt) = \mu\, dt$ and no particle $P_0(dt) = 1 - P_1(dt)$ in time dt. This yields

$$P_n(t+dt) = P_n(t)(1-\mu\, dt) + P_{n-1}(t)\mu\, dt$$

so that, after rearranging and dividing by dt, we get

$$\frac{dP_n(t)}{dt} = \frac{P_n(t+dt) - P_n(t)}{dt} = \mu P_{n-1}(t) - \mu P_n(t). \tag{17.47}$$

For $n = 0$ this differential recursion relation simplifies because there is no particle in times t and dt, giving

$$\frac{dP_0(t)}{dt} = -\mu P_0(t). \tag{17.48}$$

This ordinary differential equation (ODE) integrates to $P_0(t) = e^{-\mu t}$ if the probability that no particle is emitted during a zero time interval $P_0(0) = 1$ is used.

Now we go back to Eq. (17.47) for $n = 1$

$$\dot{P}_1 = \mu(e^{-\mu t} - P_1), \quad P_1(0) = 0, \tag{17.49}$$

and solve the homogeneous equation that is the same for P_1 as Eq. (17.48). This yields $P_1(t) = \mu_1 e^{-\mu t}$. Then we solve the inhomogeneous ODE [Eq. (17.49)] by varying the constant μ_1 to find $\dot{\mu}_1 = \mu$ so that $P_1(t) = \mu t e^{-\mu t}$. The general solution is a Poisson distribution

$$P_n(t) = \frac{(\mu t)^n}{n!} e^{-\mu t}, \tag{17.50}$$

as may be confirmed by substitution into Eq. (17.47) and verifying the initial conditions $P_n(0) = 0, \ n > 0$.

The Poisson distribution is defined with the probabilities

$$p(n) = \frac{\mu^n}{n!} e^{-\mu}, \quad X = n = 0, 1, 2, \ldots \tag{17.51}$$

and is exhibited in Fig. 17.6. The random variable X is discrete. The probabilities are properly normalized because $e^{-\mu} \sum_{n=0}^{\infty} \frac{\mu^n}{n!} = 1$. The mean value and

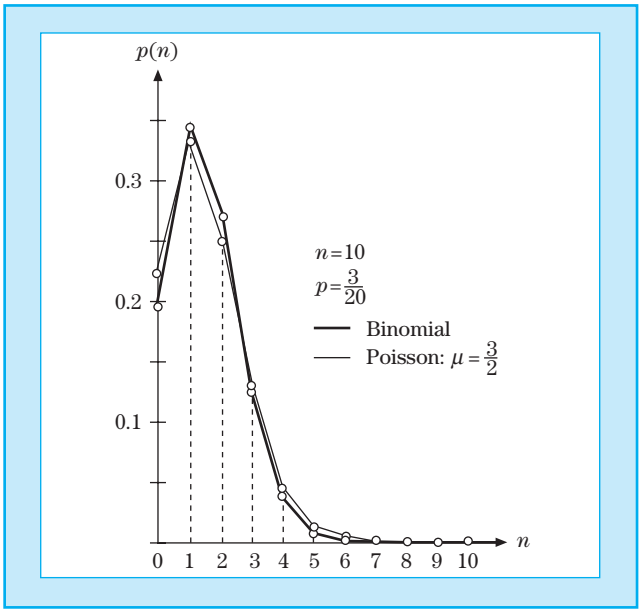


Figure 17.6

Poisson Distribution for $\mu = 3/2$ Compared with Binomial Distribution for $p = 3/20, n = 10$

variance,

$$\langle X\rangle = e^{-\mu}\sum_{n=1}^{\infty} n\frac{\mu^n}{n!} = \mu e^{-\mu}\sum_{n=0}^{\infty}\frac{\mu^n}{n!} = \mu,$$
$$\sigma^2 = \langle X^2\rangle - \langle X\rangle^2 = \mu(\mu+1) - \mu^2 = \mu, \tag{17.52}$$

follow from the characteristic function

$$\langle e^{itX}\rangle = \sum_{n=0}^{\infty} e^{itn-\mu}\frac{\mu^n}{n!} = e^{-\mu}\sum_{n=0}^{\infty}\frac{(\mu e^{it})^n}{n!} = e^{\mu(e^{it}-1)}$$

by differentiation and setting $t = 0$, using Eq. (17.17).

A Poisson distribution becomes a good approximation for the binomial distribution for a large number n of trials and small probability $p \sim \mu/n$, μ a constant.

THEOREM

> In the limit $n \to \infty$ and $p \to 0$ so that the mean value $np \to \mu$ stays finite, the binomial distribution becomes a Poisson distribution.

To prove this theorem, we apply Stirling's formula $n! \sim \sqrt{2\pi n}(n/e)^n$ for large n to the factorials in Eq. (17.42), keeping x finite while $n \to \infty$. This yields for $n \to \infty$:

$$\frac{n!}{(n-x)!} \sim \left(\frac{n}{e}\right)^n\left(\frac{e}{n-x}\right)^{n-x} \sim \left(\frac{n}{e}\right)^x\left(\frac{n}{n-x}\right)^{n-x}$$
$$\sim \left(\frac{n}{e}\right)^x\left(1+\frac{x}{n-x}\right)^{n-x} \sim \left(\frac{n}{e}\right)^x e^x \sim n^x,$$

and for $n \to \infty$, $p \to 0$, with $np \to \mu$:

$$(1-p)^{n-x} \sim \left(1-\frac{pn}{n}\right)^n \sim \left(1-\frac{\mu}{n}\right)^n \sim e^{-\mu}.$$

Finally, $p^x n^x \to \mu^x$; thus, altogether

$$\frac{n!}{x!(n-x)!}p^x(1-p)^{n-x} \to \frac{\mu^x}{x!}e^{-\mu}, \quad n \to \infty, \tag{17.53}$$

which is a Poisson distribution for the random variable $X = x$ with $0 \le x < \infty$. This limit theorem is an example of the **laws of large numbers**.

EXERCISES

17.4.1 Radioactive decays are governed by the Poisson distribution. In a Rutherford–Geiger experiment the number n_i of emitted α particles are counted in $n = 2608$ time intervals of 7.5 seconds each. In Table 17.1, n_i is the number of time intervals in which i particles were emitted. Determine the average number λ of emitted particles and compare the

n_i of Table 17.1 with np_i computed from the Poisson distribution with mean value λ.

Table 17.1

$i \rightarrow$	0	1	2	3	4	5	6	7	8	9	10
$n_i \rightarrow$	57	203	383	525	532	408	273	139	45	27	16

17.4.2 Derive the standard deviation of a Poisson distribution of mean value μ.

17.4.3 The number of α decay particles of a radium sample is counted per minute for 40 hours. The total number is 5000. How many 1-minute intervals are there with (a) 2, (b) 5 α particles?

17.4.4 For a radioactive sample, 10 decays are counted on average in 100 seconds. Use the Poisson distribution to estimate the probability of counting 3 decays in 10 seconds.

17.4.5 ^{238}U has a half-life of 4.51×10^9 years. Its decay series ends with the stable lead isotope ^{206}Pb. The ratio of the number of ^{206}Pb to ^{238}U atoms in a rock sample is measured as 0.0058. Estimate the age of the rock assuming that all the lead in the rock is from the initial decay of the ^{238}U, which determines the rate of the entire decay process because the subsequent steps take place far more rapidly.
Hint. The decay constant λ in the decay law $N(t) = Ne^{-\lambda t}$ is related to the half-life T by $T = \ln 2/\lambda$.

ANS. 3.8×10^7 years.

17.4.6 The probability of hitting a target in one shot is known to be 20%. If five shots are fired independently, what is the probability of striking the target at least once?

17.4.7 A piece of uranium is known to contain the isotopes $^{235}_{92}$U and $^{235}_{92}$U apart from 0.80 g of $^{206}_{82}$Pb per gram of uranium. Estimate the age of the piece (and thus Earth) in years.
Hint. Find out first which uranium isotope is the relevant one for the decay into lead. Use the decay constant from Exercise 17.4.5.

17.5 Gauss's Normal Distribution

The bell-shaped Gauss distribution is defined by the probability density

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{[x-\mu]^2}{2\sigma^2}\right), \quad -\infty < x < \infty, \tag{17.54}$$

with mean value μ and variance σ^2. It is by far the most important continuous probability distribution and is displayed in Fig. 17.7.

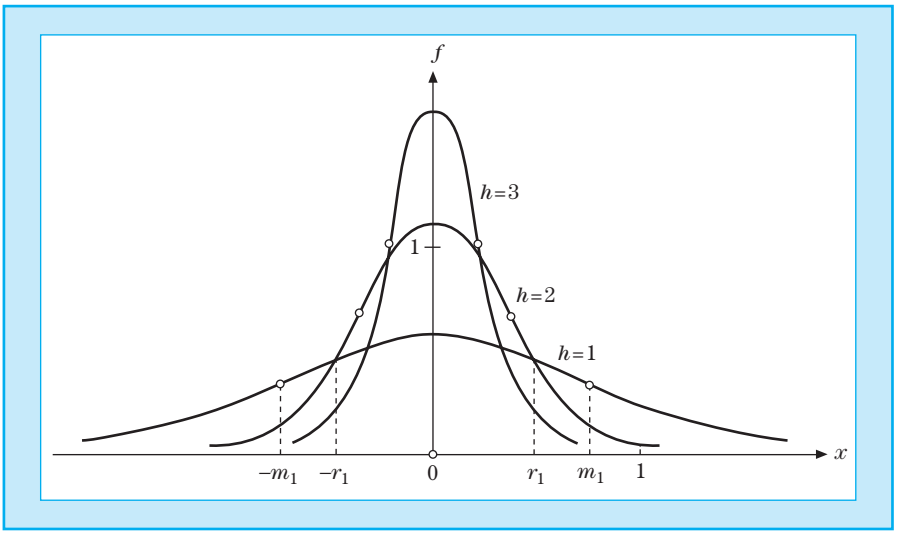


Figure 17.7

Normal Gauss Distribution for Mean Value Zero and Various Standard Deviations $h = 1/\sigma\sqrt{2}$

It is properly normalized because substituting $y = \frac{x-\mu}{\sigma\sqrt{2}}$, we obtain

$$\frac{1}{\sigma\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{-\frac{(x-\mu)^2}{2\sigma^2}}dx = \frac{1}{\sqrt{\pi}}\int_{-\infty}^{\infty} e^{-y^2}dy = \frac{2}{\sqrt{\pi}}\int_{0}^{\infty} e^{-y^2}dy = 1.$$

Similarly, substituting $y = x - \mu$, we see that

$$\langle X\rangle - \mu = \int_{-\infty}^{\infty} \frac{x-\mu}{\sigma\sqrt{2\pi}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}dx = \int_{-\infty}^{\infty} \frac{y}{\sigma\sqrt{2\pi}} e^{-\frac{y^2}{2\sigma^2}}dy = 0,$$

the integrand being odd in y so that the integral over $y > 0$ cancels that over $y < 0$. Similarly, we check that the standard deviation is σ.

From the normal distribution (by the substitution $y = \frac{x-\langle X\rangle}{\sigma}$)

$$P(|X - \langle X\rangle| > k\sigma) = P\left(\frac{|X - \langle X\rangle|}{\sigma} > k\right) = P(|Y| > k)$$
$$= \sqrt{\frac{2}{\pi}}\int_{k}^{\infty} e^{-y^2/2}dy = \sqrt{\frac{4}{\pi}}\int_{k/\sqrt{2}}^{\infty} e^{-z^2}dz = \operatorname{erfc}\frac{k}{\sqrt{2}},$$

we can evaluate the integral for $k = 1, 2, 3$ and thus extract the following numerical relations for a normally distributed random variable:

$$P(|X - \langle X\rangle| \geq \sigma) \sim 0.3173, \quad P(|X - \langle X\rangle| \geq 2\sigma) \sim 0.0455,$$
$$P(|X - \langle X\rangle| \geq 3\sigma) \sim 0.0027, \tag{17.55}$$

of which the last one is interesting to compare with Chebychev's inequality [Eq. (17.21)], giving $\leq 1/9$ for an **arbitrary** probability distribution instead of ~ 0.0027 for the 3σ rule of the **normal** distribution.

THEOREM

Addition Theorem If the random variables X, Y have the same normal distributions, that is, the same mean value and variance, then $Z = X + Y$ has normal distribution with twice the mean value and twice the variance of X and Y.

To prove this theorem, we take the Gauss density as

$$f(x) = \frac{1}{\sqrt{2\pi}} e^{-x^2/2}, \quad \text{with } \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-x^2/2} dx = 1,$$

without loss of generality. Then the probability density of (X, Y) is the product

$$f(x, y) = \frac{1}{\sqrt{2\pi}} e^{-x^2/2} \frac{1}{\sqrt{2\pi}} e^{-y^2/2} = \frac{1}{2\pi} e^{-(x^2+y^2)/2}.$$

Also, Eq. (17.36) gives the density for $Z = X + Y$ as

$$g(z) = \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}} e^{-x^2/2} \frac{1}{\sqrt{2\pi}} e^{-(x-z)^2/2} dx.$$

Completing the square in the exponent

$$2x^2 - 2xz + z^2 = \left(x\sqrt{2} - \frac{z}{\sqrt{2}}\right)^2 + \frac{z^2}{2},$$

we obtain

$$g(z) = \frac{1}{2\pi} e^{-z^2/4} \int_{-\infty}^{\infty} \exp\left(-\frac{1}{2}\left(x\sqrt{2} - \frac{z}{\sqrt{2}}\right)^2\right) dx.$$

Using the substitution $u = x - \frac{z}{2}$, the integral transforms into

$$\int_{-\infty}^{\infty} \exp\left(-\frac{1}{2}\left(x\sqrt{2} - \frac{z}{\sqrt{2}}\right)^2\right) dx = \int_{-\infty}^{\infty} e^{-u^2} du = \sqrt{\pi}$$

so that the density for $Z = X + Y$ is

$$g(z) = \frac{1}{2\sqrt{\pi}} e^{-z^2/4}, \tag{17.56}$$

which means it has mean value zero and the variance 2, twice that of X and Y.

In a special limit the discrete Poisson probability distribution is closely related to the continuous Gauss distribution. This limit theorem is another example of the **laws of large numbers** that are often dominated by the bell-shaped normal distribution.

THEOREM

For large n and mean value μ, the Poisson distribution approaches a Gauss distribution.

To prove this theorem for $n \to \infty$, we approximate the factorial in the Poisson's probability $p(n)$ of Eq. (17.51) by Stirling's asymptotic formula (see Chapter 5),

$$n! \sim \sqrt{2n\pi}\left(\frac{n}{e}\right)^n, \quad n \to \infty,$$

and choose the deviation $v = n - \mu$ from the mean value as the new variable. We let the mean value $\mu \to \infty$ and treat v/μ as small but v^2/μ as finite. Substituting $n = \mu + v$ and expanding the logarithm in a Maclaurin series keeping two terms, we obtain

$$\begin{aligned}
\ln p(n) &= -\mu + n\ln\mu - n\ln n + n - \ln\sqrt{2n\pi} \\
&= (\mu+v)\ln\mu - (\mu+v)\ln(\mu+v) + v - \ln\sqrt{2\pi(\mu+v)} \\
&= (\mu+v)\ln\left(1 - \frac{v}{\mu+v}\right) + v - \ln\sqrt{2\pi\mu} \\
&= (\mu+v)\left(-\frac{v}{\mu+v} - \frac{v^2}{2(\mu+v)^2}\right) + v - \ln\sqrt{2\pi\mu} \\
&\sim -\frac{v^2}{2\mu} - \ln\sqrt{2\pi\mu},
\end{aligned}$$

discarding $\ln\sqrt{2\pi v}$ because $|v| \ll \mu$. Exponentiating this result, we find that for large n and μ

$$p(n) \to \frac{1}{\sqrt{2\pi\mu}} e^{-\frac{v^2}{2\mu}}, \tag{17.57}$$

which is a Gauss distribution of the continuous variable v with mean value 0 and standard deviation $\sigma = \sqrt{\mu}$.

In a special limit the discrete binomial probability distribution is also closely related to the continuous Gauss distribution. This limit theorem is another example of the **laws of large numbers**.

THEOREM

In the limit $n \to \infty$, so the mean value $np \to \infty$, the binomial distribution becomes Gauss's normal distribution. Recall from Section 17.4 that when $np \to \mu < \infty$, the binomial distribution becomes a Poisson distribution.

Instead of the large number x of trials, we use the deviation $v = x - pn$ from the (large) mean value pn as our new continuous random variable under the condition that $|v| \ll pn$, but v^2/n is finite as $n \to \infty$. Thus, we replace x by $v + pn$ and $n - x$ by $qn - v$ in the factorials of Eq. (17.42), $f(x) \to W(v)$ as

$n \to \infty$, and then apply Stirling's formula. This yields

$$W(v) = \frac{p^x q^{n-x} n^{n+1/2} e^{-n+x+(n-x)}}{\sqrt{2\pi}(v+pn)^{x+1/2}(qn-v)^{n-x+1/2}}.$$

Here, we factor out the dominant powers of n and cancel powers of p and q to find

$$W(v) = \frac{1}{\sqrt{2\pi pqn}} \left(1 + \frac{v}{pn}\right)^{-(v+pn+1/2)} \left(1 - \frac{v}{qn}\right)^{-(qn-v+1/2)}.$$

In terms of the logarithm, we have

$$\begin{aligned}
\ln W(v) &= \ln \frac{1}{\sqrt{2\pi pqn}} - (v + pn + 1/2) \ln \left(1 + \frac{v}{pn}\right) \\
&\quad - (qn - v + 1/2) \ln \left(1 - \frac{v}{qn}\right) \\
&= \ln \frac{1}{\sqrt{2\pi pqn}} - (v + pn + 1/2) \left(\frac{v}{pn} - \frac{v^2}{2p^2n^2} + \cdots\right) \\
&\quad - (qn - v + 1/2) \left(-\frac{v}{qn} - \frac{v^2}{2q^2n^2} + \cdots\right) \\
&= \ln \frac{1}{\sqrt{2\pi pqn}} - \left[\frac{v}{n}\left(\frac{1}{2p} - \frac{1}{2q}\right) + \frac{v^2}{n}\left(\frac{1}{2p} + \frac{1}{2q}\right) + \cdots\right],
\end{aligned}$$

where

$$v/n \to 0, \quad v^2/n$$

is finite and

$$\left(\frac{1}{2p} + \frac{1}{2q}\right) = \frac{p+q}{2pq} = \frac{1}{2pq}.$$

Neglecting higher orders in v/n, such as v^2/p^2n^2, v^2/q^2n^2, we find the large n limit

$$W(v) = \frac{1}{\sqrt{2\pi pqn}} e^{-\frac{v^2}{2pqn}}, \tag{17.58}$$

which is a Gaussian distribution in the deviations $x - pn$ with mean value 0 and standard deviation $\sigma = \sqrt{npq}$. The large mean value pn (and the discarded terms) restricts the validity of the theorem to the central part of the Gaussian bell shape, excluding the tails.

EXERCISES

17.5.1 What is the probability for a normally distributed random variable to differ by more than 4σ from its mean value? Compare your result with the corresponding one from Chebychev's inequality. Explain the difference in your own words.

17.5.2 Let $X_1, X_2, \ldots, X_n$ be independent normal random variables with the same mean $\bar{x}$ and variance σ^2. Show that $\frac{\sum_i X_i/n - \bar{x}}{\sqrt{n}\sigma}$ is normal with mean zero and variance 1.

17.5.3 An instructor grades a final exam of a large undergraduate class, obtaining the mean value of points M and the variance σ^2. Assuming a normal distribution for the number M of points, he defines a grade F when $M < m - 3\sigma/2$, D when $m - 3\sigma/2 < M < m - \sigma/2$, C when $m - \sigma/2 < M < m + \sigma/2$, B when $m + \sigma/2 < M < m + 3\sigma/2$, and A when $M > m + 3\sigma/2$. What is the percentage of A, F; B, D; C? Redesign the cutoffs so that there are equal percentages of As and Fs (5%), 25% B and Ds, and 40% Cs.

17.5.4 If the random variable X is normal with mean value 29 and standard deviation 3, what are the distributions of $2X - 1$ and $3X + 2$?

17.5.5 For a normal distribution of mean value m and variance σ^2, find the distance r that half the area under the bell shape is between $m - r$ and $m + r$.

17.6 Statistics

In statistics, probability theory is applied to the evaluation of data from random experiments or to samples to test some hypothesis because the data have random fluctuations due to lack of complete control over the experimental conditions. Typically, one attempts to estimate the mean value and variance of the distributions, from which the samples derive, and generalize properties valid for a sample to the rest of the events at a prescribed confidence level. Any assumption about an unknown probability distribution is called a statistical hypothesis. The concepts of tests and confidence intervals are among the most important developments of statistics.

Error Propagation

When we measure a quantity x repeatedly obtaining the values x_j at random, or select a sample for testing, we determine the mean value [Eq. (17.10)] and the variance

$$\bar{x} = \frac{1}{n}\sum_{j=1}^{n} x_j, \qquad \sigma^2 = \frac{1}{n}\sum_{j=1}^{n}(x_j - \bar{x})^2$$

as a measure for the error or spread from the mean value $\bar{x}$. We can write $x_j = \bar{x} + e_j$, where the error e_j is the deviation from the mean value, and we know that $\sum_j e_j = 0$. [See the discussion after Eq. (17.15).]

Now suppose we want to determine a known function $f(x)$ from these measurements; that is, we have a set $f_j = f(x_j)$ from the measurements of x.

Substituting $x_j = \bar{x} + e_j$ and forming the mean value from

$$\begin{aligned}\bar{f} &= \frac{1}{n}\sum_j f(x_j) = \frac{1}{n}\sum_j f(\bar{x}+e_j)\\ &= f(\bar{x}) + \frac{1}{n}f'(\bar{x})\sum_j e_j + \frac{1}{2n}f''(\bar{x})\sum_j e_j^2 + \cdots\\ &= f(\bar{x}) + \frac{1}{2}\sigma^2 f''(\bar{x}) + \cdots,\end{aligned} \tag{17.59}$$

we obtain the average value $\bar{f}$ as $f(\bar{x})$ in lowest order as expected. However, in second order there is a correction given by half the variance with a scale factor $f''(\bar{x})$. It is interesting to compare this correction of the mean value with the average spread of individual f_j from the mean value $\bar{f}$, the variance of f. To lowest order, this is given by the average of the sum of squares of the deviations, in which we approximate $f_j \approx \bar{f} + f'(\bar{x})e_j$, yielding

$$\sigma^2(f) \equiv \frac{1}{n}\sum_j (f_j - \bar{f})^2 = (f'(\bar{x}))^2\frac{1}{n}\sum_j e_j^2 = (f'(\bar{x}))^2\sigma^2. \tag{17.60}$$

In summary, we may formulate somewhat symbolically

$$f(\bar{x} \pm \sigma) = f(\bar{x}) \pm f'(\bar{x})\sigma$$

as the simplest form of error propagation by a function of one measured variable.

For a function $f(x_j, y_k)$ of two measured quantities $x_j = \bar{x} + u_j$, $y_k = \bar{y} + v_k$, we similarly obtain

$$\begin{aligned}\bar{f} &= \frac{1}{rs}\sum_{j=1}^{r}\sum_{k=1}^{s} f_{jk} = \frac{1}{rs}\sum_{j=1}^{r}\sum_{k=1}^{s} f(\bar{x}+u_j, \bar{y}+v_k)\\ &= f(\bar{x}, \bar{y}) + \frac{1}{r}f_x\sum_j u_j + \frac{1}{s}f_x\sum_k v_k + \cdots,\end{aligned}$$

where $\sum_j u_j = 0 = \sum_k v_k$ so that again $\bar{f} = f(\bar{x}, \bar{y})$ in lowest order. Here,

$$f_x = \frac{\partial f}{\partial x}(\bar{x}, \bar{y}), \qquad f_y = \frac{\partial f}{\partial y}(\bar{x}, \bar{y}) \tag{17.61}$$

denote partial derivatives. The sum of squares of the deviations from the mean value is given by

$$\sum_{j=1}^{r}\sum_{k=1}^{s}(f_{jk} - \bar{f})^2 = \sum_{j,k}(u_j f_x + v_k f_y)^2 = s f_x^2\sum_j u_j^2 + r f_y^2\sum_k v_k^2$$

because $\sum_{j,k} u_j v_k = \sum_j u_j \sum_k v_k = 0$. Therefore, the variance is

$$\sigma^2(f) = \frac{1}{rs}\sum_{j,k}(f_{jk} - \bar{f})^2 = f_x^2\sigma_x^2 + f_y^2\sigma_y^2, \tag{17.62}$$

with f_x, f_y from Eq. (17.61), and

$$\sigma_x^2 = \frac{1}{r}\sum_j u_j^2, \qquad \sigma_y^2 = \frac{1}{s}\sum_k v_k^2$$

are the variances of the x and y data points. Symbolically, the error propagation for a function of two measured variables may be summarized as

$$f(\bar{x} \pm \sigma_x, \bar{y} \pm \sigma_y) = f(\bar{x}, \bar{y}) \pm \sqrt{f_x^2\sigma_x^2 + f_y^2\sigma_y^2}.$$

As an application and generalization of the last result, we now calculate the error of the mean value $\bar{x} = \frac{1}{n}\sum_{j=1}^{n} x_j$ of a sample of n individual measurements x_j, each with spread σ. In this case, the partial derivatives are given by $f_x = \frac{1}{n} = f_y = \cdots$ and $\sigma_x = \sigma = \sigma_y = \cdots$. Thus, our last error propagation rule tells us that errors of a sum of variables add quadratically, so the uncertainty of the arithmetic mean is given by

$$\bar{\sigma} = \frac{1}{n}\sqrt{n\sigma^2} = \frac{\sigma}{\sqrt{n}}, \tag{17.63}$$

decreasing with the number of measurements n.

As the number n of measurements increases, we expect the arithmetic mean $\bar{x}$ to converge to some true value x. Let $\bar{x}$ differ from x by α and $v_j = x_j - x$ be the true deviations; then

$$\sum_j (x_j - \bar{x})^2 = \sum_j e_j^2 = \sum_j v_j^2 + n\alpha^2.$$

Taking into account the error of the arithmetic mean, we determine the spread of the individual points about the unknown true mean value to be

$$\sigma^2 = \frac{1}{n}\sum_j e_j^2 = \frac{1}{n}\sum_j v_j^2 + \alpha^2.$$

According to our earlier discussion leading to Eq. (17.63), $\alpha^2 = \frac{1}{n}\sigma^2$. As a result,

$$\sigma^2 = \frac{1}{n}\sum_j v_j^2 + \frac{\sigma^2}{n},$$

from which the **standard deviation of a sample in statistics** follows:

$$\sigma = \sqrt{\frac{\sum_j v_j^2}{n-1}} = \sqrt{\frac{\sum_j (x_j - x)^2}{n-1}}, \tag{17.64}$$

with $n - 1$ being the number of control measurements of the sample. This modified mean error includes the expected error in the arithmetic mean.

Because the spread is not well defined when there is no comparison measurement (i.e., $n = 1$), the variance is sometimes defined by Eq. (17.64) replacing the number n of measurements by the number $n - 1$ of control measurements in statistics.

Fitting Curves to Data

Suppose we have a sample of measurements y_j (e.g., a particle moving freely—that is, no force) taken at known times t_j (which are taken to be practically free of errors; that is, the time t is an ordinary independent variable) that we expect to be linearly related as $y = at$, our hypothesis. We want to fit this line to the data.

First, we minimize the sum of deviations $\sum_j (at_j - y_j)^2$ to determine the slope parameter a, also called regression coefficient, using the method of least squares. Differentiating with respect to a, we obtain

$$2\sum_j (at_j - y_j)t_j = 0,$$

from which

$$a = \frac{\sum_j t_j y_j}{\sum_j t_j^2} \tag{17.65}$$

follows. Note that the numerator is built like a sample covariance—the scalar product of the variables t, y of the sample. As shown in Fig. 17.8, the measured values y_j do not lie on the line as a rule. They have the spread (or root mean square deviation from the fitted line)

$$\sigma = \sqrt{\frac{\sum_j (y_j - at_j)^2}{n - 1}}.$$

Alternatively, let the y_j values be known (without error) while t_j are measurements. As suggested by Fig. 17.9, in this case, we need to interchange the role of t and y and fit the line $t = by$ to the data points. We minimize

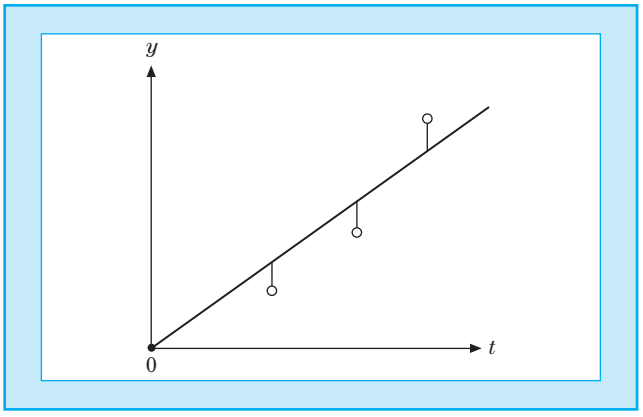


Figure 17.8

Straight Line Fit to Data Points (t_j, y_j) with t_j Known, y_j Measured

Figure 17.9

Straight Line Fit to Data Points (t_j, y_j) with y_j Known, t_j Measured

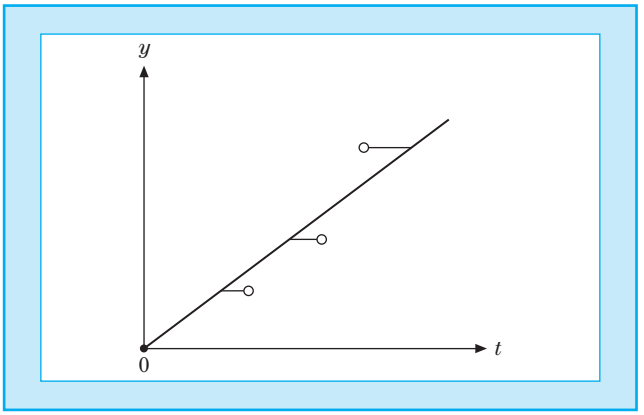
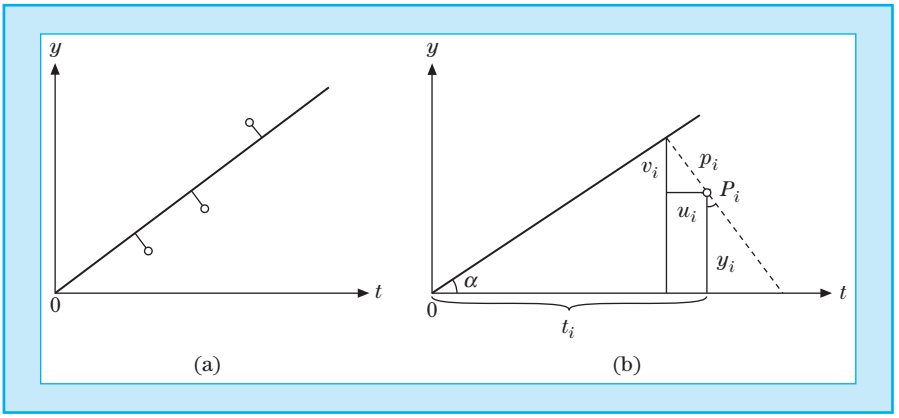


Figure 17.10

(a) Straight Line Fit to Data Points (t_j, y_j). (b) Geometry of Deviations u_j, v_j, d_j



$\sum_j (by_j - t_j)^2$, set the derivative with respect to b equal to zero, and similarly find the slope parameter

$$b = \frac{\sum_j t_j y_j}{\sum_j y_j^2}. \tag{17.66}$$

In case both t_j and y_j have errors (we take t and y to have the same units), we have to minimize the sum of squares of the deviations of both variables and fit to a parameterization $t \sin\alpha - y\cos\alpha = 0$, where t and y occur on an equal footing. As displayed in Fig. (17.10a), this means geometrically that the line has to be drawn so that the sum of the squares of the distances d_j of the points (t_j, y_j) from the line becomes a minimum. (See Fig. 17.10b and Chapter 1.) Here, $d_j = t_j \sin\alpha - y_j \cos\alpha$, so $\sum_j d_j^2 =$ minimum must be solved for the angle α. Setting the derivative with respect to the angle equal to zero,

$$\sum_j (t_j \sin\alpha - y_j \cos\alpha)(t_j \cos\alpha + y_j \sin\alpha) = 0$$

yields

$$\sin\alpha\cos\alpha\sum_j\left(t_j^2-y_j^2\right)-\left(\cos^2\alpha-\sin^2\alpha\right)\sum_j t_j y_j=0.$$

Therefore, the angle of the straight line fit is given by

$$\tan 2\alpha=\frac{2\sum_j t_j y_j}{\sum_j\left(t_j^2-y_j^2\right)}. \tag{17.67}$$

SUMMARY

This least squares fitting applies when the measurement errors are unknown. It allows assigning at least some kind of error bar to the measured points. Recall that we did not use errors for the points. Our parameter a (or α) is most likely to reproduce the data in these circumstances. More precisely, the least squares method is a **maximum likelihood** estimate of the fitted parameters when it is reasonable to assume that the errors are independent and normally distributed with **the same deviation for all points**. This fairly strong assumption can be relaxed in "weighted" least squares fits called chi square fits.[4] (See also Example 17.6.1.)

The χ^2 Distribution

This distribution is typically applied to fits of a curve $y(t, a, \ldots)$ with parameters $a, \ldots$ to data t_j using the method of least squares involving the **weighted** sum of squares of deviations; that is,

$$\chi^2=\sum_{j=1}^{N}\left(\frac{y_j-y(t_j,a,\ldots)}{\Delta y_j}\right)^2$$

is minimized, where N is the number of points and r the number of adjusted parameters $a, \ldots$. This quadratic merit function gives more weight to points with small deviation Δy_j.

We represent each point by a normally distributed random variable X with zero mean value and variance $\sigma^2=1$, the latter in view of the weights in the χ^2 function. In a first step, we determine the probability density for the random variable $Y=X^2$ of a single point that takes only positive values. Assuming a zero mean value is no loss of generality because if $\langle X\rangle=m\neq 0$, we would consider the shifted variable $Y=X-m$, whose mean value is zero. We show that if X has a Gauss normal density

$$f(x)=\frac{1}{\sigma\sqrt{2\pi}}e^{-\frac{x^2}{2\sigma^2}},\quad -\infty<x<\infty,$$

then the probability of the random variable Y is zero if $y\leq 0$, and

$$P(Y<y)=P(X^2<y)=P(-\sqrt{y}<X<\sqrt{y})\quad \text{if}\quad y>0.$$

[4]For more details, see Chapter 14 of Press et al. in Additional Reading of Chapter 8.

