Mathematical Methods in Science and Engineering

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Selçuk Ş. Bayın
Institute of Applied Mathematics
Middle East Technical University
Ankara Turkey

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Contents

Preface

Courses on mathematical methods of physics are among the essential courses for graduate programs in physics, which are also offered by most engineering departments. Considering that the audience in these courses comes from all subdisciplines of physics and engineering, the content and the level of mathematical formalism has to be chosen very carefully. Recently, the growing interest in interdisciplinary studies has brought scientists together from physics, chemistry, biology, economy, and finance and has increased the demand for these courses in which upper-level mathematical techniques are taught. It is for this reason that the mathematics departments, who once overlooked these courses, are now themselves designing and offering them.

Most of the available books for these courses are written with theoretical physicists in mind and thus are somewhat insensitive to the needs of this new multidisciplinary audience. Besides, these books should not only be tuned to the existing practical needs of this multidisciplinary audience but should also play a lead role in the development of new interdisciplinary science by introducing new techniques to students and researchers.

About the Book

We give a coherent treatment of the selected topics with a style that makes advanced mathematical tools accessible to a multidisciplinary audience. The book is written in a modular way so that each chapter is actually a review of its subject and can be read independently. This makes the book very useful not only as a self-study book for students and beginning researchers but also as a reference for scientists. We emphasize physical motivation and the multidisciplinary nature of the methods discussed. Whenever possible, we prefer to introduce mathematical techniques through physical applications. Examples are often used to extend discussions of specific techniques rather than as mere exercises.

Topics are introduced in a logical sequence and discussed thoroughly. Each sequence climaxes with a part where the material of the previous chapters is unified in terms of a general theory, as in Chapter 7 on the Sturm–Liouville theory, or as in Chapter 18 on Green's functions, where the gains of the previous chapters are utilized. Chapter 8 is on factorization method. It is a natural extension of our discussion on the Sturm–Liouville theory. It also presents a different and an advanced treatment of special functions. Similarly, Chapter 19 on path integrals is a natural extension of our chapter on Green's functions. Chapters 9 and 10 on coordinates, tensors, and continuous groups have been located after Chapter 8 on the Sturm–Liouville theory and the factorization method. Chapters 11 and 12 are on complex techniques, and they are self-contained. Chapter 13 on fractional calculus can either be integrated into the curriculum of the mathematical methods of physics courses or used independently to design a one-semester course.

Since our readers are expected to be at least at the graduate or the advanced undergraduate level, a background equivalent to the contents of our undergraduate text book *Essentials of Mathematical Methods in Science and Engineering* (Bayin, 2008) is assumed. In this regard, the basics of some of the methods discussed here can be found there. For communications about the book, we will use the website http://users.metu.edu.tr/bayin/

The entire book contains enough material for a three-semester course meeting three hours a week. The modular structure of the book gives enough flexibility to adopt the book for two- or even a one-semester course. Chapters 1–7, 11, 12, and 14–18 have been used for a two-semester compulsory graduate course meeting three hours a week at METU, where students from all subdisciplines of physics meet. In other universities, colleagues have used the book for their two or one semester courses.

During my lectures and first reading of the book, I recommend that readers view equations as statements and concentrate on the logical structure of the arguments. Later, when they go through the derivations, technical details will be understood, alternate approaches will appear, and some of the questions will be answered. Sufficient numbers of problems are given at the back of each chapter. They are carefully selected and should be considered an integral part of the learning process. Since some of the problems may require a good deal of time, we recommend the reader to skim through the entire problem section before attempting them. Depending on the level and the purpose of the reader, certain parts of the book can be skipped in first reading. Since the modular structure of the book makes it relatively easy for the readers to decide on which chapters or sections to skip, we will not impose a particular selection.

In a vast area like mathematical methods in science and engineering, there is always room for new approaches, new applications, and new topics. In fact, the number of books, old and new, written on this subject shows how dynamic this field is. Naturally, this book carries an imprint of my style and lectures. Because the main aim of this book is pedagogy, occasionally I have followed other books when their approaches made perfect sense to me. Main references are given at the back of each chapter. Additional references can be found at the back. Readers of this book will hopefully be well prepared for advanced graduate studies and research in many areas of physics. In particular, as we use the same terminology and style, they should be ready for full-term graduate courses based on the books: *The Fractional Calculus* by Oldham and Spanier and *Path Integrals in Physics, Volumes I and II* by Chaichian and Demichev, or they could jump to the advanced sections of these books, which have become standard references in their fields. Our list of references, by all means, is not meant to be complete or up to date. There are many other excellent sources that nowadays the reader can locate by a simple internet search. Their exclusion here is simply ignorance on my part and not a reflection on their quality or importance.

About the Second Edition

The challenge in writing a mathematical methods text book is that for almost every chapter an entire book can be devoted. Sometimes, even sections could be expanded into another book. In this regard, it is natural that books with such broad scope need at least another edition to settle down. The second edition of *Mathematical Methods in Science and Engineering* corresponds to a major overhaul of the entire book. In addition to 34 new examples, 34 new figures, and 48 new problems, over 60 new sections/subsections have been included on carefully selected topics that make the book more appealing and useful to its multidisciplinary audience.

Among the new topics introduced, we have the discrete and fast Fourier transforms; Cartesian tensors and the theory of elasticity; curvature; Caputo and Riesz fractional derivatives; method of steepest descent and saddle-point integrals; Padé approximants; Radon transforms; optimum control theory and controlled dynamics; diffraction; time independent perturbation theory; the anharmonic oscillator problem; anomalous diffusion; Fox's H-functions and many others. As Socrates has once said *education is the kindling of a flame, not the filling of a Vessel*, all topics are selected and written, not to fill a vessel but to inform, provoke further thought, and interest among the multidisciplinary audience we address.

Besides these, throughout the book, countless changes have been made to assure easy reading and smooth flow of the complex mathematical arguments. Derivations are given in sufficient detail so that the reader will not be distracted by searching for results in other parts of the book or by needing to write down equations. We have shown carefully selected keywords in boldface and framed key results so that information can be located easily as the reader scans through the pages. Also, using the new Wiley style and a more efficient way of displaying equations, we were able to keep the book at an optimum size.

Acknowledgments

I would again like to start by paying tribute to all the scientists and mathematicians whose works contributed to the subjects discussed in this book. I would also like to compliment the authors of the existing books on mathematical methods of physics. I appreciate the time and dedication that went into writing them. Most of them existed even before I was a graduate student and I have benefitted from them greatly. As in the first edition, I am indebted to Prof. K. T. Hecht of the University of Michigan, whose excellent lectures and clear style had a great influence on me. I am grateful to Prof. P. G. L. Leach for sharing his wisdom with me and for meticulously reading Chapters 8, 13, and 19. I also thank Prof. N. K. Pak for many interesting and stimulating discussions, encouragement, and critical reading of the chapter on path integrals. Their comments kept illuminating my way during the preparation of this edition as well. I thank Prof. E. Akyıldız and Prof. B. Karasözen for encouragement and support at the Institute of Applied Mathematics at METU, which became home to me. I also thank my editors Jon Gurstelle and Kathleen Pagliaro, and the publication team at Wiley for sharing my excitement and their utmost care in bringing this book into existence. Finally, I thank my beloved wife Adalet and darling daughter Sumru. Without their endless love and support, this project, which spanned over a decade, would not have been possible.

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1

Legendre Equation and Polynomials

Legendre polynomials, $P_n(x)$, are the solutions of the Legendre equation:

$$\frac{d}{dx}\left[(1-x^2)\frac{dP_l(x)}{dx}\right] + n(n+1)P_n(x) = 0, \quad n = 0, 1, 2, \ldots . \tag{1.1}$$

They are named after the French mathematician **Adrien-Marie Legendre** (1752–1833). They are frequently encountered in physics and engineering applications. In particular, they appear in the solutions of the Laplace equation in spherical polar coordinates.

1.1 Second-Order Differential Equations of Physics

Many of the **second-order** partial differential equations of physics and engineering can be written as

$$\boxed{\vec{\nabla}^2\Psi(x, y, z) + k^2(x, y, z)\,\Psi(x, y, z) = F(x, y, z),} \tag{1.2}$$

where some of the frequently encountered cases are:

1. When $k(x, y, z)$ and $F(x, y, z)$ are zero, we have the **Laplace equation**:

$$\boxed{\vec{\nabla}^2\Psi(x, y, z) = 0,} \tag{1.3}$$

   which is encountered in many different areas of science like electrostatics, magnetostatics, laminar (irrotational) flow, surface waves, heat transfer and gravitation.
2. When the right-hand side of the Laplace equation is different from zero, we have the **Poisson equation**:

$$\boxed{\vec{\nabla}^2\Psi = F(x, y, z),} \tag{1.4}$$

   where $F(x, y, z)$ represents sources or sinks in the system.

Mathematical Methods in Science and Engineering, Second Edition. Selçuk Ş. Bayın.

3. The **Helmholtz wave equation** is written as

$$\boxed{\vec{\nabla}^2\Psi(x,y,z) \pm k_0^2\Psi(x,y,z) = 0,} \tag{1.5}$$

   where k_0 is a constant.
4. Another important example is the time-independent **Schrödinger equation**:

$$\boxed{-\frac{\hbar^2}{2m}\vec{\nabla}^2\Psi(x,y,z) + V(x,y,z)\Psi(x,y,z) = E\Psi(x,y,z),} \tag{1.6}$$

   where $F(x,y,z)$ in Eq. (1.2) is zero and $k(x,y,z)$ is given as

$$k(x,y,z) = \sqrt{(2m/\hbar^2)[E - V(x,y,z)]}. \tag{1.7}$$

A common property of all these equations is that they are linear and second-order partial differential equations. Separation of variables, Green's functions and integral transforms are among the frequently used analytic techniques for obtaining solutions. When analytic methods fail, one can resort to numerical techniques like Runge–Kutta. Appearance of similar differential equations in different areas of science allows one to adopt techniques developed in one area into another. Of course, the variables and interpretation of the solutions will be very different. Also, one has to be aware of the fact that boundary conditions used in one area may not be appropriate for another. For example, in electrostatics, charged particles can only move perpendicular to the conducting surfaces, whereas in laminar (irrotational) flow, fluid elements follow the contours of the surfaces; thus even though the Laplace equation is to be solved in both cases, solutions obtained in electrostatics may not always have meaningful counterparts in laminar flow.

1.2 Legendre Equation

We now solve Eq. (1.2) in spherical polar coordinates using the method of **separation of variables**. We consider cases where $k(x,y,z)$ is only a function of the radial coordinate and also set $F(x,y,z)$ to zero. The time-independent Schrödinger equation (1.6) for the central force problems, $V(x,y,z) = V(r)$, is an important example for such cases. We first separate the radial, r, and the angular (θ,ϕ) variables and write the solution as $\Psi(r,\theta,\phi) = R(r)Y(\theta,\phi)$. This basically assumes that the radial dependence of the solution is independent of the angular coordinates and vice versa. Substituting this in Eq. (1.2), we get

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left[r^2\frac{\partial}{\partial r}R(r)Y(\theta,\phi)\right]+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left[\sin\theta\frac{\partial}{\partial\theta}R(r)Y(\theta,\phi)\right] + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}R(r)Y(\theta,\phi)+k^2(r)R(r)Y(\theta,\phi)=0. \tag{1.8}$$

After multiplying by $r^2/R(r)Y(\theta,\phi)$ and collecting the (θ,ϕ) dependence on the right-hand side, we obtain

$$\frac{1}{R(r)}\frac{\partial}{\partial r}\left[r^2\frac{\partial}{\partial r}R(r)\right]+k^2(r)r^2=-\frac{1}{\sin\theta}\frac{1}{Y(\theta,\phi)}\frac{\partial}{\partial\theta}\left[\sin\theta\frac{\partial}{\partial\theta}Y(\theta,\phi)\right] -\frac{1}{\sin^2\theta Y(\theta,\phi)}\frac{\partial^2 Y(\theta,\phi)}{\partial\phi^2}. \tag{1.9}$$

Since r and (θ,ϕ) are independent variables, this equation can be satisfied for all r and (θ,ϕ) only when both sides of the equation are equal to the same constant. We show this constant with λ, which is also called the **separation constant**. Now Eq. (1.9) reduces to the following two equations:

$$\boxed{\frac{d}{dr}\left(r^2\frac{dR(r)}{dr}\right)+r^2k^2(r)R(r)-\lambda R(r)=0,} \tag{1.10}$$

$$\boxed{\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left[\sin\theta\frac{\partial Y(\theta,\phi)}{\partial\theta}\right]+\frac{1}{\sin^2\theta}\frac{\partial^2 Y(\theta,\phi)}{\partial\phi^2}+\lambda Y(\theta,\phi)=0,} \tag{1.11}$$

where Eq. (1.10) for $R(r)$ is an ordinary differential equation. We also separate the θ and the ϕ variables in $Y(\theta,\phi)$ as $Y(\theta,\phi)=\Theta(\theta)\Phi(\phi)$ and call the new separation constant m^2, and write

$$\frac{\sin\theta}{\Theta(\theta)}\frac{d}{d\theta}\left[\sin\theta\frac{d\Theta}{d\theta}\right]+\lambda\sin^2\theta=-\frac{1}{\Phi(\phi)}\frac{d^2\Phi(\phi)}{d\phi^2}=m^2. \tag{1.12}$$

The differential equations to be solved for $\Theta(\theta)$ and $\Phi(\phi)$ are now found, respectively, as

$$\boxed{\sin^2\theta\frac{d^2\Theta(\theta)}{d\theta^2}+\cos\theta\sin\theta\frac{d\Theta(\theta)}{d\theta}+[\lambda\sin^2\theta-m^2]\,\Theta(\theta)=0,} \tag{1.13}$$

$$\boxed{\frac{d^2\Phi(\phi)}{d\phi^2}+m^2\Phi(\phi)=0.} \tag{1.14}$$

In summary, using the method of separation of variables, we have reduced the partial differential equation [Eq. (1.8)] to three ordinary differential equations

[Eqs. (1.10), (1.13), and (1.14)]. During this process, two constant parameters, λ and m, called the **separation constants** have entered into our equations, which so far have no restrictions on them.

1.2.1 Method of Separation of Variables

In the above discussion, the fact that we are able to separate the solution is closely related to the use of the spherical polar coordinates, which reflect the symmetry of the central force problem, where the potential, $V(r)$, depends only on the radial coordinate. In Cartesian coordinates, the potential would be written as $V(x, y, z)$ and the solution would not be separable as $\Psi(x, y, z) \neq X(x)Y(y)Z(z)$. Whether a given partial differential equation is separable or not is closely linked to the symmetries of the physical system. Even though a proper discussion of this point is beyond the scope of this book, we refer the reader to [9] and suffice by saying that if a partial differential equation is not separable in a given coordinate system, it is possible to check the existence of a coordinate system in which it would be separable. If such a coordinate system exists, then it is possible to construct it from the generators of the symmetries.

Among the three ordinary differential equations [Eqs. (1.10), (1.13), and (1.14)], Eq. (1.14) can be solved immediately with the general solution

$$\Phi(\phi) = Ae^{im\phi} + Be^{-im\phi}, \tag{1.15}$$

where the separation constant, m, is still unrestricted. Imposing the periodic boundary condition $\Phi(\phi + 2\pi) = \Phi(\phi)$, we restrict m to integer values: $0, \pm 1, \pm 2, \ldots$. Note that in anticipation of applications to quantum mechanics, we have taken the two linearly independent solutions as $e^{\pm im\phi}$. For the other problems, $\sin m\phi$ and $\cos m\phi$ could be used.

For the differential equation to be solved for $\Theta(\theta)$ [Eq. (1.13)], we define a new independent variable, $x = \cos\theta$, $\Theta(\theta) = Z(x)$, $\theta \in [0, \pi]$, $x \in [-1, 1]$, and write

$$(1 - x^2)\frac{d^2Z(x)}{dx^2} - 2x\frac{dZ(x)}{dx} + \left[\lambda - \frac{m^2}{(1 - x^2)}\right] Z(x) = 0. \tag{1.16}$$

For $m = 0$, this equation is called the **Legendre equation**. For $m \neq 0$, it is known as the **associated Legendre equation**.

1.2.2 Series Solution of the Legendre Equation

Starting with the $m = 0$ case, we write the **Legendre equation** as

$$\boxed{(1 - x^2)\frac{d^2Z(x)}{dx^2} - 2x\frac{dZ(x)}{dx} + \lambda Z(x) = 0, \quad x \in [-1, 1].} \tag{1.17}$$

This has two regular **singular points** at $x = -1$ and 1. Since these points are at the end points of our interval, we use the **Frobenius method** [8] and try a series solution about the regular point $x = 0$ as $Z(x) = \sum_{k=0}^{\infty} a_k x^{k+\alpha}$, where α is a constant. Substituting this into Eq. (1.17), we get

$$\sum_{k=0}^{\infty} a_k (k+\alpha)(k+\alpha-1)x^{k+\alpha-2} - \sum_{k=0}^{\infty} x^{k+\alpha} \left[(k+\alpha)(k+\alpha-1) + 2(k+\alpha) - \lambda\right] a_k = 0. \tag{1.18}$$

We now write the first two terms of the first series explicitly:

$$a_0\alpha(\alpha-1)x^{\alpha-2} + a_1(\alpha+1)\alpha x^{\alpha-1} + \sum_{k'=2}^{\infty} a_{k'}(k'+\alpha)(k'+\alpha-1)x^{k'+\alpha-2} \tag{1.19}$$

and make the variable change $k' = k + 2$, to write Eq. (1.18) as

$$a_0\alpha(\alpha-1)x^{\alpha-2} + a_1(\alpha+1)\alpha x^{\alpha-1} + \sum_{k=0}^{\infty} x^{k+\alpha} \left\{a_{k+2}(k+2+\alpha)(k+1+\alpha) - a_k\left[(k+\alpha)(k+\alpha+1) - \lambda\right]\right\} = 0. \tag{1.20}$$

From the uniqueness of power series, this equation cannot be satisfied for all x unless the coefficients of all the powers of x vanish simultaneously. This gives the following relations among the coefficients:

$$\boxed{a_0\alpha(\alpha-1) = 0, \quad a_0 \neq 0,} \tag{1.21}$$

$$\boxed{a_1(\alpha+1)\alpha = 0,} \tag{1.22}$$

$$\boxed{\frac{a_{k+2}}{a_k} = \frac{\left[(k+\alpha)(k+\alpha+1) - \lambda\right]}{(k+1+\alpha)(k+\alpha+2)}, \quad k = 0, 1, 2, \ldots .} \tag{1.23}$$

Equation (1.21), which is obtained by setting the coefficient of the lowest power of x to zero, is called the **indicial equation**. Assuming $a_0 \neq 0$, the two roots of the indicial equation give the values $\alpha = 0$ and $\alpha = 1$, while the remaining Eqs. (1.22) and (1.23) give the **recursion relation** among the coefficients.

Starting with the root $\alpha = 1$, we write

$$a_{k+2} = a_k \frac{(k+1)(k+2) - \lambda}{(k+2)(k+3)}, \quad k = 0, 1, 2, \ldots , \tag{1.24}$$

and obtain the remaining coefficients as

$$a_2 = a_0 \frac{(2-\lambda)}{6}, \tag{1.25}$$

$$a_3 = a_1 \frac{(6-\lambda)}{12}, \tag{1.26}$$

$$a_4 = a_2 \frac{(12-\lambda)}{20}, \tag{1.27}$$

$$\vdots \tag{1.28}$$

Since Eq. (1.22) with $\alpha = 1$ implies $a_1 = 0$, all the odd coefficients vanish, $a_3 = a_5 = \cdots = 0$, thus yielding the following series solution for $\alpha = 1$:

$$Z_1(x) = a_0 \left[x + \frac{(2-\lambda)}{6} x^3 + \frac{(2-\lambda)(12-\lambda)}{120} x^5 + \cdots \right]. \tag{1.29}$$

For the other root, $\alpha = 0$, Eqs. (1.21) and (1.22) imply $a_0 \neq 0$ and $a_1 \neq 0$, thus the recursion relation:

$$a_{k+2} = a_k \frac{k(k+1) - \lambda}{(k+1)(k+2)}, \quad k = 0, 1, 2, \ldots, \tag{1.30}$$

determines the nonzero coefficients as

$$\begin{aligned} a_2 &= a_0 \left(-\frac{\lambda}{2} \right), \\ a_3 &= a_1 \left(\frac{2-\lambda}{6} \right), \\ a_4 &= a_2 \left(\frac{6-\lambda}{12} \right), \\ a_5 &= a_3 \left(\frac{12-\lambda}{20} \right), \\ &\vdots \end{aligned} \tag{1.31}$$

Now the series solution for $\alpha = 0$ is obtained as

$$\begin{aligned} Z_2(x) = a_0 &\left[1 - \frac{\lambda}{2} x^2 - \frac{\lambda}{2} \frac{(6-\lambda)}{12} x^4 + \cdots \right] \\ &+ a_1 \left[x + \frac{(2-\lambda)}{6} x^3 + \frac{(2-\lambda)(12-\lambda)}{120} x^5 + \cdots \right]. \end{aligned} \tag{1.32}$$

The Legendre equation is a second-order linear ordinary differential equation, which in general has two linearly independent solutions. Since a_0 and a_1 are arbitrary, we note that the solution for $\alpha = 0$ also contains the solution for $\alpha = 1$; hence the general solution can be written as

$$\boxed{\begin{aligned} Z(x) = C_0 &\left[1 - \left(\frac{\lambda}{2} \right) x^2 - \left(\frac{\lambda}{2} \right) \left(\frac{6-\lambda}{12} \right) x^4 + \cdots \right] \\ &+ C_1 \left[x + \frac{(2-\lambda)}{6} x^3 + \frac{(2-\lambda)(12-\lambda)}{120} x^5 + \cdots \right], \end{aligned}} \tag{1.33}$$

where C_0 and C_1 are two integration constants to be determined from the boundary conditions. These series are called the **Legendre series**.

1.2.3 Frobenius Method – Review

A second-order linear homogeneous ordinary differential equation with two linearly independent solutions may be put in the form

$$\boxed{\frac{d^2y}{dx^2} + P(x)\frac{dy}{dx} + Q(x)y(x) = 0.} \tag{1.34}$$

If x_0 is no worse than a **regular singular point**, that is, when

$$\lim_{x \to x_0} (x - x_0)P(x) \to \text{finite} \tag{1.35}$$

and

$$\lim_{x \to x_0} (x - x_0)^2 Q(x) \to \text{finite}, \tag{1.36}$$

we can seek a **series solution** of the form

$$y(x) = \sum_{k=0}^{\infty} a_k (x - x_0)^{k+\alpha}, \quad a_0 \neq 0. \tag{1.37}$$

Substituting this series into the above differential equation and setting the coefficient of the lowest power of $(x - x_0)$ with $a_0 \neq 0$ gives us a quadratic equation for α called the **indicial equation**. For almost all the physically interesting cases, the indicial equation has two real roots. This gives us the following possibilities for the two linearly independent solutions of the differential equation [8]:

1. If the two roots $(\alpha_1 > \alpha_2)$ differ by a noninteger, then the two linearly independent solutions, $y_1(x)$ and $y_2(x)$, are given as

$$\boxed{y_1(x) = |x - x_0|^{\alpha_1} \sum_{k=0}^{\infty} a_k (x - x_0)^k, \quad a_0 \neq 0,} \tag{1.38}$$

$$\boxed{y_2(x) = |x - x_0|^{\alpha_2} \sum_{k=0}^{\infty} b_k (x - x_0)^k, \quad b_0 \neq 0.} \tag{1.39}$$

2. If $(\alpha_1 - \alpha_2) = N$, where $\alpha_1 > \alpha_2$ and N is a positive integer, then the two linearly independent solutions, $y_1(x)$ and $y_2(x)$, are given as

$$\boxed{y_1(x) = |x - x_0|^{\alpha_1} \sum_{k=0}^{\infty} a_k (x - x_0)^k, \quad a_0 \neq 0,} \tag{1.40}$$

$$y_2(x) = |x - x_0|^{\alpha_2} \sum_{k=0}^{\infty} b_k (x - x_0)^k + C y_1(x) \ln |x - x_0|, \quad b_0 \neq 0. \tag{1.41}$$

The second solution contains a logarithmic singularity, where C is a constant that may or may not be zero. Sometimes, α_2 will contain both solutions; hence it is advisable to start with the smaller root with the hopes that it might provide the general solution.

3. If the indicial equation has a double root, $\alpha_1 = \alpha_2$, then the Frobenius method yields only one series solution. In this case, the two linearly independent solutions can be taken as

$$y(x, \alpha_1) \quad \text{and} \quad \left. \frac{\partial y(x, \alpha)}{\partial \alpha} \right|_{\alpha=\alpha_1}, \tag{1.42}$$

where the second solution diverges logarithmically as $x \to x_0$. In the presence of a double root, the Frobenius method is usually modified by taking the two linearly independent solutions, $y_1(x)$ and $y_2(x)$, as

$$y_1(x) = |x - x_0|^{\alpha_1} \sum_{k=0}^{\infty} a_k (x - x_0)^k, \quad a_0 \neq 0, \tag{1.43}$$

$$y_2(x) = |x - x_0|^{\alpha_1 + 1} \sum_{k=0}^{\infty} b_k (x - x_0)^k + y_1(x) \ln |x - x_0|. \tag{1.44}$$

In all these cases, the general solution is written as $y(x) = A_1 y_1(x) + A_2 y_2(x)$.

1.3 Legendre Polynomials

Legendre series are convergent in the interval $(-1, 1)$. This can be checked easily by the ratio test. To see how they behave at the end points, $x = \pm 1$, we take the $k \to \infty$ limit of the recursion relation in Eq. (1.30) to obtain $\frac{a_{k+2}}{a_k} \to 1$. For sufficiently large k values, this means that both series behave as

$$Z(x) = \cdots + a_k x^k \left(1 + x^2 + x^4 + \cdots\right). \tag{1.45}$$

The series inside the parentheses is nothing but the geometric series:

$$\left(1 + x^2 + x^4 + \cdots\right) = \frac{1}{1 - x^2}. \tag{1.46}$$

Hence both of the Legendre series diverge at the end points as $1/(1-x^2)$. However, the end points correspond to the north and the south poles of a sphere. Because the problem is spherically symmetric, there is nothing special about these points. Any two diametrically opposite points can be chosen to serve as the end points. Hence we conclude that the physical solution should be finite everywhere on a sphere. To avoid the divergence at the end points we terminate the Legendre series after a finite number of terms. This is accomplished by restricting the separation constant λ to integer values:

$$\lambda = l(l+1), \quad l = 0, 1, 2, \ldots . \tag{1.47}$$

With this restriction on λ, one of the Legendre series in Eq. (1.33) terminates after a finite number of terms while the other one still diverges at the end points. Choosing the coefficient of the divergent series in the general solution as zero, we obtain the polynomial solutions of the Legendre equation as

$$Z(x) = P_l(x), \quad l = 0, 1, 2, \ldots . \tag{1.48}$$

These polynomials are called the **Legendre polynomials**, which are finite everywhere on a sphere. They are defined so that their value at $x = 1$ is one. In general, they can be expressed as

$$\boxed{P_l(x) = \sum_{n=0}^{[l/2]} \frac{(-1)^n (2l-2n)!}{2^l (l-2n)!(l-n)!n!} x^{l-2n},} \tag{1.49}$$

where $[l/2]$ means the greatest integer in the interval $\left(\frac{l}{2}, \frac{l}{2}-1\right]$. Restriction of λ to certain integer values for finite solutions everywhere is a physical (boundary) condition and has very significant physical consequences. For example, in quantum mechanics, it means that magnitude of the angular momentum is quantized. In wave mechanics, like the standing waves on a string fixed at both ends, it means that waves on a sphere can only have certain wavelengths.

Legendre Polynomials

$$\begin{aligned}
P_0(x) &= 1, \\
P_1(x) &= x, \\
P_2(x) &= (1/2)[3x^2 - 1], \\
P_3(x) &= (1/2)[5x^3 - 3x], \\
P_4(x) &= (1/8)[35x^4 - 30x^2 + 3], \\
P_5(x) &= (1/8)[63x^5 - 70x^3 + 15x].
\end{aligned} \tag{1.50}$$

1.3.1 Rodriguez Formula

Another definition of the Legendre polynomials is given by the **Rodriguez formula**:

$$\boxed{P_l(x) = \frac{1}{2^l l!} \frac{d^l}{dx^l} \left(x^2 - 1\right)^l.} \tag{1.51}$$

To show that this is equivalent to the previous definition in Eq. (1.49), we use the binomial formula [4]:

$$(x + y)^m = \sum_{n=0}^{\infty} \frac{m!}{n!(m - n)!} x^n y^{m-n}, \tag{1.52}$$

to write Eq. (1.51) as

$$P_l(x) = \frac{1}{2^l l!} \frac{d^l}{dx^l} \sum_{n=0}^{l} \frac{l!(-1)^n}{n!(l - n)!} x^{2l-2n}. \tag{1.53}$$

We now use the formula

$$\frac{d^l x^m}{dx^l} = \frac{m!}{(m - l)!} x^{m-l}, \tag{1.54}$$

to obtain

$$P_l(x) = \sum_{n=0}^{\left[\frac{l}{2}\right]} \frac{(-1)^n}{2^l} \frac{(2l - 2n)!}{n!(l - n)!(l - 2n)!} x^{l-2n}, \tag{1.55}$$

thus proving the equivalence of Eqs. (1.51) and (1.49).

1.3.2 Generating Function

Another way to define the Legendre polynomials is using a **generating function**, $T(x, t)$, which is given as

$$\boxed{T(x, t) = \frac{1}{\sqrt{1 - 2xt + t^2}} = \sum_{l=0}^{\infty} P_l(x) t^l, \quad |t| < 1.} \tag{1.56}$$

To show that $T(x, t)$ generates the Legendre polynomials, we write $T(x, t)$ as

$$T(x, t) = \frac{1}{[1 - t(2x - t)]^{\frac{1}{2}}} \tag{1.57}$$

and use the binomial expansion

$$(1 - x)^{-\frac{1}{2}} = \sum_{l=0}^{\infty} \frac{(-1/2)!(-1)^l x^l}{l! \left(-\frac{1}{2} - l\right)!}. \tag{1.58}$$

Deriving the useful relation:

$$\frac{\left(-\frac{1}{2}\right)!}{\left(-\frac{1}{2}-l\right)!} = \frac{\left(-\frac{1}{2}\right)\left(-\frac{1}{2}-1\right)\left(\frac{1}{2}-2\right)\cdots}{\left(-\frac{1}{2}-l\right)\left(-\frac{1}{2}-l-1\right)\cdots} \tag{1.59}$$

$$= \frac{(-1)^l \quad \left[\left(\frac{1}{2}\right)\left(\frac{1}{2}+1\right)\cdots\left(-\frac{1}{2}-l\right)\left(-\frac{1}{2}-l-1\right)\cdots\right]}{\left[\left(-\frac{1}{2}-l\right)\left(-\frac{1}{2}-l-1\right)\cdots\right]} \tag{1.60}$$

$$= (-1)^l \left[\left(\frac{1}{2}\right)\left(\frac{1}{2}+1\right)\left(\frac{1}{2}+2\right)\cdots\left(\frac{1}{2}+l-1\right)\right] \tag{1.61}$$

$$= (-1)^l \frac{1\cdot 3\cdot 5\cdots(2l-1)}{2^l} = (-1)^l \frac{(2l)!}{2^{2l} l!}, \tag{1.62}$$

we write Eq. (1.58) as

$$(1-x)^{-\frac{1}{2}} = \sum_{l=0}^{\infty} \frac{(2l)!(-1)^{2l}}{2^{2l}(l!)^2} x^l, \tag{1.63}$$

which after substituting in Eq. (1.57) gives

$$\frac{1}{(1-t(2x-t))^{\frac{1}{2}}} = \sum_{l=0}^{\infty} \frac{(2l)!(-1)^{2l} t^l}{2^{2l}(l!)^2} (2x-t)^l. \tag{1.64}$$

Employing the binomial formula once again to expand the factor $(2x-t)^l$, we rewrite the right-hand side as

$$\sum_{l=0}^{\infty} \frac{(2l)!(-1)^{2l} t^l}{2^{2l}(l!)^2} \sum_{k=0}^{l} \frac{l!}{k!(l-k)!} (2x)^{l-k}(-t)^k$$

$$= \sum_{l=0}^{\infty} \sum_{k=0}^{l} \frac{(2l)!(-1)^k (2x)^{l-k} t^{k+l}}{2^{2l} l! k! (l-k)!}. \tag{1.65}$$

We now rearrange the double sum by the substitutions $k \to n$ and $l \to l-n$ to write the generating function as

$$T(x,t) = \sum_{l=0}^{\infty} \left[\sum_{n=0}^{[l/2]} \frac{(-1)^n (2l-2n)!}{2^l (l-n)! n! (l-2n)!} x^{l-2n}\right] t^l. \tag{1.66}$$

Comparing this with the right-hand side of Eq. (1.56), which is $\sum_{l=0}^{\infty} P_l(x) t^l$, we obtain the desired result:

$$P_l(x) = \sum_{n=0}^{[l/2]} \frac{(-1)^n (2l-2n)!}{2^l (l-n)! n! (l-2n)!} x^{l-2n}. \tag{1.67}$$

1.3.3 Recursion Relations

Recursion relations are very helpful in operations with Legendre polynomials. Let us differentiate the generating function [Eq. (1.56)] with respect to t:

$$\frac{\partial}{\partial t}T(x,t) = -\frac{-2(x-t)}{2(1-2xt+t^2)^{\frac{3}{2}}} \tag{1.68}$$

$$= \sum_{l=1}^{\infty} P_l(x) l\, t^{l-1}. \tag{1.69}$$

We rewrite this as

$$(x-t)\sum_{l=0}^{\infty} P_l(x)t^l = \sum_{l=1}^{\infty} P_l(x) l\, t^{l-1}\left(1-2xt+t^2\right) \tag{1.70}$$

and expand in powers of t to get

$$\sum_{l=0}^{\infty} t^l(2l+1)xP_l(x) = \sum_{l'=1}^{\infty} P_{l'} l' t^{l'-1} + \sum_{l''=0}^{\infty} t^{l''+1}(l''+1)P_{l''}(x). \tag{1.71}$$

We now make the substitutions $l' = l+1$ and $l'' = l-1$ and collect equal powers of t^l to write

$$\sum_{l=0}^{\infty}\left[(2l+1)xP_l(x) - P_{l+1}(x)(l+1) - lP_{l-1}(x)\right]t^l = 0. \tag{1.72}$$

This equation can only be satisfied for all values of t when the expression inside the square brackets is zero for all l, thus giving the **recursion relation**

$$\boxed{(2l+1)xP_l(x) = (l+1)P_{l+1}(x) + lP_{l-1}(x).} \tag{1.73}$$

Another useful recursion relation is obtained by differentiating $T(x,t)$ with respect to x and following similar steps as

$$\boxed{P_l(x) = P'_{l+1}(x) + P'_{l-1}(x) - 2xP'_l(x).} \tag{1.74}$$

It is also possible to find other recursion relations.

1.3.4 Special Values

In various applications, one needs special values of the Legendre polynomials at the points $x = \pm 1$ and $x = 0$. If we write $x = \pm 1$ in the generating function [Eq. (1.56)], we find

$$1/(1 \mp t) = \sum_{l=0}^{\infty} P_l(1)t^l(\pm 1)^l. \tag{1.75}$$

Expanding the left-hand side using the binomial formula and comparing equal powers of t, we obtain

$$\boxed{P_l(1) = 1, \quad P_l(-1) = (-1)^l.} \tag{1.76}$$

We now set $x = 0$ in the generating function:

$$\frac{1}{\sqrt{1+t^2}} = \sum_{l=0}^{\infty} P_l(0)t^l = \sum_{t=0}^{\infty} (-1)^l \frac{(2l)!}{2^{2l}(l!)^2} t^{2l}, \tag{1.77}$$

to obtain the special values:

$$\boxed{P_{2s+1}(0) = 0, \quad P_{2l}(0) = \frac{(-1)^l(2l)!}{2^{2l}(l!)^2}.} \tag{1.78}$$

1.3.5 Special Integrals

1. In applications, we frequently encounter the integral $\int_0^1 dx\, P_l(x)$. Using the recursion relation in Eq. (1.74), we can rewrite this integral as

$$\int_0^1 dx\ P_l(x) = \int_0^1 dx \left[P'_{l+1}(x) + P'_{l-1}(x) - 2xP'_l(x)\right]. \tag{1.79}$$

The right-hand side can be integrated to write

$$\int_0^1 dx\ P_l(x) = P_{l+1}(1) + P_{l-1}(1) - P_{l+1}(0) - P_{l-1}(0) - 2xP_l(x)|_0^1 + 2\int_0^1 dx\ P_l(x). \tag{1.80}$$

This is simplified using the special values and leads to $\int_0^1 dx\ P_l(x) = P_{l+1}(0) + P_{l-1}(0)$, thus yielding

$$\boxed{\int_0^1 dx\ P_l(x) = \begin{cases} 0, & l \geq 2 \text{ and even}, \\ 1, & l = 0, \\ \dfrac{1}{2(s+1)} P_{2s}(0), & l = 2s+1,\ s = 0, 1, \ldots . \end{cases}} \tag{1.81}$$

2. Another integral useful in dipole calculations is $\int_{-1}^1 dx\, xP_l(x)P_k(x)$. Using the recursion relation in Eq. (1.73), we can rewrite this as

$$\int_{-1}^1 dx\ xP_l(x)P_k(x) = \int_{-1}^1 dx \frac{P_l(x)}{(2k+1)} \left[(k+1)P_{k+1}(x) + kP_{k-1}(x)\right], \tag{1.82}$$

which leads to

$$\int_{-1}^{1} dx\, xP_l(x)P_k(x) = \begin{cases} 0, & k \neq l \pm 1, \\ \dfrac{l}{(2l-1)}\dfrac{2}{(2l+1)}, & k = l-1, \\ \dfrac{l+1}{(2l+3)}\dfrac{2}{(2l+1)}, & k = l+1. \end{cases} \tag{1.83}$$

One can also show the useful integral

$$\int_{-1}^{1} dx\, x^l P_n(x) = \frac{2^{n+1} l! \left(\dfrac{l+n}{2}\right)!}{(l+n+1)!\left(\dfrac{l-n}{2}\right)!}, \quad l-n = |\text{even integer}|. \tag{1.84}$$

1.3.6 Orthogonality and Completeness

We can also write the Legendre equation [Eq. (1.17)] as

$$\frac{d}{dx}\left[\left(1-x^2\right)\frac{dP_l(x)}{dx}\right] + l(l+1)P_l(x) = 0. \tag{1.85}$$

Multiplying this with $P_{l'}(x)$ and integrating over x in the interval $[-1, 1]$, we get

$$\int_{-1}^{1} P_{l'}(x)\left\{\frac{d}{dx}\left[\left(1-x^2\right)\frac{dP_l(x)}{dx}\right] + l(l+1)P_l(x)\right\} dx = 0. \tag{1.86}$$

Using integration by parts, this can be written as

$$\int_{-1}^{1}\left[\left(x^2-1\right)\frac{dP_l(x)}{dx}\frac{dP_{l'}(x)}{dx} + l(l+1)P_{l'}(x)P_l(x)\right] dx = 0. \tag{1.87}$$

Interchanging l and l' and subtracting from Eq. (1.87), we get

$$\left[l(l+1) - l'(l'+1)\right]\int_{-1}^{1} P_{l'}(x)P_l(x)\, dx = 0. \tag{1.88}$$

For $l \neq l'$, this gives $\int_{-1}^{1} P_{l'}(x)P_l(x)\, dx = 0$ and for $l = l'$, it becomes

$$\int_{-1}^{1}\left[P_l(x)\right]^2 dx = N_l, \tag{1.89}$$

where N_l is a finite **normalization constant**.