From the continuous normal distribution $P(y) = \int_{-\infty}^{y} f(x)dx$, we obtain the probability density $g(y)$ by differentiation:

$$g(y) = \frac{d}{dy}[P(\sqrt{y}) - P(-\sqrt{y})] = \frac{1}{2\sqrt{y}}(f(\sqrt{y}) + f(-\sqrt{y}))$$
$$= \frac{1}{\sigma\sqrt{2\pi y}} e^{-\frac{y}{2\sigma^2}}, \quad y > 0. \tag{17.68}$$

This density, $\sim e^{-\frac{y}{2\sigma^2}}/\sqrt{y}$, corresponds to the integrand of the Euler integral of the gamma function. Such a probability distribution

$$g(y) = \frac{y^{p-1}}{\Gamma(p)(2\sigma^2)^p} e^{-\frac{y}{2\sigma^2}}$$

is called a **gamma distribution** with parameters p and σ. Its characteristic function for our case, $p = 1/2$, is given by the Fourier transform

$$\langle e^{itY}\rangle = \frac{1}{\sigma\sqrt{2\pi}} \int_0^\infty e^{-y(\frac{1}{2\sigma^2} - it)} \frac{dy}{\sqrt{y}} = \frac{1}{\sigma\sqrt{2\pi}\left(\frac{1}{2\sigma^2} - it\right)^{1/2}} \int_0^\infty e^{-x} \frac{dx}{\sqrt{x}}$$
$$= (1 - 2it\sigma^2)^{-1/2}.$$

Since the χ^2 sample function contains a sum of squares, we need an **addition theorem** for the gamma distributions: If the independent random variables Y_1 and Y_2 have a gamma distribution with $p = 1/2$, then $Y_1 + Y_2$ has a gamma distribution with $p = 1$. Since Y_1 and Y_2 are independent, the product of their densities [Eq. (17.36)] generates the characteristic function

$$\langle e^{it(Y_1+Y_2)}\rangle = \langle e^{itY_1} e^{itY_2}\rangle = \langle e^{itY_1}\rangle\langle e^{itY_2}\rangle = (1 - 2it\sigma^2)^{-1}. \tag{17.69}$$

Now we come to the second step. We assess the quality of the fit by the random variable $Y = \sum_{j=1}^{n} X_j^2$, where $n = N - r$ is the number of degrees of freedom for N data points and r fitted parameters. The independent random variables X_j are taken to be normally distributed with the (sample) variance σ^2. (In our case, $r = 1$ and $\sigma = 1$.) The χ^2 analysis does not really test the assumptions of normality and independence, but if these are not approximately valid, there will be many outlier points in the fit. The addition theorem gives the probability density (Fig. 17.11) for Y,

$$g_n(y) = \frac{y^{\frac{n}{2}-1}}{2^{n/2}\sigma^n \Gamma\left(\frac{n}{2}\right)} e^{-y/2\sigma^2}, \quad y > 0,$$

and $g_n(y) = 0$ if $y < 0$, which is the χ^2 distribution corresponding to n degrees of freedom. Its characteristic function is

$$\langle e^{itY}\rangle = (1 - 2it\sigma^2)^{-n/2}.$$

Table 17.2

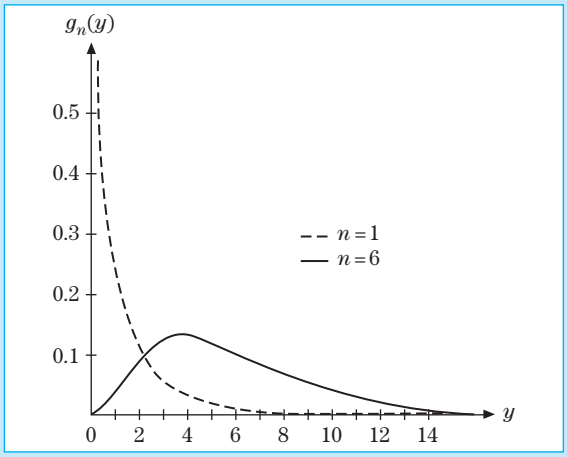
χ^2 Distribution[a]

n	$v = 0.8$	$v = 0.7$	$v = 0.5$	$v = 0.3$	$v = 0.2$	$v = 0.1$
1	0.064	0.148	0.455	1.074	1.642	2.706
2	0.446	0.713	1.386	2.408	3.219	4.605
3	1.005	1.424	2.366	3.665	4.642	6.251
4	1.649	2.195	3.357	4.878	5.989	7.779
5	2.343	3.000	4.351	6.064	7.289	9.236
6	3.070	3.828	5.348	7.231	8.558	10.645

[a] Entries are χ_v for the probabilities $v = P(\chi^2 \geq \chi_v^2) = \frac{1}{2^{n/2}\Gamma(n/2)} \int_{\chi_v^2}^{\infty} e^{-y/2} y^{(n/2)-1} dy$ for $\sigma = 1$.

Figure 17.11

χ^2 Probability Density $g_n(y)$



Differentiating and setting $t = 0$, we obtain its mean value and variance

$$\langle Y \rangle = n\sigma^2, \qquad \sigma^2(Y) = 2n\sigma^4. \tag{17.70}$$

Tables give values for the χ^2 probability for n degrees of freedom,

$$P(\chi^2 \geq y_0) = \frac{1}{2^{n/2}\sigma^n \Gamma\left(\frac{n}{2}\right)} \int_{y_0}^{\infty} y^{\frac{n}{2}-1} e^{-\frac{y}{2\sigma^2}} dy$$

for $\sigma = 1$ and $y_0 > 0$. To use Table 17.2 for $\sigma \neq 1$, rescale $y_0 = v_0\sigma^2$ so that $P(\chi^2 \geq v_0\sigma^2)$ corresponds to $P(\chi^2 \geq v_0)$ of Table 17.2. The following example illustrates the whole process.

EXAMPLE 17.6.1

Let us apply the χ^2 function to the fit in Fig. 17.8. The measured points $(t_j, y_j \pm \Delta y_j)$ with errors Δy_j are

$$(1, 0.8 \pm 0.1), \quad (2, 1.5 \pm 0.05), \quad (3, 3 \pm 0.2).$$

For comparison, the maximum likelihood fit [Eq. (17.65)] gives

$$a = \frac{1 \cdot 0.8 + 2 \cdot 1.5 + 3 \cdot 3}{1 + 4 + 9} = \frac{12.8}{14} = 0.914.$$

Minimizing instead

$$\chi^2 = \sum_j \left(\frac{y_j - a t_j}{\Delta y_j} \right)^2,$$

gives

$$0 = \frac{\partial \chi^2}{\partial a} = -2 \sum_j \frac{t_j (y_j - a t_j)}{(\Delta y_j)^2}$$

or

$$a = \frac{\sum_j \frac{t_j y_j}{(\Delta y_j)^2}}{\sum_j \frac{t_j^2}{(\Delta y_j)^2}}.$$

In our case,

$$a = \frac{\frac{1 \cdot 0.8}{0.1^2} + \frac{2 \cdot 1.5}{0.05^2} + \frac{3 \cdot 3}{0.2^2}}{\frac{1^2}{0.1^2} + \frac{2^2}{0.05^2} + \frac{3^2}{0.2^2}} = \frac{1505}{1925} = 0.782$$

is dominated by the middle point with the smallest error $\Delta y_2 = 0.05$. The error propagation formula [Eq. (17.62)] gives us the variance σ_a^2 of the estimate of a,

$$\sigma_a^2 = \sum_j (\Delta y_j)^2 \left(\frac{\partial a}{\partial y_j} \right)^2 = \sum_j \frac{\frac{t_j^2}{(\Delta y_j)^2}}{\left(\sum_k \frac{t_k^2}{(\Delta y_k)^2} \right)^2} = \frac{1}{\sum_j \frac{t_j^2}{(\Delta y_j)^2}}$$

using

$$\frac{\partial a}{\partial y_j} = \frac{\frac{t_j}{(\Delta y_j)^2}}{\sum_k \frac{t_k^2}{(\Delta y_k)^2}}.$$

For our case, $\sigma_a = 1/\sqrt{1925} = 0.023$; that is, our slope parameter is $a = 0.782 \pm 0.023$.

To estimate the quality of this fit of a, we compute the χ^2 probability that the two independent (control) points miss the fit by two standard deviations; that is, on average each point misses by one standard deviation. We apply the χ^2 distribution to the fit involving $N = 3$ data points and $r = 1$ parameter; that is, for $n = 3 - 1 = 2$ degrees of freedom. From Eq. (17.70), the χ^2 distribution has a mean value 2 and a variance 4. A rule of thumb is that $\chi^2 \approx n$ for a reasonably good fit. Then $P(\chi^2 \geq 2) \sim 0.496$ is read off Table 17.2, where we interpolate

between $P(\chi^2 \geq 1.386^2) = 0.50$ and $P(\chi^2 \geq 2.408^2) = 0.30$ as follows:

$$\begin{aligned} P(\chi^2 \geq 2) &= P(\chi^2 \geq 1.386^2) - \frac{2 - 1.386^2}{2.408^2 - 1.386^2} \\ &\quad \times [P(\chi^2 \geq 1.386^2) - P(\chi^2 \geq 2.408^2)] \\ &= 0.5 - 0.02 \cdot 0.2 = 0.496. \end{aligned}$$

Thus, the χ^2 probability that, on average, each point misses by one standard deviation is approximately 50% and fairly large. ■

Our next goal is to compute a **confidence interval** for the slope parameter of our fit. A confidence interval for an a priori unknown parameter of some distribution (e.g., a determined by our fit) is an interval that contains a not with certainty but with a high **probability** p, the **confidence level**, which we can choose. Such an interval is computed for a given sample. Such an analysis involves the Student t distribution.

The Student *t* Distribution

Because we always compute the arithmetic mean of measured points, we now consider the sample function

$$\bar{X} = \frac{1}{n} \sum_{j=1}^{n} X_j,$$

where the random variables X_j are assumed independent with a normal distribution of the same mean value m and variance σ^2. The addition theorem for the Gauss distribution tells us that $X_1 + \cdots + X_n$ has the mean value nm and variance $n\sigma^2$. Therefore, $(X_1 + \cdots + X_n)/n$ is normal with mean value m and variance $n\sigma^2/n^2 = \sigma^2/n$. The probability density of the variable $\bar{X} - m$ is the Gauss distribution

$$\bar{f}(\bar{x} - m) = \frac{\sqrt{n}}{\sigma\sqrt{2\pi}} \exp\left(-\frac{n(\bar{x} - m)^2}{2\sigma^2}\right). \tag{17.71}$$

The key problem solved by the Student t distribution is to provide estimates for the mean value m, when σ **is not known**, in terms of a sample function whose distribution is **independent** of σ. To this end, we define a rescaled sample function t:

$$t = \frac{\bar{X} - m}{S}\sqrt{n-1}, \qquad S^2 = \frac{1}{n}\sum_{j=1}^{n}(X_j - \bar{X})^2. \tag{17.72}$$

It can be shown that t and S are independent random variables. Following the arguments leading to the χ^2 distribution, the density of the denominator variable S is given by the gamma distribution

$$d(s) = \frac{n^{\frac{n-1}{2}} s^{n-2} e^{-\frac{ns^2}{2\sigma^2}}}{2^{\frac{n-3}{2}} \Gamma\left(\frac{n-1}{2}\right) \sigma^{n-1}}. \tag{17.73}$$

The probability for the ratio $Z = X/Y$ of two independent random variables X, Y with normal density for $\bar{f}$, and d is given by Eq. (17.73), is [Eq. (17.40)]

$$R(z) = \int_{-\infty}^{z}\int_{-\infty}^{\infty} f(yz)d(y)|y|dy\,dz \tag{17.74}$$

so that the variable $V = (\bar{X} - m)/S$ has the density

$$\begin{aligned} r(v) &= \int_0^\infty \frac{\sqrt{n}}{\sigma\sqrt{2\pi}} \exp\left(-\frac{nv^2s^2}{2\sigma^2}\right) \frac{n^{\frac{n-1}{2}}s^{n-2}e^{-\frac{ns^2}{2\sigma^2}}}{2^{\frac{n-3}{2}}\Gamma\left(\frac{n-1}{2}\right)\sigma^{n-1}} sds \\ &= \frac{n^{n/2}}{\sigma^n\sqrt{\pi}2^{\frac{n-2}{2}}\Gamma\left(\frac{n-1}{2}\right)} \int_0^\infty e^{-\frac{ns^2(v^2+1)}{2\sigma^2}} s^{n-1}ds. \end{aligned}$$

Here, we substitute $z = s^2$ and obtain

$$r(v) = \frac{n^{n/2}}{\sigma^n\sqrt{\pi}2^{n/2}\Gamma\left(\frac{n-1}{2}\right)} \int_0^\infty e^{-\frac{nz(v^2+1)}{2\sigma^2}} z^{\frac{n-2}{2}} dz.$$

Now we substitute $\Gamma(1/2) = \sqrt{\pi}$, define the parameter

$$a = \frac{n(v^2+1)}{2\sigma^2},$$

and transform the integral into $\Gamma(n/2)/a^{n/2}$ to find

$$r(v) = \frac{\Gamma(n/2)}{\sqrt{\pi}\Gamma\left(\frac{n-1}{2}\right)(v^2+1)^{n/2}}, \quad -\infty < v < \infty.$$

Finally, we rescale this expression to the variable t in Eq. (17.72) with the density (Fig. 17.12)

$$g(t) = \frac{\Gamma(n/2)}{\sqrt{\pi(n-1)}\Gamma\left(\frac{n-1}{2}\right)\left(1+\frac{t^2}{n-1}\right)^{n/2}}, \quad -\infty < t < \infty \tag{17.75}$$

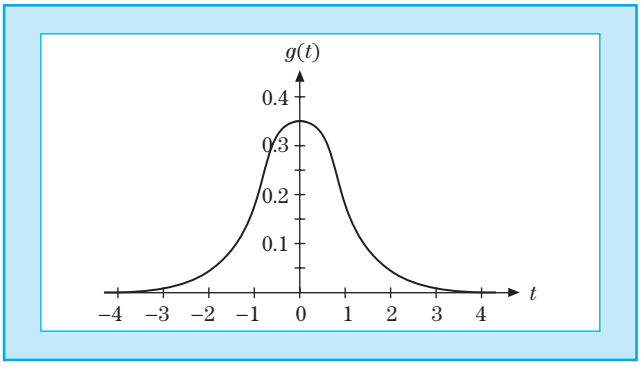


Figure 17.12

Student *t* Probability Density $g_n(t)$ for $n = 3$

Table 17.3

Student t Distribution[a]

p	$n=1$	$n=2$	$n=3$	$n=4$	$n=5$
0.8	1.38	1.06	0.98	0.94	0.92
0.9	3.08	1.89	1.64	1.53	1.48
0.95	6.31	2.92	2.35	2.13	2.02
0.975	12.7	4.30	3.18	2.78	2.57
0.99	31.8	6.96	4.54	3.75	3.36
0.999	318.3	22.3	10.2	7.17	5.89

[a] Entries are the values C in $P(C) = K_n \int_{-\infty}^{C} (1 + \frac{t^2}{n})^{-(n+1)/2} dt = p$, n is the number of degrees of freedom.

for the Student t distribution, which manifestly does not depend on m or σ. The probability for $t_1 < t < t_2$ is given by the integral

$$P(t_1, t_2) = \frac{\Gamma(n/2)}{\sqrt{\pi(n-1)}\Gamma\left(\frac{n-1}{2}\right)} \int_{t_1}^{t_2} \frac{dt}{\left(1 + \frac{t^2}{n-1}\right)^{n/2}}, \tag{17.76}$$

and $P(z) \equiv P(-\infty, z)$ is tabulated. (See Table 17.3.) Also, $P(\infty, -\infty) = 1$ and $P(-z) = 1 - P(z)$ because the integrand in Eq (17.76) is even in t, so

$$\int_{-\infty}^{-z} \frac{dt}{\left(1 + \frac{t^2}{n-1}\right)^{n/2}} = \int_{z}^{\infty} \frac{dt}{\left(1 + \frac{t^2}{n-1}\right)^{n/2}}$$

and

$$\int_{z}^{\infty} \frac{dt}{\left(1 + \frac{t^2}{n-1}\right)^{n/2}} = \int_{-\infty}^{\infty} \frac{dt}{\left(1 + \frac{t^2}{n-1}\right)^{n/2}} - \int_{-\infty}^{z} \frac{dt}{\left(1 + \frac{t^2}{n-1}\right)^{n/2}}.$$

Multiplying this by the factor preceding the integral in Eq. (17.76) yields $P(-z) = 1 - P(z)$. In the following example, we show how to apply the Student t distribution to our fit of Example 17.6.1.

EXAMPLE 17.6.2

Confidence Interval Here, we want to determine a confidence interval for the slope a in the linear $y = at$ fit of Fig. 17.8. We assume

- first that the sample points (t_j, y_j) are random and independent; and
- second that, for each fixed value t, the random variable Y is normal with mean $\mu(t) = at$ and variance σ^2 independent of t.

These values y_j are measurements of the random variable Y, but we will regard them as single measurements of the independent random variables Y_j with the same normal distribution as Y (whose variance we do not know).

We choose a confidence level, for example, $p = 95\%$. Then the Student probability is

$$P(-C, C) = P(C) - P(-C) = p = -1 + 2P(C), \quad \text{hence } P(C) = \frac{1}{2}(1 + p),$$

using $P(-C) = 1 - P(C)$, and

$$P(C) = \frac{1}{2}(1 + p) = 0.975 = K_n \int_{-\infty}^{C} \left(1 + \frac{t^2}{n}\right)^{-(n+1)/2} dt,$$

where K_{n-1} is the factor preceding the integral in Eq. (17.76). Now we determine a solution $C = 4.3$ from Table 17.3 of Student's t distribution with $n = N - r = 3 - 1 = 2$ the number of degrees of freedom, noting that $(1 + p)/2$ corresponds to p in Table 17.3.

Then we compute $A = C\sigma_a/\sqrt{N}$ for sample size $N = 3$. The confidence interval is given by

$$a - A \le a \le a + A, \qquad \text{at } p = 95\% \text{ confidence level.}$$

From the χ^2 analysis of Example 17.6.1, we use the slope $a = 0.782$ and variance $\sigma_a^2 = 0.023^2$ so that $A = 4.3\frac{0.023}{\sqrt{3}} = 0.057$, and the confidence interval is determined by $a - A = 0.782 - 0.057 = 0.725$, $a + A = 0.839$, or

$$0.725 < a < 0.839 \quad \text{at } 95\% \text{ confidence level.}$$

Compared to σ_a, the uncertainty of a has increased due to the high confidence level. Table 17.3 shows that a decrease in confidence level, p, reduces the uncertainty interval, and increasing the number of degrees of freedom, n, would also lower the range of uncertainty. ■

EXERCISES

17.6.1 Let ΔA be the error of a measurement of A, etc. Use error propagation to show that $(\frac{\sigma(C)}{C})^2 = (\frac{\sigma(A)}{A})^2 + (\frac{\sigma(B)}{B})^2$ holds for the product $C = AB$ and the ratio $C = A/B$.

17.6.2 Find the mean value and standard deviation of the sample of measurements $x_1 = 6.0$, $x_2 = 6.5$, $x_3 = 5.9$, $x_5 = 6.2$. If the point $x_6 = 6.1$ is added to the sample, how does the change affect the mean value and standard deviation?

17.6.3 (a) Carry out a χ^2 analysis of the fit of case b in Fig. 17.9 assuming the same errors for the t_i, $\Delta t_i = \Delta y_i$, as for the y_i used in the χ^2 analysis of the fit in Fig. 17.8.
(b) Determine the confidence interval at the 95% confidence level.

17.6.4 If $x_1, x_2, \ldots, x_n$ are a sample of measurements with its mean value given by the arithmetic mean $\bar{x}$, and the corresponding random variables X_j that take the values x_j with the same probability are independent and have mean value μ and variance σ^2, then show that $\langle \bar{x} \rangle = \mu$ and

$\sigma^2(\bar{x}) = \sigma^2/n$. If $\bar{\sigma}^2 = \frac{1}{n}\sum_j (x_j - \bar{x})^2$ is the sample variance, show that $\langle \bar{\sigma}^2 \rangle = \frac{n-1}{n}\sigma^2$.

Biographical Data

Pascal, Blaise. Pascal, a French mathematician, was born in 1623 and died in 1662. A prodigy in mathematics, he mastered Euclidean geometry at age 12 and later contributed to the conic sections using methods of Desargues. He invented and built the first mechanical calculator in 1645, which was capable of adding, subtracting, and multiplying. His contributions to probability theory originated from his interest in calculating odds involved in various games he played in Paris while seeking diversions from his chronic ill health. After a religious period in a monastery, he continued his mathematical work, partly in collaboration with Pierre de Fermat.

Additional Reading

Bevington, P. R., and Robinson, D. K. (2003). *Data Reduction and Error Analysis for the Physical Sciences*, 3rd ed. McGraw-Hill, New York.

Chung, K. L. (2000). *A Course in Probability Theory Revised*, 3rd ed. Academic Press, New York.

Degroot, M. H. (1986). *Probability and Statistics*, 2nd ed. Addison-Wesley, New York.

Devore, J. L. (1999). *Probability and Statistics for Engineering and the Sciences*, 5th ed. Duxbury, New York.

Kreyszig, E. (1970). *Introductory Mathematical Statistics. Principles and Methods.* Wiley, New York.

Montgomery, D. C., and Runger, G. C. (1998). *Applied Statistics and Probability for Engineers*, 2nd ed. Wiley, New York.

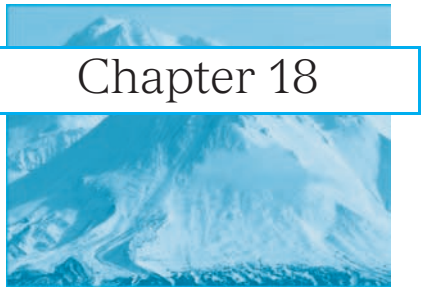
Papoulis, A. (1991). *Probability, Random Variables, and Stochastic Processes*, 3rd ed. McGraw-Hill, New York.

Ross, S. M. (1997). *First Course in Probability*, 5th ed., Vol. A. Prentice-Hall, New York.

Ross, S. M. (1999). *Introduction to Probability and Statistics for Engineers and Scientists*, 2nd ed. Academic Press, New York.

Ross, S. M. (2000). *Introduction to Probability Models*, 7th ed. Academic Press, New York.

Suhir, E. (1997). *Applied Probability for Engineers and Scientists.* McGraw-Hill, New York.



Chapter 18

Calculus of Variations

Uses of the Calculus of Variations

In this chapter, we address a different class of minimum/maximum problems where we search for an appropriate function or curve, rather than a value of some variable, that makes a given quantity stationary, usually an energy or action integral. Because a function is varied, these problems are called variational. Variational principles, such as D'Alembert's or Hamilton's, have been developed in classical mechanics, and Lagrangian techniques occur in quantum mechanics and field theory, but they also appear in electrodynamics (e.g., Fermat's principle of the shortest optical path). Before plunging into this different branch of mathematical physics, let us summarize some of its uses in both physics and mathematics.

1. In existing physical theories:
   a. Unification of diverse areas of physics using energy and action as key concepts.
   b. Convenience in analysis—Lagrange equations Section 18.2.
   c. Elegant treatment of constraints, Section 18.5.
2. Starting point for new, complex areas of physics and engineering: In general relativity the geodesic is taken as the minimum path of a light pulse or the free fall path of a particle in curved Riemannian space. Variational principles appear in quantum field theory and have been applied extensively in control theory.
3. Mathematical unification: Variational analysis provides a proof of the completeness of the Sturm–Liouville eigenfunctions (Chapter 9), and establishes a lower bound for the eigenvalues.
4. Calculation techniques (Section 18.6): Calculation of the eigenfunctions and eigenvalues of the Sturm–Liouville equation.

18.1 A Dependent and an Independent Variable

Concept of Variation

The calculus of variations involves problems in which the quantity to be minimized (or maximized) appears as a stationary integral, a functional because a function $y(x)$ needs to be determined. As the simplest case, let

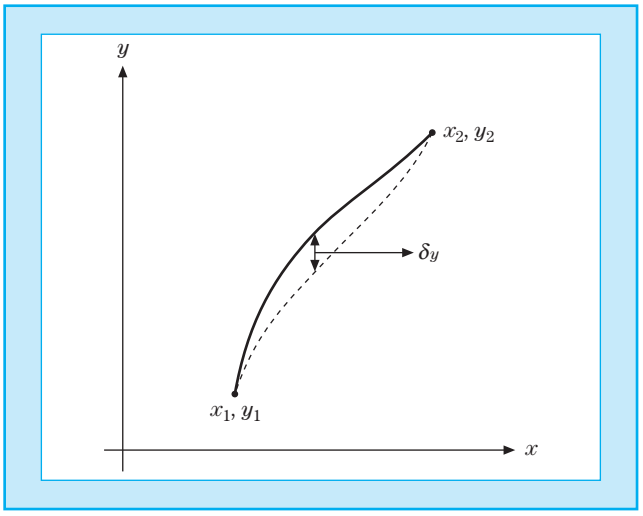
$$J = \int_{x_1}^{x_2} f\left(y, \frac{dy}{dx}, x\right) dx, \tag{18.1}$$

where J is the quantity that takes on a stationary value. Under the integral sign, f is a known function of the indicated variables $y(x)$, $dy(x)/dx$, x but the dependence of y on x is not yet known; that is, $y(x)$ is **unknown**. This means that although the integral is from x_1 to x_2, the exact path of integration is not known (Fig. 18.1). We are to choose the path of integration through points (x_1, y_1) and (x_2, y_2) to minimize J. Strictly speaking, we determine stationary values of J: minima, maxima, or saddle points. In most cases of physical interest the stationary value will be a minimum.

This problem is considerably more difficult than the corresponding problem of a function $y(x)$ in differential calculus. Indeed, there may be no solution. In differential calculus, the minimum is determined by comparing $y(x_0)$ with $y(x)$, where x ranges over neighboring points. Here, we assume the existence of an optimum path—that is, an acceptable path for which J is stationary—and then compare J for our (unknown) optimum path with that obtained from neighboring paths. In Fig. 18.1 two possible paths are shown. (There are an infinitely many.) The difference between these two for a given x is called the variation of y, δy, and is conveniently described by introducing a new function

Figure 18.1

A Varied Path



$\eta(x)$ to define the arbitrary deformation of the path and a scale factor α to give the magnitude of the variation. The function $\eta(x)$ is arbitrary except for two restrictions. First,

$$\eta(x_1) = \eta(x_2) = 0, \tag{18.2}$$

which means that all varied paths must pass through the fixed end points. Second, as will be seen soon, $\eta(x)$ must be differentiable; that is, we may **not** use

$$\begin{aligned} \eta(x) &= 1, \quad x = x_0, \\ &= 0, \quad x \neq x_0, \end{aligned} \tag{18.3}$$

but we can choose $\eta(x)$ to have a form similar to the functions used to represent the Dirac delta function (Chapter 1) so that $\eta(x)$ differs from zero only over an infinitesimal region.[1] Then, with a path described by α and $\eta(x)$,

$$y(x, \alpha) = y(x, 0) + \alpha\eta(x) \tag{18.4}$$

and

$$\delta y = y(x, \alpha) - y(x, 0) = \alpha\eta(x). \tag{18.5}$$

Let us choose $y(x, 0)$ as the unknown path that will minimize or maximize J. Then $y(x, \alpha)$ with $\alpha \neq 0$ describes a neighboring path. In Eq. (18.1), J is now a function[2] of our parameter α [and of the $\eta(x)$]:

$$J(\alpha) = \int_{x_1}^{x_2} f[y(x, \alpha), y_x(x, \alpha), x]dx, \tag{18.6}$$

with $y_x \equiv \partial y/\partial x$, and our condition for an extreme value is that

$$\left[\frac{\partial J(\alpha)}{\partial \alpha}\right]_{\alpha=0} = 0, \tag{18.7}$$

analogous to the vanishing of the derivative dy/dx in differential calculus.

Now the α-dependence of the integral is contained in $y(x, \alpha)$ and $y_x(x, \alpha) = (\partial/\partial x)y(x, \alpha)$. Therefore,[3]

$$\frac{\partial J(\alpha)}{\partial \alpha} = \int_{x_1}^{x_2} \left[\frac{\partial f}{\partial y}\frac{\partial y}{\partial \alpha} + \frac{\partial f}{\partial y_x}\frac{\partial y_x}{\partial \alpha}\right]dx. \tag{18.8}$$

From Eq. (18.4),

$$\frac{\partial y(x, \alpha)}{\partial \alpha} = \eta(x) \tag{18.9}$$

$$\frac{\partial y_x(x, \alpha)}{\partial \alpha} = \frac{d\eta(x)}{dx} \tag{18.10}$$

[1] Compare H. Jeffreys and B. S. Jeffreys, *Methods of Mathematical Physics*, 3rd ed. Cambridge Univ. Press, Cambridge, UK (1966), Chapter 10, for a more complete discussion of this point.

[2] Technically, J is a **functional**, depending on the functions $y(x, \alpha)$ and $\partial y/\partial x = y_x(x, \alpha)$: $J[y(x, \alpha), y_x(x, \alpha)]$.

[3] Note that y and y_x are being treated as **independent** variables.

so that Eq. (18.8) becomes

$$\frac{\partial J(\alpha)}{\partial \alpha} = \int_{x_1}^{x_2} \left(\frac{\partial f}{\partial y}\eta(x) + \frac{\partial f}{\partial y_x}\frac{d\eta(x)}{dx} \right) dx. \tag{18.11}$$

Integrating the second term by parts to get $\eta(x)$ as a common and arbitrary nonvanishing factor, we obtain

$$\int_{x_1}^{x_2} \frac{d\eta(x)}{dx}\frac{\partial f}{\partial y_x}\,dx = \eta(x)\frac{\partial f}{\partial y_x}\bigg|_{x_1}^{x_2} - \int_{x_1}^{x_2} \eta(x)\frac{d}{dx}\frac{\partial f}{\partial y_x}\,dx. \tag{18.12}$$

The integrated part vanishes by Eq. (18.2) and, setting $\partial J(\alpha)/\partial\alpha = 0$ at $\alpha = 0$, Eq. (18.11) leads to

$$\int_{x_1}^{x_2} \left[\frac{\partial f}{\partial y} - \frac{d}{dx}\frac{\partial f}{\partial y_x} \right] \eta(x)\,dx = 0. \tag{18.13}$$

Occasionally, Eq. (18.13) is multiplied by α, which gives

$$\int_{x_1}^{x_2} \left(\frac{\partial f}{\partial y} - \frac{d}{dx}\frac{\partial f}{\partial y_x} \right) \delta y\,dx = \delta J = 0. \tag{18.14}$$

Since $\eta(x)$ is arbitrary, we may choose it to have the same sign as the remainder of the integrand of Eq. (18.13), whenever the latter differs from zero. Hence, the integrand is always nonnegative. Equation (18.13), our condition for the existence of a stationary value, can then be satisfied only if [4]

$$\frac{\partial f}{\partial y} - \frac{d}{dx}\frac{\partial f}{\partial y_x} = 0. \tag{18.15}$$

This partial differential equation (PDE) is known as the Euler equation and can be expressed in various other forms. Sometimes, solutions are missed when they are not twice differentiable as required by Eq. (18.15). It is clear that Eq. (18.15) must be satisfied for J to take on a stationary value, that is, for Eq. (18.14) to be satisfied. Equation (18.15) is necessary, but it is by no means sufficient.[5] Courant and Robbins illustrate this very well by considering the distance over a sphere between points on the sphere, A and B (Fig. 18.2). Path 1, a great circle, is found from Eq. (18.15). However, path 2, the remainder of the great circle through points A and B, also satisfies the Euler equation. Path 2 is a maximum but only if we demand that it be a great circle and then only if we make less than one circuit; that is, path 2 plus n complete revolutions is also a solution. If the path is not required to be a great circle, any deviation from path 2 will increase the length. This is hardly the property of a local maximum, and

[4] It is important to watch the meaning of $\partial/\partial x$ and d/dx closely. For example, if $f = f[y(x), y_x, x]$,

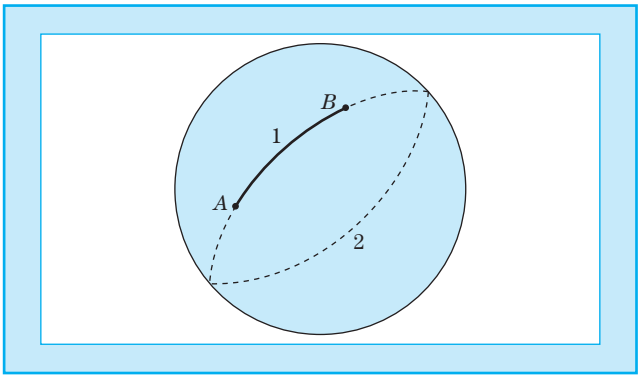
$$\frac{df}{dx} = \frac{\partial f}{\partial x} + \frac{\partial f}{\partial y}\frac{dy}{dx} + \frac{\partial f}{\partial y_x}\frac{d^2y}{dx^2}.$$

The first term on the right gives the **explicit** x-dependence. The second and third terms give the **implicit** x-dependence via y and y_x.

[5] For a discussion of sufficiency conditions and the development of the calculus of variations as a part of mathematics, see G. M. Ewing, *Calculus of Variations with Applications* [Norton, New York (1969)]. Sufficiency conditions are also covered by Sagan (see Additional Reading).

Figure 18.2

Stationary Paths over a Sphere



that is why it is important to check the properties of solutions of Eq. (18.15) to see if they satisfy the physical conditions of the given problem.

EXAMPLE 18.1.1

Straight Line Perhaps the simplest application of the Euler equation is in the determination of the shortest distance between two points in the Euclidean xy-plane in terms of a straight line. Because the element of distance is

$$ds = [(dx)^2 + (dy)^2]^{1/2} = \left[1 + y_x^2\right]^{1/2} dx, \tag{18.16}$$

the distance, J, may be written as

$$J = \int_{(x_1, y_1)}^{(x_2, y_2)} ds = \int_{x_1}^{x_2} \left[1 + y_x^2\right]^{1/2} dx. \tag{18.17}$$

Comparison with Eq. (18.1) shows that

$$f(y, y_x, x) = \left(1 + y_x^2\right)^{1/2} \tag{18.18}$$

depends only on $y_x = \partial y/\partial x$ but not on y or x. Substituting into Eq. (18.15) and using $\partial f/\partial y \equiv 0$, we obtain

$$\frac{d}{dx}\frac{\partial f}{\partial y_x} = 0,$$

which can be integrated to yield

$$\frac{\partial f}{\partial y_x} = \frac{y_x}{\left(1 + y_x^2\right)^{1/2}} = C, \tag{18.19}$$

with C a constant. This can only be satisfied by

$$y_x = a, \quad \text{with } a \text{ a constant}, \tag{18.20}$$

which has solution

$$y = ax + b, \tag{18.21}$$

the familiar equation for a straight line. The integration constants a and b are now chosen so that the line passes through the two points (x_1, y_1) and (x_2, y_2). Hence, the Euler equation predicts that the shortest[6] distance between two fixed points in Euclidean space is a straight line.

The generalization of this example in curved four-dimensional space–time leads to the important concept of the geodesic in general relativity and its differential equation (see Chapter 2). ■

EXAMPLE 18.1.2

Optical Path Near Event Horizon of a Black Hole Determine the optical path in an atmosphere in which the velocity of light increases in proportion to the height, $v(y) = y/b$, with $b > 0$ some parameter describing the light speed. Therefore, $v = 0$ at $y = 0$, which simulates the conditions at the surface of a black hole, called its event horizon, where the gravitational force is so strong that the velocity of light goes to zero, thus even trapping light.

Because light takes the shortest time, the variational problem takes the form

$$\Delta t = \int_{t_1}^{t_2} dt = \int_{s_1}^{s_2} \frac{ds}{v} = b \int_{t_1}^{t_2} \frac{\sqrt{dx^2 + dy^2}}{y} dt = \text{minimum},$$

where $v = ds/dt = y/b$ is the velocity of light in this environment, with the y coordinate being the height. A look at the variational functional suggests choosing y as the independent variable because x does not appear in the integrand. We can bring dy outside the radical and change the role of x and y in J of Eq. (18.1) and the resulting Euler equation. With $x = x(y)$, $x' = dx/dy$, we obtain

$$b \int_{y_1}^{y_2} \frac{\sqrt{x'^2 + 1}}{y} dy = \text{minimum}$$

and the Euler equation becomes

$$\frac{\partial f}{\partial x} - \frac{d}{dy} \frac{\partial f}{\partial x'} = 0. \tag{18.22}$$

Since $\partial f/\partial x = 0$, this can be integrated, giving

$$\frac{x'}{y\sqrt{x'^2 + 1}} = C_1 = \text{ const.} \quad \text{or} \quad x'^2 = C_1^2 y^2 (x'^2 + 1).$$

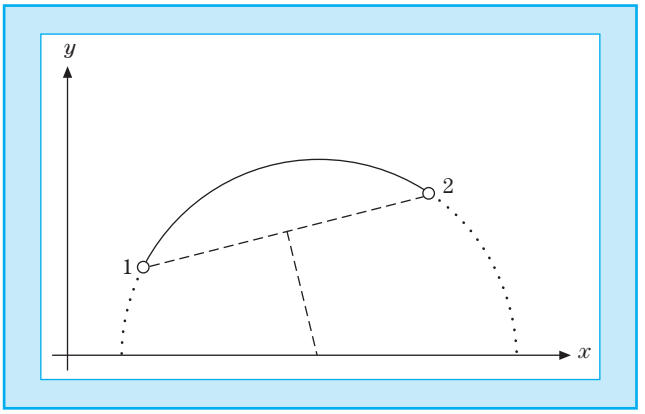
Separating dx and dy in this first-order ordinary differential equation (ODE), we find the integral

$$\int^x dx = \int^y \frac{C_1 y\, dy}{\sqrt{1 - C_1^2 y^2}},$$

[6]Technically, we have a stationary value. From the α^2 terms it can be identified as a minimum (Exercise 18.1.5).