We can evaluate N_l using the Rodriguez formula [Eq. (1.51)]. We first write

$$N_l = \int_{-1}^{1} P_l^2(x)\,dx = \frac{1}{2^{2l}(l!)^2}\int_{-1}^{1}\frac{d^l}{dx^l}\left(x^2-1\right)^l\frac{d^l}{dx^l}\left(x^2-1\right)^l dx \tag{1.90}$$

and after l-fold integration by parts, we obtain

$$N_l = \frac{(-1)^l}{2^{2l}(l!)^2}\int_{-1}^{1}\left(x^2-1\right)^l\frac{d^{2l}}{dx^{2l}}\left(x^2-1\right)^l dx. \tag{1.91}$$

Using the Leibniz formula:

$$\frac{d^m}{dx^m}A(x)\,B(x) = \sum_{s=0}^{m}\frac{m!}{s!(m-s)!}\frac{d^sA}{dx^s}\frac{d^{m-s}B}{dx^{m-s}}, \tag{1.92}$$

we evaluate the $2l$-fold derivative of $(x^2-1)^l$ as $(2l)!$, thus Eq. (1.91) becomes

$$N_l = \frac{(2l)!}{2^{2l}(l!)^2}\int_{-1}^{1}\left(1-x^2\right)^l dx. \tag{1.93}$$

We now write $(1-x^2)^l$ as

$$\left(1-x^2\right)^l = \left(1-x^2\right)\left(1-x^2\right)^{l-1} = \left(1-x^2\right)^{l-1} + \frac{x}{2l}\frac{d}{dx}\left(1-x^2\right)^l \tag{1.94}$$

to obtain

$$N_l = \frac{(2l-1)}{2l}N_{l-1} + \frac{(2l-1)!}{2^{2l}(l!)^2}\int_{-1}^{1}xd\left[(1-x^2)^l\right], \tag{1.95}$$

which gives

$$N_l = \frac{(2l-1)}{2l}N_{l-1} - \frac{1}{2l}N_l, \tag{1.96}$$

or

$$(2l+1)N_l = (2l-1)N_{l-1}. \tag{1.97}$$

This means that the value of $(2l+1)N_l$ is a constant independent of l. Evaluating the integral in Eq. (1.93) for $l = 0$ gives 2, which determines the normalization constant as

$$\boxed{N_l = \frac{2}{(2l+1)}.} \tag{1.98}$$

Using N_l, we can now define the set of polynomials

$$\boxed{\{U_l(x),\, l = 0, 1, \ldots\},\, U_l(x) = \sqrt{\frac{2l+1}{2}}P_l(x),} \tag{1.99}$$

which satisfies the **orthogonality relation**

$$\boxed{\int_{-1}^{1} U_{l'}(x)U_l(x)\,dx = \delta_{l'l}.} \tag{1.100}$$

At this point, we suffice by saying that this set is also **complete**, that is, in terms of this set any sufficiently well-behaved and at least piecewise continuous function, $\Psi(x)$, can be expressed as an infinite series in the interval $[-1, 1]$ as

$$\Psi(x) = \sum_{l=0}^{\infty} C_l U_l(x). \tag{1.101}$$

We will be more specific about what is meant by sufficiently well-behaved when we discuss the **Sturm–Liouville theory** in Chapter 7. To evaluate the expansion constants C_l, we multiply both sides by $U_{l'}(x)$ and integrate over $[-1, 1]$:

$$\int_{-1}^{1} U_{l'}(x)\Psi(x)\,dx = \sum_{l=0}^{\infty} C_l \int U_{l'}(x)U_l(x)\,dx. \tag{1.102}$$

Using the orthogonality relation [Eq. (1.100)], we can free the constants C_l under the summation sign and obtain

$$C_l = \int_{-1}^{1} U_l(x)\Psi(x)\,dx. \tag{1.103}$$

Orthogonality and the completeness of the Legendre polynomials are very useful in applications.

Example 1.1 ***Legendre polynomials and electrostatics problems***
To find the electric potential in vacuum, we solve the Laplace equation:

$$\vec{\nabla}^2\Psi(\vec{r}) = 0, \tag{1.104}$$

with the appropriate boundary conditions. For problems with azimuthal symmetry, it is advantageous to use the spherical polar coordinates, where the potential does not have any ϕ dependence. Therefore, in the ϕ-dependent part of the solution [Eq. (1.15)], we set $m = 0$. The differential equation to be solved for the r-dependent part is now found by setting $k = 0$ in Eq. (1.10) as

$$\frac{d^2R}{dr^2} + \frac{2}{r}\frac{dR}{dr} - \frac{l(l+1)}{r^2}R(r) = 0. \tag{1.105}$$

The linearly independent solutions of this equation are easily found as r^l and $\frac{1}{r^{l+1}}$, thus giving the general solution of Eq. (1.104) as

$$\Psi(r,\theta) = \sum_{l=0}^{\infty}\left[A_l r^l + \frac{B_l}{r^{l+1}}\right]P_l(x), \quad x = \cos\theta, \tag{1.106}$$

where the constants A_l and B_l are to be determined from the boundary conditions. For example, let us calculate the electric potential outside two semi-spherical conductors with radius a and that are connected by an insulator at the center, where the upper hemisphere is held at potential V_0 and the lower hemisphere is held at potential $-V_0$. Since the potential cannot diverge at infinity, we set the coefficients A_l to zero and write the potential for the outside as

$$\Psi(r,\theta) = \sum_{l=0}^{\infty} \frac{B_l}{r^{l+1}} P_l(x), \quad r \geq a. \tag{1.107}$$

To find the coefficients B_l, we use the boundary conditions at $r = a$ as

$$\Psi(a,\theta) = \sum_{l=0}^{\infty} \frac{B_l}{a^{l+1}} P_l(x) = \begin{cases} V_0, & 0 < x \leq 1, \\ -V_0, & -1 \leq x < 0. \end{cases} \tag{1.108}$$

We multiply both sides by $P_{l'}(x)$ and integrate over x and use the orthogonality relation to get

$$\int_{-1}^{1} \Psi(a,x) P_l(x)\, dx = \frac{B_l}{a^{l+1}} \frac{2}{(2l+1)}, \tag{1.109}$$

$$V_0 \int_0^1 dx\, P_l(x) - V_0 \int_{-1}^0 dx\, P_l(x) = \frac{2B_l}{(2l+1)a^{l+1}}, \tag{1.110}$$

$$B_l = \frac{(2l+1)a^{l+1}}{2} V_0 \int_0^1 \left[1 - (-1)^l\right] P_l(x)\, dx. \tag{1.111}$$

For the even values of l, the expansion coefficients are zero, $B_{2s} = 0$. For the odd values of l, we use the result in Eq. (1.81) to write

$$B_{2s+1} = \frac{(4s+3)}{2} \frac{P_{2s}(0)}{(2s+2)} a^{2s+2}(2V_0), \quad s = 0, 1, 2, \ldots. \tag{1.112}$$

Substituting B_{2s+1} in Eq. (1.107), we finally obtain the potential outside the sphere as

$$\Psi(r,\theta) = V_0 \sum_{s=0}^{\infty} (4s+3) \frac{P_{2s}(0)}{(2s+2)} \frac{a^{2s+2}}{r^{2s+2}} P_{2s+1}(\cos\theta). \tag{1.113}$$

Potential inside can be found similarly.

1.3.7 Asymptotic Forms

In many applications and in establishing the convergence properties of the Legendre series, we need the asymptotic form of the Legendre polynomials for large l. We first write the Legendre Eq. (1.13) with $\Theta(\theta) = P_l(\cos\theta)$, $\lambda = l(l+1)$, and $m = 0$ as

$$P_l''(\cos\theta) + \cot\theta P_l'(\cos\theta) + l(l+1)P_l(\cos\theta) = 0, \tag{1.114}$$

and substitute $P_l(\cos\theta) = u(\theta)/\sqrt{\sin\theta}$, to obtain

$$u''(\theta) + \left[\left(l + \frac{1}{2}\right)^2 + \frac{1}{4\sin^2\theta}\right] u(\theta) = 0. \tag{1.115}$$

For sufficiently large values of l, we can neglect $1/4\sin^2\theta$ and write the above equation as

$$u''(\theta) + \left(l + \frac{1}{2}\right)^2 u(\theta) \approx 0, \tag{1.116}$$

the solution of which is

$$P_l(\cos\theta) \approx \frac{A_l \cos\left[\left(l + \frac{1}{2}\right)\theta + \delta_l\right]}{\sqrt{\sin\theta}}. \tag{1.117}$$

In this asymptotic solution, the amplitude, A_l, and the phase, δ_l, may depend on l. To determine A_l, we use the asymptotic solution in the normalization condition [Eq. (1.89)]:

$$\int_0^{\pi} \sin\theta \left[P_l(\cos\theta)\right]^2 d\theta = \frac{2}{2l+1}, \tag{1.118}$$

to find $A_l \approx \sqrt{\frac{2}{\pi l}}$. To determine the phase, δ_l, we make use of the generating function definition [Eq. (1.56)] for $\theta = \pi/2$:

$$\frac{1}{\sqrt{1+t^2}} = \sum_{l=0}^{\infty} P_l(0)t^n. \tag{1.119}$$

If we use the binomial expansion for the left-hand side, for the odd values of l, we find $P_l(0) = 0$ and for the even values of l, the sign of $P_l(0)$ alternates. This allows us to deduce the value of δ_l as $-\pi/4$, thus allowing us to write the asymptotic solution for the sufficiently large values of l and for a given θ as

$$\boxed{P_l(\cos\theta) \approx \sqrt{\frac{2}{l\pi\sin\theta}} \cos\left[\left(l + \frac{1}{2}\right)\theta - \frac{\pi}{4}\right].} \tag{1.120}$$

1.4 Associated Legendre Equation and Polynomials

We now consider the **associated Legendre equation** (1.16):

$$\boxed{(1-x^2)\frac{d^2Z(x)}{dx^2} - 2x\frac{dZ(x)}{dx} + \left[\lambda - \frac{m^2}{(1-x^2)}\right] Z(x) = 0} \tag{1.121}$$

and try a series solution around $x = 0$ of the form $Z(x) = \sum_{k=0}^{\infty} a_k x^k$, which yields the following recursion relation:

$$(k+4)(k+3)\,a_{k+4} + \left[\left(\lambda - m^2\right) - 2(k+2)^2\right] a_{k+2} + \left[k(k+1) - \lambda\right] a_k = 0. \tag{1.122}$$

Compared with the two-term recursion relation of the Legendre equation [Eq. (1.23)], this has three terms, which makes it difficult to manipulate.

In such situations, in order to get a two-term recursion relation, we study the behavior of the differential equation near the end points. For points near $x = 1$, we introduce a new variable $y = (1 - x)$. Now Eq. (1.121) becomes

$$(2-y)y\frac{d^2Z(y)}{dy^2} + 2(1-y)\frac{dZ(y)}{dy} + \left[\lambda - \frac{m^2}{y(2-y)}\right] Z(y) = 0. \tag{1.123}$$

In the limit as $y \to 0$, this equation can be approximated by

$$2y\frac{d^2Z(y)}{dy^2} + 2\frac{dZ(y)}{dy} - m^2\frac{Z(y)}{2y} = 0. \tag{1.124}$$

To find the solution, we try a power dependence of the form $Z(y) = y^n$ and determine n as $\pm m/2$. Hence, the two linearly independent solutions are $y^{m/2}$ and $y^{-m/2}$. For $m \geq 0$, the solution that remains finite as $y \to 0$ is $y^{\frac{m}{2}}$. Similarly, for points near $x = -1$, we use the substitution $y = (1 + x)$ and obtain the finite solution in the limit $y \to 0$ as $y^{\frac{m}{2}}$. We now substitute in the associated Legendre Eq. (1.121), a solution of the form

$$Z(x) = (1+x)^{m/2}(1-x)^{m/2} f(x) \tag{1.125}$$

$$= (1-x^2)^{m/2} f(x), \tag{1.126}$$

which gives the differential equation to be solved for $f(x)$ as

$$(1-x^2)\frac{d^2f}{dx^2} - 2x(m+1)\frac{df(x)}{dx} + [\lambda - m(m+1)]\,f(x) = 0. \tag{1.127}$$

Note that this equation is valid for both the positive and the negative values of m. We now try a series solution in this equation, $f(x) = \sum_k a_k x^{k+\alpha}$, and obtain a two-term recursion relation as

$$a_{k+2} = a_k \frac{\left[(k+m)(k+m+1) - \lambda\right]}{(k+2)(k+1)}. \tag{1.128}$$

Since in the limit as k goes to infinity, the ratio of two successive terms, $\frac{a_{k+2}}{a_k}$, goes to 1, this series also diverges at the end points. For a finite solution, we restrict the separation constant λ to the values

$$\lambda = (k+m)\left[(k+m) + 1\right]. \tag{1.129}$$

Defining a new integer, $l = k + m$, we obtain

$$\lambda = l(l+1) \quad \text{and} \quad k = l - m. \tag{1.130}$$

Since k takes only positive integer values, m can only take the values $m = -l, \dots, 0, \dots, l$.

1.4.1 Associated Legendre Polynomials $P_l^m(x)$

To obtain the associated Legendre polynomials, we start with the equation that the Legendre polynomials satisfy as

$$(1-x^2)\frac{d^2P_l(x)}{dx^2} - 2x\frac{dP_l(x)}{dx} + l(l+1)P_l(x) = 0. \tag{1.131}$$

Using the **Leibniz formula**:

$$\frac{d^m}{dx^m}[A(x)B(x)] = \sum_{s=0}^{m} \frac{m!}{s!(m-s)!}\left[\frac{d^sA}{dx^s}\right]\left[\frac{d^{m-s}B}{dx^{m-s}}\right], \tag{1.132}$$

m-fold differentiation of Eq. (1.131) yields

$$\begin{aligned}(1-x^2)P_l^{(m+2)}(x) - 2xmP_l^{(m+1)}(x) - \frac{2m(m-1)}{2}P_l^{(m)}(x) \\ = 2xP_l^{(m+1)}(x) + 2mP_l^{(m)}(x) - l(l+1)P_l^{(m)}(x).\end{aligned} \tag{1.133}$$

After simplification, this becomes

$$(1-x^2)P_l^{(m+2)}(x) - 2x(m+1)P_l^{(m+1)}(x) + \left[l(l+1) - m(m+1)\right]P_l^{(m)}(x) = 0, \tag{1.134}$$

where

$$P_l^{(m)}(x) = \frac{d^m}{dx^m}P_l(x). \tag{1.135}$$

Comparing Eq. (1.134) with Eq. (1.127), we obtain $f(x)$ as

$$f(x) = \frac{d^m}{dx^m}P_l(x). \tag{1.136}$$

Using Eq. (1.126), we can now write the finite solutions of the **associated Legendre equation** [Eq. (1.121)] as

$$\boxed{P_l^m(x) = (1-x^2)^{m/2}\frac{d^m}{dx^m}P_l(x), \quad m \geq 0,} \tag{1.137}$$

where the polynomials $P_l^m(x)$ are called the **associated Legendre polynomials**.

For the negative values of m, the associated Legendre polynomials are defined as

$$\boxed{P_l^{-m}(x) = (-1)^m\frac{(l-m)!}{(l+m)!}P_l^m(x), \quad m \geq 0.} \tag{1.138}$$

We will see how this is obtained in Section 1.4.5.

1.4.2 Orthogonality

To derive the orthogonality relation of the associated Legendre polynomials, we use the Rodriguez formula [Eq. (1.51)] for the Legendre polynomials to write

$$\int_{-1}^{1} P_l^m(x)P_{l'}^m(x)dx = \frac{(-1)^m}{2^{l+l'}l!l'!}\left\{\int_{-1}^{1} X^m \left[\frac{d^{l+m}}{dx^{l+m}}X^l\right]\left[\frac{d^{l'+m}}{dx^{l'+m}}X^{l'}\right]dx\right\} \tag{1.139}$$

$$= \frac{(-1)^m}{2^{l+l'}l!l'!}I, \tag{1.140}$$

where

$$I = \int_{-1}^{1} X^m \left[\frac{d^{l+m}}{dx^{l+m}}X^l\right]\left[\frac{d^{l'+m}}{dx^{l'+m}}X^{l'}\right]dx, \quad X = x^2 - 1, \tag{1.141}$$

$$P_l^m(x) = \left(1-x^2\right)^{\frac{m}{2}}\frac{d^m}{dx^m}P_l(x); \quad P_l(x) = \frac{1}{2^l l!}\frac{d^l}{dx^l}\left(x^2-1\right)^l. \tag{1.142}$$

The integral, I, in Eq. (1.141), after $(l'+m)$-fold integration by parts, becomes

$$I = (-1)^{l'+m}\int_{-1}^{1}\frac{d^{l'+m}}{dx^{l'+m}}\left[X^m\frac{d^{l+m}}{dx^{l+m}}X^l\right]X^{l'}\,dx. \tag{1.143}$$

Using the Leibniz formula [Eq. (1.132)], we get

$$I = (-1)^{l'+m}\int_{-1}^{1} X^{l'}\sum_{\lambda}\binom{l'+m}{\lambda}\left[\frac{d^{l'+m-\lambda}}{dx^{l'+m-\lambda}}X^m\right]\left[\frac{d^{l+m+\lambda}}{dx^{l+m+\lambda}}X^l\,dx\right]. \tag{1.144}$$

Since the highest power in X^m is x^{2m} and the highest power in X^l is x^{2l}, the summation is empty unless the inequalities

$$l'+m-\lambda \le 2m \quad \text{and} \quad l+m+\lambda \le 2l \tag{1.145}$$

are simultaneously satisfied. The first inequality gives $\lambda \ge l'-m$, while the second one gives $\lambda \le l-m$. For $m \ge 0$, if we assume $l < l'$, the summation [Eq. (1.144)] does not contain any term that is different from zero; hence the integral is zero. Since the expression in Eq. (1.139) is symmetric with respect to l' and l, this result is also valid for $l > l'$. When $l = l'$, these inequalities can be satisfied only for the single value of $\lambda = l-m$. Now the summation contains only one term, and Eq. (1.144) becomes

$$I = (-1)^{l+m}\int_{-1}^{1} X^l\binom{l+m}{l-m}\left[\frac{d^{2m}}{dx^{2m}}X^m\right]\left[\frac{d^{2l}}{dx^{2l}}X^l\right]dx \tag{1.146}$$

$$= (-1)^{l+m}\binom{l+m}{l-m}(2l)!(2m)!\int_{-1}^{1} X^l\,dx. \tag{1.147}$$

The integral in I can be evaluated as

$$\int_{-1}^{1} X^l \, dx = \int_{-1}^{1} (x^2 - 1)^l dx \tag{1.148}$$

$$= 2(-1)^l \int_0^{\pi/2} (\sin\theta)^{2l+1} d\theta \tag{1.149}$$

$$= \frac{(-1)^l 2^{l+1} l!}{3.5 \ldots (2l+1)} \tag{1.150}$$

$$= \frac{(-1)^l 2^{2l+1} (l!)^2}{(2l+1)!}. \tag{1.151}$$

Since the binomial coefficients are given as

$$\binom{l+m}{l-m} = \frac{(l+m)!}{(l-m)!(2m)!}, \tag{1.152}$$

we write

$$\int_{-1}^{1} P_l^m(x) P_{l'}^m(x) \, dx = \frac{(-1)^m}{2^{2l}(l!)^2} \frac{(l+m)!(-1)^{l+m}}{(l-m)!(2m)!} (2l)!(2m)! \frac{(-1)^l 2^{2l+1} (l!)^2}{(2l+1)!} \delta_{ll'}, \tag{1.153}$$

which after simplifying gives the **orthogonality relation** of the associated Legendre polynomials as

$$\boxed{\int_{-1}^{1} P_l^m(x) P_{l'}^m(x) dx = \frac{(l+m)!}{(l-m)!} \left[\frac{2}{(2l+1)}\right] \delta_{ll'}.} \tag{1.154}$$

Associated Legendre Polynomials

$$\begin{aligned} P_0^0(x) &= 1, \\ P_1^1(x) &= (1-x^2)^{1/2} = \sin\theta, \\ P_2^1(x) &= 3x(1-x^2)^{1/2} = 3\cos\theta\sin\theta, \\ P_2^2(x) &= 3(1-x^2) = 3\sin^2\theta, \\ P_3^1(x) &= \frac{3}{2}(5x^2-1)(1-x^2)^{1/2} = \frac{3}{2}(5\cos^2\theta - 1)\sin\theta, \\ P_3^2(x) &= 15x(1-x^2) = 15\cos\theta\sin^2\theta, \\ P_3^3(x) &= 15(1-x^2)^{3/2} = 15\sin^3\theta. \end{aligned} \tag{1.155}$$

1.4.3 Recursion Relations

Operating on the recursion relation [Eq. (1.73)]:

$$(l+1)P_{l+1}(x) - (2l+1)x\, P_l(x) + lP_{l-1}(x) = 0 \tag{1.156}$$

with

$$(1-x^2)^{m/2}\frac{d^m}{dx^m} \tag{1.157}$$

and using the relation

$$(1-x^2)^{m/2}\frac{d^m P_l}{dx^m} = P_l^m(x), \tag{1.158}$$

we obtain a recursion relation for $P_l^m(x)$ as

$$\boxed{\begin{aligned}(l+1)P_{l+1}^m(x) - (2l+1)xP_l^m(x) + lP_{l-1}^m(x)\\ + m(2l+1)\sqrt{1-x^2}P_{l-1}^{m-1}(x) = 0.\end{aligned}} \tag{1.159}$$

Two other useful recursion relations for $P_l^m(x)$ can be obtained as follows:

$$\boxed{(l+1-m)P_{l+1}^m(x) - (2l+1)xP_l^m(x) + (l+m)P_{l-2}^m(x) = 0,} \tag{1.160}$$

$$\boxed{P_l^{m+2} + \frac{2(m+1)x}{\sqrt{1-x^2}}P_l^{m+1}(x) + (l-m)(l+m+1)P_l^m(x) = 0.} \tag{1.161}$$

To prove the first recursion relation [Eq. (1.160)], we write

$$\frac{d}{dx}\left[P_{l+1}(x) - P_{l-1}(x)\right] = \sum_{k=0}^{l} a_k P_k(x), \tag{1.162}$$

which follows from the fact that the left-hand side is a polynomial of order l. Using the orthogonality relation of the Legendre polynomials [Eq. (1.100)], we can evaluate a_k as

$$a_k = \frac{2k+1}{2}\int_{-1}^{1} P_k(x)\frac{d}{dx}\left[P_{l+1}(x) - P_{l-1}(x)\right] dx. \tag{1.163}$$

After integration by parts and using the special values [Eq. (1.76)]:

$$P_l(1) = 1, \quad P_l(-1) = (-1)^l, \tag{1.164}$$

we obtain

$$a_k = -\frac{2k+1}{2}\int_{-1}^{1} P_k'(x)\left[P_{l+1}(x) - P_{l-1}(x)\right] dx. \tag{1.165}$$

In this expression, $P_k'(x)$ is of order $k-1$. Since $P_{l+1}(x)$ and $P_{l-1}(x)$ are orthogonal to all polynomials of order $l-2$ or lower, $a_k = 0$ for $k = 0, 1, \ldots, (l-1)$, hence we obtain

$$a_l = -\frac{2l+1}{2}\int_{-1}^{1} P_l'(x)[P_{l+1}(x) - P_{l-1}(x)]dx \tag{1.166}$$

$$= \frac{2l+1}{2}\int_{-1}^{1} P_l'(x)P_{l-1}(x)dx \tag{1.167}$$

$$= \frac{2l+1}{2}\left[P_l(x)P_{l-1}(x)|_{-1}^{1} - \int_{-1}^{1} P_l(x)P_{l-1}'(x)dx\right] \tag{1.168}$$

$$= 2l + 1. \tag{1.169}$$

Substituting this into Eq. (1.162) gives

$$\frac{d}{dx}\left[P_{l+1}(x) - P_{l-1}(x)\right] = (2l+1)P_l(x). \tag{1.170}$$

Operating on this with d^{m-1}/dx^{m-1} and multiplying with $(1-x^2)^{m/2}$, we finally obtain the desired result:

$$(l+1-m)P_{l+1}^m(x) - (2l+1)xP_l^m(x) + (l+m)P_{l-2}^m(x) = 0. \tag{1.171}$$

The second recursion relation [Eq. (1.161)] can be obtained using the Legendre Eq. (1.131):

$$(1-x^2)P_l''(x) - 2xP_l'(x) + l(l+1)P_l(x) = 0, \tag{1.172}$$

and by operating on it with $(1-x^2)^{m/2}d^m/dx^m$.

1.4.4 Integral Representations

1) Using the Cauchy integral formula:

$$\frac{d^n f(z_0)}{dz_0^n} = \frac{n!}{2\pi i}\oint_C \frac{f(z)dz}{(z-z_0)^{n+1}}, \tag{1.173}$$

where $f(z)$ is analytic on and within the closed contour C, and where z_0 is a point within C, we can obtain an integral representation of $P_l(x)$ and $P_l^m(x)$. Using any closed contour C enclosing the point $z_0 = x$ on the real axis and the Rodriguez formula for $P_l(x)$ [Eq. (1.51)]:

$$P_l(x) = \frac{1}{2^l l!}\frac{d^l}{dx^l}(x^2-1)^l, \tag{1.174}$$

we can write

$$P_l(x) = \frac{2^{-l}}{2\pi i}\oint_C \frac{(z^2-1)^l}{(z-x)^{l+1}}dz. \tag{1.175}$$

Using the definition [Eq. (1.142)]:

$$P_l^m(x) = (1-x^2)^{m/2}\frac{d^m}{dx^m}P_l(x), \tag{1.176}$$

we finally obtain

$$P_l^m(x) = \frac{(l+m)!(1-x^2)^{m/2}}{2^l(2\pi i)l!} \oint_C \frac{(z^2-1)^l}{(z-x)^{l+m+1}} dz. \tag{1.177}$$

2) In Eq. (1.173), C is any closed contour enclosing the point x. Now let C be a circle with the radius $\sqrt{1-x^2}$ and centered at x with the parametrization

$$z = \cos\theta + i \sin\theta e^{i\phi}. \tag{1.178}$$

Using ϕ as the new integration variable, we obtain the following integral representation:

$$P_l^m(\cos\theta) = \frac{(-1)^m i^m (l+m)!}{2\pi l!} \int_{-\pi}^{\pi} [\cos\theta + i\sin\theta\cos\phi]^l e^{-im\phi}\, d\phi. \tag{1.179}$$

The advantage of this representation is that the definite integral is taken over the real domain.

Proof: Using Eq. (1.178), we first write the following relations:

$$(z - \cos\theta)^{l+m+1} = i^{l+m+1} \sin^{l+m+1}\theta e^{i(l+m+1)\phi}, \tag{1.180}$$

$$(z^2 - 1) = 2i \sin\theta e^{i\phi} [\cos\theta + i \sin\theta \cos\phi], \tag{1.181}$$

$$dz = -\sin\theta e^{i\phi}\, d\phi, \tag{1.182}$$

which when substituted into Eq. (1.177) gives the desired result [Eq. (1.179)]. Note that $x = \cos\theta$.

Example 1.2 ***Integral representation***

Show that the function $V(x, y, z) = [z + ix\cos u + iy\sin u]^l$, where (x, y, z) are the Cartesian coordinates of a point and u is a real parameter, is a solution of the Laplace equation. Next, show that an integral representation of $P_l^m(\cos\theta)$ given in terms of the angles, θ and ϕ, of the spherical polar coordinates also yields Eq. (1.179) up to a proportionality constant.

Solution

First evaluate the derivatives V_{xx}, V_{yy}, and V_{yy} to show that

$$\vec{\nabla}^2 V = V_{xx} + V_{yy} + V_{zz} = 0. \tag{1.183}$$

Since u is just a real parameter,

$$\int_{-\pi}^{\pi} [z + ix\cos u + iy\sin u]^l e^{imu}\, du \tag{1.184}$$

is also a solution of the Laplace equation. We now transform Cartesian coordinates (x, y, z) to spherical polar coordinates (r, θ, ϕ) and let $\phi - u = \psi$, to obtain

$$r^l e^{im\phi} \int_{-\pi}^{+\pi} [\cos\theta + i \sin\theta \cos\psi]^l e^{-im\psi} (-d\psi). \tag{1.185}$$

Comparing with the solution of the Laplace equation, $r^l e^{im\phi} P_l^m(\cos\theta)$, we see that the integral

$$\int_{-\pi}^{+\pi} [\cos\theta + i \sin\theta \cos\psi]^l e^{-im\psi} \, d\psi, \tag{1.186}$$

must be proportional to $P_l^m(\cos\theta)$. Inserting the proportionality constant [Eq. (1.179)] gives

$$P_l^m(\cos\theta) = \frac{(-1)^m i^m}{2\pi} \frac{(l+m)!}{l!} \int_{-\pi}^{+\pi} [\cos\theta + i \sin\theta \cos\psi]^l e^{-im\psi} \, d\psi. \tag{1.187}$$

If we write $e^{-im\psi} = \cos m\psi - i \sin m\psi$, from symmetry, the integral corresponding to $-i \sin m\psi$ vanishes, thus allowing us to write

$$P_l^m(\cos\theta) = \frac{(-1)^m i^m}{2\pi} \frac{(l+m)!}{l!} \int_{-\pi}^{+\pi} [\cos\theta + i \sin\theta \cos\psi]^l \cos m\psi \, d\psi. \tag{1.188}$$

1.4.5 Associated Legendre Polynomials for $m < 0$

The differential equation that $P_l^m(x)$ satisfies [Eq. (1.16)], where $\lambda = l(l+1)$, depends on l as $l(l+1)$, which is unchanged when we let $l \to -l-1$. In other words, if we replace l with $-l-1$ in the right-hand side of Eq. (1.188), we should get the same solution. Under the same replacement,

$$\frac{(l+m)!}{l!} = (l+m)(l+m-1)\cdots(l+1) \tag{1.189}$$

becomes

$$(-l-1+m)(-l-1+m-1)\cdots(-l) = (-1)^m \frac{l!}{(l-m)!}, \tag{1.190}$$

hence we can write

$$P_l^m(x) = \frac{(-1)^m (-i)^m l!}{2\pi (l-m)!} \int_{-\pi}^{+\pi} \frac{\cos m\psi \, d\psi}{[\cos\theta + i \sin\theta \cos\psi]^{l+1}}. \tag{1.191}$$

Since m appears in the differential equation [Eq. (1.16)] as m^2, we can also replace m by $-m$ in Eq. (1.188), thus allowing us to write

$$P_l^{-m}(x) = \frac{(-1)^m i^{-m}}{2\pi} \frac{(l-m)!}{l!} \int_{-\pi}^{+\pi} [\cos\theta + i \sin\theta \cos\psi]^l \cos m\psi \, d\psi \tag{1.192}$$

$$= \frac{(-1)^m (i)^m l!}{2\pi(l+m)!} \int_{-\pi}^{+\pi} \frac{\cos m\psi \; d\psi}{[\cos\theta + i \sin\theta \cos\psi]^{l+1}}. \tag{1.193}$$

Comparing Eq. (1.193) with Eq. (1.191), we obtain

$$\boxed{P_l^{-m}(x) = (-1)^m \frac{(l-m)!}{(l+m)!} P_l^m(x).} \tag{1.194}$$

1.5 Spherical Harmonics

We have seen that the solution of Eq. (1.14) with respect to the independent variable ϕ is given as

$$\Phi(\phi) = Ae^{im\phi} + Be^{-im\phi}. \tag{1.195}$$

Imposing the periodic boundary condition:

$$\Phi_m(\phi + 2\pi) = \Phi_m(\phi), \tag{1.196}$$

we see that the separation constant m has to take ±integer values. However, in Section 1.4, we have also seen that m must be restricted further to the integer values $-l, \ldots, 0, \ldots, l$. We can now define another complete and orthonormal set as

$$\left\{ \Phi_m(\phi) = \frac{1}{\sqrt{2\pi}} e^{im\phi}, \; m = -l, \ldots, 0, \ldots, l \right\}. \tag{1.197}$$

This set satisfies the orthogonality relation

$$\int_0^{2\pi} d\phi \Phi_{m'}(\phi) \Phi_m^*(\phi) = \delta_{mm'}. \tag{1.198}$$

We now combine the two sets, $\{\Phi_m(\phi)\}$ and $\{P_l^m(\theta)\}$, to define a new complete and orthonormal set called the **spherical harmonics** as

$$\boxed{Y_l^m(\theta, \phi) = (-1)^m \sqrt{\frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!}} e^{im\phi} P_l^m(\cos\theta), \quad m \geq 0.} \tag{1.199}$$

In conformity with applications to quantum mechanics and atomic spectroscopy, we have introduced the factor $(-1)^m$. It is also called the **Condon-Shortley phase**. The definition of spherical harmonics can be extended to the negative m values as

$$\boxed{Y_l^{-m}(\theta, \phi) = (-1)^m Y_l^{m*}(\theta, \phi), \quad m \geq 0.} \tag{1.200}$$

The **orthogonality relation** of $Y_l^m(\theta, \phi)$ is given as

$$\boxed{\int_0^{2\pi} d\varphi \int_0^{\pi} d\theta \ \sin\theta Y_{l'}^{m'*}(\theta, \phi) Y_l^m(\theta, \phi) = \delta_m^{m'} \delta_l^{l'}.} \tag{1.201}$$

Since they also form a complete set, any sufficiently well-behaved and at least piecewise continuous function $g(\theta, \phi)$ can be expressed in terms of $Y_l^m(\theta, \phi)$ as

$$g(\theta, \phi) = \sum_{l=0}^{\infty} \sum_{m=-l}^{m=l} A_m^l Y_l^m(\theta, \phi), \tag{1.202}$$

where the expansion coefficients A_m^l are given as

$$A_m^l = \int\int d\phi \ d\theta \ \sin\theta g(\theta, \phi) Y_l^{m*}(\theta, \phi). \tag{1.203}$$

Looking back at Eq. (1.11) with $\lambda = l(l+1)$, we see that the spherical harmonics satisfy the differential equation

$$\boxed{\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left[\sin\theta\frac{\partial Y_l^m(\theta, \phi)}{\partial\theta}\right] + \frac{1}{\sin^2\theta}\frac{\partial^2 Y_l^m(\theta, \phi)}{\partial\phi^2} + l(l+1)Y_l^m(\theta, \phi) = 0.} \tag{1.204}$$

If we rewrite this equation as

$$\boxed{\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left[\sin\theta\frac{\partial}{\partial\theta}\right] + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right] Y_l^m(\theta, \phi) = -l(l+1)Y_l^m(\theta, \phi),} \tag{1.205}$$

aside from a factor of $\hbar$, the left-hand side is nothing but the square of the angular momentum operator in quantum mechanics:

$$\vec{L}^2 = (\vec{r} \times \vec{p})^2 = \left(\vec{r} \times \frac{\hbar}{i}\vec{\nabla}\right)^2, \tag{1.206}$$

where in spherical polar coordinates

$$\boxed{\vec{L}^2 = -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left[\sin\theta\frac{\partial}{\partial\theta}\right] + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right].} \tag{1.207}$$

The fact that the separation constant λ is restricted to integer values, in quantum mechanics means that the magnitude of the angular momentum is quantized. From Eq. (1.205), it is seen that the spherical harmonics are also the eigenfunctions of the $\vec{L}^2$ operator.