Figure 18.3

Circular Optical Path in Medium



which yields

$$x + C_2 = \frac{-1}{C_1}\sqrt{1 - C_1^2 y^2} \quad \text{or} \quad (x + C_2)^2 + y^2 = \frac{1}{C_1^2}.$$

This is a circular light path with center on the x-axis along the event horizon (Fig. 18.3). This example may be adapted to a mirage (Fata Morgana) in a desert with hot air near the ground and cooler air aloft (the index of refraction changes with height in cool versus hot air), thus changing the velocity law from $v = y/b \to v_0 - y/b$. In this case, the circular light path is no longer convex with center on the x-axis but rather becomes concave. ■

EXAMPLE 18.1.3

Soap Film As a second illustration (Fig. 18.4), consider two parallel coaxial wire circles to be connected by a surface of minimum area that is generated by revolving a curve $y(x)$ about the x-axis. Physically, this will minimize the energy due to surface tension. The curve is required to pass through fixed end points (x_1, y_1) and (x_2, y_2). The variational problem is to choose the curve $y(x)$ so that the area of the resulting surface will be a minimum.

For the element of area shown in Fig. 18.4,

$$dA = 2\pi y\, ds = 2\pi y(dx^2 + dy^2)^{1/2}, \tag{18.23}$$

where we keep x as the independent variable and bring dx outside the radical. The variational functional is then

$$A = J = \int_{x_1}^{x_2} 2\pi y\left(1 + y_x^2\right)^{1/2} dx, \quad y_x = \frac{dy}{dx}.$$

Neglecting the 2π, we obtain

$$f(y, y_x, x) = y\left(1 + y_x^2\right)^{1/2}.$$

Since $\partial f/\partial x = 0$, instead of choosing y as an independent variable as in Example 18.1.2, which would be inconvenient here, we apply the following variant

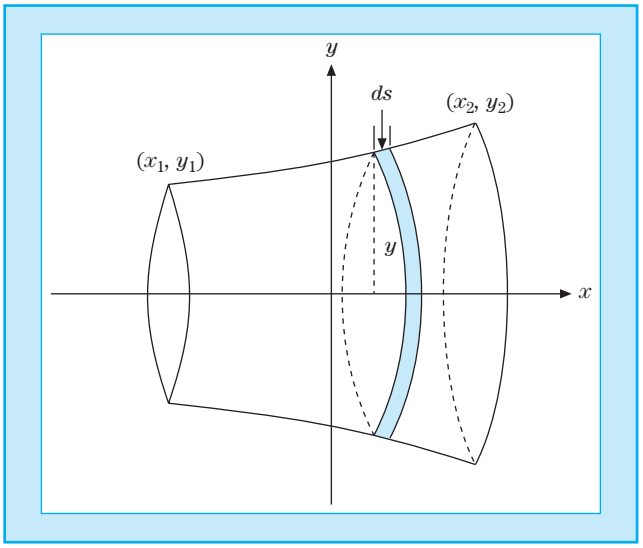


Figure 18.4

Surface of Rotation-Soap Film Problem

of the Euler Eq. (18.15):

$$\frac{\partial f}{\partial x} - \frac{d}{dx}\left(f - y_x \frac{\partial f}{\partial y_x}\right) = 0. \tag{18.24}$$

To prove this, we first carry out the differentiation explicitly:

$$\begin{aligned}\frac{d}{dx}\left(f - y_x \frac{\partial f}{\partial y_x}\right) &= \frac{\partial f}{\partial x} + y_x \frac{\partial f}{\partial y} + y_{xx} \frac{\partial f}{\partial y_x} - y_{xx} \frac{\partial f}{\partial y_x} - y_x \frac{d}{dx} \frac{\partial f}{\partial y_x} \\ &= \frac{\partial f}{\partial x} + y_x \left(\frac{\partial f}{\partial y} - \frac{d}{dx} \frac{\partial f}{\partial y_x}\right) = \frac{d}{dy} \frac{\partial f}{\partial x'}.\end{aligned}$$

Bringing f_x to the left-hand side, we obtain

$$-\frac{\partial f}{\partial x} + \frac{d}{dx}\left(f - y_x \frac{\partial f}{\partial y_x}\right) = y_x \left(\frac{\partial f}{\partial y} - \frac{d}{dx} \frac{\partial f}{\partial y_x}\right),$$

thus verifying the equivalence of the Euler variant [Eq. (18.24)] and Eq. (18.15) for $y_x \neq 0$. Then, in the last equality, we enforce the equivalence of the Euler Eqs. (18.22) and (18.15), which can now be written as

$$\frac{\partial f}{\partial x} - \frac{d}{dy} \frac{\partial f}{\partial x'} = -y_x \left(\frac{\partial f}{\partial y} - \frac{d}{dx} \frac{\partial f}{\partial y_x}\right).$$

For $y_x \neq 0$ the equivalence of both Euler equations is manifest. From this form [Eq. (18.24)], we get, with $\frac{\partial f}{\partial x} = 0$,

$$\frac{d}{dx}\left(f - y_x \frac{\partial f}{\partial x}\right) = 0,$$

which we integrate to yield

$$f - y_x \frac{\partial f}{\partial x} = c_1 = \text{const.}$$

In our case, this is

$$y\left(1 + y_x^2\right)^{1/2} - y y_x^2 \frac{1}{\left(1 + y_x^2\right)^{1/2}} = c_1 \tag{18.25}$$

or

$$\frac{y}{\left(1 + y_x^2\right)^{1/2}} = c_1. \tag{18.26}$$

Squaring, we get

$$\frac{y^2}{1 + y_x^2} = c_1^2. \tag{18.27}$$

Since $y_x^2 \geq 0$, Eq. (18.26) implies that $y^2 \geq c_1^2$ so that

$$(y_x)^{-1} = \frac{dx}{dy} = \frac{c_1}{\sqrt{y^2 - c_1^2}}. \tag{18.28}$$

This may be integrated to give

$$x = c_1 \cosh^{-1} \frac{y}{c_1} + c_2. \tag{18.29}$$

Solving for y, we have

$$y = c_1 \cosh\left(\frac{x - c_2}{c_1}\right). \tag{18.30}$$

The constants c_1 and c_2 are determined by requiring this curve to pass through the points (x_1, y_1) and (x_2, y_2). Our "minimum" area surface is a special case of a catenary of revolution or a **catenoid**.

For an excellent discussion of both the mathematical problems and experiments with soap films, we refer to Courant and Robbins in Additional Reading. ■

Biographical Data

d'Alembert, Jean Le Rond. d'Alembert, a French physicist and mathematician, was born in 1717 in Paris and died in 1783 in Paris. Illegitimate son of a Paris salon hostess and a cavalry officer, he was abandoned at the church of St. Jean-le-Rond (whence his name) and raised by a foster family, his education being supported by his father. Besides the famous variational principle of analytical mechanics named after him, he developed the precession of the equinoxes in celestial mechanics, fluid dynamics, and vibrating strings, introducing the separation of variables.

EXERCISES

18.1.1 Derive Euler's equation by expanding the integrand of

$$J(\alpha) = \int_{x_1}^{x_2} f[y(x, \alpha), y_x(x, \alpha), x]dx$$

in powers of a using a Taylor (Maclaurin) expansion with y and y_x as the two variables (Section 5.6).
Note. The stationary condition is $\partial J(\alpha)/\partial\alpha = 0$, evaluated at $\alpha = 0$. The terms quadratic in α may be useful in establishing the nature of the stationary solution (maximum, minimum, or saddle point).

18.1.2 Find the Euler equation corresponding to Eq. (18.15) if $f = f(y_{xx}, y_x, y, x)$.

ANS.
$$\frac{d^2}{dx^2}\left(\frac{\partial f}{\partial y_{xx}}\right) - \frac{d}{dx}\left(\frac{\partial f}{\partial y_x}\right) + \frac{\partial f}{\partial y} = 0,$$
$$\eta(x_1) = \eta(x_2) = 0, \quad \eta_x(x_1) = \eta_x(x_2) = 0.$$

18.1.3 The integrand $f(y, y_x, x)$ of Eq. (18.1) has the form

$$f(y, y_x, x) = f_1(x, y) + f_2(x, y)y_x.$$

(a) Show that the Euler equation leads to

$$\frac{\partial f_1}{\partial y} - \frac{\partial f_2}{\partial x} = 0.$$

(b) What does this imply for the dependence of the integral J upon the choice of path?

18.1.4 Show that the condition that

$$J = \int f(x, y)dx$$

has a stationary value
(a) leads to $f(x, y)$ independent of y and
(b) yields no information about any x-dependence.
We get no (continuous, differentiable) solution. To be a meaningful variational problem, dependence on y or higher derivatives is essential.
Note. The situation will change when constraints are introduced.

18.1.5 In Example 18.1.1, expand $J[y(x, \alpha)] - J[y(x, 0)]$ in powers of α. The term linear in α leads to the Euler equation and to the straight-line solution [Eq. (18.21)]. Investigate the α^2 term and show that the stationary value of J, the straight-line distance, is a **minimum**.

18.1.6 (a) Show that the integral

$$J = \int_{x_1}^{x_2} f(y, y_x, x)\, dx, \quad \text{with} \quad f = y(x),$$

has **no** extreme values.
(b) If $f(y, y_x, x) = y^2(x)$, find a discontinuous solution.

18.1.7 Fermat's principle of optics states that a light ray will follow the path $y(x)$, for which

$$\int_{x_1, y_1}^{x_2, y_2} n(y, x) ds$$

is a minimum when n is the index of refraction. For $y_2 = y_1 = 1$, $-x_1 = x_2 = 1$, find the ray path if
(a) $n = e^y$, (b) $n = a(y - y_0)$, $y > y_0$.

18.1.8 A frictionless particle moves from point A on the surface of the earth to point B by sliding through a tunnel under the gravitational force. Find the differential equation to be satisfied if the transit time is to be a minimum.
Note. Assume the earth to be a nonrotating sphere of uniform density and the depth of the tunnel to be small compared to the radius of the earth.

ANS. [Eq. (18.15)] $r_{\varphi\varphi}(r^3 - ra^2) + r_\varphi^2(2a^2 - r^2) + a^2r^2 = 0$,
$r(\varphi = 0) = r_0$, $r_\varphi(\varphi = 0) = 0$, $r(\varphi = \varphi_A) = a$,
$r(\varphi = \varphi_B) = a$. Or: $r_\varphi^2 = \dfrac{a^2r^2}{r_0^2} \cdot \dfrac{r^2 - r_0^2}{a^2 - r^2}$

The solution of these equations is a hypocycloid, generated by a circle of radius $\frac{1}{2}(a - r_0)$ rolling inside the circle of radius a. You might want to show that the transit time is

$$t = \pi \frac{(a^2 - r_0^2)^{1/2}}{(ag)^{1/2}}.$$

For details, see P. W. Cooper, *Am. J. Phys.* **34**, 68 (1966); G. Veneziano *et al.*, *Am. J. Phys.* **34**, 701–704 (1966).

18.1.9 A ray of light follows a straight-line path in a first homogeneous medium, is refracted at an interface, and then follows a new straight-line path in the second medium. Use Fermat's principle of optics to derive Snell's law of refraction:

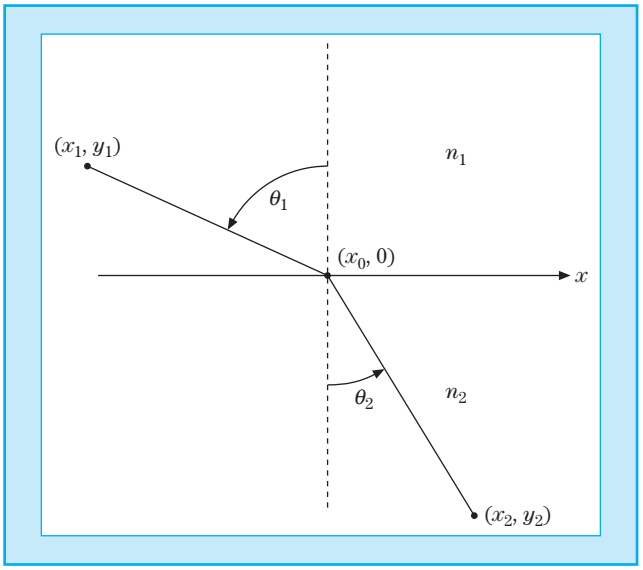
$$n_1 \sin\theta_1 = n_2 \sin\theta_2.$$

Hint. Keep the points (x_1, y_1) and (x_2, y_2) fixed and vary x_0 to satisfy Fermat (Fig. 18.5). This is **not** a Euler equation problem. (The light path is not differentiable at x_0.)

18.1.10 Find the curve of quickest descent from $(0, 0)$ to (x_0, y_0) for a particle sliding under gravity and without friction. Show that the ratio of times taken by the particle along a straight line joining the two points compared to along the curve of quickest descent is $(1 + 4/\pi^2)^{1/2}$.
Hint. Take y to increase downwards. Obtain $y_x^2 = (1 - c^2y)/c^2y$, where c is an integration constant. Then make the substitution

Figure 18.5

Snell's Law



$y = (\sin^2 \varphi/2)/c^2$ to parameterize the cycloid and take $(x_0, y_0) = (\pi/2c^2, 1/c^2)$.

18.1.11 What is the shortest distance between two points on a cylinder?

18.2 Several Dependent Variables

Our original variational problem, Eq. (18.1), may be generalized in several respects. In this section, we consider the integrand, f, to be a function of several **dependent** variables, $y_1(x)$, $y_2(x)$, $y_3(x)$, . . ., all of which depend on x, the independent variable. In Section 18.3, f again will contain only one unknown function y, but y will be a function of several independent variables (over which we integrate). In Section 18.4, these two generalizations are combined. Finally, in Section 18.5 the stationary value is restricted by one or more constraints.

For more than one dependent variable, Eq. (18.1) becomes

$$J = \int_{x_1}^{x_2} f[y_1(x), y_2(x), \ldots, y_n(x), y_{1x}(x), y_{2x}(x), \ldots, y_{nx}(x), x]dx. \quad (18.31)$$

As in Section 18.1, we determine the extreme value of J by comparing neighboring paths. Let

$$y_i(x, \alpha) = y_i(x, 0) + \alpha\eta_i(x), \qquad i = 1, 2, \ldots, n, \quad (18.32)$$

with the η_i independent of one another but subject to the restrictions discussed in Section 18.1. By differentiating Eq. (18.31) with respect to α and setting

$\alpha = 0$, since Eq. (18.6) still applies, we obtain

$$\int_{x_1}^{x_2} \sum_i \left(\frac{\partial f}{\partial y_i} \eta_i + \frac{\partial f}{\partial y_{ix}} \eta_{ix} \right) dx = 0, \tag{18.33}$$

the subscript x denoting partial differentiation with respect to x; that is, $y_{ix} = \partial y_i / \partial x$, and so on. Again, each of the terms $(\partial f / \partial y_{ix}) \eta_{ix}$ is integrated by parts. The integrated part vanishes and Eq. (18.33) becomes

$$\sum_i \int_{x_1}^{x_2} \left(\frac{\partial f}{\partial y_i} - \frac{d}{dx} \frac{\partial f}{\partial y_{ix}} \right) \eta_i \, dx = 0. \tag{18.34}$$

Since the η_i are arbitrary and **independent** of one another,[7] each of the terms in the sum must vanish **independently**. We have

$$\frac{\partial f}{\partial y_i} - \frac{d}{dx} \frac{\partial f}{\partial (\partial y_i / \partial x)} = 0, \quad i = 1, 2, \ldots, n, \tag{18.35}$$

a whole set of Euler equations, each of which must be satisfied for an extreme value.

EXAMPLE 18.2.1

Missing Dependent Variables Consider the variational problem $\int f(\dot{\mathbf{r}}) dt =$ minimum. Here, $\dot{\mathbf{r}} = d\mathbf{r}/dt$ and $\mathbf{r}$ is absent from the integrand. Therefore, the Euler equations become

$$\frac{d}{dt} \frac{\partial f}{\partial \dot{x}} = 0, \qquad \frac{d}{dt} \frac{\partial f}{\partial \dot{y}} = 0, \qquad \frac{d}{dt} \frac{\partial f}{\partial \dot{z}} = 0,$$

with $\mathbf{r} = (x, y, z)$ so that $f_{\dot{\mathbf{r}}} = (\frac{\partial f}{\partial \dot{x}}, \frac{\partial f}{\partial \dot{y}}, \frac{\partial f}{\partial \dot{z}}) = \mathbf{c} =$ const. Solving these three equations for the three unknowns $\dot{x}, \dot{y}, \dot{z}$ yields $\dot{\mathbf{r}} = \mathbf{c}_1 =$ const. Integrating this constant velocity gives $\mathbf{r} = \mathbf{c}_1 t + \mathbf{c}_2$. The solutions are straight lines despite the general nature of the function f.

A physical example illustrating this case is the propagation of light in a crystal, where the velocity of light depends on the (crystal) directions but not on the location in the crystal because a crystal is an anisotropic **homogeneous medium**. The variational problem

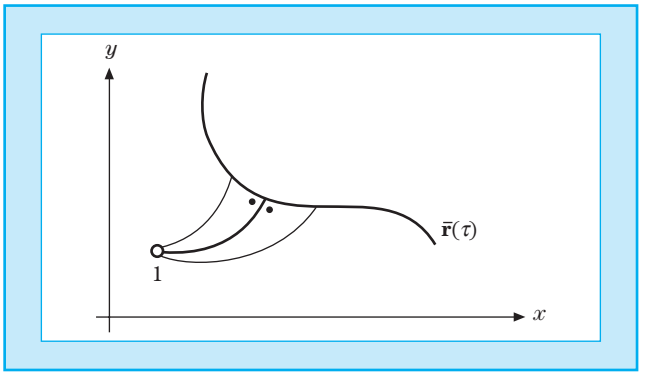
$$\int \frac{ds}{v} = \int \frac{\sqrt{\dot{\mathbf{r}}^2}}{v(\dot{\mathbf{r}})} dt = \text{ minimum}$$

has the form of our example. Note that t need not be the time, but it parameterizes the light path. ■

[7] For example, we could set $\eta_2 = \eta_3 = \eta_4 \cdots = 0$, eliminating all but one term of the sum, and then treat η_1 exactly as in Section 18.1.

Figure 18.6

Transversality Condition



Transversality Condition

So far in our variational problems we have held the end points of the varied curves fixed (see Fig. 18.1). Now we relax this condition and let one end point move on a given path for the following reason: We anticipate using the variational calculus to deal with problems such as Examples 1.2.2 and 1.3.1, where we seek the shortest distance from an observer to a rocket in flight or between two rockets in free flight. We shall find and confirm the result of these examples that the line of shortest distance is perpendicular to the rocket path, which is called transversality condition. It may be used to determine the location of the end point.

Let $\mathbf{r} = \bar{\mathbf{r}}(\tau)$ be the rocket path that, in general, will not be a straight line, and $\mathbf{r}_0$ the position of the observer. Let $\mathbf{r} = \mathbf{r}_1(t, \tau)$ be a family of curves from any point τ on the rocket path to the observer covering a surface area so that $\mathbf{r}_1(t = 0, \tau) = \mathbf{r}_0$ (for all τ values) is the observer's location and $\mathbf{r}_1(t = 1, \tau) = \bar{\mathbf{r}}(\tau)$, its intersection with the rocket path (Fig. 18.6). Let $\tau = \tau_0$ denote the curve of shortest distance (the extremal solution) so that $\mathbf{r}_1(t = 1, \tau_0) = \mathbf{r}_s$ is the intersection of the shortest distance curve with the rocket path. Now we vary the intersection point $\mathbf{r}_s$ so that $\mathbf{r}_1(t, \tau_0)$ becomes $\mathbf{r}_1(t, \tau_0) + \alpha\mathbf{T}(t)$ for small enough α. Here, $\mathbf{T} = \partial\mathbf{r}_1/\partial\tau$, and for $t = 1$, $\tau = \tau_0$, it is the tangent vector $d\bar{\mathbf{r}}/d\tau = \mathbf{T}_0$ of the rocket path at $\mathbf{r}_s$. At the observer's point we have $\mathbf{T} \to 0$ because this point is fixed. Now we substitute this curve into the variational integral

$$J(\alpha) = \int_0^1 f(\mathbf{r}_1 + \alpha\mathbf{T}, \dot{\mathbf{r}}_1 + \alpha\dot{\mathbf{T}})dt$$

and set $\frac{\partial J(\alpha)}{\partial \alpha}|_{\alpha=0} = 0$ (see Eq. 18.7), expand to first order in α, and integrate by parts as usual to find

$$0 = J'(0) = \int_0^1 [f_{\mathbf{r}} \cdot \mathbf{T} + f_{\dot{\mathbf{r}}} \cdot \dot{\mathbf{T}}]dt = \int_0^1 \left[f_{\mathbf{r}} - \frac{d}{dt} f_{\dot{\mathbf{r}}}\right] \cdot \mathbf{T}dt + f_{\dot{\mathbf{r}}} \cdot \mathbf{T}\Big|_{t=0}^1,$$

where $f_{\mathbf{r}} = (\partial f/\partial x, \partial f/\partial y, \partial f/\partial z)$ and $f_{\dot{\mathbf{r}}} = (\partial f/\partial \dot{x}, \partial f/\partial \dot{y}, \partial f/\partial \dot{z})$. Here, the integral vanishes because for $\alpha = 0$ we have $\tau = \tau_0$, and the shortest distance curve satisfies Euler's equation. Thus, the term from the integration by parts must vanish as well. Since at $t = 0$ (the observer's location) $\mathbf{T} = 0$, and at $t = 1$ (the intersection with the rocket path) $\mathbf{T} = \mathbf{T}_0$ is the tangent vector of the rocket path, we end up with the **transversality condition**

$$f_{\dot{\mathbf{r}}}|_{\mathbf{r}_s} \cdot \mathbf{T}_0 = 0 = f_{\dot{\mathbf{r}}}|_{\mathbf{r}_s} \cdot \frac{d\bar{\mathbf{r}}}{d\tau}.$$

When we seek the shortest distance between two curves, the transversality condition holds at both ends because we may hold one end fixed while we determine one end point and then treat the second end point similarly.

EXAMPLE 18.2.2 **Shortest Distance of an Observer from a Rocket** Now we are ready to reconsider Example 1.2.2 using the variational calculus. The observer is at $\mathbf{r}_0 = (2, 1, 3)$ and the rocket path is the line

$$\bar{\mathbf{r}}(\tau) = \mathbf{r}_1 + \mathbf{v}\tau, \quad \mathbf{r}_1 = (1, 1, 1), \quad \mathbf{v} = (1, 2, 3).$$

We want to minimize the distance

$$s = \int \sqrt{\dot{x}^2 + \dot{y}^2}\, dt = \text{minimum},$$

which we expect to be a straight line $\mathbf{r} = t\mathbf{d} + \mathbf{r}_0$ from the observer at $t = 0$ to the point $\mathbf{r}_s$ on the path of the rocket. This is confirmed by applying Example 18.2.1 to this problem because the variational integrand only depends on the slope of the line from the observer to the rocket path. With $f = \sqrt{\dot{x}^2 + \dot{y}^2}$, $f_{\dot{\mathbf{r}}} \sim \dot{\mathbf{r}} = (\dot{x}, \dot{y}) = \mathbf{d}$. The transversality condition becomes $\mathbf{d} \cdot \mathbf{v} = 0$ because $d\bar{\mathbf{r}}/d\tau = \mathbf{v}$. We denote the intersection of the shortest distance line with the rocket path by $\mathbf{r}_s = \mathbf{v}\tau_s + \mathbf{r}_1$, where τ_s will be determined from the transversality condition $(\mathbf{r}_1 - \mathbf{r}_0 + \mathbf{v}\tau_s) \cdot \mathbf{v} = 0$. Thus,

$$\tau_s = \frac{(\vec{\mathbf{r}}_0 - \vec{\mathbf{r}}_1) \cdot \vec{\mathbf{v}}}{\vec{\mathbf{v}}^2} = \frac{(1, 0, 2) \cdot (1, 2, 3)}{14} = \frac{7}{14} = \frac{1}{2},$$

in agreement with Example 1.2.2. This gives

$$\mathbf{r}_s = \mathbf{r}_1 + \mathbf{v}\tau_s = (1, 1, 1) + \frac{1}{2}(1, 2, 3) = \left(\frac{3}{2}, 2, \frac{5}{2}\right)$$

or

$$\mathbf{r}_s - \mathbf{r}_0 = \left(\frac{3}{2} - 2, 2 - 1, \frac{5}{2} - 3\right) = \left(-\frac{1}{2}, 1, -\frac{1}{2}\right).$$

The shortest distance is $|\mathbf{r}_s - \mathbf{r}_0| = \sqrt{\frac{2}{4} + 1} = \sqrt{3/2}$.

The shortest distance between two rockets in free flight in Example 1.3.1 can be treated similarly. Here, the two transversality conditions become

$$(\mathbf{r}_{10} - \mathbf{r}_{20}) \cdot \mathbf{t}_1 = 0 = (\mathbf{r}_{10} - \mathbf{r}_{20}) \cdot \mathbf{t}_2,$$

with the tangent vectors

$$\mathbf{t}_1 = \mathbf{r}_2 - \mathbf{r}_1 = (2 - 1, 3 - 1, 4 - 1) = (1, 2, 3),$$
$$\mathbf{t}_2 = \mathbf{r}_4 - \mathbf{r}_3 = (4 - 5, 1 - 2, 2 - 1) = (-1, -1, 1).$$

Therefore, the direction of the shortest distance $\mathbf{r}_{10} - \mathbf{r}_{20}$ is

$$\mathbf{n} = \frac{\mathbf{t}_1 \times \mathbf{t}_2}{|\mathbf{t}_1 \times \mathbf{t}_2|} = \frac{1}{\sqrt{42}}(5, -4, 1).$$

The shortest distance is obtained by projecting the distance between two points on the rocket paths, one on each path, onto $\mathbf{n}$; that is,

$$d = (\mathbf{r}_3 - \mathbf{r}_1) \cdot \mathbf{n} = \frac{1}{\sqrt{42}}(5 - 1, 2 - 1, 1 - 1) \cdot (5, -4, 1)$$
$$= \frac{1}{\sqrt{42}}(4, 1, 0) \cdot (5, -4, 1) = \frac{16}{\sqrt{42}}. \quad \blacksquare$$

Hamilton's Principle

The most important application of Eq. (18.31) occurs when the integrand f is taken to be a Lagrangian L. The Langrangian (for nonrelativistic systems; see Exercise 18.2.5 for a relativistic particle) is defined as the **difference** of kinetic and potential energies of a system:

$$L \equiv T - V. \tag{18.36}$$

Using time as an independent variable instead of x and $x_i(t)$ as the dependent variables,

$$x \to t, \quad y_i \to x_i(t), \quad y_{ix} \to \dot{x}_i(t);$$

$x_i(t)$ is the location and $\dot{x}_i = dx_i/dt$, the velocity of particle i as a function of time. The equation $\delta J = 0$ is then a mathematical statement of Hamilton's principle of classical mechanics,

$$\delta \int_{t_1}^{t_2} L(x_1, x_2, \ldots, x_n, \dot{x}_1, \dot{x}_2, \ldots, \dot{x}_n; t)dt = 0. \tag{18.37}$$

In words, Hamilton's principle asserts that the motion of the system from time t_1 to t_2 is such that the time integral of the Lagrangian L, or action, has a stationary value. The resulting Euler equations are usually called the Lagrangian equations of motion,

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{x}_i} - \frac{\partial L}{\partial x_i} = 0, \tag{18.38}$$

the first term being the kinetic part and the second the generalized force component. These Lagrangian equations can be derived from Newton's equations of motion, and Newton's equations can be derived from Lagrange's. The two sets of equations are equally "fundamental."

The Lagrangian formulation has advantages over the conventional Newtonian laws. Whereas Newton's equations are vector equations, Lagrange's equations involve only scalar quantities. The coordinates $x_1, x_2, \ldots$ need not be any standard set of coordinates or lengths. They can be selected to match the conditions of the physical problem. The Lagrange equations are invariant with respect to the choice of coordinate system. Newton's equations (in component form) are not manifestly invariant. Exercise 2.5.6 shows what happens to $\mathbf{F} = m\mathbf{a}$ resolved in spherical polar coordinates.

Exploiting the concept of action, we may easily extend the Lagrangian formulation from mechanics to diverse fields, such as electrical networks and acoustical systems. Extensions to electromagnetism appear in the exercises. The result is a unity of otherwise separate areas of physics. In the development of new areas the quantization of Lagrangian particle mechanics provided a model for the quantization of electromagnetic fields and led to the gauge theory of quantum electrodynamics.

One of the most valuable advantages of the Hamilton principle–Lagrange equation formulation is the ease in seeing a relation between a symmetry and a conservation law. For example, let $x_i = \varphi$, an azimuthal angle. If our Lagrangian is independent of φ (i.e., φ is an ignorable coordinate), there are two consequences: (i) an axial (rotational) symmetry from which $\partial L/\partial\varphi = 0$ follows, and (ii) from Eq. (18.38) $\partial L/\partial\dot{\varphi} =$ constant. Physically, this corresponds to the conservation or invariance of a component of angular momentum because the kinetic part of Eq. (18.38) corresponding to an angular coordinate represents the torque. Similarly, invariance under translation leads to conservation of linear momentum. Noether's theorem (see Additional Reading in Chapter 4) is a generalization of this invariance (symmetry)—the conservation law relation.

Biographical Data

Hamilton, William R. Hamilton, an English mathematician and physicist, was born in 1805 in Dublin, Ireland, and died in 1865 near Dublin. At age 22, he became a professor of astronomy of Trinity College of Dublin while still an undergraduate. In 1843, he discovered (noncommuting) quaternions, developing them lifelong in addition to the famous variational principle of analytical mechanics named after him.

EXAMPLE 18.2.3

Moving Particle—Cartesian Coordinates Consider Eq. (18.36) for one particle with kinetic energy

$$T = \frac{1}{2}m\dot{x}^2 \tag{18.39}$$

and potential energy $V(x)$, in which, as usual, the force is given by the negative gradient of the potential,

$$F(x) = -\frac{dV(x)}{dx}. \tag{18.40}$$

From Eq. (18.38),

$$\frac{d}{dt}(m\dot{x}) - \frac{\partial(T-V)}{\partial x} = m\ddot{x} - F(x) = 0, \tag{18.41}$$

which is Newton's second law of motion. ■

EXAMPLE 18.2.4

Moving Particle—Circular Cylindrical Coordinates Now consider a particle in the xy-plane described in cylindrical coordinates. The kinetic energy is

$$T = \frac{1}{2}m(\dot{x}^2 + \dot{y}^2) = \frac{m}{2}(\dot{\rho}^2 + \rho^2\dot{\varphi}^2), \tag{18.42}$$

and we take $V = 0$ for simplicity.

The transformation of $\dot{x}^2 + \dot{y}^2$ into circular cylindrical coordinates could be carried out by taking $x(\rho, \varphi)$ and $y(\rho, \varphi)$ [Eq. (2.7)] and differentiating with respect to time and squaring. It is much easier to interpret $\dot{x}^2 + \dot{y}^2$ as v^2 and write the components of $\mathbf{v}$ as $\hat{\boldsymbol{\rho}}(ds_\rho/dt) = \hat{\boldsymbol{\rho}}\dot{\rho}$, and so on. (The ds_ρ is an increment of **length**, with ρ changing by $d\rho$ and φ remaining constant. See Example 2.2.1.)

The Lagrangian equations for ρ and φ yield, respectively,

$$\frac{d}{dt}(m\dot{\rho}) - m\rho\dot{\varphi}^2 = 0, \qquad \frac{d}{dt}(m\rho^2\dot{\varphi}) = 0. \tag{18.43}$$

The second equation is a statement of conservation of angular momentum. The first may be interpreted as radial acceleration[8] equated to centrifugal force (a "generalized force"). ■

EXERCISES

18.2.1 (a) Develop the equations of motion for the Lagrangian

$$L = \tfrac{1}{2}m(\dot{x}^2 + \dot{y}^2).$$

(b) In what sense do your solutions minimize the integral $\int_{t_1}^{t_2} L\,dt$? Compare the result for your solution with $x = \text{const.}$, $y = \text{const.}$

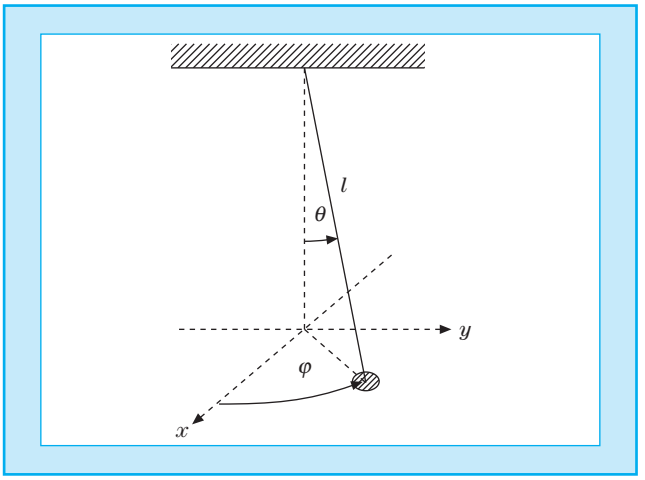
18.2.2 From Lagrange's equations of motion [Eq. (18.38)], show that a system in stable equilibrium has a minimum potential energy.

18.2.3 Write out Lagrange's equations of motion of a particle in spherical polar coordinates for a potential V equal to a constant. Identify the terms corresponding to (a) centrifugal force and (b) Coriolis force.

[8] Here is a second method of handling Exercise 2.2.8.

Figure 18.7

Spherical Pendulum



18.2.4 The spherical pendulum consists of a mass on a wire of length l, free to move in polar angle θ and azimuth angle φ (Fig. 18.7).
(a) Set up the Lagrangian for this physical system.
(b) Develop Lagrange's equations of motion.

18.2.5 Show that the Lagrangian

$$L = m_0c^2\left(1 - \sqrt{1 - \frac{v^2}{c^2}}\right) - V(\mathbf{r})$$

leads to a relativistic form of Newton's second law of motion,

$$\frac{d}{dt}\left(\frac{m_0v_i}{\sqrt{1 - v^2/c^2}}\right) = F_i,$$

in which the force components are $F_i = -\partial V/\partial x_i$. (Compare with Chapter 4, Vector Analysis in Minkowski Space–Time.)

18.2.6 The Lagrangian for a particle with charge q in an electromagnetic field described by scalar potential φ and vector potential $\mathbf{A}$ is

$$L = \tfrac{1}{2}mv^2 - q\varphi + q\mathbf{A}\cdot\mathbf{v}.$$

Find the equation of motion of the charged particle.
Hint. $(d/dt)A_j = \partial A_j/\partial t + \sum_i(\partial A_j/\partial x_i)\dot{x}_i$. The dependence of the force fields $\mathbf{E}$ and $\mathbf{B}$ on the potentials φ and $\mathbf{A}$ is developed in Section 1.12 (compare Exercise 1.12.6).