Spherical Harmonics $Y_l^m(\theta, \phi)$

$$l = 0 \left\{ Y_0^0 = \frac{1}{\sqrt{4\pi}} \right. ,$$

$$l = 1 \left\{ \begin{aligned} Y_1^1 &= -\sqrt{\frac{3}{8\pi}} \sin\theta e^{i\phi}, \\ Y_1^0 &= +\sqrt{\frac{3}{4\pi}} \cos\theta, \\ Y_1^{-1} &= +\sqrt{\frac{3}{8\pi}} \sin\theta e^{-i\phi}, \end{aligned} \right.$$

$$l = 2 \left\{ \begin{aligned} Y_2^2 &= +\frac{1}{4}\sqrt{\frac{15}{2\pi}} \sin^2\theta e^{2i\phi}, \\ Y_2^1 &= -\sqrt{\frac{15}{8\pi}} \sin\theta \cos\theta e^{i\phi}, \\ Y_2^0 &= +\sqrt{\frac{5}{4\pi}} \left(\frac{3}{2}\cos^2\theta - \frac{1}{2}\right), \\ Y_2^{-1} &= +\sqrt{\frac{15}{8\pi}} \sin\theta \cos\theta e^{-i\phi}, \\ Y_2^{-2} &= +\frac{1}{4}\sqrt{\frac{15}{2\pi}} \sin^2\theta e^{-2i\phi}, \end{aligned} \right.$$

$$l = 3 \left\{ \begin{aligned} Y_3^3 &= -\frac{1}{4}\sqrt{\frac{35}{4\pi}} \sin^3\theta e^{3i\phi}, \\ Y_3^2 &= +\frac{1}{4}\sqrt{\frac{105}{2\pi}} \sin^2\theta \cos\theta e^{2i\phi}, \\ Y_3^1 &= -\frac{1}{4}\sqrt{\frac{21}{4\pi}} \sin\theta \left(5\cos^2\theta - 1\right) e^{i\phi}, \\ Y_3^0 &= +\sqrt{\frac{7}{4\pi}} \left(\frac{5}{2}\cos^3\theta - \frac{3}{2}\cos\theta\right), \\ Y_3^{-1} &= +\frac{1}{4}\sqrt{\frac{21}{4\pi}} \sin\theta \left(5\cos^2\theta - 1\right) e^{-i\phi}, \\ Y_3^{-2} &= +\frac{1}{4}\sqrt{\frac{105}{2\pi}} \sin^2\theta \cos\theta e^{-2i\phi}, \\ Y_3^{-3} &= +\frac{1}{4}\sqrt{\frac{35}{4\pi}} \sin^3\theta e^{-3i\phi}. \end{aligned} \right.$$

1.5.1 Addition Theorem of Spherical Harmonics

Spherical harmonics are defined as [Eq. (1.199)]

$$Y_l^m(\theta, \phi) = (-1)^m \sqrt{\frac{(2l+1)}{4\pi}\frac{(l-m)!}{(l+m)!}} e^{im\phi} P_l^m(\cos\theta), \tag{1.208}$$

where the orthogonality relation is given as

$$\int_0^{2\pi}\int_0^{\pi} d\phi' \, d\theta' \sin\theta' Y_l^{m*}(\theta', \phi') Y_{l'}^{m'}(\theta', \phi') = \delta_{mm'}\delta_{ll'}. \tag{1.209}$$

Since the spherical harmonics form a complete and an orthonormal set, any sufficiently smooth function $g(\theta, \phi)$ can be represented as the series

$$g(\theta, \phi) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} A_m^l Y_l^m(\theta, \phi), \tag{1.210}$$

where the expansion coefficients are given as

$$A_m^l = \int_0^{2\pi}\int_0^{\pi} d\phi \, d\theta \sin\theta g(\theta, \phi) Y_l^{m*}(\theta, \phi). \tag{1.211}$$

Substituting A_m^l back into $g(\theta, \phi)$, we write

$$g(\theta, \phi) = \int_0^{2\pi}\int_0^{\pi} d\phi' \, d\theta' \sin\theta' g(\theta', \phi') \sum_{l=0}^{\infty}\sum_{m=-l}^{l} Y_l^m(\theta, \phi) Y_l^{m*}(\theta', \phi'). \tag{1.212}$$

Substituting the definition of spherical harmonics, this also becomes

$$g(\theta, \phi) = \int_0^{2\pi}\int_0^{\pi} d\phi' \, d\theta' \sin\theta' g(\theta', \phi') \times \sum_{l=0}^{\infty}\sum_{m=-l}^{l} \frac{(2l+1)}{4\pi}\frac{(l-m)!}{(l+m)!} e^{im\phi} P_l^m(\cos\theta) e^{-im\phi'} P_l^m(\cos\theta'), \tag{1.213}$$

$$g(\theta, \phi) = \int_0^{2\pi}\int_0^{\pi} d\phi' \, d\theta' \sin\theta' g(\theta', \phi') \times \sum_{l=0}^{\infty} \frac{(2l+1)}{4\pi} \sum_{m=-l}^{l} \frac{(l-m)!}{(l+m)!} e^{im(\phi-\phi')} P_l^m(\cos\theta) P_l^m(\cos\theta'). \tag{1.214}$$

In this equation, angular coordinates (θ, ϕ) give the orientation of the position vector $\overrightarrow{r} = (r, \theta, \phi)$ which is also called the field point and $\overrightarrow{r}' = (r', \theta', \phi')$ represents the source point. We now orient our axes so that the field point $\overrightarrow{r}$ aligns with the $\overline{z}$-axis of the new coordinates. Hence, θ in the new coordinates is 0 and the angle θ' that $\overrightarrow{r}'$ makes with the $\overline{z}$-axis is γ (Figure 1.1).

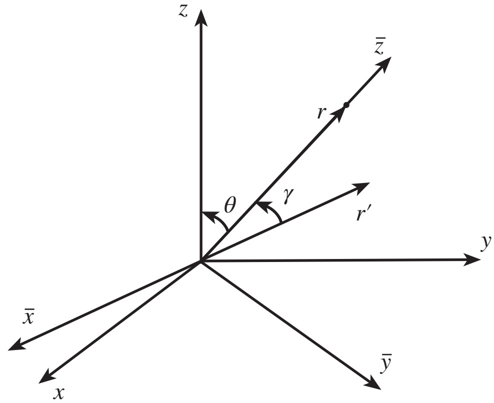

Figure 1.1 Addition theorem.

We first make a note of the following special values:

$$P_l(\cos 0) = P_l(1) = 1, \tag{1.215}$$

$$P_l^m(\cos 0) = P_l^m(1) = 0, \quad m > 0. \tag{1.216}$$

From spherical trigonometry, the angle γ between the vectors $\vec{r}$ and $\vec{r}'$ is related to (θ, ϕ) and (θ', ϕ') as $\cos\gamma = \cos\theta\cos\theta' + \sin\theta\sin\theta'\cos(\phi - \phi')$. In terms of the new orientation of our axes, we now write Eq. (1.214) as

$$\begin{aligned} g(0, -) = \int_0^{2\pi}\int_0^{\pi} d\phi'\, d\theta' \sin\theta' g(\theta', \phi') \sum_{l=0}^{\infty} \frac{(2l+1)}{4\pi} \Bigg\{ P_l^0(\cos 0) P_l^0(\cos\theta') \\ + \sum_{m=1}^{l} \frac{(l-m)!}{(l+m)!} e^{-im\phi'} P_l^m(\cos 0) P_l^m(\cos\theta') \\ + \sum_{m=-l}^{-1} \frac{(l-m)!}{(l+m)!} e^{-im\phi'} P_l^m(\cos 0) P_l^m(\cos\theta') \Bigg\}. \end{aligned} \tag{1.217}$$

Note that in the new orientation of our axes, we are still using primes to denote the coordinates of the source point $\vec{r}'$. In other words, the angular variables, θ' and ϕ', in Eq. (1.217) are now measured in terms of the new orientation of our axes. Naturally, rotation does not affect the magnitudes of $\vec{r}$ and $\vec{r}'$. Since $g(\theta, \phi)$ is a scalar function on the surface of a sphere, its numerical value at a given point on the sphere is also independent of the orientation of our axes. Hence, in the new orientation of our axes, the numerical value of g, that is, $g(0, -)$, is still equal to $g(\theta, \phi)$, where in $g(\theta, \phi)$ the angles are measured in terms of the original orientation of our axes. Hence we can write

$$g(\theta,\phi) = g(0,-) = \int_0^{2\pi}\int_0^{\pi} d\phi'\ d\theta' \sin\theta' g(\theta',\phi') \sum_{l=0}^{\infty} \frac{(2l+1)}{4\pi} \left\{ P_l(1)P_l(\cos\gamma) + \sum_{m=1}^{l} \frac{(l-m)!}{(l+m)!} e^{-im\phi'} P_l^m(1) P_l^m(\cos\gamma) + \sum_{m=-l}^{-1} \frac{(l-m)!}{(l+m)!} e^{-im\phi'} P_l^m(1) P_l^m(\cos\gamma) \right\}. \tag{1.218}$$

Substituting the special values in Eqs. (1.215) and (1.216), this becomes

$$g(\theta,\phi) = \int_0^{2\pi}\int_0^{\pi} d\phi'\ d\theta' \sin\theta' g(\theta',\phi') \sum_{l=0}^{\infty} \frac{(2l+1)}{4\pi} P_l(\cos\gamma). \tag{1.219}$$

Comparison of Eqs. (1.219) and (1.212) gives the **addition theorem** of spherical harmonics:

$$\boxed{\frac{(2l+1)}{4\pi} P_l(\cos\gamma) = \sum_{m=-l}^{l} Y_l^m(\theta,\phi) Y_l^{m*}(\theta',\phi').} \tag{1.220}$$

Sometimes we need the addition theorem written in terms of $P_l^m(\cos\theta)$ as

$$P_l(\cos\gamma) = P_l(\cos\theta)P_l(\cos\theta') + 2\sum_{m=1}^{l} \frac{(l-m)!}{(l+m)!} P_l^m(\cos\theta) P_l^m(\cos\theta') \cos m(\phi-\phi'). \tag{1.221}$$

If we set $\gamma = 0$, the result is the **sum rule**:

$$\boxed{\frac{(2l+1)}{4\pi} = \sum_{m=-l}^{l} |Y_l^m(\theta,\phi)|^2.} \tag{1.222}$$

Another derivation of the addition theorem using the rotation matrices is given in Section 10.8.13.

Note: In spherical coordinates, a general solution of Laplace equation, $\vec{\nabla}^2\Phi(r,\theta,\phi) = 0$, can be written as

$$\boxed{\Phi(r,\theta,\phi) = \sum_{l=0}^{\infty}\sum_{m=-l}^{m=l} \left[A_{lm} r^l + B_{lm} r^{-(l+1)}\right] Y_{lm}(\theta,\phi),} \tag{1.223}$$

where A_{lm} and B_{lm} are to be evaluated using the appropriate boundary conditions and the orthogonality condition of the spherical harmonics. The fact that under rotations $\Phi(r,\theta,\phi)$ remains to be solution of the Laplace operator follows from the fact that the Laplace operator, $\overrightarrow{\nabla}^2 = \overrightarrow{\nabla} \cdot \overrightarrow{\nabla}$, is invariant under rotations. That is, $\overrightarrow{\nabla}^2 = \overrightarrow{\nabla}'^2$. On the surface of a sphere, $r = R$, the angular part of the Laplace equation reduces to

$$\boxed{\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right] Y_{lm}(\theta,\phi) + l(l+1)Y_{lm}(\theta,\phi) = 0,} \tag{1.224}$$

which is the differential equation that the spherical harmonics satisfy.

1.5.2 Real Spherical Harmonics

Aside from applications to classical physics and quantum mechanics, spherical harmonics have found interesting applications in **computer graphics** and **cinematography** in terms of a technique called the **spherical harmonic lighting**. As in spherical harmonic lighting, in some applications, we require only the real-valued spherical harmonics:

$$y_l^m = \begin{cases} \sqrt{2}\mathrm{Re}(Y_l^m) = \sqrt{2}N_l^m \cos(m\phi)P_l^m(\cos\theta), & m > 0, \\ Y_l^0 = N_l^0 P_l^0(\cos\theta), & m = 0, \\ \sqrt{2}\mathrm{Im}(Y_l^m) = \sqrt{2}N_l^{|m|} \sin(|m|\phi)P_l^{|m|}(\cos\theta), & |m| < 0, \end{cases} \tag{1.225}$$

where

$$N_l^m = \sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}}. \tag{1.226}$$

Since the spherical harmonics with $m = 0$ define zones parallel to the equator on the unit sphere, they are called **zonal harmonics**. Spherical harmonics of the form $Y_{|m|}^m$ are called **sectoral harmonics**, while all the other spherical harmonics are called **tesseral harmonics**, which usually divide the unit sphere into several blocks in latitude and longitude.

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Problems

1 Locate and classify the singular points of each of the following differential equations:

(i) Laguerre equation:

$$x\frac{d^2y_n}{dx^2} + (1-x)\frac{dy_n}{dx} + ny_n = 0.$$

(ii) Quantum harmonic oscillator equation:

$$\frac{d^2\Psi_\varepsilon(x)}{dx^2} + \left(\varepsilon - x^2\right)\Psi_\varepsilon(x) = 0.$$

(iii) Bessel equation:

$$x^2J''_m(x) + xJ'_m(x) + \left(x^2 - m^2\right)J_m(x) = 0.$$

(iv)

$$\left(x^2 - 4x\right)\frac{d^2y}{dx^2} + (x+8)\frac{dy}{dx} + 2y = 0.$$

(v)

$$\left(x^4 - 2x^3 + x^2\right)\frac{d^2y}{dx^2} + (x-1)\frac{dy}{dx} + 2x^2y = 0.$$

(vi) Chebyshev equation:

$$\left(1 - x^2\right)\frac{d^2y}{dx^2} - x\frac{dy}{dx} + n^2y = 0.$$

(vii) Gegenbauer equation:

$$\left(1 - x^2\right)\frac{d^2C_n^\lambda(x)}{dx^2} - (2\lambda+1)x\frac{dC_n^\lambda(x)}{dx} + n(n+2\lambda)C_n^\lambda(x) = 0.$$

(viii) Hypergeometric equation:

$$x(1-x)\frac{d^2y(x)}{dx^2} + [c-(a+b+1)x]\frac{dy(x)}{dx} - aby(x) = 0.$$

(ix) Confluent Hypergeometric equation:

$$z\frac{d^2y(z)}{dz^2} + [c-z]\frac{dy(z)}{dz} - ay(z) = 0.$$

2 For the following differential equations, use the Frobenius method to find solutions about $x = 0$:

(i) $$2x^3\frac{d^2y}{dx^2} + 5x^2\frac{dy}{dx} + x^3y = 0.$$

(ii) $$x^3\frac{d^2y}{dx^2} + 3x^2\frac{dy}{dx} + \left(x^3 + \frac{8}{9}x\right)y = 0.$$

(iii) $$x^3\frac{d^2y}{dx^2} + 3x^2\frac{dy}{dx} + \left(x^3 + \frac{3}{4}x\right)y = 0.$$

(iv) $$x^2\frac{d^2y}{dx^2} + 3x\frac{dy}{dx} + (2x+1)\,y = 0.$$

(v) $$x^3\frac{d^2y}{dx^2} + x^2\frac{dy}{dx} + \left(8x^3 - 9x\right)y = 0.$$

(vi) $$x^2\frac{d^2y}{dx^2} + x\frac{dy}{dx} + x^2y = 0.$$

(vii) $$x\frac{d^2y}{dx^2} + (1-x)\frac{dy}{dx} + 4y = 0.$$

(viii) $$2x^3\frac{d^2y}{dx^2} + 5x^2\frac{dy}{dx} + \left(x^3 - 2x\right)y = 0.$$

3 In the interval $x \in [-1, 1]$ for $n =$ integer, find finite solutions of the equation

$$\left(1 - x^2\right)\frac{d^2y}{dx^2} - x\frac{dy}{dx} + n^2y = 0.$$

4 Consider a spherical conductor with radius a, with the upper hemisphere held at potential V_0 and the lower hemisphere held at potential $-V_0$, which are connected by an insulator at the center. Show that the electric potential inside the sphere is given as

$$\Psi(r,\theta) = V_0\sum_{l=0}^{\infty}(-1)^l\left(\frac{r}{a}\right)^{2l+1}\frac{(2l)!}{(2^l l!)^2}\frac{4l+3}{2l+2}P_{2l+1}(\cos\theta).$$

5 Using the Frobenius method, show that the two linearly independent solutions of

$$\frac{d^2R}{dr^2} + \frac{2}{r}\frac{dR}{dr} - \frac{l(l+1)}{r^2}R = 0$$

are given as r^l and $r^{-(l+1)}$.

6 The amplitude of a scattered wave is given as

$$f(\theta) = \gamma \sum_{l=0}^{\infty}(2l+1)(e^{i\delta_l}\sin\delta_l)P_l(\cos\theta),$$

where θ is the scattering angle, l is the angular momentum, and δ_l is the phase shift caused by the central potential causing the scattering. If the total scattering cross section is $\sigma_{\text{total}} = \int_0^{2\pi}\int_0^{\pi} d\phi\, d\theta \sin\theta |f(\theta)|^2$, show that

$$\sigma_{\text{total}} = 4\pi\gamma^2 \sum_{l=0}^{\infty}(2l+1)\sin^2\delta_l.$$

7 Prove the following recursion relations:

(i) $$P_l(x) = P'_{l+1}(x) + P'_{l-1}(x) - 2xP'_l(x).$$

(ii) $$P'_{l+1}(x) - P'_{l-1}(x) = (2l+1)P_l(x).$$

(iii) $$P'_{l+1}(x) - xP'_l(x) = (l+1)P_l(x).$$

8 Use the Rodriguez formula to prove the following recursion relations:

(i) $$P'_l(x) = xP'_{l-1}(x) + lP_{l-1}(x),\ l = 1, 2, \ldots.$$

(ii) $$P_l(x) = xP_{l-1}(x) + \frac{x^2-1}{l}P'_{l-1}(x),\ l = 1, 2, \ldots.$$

9 Show that the Legendre polynomials satisfy the following relations:

(i) $$\frac{d}{dx}\left[(1-x^2)P'_l(x)\right] + l(l+1)P_l(x) = 0.$$

(ii) $$P_{l+1}(x) = \frac{(2l+1)xP_l(x) - lP_{l-1}(x)}{l+1},\quad l \geq 1.$$

10 Derive the normalization constant, N_l, in the orthogonality relation, $\int_{-1}^{1} P_{l'}(x)P_l(x)\,dx = N_l\delta_{ll'}$, of the Legendre polynomials using the generating function.

11 Show the integral

$$\int_{-1}^{1} dx\, x^l P_n(x) = \frac{2^{n+1} l! \left(\frac{l+n}{2}\right)!}{(l+n+1)! \left(\frac{l-n}{2}\right)!}, \quad (l-n) = |\text{even integer}|.$$

12 Show that the associated Legendre polynomials with negative m values are given as

$$P_l^{-m}(x) = (-1)^m \frac{(l-m)!}{(l+m)!} P_l^m(x), \quad m \geq 0.$$

13 Expand the Dirac delta function in a series of Legendre polynomials in the interval $[-1, 1]$.

14 A metal sphere is cut into sections that are separated by a very thin insulating material. One section extending from $\theta = 0$ to $\theta = \theta_0$ at potential V_0 and the second section extending from $\theta = \theta_0$ to $\theta = \pi$ is grounded. Find the electrostatic potential outside the sphere.

15 The equation for the surface of a liquid drop (nucleus) is given by

$$r^2 = a^2 \left(1 + \varepsilon_2 \frac{Z^2}{r^2} + \varepsilon_4 \frac{Z^4}{r^4}\right),$$

where Z, ε_2, and ε_4 are given constants. Express this in terms of the Legendre polynomials as $r^2 = a^2 \sum_l C_l P_l(\cos\theta)$.

16 Show that the inverse distance between two points in three dimensions can be expressed in terms of the Legendre polynomials as

$$\frac{1}{|\vec{x} - \vec{x}'|} = \frac{1}{\sqrt{r^2 + r'^2 - 2rr'\cos\theta}} = \sum_{l=0} \frac{r_<^l}{r_>^{l+1}} P_l(\cos\theta),$$

where $r_<$ and $r_>$ denote the lesser and the greater of r and r', respectively.