ANS. $m\ddot{x}_i = q[\mathbf{E} + \mathbf{v}\times\mathbf{B}]_i$.

18.2.7 Consider a system in which the Lagrangian is given by

$$L(q_i, \dot{q}_i) = T(q_i, \dot{q}_i) - V(q_i),$$

where q_i and $\dot{q}_i$ represent sets of variables. The potential energy V is independent of velocity and neither T nor V have any explicit time dependence.

(a) Show that

$$\frac{d}{dt}\left(\sum_j \dot{q}_j \frac{\partial L}{\partial \dot{q}_j} - L\right) = 0.$$

(b) The constant quantity

$$\sum_j \dot{q}_j \frac{\partial L}{\partial \dot{q}_j} - L$$

defines the Hamiltonian H. Show that under the preceding assumed conditions, $H = T + V$, the total energy.

Note. The kinetic energy T is a quadratic function of the $\dot{q}_i$.

18.3 Several Independent Variables

Sometimes, the integrand f of Eq. (18.1) will contain one unknown function u, which is a function of several independent variables, $u = u(x, y, z)$, for the three-dimensional case, for example. Equation (18.1) becomes

$$J = \iiint f[u, u_x, u_y, u_z, x, y, z]dx\,dy\,dz, \tag{18.44}$$

$u_x = \partial u/\partial x$, and so on. The variational problem is to find the function $u(x, y, z)$ for which J is stationary,

$$\delta J = \alpha \frac{\partial J}{\partial \alpha}\bigg|_{\alpha=0} = 0. \tag{18.45}$$

Generalizing Section 18.1, we let

$$u(x, y, z, \alpha) = u(x, y, z, 0) + \alpha\eta(x, y, z), \tag{18.46}$$

where $u(x, y, z, \alpha = 0)$ represents the (unknown) function for which Eq. (18.45) is satisfied, whereas again $\eta(x, y, z)$ is the arbitrary deviation that describes the varied function $u(x, y, z, \alpha)$. This deviation, $\eta(x, y, z)$, is required to be differentiable and to vanish at the end points. Then from Eq. (18.46),

$$u_x(x, y, z, \alpha) = u_x(x, y, z, 0) + \alpha\eta_x, \tag{18.47}$$

and similarly for u_y and u_z.

Differentiating the integral Eq. (18.44) with respect to the parameter α and then setting $\alpha = 0$, we obtain

$$\frac{\partial J}{\partial \alpha}\bigg|_{\alpha=0} = \iiint \left(\frac{\partial f}{\partial u}\eta + \frac{\partial f}{\partial u_x}\eta_x + \frac{\partial f}{\partial u_y}\eta_y + \frac{\partial f}{\partial u_z}\eta_z\right)dx\,dy\,dz = 0. \tag{18.48}$$

Again, we integrate each of the terms $(\partial f/\partial u_i)\eta_i$ by parts. The integrated part vanishes at the end points (because the deviation η is required to go to zero at the end points) and[9]

$$\iiint \left(\frac{\partial f}{\partial u} - \frac{\partial}{\partial x}\frac{\partial f}{\partial u_x} - \frac{\partial}{\partial y}\frac{\partial f}{\partial u_y} - \frac{\partial}{\partial z}\frac{\partial f}{\partial u_z} \right) \eta(x, y, z)dx\, dy\, dz = 0. \tag{18.49}$$

Since the variation $\eta(x, y, z)$ is arbitrary, the term in large parentheses is set equal to zero. This yields the Euler equation for (three) independent variables,

$$\frac{\partial f}{\partial u} - \frac{\partial}{\partial x}\frac{\partial f}{\partial u_x} - \frac{\partial}{\partial y}\frac{\partial f}{\partial u_y} - \frac{\partial}{\partial z}\frac{\partial f}{\partial u_z} = 0. \tag{18.50}$$

EXAMPLE 18.3.1

Laplace's Equation An example of this sort of variational problem is provided by electrostatics. The energy of an electrostatic field is

$$\text{energy density} = \tfrac{1}{2}\varepsilon \mathbf{E}^2, \tag{18.51}$$

where $\mathbf{E}$ is the usual electrostatic force field. In terms of the static potential φ,

$$\text{energy density} = \tfrac{1}{2}\varepsilon(\boldsymbol{\nabla}\varphi)^2. \tag{18.52}$$

Now let us impose the requirement that the electrostatic energy (associated with the field) in a given volume be a minimum. (Boundary conditions on $\mathbf{E}$ and φ must still be satisfied.) We have the volume integral[10]

$$J = \iiint (\boldsymbol{\nabla}\varphi)^2\, dx\, dy\, dz = \iiint \left(\varphi_x^2 + \varphi_y^2 + \varphi_z^2\right) dx\, dy\, dz. \tag{18.53}$$

With

$$f(\varphi, \varphi_x, \varphi_y, \varphi_z, x, y, z) = \varphi_x^2 + \varphi_y^2 + \varphi_z^2, \tag{18.54}$$

the function φ replacing the u of Eq. (18.50), Euler's equation [Eq. (18.50)] yields

$$-2(\varphi_{xx} + \varphi_{yy} + \varphi_{zz}) = 0 \tag{18.55}$$

or

$$\boldsymbol{\nabla}^2\varphi(x, y, z) = 0, \tag{18.56}$$

which is Laplace's equation of electrostatics.

Closer investigation shows that this stationary value is indeed a minimum. Thus, the demand that the field energy be minimized leads to Laplace's PDE. ■

[9]Recall that $\partial/\partial x$ is a partial derivative, where y and z are held constant. However, $\partial/\partial x$ is also a total derivative in that it acts on **implicit** x-dependence as well as on **explicit** x-dependence. In this sense,

$$\frac{\partial}{\partial x}\left(\frac{\partial f}{\partial u_x}\right) = \frac{\partial^2 f}{\partial x \partial u_x} + \frac{\partial^2 f}{\partial u \partial u_x}u_x + \frac{\partial^2 f}{\partial u_x^2}u_{xx} + \frac{\partial^2 f}{\partial u_y \partial u_x}u_{xy} + \frac{\partial^2 f}{\partial u_z \partial u_x}u_{xz}.$$

[10]The subscript x indicates the x-partial derivative, not an x-component.

EXERCISES

18.3.1 The Lagrangian for a vibrating string (small-amplitude vibrations) is

$$L = \int \left(\tfrac{1}{2}\rho u_t^2 - \tfrac{1}{2}\tau u_x^2\right) dx,$$

where ρ is the (constant) linear mass density and τ is the (constant) tension. The x-integration is over the length of the string. Show that application of Hamilton's principle to the Lagrangian density (the integrand), now with two independent variables, leads to the classical wave equation

$$\frac{\partial^2 u}{\partial x^2} = \frac{\rho}{\tau}\frac{\partial^2 u}{\partial t^2}.$$

18.3.2 Show that the stationary value of the total energy of the electrostatic field of Example 18.3.1 is a **minimum**.
Hint. Use Eq. (18.48) and investigate the α^2 terms.

18.4 Several Dependent and Independent Variables

In some cases, our integrand f contains more than one dependent variable and more than one independent variable. Consider

$$f = f[p(x, y, z), p_x, p_y, p_z, q(x, y, z), q_x, q_y, q_z, r(x, y, z), r_x, r_y, r_z, x, y, z]. \tag{18.57}$$

We proceed as before with

$$\begin{aligned} p(x, y, z, \alpha) &= p(x, y, z, 0) + \alpha\xi(x, y, z), \\ q(x, y, z, \alpha) &= q(x, y, z, 0) + \alpha\eta(x, y, z), \\ r(x, y, z, \alpha) &= r(x, y, z, 0) + \alpha\zeta(x, y, z), \quad \text{and so on.} \end{aligned} \tag{18.58}$$

Keeping in mind that ξ, η, and ζ are independent of one another, as were the η_i in Section 18.3, the same differentiation and then integration by parts leads to

$$\frac{\partial f}{\partial p} - \frac{\partial}{\partial x}\frac{\partial f}{\partial p_x} - \frac{\partial}{\partial y}\frac{\partial f}{\partial p_y} - \frac{\partial}{\partial z}\frac{\partial f}{\partial p_z} = 0, \tag{18.59}$$

with similar equations for functions q and r. Replacing $p, q, r, \ldots$ with y_i and $x, y, z, \ldots$ with x_i, we can put Eq. (18.59) in a more compact form:

$$\frac{\partial f}{\partial y_i} - \sum_j \frac{\partial}{\partial x_j}\left(\frac{\partial f}{\partial y_{ij}}\right) = 0, \quad i = 1, 2, \ldots, \tag{18.60}$$

in which

$$y_{ij} \equiv \frac{\partial y_i}{\partial x_j}.$$

An application of Eq. (18.59) appears in Section 18.5.

Relation to Physics

The calculus of variations as developed so far provides an elegant description of a wide variety of physical phenomena. The physics includes classical mechanics in Section 18.2; relativistic mechanics, Exercise 18.2.5; electrostatics, Example 18.3.1; and electromagnetic theory in Exercise 18.4.1. The convenience should not be minimized, but at the same time we should be aware that in these cases the calculus of variations has only provided an alternate description of what was already known. Variational problems in quantum mechanics are applications of the calculus of variations that are essential and highly useful. The situation does change with incomplete theories.

- If the basic physics is not yet known, a postulated variational principle can be a useful starting point.

EXERCISE

18.4.1 The Lagrangian (per unit volume) of an electromagnetic field with a charge density ρ is given by

$$\mathcal{L} = \frac{1}{2}\left(\varepsilon_0 \mathbf{E}^2 - \frac{1}{\mu_0}\mathbf{B}^2\right) - \rho\varphi + \rho\mathbf{v}\cdot\mathbf{A}.$$

Show that Lagrange's equations lead to two of Maxwell's equations. (The remaining two are a consequence of the definition of **E** and **B** in terms of **A** and φ.)
Hint. Take A_1, A_2, A_3, and φ as **dependent** variables, x, y, z, and t as **independent** variables. Write **E** and **B** in terms of **A** and φ.

18.5 Lagrangian Multipliers: Variation with Constraints

In this section, the concept of a constraint is introduced. To simplify the treatment, the constraint appears first as a simple function rather than as an integral. In the initial part of this section, we are not concerned with the calculus of variations, but then, with our newly developed Lagrangian multipliers, constraints are incorporated into the calculus of variations.

Consider a function of three independent variables, $f(x, y, z)$. For the function f to be an extreme or saddle point,

$$df = 0. \tag{18.61}$$

The necessary and sufficient condition for this is

$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial y} = \frac{\partial f}{\partial z} = 0 \tag{18.62}$$

because the total variation

$$df = \frac{\partial f}{\partial x}dx + \frac{\partial f}{\partial y}dy + \frac{\partial f}{\partial z}dz, \tag{18.63}$$

where dx, dy, dz vary independently.

Often in physical problems the variables x, y, z are subjected to constraints so that they are no longer all independent. It is possible, at least in principle, to use each constraint to eliminate one variable and to proceed with a new and smaller set of independent variables.

The use of Lagrangian multipliers is an alternate technique that may be applied when this elimination of variables is inconvenient or undesirable, as shown in Example 1.5.4. Let our **equation of constraint** be

$$\varphi(x, y, z) \equiv 0, \tag{18.64}$$

from which $z(x, y)$ can be extracted as a function of x, y, if x, y are taken as the independent coordinates. Returning to Eq. (18.61), Eq. (18.62) no longer follows because there are now only two independent variables. If we take x and y as these independent variables, dz is no longer arbitrary. From the total differential $d\varphi = 0$, we then obtain

$$-\frac{\partial \varphi}{\partial z} dz = \frac{\partial \varphi}{\partial x} dx + \frac{\partial \varphi}{\partial y} dy \tag{18.65}$$

and therefore

$$df = \frac{\partial f}{\partial x} dx + \frac{\partial f}{\partial y} dy + \lambda \left(\frac{\partial \varphi}{\partial x} dx + \frac{\partial \varphi}{\partial y} dy \right), \quad \lambda = -\frac{f_z}{\varphi_z},$$

assuming that $\varphi_z \equiv \partial \varphi / \partial z \neq 0$. Here, we have written the partial derivatives as f_z, φ_z. The condition $df = 0$ that f be stationary can then be written as

$$\left(\frac{\partial f}{\partial x} + \lambda \frac{\partial \varphi}{\partial x} \right) dx + \left(\frac{\partial f}{\partial y} + \lambda \frac{\partial \varphi}{\partial y} \right) dy = 0. \tag{18.66}$$

In other words, if our Lagrangian multiplier λ is chosen so that

$$\frac{\partial f}{\partial z} + \lambda \frac{\partial \varphi}{\partial z} = 0, \tag{18.67}$$

then dx and dy are arbitrary and the quantities in parentheses in Eq. (18.66) must vanish,

$$\frac{\partial f}{\partial x} + \lambda \frac{\partial \varphi}{\partial x} = 0, \qquad \frac{\partial f}{\partial y} + \lambda \frac{\partial \varphi}{\partial y} = 0. \tag{18.68}$$

Equations (18.67) and (18.68) are equivalent to

$$df + \lambda d\varphi = \left(\frac{\partial f}{\partial x} + \lambda \frac{\partial \varphi}{\partial x} \right) dx + \left(\frac{\partial f}{\partial y} + \lambda \frac{\partial \varphi}{\partial y} \right) dy + \left(\frac{\partial f}{\partial z} + \lambda \frac{\partial \varphi}{\partial z} \right) dz = 0. \tag{18.69}$$

When Eqs. (18.67)–(18.69) are satisfied, $df = 0$ and f is an extremum. Notice that there are now four unknowns: x, y, z, and λ. The fourth equation, of course, is the constraint equation (18.64). We want only x, y, and z so that λ need not be determined. (However, often λ has a real physical meaning that depends on the problem.) For this reason, λ is sometimes called Lagrange's undetermined multiplier. This method will fail if all the coefficients of λ vanish at the extremum, $\partial \varphi / \partial x$, $\partial \varphi / \partial y$, $\partial \varphi / \partial z = 0$. It is then impossible to solve for λ.

EXAMPLE 18.5.1

Particle in a Box As an example of the use of Lagrangian multipliers, consider the quantum mechanical problem of a particle (mass m) in a box. The box is a rectangular parallelepiped with sides a, b, and c. The ground state energy of the particle is given by

$$E = \frac{h^2}{8m}\left(\frac{1}{a^2} + \frac{1}{b^2} + \frac{1}{c^2}\right). \tag{18.70}$$

We seek the shape of the box that will minimize the energy E, subject to constraint that the volume is constant,

$$V(a, b, c) = abc = k. \tag{18.71}$$

With $f(a, b, c) = E(a, b, c)$ and $\varphi(a, b, c) = abc - k = 0$, we obtain

$$\frac{\partial E}{\partial a} + \lambda\frac{\partial \varphi}{\partial a} = -\frac{h^2}{4ma^3} + \lambda bc = 0. \tag{18.72}$$

Also,

$$-\frac{h^2}{4mb^3} + \lambda ac = 0, \qquad -\frac{h^2}{4mc^3} + \lambda ab = 0.$$

Multiplying the first of these expressions by a, the second by b, and the third by c, we have

$$\lambda abc = \frac{h^2}{4ma^2} = \frac{h^2}{4mb^2} = \frac{h^2}{4mc^2}. \tag{18.73}$$

Therefore, our solution is

$$a = b = c, \quad \text{a cube.} \tag{18.74}$$

Notice that λ has not been determined but follows from Eq. (18.73). ■

Variation with Constraints

As in the preceding sections, we seek the path that will make the integral

$$J = \int f\left(y_i, \frac{\partial y_i}{\partial x_j}, x_j\right) dx_j \tag{18.75}$$

stationary. Here and in the following, a sum over the index j is understood. This is the general case in which x_j represents a set of independent variables and y_i a set of dependent variables. Again,

$$\delta J = 0. \tag{18.76}$$

Now, however, we introduce one or more constraints. This means that the y_i are no longer independent of each other. Not all the η_i may be varied arbitrarily and Eqs. (18.50) or (18.60) would not apply. The constraint may have the form

$$\varphi_k(y_i, x_j) = 0. \tag{18.77}$$

In this case we may multiply by a function of x_j, for example, $\lambda_k(x_j)$, and integrate over the same range as in Eq. (18.75) to obtain

$$\int \lambda_k(x_j)\varphi_k(y_i, x_j)dx_j = 0. \tag{18.78}$$

Then clearly

$$\delta \int \lambda_k(x_j)\varphi_k(y_i, x_j)dx_j = 0. \tag{18.79}$$

Alternatively, the constraint may appear in the form of an integral

$$\int \varphi_k(y_i, \partial y_i/\partial x_j, x_j)dx_j = \text{constant}, \tag{18.80}$$

generalizing Eq. (18.77). We may introduce any **constant** Lagrangian multiplier, and again Eq. (18.79) follows—now with λ a constant.

In either case, by adding Eqs. (18.76) and (18.79), possibly with more than one constraint, we obtain

$$\delta \int \left[f\left(y_i, \frac{\partial y_i}{\partial x_j}, x_j\right) + \sum_k \lambda_k \varphi_k \right] dx_j = 0. \tag{18.81}$$

The Lagrangian multiplier λ_k may depend on x_j when $\varphi(y_i, x_j)$ is given in the form of Eq. (18.77).

Treating the entire integrand as a new function

$$g\left(y_i, \frac{\partial y_i}{\partial x_j}, x_j\right),$$

we obtain

$$g\left(y_i, \frac{\partial y_i}{\partial x_j}, x_j\right) = f + \sum_k \lambda_k \varphi_k. \tag{18.82}$$

If we have N y_i ($i = 1, 2, \ldots, N$) and m constraints ($k = 1, 2, \ldots m$), $N - m$ of the η_i may be taken as arbitrary. For the remaining m η_i, the λ_k may, in principle, be chosen so that the remaining Euler–Lagrange equations are satisfied, completely analogous to Eq. (18.67). The result is that our composite function g must satisfy the usual Euler–Lagrange equations

$$\frac{\partial g}{\partial y_i} - \sum_j \frac{\partial}{\partial x_j} \frac{\partial g}{(\partial y_i/\partial x_j)} = 0, \tag{18.83}$$

with one such equation for each dependent variable y_i [compare Eqs. (18.50) and (18.60)]. These Euler equations and the equations of constraint are then solved simultaneously to find the function yielding a stationary value.

Note that from the form of Eqs. (18.67) and (18.69), we could identify f as the function, taking an extreme value subject to φ, the constraint, or identify f as the constraint and φ as the function.

If we have a **set of constraints** φ_k, then Eqs. (18.67) and (18.69) become

$$\frac{\partial f}{\partial x_i} + \sum_k \lambda_k \frac{\partial \varphi_k}{\partial x_i} = 0, \quad i = 1, 2, \ldots, n,$$

with a separate Lagrange multiplier λ_k for each φ_k.

EXAMPLE 18.5.2

Maximum Surface Tension Given two points $-x_0,\ x_0 \geq 0$ on the x-axis, find a curve $y(x)$ of fixed length $L > 0$ so that the area between the x-axis and the curve is a maximum. The boundary condition is $y(-x_0) = 0 = y(x_0)$.

We start from the surface formula

$$\text{area} = \int_{-x_0}^{x_0} y(x)\,dx = \text{maximum}$$

under the constraint of constant length

$$\int_{-x_0}^{x_0} \sqrt{dx^2 + dy^2} = \int_{-x_0}^{x_0} \sqrt{1 + y_x^2}\,dx = L,$$

which leads to the integrand

$$f + \lambda\varphi \equiv y + \lambda\sqrt{1 + y_x^2}$$

of the problem. Here, λ is the constant Lagrange multiplier, y is the dependent variable, and x is the independent variable. The Euler equation is

$$1 - \frac{d}{dx}\frac{\lambda y_x}{\sqrt{1 + y_x^2}} = 0.$$

Integrating it yields

$$\frac{\lambda y_x}{\sqrt{1 + y_x^2}} = x + a, \quad a = \text{const.},$$

which can be solved for y_x:

$$y_x = \pm\frac{x + a}{\sqrt{\lambda^2 - (x + a)^2}}.$$

Integrating again yields

$$y(x) = \pm\sqrt{\lambda^2 - (x + a)^2} + b, \quad b = \text{const.}$$

The boundary conditions lead to $(x_0 + a)^2 = (a - x_0)^2$; that is, $a = 0$ and $b = \mp\sqrt{\lambda^2 - x_0^2}$. Let us choose $y \geq 0$. Note that $y' = y_x$ becomes infinite at an interior point x unless $\lambda^2 \geq x_0^2$. The curve $y(x)$ is a circular arc through the points $(-x_0, 0)$, $(x_0, 0)$ of length $L = 2\lambda \arcsin(x_0/\lambda)$. When $\lambda = x_0$, then $L = 2x_0 \arcsin 1 = x_0\pi$, a half circle with maximal area. When $\lambda \to \infty$, or $x_0 \ll \lambda$, then the arc becomes the closed circle $x^2 + (y - \lambda)^2 = \lambda^2$ with radius λ and length $2\lambda\pi$ and the x-axis its tangent; that is, $x_0 \to 0$ and the points approach each other. ■

Lagrangian Equations

In the absence of constraints, Lagrange's equations of motion [Eq. (18.38)] were found to be[11]

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_i} - \frac{\partial L}{\partial q_i} = 0,$$

with t (time) the one independent variable and $q_i(t)$ (particle position) a set of dependent variables. Usually, the coordinates q_i are chosen to eliminate the forces of constraint, but this is not necessary and not always desirable. In the presence of constraints $\varphi_k(q_i, t) = 0$ that are independent of the velocities $\dot{q}_i$, Hamilton's principle is

$$\delta \int \left[L(q_i, \dot{q}_i, t) + \sum_k \lambda_k(t)\varphi_k(q_i, t) \right] dt = 0, \tag{18.84}$$

and the constrained Lagrangian equations of motion are

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_i} - \frac{\partial L}{\partial q_i} = \sum_k a_{ik}\lambda_k. \tag{18.85}$$

Here, the right-hand side is the total force of constraint corresponding to the coordinate q_i. The coefficient a_{ik} is given by

$$a_{ik} = \frac{\partial \varphi_k}{\partial q_i}. \tag{18.86}$$

If q_i is a length, then $a_{ik}\lambda_k$ (no summation) represents the force of the kth constraint in the q_i direction, appearing in Eq. (18.85) in exactly the same way as $-\partial V/\partial q_i$.

EXAMPLE 18.5.3

Simple Pendulum To illustrate, consider the simple pendulum, a mass m, constrained by a wire of length l to swing in an arc (Fig. 18.8). In the absence of the constraint

$$\varphi_1 = r - l = 0 \tag{18.87}$$

there are two generalized coordinates r and θ (motion in vertical plane). The Lagrangian is (taking the potential V to be zero when the pendulum is horizontal, $\theta = \pi/2$)

$$L = T - V = \tfrac{1}{2}m(\dot{r}^2 + r^2\dot{\theta}^2) + mgr\cos\theta. \tag{18.88}$$

By Eq. (18.85), the equations of motion are

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{r}} - \frac{\partial L}{\partial r} = \lambda_1, \quad \frac{d}{dt}\frac{\partial L}{\partial \dot{\theta}} - \frac{\partial L}{\partial \theta} = 0, \quad (a_{r1} = 1, a_{\theta 1} = 0), \tag{18.89}$$

[11] The symbol q is customary in classical mechanics. It serves to emphasize that the variable is not necessarily a Cartesian variable (and not necessarily a length).

Figure 18.8

Simple Pendulum

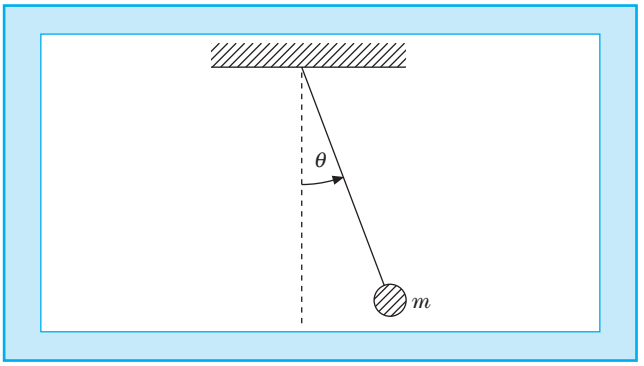
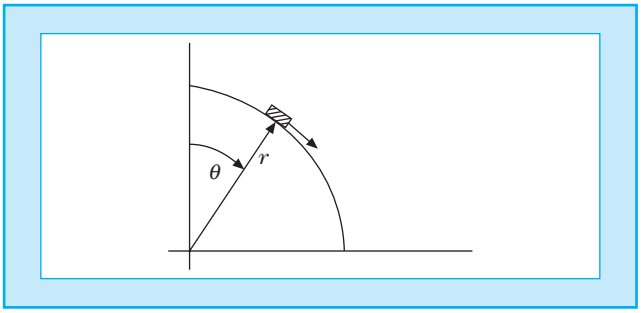


Figure 18.9

A Particle Sliding on a Cylindrical Surface



or

$$\frac{d}{dt}(m\dot{r}) - mr\dot{\theta}^2 - mg\cos\theta = \lambda_1,$$

$$\frac{d}{dt}(mr^2\dot{\theta}) + mgr\sin\theta = 0. \tag{18.90}$$

Substituting in the equation of constraint ($r = l, \dot{r} = 0$), we have

$$ml\dot{\theta}^2 + mg\cos\theta = -\lambda_1, \quad ml^2\ddot{\theta} + mgl\sin\theta = 0. \tag{18.91}$$

The second equation of Eq. (18.91) may be solved for $\theta(t)$ to yield simple harmonic motion if the amplitude is small ($\sin\theta \approx \theta$), whereas the first equation expresses the tension in the wire in terms of θ and $\dot{\theta}$.

Note that since the equation of constraint [Eq. (18.87)] is in the form of Eq. (18.77), the Lagrange multiplier λ may be (and here is) a function of t [because $\theta = \theta(t)$, a function]. ■

EXAMPLE 18.5.4

Sliding off a Log Closely related to this is the problem of a particle sliding on a cylindrical surface. The object is to find the critical angle θ_c at which the particle flies off from the surface. This critical angle is the angle at which the radial force of constraint goes to zero (Fig. 18.9).

We have (with $\theta = 0$ in the upward vertical direction)

$$L = T - V = \tfrac{1}{2}m(\dot{r}^2 + r^2\dot{\theta}^2) - mgr\cos\theta \tag{18.92}$$

and the equation of constraint

$$\varphi_1 = r - l = 0. \tag{18.93}$$

Proceeding as in Example 18.5.3 with $a_{r1} = 1$,

$$\begin{aligned} m\ddot{r} - mr\dot{\theta}^2 + mg\cos\theta &= \lambda_1(\theta), \qquad (18.94)\\ mr^2\ddot{\theta} + 2mr\dot{r}\dot{\theta} - mgr\sin\theta &= 0, \end{aligned}$$

in which the constraining force $\lambda_1(\theta)$ is a function of the angle θ.[12] Since $r = l$, $\ddot{r} = \dot{r} = 0$, the radial equation of motion reduces to

$$-ml\dot{\theta}^2 + mg\cos\theta = \lambda_1(\theta), \tag{18.95}$$

$$ml^2\ddot{\theta} - mgl\sin\theta = 0. \tag{18.96}$$

Differentiating with respect to time using the chain rule

$$\frac{df(\theta)}{dt} = \frac{df(\theta)}{d\theta}\dot{\theta},$$

we obtain

$$-2ml\ddot{\theta}\dot{\theta} - mg\sin\theta\dot{\theta} = \frac{d\lambda_1(\theta)}{d\theta}\dot{\theta}.$$

If $\dot{\theta} \neq 0$, we can drop this factor to find

$$-2ml\ddot{\theta} - mg\sin\theta = \frac{d\lambda_1(\theta)}{d\theta}.$$

Multiplying this result by $l/2$ and adding it to Eq. (18.96) eliminates the $\ddot{\theta}$ term and yields

$$-3mg\sin\theta = \frac{d\lambda_1(\theta)}{d\theta},$$

which we integrate to get

$$\lambda_1(\theta) = 3mg\cos\theta + C, \quad C = \text{const.}$$

Using the initial condition, when the particle is at rest, $\theta(0) = 0$, $\dot{\theta} = 0$ at $t = 0$, in the radial equation of motion [Eq. (18.94)] yields

$$\lambda_1(0) = mg,$$

consistent with λ_1 being the radial force, and we find

$$C = -2mg.$$

[12]Note that λ_1 is the **radial** force exerted by the cylinder on the particle. Consideration of the physical problem should show that λ_1 must depend on the angle θ. We permitted $\lambda = \lambda(t)$. Now we are replacing the time dependence by an (unknown) angular dependence.

The particle m will stay on the surface as long as the force of constraint is nonnegative; that is, as long as the surface has to push outward on the particle,

$$\lambda_1(\theta) = 3mg\cos\theta - 2mg \geq 0. \tag{18.97}$$

The critical angle lies where $\lambda_1(\theta_c) = 0$, the force of constraint going to zero:

$$\cos\theta_c = \tfrac{2}{3}, \quad \text{or} \quad \theta_c = 48^\circ 11' \tag{18.98}$$

from the vertical. At this angle (neglecting all friction) our particle takes off.

This result can be obtained more easily by considering a varying centripetal force furnished by the radial component of the gravitational force. The example was chosen to illustrate the use of Lagrange's undetermined multiplier in a simple physical system. ■

EXAMPLE 18.5.5

The Schrödinger Wave Equation As a final illustration of a constrained minimum, let us find the Euler equations for a quantum mechanical problem

$$\delta \iiint \psi^*(x, y, z) H \psi(x, y, z)\, dx\, dy\, dz = 0, \tag{18.99}$$

with the constraint

$$\iiint \psi^* \psi\, dx\, dy\, dz = 1. \tag{18.100}$$

Equation (18.99) is a statement that the energy of the system is stationary, with H being the quantum mechanical Hamiltonian for a particle of mass m, a differential operator,

$$H = -\frac{\hbar^2}{2m}\nabla^2 + V(x, y, z). \tag{18.101}$$

Equation (18.100), the constraint, is the condition that there will be exactly one particle present; ψ is the usual wave function, a dependent variable, and ψ^*, its complex conjugate, is treated as a **second** dependent variable.[13]

The integrand in Eq. (18.99) involves **second** derivatives, which can be converted to first derivatives by integrating by parts:

$$\int \psi^* \frac{\partial^2 \psi}{\partial x^2}\, dx = \psi^* \frac{\partial \psi}{\partial x}\bigg|_{-\infty}^{\infty} - \int \frac{\partial \psi^*}{\partial x}\frac{\partial \psi}{\partial x}\, dx. \tag{18.102}$$

We assume either periodic boundary conditions (as in the Sturm–Liouville theory; Chapter 9) or that the volume of integration is so large that ψ and ψ^* vanish strongly at the boundary.[14] Then the integrated part vanishes and

[13] Compare Section 6.1.

[14] $\lim_{r\to\infty} r\psi(r) = 0$.

Eq. (18.99) may be rewritten as

$$\delta \iiint \left[\frac{\hbar^2}{2m} \nabla\psi^* \cdot \nabla\psi + V\psi^*\psi \right] dx\, dy\, dz = 0. \tag{18.103}$$

The function g of Eq. (18.82) is

$$\begin{aligned} g &= \frac{\hbar^2}{2m} \nabla\psi^* \cdot \nabla\psi + V\psi^*\psi - \lambda\psi^*\psi \\ &= \frac{\hbar^2}{2m} (\psi_x^*\psi_x + \psi_y^*\psi_y + \psi_z^*\psi_z) + V\psi^*\psi - \lambda\psi^*\psi, \end{aligned} \tag{18.104}$$

again using the subscript x to denote $\partial/\partial x$. For $y_i = \psi^*$, Eq. (18.83) becomes

$$\frac{\partial g}{\partial \psi^*} - \frac{\partial}{\partial x}\frac{\partial g}{\partial \psi_x^*} - \frac{\partial}{\partial y}\frac{\partial g}{\partial \psi_y^*} - \frac{\partial}{\partial z}\frac{\partial g}{\partial \psi_z^*} = 0.$$

This yields

$$V\psi - \lambda\psi - \frac{\hbar^2}{2m}(\psi_{xx} + \psi_{yy} + \psi_{zz}) = 0$$

or

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = \lambda\psi. \tag{18.105}$$

Reference to Eq. (18.101) enables us to identify λ physically as the energy of the quantum mechanical system. With this interpretation, Eq. (18.105) is the celebrated Schrödinger wave equation. This variational approach is more than just a matter of academic curiosity. It provides a very powerful method of obtaining approximate solutions of the wave equation (Rayleigh–Ritz variational method; Section 18.6). ■

EXERCISES

The following problems are to be solved by using Lagrangian multipliers.

18.5.1 The ground state energy of a particle in a pillbox (right-circular cylinder) is given by

$$E = \frac{\hbar^2}{2m}\left(\frac{(2.4048)^2}{R^2} + \frac{\pi^2}{H^2} \right),$$

where R is the radius, H is the height of the pillbox, and 2.4048 is the first zero of $J_0(r)$. Find the ratio of R to H that will minimize the energy for a fixed volume.

18.5.2 Find the ratio of R (radius) to H (height) that will minimize the total surface area of a right-circular cylinder of fixed volume of the previous problem.

18.5.3 The U.S. Post Office limits first-class mail to Canada to a total of 36 in., length plus girth. Using a Lagrange multiplier, find the maximum volume and the dimensions of a (rectangular parallelepiped) package subject to this constraint.

18.5.4 For a lens of focal length f, the object distance p and the image distance q are related by $1/p + 1/q = 1/f$. Find the minimum object–image distance $(p + q)$ for fixed f. Assume real object and image (p and q both positive).

18.5.5 You have an ellipse $(x/a)^2 + (y/b)^2 = 1$. Find the inscribed rectangle of maximum area. Show that the ratio of the maximum rectangle area to the area of the ellipse is $(2/\pi) = 0.6366$.

18.5.6 A rectangular parallelepiped is inscribed in an ellipsoid of semiaxes a, b, and c. Maximize the volume of the inscribed rectangular parallelepiped. Show that the ratio of the maximum volume to the volume of the ellipsoid is $2/\pi\sqrt{3} \approx 0.367$.

18.5.7 A **deformed** sphere has a radius given by $r = r_0\{\alpha_0 + \alpha_2 P_2(\cos\theta)\}$, where $\alpha_0 \approx 1$ and $|\alpha_2| \ll |\alpha_0|$. Show that the area and volume are

$$A = 4\pi r_0^2 \alpha_0^2 \left\{1 + \frac{4}{5}\left(\frac{\alpha_2}{\alpha_0}\right)^2\right\}, \qquad V = \frac{4\pi r_0^3}{3}\alpha_0^3 \left\{1 + \frac{3}{5}\left(\frac{\alpha_2}{\alpha_0}\right)^2\right\}.$$

Terms of order α_2^3 have been neglected.

(a) With the constraint that the enclosed volume be held constant, $V = 4\pi r_0^3/3$, show that bounding surface of minimum area is a sphere ($\alpha_0 = 1$, $\alpha_2 = 0$).

(b) With the constraint that the area of the bounding surface be held constant (i.e., $A = 4\pi r_0^2$), show that the enclosed volume is a maximum when the surface is a sphere.

18.5.8 Find the maximum value of the directional derivative of $\varphi(x, y, z)$,

$$\frac{d\varphi}{ds} = \frac{\partial\varphi}{\partial x}\cos\alpha + \frac{\partial\varphi}{\partial y}\cos\beta + \frac{\partial\varphi}{\partial z}\cos\gamma,$$

subject to the constraint

$$\cos^2\alpha + \cos^2\beta + \cos^2\gamma = 1.$$

ANS. $\left(\dfrac{d\varphi}{ds}\right) = |\nabla\varphi|.$

Concerning the following exercises, note that in a quantum-mechanical system there are g_i distinct quantum states between energy E_i and $E_i + dE_i$. The problem is to describe how n_i particles are distributed among these states subject to two constraints:

(a) fixed number of particles,

$$\sum_i n_i = n.$$

(b) fixed total energy,

$$\sum_i n_i E_i = E.$$

18.5.9 For identical particles obeying the Pauli exclusion principle, the probability of a given arrangement is

$$W_{\text{FD}} = \prod_i \frac{g_i!}{n_i!(g_i - n_i)!}.$$

Show that maximizing W_{FD} subject to a fixed number of particles and fixed total energy leads to

$$n_i = \frac{g_i}{e^{\lambda_1 + \lambda_2 E_i} + 1}.$$

With $\lambda_1 = -E_0/kT$ and $\lambda_2 = 1/kT$, this yields Fermi–Dirac statistics. *Hint.* Try working with $\ln W$ and using Stirling's formula (Section 10.3). The justification for **differentiation** with respect to n_i is that we are dealing here with a large number of particles, $\Delta n_i/n_i \ll 1$.

18.5.10 For identical particles but no restriction on the number in a given state, the probability of a given arrangement is

$$W_{\text{BE}} = \prod_i \frac{(n_i + g_i - 1)!}{n_i!(g_i - 1)!}.$$

Show that maximizing W_{BE}, subject to a fixed number of particles and fixed total energy, leads to

$$n_i = \frac{g_i}{e^{\lambda_1 + \lambda_2 E_i} - 1}.$$

With $\lambda_1 = -E_0/kT$ and $\lambda_2 = 1/kT$, this yields Bose–Einstein statistics.
Note. Assume that $g_i \gg 1$.

18.5.11 Photons satisfy Bose–Einstein statistics and the constraint that total energy is constant. They clearly do **not** satisfy the fixed number constraint. Show that eliminating the fixed number constraint leads to the foregoing result but with $\lambda_1 = 0$.

18.5.12 A particle, mass m, is on a frictionless horizontal surface. It is constrained to move so that $\theta = \omega t$ (rotating radial arm, no friction). With the initial conditions

$$t = 0, \quad r = r_0, \quad \dot{r} = 0,$$

(a) find the radial positions as a function of time;

ANS. $r(t) = r_0 \cosh \omega t.$

(b) find the force exerted on the particle by the constraint.

ANS. $F^{(c)} = 2m\dot{r}\omega = 2mr_0\omega^2 \sinh \omega t.$

18.5.13 A point mass m is moving over a flat, horizontal, frictionless plane. The mass is constrained by a string to move radially inward at a constant rate. Using plane polar coordinates (ρ, φ), $\rho = \rho_0 - kt$,

(a) Set up the Lagrangian.

(b) Obtain the constrained Lagrange equations;

(c) Solve the φ-dependent Lagrange equation to obtain $\omega(t)$, the angular velocity. What is the physical significance of the constant of integration that you get from your "free" integration?

(d) Using the $\omega(t)$ from part (b), solve the ρ-dependent (constrained) Lagrange equation to obtain $\lambda(t)$. In other words, explain what is happening to the **force** of constraint as $\rho \to 0$.

18.5.14 A flexible cable is suspended from two fixed points. The length of the cable is fixed. Find the curve that will minimize the total gravitational potential energy of the cable.

ANS. Hyperbolic cosine.

18.5.15 A fixed volume of water is rotating in a cylinder with constant angular velocity ω. Find the water surface that will minimize the action.

ANS. Parabola.

18.5.16 (a) Show that for a fixed-length string, the figure with maximum area enclosed by it is a circle.

(b) Show that for a fixed area, the curve with minimum perimeter is a circle.

Hint. The radius of curvature R is given by

$$R = \left(r^2 + r_\theta^2\right)^{3/2} \Big/ \left(r r_{\theta\theta} - 2r_\theta^2 - r^2\right).$$

Note. The problems of this section, variation subject to constraints, are often called **isoperimetric**. The term arose from problems of maximizing area subject to a fixed perimeter, as in Exercise 18.5.16(a).

18.5.17 Show that requiring J, given by

$$J = \int_a^b \left[p(x) y_x^2 - q(x) y^2\right] dx,$$

to have a stationary value subject to the normalizing condition

$$\int_a^b y^2 w(x)\, dx = 1$$

and boundary condition

$$p y_x y \,|_a^b = 0$$

leads to the Sturm–Liouville equation of Chapter 9:

$$\frac{d}{dx}\left(p\frac{dy}{dx}\right) + qy + \lambda w y = 0.$$

Give a physical interpretation of J.

Note. The boundary condition is used in Section 9.1 in establishing the Hermitian property of the operator.

18.6 Rayleigh–Ritz Variational Technique

Exercise 18.5.17 opens up a connection between the calculus of variations and eigenfunction–eigenvalue problems. We may rewrite the expression of Exercise 18.5.17 as

$$F[y(x)] = \frac{\int_a^b \left(py_x^2 - qy^2\right)dx}{\int_a^b y^2 w\, dx}. \tag{18.106}$$

The normalization integral appears in the denominator instead of in a constraint. The quantity F, a functional of the function $y(x)$, is homogeneous in y and independent of the normalization of y, and it corresponds to the constrained stationary value of J. Then from Exercise 18.5.17, with $f = py_x^2 - qy^2 - \lambda y^2$ and Euler's equation $\frac{\partial f}{\partial y} = \frac{d}{dx}\frac{\partial f}{\partial y_x}$, we find that $y(x)$ satisfies the Sturm–Liouville equation

$$\frac{d}{dx}\left(p\frac{dy}{dx}\right) + qy + \lambda wy = 0, \tag{18.107}$$

with λ now the eigenvalue (whereas in Exercise 18.5.17 it was a Lagrangian multiplier). Our optimum function $y(x)$ is such that J and F take on a stationary value. Integrating the first term in the numerator of Eq. (18.106) by parts and using the **boundary condition**,

$$py_x y\,|_a^b = 0, \tag{18.108}$$

we obtain

$$F[y(x)] = -\int_a^b y\left\{\frac{d}{dx}\left(p\frac{dy}{dx}\right) + qy\right\} dx \Big/ \int_a^b y^2 w\, dx. \tag{18.109}$$

Then substituting in Eq. (18.107), the stationary values of $F[y(x)]$ are given by

$$F[y_n(x)] = \lambda_n, \tag{18.110}$$

with λ_n the eigenvalue corresponding to the eigenfunction y_n. Equation (18.110) with F given by either Eq. (18.106) or (18.109) forms the basis of the approximate Rayleigh–Ritz method for the computation of eigenfunctions and eigenvalues.

Biographical Data

Rayleigh, John William Strutt, Lord. Rayleigh, an English physicist, was born in 1842 in Essex, England, and died in 1919 in Essex. He developed the scattering of light by atmospheric dust, explaining the blue color of the sky; contributed to black-body radiation at long wave lengths; and analyzed sound and water waves. He was awarded the physics Nobel prize in 1904 for the discovery of argon.

Ground-State Eigenfunction

Suppose that we seek to compute the ground-state eigenfunction y_0 and eigenvalue[15] λ_0 of some Hermitian operator with a lower bound that need not be positive or zero of some complicated atomic or nuclear system. The classical example for which no exact solution exists is the helium atom problem. The eigenfunction y_0 is **unknown**, but we assume that we can make a pretty good guess at an approximate function y so that mathematically we may write[16]

$$y = y_0 + \sum_{i=1}^{\infty} c_i y_i. \tag{18.111}$$

The c_i are small quantities compared to unity. (How small depends on how good our guess y was compared to y_0.) The y_i are orthonormalized eigenfunctions (also unknown); therefore, our trial function y is not normalized.

Substituting the approximate function y into Eq. (18.109) and noting that

$$\int_a^b y_i \left\{ \frac{d}{dx}\left(p\frac{dy_j}{dx} \right) + q y_j \right\} dx = -\lambda_i \delta_{ij}, \tag{18.112}$$

$$F[y(x)] = \frac{\lambda_0 + \sum_{i=1}^{\infty} c_i^2 \lambda_i}{1 + \sum_{i=1}^{\infty} c_i^2}. \tag{18.113}$$

Here, we have taken the eigenfunctions to be orthogonal since they are solutions of the Sturm–Liouville equation [Eq. (18.107)]. We also assume that y_0 is nondegenerate. Now we convert Eq. (18.113) to the form

$$F[y(x)] = \frac{\lambda_0\left(1 + \sum_{i=1}^{\infty} c_i^2\right) + \sum_{i=1}^{\infty} c_i^2(\lambda_i - \lambda_0)}{1 + \sum_{i=1}^{\infty} c_i^2} \geq \lambda_0, \tag{18.114}$$

where we neglect the second term in the numerator, which is nonnegative because $\lambda_i \geq \lambda_0$, to get the lower bound λ_0. Equation (18.114) contains three important results:

- Whereas the error in the eigenfunction y was of order $O(c_i)$, the error in λ is only of order $\mathcal{O}(c_i^2)$. Even a poor approximation of the eigenfunctions may yield an accurate calculation of the eigenvalue.
- If λ_0 is the lowest eigenvalue (ground state), then since $\lambda_i - \lambda_0 > 0$, the expectation value of the operator,

  $$F[y(x)] = \lambda \geq \lambda_0, \tag{18.115}$$

  or our approximation is always on the high side becoming lower, converging on λ_0 as our approximate eigenfunction y improves ($c_i \to 0$). Note that Eq. (18.115) is a direct consequence of Eq. (18.113). More directly, $F[y(x)]$ in Eq. (18.113) is the positively weighted average of the λ_i and, therefore, must be no smaller than the smallest λ_i, to wit, λ_0.

[15] This means that λ_0 is the lowest eigenvalue. It is clear from Eq. (18.106) that if $p(x) \geq 0$ and $q(x) \leq 0$ (compare Table 9.1), then $F[y(x)]$ has a lower bound and this lower bound is nonnegative. Recall from Section 9.1 that $w(x) \geq 0$.

[16] We are guessing at the form of the function. The normalization is irrelevant.

- We do not know y; in practice, we invent a $y(x)$, adjusting its form to get the smallest $F[y(x)]$ possible. Often, parameters in y may be varied to minimize F and thereby improve the estimate of the ground-state energy λ_0. The method can be extended to excited states by including orthogonality constraints to the ground state and lower lying excitations.

EXAMPLE 18.6.1

Vibrating String A vibrating string clamped at $x = 0$ and 1 satisfies the eigenvalue equation

$$\frac{d^2y}{dx^2} + \lambda y = 0 \tag{18.116}$$

and the boundary condition $y(0) = y(1) = 0$. For this simple example, we recognize immediately that $y_0(x) = \sin \pi x$ (unnormalized) and $\lambda_0 = \pi^2$. However, let us try the Rayleigh–Ritz technique.

With one eye on the boundary conditions, we try

$$y(x) = x(1 - x). \tag{18.117}$$

Then with $p = 1$, $q = 0$, and $w = 1$, using $y'' = -2$, Eq. (18.116) yields

$$F[y(x)] = 2\frac{\int_0^1 x(1-x)dx}{\int_0^1 x^2(1-x)^2dx} = \frac{1/3}{1/30} = 10. \tag{18.118}$$

This result, $\lambda = 10$, is a fairly good approximation (1.3% error)[17] of $\lambda_0 = \pi^2 \approx 9.8696$. The reader may have noted that $y(x)$ [Eq. (18.110)] is not normalized to unity. The denominator in $F[y(x)]$ compensates for the lack of unit normalization. In the usual calculation the eigenfunction would be improved by introducing more terms and adjustable parameters, such as

$$y = x(1 - x) + a_2x^2(1 - x)^2. \tag{18.119}$$

It is convenient to have the additional terms orthogonal, but it is not necessary. The parameter a_2 is adjusted to **minimize** $F[y(x)]$. In this case, choosing $a_2 = 1.1353$ drives $F[y(x)]$ down to 9.8697, very close to the exact eigenvalue value. ■

EXAMPLE 18.6.2

S-Wave Particle in an Infinite Spherical Square Well We start from the radial Schrödinger equation,

$$\frac{d^2u}{dr^2} + k^2u = 0, \quad r \le a,$$

[17] The closeness of the fit may be checked by a Fourier sine expansion (compare Exercise 14.2.3 over the half interval [0, 1] or, equivalently, over the interval $[-1, 1]$, with $y(x)$ taken to be odd). Because of the even symmetry relative to $x = 1/2$, only odd n terms appear:

$$y(x) = x(1 - x) = \left(\frac{8}{\pi^3}\right)\left[\sin \pi x + \frac{\sin 3\pi x}{3^3} + \frac{\sin 5\pi x}{5^3} + \cdots\right].$$

with orbital angular momentum $l = 0$, potential $V = 0$, $r \le a$, and $V \to +\infty$ for $r \ge a$. We call the energy eigenvalue $2\mu E/\hbar^2 = k^2$, where μ is the reduced mass of the particle, and $u(r) = r\psi(r)$ is r times the radial wave function.

We take $u(r) = r(1 - r^2/a^2)$ as our unnormalized trial wave function, imposing a node at $r = a$, where the potential becomes infinite. Then we compare the ODE for u with the Sturm–Liouville ODE [Eq. (18.107)], which yields $p(x) = 1$, $q(x) = 0$, $w(x) = 1$, and

$$F[u(r)] = \frac{-\int_0^a uu''dr}{\int_0^a u^2\,dr}.$$

Integrating the numerator by parts, or Eq. (18.106), gives

$$F[u(r)] = \frac{\int_0^a (u')^2\,dr}{\int_0^a u^2\,dr} = \frac{4a/5}{8a^3/105} = \frac{21}{2a^2}$$

using

$$u' = 1 - 3r^2/a^2, \qquad \int_0^a u^2\,dr = \int_0^a r^2\left(1 - \frac{r^2}{a^2}\right)^2 dr = \left(\frac{a^3}{3} - \frac{2a^5}{5a^2} + \frac{a^7}{7a^4}\right)$$

$$= \frac{8a^3}{105},$$

$$\int_0^a \left(1 - 3\frac{r^2}{a^2}\right)^2 dr = \frac{4}{5}a.$$

Now we use the ODE $u'' = -k^2u$ in the numerator of F to get the eigenvalue k^2:

$$F[u(r)] = \frac{-\int_0^a u\,u''dr}{\int_0^a u^2\,dr} = k^2 = \frac{21}{2a^2}.$$

Comparing to the exact solution $k^2 = \pi^2/a^2$, our estimate is 6% off. Exercise 18.6.5 addresses possible improvements. ■

EXERCISES

18.6.1 The wave equation for the quantum-mechanical oscillator may be written as

$$\frac{d^2\psi(x)}{dx^2} + (\lambda - x^2)\psi(x) = 0,$$

with $\lambda = 1$ for the ground state [Eq. (13.4)]. Take

$$\psi_{\text{trial}} = \begin{cases} 1 - (x^2/a^2), & x^2 \le a^2 \\ 0, & x^2 > a^2 \end{cases}$$

for the ground-state wave function (with a^2 an adjustable parameter) and calculate the corresponding ground-state energy. How much error do you have?

Note. Your parabola is really not a very good approximation to a Gaussian solution. What improvements can you suggest?

18.6.2 The Schrödinger equation for a central potential may be written as

$$\mathcal{L}u(r) + \frac{\hbar^2 l(l+1)}{2Mr^2}u(r) = Eu(r).$$

The $l(l+1)$ term is the angular momentum barrier; it is derived from splitting off the angular dependence (Example 9.1.1). Treating this term as a perturbation, use the variational technique to show that $E > E_0$, where E_0 is the energy eigenvalue of $\mathcal{L}u_0 = E_0u_0$ corresponding to $l = 0$. This means that the minimum energy state will have $l = 0$, zero angular momentum.
Hint. You can expand $u(r)$ as $u_0(r) + \sum_{i=1}^{\infty} c_i u_i$, where $\mathcal{L}u_i = E_i u_i$, $E_i > E_0$.

18.6.3 In the matrix eigenvector, eigenvalue equation

$$\mathsf{A}\mathbf{r}_i = \lambda_i \mathbf{r}_i,$$

where λ is an $n \times n$ Hermitian matrix. For simplicity, assume that its n real eigenvalues (Section 3.5) are distinct, λ_1 being the largest. If r is an approximation to $\mathbf{r}_1$,

$$\mathbf{r} = \mathbf{r}_1 + \sum_{i=2}^{n} \delta_i \, \mathbf{r}_i,$$

show that

$$\frac{\mathbf{r}^\dagger \mathsf{A}\mathbf{r}}{\mathbf{r}^\dagger \mathbf{r}} \le \lambda_1$$

and that the error in λ_1 is of the order $|\delta_i|^2$. Take $|\delta_i| \ll 1$.
Hint. The $n\mathbf{r}_i$ form a complete orthogonal set spanning the n-dimensional (complex) space.

18.6.4 The variational solution of Example 18.6.1 may be refined by taking $y = x(1-x) + a_2x^2(1-x)^2$. Using a numerical quadrature, calculate $\lambda_{\text{approx}} = F[y(x)]$ [Eq. (18.106)] for a fixed value of a_2. Vary a_2 to minimize λ. Calculate the value of a_2 that minimizes λ and λ itself to five significant figures. Compare your eigenvalue λ with π^2.

18.6.5 (a) Improve the eigenvalue estimate of Example 18.6.2 using the trial wave function $u = r(1 - r/a)(1 - r/b)$, b a parameter. Then determine b by minimizing $F[u]$. The result is expected to satisfy $\pi^2/a^2 \le k^2 \le 10.5/a^2$. Explain why this is not the case. Plot $F[u]$ versus b and determine its minimum value by eye. Which alternative trial wave function does your result suggest?

(b) Use the trial wave function $u = r(1 - r/a)$ and show $F[u] = k^2 = 10/a^2$, improving Example 18.6.2 from 6 to 1.3%. Also use the trial wave function $u = r[1 - (r/a)^b]$, b a parameter, to improve the estimate further.

Additional Reading

Bliss, G. A. (1925). *Calculus of Variations*. Mathematical Association of America Open Court, LaSalle, IL. As one of the older texts, this is still a valuable reference for details of problems such as minimum area problems.

Courant, R., and Robbins, H. (1996). *What Is Mathematics?*, 2nd ed. Oxford Univ. Press, New York. Chapter 7 contains a fine discussion of the calculus of variations, including soap film solutions to minimum area problems.

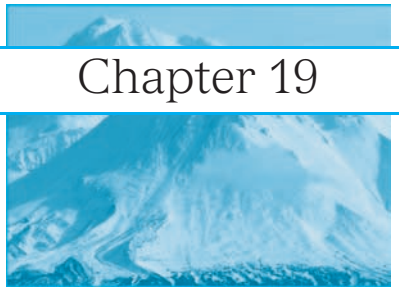
Lanczos, C. (1970). *The Variational Principles of Mechanics*, 4th ed. Univ. of Toronto Press, Toronto. Reprinted, Dover, New York (1986). This book is a very complete treatment of variational principles and their applications to the development of classical mechanics.

Sagan, H. (1961). *Boundary and Eigenvalue Problems in Mathematical Physics*. Wiley, New York. Reprinted, Dover, New York (1989). This delightful text could also be listed as a reference for Sturm–Liouville theory, Legendre and Bessel functions, and Fourier series. Chapter 1 is an introduction to the calculus of variations with applications to mechanics. Chapter 7 picks up the calculus of variations again and applies it to eigenvalue problems.

Sagan, H. (1969). *Introduction to the Calculus of Variations*. McGraw-Hill, New York. Reprinted, Dover, New York (1983). This is an excellent introduction to the modern theory of the calculus of variations, which is more sophisticated and complete than his 1961 text. Sagan covers sufficiency conditions and relates the calculus of variations to problems of space technology.

Weinstock, R. (1952). *Calculus of Variations*. McGraw-Hill, New York. Reprinted, Dover, New York (1974). A detailed, systematic development of the calculus of variations and applications to Sturm–Liouville theory and physical problems in elasticity, electrostatics, and quantum mechanics.

Yourgrau, W., and Mandelstam, S. (1968). *Variational Principles in Dynamics and Quantum Theory*, 3rd ed. Saunders, Philadelphia. Reprinted, Dover, New York (1979). This is a comprehensive, authoritative treatment of variational principles. The discussions of the historical development and the many metaphysical pitfalls are of particular interest.



Chapter 19

Nonlinear Methods and Chaos

Our mind would lose itself in the complexity of the world if that complexity were not harmonious; like the short-sighted, it would only see the details, and would be obliged to forget each of these details before examining the next, because it would be incapable of taking in the whole. The only facts worthy of our attention are those which introduce order into this complexity and so make it accessible to us.

—Henri Poincaré

19.1 Introduction

The origin of nonlinear dynamics goes back to the work of the renowned French mathematician Henri Poincaré on celestial mechanics at the turn of the century. Classical mechanics is, in general, nonlinear in its dependence on the coordinates of the particles and the velocities. Examples are vibrations with a nonlinear restoring force. The Navier–Stokes equations (see Yourgrau and Mandelstam in Additional Reading of Chapter 18) are nonlinear, which makes hydrodynamics difficult to handle. For almost four centuries, however, following the lead of Galilei, Newton, and others, physicists have focused on predictable, effectively linear responses of classical systems that usually have linear and nonlinear properties.

Poincaré was the first to understand the possibility of completely irregular or "chaotic" behavior of solutions of nonlinear differential equations (more precise definitions of chaos will be developed later) that are characterized by an extreme sensitivity to initial conditions: Given slightly different initial conditions, from small perturbations or errors in measurements, for example, solutions can grow exponentially apart with time so that the system soon

becomes effectively unpredictable or chaotic. This property of chaos is often called the "butterfly" effect and will be discussed in Section 19.3. Since the rediscovery of this effect by Lorenz in meteorology in the early 1960s, the field of nonlinear dynamics has grown tremendously. Thus, nonlinear dynamics and chaos theory have entered the mainstream of physics.

Numerous examples of nonlinear systems have been found to display irregular behavior. Surprisingly, order in the sense of quantitative similarities as universal properties or other regularities may arise spontaneously in chaos; a first example, Feigenbaum's universal numbers α and δ will be discussed in Section 19.2. Dynamical chaos is not a rare phenomenon but ubiquitous in nature. It includes irregular shapes of clouds, coastlines, and other landscapes, which are examples of fractals (discussed in Section 19.3), and turbulent flow of fluids, water dripping from a faucet, and the weather. The damped, driven pendulum is among the simplest systems displaying chaotic motion. As a rule, we take the time as the independent dynamic variable.

Necessary conditions for chaotic (defined for now as completely irregular so as to be unpredictable) motion in dynamical systems described by **first-order** differential equations are known to be

- at least three dynamical variables; and
- one or more nonlinear terms coupling two or several of them.

That is, external noise, perturbations, or complexity are not needed to generate random behavior.

As in classical mechanics, the space of the time-dependent dynamical variables of a system of coupled differential equations is called its **phase space**. In such deterministic systems, trajectories in phase space are not allowed to cross. If they did, the system would have a choice at each intersection and would not be deterministic. If the phase space has only two dimensions, such nonlinear systems allow only for fixed points, defined as equilibrium points where iterations (or the motion) stop. An example is a damped pendulum [which can be described by a set of two first-order ordinary differential equations (ODEs) involving two first-order derivatives $\omega = \dot{\theta}$, $\dot{\omega} = f(\omega, \theta)$; that is, only two dynamic variables $\omega(t)$ and $\theta(t)$]. In the undamped case, there are only periodic motion and equilibrium points (e.g., the turning points if there is a maximal angle). These systems are predictable and deterministic. If there is a time-dependent driving term (e.g., $\sin \omega t$), we define a third variable $\varphi = \omega t$ so that the coupled ODEs do not depend on time explicitly. This adds one more dimension to the phase space because $\dot{\varphi} = \omega = \text{const}$. With three (or more) dynamic variables (e.g., **damped**, **driven** pendulum written as first-order coupled ODEs again), more complicated nonintersecting trajectories are possible. These can be shown to include chaotic motion and are called **deterministic chaos**.

A central theme in chaos is the evolution of **complex** forms from the repetition of **simple** but **nonlinear** operations; this is recognized as a **fundamental organizing principle of nature**. Although nonlinear differential equations are a natural place in physics for chaos to occur, the mathematically simpler

iteration of nonlinear functions provides a quicker entry to chaos theory, which we will pursue first in Section 19.2.

Biographical Data

Poincaré, Jules Henri. Poincaré, a French mathematician, was born in 1854 in Nancy, France, and died in 1912 in Paris. Like Hilbert, he made major contributions to most branches of mathematics. In celestial mechanics he worked on the three-body problem, tides and the tidal origin of the moon. Independent of Lorentz, he developed Lorentz transformations from electrodynamics.

19.2 The Logistic Map

The nonlinear, one-dimensional iteration or difference equation

$$x_{n+1} = \mu x_n(1 - x_n), \quad x_n \in [0, 1]; \quad 1 < \mu < 4, \tag{19.1}$$

is sometimes called the logistic map. It is patterned after the nonlinear differential equation $dx/dt = \mu x(1 - x)$, used by P. F. Verhulst in 1845 to model the development of a breeding population whose generations do not overlap. The density of the population at time n is x_n. The positive linear term simulates the birth rate and the nonlinear negative term the death rate of the species in a constant environment that is controlled by the parameter μ.

The quadratic function $f_\mu(x) = \mu x(1 - x)$ is chosen because it has one maximum in the interval [0, 1] and is zero at the end points, $f_\mu(0) = 0 = f_\mu(1)$. The maximum at $x_m = 1/2$ is determined from $f'(x) = 0$; that is,

$$f'_\mu(x_m) = \mu(1 - 2x_m) = 0, \qquad x_m = \frac{1}{2}, \tag{19.2}$$

where $f_\mu(1/2) = \mu/4$.

- Varying the single parameter μ controls a rich and complex behavior including one-dimensional chaos, as we shall see. More parameters or additional variables are hardly necessary at this point to increase the complexity. In a qualitative sense, the simple **logistic** map of Eq. (19.1) is representative of many dynamical systems in biology, chemistry, and physics.

Starting with some $x_0 \in [0, 1]$ in Eq. (19.1), we get x_1, then $x_2, \ldots$, defined as a **cycle**. Plotting $f_\mu(x) = \mu x(1-x)$ along with the diagonal, straight vertical lines to show the intersections with the curve f_μ and horizontal lines to convert $f_\mu(x_i) = x_{i+1}$ to the next x-coordinate, we can construct Fig. 19.1. Choosing μ (= 2 in Fig. 19.1) and x_0 (= 0.1), the vertical line $x = x_0$ meets the curve $f_\mu(x)$ in x_1 (= 0.18), and a horizontal line from (x_0, x_1) intersects the diagonal in (x_1, x_1). The vertical line through (x_1, x_1) meets the curve in x_2 (= 0.2952 in Fig. 19.1), etc.

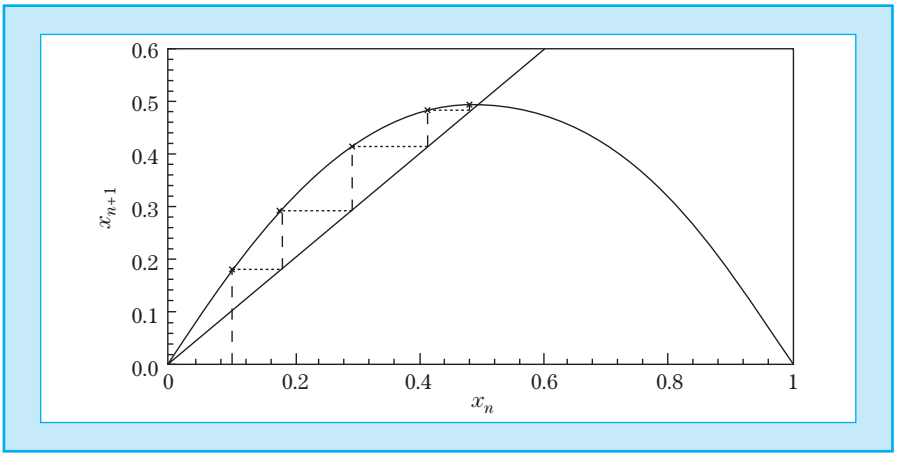


Figure 19.1

Cycle $(x_0, x_1, \ldots)$ for the Logistic Map for $\mu = 2$, Starting Value $x_0 = 0.1$ and Attractor $x^* = 1/2$

The x_i converge toward (0.5, 0.5), a fixed point. A **fixed point** is defined by $f_\mu(x) = x$. Thus, at the fixed point labeled x^*, **the iteration stops** so that

$$f_\mu(x^*) = \mu x^*(1 - x^*) = x^*, \qquad \text{i.e.,}\ x^* = 1 - 1/\mu. \tag{19.3}$$

For any initial x_0 satisfying $f_\mu(x_0) < x^*$, or $0 < x_0 < 1/\mu$, the x_i converge to x^*; such a fixed point is defined as stable. Such fixed points are also called **attractor** or **sink**. The interval $(0, 1/\mu)$ defines a **basin of attraction** for the fixed point x^*. The attractor x^* is **stable** provided the slope $|f'_\mu(x^*)| < 1$, or $1 < \mu < 3$. This can be seen from a Taylor expansion of an iteration near the attractor

$$x_{n+1} = f_\mu(x_n) = f_\mu(x^*) + f'_\mu(x^*)(x_n - x^*) + \cdots,$$

from which follows

$$\frac{x_{n+1} - x^*}{x_n - x^*} = f'_\mu(x^*),$$

upon dropping all higher order terms. Thus, if $|f'_\mu(x^*)| < 1$, the next iterate x_{n+1} lies closer to x^* than x_n, implying convergence to and stability of the fixed point. However, if $|f'_\mu(x^*)| > 1$, x_{n+1} moves farther from x^* than x_n, implying instability. Given the continuity of f'_μ in μ, the fixed point and its properties persist when the parameter (here μ) is slightly varied.

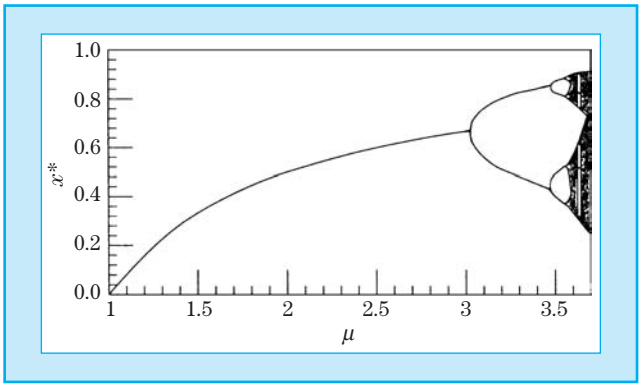
For $\mu > 1$ and $x_0 < 0$ or $x_0 > 1$, it is easy to verify graphically or analytically that the $x_i \to -\infty$. The origin $x = 0$ is a second fixed point. Since $f'_\mu(0) = \mu(1 - 2x)|_{x=0} = \mu > 1$, the iterates x_i move away from it. Such a fixed point is called a **repellor**.

When

$$f'_\mu(x^*) = \mu(1 - 2x^*) = 2 - \mu = -1$$

Figure 19.2

Part of the Bifurcation Plot for the Logistic Map: Fixed Points x^* Versus Parameter μ



is reached for $\mu = 3$, **two fixed points occur**, shown as the two branches in Fig. 19.2 as μ increases beyond the value 3. They can be located by solving

$$x_2^* = f_\mu(f_\mu(x_2^*)) = \mu^2 x_2^*(1 - x_2^*)[1 - \mu x_2^*(1 - x_2^*)]$$

for x_2^*. Here, it is convenient to abbreviate $f^{(1)}(x) = f_\mu(x)$, $f^{(2)}(x) = f_\mu(f_\mu(x))$ for the second iterate, etc. Now we drop the common x_2^* and then reduce the remaining third-order polynomial to second order by recalling that a fixed point of f_μ is also a fixed point of $f^{(2)}$ as $f_\mu(f_\mu(x^*)) = f_\mu(x^*) = x^*$. Therefore, $x_2^* = x^*$ is one solution. Solving for the quadratic polynomial, we obtain

$$\begin{aligned} 0 &= \mu^2[1 - (\mu + 1)x_2^* + 2\mu(x_2^*)^2 - \mu(x_2^*)^3] - 1 \\ &= (\mu - 1 - \mu x_2^*)[\mu + 1 - \mu(\mu + 1)x_2^* + \mu^2(x_2^*)^2]. \end{aligned}$$

The roots of the quadratic polynomial are

$$x_2^* = \frac{1}{2\mu}\left(\mu + 1 \pm \sqrt{(\mu + 1)(\mu - 3)}\right),$$

which are the two branches in Fig. 19.2 for $\mu > 3$ starting at $x_2^* = 2/3$ at $\mu = 3$. Each x_2^* is a point of period 2 and invariant under two iterations of the map f_μ. The iterates oscillate between both branches of fixed points x_2^*. A point x_n is defined as a **periodic point of period** n for f_μ if $f^{(n)}(x_0) = x_0$ but $f^{(i)}(x_0) \neq x_0$ for $0 < i < n$. Thus, for $3 < \mu < 3.45$ (Fig. 19.2) the stable attractor **bifurcates** into two fixed points x_2^*. The bifurcation for $\mu = 3$, where the doubling occurs, is called a **pitchfork** bifurcation because of its characteristic (rounded Y) shape. A bifurcation is a sudden change in the evolution of the system, such as a splitting into two regions.

As μ increases beyond 3, the derivative $df^{(2)}/dx$ decreases from unity to -1. For $\mu = 1 + \sqrt{6} \sim 3.44949$, which can be derived from

$$\left.\frac{df^{(2)}}{dx}\right|_{x=x^*} = -1, \quad f^{(2)}(x^*) = x^*,$$

each branch of fixed points bifurcates again so that $x_4^* = f^{(4)}(x_4^*)$ (i.e., it has period 4). For $\mu = 1 + \sqrt{6}$, these are $x_4^* = 0.43996$ and $x_4^* = 0.849938$. With increasing period doublings it becomes impossible to obtain analytic solutions. The iterations are better done by computer, whose rapid improvements (computer-driven graphics, in particular) and wide distribution starting in the 1970s and 1980s have accelerated the development of chaos theory. As the μ values where bifurcations occur become increasingly more closely spaced, the sequence of bifurcations continues with ever longer periods until it converges to $\mu_\infty = 3.5699456\ldots$, where an infinite number of bifurcations occur. Near bifurcation points, fluctuations, rounding errors in initial conditions, etc. play an increasing role because the system has to choose between two possible branches and becomes much more **sensitive to small perturbations**, a characteristic feature on the road to chaos. In the present case, for most $\mu > \mu_\infty$ the x_n never repeat, except for narrow periodic windows (that are unshaded in Fig. 19.2). The bands of fixed points x^* begin forming a continuum (shown dark in Fig. 19.2): This is where chaos starts and what is defined as chaos. This increasing period doubling is the route to chaos for the logistic map that is characterized by a constant δ, called a Feigenbaum number. The first bifurcation occurs at $\mu_1 = 3$, the second at $\mu_2 = 3.44949, \ldots$, and the ratios of spacings between the μ_n can be shown to converge to δ:

$$\lim_{n\to\infty} \frac{\mu_n - \mu_{n-1}}{\mu_{n+1} - \mu_n} = \delta = 4.66920161\ldots. \tag{19.4}$$

From the bifurcation plot Fig. 19.2, we obtain

$$(\mu_2 - \mu_1)/(\mu_3 - \mu_2) = (3.45 - 3.00)/(3.54 - 3.45) = 4.97$$

as a first approximation for the dimensionless δ.