17 Evaluate the sum

$$S = \sum_{l=0}^{\infty} \frac{x^{l+1}}{l+1} P_l(x).$$

Hint: Try using the generating function of the Legendre polynomials.

18 If two solutions, $y_1(x)$ and $y_2(x)$, are linearly dependent, then their Wronskian, $W[y_1(x), y_2(x)] = y_1(x)y_2'(x) - y_1'(x)y_2(x)$, vanishes identically. What is the Wronskian of the two solutions of the Legendre equation?

19 The Jacobi polynomials $P_n^{(a,b)}(\cos\theta)$, where $n =$ positive integer and a, b are arbitrary real numbers, are defined by the Rodriguez formula

$$P_n^{(a,b)}(x) = \frac{(-1)^n}{2^n n!(1-x)^a(1+x)^b}\frac{d^n}{dx^n}\left[(1-x)^{n+a}(1+x)^{n+b}\right], \quad |x| < 1.$$

Show that the polynomial can be expanded as

$$P_n^{(a,b)}(\cos\theta) = \sum_{k=0}^{n} A(n,a,b,k)\left(\sin\frac{\theta}{2}\right)^{2n-2k}\left(\cos\frac{\theta}{2}\right)^{2k}.$$

Determine the coefficients $A(n,a,b,k)$ for the special case, where a and b are both integers.

20 Find solutions of the differential equation

$$2x(x-1)\frac{d^2y}{dx^2} + (10x-3)\frac{dy}{dx} + \left[8 + \frac{1}{x} - 2\lambda\right]y(x) = 0,$$

satisfying the condition $y(x) =$ finite in the entire interval $x \in [0,1]$. Write the solution explicitly for the third lowest value of λ.

21 Show that the Jacobi polynomials:

$$P_n^{(a,b)}(x) = 2^{-n}\sum_{k=0}^{n}\binom{n+a}{k}\binom{n+b}{n-k}(x-1)^{n-k}(x+1)^k, \quad |x| < 1,$$

satisfy the differential equation

$$(1-x^2)\frac{dy^2}{dx^2} + \left[b - a - (a+b+2)x\right]\frac{dy}{dx} + n(n+a+b+1)y(x) = 0.$$

22 Show that the Jacobi Polynomials satisfy the orthogonality condition

$$\int_{-1}^{1}(1-x)^a(1+x)^b P_n^{(a,b)}(x)P_m^{(a,b)}(x)dx$$
$$= \frac{2^{a+b+1}}{2n+a+b+1}\frac{\Gamma(n+a+1)\Gamma(n+b+1)}{\Gamma(n+1)\Gamma(n+a+b+1)}\delta_{nm}.$$

Note that the Jacobi polynomials are normalized so that

$$P_n^{(a,b)}(1) = \binom{n+a}{n}.$$

2

Laguerre Polynomials

Laguerre polynomials, $L_n(x)$, are named after the French mathematician **Edmond Laguerre** (1834–1886). They are the solutions of the Laguerre equation:

$$xL_n''(x) + (1 - x)L_n'(x) + nL_n(x) = 0, \tag{2.1}$$

where nonsingular solutions exist only for the non-negative integer values of n. We encounter them in quantum mechanics in the solutions of the hydrogen atom problem.

2.1 Central Force Problems in Quantum Mechanics

For the central force problems solutions of the time-independent **Schrödinger equation**:

$$\boxed{-\frac{\hbar^2}{2m}\vec{\nabla}^2\Psi(x,y,z) + V(x,y,z)\Psi(x,y,z) = E\Psi(x,y,z),} \tag{2.2}$$

can be separated in spherical polar coordinates as $\Psi(r,\theta,\phi) = R_l(r)Y_l^m(\theta,\phi)$. The angular part of the solution, $Y_l^m(\theta,\phi)$, is the **spherical harmonics** and the **radial part**, $R_l(r)$, comes from the solutions of the differential equation

$$\frac{d}{dr}\left(r^2\frac{dR_l(r)}{dr}\right) + r^2k^2(r)R_l(r) - l(l+1)R_l(r) = 0, \quad k^2(r) = \frac{2m}{\hbar^2}[E - V(r)]. \tag{2.3}$$

Here, m is the mass of the particle, $V(r)$ is the potential, E is the energy, and $\hbar$ is the Planck constant. Substituting $R_l(r) = u_{E,l}(r)/r$, the differential equation to be solved for $u_{E,l}(r)$ is obtained as

$$\boxed{-\frac{\hbar^2}{2m}\frac{d^2u_{E,l}}{dr^2} + \left[\frac{\hbar^2 l(l+1)}{2mr^2} + V(r)\right]u_{E,l}(r) = Eu_{E,l}(r).} \tag{2.4}$$

Mathematical Methods in Science and Engineering, Second Edition. Selçuk Ş. Bayın.

To indicate that the solutions depend on the energy and the angular momentum values, we have written $u_{E,l}(r)$.

For **single-electron atoms**, the potential energy is given as the Coulomb's law, $V(r) = -Ze^2/r$, where Z is the atomic number and e is the electron charge. A series solution in Eq. (2.4) yields a three-term recursion relation, which is not easy to manipulate. For a two-term recursion relation, we investigate the behavior of the differential equation near the end points, 0 and ∞, and try a solution of the form

$$\boxed{u_{E,l}(\rho) = \rho^{l+1} e^{-\rho} w(\rho),} \tag{2.5}$$

where $\rho = (2m|E|/\hbar^2)^{1/2} r$ is a dimensionless variable. Since electrons in an atom are bounded, their energy values are negative, hence we can simplify the differential equation for $w(\rho)$ further with the definitions $\rho_0 = \sqrt{2m/|E|}(Ze^2/\hbar)$ and $E/V = \rho/\rho_0$, to write

$$\boxed{\rho \frac{d^2 w}{d\rho^2} + 2(l + 1 - \rho)\frac{dw}{d\rho} + [\rho_0 - 2(l+1)]w(\rho) = 0.} \tag{2.6}$$

We now try the following **series solution** in Eq. (2.6):

$$w(\rho) = \sum_{k=0}^{\infty} a_k \rho^k, \tag{2.7}$$

which has a two-term **recursion relation**:

$$\boxed{\frac{a_{k+1}}{a_k} = \frac{2(k + l + 1) - \rho_0}{(k+1)(k+2l+2)}.} \tag{2.8}$$

In the limit as $k \to \infty$, the ratio of two successive terms, a_{k+1}/a_k, goes as $2/k$; hence the infinite series in Eq. (2.7) diverges as $e^{2\rho}$, which also implies that $R_{E,l}(r)$ diverges as $r^l e^{(2m|E|/\hbar^2)^{1/2} r}$. Although the wave function $\Psi(r,\theta,\phi)$ is complex,

$$|\Psi(r,\theta,\phi)|^2 = |R_{E,l}(r)|^2 |Y_l^m(\theta,\varphi)|^2 \tag{2.9}$$

is real and represents the probability density of the electron. Therefore, for physically acceptable solutions, $R_{E,l}(r)$ must be finite everywhere. In particular, as $r \to \infty$, probability should vanish. Hence for a finite solution, in the interval $[0,\infty)$, we **terminate** the series [Eq. (2.7)] by restricting ρ_0 to integer values as

$$\rho_0 = 2(N + l + 1), \qquad N = 0, 1, 2, \dots. \tag{2.10}$$

Since l takes integer values, we introduce a new quantum number, n, and write the energy levels of a single-electron atom as

$$\boxed{E_n = -\frac{Z^2 m e^4}{2\hbar^2 n^2}, \qquad n = 1, 2, \dots.} \tag{2.11}$$

These are nothing but the **Bohr energy** levels.

Substituting ρ_0 [Eq. (2.10)] in Eq. (2.6), the differential equation to be solved for $w(\rho)$ becomes

$$\frac{\rho}{2}\frac{d^2w}{d\rho^2} + (l + 1 - \rho)\frac{dw}{d\rho} + Nw(\rho) = 0. \tag{2.12}$$

The solutions of this equation can be expressed in terms of the **associated Laguerre polynomials.**

2.2 Laguerre Equation and Polynomials

The **Laguerre equation** is defined as

$$\boxed{x\frac{d^2y}{dx^2} + (1 - x)\frac{dy}{dx} + ny = 0,} \tag{2.13}$$

where n is a constant. Using the **Frobenius method**, we substitute a series solution about the regular singular point $x = 0$ as

$$y(x, s) = \sum_{r=0}^{\infty} a_r x^{s+r} \tag{2.14}$$

and obtain a two-term recursion relation:

$$a_{r+1} = a_r \frac{(s + r - n)}{(s + r + 1)^2}. \tag{2.15}$$

In this case, the indicial equation has a double root, $s = 0$, where the two linearly independent solutions are given as

$$y(x, 0) \quad \text{and} \quad \left.\frac{\partial y(x, s)}{\partial s}\right|_{s=0}. \tag{2.16}$$

The second solution diverges logarithmically as $x \to 0$ (Section 1.2.3). Hence for finite solutions everywhere, we keep only the first solution, $y(x, 0)$, which has the recursion relation

$$a_{r+1} = -a_r \frac{(n - r)}{(r + 1)^2}. \tag{2.17}$$

This gives the infinite series solution as

$$y(x) = a_0 \left\{ 1 - \frac{nx}{1^2} + \frac{n(n-1)}{(2!)^2}x^2 + \cdots + \frac{(-1)^r n(n-1)\cdots(n-r+1)}{(r!)^2}x^r + \cdots \right\}. \tag{2.18}$$

From the recursion relation [Eq. (2.17)], it is seen that in the limit as $r \to \infty$, the ratio of two successive terms has the limit $a_{r+1}/a_r \to 1/r$, hence this series diverges as e^x for large x. We now restrict n to integer values to obtain finite polynomial solutions as

$$\begin{aligned} y(x) &= a_0 \sum_{r=0}^{n} (-1)^r \frac{n(n-1)\cdots(n-r+1)}{(r!)^2} x^r \\ &= a_0 \sum_{r=0}^{n} (-1)^r \frac{n! x^r}{(n-r)!(r!)^2}. \end{aligned} \tag{2.19}$$

Laguerre polynomials are defined by setting $a_0 = 1$ in Eq. (2.19) as

$$\boxed{L_n(x) = \sum_{r=0}^{n} (-1)^r \frac{n! x^r}{(n-r)!(r!)^2}.} \tag{2.20}$$

2.2.1 Generating Function

The **generating function**, $T(x, t)$, of the Laguerre polynomials is defined as

$$\boxed{T(x,t) = \frac{e^{-xt/(1-t)}}{(1-t)} = \sum_{n=0}^{\infty} L_n(x) t^n, \quad |t| < 1.} \tag{2.21}$$

To see that this gives the same polynomials as Eq. (2.20), we expand the left-hand side as power series:

$$\begin{aligned} \frac{e^{-xt/(1-t)}}{(1-t)} &= \frac{1}{(1-t)} \sum_{r=0}^{\infty} \frac{1}{r!} \left[-\frac{xt}{1-t} \right]^r \\ &= \sum_{r=0}^{\infty} \frac{(-1)^r}{r!} \frac{x^r t^r}{(1-t)^{r+1}}. \end{aligned} \tag{2.22}$$

Using the binomial formula:

$$\begin{aligned} \frac{1}{(1-t)^{r+1}} &= 1 + (r+1)t + \frac{(r+1)(r+2)}{2!} t^2 + \cdots \\ &= \sum_{s=0}^{\infty} \frac{(r+s)!}{r!s!} t^s, \end{aligned} \tag{2.23}$$

Equation (2.22) becomes

$$\frac{1}{(1-t)} \exp\left\{ -\frac{xt}{(1-t)} \right\} = \sum_{r,s=0}^{\infty} (-1)^r \frac{(r+s)!}{(r!)^2 s!} x^r t^{r+s}. \tag{2.24}$$

Defining a new dummy variable:

$$n = r + s, \tag{2.25}$$

we now write

$$\sum_{n=0}^{\infty}\left[\sum_{r=0}^{\infty}(-1)^r\frac{n!}{(r!)^2(n-r)!}x^r\right]t^n=\sum_{n=0}^{\infty}L_n(x)t^n \tag{2.26}$$

and compare equal powers of t. Since $s=n-r\geq 0$, $r\leq n$, we obtain the Laguerre polynomials $L_n(x)$ as

$$L_n(x)=\sum_{r=0}^{n}(-1)^r\frac{n!}{(r!)^2(n-r)!}x^r. \tag{2.27}$$

2.2.2 Rodriguez Formula

Another definition of the Laguerre polynomials is given in terms of the **Rodriguez formula**:

$$\boxed{L_n(x)=\frac{e^x}{n!}\frac{d^n}{dx^n}(x^n e^{-x}).} \tag{2.28}$$

To show the equivalence of this formula with the other definitions, we use the **Leibniz formula:**

$$\frac{d^n}{dx^n}\left(fg\right)=\sum_{r=0}^{n}\frac{n!}{(n-r)!r!}\frac{d^{n-r}f}{dx^{n-r}}\frac{d^r g}{dx^r}, \tag{2.29}$$

to write

$$\frac{e^x}{n!}\frac{d^n}{dx^n}(x^n e^{-x})=\frac{e^x}{n!}\sum_{r=0}^{n}\frac{n!}{(n-r)!r!}\frac{d^{n-r}x^n}{dx^{n-r}}\frac{d^r e^{-x}}{dx^r}. \tag{2.30}$$

We now use

$$\begin{aligned}\frac{d^p x^q}{dx^p}&=q(q-1)\cdots(q-p+1)x^{q-p}\\&=\frac{q!}{(q-p)!}x^{q-p},\end{aligned} \tag{2.31}$$

to obtain

$$\begin{aligned}\frac{e^x}{n!}\frac{d^n}{dx^n}(x^n e^{-x})&=\frac{e^x}{n!}\sum_{r=0}^{n}\frac{n!}{(n-r)!r!}\frac{n!}{r!}x^r(-1)^r e^{-x}\\&=\sum_{r=0}^{n}(-1)^r\frac{n!x^r}{(r!)^2(n-r)!}\\&=L_n(x).\end{aligned} \tag{2.32}$$

2.2.3 Orthogonality

To show that the Laguerre polynomials form an **orthogonal set**, we evaluate the integral

$$I_{nm} = \int_0^{\infty} e^{-x} L_n(x) L_m(x) dx. \tag{2.33}$$

Using the generating function definition of the Laguerre polynomials, we write

$$\frac{1}{1-t} \exp\left\{-\frac{xt}{(1-t)}\right\} = \sum_{n=0}^{\infty} L_n(x) t^n \tag{2.34}$$

and

$$\frac{1}{1-s} \exp\left\{-\frac{xs}{(1-s)}\right\} = \sum_{n=0}^{\infty} L_m(x) s^m. \tag{2.35}$$

We first multiply Eq. (2.34) with Eq. (2.35) and then the result with e^{-x} to write

$$\sum_{n,m=0}^{\infty} e^{-x} L_n(x) L_m(x) t^n s^m = \frac{e^{-x} \exp\left\{-\frac{xt}{(1-t)}\right\}}{(1-t)} \frac{\exp\left\{-\frac{xs}{(1-s)}\right\}}{(1-s)}. \tag{2.36}$$

Interchanging the integral and the summation signs and integrating with respect to x gives

$$\sum_{n,m=0}^{\infty} \left[\int_0^{\infty} e^{-x} L_n(x) L_m(x) dx\right] t^n s^m = \int_0^{\infty} \frac{e^{-x} \exp\left\{-\frac{xt}{(1-t)}\right\}}{(1-t)} \frac{\exp\left\{-\frac{xs}{(1-s)}\right\}}{(1-s)} dx. \tag{2.37}$$

It is now seen that the value of the integral, I_{nm}, in Eq. (2.33) can be obtained by expanding

$$I = \int_0^{\infty} \frac{e^{-x} \exp\left\{-\frac{xt}{(1-t)}\right\}}{(1-t)} \frac{\exp\left\{-\frac{xs}{(1-s)}\right\}}{(1-s)} dx \tag{2.38}$$

in powers of t and s and then by comparing the equal powers of $t^n s^m$ with the left-hand side of Eq. (2.37). If we write I as

$$I = \frac{1}{(1-t)(1-s)} \int_0^{\infty} \exp\left\{-x\left(1 + \frac{t}{1-t} + \frac{s}{1-s}\right)\right\} dx, \tag{2.39}$$

the integral can be taken to yield

$$I = \frac{1}{(1-t)(1-s)} \left[\frac{-\exp\left\{-x\left(1 + \frac{t}{1-t} + \frac{s}{1-s}\right)\right\}}{1 + \left[\frac{t}{(1-t)}\right] + \left[\frac{s}{(1-s)}\right]}\right]_0^{\infty} \tag{2.40}$$

$$= \frac{1}{(1-t)(1-s)} \left[\frac{1}{1 + \left[\frac{t}{(1-t)}\right] + \left[\frac{s}{(1-s)}\right]} \right] \tag{2.41}$$

$$= \frac{1}{1-st} \tag{2.42}$$

$$= \sum_{n=0}^{\infty} s^n t^n. \tag{2.43}$$

This leads us to the orthogonality relation of the Laguerre polynomials as

$$\boxed{\int_0^{\infty} e^{-x} L_n(x) L_m(x)\, dx = \delta_{nm}.}$$

Compared with the Legendre polynomials, we say that the Laguerre polynomials are **orthogonal** with respect to the **weight function** e^{-x}.

2.2.4 Recursion Relations

Using the method that we used for the Legendre polynomials, we can obtain two **recursion relations** for the Laguerre polynomials. We first differentiate the generating function with respect to t to obtain

$$\boxed{(n+1)L_{n+1}(x) = (2n+1-x)L_n(x) - nL_{n-1}(x).} \tag{2.44}$$

Differentiating the generating function with respect to x gives the second recursion relation:

$$\boxed{xL'_n(x) = nL_n(x) - nL_{n-1}(x).} \tag{2.45}$$

Another useful recursion relation is given as

$$\boxed{L'_n(x) = -\sum_{r=0}^{n-1} L_r(x).} \tag{2.46}$$

Laguerre polynomials

$$L_0(x) = 1,$$
$$L_1(x) = -x + 1,$$
$$L_2(x) = (1/2!)(x^2 - 4x + 2),$$
$$L_3(x) = (1/3!)(-x^3 + 9x^2 - 18x + 6),$$
$$L_4(x) = (1/4!)(x^4 - 16x^3 + 72x^2 - 96x + 24),$$
$$L_5(x) = (1/5!)(-x^5 + 25x^4 - 200x^3 + 600x^2 - 600x + 120). \tag{2.47}$$

2.2.5 Special Values

In the generating function, we set $x = 0$:

$$\sum_{n=0}^{\infty} L_n(0)t^n = \frac{1}{1-t} = \sum_{n=0}^{\infty} t^n. \tag{2.48}$$

This gives the **special value**

$$\boxed{L_n(0) = 1.} \tag{2.49}$$

Another special value is obtained by writing the Laguerre equation at $x = 0$:

$$\left[x\frac{d^2L_n(x)}{dx^2} + (1-x)\frac{d}{dx}L_n(x) + nL_n(x)\right]_{x=0} = 0, \tag{2.50}$$

which gives

$$\boxed{L_n'(0) = -n.} \tag{2.51}$$

2.3 Associated Laguerre Equation and Polynomials

The **associated Laguerre equation** is given as

$$\boxed{x\frac{d^2y}{dx^2} + (k+1-x)\frac{dy}{dx} + ny = 0.} \tag{2.52}$$

This reduces to the Laguerre equation for $k = 0$. Solution of Eq. (2.52) can be found by the following theorem:

Theorem 2.1 Let $Z(x)$ be a solution of the Laguerre equation of order $(n+k)$, then $\frac{d^kZ(x)}{dx^k}$ satisfies the associated Laguerre equation.