We recognize that each successive period-doubling bifurcation is a smaller replica of the sidewise cup shape, with twice the number of cups of the bifurcation just before it. We can measure the width of successive cups, calling them d_n, going along a definite branch. The ratios of widths of these self-similar cup shapes can be shown to converge to another dimensionless quantity α:

$$\lim_{n\to\infty} \frac{d_n}{d_{n+1}} = \alpha = 2.5029\ldots. \tag{19.5}$$

Using our earlier bifurcation points $x_4^* = 0.849938$ and $x_4^* = 0.43996$ and reading off Fig. 19.2 approximate values for the next bifurcation values x^* from the lower branch, we obtain

$$d_1 = 0.849938 - 0.43996 = 0.409978 \approx 0.41, \quad d_2 \approx 0.51 - 0.35 = 0.16,$$
$$\frac{d_1}{d_2} \approx \frac{0.41}{0.16} = 2.56$$

as a first approximation for α. Further details are discussed in Section 19.3.

The Feigenbaum numbers δ and α are the same, and in this sense universal, for the route to chaos via period doublings for all maps with a **quadratic** maximum such as the logistic map. This is an example of order in chaos. Experience shows that its validity is even wider, including two-dimensional (dissipative) systems with twice continuously differentiable functions.[1] When the maps behave like $|x-x_m|^{1+\varepsilon}$ near their maximum x_m for some ε between 0 and 1, the Feigenbaum number will depend on the exponent ε; thus, $\delta(\varepsilon)$ varies between $\delta(1) = \delta$ given in Eq. (19.4) for quadratic maps and $\delta(0) = 2$ for $\varepsilon = 0$.[2] Solutions of (nonlinear) differential equations can often be analyzed in terms of discrete maps (i.e., cycles of iterates, fixed points, and bifurcations) that are generated by placing a tranverse plane into a trajectory that then intersects the plane in a series of points at increasing times.

EXERCISES

19.2.1 Show that $x^* = 1$ is a nontrivial fixed point of the map $x_{n+1} = x_n \exp[r(1-x_n)]$ with a slope $1-r$ so that the equilibrium is stable if $0 < r < 2$.

19.2.2 Draw a bifurcation diagram for the exponential map of Exercise 19.2.1 for $r > 1.9$.

19.2.3 Determine fixed points of the cubic map $x_{n+1} = a x_n^3 + (1-a)x_n$ for $0 < a < 4$ and $0 < x_n < 1$.

19.2.4 Write the time-delayed logistical map $x_{n+1} = \mu x_n(1-x_{n-1})$ as a two-dimensional map, $x_{n+1} = \mu x_n(1-y_n)$, $y_{n+1} = x_n$, and determine some of its fixed points.

19.2.5 Show that the second bifurcation for the logistical map that leads to cycles of period 4 is located at $\mu = 1+\sqrt{6}$.

19.2.6 Construct a nonlinear iteration function with Feigenbaum δ in the interval $2 < \delta < 4.6692\ldots$.

19.2.7 Determine the Feigenbaum δ for (a) the exponential map of Exercise 18.2.1, (b) some cubic map of Exercise 19.2.3, (c) the time-delayed logistic map of Exercise 19.2.4.

19.2.8 Repeat Exercise 19.2.7 for Feigenbaum's α instead of δ.

19.2.9 Find numerically the first four points μ for period doubling of the logistic map and then obtain the first two approximations to the Feigenbaum δ. Compare with Fig. 19.2 and Eq. (19.4).

[1] More details and computer codes for the logistic map are given by G. L. Baker and J. P. Gollub, *Chaotic Dynamics: An Introduction*, 2nd ed. Cambridge Univ. Press, Cambridge, UK (1996).

[2] For other maps and a discussion of the fascinating history of how chaos became again a hot research topic, see D. Holton and R. M. May in *The Nature of Chaos* (T. Mullin, Ed.), Section 5, p. 95. Clarendon, Oxford, UK (1993); and Gleick's *Chaos* (1987).

19.2.10 Find numerically the values μ where the cycle of period 1,3,4,5,6 begins and then where it becomes unstable.

Check values. For period $\begin{matrix} 3, & \mu = 3.8284, \\ 4, & \mu = 3.9601, \\ 5, & \mu = 3.7382, \\ 6, & \mu = 3.6265. \end{matrix}$

19.2.11 Repeat Exercise 19.2.9 for Feigenbaum's α.

19.3 Sensitivity to Initial Conditions and Parameters

Lyapunov Exponents

In Section 19.2, we described how, as we approach the period doubling accumulation parameter value $\mu_\infty = 3.5699\ldots$ from below, the period $n+1$ of cycles $(x_0, x_1, \ldots, x_n)$ with $x_{n+1} = x_0$ gets longer. The logistic map is defined to be chaotic at all values of μ where fixed points with cycles of infinite length occur. Thus, chaos starts with $\mu_\infty = 3.5699\ldots$. For most $\mu \geq \mu_\infty$ it is also easy to check numerically that the distances between neighboring iterates x_0 and $x_0 + \varepsilon$,

$$d_n = |f^{(n)}(x_0 + \varepsilon) - f^{(n)}(x_0)|, \tag{19.6}$$

grow as well for small $\varepsilon > 0$. With chaotic behavior this distance increases exponentially with $n \to \infty$; that is, $d_n/\varepsilon = e^{\lambda n}$, or

$$\lambda = \frac{1}{n} \ln \left(\frac{|f^{(n)}(x_0 + \varepsilon) - f^{(n)}(x_0)|}{\varepsilon} \right), \tag{19.7}$$

where λ is the **Lyapunov exponent**. For $\varepsilon \to 0$, we may rewrite Eq. (19.7) in terms of derivatives as

$$\lambda(x_0) = \frac{1}{n} \ln \left| \frac{df^{(n)}(x_0)}{dx} \right| = \frac{1}{n} \sum_{i=0}^{n} \ln |f'(x_i)| \tag{19.8}$$

using the chain rule of differentiation for $df^{(n)}(x)/dx$, where

$$\frac{df^{(2)}(x_0)}{dx} = \frac{df_\mu}{dx}\bigg|_{x=f_\mu(x_0)} \frac{df_\mu}{dx}\bigg|_{x=x_0} = f'_\mu(x_1) f'_\mu(x_0) \tag{19.9}$$

and $f'_\mu = df_\mu/dx$, $x_1 = f_\mu(x_0)$, etc. Our Lyapunov exponent has been calculated at the point x_0. To understand whether or not an attractor x^* is chaotic, one needs to determine λ_j for several starting points x_j near x^* and calculate the average λ. If the average turns out to be positive, the attractor (and its parameter μ) is defined to be chaotic. This is particularly relevant in higher dimensional dynamical systems in which the motion is often bounded so that

the d_n cannot go to ∞. In general, one point is not enough to determine λ as a measure of the sensitivity of the system to changes in initial conditions. In such cases, we repeat the procedure for several points on the trajectory and average over them. This way, we obtain the **average Lyapunov exponent** for the sample. This average value is often called and taken as the Lyapunov exponent.

The Lyapunov exponent λ is a quantitative measure of chaos: A one-dimensional iterated function such as the logistic map has **chaotic** iterates $(x_0, x_1, \ldots)$ for the parameter μ **if the average Lyapunov exponent is positive** for that value of μ (the shaded region in Fig. 19.2). For cycles of finite period, λ is negative. This is the case for $\mu < 3$, for $\mu < \mu_\infty$, and even in the periodic window at $\mu \sim 3.627$ inside the chaotic region of Fig. 19.2. A negative Lyapunov exponent does not necessarily correspond to periodicity of iterates. At bifurcation points, $\lambda = 0$. For $\mu > \mu_\infty$, the Lyapunov exponent is positive, except in the periodic windows where $\lambda < 0$, and λ grows with μ. In other words, the logistic map becomes more chaotic as the control parameter μ increases.

In the chaos region of the logistic map there is a scaling law for the average Lyapunov exponent (that we do not derive here),

$$\lambda(\mu) = \lambda_0(\mu - \mu_\infty)^{\ln 2/\ln \delta}, \tag{19.10}$$

where $\ln 2/\ln \delta \sim 0.445$, δ is the universal Feigenbaum number of Section 19.2, and λ_0 is a constant. This relation is reminiscent of a physical observable at a (second-order) phase transition. The exponent in Eq. (19.10) is a universal number; the Lyapunov exponent plays the role of an **order parameter**, whereas $\mu - \mu_\infty$ is the analog of $T - T_c$, where T_c is the **critical** temperature at which the phase transition occurs.

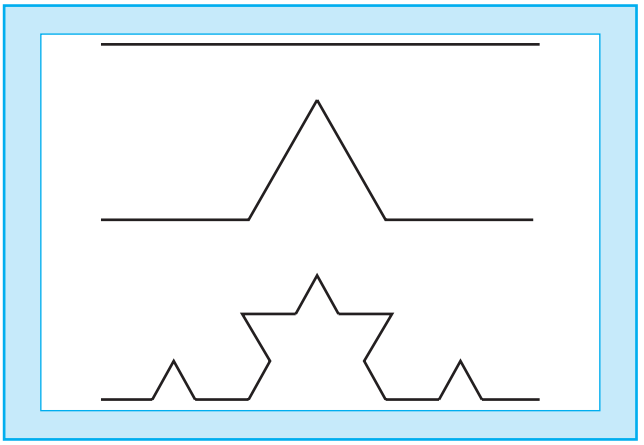
Fractals

In dissipative chaotic systems (but rarely in conservative Hamiltonian systems), often new geometric objects with intricate shapes appear that are called fractals. Fractals are irregular geometric objects that exist at many scales like cauliflowers so that their smaller parts resemble their larger parts. Intuitively, a fractal is a set that is (approximately) **self-similar** under magnification. The dimension is not a conventional positive integer. The clarification and definition of the concept of dimension is our next topic.

We need a quantitative measure of dimensionality in order to describe fractals. Unfortunately, there are several definitions with usually different numerical values, none of which has become a standard. For strictly self-similar sets one measure suffices, of course. More complicated (e.g., only approximately self-similar) sets require more measures for their complete description. The simplest is the **box-counting dimension** of Kolmogorov and Hausdorff. For a one-dimensional set, cover the curve by line segments of length R; in two dimensions, cover the surface by boxes, squares of area R^2; in three dimensions, cover the volume by cubes of volume R^3; etc. Count the number $N(R)$ of boxes needed to cover the set. Letting R go to zero, we

Figure 19.3

Construction of the Koch Curve by Iterations



expect N to scale as $N(R) \sim R^{-d}$. Taking the logarithm, the **box-counting dimension** is defined as

$$d = \lim_{R \to 0} [-\ln N(R)/\ln R]. \tag{19.11}$$

For example, in a two-dimensional space a single point is covered by one square so that $\ln N(R) = 0$ and $d = 0$. A finite set of isolated points also has dimension $d = 0$. For a differentiable curve of length L, $N(R) \sim L/R$ as $R \to 0$ so that $d = 1$ from Eq. (19.11), as expected.

Let us now construct a more irregular set, the **Koch curve**. We start with a line segment of unit length in Fig. 19.3 and remove the middle one-third. Then we replace it with two segments of length one-third that form a triangle in Fig. 19.3. We iterate this procedure with each segment ad infinitum. The resulting Koch curve is infinitely long and is nowhere differentiable because of the infinitely many discontinuous changes of slope. At the nth step each line segment has length $R_n = 3^{-n}$ and there are $N(R_n) = 4^n$ segments. Hence, its dimension is $d = \ln 4/\ln 3 = 1.26\ldots$, which is more than a curve but less than a surface. As the Koch curve results from iteration of the first step, it is strictly self-similar.

A two-dimensional Koch-type construction conserves area and starts from a square, adding in the middle of each side a narrow triangle and cutting one out of the square next to it, repeating the process over and over to make it self-similar. Or starting from a rectangle, adding a small rectangle in the middle of each side and cutting one out next to it, repeating the construction at smaller scales over and over.

For the logistic map the box-counting dimension at a period-doubling accumulation point μ_∞ is $0.5388\ldots$, which is a universal number for iterations of functions in one variable with a quadratic maximum. To see how this comes about, consider the pairs of line segments originating from successive bifurcation points for a given parameter μ in the chaos regime (see Fig. 19.2).

Imagine removing the interior space from the chaotic bands. When we go to the next bifurcation the relevant scale parameter is $\alpha = 2.5029\ldots$ from Eq. (19.5). Suppose we need 2^n line segments of length R to cover 2^n bands. In the next stage, we need 2^{n+1} segments of length R/α to cover the bands. This yields a dimension $d = -\ln(2^n/2^{n+1})/\ln\alpha = 0.4498\ldots$. This crude estimate can be improved by taking into account that the width between neighboring pairs of line segments differs by $1/\alpha$ (see Fig. 19.2). The improved estimate, 0.543, is closer to $0.5388\ldots$. A more accurate analysis of the logistic map and other examples shows that when the fractal set does not have a strictly self-similar structure, the box-counting dimension depends on the box construction method.

A set of attracting points in the phase space of the (dissipative) dynamics with noninteger dimension is called a **strange attractor**. Such strange attractors play a pivotal role in the theory of chaos.

Finally, we turn to the beautiful fractals that are surprisingly easy to generate and whose color pictures had considerable impact. For complex $c = a+ib$, the quadratic complex map involving the complex variable $z = x + iy$,

$$z_{n+1} = z_n^2 + c, \tag{19.12}$$

looks deceptively simple, but the equivalent two-dimensional map in terms of the real variables

$$x_{n+1} = x_n^2 - y_n^2 + a, \qquad y_{n+1} = 2x_n y_n + b \tag{19.13}$$

reveals more of its complexity. This map forms the basis for some of Mandelbrot's beautiful multicolor fractal pictures (see Mandelbrot and Peitgen in Additional Reading), and it has been found to generate intricate shapes for various $c \neq 0$. For example, the **Julia set** of a map $z_{n+1} = F(z_n)$ is defined as the set of all its repellors or periodic points. Thus, it forms the boundary between initial points of a two-dimensional iterated map leading to iterates that diverge and those that stay within some finite region of the complex plane. For the case $c = 0$ and $F(z) = z^2$, the Julia set can be shown to be a circle about the origin of the complex plane. However, just by adding a constant $c \neq 0$, the Julia set becomes fractal. For example, for $c = -1$ one finds a fractal necklace with infinitely many loops (see Devaney in Additional Reading).

While the Julia set is drawn in the complex plane, the **Mandelbrot set** is constructed in the two-dimensional parameter space $c = (a, b) = a + bi$. It is constructed as follows. Starting from the initial value $z_0 = 0 = (0, 0)$, one searches Eq. (19.12) for parameter values c so that the iterated $\{z_n\}$ do **not** diverge to ∞. Each color outside the fractal boundary of the Mandelbrot set represents a given number of iterations, m, needed for the z_n to go beyond a specified absolute (real) value R, $|z_m| > R > |z_{m-1}|$. For real parameter value $c = a$, the resulting map $x_{n+1} = x_n^2 + a$ is equivalent to the logistic map with period-doubling bifurcations (see Section 19.2) as a increases on the real axis inside the Mandelbrot set.

Fractals are ubiquitous in nature, as seen in eroded steep mountain aretes, coastlines, and cumulus cloud shapes because nonlinear iterations occur in the dynamics shaping these formations.

EXERCISES

19.3.1 Use a computer with BASIC or FORTRAN or symbolic software such as Mathematica or Maple or a website to obtain the iterates x_i of an initial $0 < x_0 < 1$ and $f'_\mu(x_i)$ for the logistic map. Then calculate the Lyapunov exponent for cycles of period 2,3,... of the logistic map for $2 < \mu < 3.7$. Show that for $\mu < \mu_\infty$ the Lyapunov exponent $\lambda = 0$ at bifurcation points and negative elsewhere, whereas for $\mu > \mu_\infty$ it is positive except in periodic windows.
Hint. See Fig. 9.3 of Hilborn in Additional Reading.

19.3.2 Consider the map $x_{n+1} = F(x_n)$ with

$$F(x) = \begin{cases} a + bx, & x < 1, \\ c + dx, & x > 1, \end{cases}$$

for $b > 0$ and $d < 0$. Show that its Lyapunov exponent is positive when $b > 1,\ d < -1$. Plot a few iterations in the (x_{n+1}, x_n) plane.

19.4 Nonlinear Differential Equations

In Section 19.1, we mentioned nonlinear differential equations (NDEs) as the natural place in physics for chaos to occur but continued with the simpler iteration of nonlinear functions of one variable (maps). Here, we briefly address the much broader area of NDEs and the far greater complexity in the behavior of their solutions. However, maps and systems of solutions of NDEs are closely related. The latter can often be analyzed in terms of discrete maps. One prescription is the **Poincaré section** (or map) of a system of NDE solutions. Placing a plane transverse into a trajectory (of a solution of a NDE), it intersects the plane in a series of points at increasing discrete times [e.g., in Fig. 19.4, $(x(t_1), y(t_1)) \equiv (x_1, y_1), (x_2, y_2), \ldots$], which are recorded and graphically or numerically analyzed for fixed points, period-doubling bifurcations, etc. This method is useful when solutions of NDEs are obtained numerically in computer simulations so that one can generate Poincaré sections at various locations and with different orientations with further analysis leading to two-dimensional iterated maps

$$x_{n+1} = F_1(x_n, y_n), \qquad y_{n+1} = F_2(x_n, y_n) \tag{19.14}$$

stored by the computer. Extracting the functions F_j analytically or graphically is not always easy, though.

Let us start with a few classical examples of NDEs.

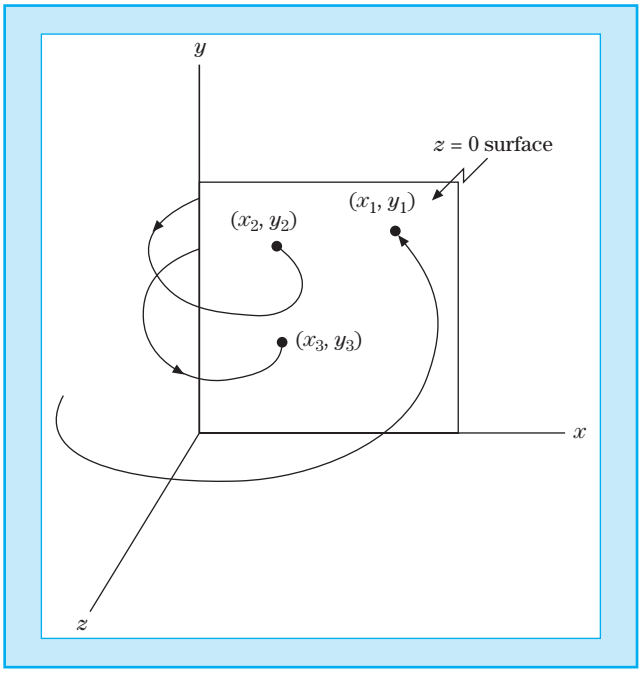


Figure 19.4
Schematic of a Poincaré Section

Bernoulli and Riccati Equations

Bernoulli equations are also nonlinear, having the form

$$y'(x) = p(x)y(x) + q(x)[y(x)]^n, \tag{19.15}$$

where p and q are real functions and $n \neq 0, 1$ to exclude first-order linear ODEs. They are an example of a nonlinear ODE that can be solved analytically, but being one-dimensional, they do not generate chaos and their solutions do not diverge exponentially. If we substitute

$$u(x) = [y(x)]^{1-n}, \tag{19.16}$$

then Eq. (19.15) becomes a first-order linear ODE

$$u' = (1-n)y^{-n}y' = (1-n)[p(x)u(x) + q(x)], \tag{19.17}$$

which we can solve as described in Section 8.2.

EXAMPLE 19.4.1

Bernoulli NDE Solve $\dot{y} = y - 2y^2$ for $y(t = 0) = 1/3$, an NDE that models animal (and human) population growth similar to Verhulst's (or the logistic) NDE. Here, the quadratic term with its negative sign prevents the population from exploding. Neglecting it, one obtains exponential growth $y(t) = e^t$ (Malthus's law) with increasing time. Substituting $u = 1/y,\ \dot{u} = -\dot{y}/y^2$ into

the NDE $\frac{\dot{y}}{y^2} = \frac{1}{y} - 2$, we obtain $\dot{u} = 2 - u$. Separating variables and integrating yields

$$\ln(u-2) = \int^u \frac{du}{u-2} = -\int^t dt = -t + \ln C.$$

Exponentiating, this result gives $u = 2 + Ce^{-t}$, or $y(t) = \frac{1}{2+Ce^{-t}}$. Upon varying C the solutions do not diverge exponentially, and there is no chaos. The initial condition $y(0) = 1/3$ fixes $C = 1$. This solution $y(t) = \frac{1}{2+e^{-t}}$ increases from $1/3$ at $t = 0$ to $1/2$ for $t \to \infty$. ■

Riccati equations[3] are quadratic in $y(x)$:

$$y' = p(x)y^2 + q(x)y + r(x), \tag{19.18}$$

where $p \neq 0$ to exclude linear ODEs and $r \neq 0$ to exclude Bernoulli equations. There is no general method for solving Riccati equations. However, when a special solution $y_0(x)$ of Eq. (19.18) is known by guess or inspection, then the substitution $y = y_0 + u$ leads to the Bernoulli equation for $u(x)$,

$$u' = pu^2 + (2py_0 + q)u, \tag{19.19}$$

because substitution of $y = y_0 + u$ into Eq. (19.18) removes $r(x)$ from Eq. (19.18).

Finally, we prove the following theorem: The substitution $y = -z'/pz(x)$ transforms the Riccati NDE into the homogeneous **linear** second-order ODE

$$z'' - \left(q + \frac{p'}{p}\right)z' + prz(x) = 0. \tag{19.20}$$

We show this by substituting y' expressed in terms of z into the NDE

$$y' = -\frac{z''}{pz} + \frac{z'p'}{p^2z} + \frac{z'^2}{pz^2} = \frac{z'^2}{pz^2} - \frac{qz'}{pz} + r,$$

which yields

$$z'' = z'\left(q + \frac{p'}{p}\right) - prz.$$

If this ODE cannot be solved analytically, it may be solved by the power series method.

EXAMPLE 19.4.2

Riccati NDE Solve $y' = 1/2 - x^2y + 2xy^2$ with initial condition $y(0) = 1$.

We start by guessing a solution (there are no rules to find one—just trial and error), namely $y = x/2$, and verify it by $1/2 = 1/2 - x^3/2 + 2x(x^2/4)$. Then we substitute $y = \frac{x}{2} + u$, $y' = \frac{1}{2} + u'$ into the Riccati NDE to obtain the

[3]Riccati's NDE has been used for solving the Schrödinger equation by S. B. Haley, *Am. J. Phys.* **65,** 237 (1997).

Bernoulli NDE

$$u' = x^2 u + 2xu^2.$$

We solve this by setting $v = 1/u$, $v' = -u'/u^2$. This gives the ODE

$$-v' = x^2 v + 2x.$$

We solve first the homogeneous ODE $-v' = x^2 v$ by separating variables and integrating

$$\int^v \frac{dv}{v} = -\int^x x^2\, dx = -x^3/3 + \ln C.$$

Exponentiating gives $v = Ce^{-x^3/3}$. Now we vary the constant $C \to C(x)$ and substitute $v = C(x)e^{-x^3/3}$ into the inhomogeneous ODE, getting $C' = -2xe^{x^3/3}$. Hence, $v = e^{-x^3/3}(c - 2\int^x xe^{x^3/3}dx)$, $u = 1/v$, and finally $y = x/2 + u$. The initial condition fixes the integration constant $c = 1$ from $y(0) = 1 = 1/c$. ■

Just as for Riccati equations, **there are no general methods for obtaining exact solutions of other nonlinear ODEs**. It is more important to develop methods for finding the **qualitative behavior of solutions by numerical integration**, where chaos occurs, etc. In Chapter 8, we described that power series solutions of ODEs exist except (possibly) at essential singularities. The locations of the latter are directly given by the properties of the coefficient functions of the ODE. Such a local analysis provides us with the asymptotic behavior of solutions as well.

Fixed and Movable Singularities, Special Solutions

Solutions of NDEs also have such singular points that are independent of the initial or boundary conditions and are called **fixed singularities**. In addition, they may have **spontaneous** or **movable** singularities that vary with the initial or boundary conditions. They complicate the (asymptotic) analysis of NDEs.

EXAMPLE 19.4.3 **Movable Singularity** This point is illustrated by a comparison of the linear ODE

$$y' + \frac{y}{x-1} = 0, \tag{19.21}$$

which has an obvious regular singularity at $x = 1$, with the NDE $y' = y^2$. Both have the same solution with initial condition $y(0) = 1$, namely $y(x) = 1/(1-x)$. For $y(0) = 2$, though, the pole in the (obvious, but check) solution $y(x) = 2/(1-2x)$ of the NDE has moved to $x = 1/2$. More generally, $y(x) = y_0/(1 - y_0 x)$ is a solution of $y' = y^2$ with $y(0) = y_0$, which in this case shows how the singularity moves with the initial condition. ■

For a linear second-order ODE we have a complete description of (the asymptotic behavior of) its solutions when (that of) two linearly independent

solutions are known. For NDEs there may still be **special solutions** whose asymptotic behavior is not obtainable from two independent solutions. This is another **characteristic** property of NDEs, which we illustrate again by an example.

EXAMPLE 19.4.4

Special Solution The class of solutions of the NDE $y'' = yy'/x$ that depends on two parameters to satisfy initial conditions $y(0) = y_0$ and $y'(0) = y_0'$, for example, is given by

$$y(x) = 2c_1 \tan(c_1 \ln x + c_2) - 1, \tag{19.22}$$

where c_i are integration constants. An obvious (check it) special solution is $y = c_3 =$ constant, which cannot be obtained from Eq. (19.22) for any choice of the parameters c_1, c_2 for $c_3 \neq -1$. Note that using the substitution $x = e^t$, $Y(t) = y(e^t)$ so that $x\,dy/dx = dY/dt$, we obtain the ODE $Y'' = Y'(Y+1)$. This ODE can be integrated once to give $Y' = \frac{1}{2}Y^2 + Y + c$, with $c = 2(c_1^2 + 1/4)$ an integration constant, and again according to Section 8.2 to lead to the solution of Eq. (19.22). ■

Autonomous Differential Equations

Differential equations that do not explicitly contain the independent variable taken to be the time t here are called **autonomous**. Verhulst's NDE $\dot{y} = dy/dt = \mu y(1 - y)$, which we discussed briefly in Section 19.2 as motivation for the logistic map, is a special case of this wide and important class of ODEs.[4] For one dependent variable $y(t)$, they can be written as

$$\dot{y} = f(y) \tag{19.23a}$$

and for several dependent variables as a system

$$\dot{y}_i = f_i(y_1, y_2, \ldots, y_n), \quad i = 1, 2, \ldots, n \tag{19.23b}$$

with sufficiently differentiable functions f, f_i. A solution of Eq. (19.23a) is a curve or trajectory $y(t)$ for $n = 1$ and, for $n > 1$, a trajectory $(y_1(t), y_2(t), \ldots, y_n(t))$ in **phase space**. As discussed in Section 19.1, two trajectories cannot cross because of the uniqueness of the solutions of ODEs. Clearly, solutions of the algebraic system

$$f_i(y_1, y_2, \ldots, y_n) = 0, \quad i = 1, 2, \ldots, n \tag{19.24}$$

are special points in phase space, where the position vector $(y_1, y_2, \ldots, y_n)$ does not move on the trajectory; they are called **critical** (or **fixed**) **points**, just like fixed points for nonlinear maps. A local analysis of solutions near critical points leads to an understanding of the global behavior of the solutions. First, let us discuss a simple example.

[4] Solutions of nonautonomous equations can be more complicated.

EXAMPLE 19.4.5

Verhulst's NDE For Verhulst's ODE $\dot{y} = f(y) = \mu y(1-y) = 0$ with $\mu > 0$ gives $y = 0$ and $y = 1$ as the critical points; for the logistic map $y = 0$ is a repellor as $df/dy = \mu > 1$, whereas $x^* = 1 - 1/\mu$ is an attractor as $|df(x^*)/dy| = |2 - \mu| < 1$ for $\mu < 3$.

At $y = 0$ we expand $\dot{y} = f(0) + f'(0)y + \cdots = \mu y + \cdots$ so that y moves to the right for $y > 0$ and to the left for $y < 0$. This behavior $\cdots \leftarrow \cdot \rightarrow \cdots$ characterizes $y = 0$ as a repellor. At $y = 1$, we expand

$$\dot{y} = f(1) + f'(1)(y-1) + \cdots = -\mu(y-1) + \cdots$$

so that y moves to the right for $y < 1$ and to the left for $y > 1$. This behavior $\cdots \rightarrow \cdot \leftarrow \cdots$ describes an attractor.

This local analysis near $y = 0$ suggests neglecting the y^2 term and solving $\dot{y} = \mu y$ instead. Integrating $\int dy/y = \mu t + \ln c$ gives the solution $y(t) = ce^{\mu t}$, which diverges as $t \to \infty$ so that $y = 0$ is a repellor. Similarly, at $y = 1$, $\int dy/(1-y) = \mu t - \ln c$ leads to $y(t) = 1 - ce^{-\mu t} \to 1$ for $t \to \infty$. Hence, $y = 1$ is an attractor. Because the NDE is separable, its general solution is given by

$$\int \frac{dy}{y(1-y)} = \int dy \left[\frac{1}{y} + \frac{1}{1-y}\right] = \ln \frac{y}{1-y} = \mu t + \ln c.$$

Hence, $y(t) = ce^{\mu t}/[1 + ce^{\mu t}]$ for $t \to \infty$ converges to unity, thus confirming the local analysis. No chaos is found here because the NDE has only one dynamical variable, and as c is varied there is no exponential divergence. ■

This example motivates us to examine the properties of fixed points in more detail. In general, it is easy to see that

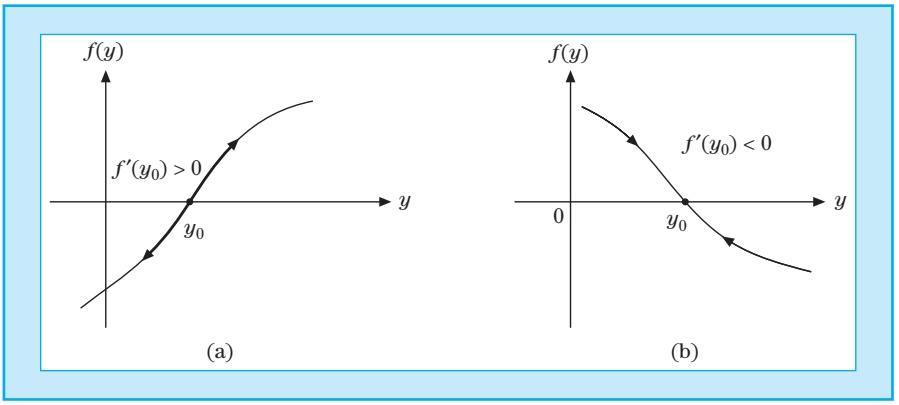
- in **one dimension** fixed points y_i with $f(y_i) = 0$ divide the y-axis into dynamically separate intervals because, given an initial value in one of the intervals, the trajectory $y(t)$ will stay there since it cannot go beyond either fixed point where $\dot{y} = 0$.

If $f'(y_0) > 0$ at the fixed point y_0 where $f(y_0) = 0$, then at $y_0 + \varepsilon$ for $\varepsilon > 0$ sufficiently small, $\dot{y} = f'(y_0)\varepsilon + \mathcal{O}(\varepsilon^2) > 0$ in a neighborhood to the right of y_0 so that the trajectory $y(t)$ keeps moving to the right, away from the fixed point y_0. To the left of y_0, $\dot{y} = -f'(y_0)\varepsilon + \mathcal{O}(\varepsilon^2) < 0$ so that the trajectory moves away from the fixed point here as well. Hence,

- a fixed point [with $f(y_0) = 0$] at y_0 with $f'(y_0) > 0$ as shown in Fig. 19.5a repels trajectories (i.e., all trajectories move away from the critical point): $\cdots \leftarrow \cdot \rightarrow \cdots$. It is a **repellor**. Similarly, we see that
- a fixed point at y_0 with $f'(y_0) < 0$ as shown in Fig. 19.5b attracts trajectories (i.e., all trajectories converge toward the critical point y_0): $\cdots \rightarrow \cdot \leftarrow \cdots$. It is a **sink**.

Figure 19.5

Fixed Points. (a) Repellor; (b) Sink



Let us now consider the remaining case in which also $f'(y_0) = 0$. Let us assume $f''(y_0) > 0$. Then at $y_0 + \varepsilon$ to the right of fixed point y_0,

$$\dot{y} = f''(y_0)\varepsilon^2/2 + \mathcal{O}(\varepsilon^3) > 0$$

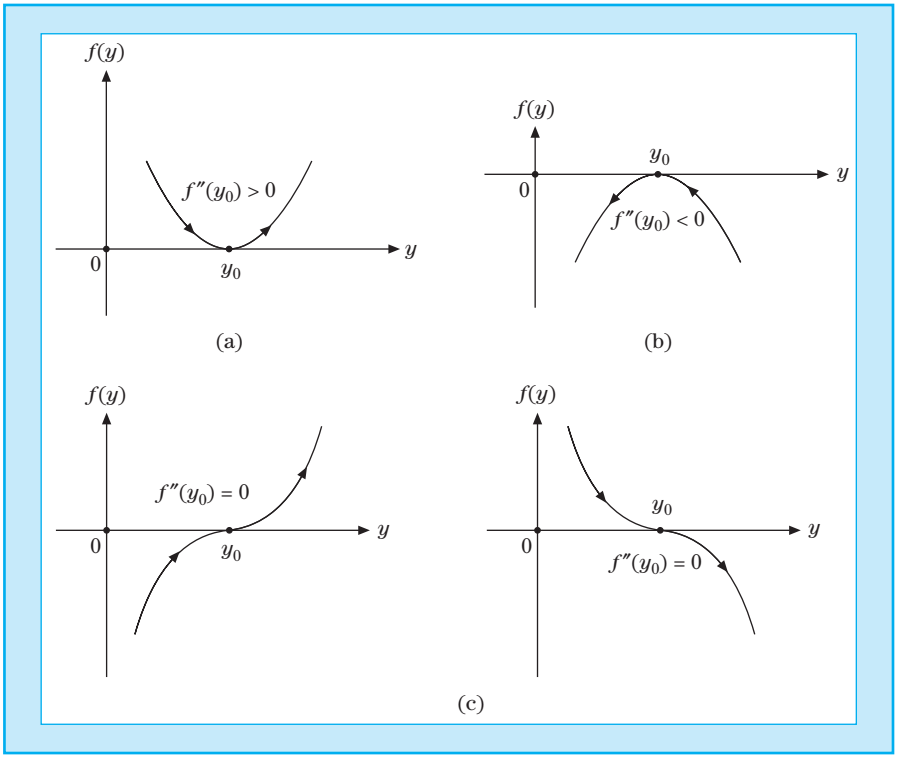
so that the trajectory moves away from the fixed point there, whereas to the left it moves closer to y_0. This is defined as a **saddle point in one dimension**. For $f''(y_0) < 0$, the sign of $\dot{y}$ is reversed so that we deal again with a saddle point with the motion to the right of y_0 toward the fixed point and at left away from it. Let us summarize the local behavior of trajectories near such a fixed point y_0: We have

- a saddle point at y_0 when $f(y_0) = 0$, and $f'(y_0) = 0$, as shown in Figs. 19.6a and 19.6b corresponding to the cases in which (a) $f''(y_0) > 0$ and trajectories on one side of the critical point converge toward it and diverge from it on the other side ($\cdots \to \cdot \to \cdots$) and (b) $f''(y_0) < 0$. Here, the direction is simply reversed compared to (a). Fig. 19.6(c) shows the cases in which $f''(y_0) = 0$.

So far, we have ignored the additional dependence of $f(y)$ on one or more parameters, such as μ for the logistic map. When a critical point maintains its properties qualitatively as we adjust a parameter slightly, we call it structurally stable. This definition makes sense in practice: Structurally unstable objects are unlikely to occur in reality because noise and other neglected degrees of freedom act as perturbations on the system that effectively prevent unstable points from being observed. Let us now examine fixed points from this point of view. Upon varying such a control parameter slightly, we deform the function f, or we may just shift f up or down or sideways in Fig. 19.5. This will slightly move the location y_0 of the fixed point with $f(y_0) = 0$ but maintain the sign of $f'(y_0)$. Thus, both **attractors and repellors are structurally stable**, whereas a saddle point in general is not. For example, shifting f in Fig. 19.6a down creates two fixed points, one a sink and the other a repellor, and removes the saddle point. However, saddle points mark the border between different

Figure 19.6

Saddle Points



types of dynamics and are useful and meaningful for the global analysis of the dynamics. We are now ready to consider the richer, but more complicated, higher dimensional cases.

Local and Global Behavior in Higher Dimensions

In two or more dimensions we start the local analysis at a fixed point

$$(y_1^0, y_2^0, \ldots, y_n^0) \quad \text{with} \quad \dot{y}_i = f_i(y_1^0, y_2^0, \ldots, y_n^0) = 0,$$

using the same Taylor expansion of the f_i in Eq. (19.23b) as for the one-dimensional case. Retaining only the first-order derivatives, this approach **linearizes the coupled NDEs** of Eq. (19.23b) and reduces their solution to linear algebra as follows. We abbreviate the constant derivatives at the fixed point as a matrix F with elements

$$f_{ij} \equiv \left.\frac{\partial f_i}{\partial y_j}\right|_{(y_1^0, y_2^0, \ldots, y_n^0)}. \tag{19.25}$$

In contrast to the standard linear algebra in Chapter 3, however, F is neither symmetric nor Hermitian in general. If we shift the fixed point to the origin and call the shifted coordinates $x_i = y_i - y_i^0$, then the coupled NDEs of

Eq. (19.23b) become

$$\dot{x}_i = f_{ij}x_j, \tag{19.26}$$

that is, coupled linear ODEs with constant coefficients. Here, a summation over the repeated index j is understood. This expansion is the linearized dynamics around one fixed point in the multidimensional space. We solve Eq. (19.26) with the standard exponential Ansatz (Sections 8.3 and 15.9)

$$x_i(t) = c_{ij}e^{\lambda_j t}, \tag{19.27}$$

with constant exponents λ_j and a constant matrix C of coefficients c_{ij} so that $\mathbf{c}_j = (c_{ij}, i = 1, 2, \ldots)$ forms the jth column vector of C. Substituting Eq. (19.27) into Eq. (19.26) yields a linear combination of exponential functions,

$$c_{ij}\lambda_j e^{\lambda_j t} = f_{ik}c_{kj}e^{\lambda_j t}, \tag{19.28}$$

which are independent if $\lambda_i \neq \lambda_j$. This is the general case on which we focus. Degeneracies in which two or more λ are equal require special treatment, as in the case of saddle points in one dimension. Comparing coefficients of exponential functions with the same exponent yields the linear eigenvalue equations

$$f_{ik}c_{kj} = \lambda_j c_{ij} \quad \text{or} \quad \mathsf{F}\mathbf{c}_j, = \lambda_j \mathbf{c}_j, \tag{19.29}$$

where the repeated index k on the left-hand side is summed, but j on the right-hand side is held fixed. A nontrivial solution comprising the eigenvalue λ_j and eigenvector $\mathbf{c}_j$ of the homogeneous linear equations (19.29) requires λ_j to be a root of the secular polynomial (compare with Section 3.5)

$$\det(\mathsf{F} - \lambda\, 1) = 0. \tag{19.30}$$

Equation (19.29) states that C diagonalizes F so that we can write Eq. (19.29) as

$$\mathsf{C}^{-1}\mathsf{F}\mathsf{C} = [\lambda_1, \lambda_2, \ldots], \tag{19.31}$$

a diagonal matrix with diagonal matrix elements λ_i in the notation of Chapter 3. In the new, but generally nonorthogonal, coordinates ξ_j defined as $\mathsf{C}\boldsymbol{\xi} = \mathbf{x}$ we have a **characteristic exponent** for each direction ξ_j, as $\dot{\xi}_j = \lambda_j \xi_j$, where the λ_j play the role of $f'(y_0)$ in the one-dimensional case. The λ are complex numbers in general. (There are no other directions in the solutions.) This is seen by substituting $\mathbf{x} = \mathsf{C}\boldsymbol{\xi}$ into Eq. (19.26) in conjunction with Eqs. (19.29) and (19.31). Thus, this solution represents the independent combination of one-dimensional fixed points, one for each component of $\boldsymbol{\xi}$ and each independent of the other components. In two dimensions for $\lambda_1 < 0$ and $\lambda_2 < 0$, we have a sink.

EXAMPLE 19.4.6

Stable Sink The coupled ODEs

$$\dot{x} = -x, \quad \dot{y} = -x - 3y$$

have an equilibrium point at the origin. The solutions have the form

$$x(t) = c_{11}e^{\lambda_1 t}, \quad y(t) = c_{21}e^{\lambda_1 t} + c_{22}e^{\lambda_2 t}$$

so that the eigenvalue $\lambda_1 = -1$ results from $\lambda_1 c_{11} = -c_{11}$, and the solution is $x = c_{11}e^{-t}$. The determinant of Eq. (19.30),

$$\begin{vmatrix} -1-\lambda & 0 \\ -1 & -3-\lambda \end{vmatrix} = (1+\lambda)(3+\lambda) = 0,$$

yields the eigenvalues $\lambda_1 = -1,\ \lambda_2 = -3$. Because both are negative, we have a stable sink at the origin. The ODE for y gives the linear relations

$$\lambda_1 c_{21} = -c_{11} - 3c_{21} = -c_{21}, \quad \lambda_2 c_{22} = -3c_{22},$$

from which we infer $2c_{21} = -c_{11}$ or $c_{21} = -c_{11}/2$. Because the general solution will contain two constants, it is given by

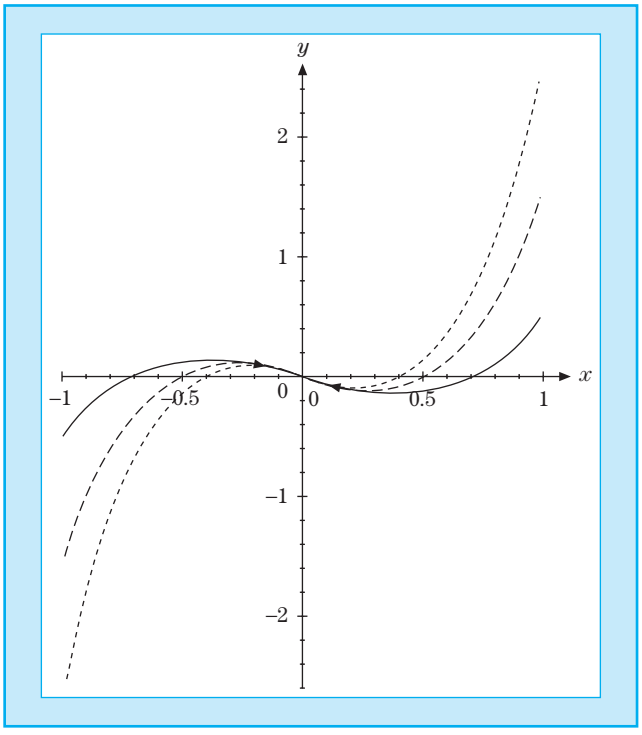
$$x(t) = c_{11}e^{-t}, \quad y(t) = -\frac{c_{11}}{2}e^{-t} + c_{22}e^{-3t}.$$

As the time $t \to \infty$, we have $y \sim -x/2$ and $x \to 0$ and $y \to 0$, whereas for $t \to -\infty$, $y \sim x^3$ and $x,\ y \to \pm\infty$. The motion toward the sink is indicated by arrows in Fig. 19.7. To find the orbit we eliminate the independent variable t and find the cubics

$$y = -\frac{x}{2} + \frac{c_{22}}{c_{11}^3}x^3. \quad \blacksquare$$

Figure 19.7

Stable Sink



When both λ are >0, we have repellor. In this case, the motion is away from the fixed point. However, when the λ have different signs we have a saddle point (i.e., a combination of a sink in one dimension and a repellor in the other).

EXAMPLE 19.4.7

Saddle Point The coupled ODEs

$$\dot{x} = -2x - y, \quad \dot{y} = -x + 2y$$

have a fixed point at the origin. The solutions have the form

$$x(t) = c_{11}e^{\lambda_1 t} + c_{12}e^{\lambda_2 t}, \quad y(t) = c_{21}e^{\lambda_1 t} + c_{22}e^{\lambda_2 t}.$$

The eigenvalues $\lambda = \pm\sqrt{5}$ are determined from

$$\begin{vmatrix} -2-\lambda & -1 \\ -1 & 2-\lambda \end{vmatrix} = \lambda^2 - 5 = 0.$$

Substituting the general solutions into the ODEs yields the linear equations

$$\lambda_1 c_{11} = -2c_{11} - c_{21} = \sqrt{5}c_{11}, \qquad \lambda_1 c_{21} = -c_{11} + 2c_{21} = \sqrt{5}c_{21},$$
$$\lambda_2 c_{12} = -2c_{12} - c_{22} = -\sqrt{5}c_{12}, \qquad \lambda_2 c_{22} = -c_{12} + 2c_{22} = -\sqrt{5}c_{22},$$

or

$$(\sqrt{5}+2)c_{11} = -c_{21}, \quad (\sqrt{5}-2)c_{12} = c_{22},$$
$$(\sqrt{5}-2)c_{21} = -c_{11}, \quad (\sqrt{5}+2)c_{22} = c_{12},$$

so that $c_{21} = -(2+\sqrt{5})c_{11}$, $c_{22} = (\sqrt{5}-2)c_{12}$. The family of solutions depends on two parameters c_{11}, c_{12}. For large time $t \to \infty$, the positive exponent prevails and $y \sim -(\sqrt{5}+2)x$, whereas for $t \to -\infty$ we have $y = (\sqrt{5}-2)x$. These straight lines are the asymptotes of the orbits. Because $-(\sqrt{5}+2)(\sqrt{5}-2) = -1$, they are orthogonal. We find the orbits by eliminating the independent variable t as follows. Substituting the c_{2j}, we write

$$y = -2x - \sqrt{5}\left(c_{11}e^{\sqrt{5}t} - c_{12}e^{-\sqrt{5}t}\right) \text{ so that } \frac{y+2x}{\sqrt{5}} = -c_{11}e^{\sqrt{5}t} + c_{12}e^{-\sqrt{5}t}.$$

Now we add and subtract the solution $x(t)$ to get

$$\frac{1}{\sqrt{5}}(y+2x) + x = 2c_{12}e^{-\sqrt{5}t}, \quad \frac{1}{\sqrt{5}}(y+2x) - x = -2c_{11}e^{\sqrt{5}t},$$

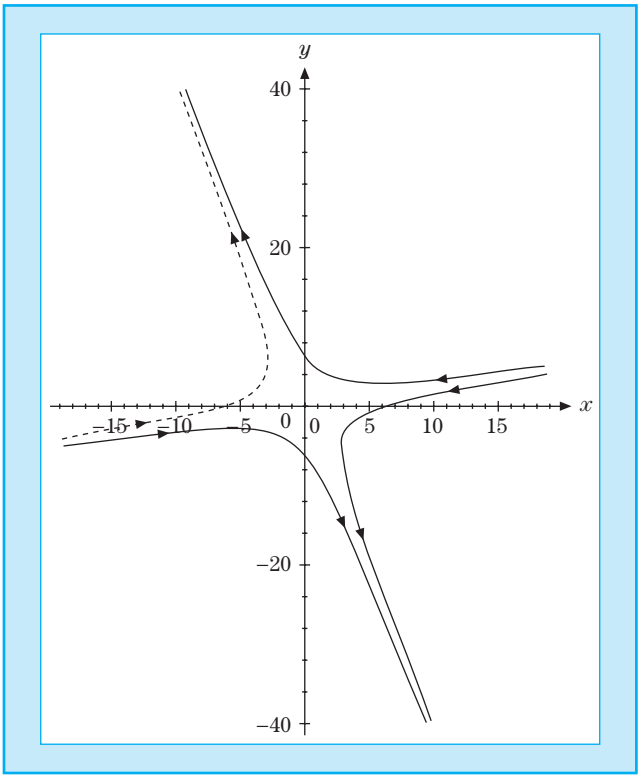
which we multiply to obtain

$$\frac{1}{5}(y+2x)^2 - x^2 = -4c_{12}c_{11} = \text{ const.}$$

The resulting quadratic form $y^2 + 4xy - x^2 = \text{const.}$ is a rotated hyperbola because of the negative sign and the mixed term. The hyperbola is rotated because its asymptotes are not aligned with the x, y-axes (Fig. 19.8).

Figure 19.8

Saddle Point



Its orientation is given by the direction of the asymptotes that we found earlier. Alternatively, we could find the direction of minimal distance from the origin proceeding as in Examples 1.5.3 and 1.5.4. That is, setting the x and y derivatives of $f + \Lambda g \equiv x^2 + y^2 + \Lambda(y^2 + 4xy - x^2)$ equal to zero, where Λ is the Lagrange multiplier for the hyperbolic constraint. The four branches of hyperbolas correspond to the different signs of the parameters c_{11} and c_{12}. Figure 19.8 is plotted for the cases $c_{11} = \pm 1,\ c_{12} = \pm 2$. ■

This type of behavior generalizes to higher dimensions.

However, a new kind of behavior arises for a pair of complex conjugate eigenvalues $\lambda_{1,2} = \rho \pm i\kappa$. If we write the complex solutions $\xi_{1,2} = \exp(\rho t \pm i\kappa t)$ in real variables $\xi_\pm = (\xi_1 \pm \xi_2)/2$ upon using the Euler identity $\exp(ix) = \cos x + i \sin x$ (see Sections 3.5 and 6.1),

$$\xi_+ = \exp(\rho t)\cos(\kappa t), \qquad \xi_- = \exp(\rho t)\sin(\kappa t) \tag{19.32}$$

describe a trajectory that spirals inward to the fixed point at the origin for $\rho < 0$, a **spiral sink**, and spirals away from the fixed point for $\rho > 0$, a **spiral repellor**.

EXAMPLE 19.4.8

Spiral Fixed Point The coupled ODEs

$$\dot{x} = -x + 3y, \quad \dot{y} = -3x + 2y$$

have a fixed point at the origin and solutions of the form

$$x(t) = c_{11}e^{\lambda_1 t} + c_{12}e^{\lambda_2 t}, \quad y(t) = c_{21}e^{\lambda_1 t} + c_{22}e^{\lambda_2 t}.$$

The exponents $\lambda_{1,2}$ are solutions of

$$\begin{vmatrix} -1-\lambda & 3 \\ -3 & 2-\lambda \end{vmatrix} = (1+\lambda)(\lambda-2) + 9 = 0,$$

or $\lambda^2 - \lambda + 7 = 0$. The eigenvalues are complex conjugate, $\lambda = 1/2 \pm i\sqrt{27}/2$, so that we deal with a spiral fixed point at the origin (a repellor because $1/2 > 0$). Substituting the general solutions into the ODEs yields the linear equations

$$\lambda_1 c_{11} = -c_{11} + 3c_{21}, \quad \lambda_1 c_{21} = -3c_{11} + 2c_{21},$$
$$\lambda_2 c_{12} = -c_{12} + 3c_{22}, \quad \lambda_2 c_{22} = -3c_{12} + 2c_{22},$$

or

$$(\lambda_1 + 1)c_{11} = 3c_{21}, \quad (\lambda_1 - 2)c_{21} = -3c_{11},$$
$$(\lambda_2 + 1)c_{12} = 3c_{22}, \quad (\lambda_2 - 2)c_{22} = -3c_{12},$$

which, using the values of $\lambda_{1,2}$, imply the family of curves

$$x(t) = e^{t/2}\left(c_{11}e^{i\sqrt{27}t/2} + c_{12}e^{-i\sqrt{27}t/2}\right),$$
$$y(t) = \frac{x}{2} + \frac{\sqrt{27}}{6}e^{t/2}i\left(c_{11}e^{i\sqrt{27}t/2} - c_{12}e^{-i\sqrt{27}t/2}\right)$$

that depend on two parameters c_{11}, c_{12}. To simplify, we can separate real and imaginary parts of $x(t)$ and $y(t)$ using the Euler identity $e^{ix} = \cos x + i \sin x$. It is equivalent, but more convenient, to choose $c_{11} = c_{12} = c/2$ and rescale $t \to 2t$ so that with the Euler identity we have

$$x(t) = ce^t \cos\left(\sqrt{27}t\right), \quad y(t) = \frac{x}{2} - \frac{\sqrt{27}}{6}ce^t \sin\left(\sqrt{27}t\right).$$

Here, we can eliminate t and find the orbit

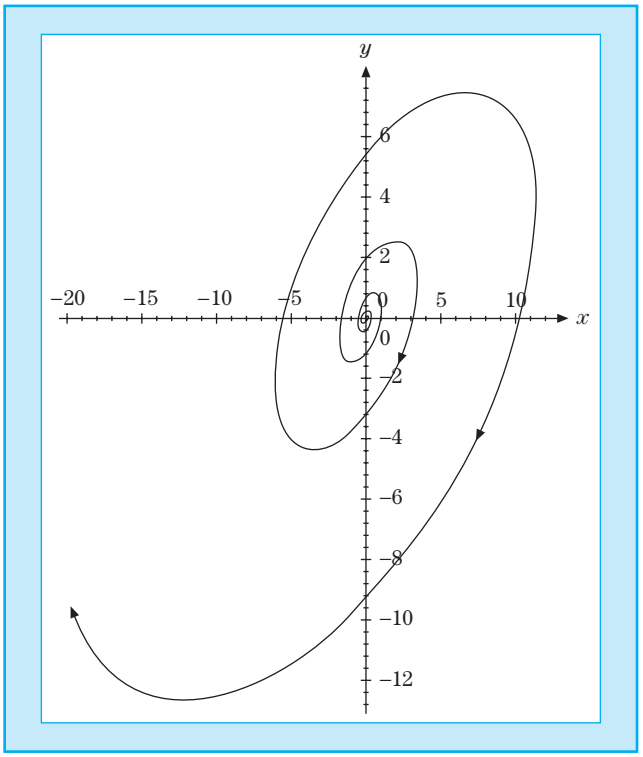
$$x^2 + \frac{4}{3}\left(y - \frac{x}{2}\right)^2 = (ce^t)^2.$$

For fixed t this is the positive definite quadratic form $x^2 - xy + y^2 = \text{const.}$ (i.e., an ellipse). However, there is no ellipse in the solutions because t is not fixed. Nonetheless, it is useful to find its orientation. We proceed as in Examples 1.5.3 and 1.5.4. With Λ the Lagrange multiplier for the elliptical constraint, we seek the directions of maximal and minimal distance from the origin, forming

$$f(x, y) + \Lambda g(x, y) \equiv x^2 + y^2 + \Lambda(x^2 - xy + y^2)$$

Figure 19.9

Spiral Point



and setting

$$\frac{\partial(f+\Lambda g)}{\partial x} = 2x + 2\Lambda x - \Lambda y = 0, \quad \frac{\partial(f+\Lambda g)}{\partial y} = 2y + 2\Lambda y - \Lambda x = 0.$$

From

$$2(\Lambda+1)x = \Lambda y, \quad 2(\Lambda+1)y = \Lambda x$$

we obtain the directions

$$\frac{x}{y} = \frac{\Lambda}{2(\Lambda+1)} = \frac{2(\Lambda+1)}{\Lambda},$$

or $\Lambda^2 + \frac{8}{3}\Lambda + \frac{4}{3} = 0$. This yields the values $\Lambda = -2/3,\ -2$ and the directions $y = \pm x$. In other words, our ellipse is centered at the origin and rotated by 45°. As we vary the independent variable t, the size of the ellipse changes so that we get the rotated spiral shown in Fig. 19.9 for $c = 1$. ■

In the special case in which $\rho = 0$, the circular trajectory is called a **cycle**.

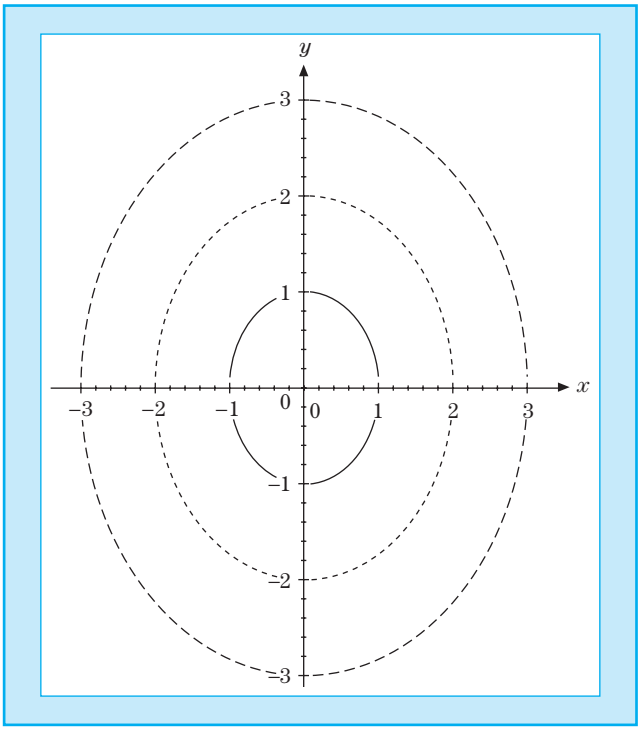
EXAMPLE 19.4.9

Center or Cycle The undamped linear harmonic oscillator ODE $\ddot{x} + \omega^2 x = 0$ can be written as two coupled ODEs:

$$\dot{x} = -\omega y, \quad \dot{y} = \omega x.$$

Figure 19.10

Center



Integrating the resulting ODE $\dot{x}x + \dot{y}y = 0$ yields the circular orbits $x^2 + y^2 = \text{const.}$, which define a center at the origin and are shown in Fig. 19.10. The solutions can be parameterized as $x = R\cos t$, $y = R\sin t$, where R is the radius parameter. They correspond to the complex conjugate eigenvalues $\lambda_{1,2} = \pm i\omega$. We can check them if we write the general solution as

$$x(t) = c_{11}e^{\lambda_1 t} + c_{12}e^{\lambda_2 t}, \quad y(t) = c_{21}e^{\lambda_1 t} + c_{22}e^{\lambda_2 t}.$$

Then the eigenvalues follow from

$$\begin{vmatrix} -\lambda & -\omega \\ \omega & -\lambda \end{vmatrix} = \lambda^2 + \omega^2 = 0. \quad \blacksquare$$

For the driven damped pendulum when trajectories near a center (closed orbit) are attracted to it as time goes on, this closed orbit is defined as a **limit cycle** representing periodic motion for autonomous systems. A damped pendulum usually spirals into the origin (the position at rest); that is, the origin is a spiral fixed point in its phase space. When we turn on a driving force, the system formally becomes nonautonomous because of its explicit time dependence but also more interesting. In this case, we can call the explicit time in a sinusoidal driving force a new variable φ, where ω_0 is a fixed rate, in the equation of motion

$$\dot{\omega} + \gamma\omega + \sin\theta = f\sin\varphi, \quad \omega = \dot{\theta}, \quad \varphi = \omega_0 t.$$

Then we increase the dimension of our phase space by one (adding one variable φ) because $\dot{\varphi} = \omega_0 = \text{const.}$, but we keep the coupled ODEs autonomous. This driven damped pendulum has trajectories that cross a closed orbit in phase space and spiral back to it: It is called a limit cycle. This happens for a range of strength f of the driving force, the control parameter of the system. As we increase f, the phase space trajectories go through several neighboring limit cycles and eventually become aperiodic and chaotic. Such closed limit cycles are called Hopf bifurcations of the pendulum on its road to chaos after the mathematician E. Hopf, who generalized Poincaré's results on such bifurcations to higher dimensions of phase space.

Another classic attractor is quasiperiodic motion, such as the trajectory

$$x(t) = A_1 \sin(\omega_1 t + b_1) + A_2 \sin(\omega_2 t + b_2), \tag{19.33}$$

where the ratio ω_1/ω_2 is an irrational number. In the phase plane $(x,\ y = \dot{x})$ the orbit forms a closed figure. Such combined oscillations in Eq. (19.33) occur as solutions of a damped anharmonic oscillator (Van der Pol nonautonomous system)

$$\ddot{x} + 2\gamma\dot{x} + \omega_2^2 x + \beta x^3 = f\cos(\omega_1 t). \tag{19.34}$$

The importance of the ratio of frequencies being rational is illustrated with the closed curve $(x = \sin t,\ y = \cos(3t))$ in Fig. 19.11, whereas for the irrational ratio in Fig. 19.12 the curve $(x = \sin t,\ y = \cos(\sqrt{2}t))$ stays open, no matter how large the time t grows.

Figure 19.11

The Curve $(x = \sin t, \cos(3t))$ Is Closed

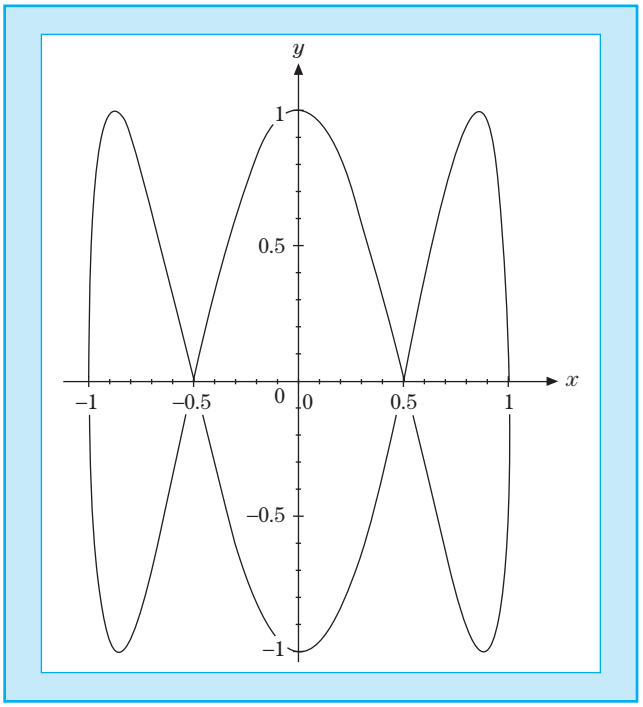
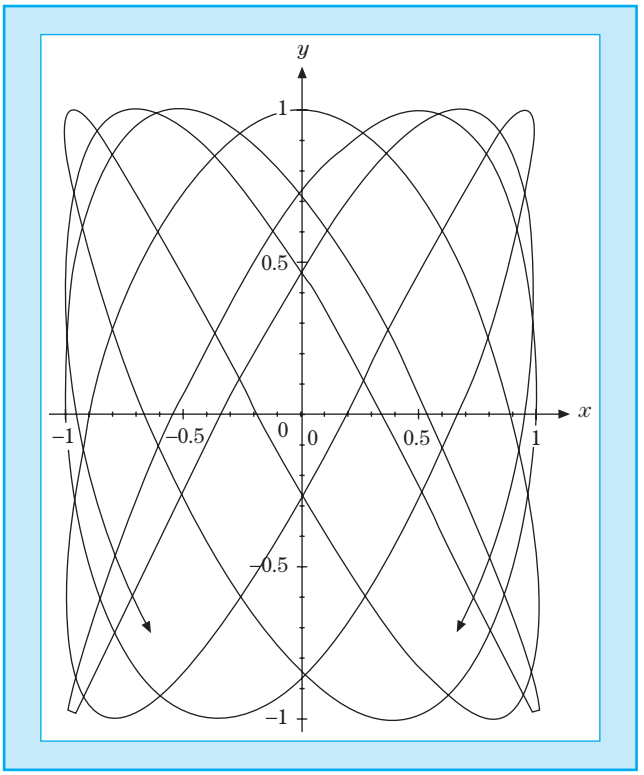


Figure 19.12

The Curve $(x = \sin t, \cos(\sqrt{2}t))$ Is Not Closed



In three dimensions, when there is a positive characteristic exponent and an attracting complex conjugate pair in the other directions, we have a **spiral saddle point** as a new feature. Conversely, a negative characteristic exponent in conjunction with a repelling pair also gives rise to a spiral saddle point, where trajectories spiral out in two dimensions but are attracted in a third direction. This is illustrated in Example 19.4.10 and shown in Fig. 19.13.

EXAMPLE 19.4.10 **Repelling Spiral Saddle Point** The coupled ODEs

$$\dot{x} = y, \quad \dot{y} = z, \quad \dot{z} = -x$$

have the general solutions

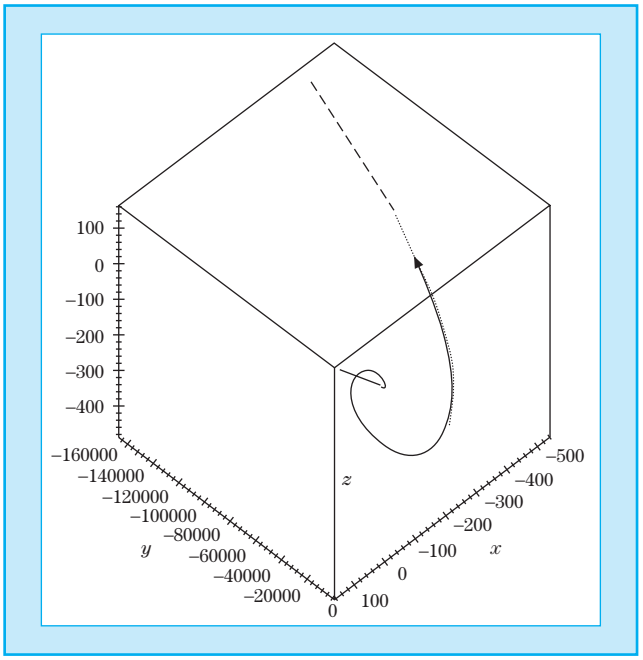
$$x = \sum_j c_{1j} e^{\lambda_j t}, \quad y = \sum_j c_{2j} e^{\lambda_j t}, \quad z = \sum_j c_{3j} e^{\lambda_j t}.$$

Substituting them into the ODEs yields the linear relations

$$\lambda_j c_{1j} = c_{2j}, \quad \lambda_j c_{2j} = c_{3j}, \quad \lambda_j c_{3j} = -c_{1j}$$

Figure 19.13

Repelling Spiral Saddle Point



and the eigenvalue condition

$$\begin{vmatrix} -\lambda & 1 & 0 \\ 0 & -\lambda & 1 \\ -1 & 0 & -\lambda \end{vmatrix} = -\lambda^3 - 1 = 0.$$

The exponents of the solution are given by the eigenvalues

$$\lambda_1 = -1, \quad \lambda_{2,3} = e^{\pm \pi i/3} = \frac{1}{2} \pm i\frac{\sqrt{3}}{2},$$

which correspond to a spiral repellor for positive time. The linear relations imply

$$c_{21} = \lambda_1 c_{11} = -c_{11}, \quad c_{22} = \lambda_2 c_{12}, \quad c_{23} = \lambda_3 c_{13},$$

$$c_{31} = \lambda_1 c_{21} = -c_{21} = c_{11}, \quad \lambda_1 c_{31} = -c_{11} = -c_{31},$$

$$\lambda_2 c_{32} = -c_{12}, \quad \lambda_3 c_{33} = -c_{13}.$$

Therefore, the solutions

$$x(t) = c_{11}e^{-t} + c_{12}e^{(1/2+i\sqrt{3}/2)t} + c_{13}e^{(1/2-i\sqrt{3}/2)t},$$

$$y(t) = -c_{11}e^{-t} + c_{12}\left(\frac{1}{2} + i\frac{\sqrt{3}}{2}\right)e^{(1/2+i\sqrt{3}/2)t} + c_{13}\left(\frac{1}{2} + i\frac{\sqrt{3}}{2}\right)e^{(1/2-i\sqrt{3}/2)t}$$

$$z(t) = c_{11}e^{-t} - \frac{c_{12}}{\frac{1}{2} + i\frac{\sqrt{3}}{2}}e^{(1/2+i\sqrt{3}/2)t} - \frac{c_{13}}{\frac{1}{2} - i\frac{\sqrt{3}}{2}}e^{(1/2-i\sqrt{3}/2)t}$$

depend on three parameters $c_{11},\ c_{12},\ c_{13}$. To simplify them, we use the Euler identity and keep the real part only. This yields the solution

$$x = c_{11}e^{-t} + (c_{12} + c_{13})e^{t/2}\cos\left(\frac{1}{2}\sqrt{3}t\right),$$

$$y = -c_{11}e^{-t} + \frac{1}{2}(c_{12} + c_{13})e^{t/2}\cos\left(\frac{1}{2}\sqrt{3}t\right) + \frac{\sqrt{3}}{2}(c_{12} - c_{13})e^{t/2}\sin\left(\frac{1}{2}\sqrt{3}t\right),$$

$$z = c_{11}e^{-t} + (c_{12} + c_{13})e^{t/2}\cos\left(\frac{1}{2}\sqrt{3}t\right) - \frac{\sqrt{3}}{2}(c_{12} - c_{13})e^{t/2}\sin\left(\frac{1}{2}\sqrt{3}t\right),$$

which is plotted in Fig. 19.13 for $c_{11} = 1,\ c_{12} + c_{13} = 1,\ c_{12} - c_{13} = 1$. For $t \to -\infty$, only the e^{-t} terms survive so that $y \sim -x,\ z \sim x$ is the straight line section in Fig. 19.13 ending near the origin. For $t \to \infty$, only the terms involving $e^{t/2}$ survive so that $(y - x/2)/(z - x) \sim -1$, which is the plane $z = y - 3x/2$. Between these asymptotic limits we recognize the spiral behavior that changes with the parameters c_{1j} of the curves. The asymptotes do not depend on the parameters. ■

Of course, such spiral sinks or saddle points cannot occur in one dimension, but we might ask if they are stable when they occur in higher dimensions. An answer is given by the Poincaré–Bendixson theorem, which states that either trajectories (in the finite region to be specified in a moment) are attracted to a fixed point as time goes on or they approach a limit cycle provided the relevant two-dimensional subsystem stays inside a finite region (i.e., does not diverge there as $t \to \infty$). For a proof, we refer to Hirsch and Smale and Jackson in Additional Reading.

In general, when some form of damping is present the transients decay and the system settles either in equilibrium (i.e., a single point) or in periodic or quasiperiodic motion. Chaotic motion is now recognized as a fourth state, and its attractors are often called strange.