Proof: We write the Laguerre equation of order $(n+k)$ as

$$x\frac{d^2Z}{dx^2} + (1-x)\frac{dZ}{dx} + (n+k)Z(x) = 0. \tag{2.53}$$

Using the Leibniz formula [Eq. (2.29)], k-fold differentiation of Eq. (2.53) gives

$$x\frac{d^{k+2}Z}{dx^{k+2}} + k\frac{d^{k+1}Z}{dx^{k+1}} + (1-x)\frac{d^{k+1}Z}{dx^{k+1}} + k(-1)\frac{d^kZ}{dx^k} + (n+k)\frac{d^kZ}{dx^k} = 0. \tag{2.54}$$

Rearranging this, we obtain the desired result:

$$x\frac{d^2}{dx^2}\left[\frac{d^kZ}{dx^k}\right] + (k+1-x)\frac{d}{dx}\left[\frac{d^kZ}{dx^k}\right] + n\left[\frac{d^kZ}{dx^k}\right] = 0. \tag{2.55}$$

Using the definition of the Laguerre polynomials [Eq. (2.27)], we can now write the associated Laguerre polynomials as

$$L_n^k(x) = (-1)^k \frac{d^k}{dx^k} \sum_{r=0}^{n+k} (-1)^r \frac{(n+k)!x^r}{(n+k-r)!(r!)^2}. \tag{2.56}$$

Since k-fold differentiation of x^r is going to give zeroes for the $r < k$ values, we can write

$$L_n^k(x) = (-1)^k \frac{d^k}{dx^k} \sum_{r=k}^{n+k} (-1)^r \frac{(n+k)!x^r}{(n+k-r)!(r!)^2}, \tag{2.57}$$

$$L_n^k(x) = (-1)^k \sum_{r=k}^{n+k} (-1)^r \frac{(n+k)!}{(n+k-r)!(r!)^2} \frac{r!}{(r-k)!} x^{r-k}. \tag{2.58}$$

Defining a new dummy variable s as $s = r - k$, we find the final form of the **associated Laguerre polynomials**:

$$\boxed{L_n^k(x) = \sum_{s=0}^{n} (-1)^s \frac{(n+k)!x^s}{(n-s)!(k+s)!s!}.} \tag{2.59}$$

Example 2.1 ***Associated Laguerre Polynomials***
In quantum mechanics, the radial part of the Schrödinger equation for the three-dimensional harmonic oscillator is given as

$$\frac{d^2R(x)}{dx^2} + \frac{2}{x}\frac{dR(x)}{dx} + \left(\epsilon - x^2 - \frac{l(l+1)}{x^2}\right) R(x) = 0, \tag{2.60}$$

where $l = 0, 1, 2 \ldots$ and x and ϵ are defined in terms of the radial distance r and the energy E as

$$x = \frac{r}{\sqrt{\hbar/m\omega}}, \quad \epsilon = \frac{E}{\hbar\omega/2}. \tag{2.61}$$

A series solution about the regular singular point at $x = 0$ gives a three-term recursion relation. To obtain a two-term recursion relation, we analyze the behavior of the differential equation about the singular points $x = 0$ and $x = \infty$, and try a solution of the form

$$R(x) = x^l e^{-x^2/2} w(x). \tag{2.62}$$

Substituting this into Eq. (2.60) gives the differential equation to be solved for $w(x)$ as

$$w'' + \left(\frac{2(l+1)}{x} - 2x\right) w' + (-3 + \epsilon - 2l)w = 0. \tag{2.63}$$

Associated Laguerre polynomials with the argument x^2 satisfies

$$\frac{d^2}{dx^2}L_n^k(x^2) + \left[(2k+1)\frac{1}{x} - 2x\right]\frac{d}{dx}L_n^k(x^2) + nL_n^k(x^2) = 0, \tag{2.64}$$

which when compared with Eq. (2.63) allows us to write the solution for $w(x)$ as

$$w(x) = L_{-3+\epsilon-2l}^{l+1/2}(x^2). \tag{2.65}$$

Thus the solution for Eq. (2.60) is obtained as

$$R(x) = x^l e^{-x^2/2} L_{-3+\epsilon-2l}^{l+1/2}(x^2). \tag{2.66}$$

2.3.1 Generating Function

The **generating function** of the associated Laguerre polynomials is defined as

$$\boxed{T(x,t) = \frac{\exp\left[-\frac{xt}{(1-t)}\right]}{(1-t)^{k+1}} = \sum_{n=0} L_n^k(x)t^n, \quad |t| < 1.} \tag{2.67}$$

To prove this, we write the generating function of the Laguerre polynomials:

$$\frac{\exp\left[-\frac{xt}{(1-t)}\right]}{(1-t)^{k+1}} = \sum_{n=0}^{\infty} L_n(x)t^n, \tag{2.68}$$

which after k-fold differentiation:

$$\frac{d^k}{dx^k}\left[\frac{\exp\left[-\frac{xt}{(1-t)}\right]}{(1-t)}\right] = \frac{d^k}{dx^k}\sum_{n=k}^{\infty} L_n(x)t^n, \tag{2.69}$$

yields

$$\left[\frac{-t}{(1-t)}\right]^k \frac{\exp\left[-\frac{xt}{(1-t)}\right]}{(1-t)} = \sum_{n=0}^{\infty} \frac{d^k}{dx^k} L_{n+k}(x)t^{n+k}. \tag{2.70}$$

We now use the relation

$$L_n^k(x) = (-1)^k \frac{d^k}{dx^k} L_{n+k}(x), \tag{2.71}$$

to write

$$(-1)^k \frac{t^k}{(1-t)^{k+1}} \exp\left[-\frac{xt}{(1-t)}\right] = \sum_{n=0}^{\infty} (-1)^k L_n^k(x)t^{n+k}, \tag{2.72}$$

which leads to the desired result:

$$\frac{\exp\left[-\frac{xt}{(1-t)}\right]}{(1-t)^{k+1}} = \sum_{n=0}^{\infty} L_n^k(x)t^n. \tag{2.73}$$

2.3.2 Rodriguez Formula and Orthogonality

The **Rodriguez formula** for the associated Laguerre polynomials is given as

$$\boxed{L_n^k(x) = \frac{e^x x^{-k}}{n!}\frac{d^n}{dx^n}\left[e^{-x}x^{n+k}\right].} \tag{2.74}$$

Their orthogonality relation is

$$\boxed{\int_0^{\infty} e^{-x}x^k L_n^k(x)L_m^k(x)dx = \frac{(n+k)!}{n!}\delta_{nm},} \tag{2.75}$$

where the weight function is given as $(e^{-x}x^k)$.

2.3.3 Recursion Relations

Some frequently used **recursion relations** of the associated Laguerre polynomials are given as follows:

$$\boxed{(n+1)L_{n+1}^k(x) = (2n+k+1-x)L_n^k(x) - (n+k)L_{n-1}^k(x),} \tag{2.76}$$

$$\boxed{x\frac{d}{dx}L_n^k(x) = nL_n^k(x) - (n+k)L_{n-1}^k(x),} \tag{2.77}$$

$$\boxed{L_{n-1}^k(x) + L_n^{k-1}(x) = L_n^k(x).} \tag{2.78}$$

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Problems

1 We have seen that the Schrödinger equation for a single-electron atom is written as

$$-\frac{\hbar^2}{2m}\frac{d^2 u_{E,l}}{dr^2} + \left[\frac{\hbar^2 l(l+1)}{2mr^2} - \frac{Ze^2}{r}\right] u_{E,l}(r) = E u_{E,l}(r).$$

(i) Without any substitutions, convince yourself that the above equation gives a three-term recursion relation and then derive the substitution

$$u_{E,l}(\rho) = \rho^{l+1} e^{-\rho} w(\rho),$$

which leads to a differential equation with a two-term recursion relation for $w(\rho)$. We have defined a dimensionless variable $\rho = r\sqrt{2m|E|/\hbar^2}$. Hint: Study the asymptotic forms and the solutions of the differential equation at the end points of the interval $[0, \infty)$.

(ii) Show that the differential equation for $w(\rho)$ has the recursion relation

$$\frac{a_{k+1}}{a_k} = \frac{2(k+l+1) - \rho_0}{(k+1)(k+2l+2)}, \qquad \rho_0 = \sqrt{\frac{2m}{|E|}}\frac{Ze^2}{\hbar}.$$

2 Derive the following recursion relations:

(i) $(n+1)L_{n+1}(x) = (2n+1-x)L_n(x) - nL_{n-1}(x)$,

(ii) $xL'_n(x) = nL_n(x) - nL_{n-1}(x)$,

(iii) $L'_n(x) = -\sum_{r=0}^{n-1} L_r(x)$.

3 Show that the associated Laguerre polynomials satisfy the orthogonality relation

$$\int_0^\infty e^{-x}x^k L_n^k(x)L_m^k(x)dx = \frac{(n+k)!}{n!}\delta_{nm}.$$

4 Write the normalized wave function of the hydrogen atom in terms of the spherical harmonics and the associated Laguerre polynomials.

5 Using the generating function

$$\frac{\exp\left[-\frac{xt}{(1-t)}\right]}{(1-t)^{k+1}} = \sum_{n=0}^{\infty} L_n^k(x)t^n,$$

derive the Rodriguez formula for $L_n^k(x)$.

6 Find the expansion of $\exp(-kx)$ in terms of the associated Laguerre polynomials.

7 Show the special value

$$L_n^k(0) = \frac{(n+k)!}{n!k!}$$

for the associated Laguerre polynomials.

8 (i) Using the Frobenius method, find a series solution about $x = 0$ to the differential equation

$$x\frac{d^2C}{dx^2} + \frac{dC}{dx} + (\lambda - \frac{x}{4})C = 0, \quad x \in [0, \infty].$$

(ii) Show that solutions regular in the entire interval $[0, \infty)$ must be of the form

$$C_n(x) = e^{-x/2}\overline{L}_n(x),$$

with $\lambda = n + 1/2$, $n = 0, 1, 2, \ldots$, where $\overline{L}_n(x)$ satisfies the differential equation

$$x\frac{d^2\overline{L}_n}{dx^2} + (1-x)\frac{d\overline{L}_n}{dx} + n\overline{L}_n = 0.$$

(iii) With the integration constant

$$a_n = (-1)^n,$$

find the general expression for the coefficients a_{n-j} of $\overline{L}_n(x)$.

(iv) Show that this polynomial can also be defined by the generating function

$$T(x,t) = \frac{\exp\left[-\frac{xt}{(1-t)}\right]}{(1-t)} = \sum_{n=0}^{\infty} \frac{\overline{L}_n(x)}{n!}t^n$$

or the Rodriguez formula

$$\overline{L}_n(x) = e^x \frac{d^n}{dx^n}(x^n e^{-x}).$$

(v) Derive two recursion relations connecting

$$\overline{L}_{n+1}, \overline{L}_n \quad \text{and} \quad \overline{L}_{n-1}$$

and

$$\overline{L}_n' \quad \text{with} \quad \overline{L}_n, \overline{L}_{n-1}.$$

(vi) Show that $C_n(x)$ form an orthogonal set, that is,

$$\int_0^\infty dx e^{-x}\overline{L}_n(x)\overline{L}_m(x) = 0 \quad \text{for} \quad n \neq m$$

and calculate the integral

$$\int_0^{\infty} dx e^{-x} [\overline{L}_n(x)]^2.$$

Note: Some books use $\overline{L}_n$ for their definition of Laguerre polynomials.

9 Starting with the generating function definition:

$$\exp(-xt/(1-t))/(1-t) = \sum_{n=0}^{\infty} L_n(x) t^n,$$

derive the Rodriguez formula, $L_n(x) = \frac{e^x}{n!} \frac{d^n}{dx^n}(x^n e^{-x})$, for the Laguerre polynomials.

10 Using the series definition of the Laguerre polynomials show that

$$L_n'(0) = -n \quad \text{and} \quad L_n''(0) = \frac{1}{2} n(n-1).$$

11 In quantum mechanics, the radial part of Schrödinger's equation for the three-dimensional harmonic oscillator is given as

$$\frac{d^2R(x)}{dx^2} + \frac{2}{x}\frac{dR(x)}{dx} + \left(\epsilon - x^2 - \frac{l(l+1)}{x^2}\right) R(x) = 0,$$

where x and ϵ are defined in terms of the radial distance r and the energy E as

$$x = r/\sqrt{\hbar\omega/2} \quad \text{and} \quad \epsilon = E/\hbar\omega/2.$$

l takes the integer values $l = 0, 1, 2 \ldots$. Analyze the behavior of this equation about its singular points and show that its solution can be expressed in terms of the associated Laguerre polynomials.

3

Hermite Polynomials

Hermite polynomials appear in many different branches of science like the probability theory, combinatorics, and numerical analysis. We also encounter them in quantum mechanics in conjunction with the harmonic oscillator problem and in systems theory in connection with Gaussian noise. They are named after the French mathematician **Charles Hermite** (1822–1901).

3.1 Harmonic Oscillator in Quantum Mechanics

In terms of the Hamiltonian operator, **H**, the time-independent **Schrödinger equation** is written as

$$\mathbf{H}\Psi(\overrightarrow{x}) = E\Psi(\overrightarrow{x}), \tag{3.1}$$

where $\Psi(\overrightarrow{x})$ is the wave function and E stands for the energy eigenvalues. In general, **H** is obtained from the classical Hamiltonian by replacing the position, $\overrightarrow{x}$, and the momentum, $\overrightarrow{p}$, with their operator counterparts:

$$\overrightarrow{x} \to \overrightarrow{x}, \quad \overrightarrow{p} \to \frac{\hbar}{i}\overrightarrow{\nabla}. \tag{3.2}$$

In one-dimension, the **Hamiltonian operator** for the **harmonic oscillator** is obtained from the classical Hamiltonian, $H = p^2/2m + m\omega^2x^2/2$, as

$$\mathbf{H}(x) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{m\omega^2x^2}{2}. \tag{3.3}$$

This leads us to the following **Schrödinger equation**:

$$\frac{d^2\Psi(x)}{dx^2} + \frac{2m}{\hbar^2}\left(E - \frac{m\omega^2x^2}{2}\right)\Psi(x) = 0. \tag{3.4}$$

Defining two dimensionless variables, $x' = x/\sqrt{\hbar/m\omega}$, $\varepsilon = E/(\hbar\omega/2)$, and dropping the prime in x', we obtain the differential equation to be solved for

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the wave function as

$$\boxed{\frac{d^2\Psi(x)}{dx^2} + (\varepsilon - x^2)\Psi(x) = 0, \quad x \in (-\infty, \infty).} \tag{3.5}$$

This is closely related to the **Hermite equation,** and its solutions are given in terms of the **Hermite polynomials**.

3.2 Hermite Equation and Polynomials

We seek a finite solution to the above differential equation (3.5) in the entire interval $(-\infty, \infty)$. However, direct application of the **Frobenius method** gives a three-term recursion relation. To get a two-term recursion relation, we look at the behavior of the solution near the singularity at infinity.

First, we make the substitution $x = 1/\xi$, which transforms the differential equation into the form

$$\frac{d^2\Psi(\xi)}{d\xi^2} + \frac{2}{\xi}\frac{d\Psi(\xi)}{d\xi} + \frac{1}{\xi^4}\left[\varepsilon - \frac{1}{\xi^2}\right]\Psi(\xi) = 0. \tag{3.6}$$

It is clear that the **singularity** at infinity is **essential**. However, since it is at the end points of our interval, it does not pose any difficulty in finding a series solution about the origin. We now consider the differential equation (3.5) in the limit as $x \to \mp\infty$, where it behaves as

$$\frac{d^2\Psi(x)}{dx^2} - x^2\Psi(x) = 0. \tag{3.7}$$

This has two solutions, $\exp(-x^2/2)$ and $\exp(x^2/2)$. Since $\exp(x^2/2)$ blows up at infinity, we use the first solution and substitute into Eq. (3.5) a solution of the form $\Psi(x) = h(x)\exp(-x^2/2)$, which leads to the following differential equation for $h(x)$:

$$\boxed{\frac{d^2h}{dx^2} - 2x\frac{dh}{dx} + (\varepsilon - 1)h(x) = 0.} \tag{3.8}$$

We now try a **series solution,** $h(x) = \sum_{k=0}^{\infty} a_k x^k$, which gives a two-term recursion relation:

$$a_{k+2} = a_k \frac{(2k + 1 - \varepsilon)}{(k + 2)(k + 1)}. \tag{3.9}$$

Since the ratio of two successive terms, a_{k+2}/a_k, has the limit $2k$ as k goes to infinity, this series asymptotically behaves as e^{x^2}. Thus the wave function $\Psi(x)$ diverges as $e^{x^2/2}$ as $x \to \mp\infty$. A physically meaningful solution must be finite in the entire interval $(-\infty, \infty)$; hence we terminate the series after a finite number of terms. This is accomplished by restricting the energy of the system to certain integer values as $\varepsilon - 1 = 2n$, $n = 0, 1, 2, \ldots$. Now the recursion relation [Eq. (3.9)] becomes

$$a_{k+2} = a_k \frac{(2k - 2n)}{(k + 2)(k + 1)}, \tag{3.10}$$

which yields the polynomial solutions of Eq. (3.8) as

$$\begin{array}{lll} n = 0 & h_0(x) = & a_0, \\ n = 1 & h_1(x) = & a_1 x, \\ n = 2 & h_2(x) = & a_0(1 - 2x^2), \\ \vdots & \vdots & \vdots \end{array} \tag{3.11}$$

Using the recursion relation [Eq. (3.10)], we can write the coefficients of the decreasing powers of x for the nth-order polynomial as

$$a_{n-2j} = (-1)^j \frac{n(n-1)(n-2)(n-3)\cdots(n-2j+1)}{2^j 2.4 \ldots (2j)} a_n, \tag{3.12}$$

$$a_{n-2j} = \frac{(-1)^j n!}{(n-2j)!} \frac{1}{2^j 2^j j!} a_n. \tag{3.13}$$

When we take a_n as $a_n = 2^n$, we obtain the **Hermite polynomials:**

$$\boxed{H_n(x) = \sum_{j=0}^{[n/2]} \frac{(-1)^j 2^{n-2j} n!}{(n-2j)! j!} x^{n-2j},} \tag{3.14}$$

which satisfy the **Hermite equation:**

$$\boxed{H_n''(x) - 2xH_n'(x) + 2nH_n(x) = 0.} \tag{3.15}$$

Hermite Polynomials

$$H_0(x) = 1,$$
$$H_1(x) = 2x,$$
$$H_2(x) = -2 + 4x^2,$$
$$H_3(x) = -12x + 8x^3,$$
$$H_4(x) = 12 - 48x^2 + 16x^4,$$
$$H_5(x) = 120x - 160x^3 + 32x^5.$$

Going back to the energy parameter E, we find

$$E = \frac{\hbar\omega}{2}\varepsilon = \hbar\omega\left(n + \frac{1}{2}\right), \quad n = 0, 1, 2, \ldots. \tag{3.16}$$

This means that in quantum mechanics, the energy of the harmonic oscillator is quantized, hence a one-dimensional harmonic oscillator can only oscillate with the energy values given above.