Dissipation in Dynamical Systems

Dissipative forces, in two dimensions for simplicity, entail changes of area in phase space. An example is the parachutist in Example 8.2.2, where $v \to v_0$ with increasing time, while $\dot{v} \to 0$. The area in phase space spanned by $v, \dot{v}$ shrinks to zero due to drag. As particles on such trajectories carry energy, changing areas involve loss or gain of energy; they often involve velocities—that is first-order time derivatives such as friction (e.g., for the damped oscillator). Let us look for a measure of dissipation; that is, how a small area $A = c_{1,2}\Delta\xi_1\Delta\xi_2$ at a fixed point shrinks or expands. Here, $c_{1,2} = \sin(\hat{\xi}_1, \hat{\xi}_2)$ is a time-independent angular factor that takes into account the nonorthogonality of the characteristic directions $\hat{\xi}_1$ and $\hat{\xi}_2$ of Eq. (19.29). If we take the time derivative of A and use $\dot{\xi}_j = \lambda_j\xi_j$ of the characteristic coordinates, implying

$\dot{\Delta\xi}_j = \lambda_j \Delta\xi_j$, we obtain, to lowest order in the $\Delta\xi_j$,

$$\dot{A} = c_{1,2}[\Delta\xi_1\lambda_2\Delta\xi_2 + \Delta\xi_2\lambda_1\Delta\xi_1] = c_{1,2}\Delta\xi_1\Delta\xi_2(\lambda_1 + \lambda_2). \tag{19.35}$$

In the limit $\Delta\xi_j \to 0$, we find from Eq. (19.35) that the rate

$$\frac{\dot{A}}{A} = \lambda_1 + \lambda_2 = \text{tr}(\mathsf{F}) = \boldsymbol{\nabla} \cdot \mathbf{f}|_{\mathbf{y}_0} \tag{19.36}$$

with $\mathbf{f} = (f_1, f_2)$ the vector of time derivatives in Eq. (19.23b) at the fixed point. Note that the time-independent sine of the angle between ξ_1 and ξ_2 drops out of the rate. The generalization to higher dimensions is obvious. Moreover, in n dimensions,

$$\text{trace}(\mathsf{F}) = \sum_i \lambda_i. \tag{19.37}$$

Although F is not hermitian, this trace formula follows from the invariance of the secular polynomial in Eq. (19.30) under a linear transformation, $\mathsf{C}\boldsymbol{\xi} = \mathbf{x}$ in particular, and it is a result of its determinental form using the product theorem for determinants (see Section 3.2), viz.,

$$\det(\mathsf{F} - \lambda \cdot 1) = [\det(\mathsf{C})]^{-1} \det(\mathsf{F} - \lambda \cdot 1)[\det(\mathsf{C})] = \det(\mathsf{C}^{-1}(\mathsf{F} - \lambda \cdot 1)\mathsf{C})$$

$$= \det(\mathsf{C}^{-1}\mathsf{F}\mathsf{C} - \lambda \cdot 1) = \prod_{i=1}^{n}(\lambda_i - \lambda). \tag{19.38}$$

Here, the product form derives by substituting Eq. (19.31). Now tr(F) is the coefficient of $(-\lambda)^{n-1}$ upon expanding $\det(\mathsf{F} - \lambda \cdot 1)$ in powers of λ, whereas it is $\sum_i \lambda_i$ from the product form $\prod_i(\lambda_i - \lambda)$, which proves Eq. (19.37). Clearly, according to Eqs. (19.36) and (19.37),

- it is the sign (more precisely the trace) of the characteristic exponents of the derivative matrix at the fixed point that determines whether there is expansion or shrinkage of areas and volumes in higher dimensions near a critical point.

SUMMARY

Equation (19.36) clearly states that dissipation requires $\boldsymbol{\nabla} \cdot \mathbf{f}(\mathbf{y}) \neq 0$, where $\dot{y}_j = f_j$ and does not occur in Hamiltonian systems where $\boldsymbol{\nabla} \cdot \mathbf{f} = 0$.

Moreover, in two or more dimensions, there are the following global possibilities:

- The trajectory may describe a closed orbit (center or cycle).
- The trajectory may approach a closed orbit (spiraling inward or outward toward the orbit) as $t \to \infty$. In this case, we have a limit cycle.

The local behavior of a trajectory near a critical point is also more varied in general than in one dimension: At a stable critical point all trajectories may approach the critical point along straight lines, curve in as in Example 19.4.6

with $trace(\lambda) = -4$, spiral inward (toward the **spiral sink**), or may follow a more complicated path. If all time-reversed trajectories move toward the critical point in spirals as $t \to -\infty$, then the critical point is a divergent spiral point or **spiral repellor**. This is the case in Example 19.4.8 with $trace(\lambda) = 1$. When some trajectories approach the critical point while others move away from it, as in Example 19.4.7 with $trace(\lambda) = 0$ (in general, the trace can be positive or negative at a saddle point), then it is called a **saddle point**. When all trajectories form closed orbits about the critical point, it is called a **center**, as in Example 19.4.9, where $trace(\lambda) = 0$.

Bifurcations in Dynamical Systems

As in one dimension, such as bifurcations of the logistic map, a bifurcation in two or more dimensions is a sudden change in dynamics for specific parameter values, such as the birth of a sink–repellor pair of fixed points or their disappearance upon adjusting a control parameter (i.e., the motions before and after the bifurcation are topologically different). At a bifurcation point, not only are solutions unstable when one or more parameters are changed slightly but also the character of the bifurcation in phase space or in the parameter manifold may change. Sudden changes from regular to random behavior of trajectories are characteristic of bifurcations, as is sensitive dependence on initial conditions: Nearby initial conditions can lead to very different long-term behavior. If a bifurcation does not change qualitatively with parameter adjustments, it is called structurally stable. Note that structurally unstable bifurcations are unlikely to occur in reality because noise and other neglected degrees of freedom act as perturbations on the system that effectively eliminate unstable bifurcations from our view. Bifurcations (such as period doublings in maps) are important as one among many routes to chaos. Others are sudden changes in trajectories associated with several critical points called **global bifurcations**. Often, they involve changes in basins of attraction and/or other global structures. The theory of global bifurcations is fairly complicated and still in its infancy.

Bifurcations that are linked to sudden changes in the qualitative behavior of dynamical systems at a single fixed point are called **local bifurcations**. Specifically, a change in stability occurs in parameter space where the real part of a characteristic exponent of the fixed point alters its sign (i.e., moves from attracting to repelling trajectories or vice versa). The **center manifold theorem** states that at a local bifurcation only those degrees of freedom matter that are involved with characteristic exponents going to zero: $\Re(\lambda_i) = 0$. Locating the set of these points is the first step in a bifurcation analysis. Another step consists in cataloguing the types of bifurcations in dynamical systems, to which we turn next.

The conventional **normal forms** of dynamical equations represent a start in classifying bifurcations. For systems with one parameter (i.e., a one dimensional center manifold), we write the general case of NDE as follows:

$$\dot{x} = \sum_{j=0}^{\infty} a_j^{(0)} x^j + c \sum_{j=0}^{\infty} a_j^{(1)} x^j + c^2 \sum_{j=0}^{\infty} a_j^{(2)} x^j + \cdots, \tag{19.39}$$

where the superscript on $a^{(m)}$ denotes the power of the parameter c with which bifurcations are associated. One-dimensional iterated nonlinear maps such as the logistic map of Section 19.2 (that occur in Poincaré sections) of nonlinear dynamical systems can be classified similarly, viz.,

$$x_{n+1} = \sum_{j=0}^{\infty} a_j^{(0)} x_n^j + c \sum_{j=0}^{\infty} a_j^{(1)} x_n^j + c^2 \sum_{j=0}^{\infty} a_j^{(2)} x_n^j + \cdots. \tag{19.40}$$

The logistic map corresponds to $c = \mu$, $a_1^{(1)} = 1, a_2^{(1)} = -1$, with all other $a_j^{(i)} = 0$. One of the simplest NDEs with a bifurcation is

$$\dot{x} = x^2 - c, \tag{19.41}$$

which corresponds to all $a_j^{(m)} = 0$ except for $a_0^{(1)} = -1$ and $a_2^{(0)} = 1$. For $c > 0$, there are two fixed points (recall $\dot{x} = 0$) $x_\pm = \pm\sqrt{c}$ with characteristic exponents $2x_\pm$ so that x_- is a sink and x_+ is a repellor. For $c < 0$, there are no fixed points. Therefore, as $c \to 0$ the fixed point pair disappears suddenly (i.e., the parameter value $c = 0$ is a repellor–sink bifurcation that is structurally unstable). This complex map (with $c \to -c$) generates the fractal Julia and Mandelbrot sets discussed in Section 19.3.

A pitchfork bifurcation (as in Fig. 19.2 at $\mu = 3$) occurs for the undamped (nondissipative and special case of the Duffing) oscillator with a cubic anharmonicity

$$\ddot{x} + ax + bx^3 = 0, \quad b > 0. \tag{19.42}$$

It has a continuous frequency spectrum and is, among others, a model for a ball bouncing between two walls. When the control parameter $a > 0$, there is only one fixed point at $x = 0$, a sink, whereas for $a < 0$ there are two more sinks at $x_\pm = \pm\sqrt{-a/b}$. Thus, we have a pitchfork bifurcation of a sink at the origin into a saddle point at the origin and two sinks at $x_\pm \neq 0$. In terms of a potential formulation, $V(x) = ax^2/2 + bx^4/4$ is a **single well** for $a > 0$ but a **double well** (with a maximum at $x = 0$) for $a < 0$.

When a pair of complex conjugate characteristic exponents $\rho \pm i\kappa$ crosses from a spiral sink ($\rho < 0$) to a repelling spiral ($\rho > 0$) and periodic motion (limit cycle) emerges, we call the qualitative change a Hopf bifurcation. They occur in the quasiperiodic route to chaos that will be discussed in the next section.

In a global analysis, we piece together the motions near various critical points, such as sinks and bifurcations, to bundles of trajectories that flow more or less together in two dimensions. (This geometric view is the current mode of analyzing solutions of dynamical systems.) However, this flow is no longer collective in the case of three dimensions, where they diverge from each other in general, because chaotic motion is possible that typically fills the plane of a Poincaré section with points.

Chaos in Dynamical Systems

Our previous summaries of intricate and complicated features of dynamical systems due to nonlinearities in **one and two dimensions do not include chaos**, although some of them, such as bifurcations, are sometimes precursors to chaos. This is why Verhulst's NDE shows no chaos, whereas the corresponding (logistic) map does. In three- or more dimensional NDEs chaotic motion may occur (but does not always), often when a constant of the motion (e.g., an energy integral for NDEs defined by a Hamiltonian) restricts the trajectories to a finite volume in phase space and when there are no critical points. Another characteristic signal for chaos is when for each trajectory there are nearby ones, some of which move away from it and others approach it with increasing time. The notion of exponential divergence of nearby trajectories is made quantitative by the Lyapunov exponent λ (Section 19.3) of iterated maps of Poincaré sections (Section 19.4) associated with the dynamical system. If two nearby trajectories are at a distance d_0 at time $t = 0$ but diverge with a distance $d(t)$ at a later time t, then $d(t) \approx d_0 e^{\lambda t}$ holds. Thus, by analyzing the series of points (i.e., iterated maps generated on Poincaré sections), one can study routes to chaos of three-dimensional dynamic systems. This is the key method for studying chaos. As one varies the location and orientation of the Poincaré plane, a fixed point on it is often recognized to originate from a limit cycle in the three-dimensional phase space whose structural stability can be checked there. For example, attracting limit cycles show up as sinks in Poincaré sections, repelling limit cycles as repellors of Poincaré maps, and saddle cycles as saddle points of associated Poincaré maps.

Three or more dimensions of phase space are required for chaos to occur because of the interplay of the necessary conditions just discussed, viz.,

- bounded trajectories (often the case for Hamiltonian systems);
- exponential divergence of nearby trajectories (guaranteed by positive Lyapunov exponents of corresponding Poincaré maps); and
- no intersection of trajectories.

The last condition is obeyed by deterministic systems in particular, as discussed in Section 19.1. A surprising feature of chaos mentioned in Section 19.1 is how prevalent it is and how universal the routes to chaos often are despite the variety of NDEs.

An example of spatially complex patterns in classical mechanics is the planar pendulum whose one-dimensional equation of motion

$$I\frac{d\theta}{dt} = L, \qquad \frac{dL}{dt} = -lmg\sin\theta \tag{19.43}$$

is nonlinear in the dynamic variable $\theta(t)$. Here, I is the moment of inertia, L is the orbital angular momentum, l is the distance to the center of mass, m is the mass, and g is the gravitational acceleration constant. When all parameters in Eq. (19.43) are constant in time and space, the solutions are given in terms of elliptic integrals (see Section 5.8) and no chaos exists. However, a pendulum

under a periodic external force can exhibit chaotic dynamics, for example, for the Lagrangian

$$\mathcal{L} = \frac{m}{2}\dot{\mathbf{r}}^2 - m\frac{g}{l}(l - z), \quad (x - x_0)^2 + y^2 + z^2 = l^2, \tag{19.44}$$
$$x_0 = \varepsilon l \cos \omega t,$$

where x_0 represents the periodic driving force (see Moon in Additional Reading).

Good candidates for chaos are multiple well potential problems

$$\frac{d^2\mathbf{r}}{dt^2} + \nabla V(\mathbf{r}) = F\left(\mathbf{r}, \frac{d\mathbf{r}}{dt}, t\right), \tag{19.45}$$

where F represents dissipative and/or driving forces. Another classic example is rigid body rotation whose nonlinear three-dimensional Euler equations are familiar, viz.,

$$\begin{aligned}
\frac{d}{dt}I_1\omega_1 &= (I_2 - I_3)\omega_2\omega_3 + M_1, \\
\frac{d}{dt}I_2\omega_2 &= (I_3 - I_1)\omega_1\omega_3 + M_2, \\
\frac{d}{dt}I_3\omega_3 &= (I_1 - I_2)\omega_1\omega_2 + M_3,
\end{aligned} \tag{19.46}$$

where (M_1, M_2, M_3) is the torque, I_j are the principal moments of inertia, and ω is the angular velocity with components ω_j about the body-fixed principal axes. Even free rigid body rotation can be chaotic because its nonlinear couplings and three-dimensional form satisfy all requirements for chaos to occur (Section 19.1). A rigid body example of chaos in our solar system is the chaotic tumbling of Hyperion, one of Saturn's moons that is highly nonspherical. It is a world in which the Saturn rise and set is so irregular as to be unpredictable. Another is Halley's comet, whose orbit is perturbed by Jupiter and Saturn. In general, when three or more celestial bodies interact gravitationally, chaotic dynamics is possible. Note, though, that computer simulations over large time intervals are required to ascertain chaotic dynamics in the solar system. For more details on chaos in such conservative Hamiltonian systems, see Chapter 8 of Hilborn in Additional Reading.

Routes to Chaos in Dynamical Systems

Let us now examine some routes to chaos. The period-doubling route to chaos is exemplified by the logistic map in Section 19.2, and the universal Feigenbaum numbers α, δ are its quantitative features along with Lyapunov exponents. It is common in dynamical systems. It may begin with limit cycle (periodic) motion, which shows up as a set of fixed points in a Poincaré section. The limit cycle may have originated in a bifurcation from a sink or some other fixed point. As a control parameter changes, the fixed point of the Poincaré

map splits into two points (i.e., the limit cycle has a characteristic exponent going through zero from attracting to repelling). The periodic motion now has a period twice as long as before, etc. We refer to Chapter 11 of Barger and Olsson in Additional Reading for period-doubling plots of Poincaré sections for the Duffing equation [Eq. (19.42)] with a periodic external force. Another example of period doubling is a forced oscillator with friction (see Helleman in Cvitanovic in Additional Reading).

The quasiperiodic route to chaos is also quite common in dynamical systems (e.g., starting from a time-independent sink, a fixed point). If we adjust a control parameter the system undergoes a Hopf bifurcation to the periodic motion corresponding to a limit cycle in phase space. With further change of the control parameter, a second frequency appears. If the frequency ratio is an irrational number, the trajectories are quasiperiodic, eventually covering the surface of a torus in phase space (i.e., quasiperiodic orbits never close or repeat). Further changes of the control parameter may lead to a third frequency or directly to chaotic motion. Bands of chaotic motion can alternate with quasiperiodic motion in parameter space. An example of such a dynamic system is a periodically driven pendulum.

A third route to chaos is via intermittency, where the dynamical system switches between two qualitatively different motions at fixed control parameters. For example, at the beginning periodic motion alternates with an occasional burst of chaotic motion. With a change of the control parameter, the chaotic bursts typically lengthen until, eventually, no periodic motion remains. The chaotic parts are irregular and do not resemble each other, but one needs to check for a positive Lyapunov exponent to demonstrate chaos. Intermittencies of various types are common features of turbulent states in fluid dynamics. The Lorenz coupled NDEs also show intermittency.

EXERCISES

19.4.1 For the damped harmonic oscillator

$$\ddot{x} + 2a\dot{x} + x = 0,$$

consider the Poincaré section $\{x > 0,\ y = \dot{x} = 0\}$. Take $0 < a \ll 1$ and show that the map is given by $x_{n+1} = bx_n$ with $b < 1$. Find an estimate for b.

19.4.2 Show that the (Rössler) coupled ODEs

$$\dot{x}_1 = -x_2 - x_3, \quad \dot{x}_2 = x_1 + a_1 x_2, \quad \dot{x}_3 = a_2 + (x_1 - a_3)x_3$$

(a) have two fixed points for $a_2 = 2,\ a_3 = 4$, and $0 < a_1 < 2$,
(b) have a spiral repellor at the origin, and
(c) have a spiral chaotic attractor for $a_1 = 0.398$.

19.4.3 Construct a Poincaré map for the Duffing oscillator in Eq. (19.42).

19.4.4 Guess a particular solution of the Riccati NDE $y' = A - ABx^2y + Bxy^2$, where A, B are constants. Then reduce the NDE to a Bernoulli NDE and solve that also.

$$\textit{ANS.} \quad y(x) = Ax + \tfrac{1}{v}, \; v(x) = C(x)e^{-AB(x^2 - x^3/3)},$$
$$C(x) = B\int^x xe^{AB(x^2 - x^3/3)}dx.$$

19.4.5 Plot the intermittency region of the logistic map at $\mu = 3.8319$. What is the period of the cycles? What happens at $\mu = 1 + 2\sqrt{2}$?

ANS. There is a (so-called) tangent bifurcation to period 3 cycles.

Additional Reading

Amann, H. (1990). *Ordinary Differential Equations: An Introduction to Nonlinear Analysis*. de Gruyter, New York.

Baker, G. L., and Gollub, J. P. (1996). *Chaotic Dynamics: An Introduction*, 2nd ed. Cambridge Univ. Press, Cambridge, UK.

Barger, V. D., and Olsson, M. G. (1995). *Classical Mechanics*, 2nd ed. McGraw-Hill, New York.

Bender, C. M., and Orszag, S. A. (1978). *Advanced Mathematical Methods for Scientists and Engineers*. McGraw-Hill, New York. See Chapter 4 in particular.

Bergé, P., Pomeau, Y., and Vidal, C. (1987). *Order within Chaos*. Wiley, New York.

Cvitanovic, P. (Ed.) (1989). *Universality in Chaos*, 2nd ed. Hilger, Bristol, PA.

Devaney, R. L. (1989). *An Introduction to Chaotic Dynamical Systems*. Benjamin/Cummings, Menlo Park, CA.

Earnshaw, J. C., and Haughey, D. (1993). Lyapunov exponents for pedestrians. *Am. J. Phys.* **61**, 401.

Gleick, J. (1987). *Chaos*. Penguin, New York.

Hilborn, R. C. (1994). *Chaos and Nonlinear Dynamics*. Oxford Univ. Press, New York.

Hirsch, M. W., and Smale, S. (1974). *Differential Equations, Dynamical Systems, and Linear Algebra*. Academic Press, New York.

Infeld, E., and Rowlands, G. (1990). *Nonlinear Waves, Solitons and Chaos*. Cambridge Univ. Press, Cambridge, UK.

Jackson, E. A. (1989). *Perspectives of Nonlinear Dynamics*. Cambridge Univ. Press, Cambridge, UK.

Jordan, D. W., and Smith, P. (1987). *Nonlinear Ordinary Differential Equations*, 2nd ed. Oxford Univ. Press, Oxford, UK.

Lyapunov, A. M. (1992). *The General Problem of the Stability of Motion*. Taylor & Francis, Bristol, PA.

Mandelbrot, B. B. (1988). *The Fractal Geometry of Nature* [Reprint]. Freeman, San Francisco.

Moon, F. C. (1992). *Chaotic and Fractal Dynamics*. Wiley, New York.

Peitgen, H.-O., and Richter, P. H. (1986). *The Beauty of Fractals*. Springer, New York.

Sachdev, P. L. (1991). *Nonlinear Differential Equations and Their Applications*. Dekker, New York.

Tufillaro, N. B., Abbott, T., and Reilly, J. (1992). *An Experimental Approach to Nonlinear Dynamics and Chaos*. Addison-Wesley, Redwood City, CA.

Appendix 1

Real Zeros of a Function

The demand for the values of the real zeros of a function occurs frequently in mathematical physics. Examples include the boundary conditions on the solution of a coaxial waveguide problem (Example 11.5.1); eigenvalue problems in quantum mechanics such as the deuteron with a square well potential (Example 9.1.2), that is, solutions of transcental equations from matching conditions in quantum mechanics; and the location of the evaluation points in Gaussian quadrature.

Most numerical methods require close initial guesses of the zero or root. How close depends on how wildly your function is varying and what accuracy you demand. All are methods for refining a good initial value. To obtain the good initial value and to locate pathological features that must be avoided (such as discontinuities or singularities), you should make a reasonably detailed graph of the function. There is no real substitute for a graph. Exercise 11.3.11 emphasizes this point.

Newton's method is often presented in differential calculus because it assumes the function $f(x)$ to have a continuous first derivative and requires its computation. If no pathologies occur, it converges rapidly. However, it is a method to **avoid** because it is treacherous: It may fail to converge or may converge to the wrong root. When iterated, it may lead to chaos for suitable initial guesses. We therefore do not discuss it in detail and refer to Chapter 9 of Press *et al.* in Additional Reading.

Bisection Method

This method assumes only that $f(x)$ is **continuous**. It requires that initial values x_l and x_r straddle the zero being sought. Thus, $f(x_l)$ and $f(x_r)$ will have opposite signs, making the product $f(x_l) \cdot f(x_r)$ negative. In the simplest form of the bisection method, take the midpoint $x_m = \frac{1}{2}(x_l + x_r)$ and test to see which interval $[x_l, x_m]$ or $[x_m, x_r]$ contains the zero. The easiest test is to see if one product, for example, $f(x_m) \cdot f(x_r) < 0$. If this product is negative, then the root is in the upper half interval $[x_m, x_r]$; if it is positive, then the root must be in the lower half interval $[x_l, x_m]$. Remember, we are assuming $f(x)$ to be continuous. The interval containing the zero is relabeled $[x_l, x_r]$ and the bisecting continues (as in Fig. A.1) until the root is located to the desired

Figure A.1

Bisection Root-Finding Method

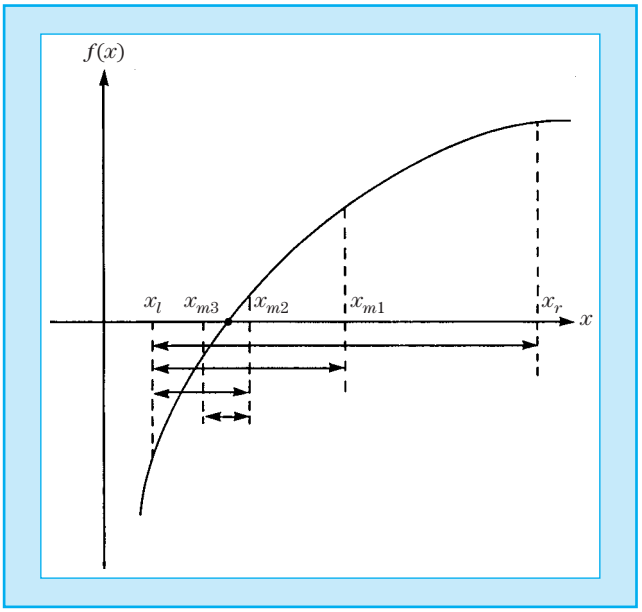
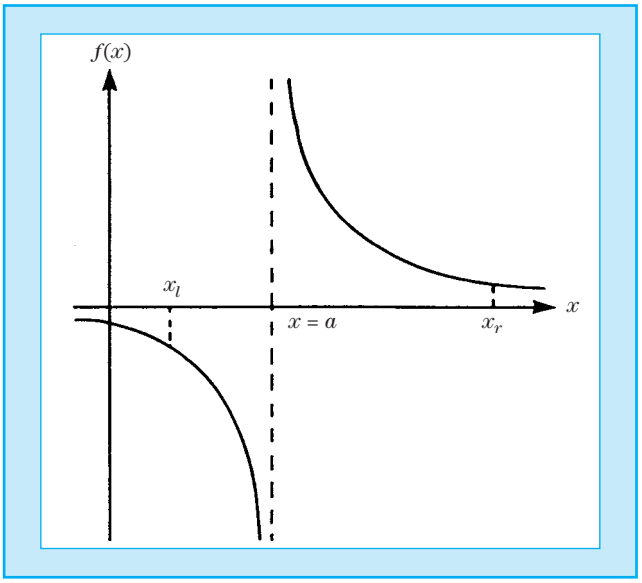


Figure A.2

A Simple Pole, $f(x_l) \cdot f(x_r) < 0$ But No Root



degree of accuracy. Of course, the better the initial choice of x_l and x_r, the fewer bisections required. However, as explained subsequently, it is important to specify the maximum number of bisections that will be permitted.

This bisection technique may not have the elegance of Newton's method, but it is reasonably fast and much more reliable—almost foolproof if you avoid discontinuous functions, such as $f(x) = 1/(x - a)$, shown in Fig. A.2. Again,

there is no substitute for knowing the detailed local behavior of your function in the vicinity of your supposed root.

In general, the bisection method is **recommended**.

Three Warnings

1. Always plot your function before performing any root finding. Compare the results from your root finding to your graph.
2. Since the computer carries only a finite number of significant figures we cannot expect to calculate a zero with infinite precision. It is necessary to specify some tolerance. When the root is located to within this tolerance, the subroutine returns control to the main calling program.
3. All the approaches mentioned here are iteration techniques. How many times do you iterate? How do you decide to stop? It is possible to program the iteration so that it continues until the desired accuracy is obtained. The danger is that some factor may prevent reasonable convergence. Then your tolerance is never achieved and you have an infinite loop. It is far safer to specify in advance a maximum number of iterations. Thus, these subroutines will stop when either a zero is determined to within your specified tolerance or the number of iterations reaches your specified maximum—whichever occurs first. With a simple bisection technique the selection of a number of iterations depends on the initial spread $x_r - x_l$ and on the precision you demand. Each iteration will cut the range by a factor of 2. Since $2^{10} = 1024 \approx 10^3$, 10 iterations should add three significant figures; 20 should add six significant figures to the location of the root.

EXERCISES

A1.1 Write a **simple** bisection root determination subroutine that will determine a simple real root once you have straddled it. Test your subroutine by determining the roots of one or more polynomials or elementary transcendental functions.

A1.2 Try the bisection method to locate a root of the following functions:
(a) $f(x) = x^2 - 1$, and $x_0 = 0.9, 1.1$
(b) $f(x) = (x^2 - 1)^{1/2}$, $x_0 = 0.9, 1.1$
(c) $f(x) = \sin x$, $x_0 = 3.0, 3.2$
(d) $f(x) = \tanh x - x/2$, $x_0 = 1.8, 2.0$.

A1.3 The theory of free radial oscillations of a homogeneous earth leads to an equation

$$\tan x = \frac{x}{1 - a^2 x^2}.$$

The parameter a depends on the velocities of the primary and secondary waves. For $a = 1.0$, find the first three positive roots of this equation.

ANS. $x_1 = 2.7437$ $x_2 = 6.1168$ $x_3 = 9.3166$.

A1.4 (a) Using the Bessel function $J_0(x)$ generated by function BESSJ0(x) of Press *et al.* in Additional Reading, locate consecutive roots of $J_0(x)$: α_n and α_{n+1} for $n = 5, 10, 15, \ldots, 30$. Tabulate α_n, α_{n+1}, $(\alpha_{n+1} - \alpha_n)$, and $(\alpha_{n+1} - \alpha_n)/\pi$. Note how this last ratio is approaching unity.

(b) Compare your values of α_n with values calculated from McMahon's expansion, AMS-55, Eq. (9.5.12).

Additional Reading

Hamming, R. W. (1971). *Introduction to Applied Numerical Analysis*. McGraw-Hill, New York. Reprinted, Hemisphere, New York (1989), especially Chapter 2. In terms of the author's insight into numerical computation and his ability to communicate to the average reader, this book is unexcelled.

Press, W. H., Flannery, B. P., Teukolsky, S. A., and Vetterling, W. T. (1996). *Numerical Recipes*, 2nd ed. Cambridge Univ. Press, Cambridge, UK.

General References

1. Whittaker, E. T., and Watson, G. N. (1962). *A Course of Modern Analysis*, 4th ed., paperback. Cambridge Univ. Press, Cambridge, UK. Although this is the oldest (original edition 1902) of the references, it still is the classic reference. It leans strongly to pure mathematics, as of 1902, with full mathematical rigor.
2. Morse, P. M., and Feshbach, H. (1953). *Methods of Theoretical Physics*, 2 vols. McGraw-Hill, New York. This work presents the mathematics of much of theoretical physics in detail but at a rather advanced level. It is recommended as the outstanding source of information for supplementary reading and advanced study.
3. Jeffreys, H. S., and Jeffreys, B. S. (1972). *Methods of Mathematical Physics*, 3rd ed. Cambridge Univ. Press, Cambridge, UK. This is a scholarly treatment of a wide range of mathematical analysis, in which considerable attention is paid to mathematical rigor. Applications are to classical physics and to geophysics.
4. Courant, R., and Hilbert, D. (1953). *Methods of Mathematical Physics*, Vol. 1 (1st English ed.). Wiley (Interscience), New York. As a reference book for mathematical physics, it is particularly valuable for existence theorems and discussions of areas such as eigenvalue problems, integral equations, and calculus of variations.
5. Byron, F. W., Jr., and Fuller, R. W. (1992). *Mathematics of Classical and Quantum Physics*, Addison-Wesley, Reading, MA. Reprinted, Dover, New York. This is an advanced text that presupposes a moderate knowledge of mathematical physics.
6. Bender, C. M., and Orszag, S. A. (1978). *Advanced Mathematical Methods for Scientists and Engineers*. McGraw-Hill, New York.

7. *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables*, Applied Mathematics Series 55 (AMS-55). National Bureau of Standards, U.S. Department of Commerce, Washington, DC. Reprinted, Dover, New York (1974). As a tremendous compilation of just what the title says, this is an extremely useful reference.

Other more specialized references are listed at the end of each chapter.

INDEX

C

D

E

F

G

H

I

J

M

N

O

P

Q

R

S

T

U

V

W

Y

Z

$$f(x) = \sum_{n=0}^{\infty} f^{(n)}(a)\frac{(x-a)^n}{n!}, \quad f(z) = f(0) + \sum_{n=0}^{\infty} b_n\left(\frac{1}{z-a_n} + \frac{1}{a_n}\right)$$

$$\frac{f'}{f}(z) = \frac{f'}{f}(0) + \sum_{n=0}^{\infty}\left(\frac{1}{z-a_n} + \frac{1}{a_n}\right), \quad f(z) = f(0)e^{z\frac{f'}{f}(0)}\prod_{n=1}^{\infty}\left(1-\frac{z}{a_n}\right)e^{z/a_n}$$

$$\frac{1}{1-x} = \sum_{n=0}^{\infty} x^n, \quad (1+x)^{\alpha} = \sum_{n=0}^{\infty}\binom{\alpha}{n}x^n, \quad e^x = \sum_{n=0}^{\infty}\frac{x^n}{n!},$$

$$\ln(1+x) = \sum_{n=1}^{\infty}\frac{(-1)^{n-1}}{n}x^n$$

$$\sin x = \sum_{n=0}^{\infty}\frac{(-1)^n x^{2n+1}}{(2n+1)!}, \quad \cos x = \sum_{n=0}^{\infty}\frac{(-1)^n x^{2n}}{(2n)!},$$

$$\frac{x}{e^x - 1} = 1 - \frac{x}{2} + \sum_{n=1}^{\infty} B_{2n}\frac{x^{2n}}{(2n)!}$$

$$x\cot x = \sum_{n=0}^{\infty}(-1)^n B_{2n}\frac{(2x)^{2n}}{(2n)!}, \quad \cot \pi x = \frac{1}{x} + \sum_{n=1}^{\infty}\left(\frac{1}{x-n} + \frac{1}{x+n}\right)$$

$$\zeta(s) = \sum_{n=1}^{\infty}\frac{1}{n^s}, \quad \zeta(2n) = (-1)^{n-1}\frac{(2\pi)^{2n}}{2(2n)!}B_{2n}$$

$$\frac{\pi^2}{\sin^2 \pi x} = \sum_{n=-\infty}^{\infty}\frac{1}{(x-n)^2}, \quad \sin \pi x = \pi x\prod_{n=1}^{\infty}\left(1-\frac{x^2}{n^2}\right)$$

$$\Gamma(z) = \int_0^{\infty} e^{-t}t^{z-1}dt, \quad \frac{1}{\Gamma(x)} = xe^{\gamma x}\prod_{n=1}^{\infty}\left(1+\frac{x}{n}\right)e^{-x/n},$$

$$\frac{\Gamma'}{\Gamma}(z+1) = -\gamma + \sum_{n=1}^{\infty}\left(\frac{1}{n} - \frac{1}{z+n}\right)$$

$$e^{iz} = e^{-y}(\cos x + i\sin x), \quad \ln z = \ln|z| + i(\arg z + 2\pi n)$$

$$J_{\nu}(x) = \sum_{n=0}^{\infty}\frac{(-1)^n}{n!(\nu+n)!}\left(\frac{x}{2}\right)^{\nu+2n}, \quad e^{(x/2)(t-1/t)} = \sum_{n=-\infty}^{\infty} J_n(x)t^n$$

$$(1-2xt+t^2)^{-1/2} = \sum_{l=0}^{\infty} P_l(x)t^l, \quad P_l(x) = \frac{1}{2^l l!}\left(\frac{d}{dx}\right)^l (x^2-1)^l,$$

$$\int_{-1}^{1} P_l(x)P_{l'}(x)dx = \frac{2\delta_{ll'}}{2l+1}$$

$$e^{i\mathbf{k}\cdot\mathbf{r}} = 4\pi \sum_{l=0}^{\infty} i^l j_l(kr) \sum_{m=-l}^{l} Y_{lm}^*(\theta_k, \varphi_k) Y_{lm}(\theta, \varphi)$$

$$e^{-t^2+2tx} = \sum_{n=0}^{\infty} H_n(x)\frac{t^n}{n!}, \quad H_n(x) = (-1)^n e^{x^2}\frac{d^n}{dx^n}e^{-x^2}$$

$$L_n(x) = \frac{e^x}{n!}\frac{d^n}{dx^n}(x^n e^{-x}), \quad \int_0^{\infty} e^{-x} L_m(x) L_n(x) dx = \delta_{mn}$$

$$f(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty}(a_n \cos nx + b_n \sin nx), \; a_n = \frac{1}{\pi}\int_0^{2\pi} f(x)\cos nx\, dx,$$

$$b_n = \frac{1}{\pi}\int_0^{2\pi} f(x)\sin nx\, dx$$

Integrals

$$F(\omega) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} f(t)e^{i\omega t}dt, \quad f(t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} F(\omega)e^{-i\omega t}d\omega$$

$$\int_{-\infty}^{\infty} F(\omega)G^*(\omega)d\omega = \int_{-\infty}^{\infty} f(t)g^*(t)dt,$$

$$\int_{-\infty}^{\infty} g(y)f(x-y)dy = \int_{-\infty}^{\infty} F(\omega)G(\omega)e^{-i\omega x}d\omega$$

$$\int g(z)e^{sf(z)}dz \sim \frac{\sqrt{2\pi}\,g(z_0)e^{sf(z_0)+i\alpha}}{|sf''(z_0)|^{1/2}}, \; f'(z_0) = 0, \; \alpha = \frac{\pi}{2} - \frac{1}{2}\arg f''(z_0)$$

$$\nabla^2 V = -\frac{\rho}{\varepsilon_0}, \quad V(\mathbf{r}) = \frac{1}{4\pi\varepsilon_0}\int \frac{\rho(\mathbf{r}')d^3r'}{|\mathbf{r}-\mathbf{r}'|}, \quad \int \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{k^2+m^2}\frac{d^3k}{(2\pi)^3}$$

$$= \frac{e^{-mr}}{4\pi r}$$

Greek Alphabet

Alpha	A	α	Nu	N	ν
Beta	B	β	Xi	Ξ	ξ
Gamma	Γ	γ	Omicron	O	o
Delta	Δ	δ	Pi	Π	π
Epsilon	E	ϵ	Rho	P	ρ
Zeta	Z	ζ	Sigma	Σ	σ
Eta	H	η	Tau	T	τ
Theta	Θ	θ	Upsilon	Υ	υ
Iota	I	ι	Phi	Φ	ϕ
Kappa	K	κ	Chi	X	χ
Lambda	Λ	λ	Psi	Ψ	ψ
Mu	M	μ	Omega	Ω	ω