3.2.1 Generating Function

The **generating function** for the Hermite polynomials is given as

$$\boxed{T(t,x) = e^{-t^2+2xt} = \sum_{n=0}^{\infty} \frac{H_n(x)}{n!} t^n.} \tag{3.17}$$

To show that this is equivalent to our former definition [Eq. (3.14)], we write the left-hand side as

$$e^{t(2x-t)} = \sum_{n=0}^{\infty} \frac{t^n(2x-t)^n}{n!} = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} (-1)^m \frac{n!2^{n-m}}{m!(n-m)!n!} x^{n-m} t^{n+m}. \tag{3.18}$$

Making the replacement $n + m \to n'$ and dropping primes, we obtain

$$e^{t(2x-t)} = \sum_{n=0}^{\infty} \sum_{m=0}^{[n/2]} (-1)^m \frac{2^{n-2m} x^{n-2m}}{m!(n-2m)!} t^n. \tag{3.19}$$

Comparing this with the right-hand side of Eq. (3.17), we see that $H_n(x)$ is the same as given in Eq. (3.14).

3.2.2 Rodriguez Formula

Another definition for the Hermite polynomials is given by the **Rodriguez formula:**

$$\boxed{H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} \left[e^{-x^2}\right].} \tag{3.20}$$

To see that this is equivalent to the generating function [Eq. (3.17)], we write the Taylor series expansion of an arbitrary function $F(t)$ as

$$F(t) = \sum_{n=0}^{\infty} \left. \frac{d^n F(t)}{dt^n} \right|_{t=0} \frac{t^n}{n!}. \tag{3.21}$$

Comparing this with Eq. (3.17), we obtain

$$H_n(x) = \left[\frac{\partial^n}{\partial t^n} e^{2tx-t^2} \right]_{t=0} \tag{3.22}$$

$$= \left. \frac{\partial^n}{\partial t^n} e^{x^2-(x-t)^2} \right|_{t=0} \tag{3.23}$$

$$= e^{x^2} \left. \frac{\partial^n}{\partial t^n} e^{-(x-t)^2} \right|_{t=0}. \tag{3.24}$$

For an arbitrary differentiable function, we can write $\frac{\partial}{\partial t} f(x-t) = -\frac{\partial}{\partial x} f(x-t)$, hence

$$\frac{\partial^n}{\partial t^n} f(x-t) = (-1)^n \frac{\partial^n}{\partial x^n} f(x-t). \tag{3.25}$$

Applying this to Eq. (3.24), we obtain the Rodriguez formula as

$$H_n(x) = (-1)^n e^{x^2} \frac{\partial^n}{\partial x^n} e^{-(x-t)^2}\bigg|_{t=0} = (-1)^n e^{x^2} \frac{d^n}{dx^n}\, e^{-x^2}. \tag{3.26}$$

3.2.3 Recursion Relations and Orthogonality

Differentiating the generating function of the Hermite polynomials [Eq. (3.17)], first with respect to x and then with respect to t, we obtain two **recursion relations**:

$$\boxed{H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x), \quad n \geq 1, \quad H_1(x) = 2xH_0(x),} \tag{3.27}$$

$$\boxed{H_n'(x) = 2nH_{n-1}(x), \quad n \geq 1, \quad H_0'(x) = 0.} \tag{3.28}$$

To show the **orthogonality** of the Hermite polynomials, we evaluate the integral

$$I_{nm} = \int_{-\infty}^{\infty} dx\, e^{-x^2} H_n(x)H_m(x), \quad n \geq m. \tag{3.29}$$

Using the Rodriguez formula, we write Eq. (3.29) as

$$I_{nm} = (-1)^n \int_{-\infty}^{\infty} dx\, e^{-x^2} e^{x^2} \left[\frac{d^n}{dx^n}\, e^{-x^2}\right] H_m(x). \tag{3.30}$$

After n-fold integration by parts and since $n > m$, we obtain

$$\begin{aligned} I_{nm} &= (-1)^n \frac{d^{n-1}}{dx^{n-1}}(e^{-x^2})H_m(x)\bigg|_{-\infty}^{\infty} + (-1)^{n+1} \int_{-\infty}^{\infty} dx \left[\frac{d^{n-1}}{dx^{n-1}} e^{-x^2}\right] H_m'(x), \\ &\;\;\vdots \\ &= (-1)^{2n} \int_{-\infty}^{\infty} dx\, e^{-x^2} \frac{d^n}{dx^n} H_m. \end{aligned} \tag{3.31}$$

Since the x dependence of the mth-order Hermite polynomial goes as

$$H_m(x) = 2^m x^m + a_{m-2}x^{m-2} + \cdots , \tag{3.32}$$

we obtain

$$I_{nm} = \begin{cases} 0, & n > m, \\ 2^n n! \sqrt{\pi}, & n = m, \end{cases} \tag{3.33}$$

where we have used $\frac{d^n H_n(x)}{dx^n} = 2^n n!$, and $2\int_0^{\infty} dx\, e^{-x^2} = \sqrt{\pi}$. We now write the **orthogonality relation** as

$$\boxed{\int_{-\infty}^{\infty} dx\, e^{-x^2} H_n(x)H_m(x) = 2^n n! \sqrt{\pi}\delta_{nm}.} \tag{3.34}$$

Using Eq. (3.34), we can define a set of polynomials, $\{\phi_n(x)\}$, where $\phi_n(x)$ are defined as

$$\boxed{\phi_n(x) = \frac{1}{\sqrt{2^n n!\sqrt{\pi}}} e^{-x^2/2} H_n(x), \quad n = 0, 1, 2, \ldots,} \tag{3.35}$$

and which satisfies the orthogonality relation $\int_{-\infty}^{\infty} dx \phi_n(x)\phi_m(x) = \delta_{nm}$. Since this set is also **complete**, any sufficiently well-behaved function in the interval $(-\infty, \infty)$ can be expanded in terms of $\{\phi_n(x)\}$ as $f(x) = \sum_{n=0}^{\infty} C_n \phi_n(x)$, where the coefficients C_n are found as

$$C_n = \int_{-\infty}^{\infty} dx' f(x')\phi_n(x'). \tag{3.36}$$

Example 3.1 ***Gaussian and the Hermite polynomials***

In quantum mechanics, the wave function of a particle localized around x_0 can be given as a Gaussian, $f(x) = Ae^{-\frac{1}{2}(x-x_0)^2}$, where A is the normalization constant, which is determined by requiring the area under $f(x)$ to be unity. Let us find the expansion of this function in terms of the Hermite polynomials as

$$f(x) = \sum_{n=0}^{\infty} C_n \frac{e^{-x^2/2} H_n(x)}{\sqrt{2^n n!\sqrt{\pi}}}. \tag{3.37}$$

This expansion corresponds to the representation of the wave function of a particle under the influence of a harmonic oscillator potential in terms of the harmonic oscillator energy eigenfunctions. Expansion coefficients C_n are determined from the integral

$$C_n = \frac{A}{\sqrt{2^n n!\sqrt{\pi}}} \int_{-\infty}^{\infty} d\xi \exp\left[-\frac{(\xi - x_0)^2}{2} - \frac{\xi^2}{2}\right] H_n(\xi). \tag{3.38}$$

Writing this as

$$C_n = \frac{A}{\sqrt{2^n n!\sqrt{\pi}}} \int_{-\infty}^{\infty} d\xi \, e^{-\xi^2} \exp\left[2\xi\left(\frac{x_0}{2}\right) - \left(\frac{x_0}{2}\right)^2\right] H_n(\xi) e^{-x_0^2/4} \tag{3.39}$$

and defining a new parameter $x_0/2 = t$, and using the generating function [Eq. (3.17)], we obtain

$$C_n = \frac{A}{\sqrt{2^n n!\sqrt{\pi}}} e^{-x_0^2/4} \int_{-\infty}^{\infty} d\xi \, e^{-\xi^2} \left[\sum_{m=0}^{\infty} \frac{H_m(\xi)}{m!}\left(\frac{x_0}{2}\right)^m\right] H_n(\xi). \tag{3.40}$$

We now use the orthogonality relation [Eq. (3.34)] of the Hermite polynomials to obtain

$$C_n = \frac{A}{\sqrt{2^n n!\sqrt{\pi}}} e^{-x_0^2/4} \left(\frac{x_0}{2}\right)^n \frac{1}{n!} \int d\xi\ e^{-\xi^2} [H_n(\xi)]^2 \tag{3.41}$$

$$= \frac{A}{\sqrt{2^n n!\sqrt{\pi}}} e^{-x_0^2/4} \left(\frac{x_0}{2}\right)^n \frac{1}{n!} 2^n n! \sqrt{\pi} \tag{3.42}$$

$$= A e^{-x_0^2/4} \left(\frac{x_0}{2}\right)^n \frac{\sqrt{2^n}}{\sqrt{n!}} \pi^{\frac{1}{4}}. \tag{3.43}$$

The probability of finding a particle in the nth energy eigenstate is given as $|C_n|^2$.

Example 3.2 ***Dipole calculations in quantum mechanics***
In quantum mechanics and in electric dipole calculations, we encounter integrals like

$$I_{nm} = e \int_{-\infty}^{\infty} x\phi_n(x)\phi_m(x)dx, \tag{3.44}$$

where e is the electric charge. Let us write this as

$$I_{nm} = \frac{e}{\sqrt{2^n n!\sqrt{\pi}}\sqrt{2^m m!\sqrt{\pi}}} \left[\int_{-\infty}^{\infty} dx\ e^{-x^2} H_n(x) H_m(x) x\right]. \tag{3.45}$$

We now use the generating function definition of the Hermite polynomials to write

$$\int_{-\infty}^{\infty} dx\ T(t,x)S(s,x)e^{-x^2}x$$
$$= \sum_{n=0}^{\infty}\sum_{m=0}^{\infty} \frac{1}{n!m!} \left[\int_{-\infty}^{\infty} dx\ e^{-x^2} H_n(x) H_m(x) x\right] t^n s^m. \tag{3.46}$$

If we show the expression inside the square brackets on the right-hand side as J_{nm}, the integral I_{nm} will be given as

$$I_{nm} = \frac{e}{\sqrt{2^n n!\sqrt{\pi}}\sqrt{2^m m!\sqrt{\pi}}} J_{nm}. \tag{3.47}$$

We now evaluate the left-hand side of Eq. (3.46) as

$$\int_{-\infty}^{\infty} dx\ e^{-t^2+2tx} e^{-s^2+2sx} e^{-x^2} x$$
$$= \int_{-\infty}^{\infty} dx\ e^{-(x-(s+t))^2} e^{2st} \{[x-(s+t)] + (s+t)\} \tag{3.48}$$

$$= e^{2st} \left\{ \int_{-\infty}^{\infty} ue^{-u^2}\, du + (s+t) \int_{-\infty}^{\infty} du\, e^{-u^2} \right\} \tag{3.49}$$

$$= e^{2st}(s+t)\sqrt{\pi}, \tag{3.50}$$

where we have defined $u = x - (s+t)$. Expanding this in power series of t and s gives

$$\int_{-\infty}^{\infty} dx\, e^{-t^2+2tx} e^{-s^2+2sx} e^{-x^2} x = \sqrt{\pi} \sum_{k=0}^{\infty} \frac{2^k s^k t^{k+1}}{k!} + \sqrt{\pi} \sum_{k=0}^{\infty} \frac{2^k s^{k+1} t^k}{k!}. \tag{3.51}$$

Finally, comparing with $\sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \frac{1}{n!m!}[J_{nm}]t^n s^m$, we obtain the desired result:

$$\begin{array}{llll} J_{nm} = 0 & \Rightarrow \quad I_{nm} = 0 & \text{for} & m \neq n \mp 1, \\ J_{n,n+1} = \sqrt{\pi}2^n(n+1)! & \Rightarrow \quad I_{n,n+1} = e[(n+1)/2]^{1/2} & \text{for} & m = n+1, \\ J_{n,n-1} = \sqrt{\pi}2^{n-1}n! & \Rightarrow \quad I_{n,n-1} = e\sqrt{n/2} & \text{for} & m = n-1. \end{array} \tag{3.52}$$

We can also write this result as

$$\boxed{J_{nm} = \sqrt{\pi}2^{n-1}n!\delta_{n-1,m} + \sqrt{\pi}2^n(n+1)!\delta_{n+1,m}.} \tag{3.53}$$

Example 3.3 ***Operations with Hermite polynomials***

Evaluate the following integral:

$$I = \int_{-\infty}^{\infty} xe^{-x^2} H_n(x)H_m(x)dx. \tag{3.54}$$

Solution

We use the following recursion relation [Eq. (3.27)]:

$$H_n(x) = \frac{1}{x}\left[\frac{1}{2}H_{n+1}(x) + nH_{n-1}(x)\right], \tag{3.55}$$

to write

$$\begin{aligned} I &= \int_{-\infty}^{\infty} xe^{-x^2} \frac{1}{x}\left[\frac{1}{2}H_{n+1}(x) + nH_{n-1}(x)\right] H_m(x)dx \\ &= \int_{-\infty}^{\infty} e^{-x^2} \left[\frac{1}{2}H_{n+1}H_m + nH_{n-1}H_m\right] \quad dx. \end{aligned} \tag{3.56}$$

Finally, using the orthogonality relation [Eq. (3.34)]:

$$\int_{-\infty}^{\infty} e^{-x^2} H_n(x)H_m(x)dx = \sqrt{\pi}2^n n!\delta_{nm}, \tag{3.57}$$

we obtain the desired result as

$$\boxed{\int_{-\infty}^{\infty} xe^{-x^2} H_n(x)H_m(x)dx = \sqrt{\pi}2^{n-1}n![2(n+1)\delta_{m,n+1} + \delta_{m,n-1}].} \quad (3.58)$$

Example 3.4 ***Operations with Hermite polynomials***
Verify the relation

$$\frac{d^m}{dx^m}H_n(x) = \frac{2^n n!}{(n-m)!}H_{n-m}(x), \quad m < n. \quad (3.59)$$

Solution:
Using the generating function, $\sum_{n=0}^{\infty} H_n(x)\frac{t^n}{n!} = e^{-t^2+2xt}$, we write

$$\sum_{n=0}^{\infty}\left[\frac{d^m}{dx^m}H_n(x)\right]\frac{t^n}{n!} = \frac{d^m}{dx^m}[e^{-t^2+2xt}] \quad (3.60)$$

$$= (2t)^m e^{-t^2+2xt} \quad (3.61)$$

$$= 2^m t^m \sum_{n=0}^{\infty} H_n(x)\frac{t^n}{n!} \quad (3.62)$$

$$= 2^m \sum_{n=0}^{\infty} H_n(x)\frac{t^{n+m}}{n!}. \quad (3.63)$$

Let $n + m = k$ to get

$$\sum_{n=0}^{\infty}\left[\frac{d^m}{dx^m}H_n(x)\right]\frac{t^n}{n!} = 2^m \sum_{k=m}^{\infty} H_{k-m}(x)\frac{t^k}{(k-m)!}, \quad (3.64)$$

which implies

$$\boxed{\frac{d^m}{dx^m}H_n(x) = \frac{2^n n!}{(n-m)!}H_{n-m}(x), \quad m < n.} \quad (3.65)$$

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Problems

1 For the Hermite polynomials, using the recursion relation

$$a_{k+2} = a_k \frac{(2k-2n)}{(k+2)(k+1)},$$

show that one can write the coefficients of the decreasing powers of x for the nth-order polynomial as

$$a_{n-2j} = (-1)^j \frac{n(n-1)(n-2)(n-3)\cdots(n-2j+1)}{2^j 2.4 \ldots (2j)} a_n,$$

or as

$$a_{n-2j} = \frac{(-1)^j n!}{(n-2j)!} \frac{1}{2^j 2^j j!} a_n.$$

2 For a three-dimensional harmonic oscillator, the Schrödinger equation is given as

$$-\frac{\hbar^2}{2m}\vec{\nabla}^2 \Psi(\vec{r}) + \frac{1}{2}m\omega^2 r^2 \Psi(\vec{r}) = E\Psi(\vec{r}).$$

Using the separation of variables technique, find the ordinary differential equations to be solved for r, θ, and ϕ.

3 Quantum mechanics of the three-dimensional harmonic oscillator leads to the following differential equation for the radial part of the wave function:

$$\frac{d^2R(x)}{dx^2} + \frac{2}{x}\frac{dR(x)}{dx} + \left[\epsilon - x^2 - \frac{l(l+1)}{x^2}\right] R(x) = 0,$$

where x and ϵ are defined in terms of the radial distance r and the energy E as $x = r/\sqrt{\hbar/m\omega}$ and $\epsilon = E/(\hbar\omega/2)$, and l takes integer values $l = 0, 1, 2, \ldots$.

(i) Examine the nature of the singular point at $x = \infty$.

(ii) Show that in the limit as $x \to \infty$, $R(x)$ behaves as $R \to e^{-x^2/2}$.

(iii) Using the Frobenius method, find an infinite series solution about $x = 0$ in the interval $[0, \infty]$. Check the convergence of your solution. Should the solution be finite everywhere including the end points, why?

(iv) For finite solutions everywhere in the interval $[0, \infty]$, what restrictions do you have to impose on the physical parameters of the system.

(v) For $l = 0, 1$, and 2, find explicitly the solutions corresponding to the three smallest values of ϵ.

4 Show the integral

$$\int_{-\infty}^{\infty} x^2 e^{-x^2} H_n(x) H_n(x) dx = \pi^{1/2} 2^n n! \left(n + \frac{1}{2}\right).$$

5 Prove the orthogonality relation

$$\int_{-\infty}^{\infty} e^{-x^2} H_m(x) H_n(x) dx = 2^n n! \sqrt{\pi} \delta_{mn}$$

using the generating function definition of $H_n(x)$.

6 Expand x^{2k} and x^{2k+1} in terms of the Hermite polynomials, to establish the results

(i) $x^{2k} = \dfrac{(2k)!}{2^{2k}} \sum_{n=0}^{k} \dfrac{H_{2n}(x)}{(2n)!(k-n)!}, \quad k = 0, 1, 2, \ldots,$

(ii) $x^{2k+1} = \dfrac{(2k+1)!}{2^{2k+1}} \sum_{n=0}^{k} \dfrac{H_{2n+1}(x)}{(2n+1)!(k-n)!}, \quad k = 0, 1, 2, \ldots.$

7 Show the following integrals:

(i) $\displaystyle\int_{-\infty}^{\infty} x e^{-x^2/2} H_n(x) dx = \left\{ \begin{array}{c} 0 \\ \dfrac{\sqrt{2\pi}(n+1)!}{[(n+1)/2]!} \end{array} \right\} \quad \text{for} \quad \left\{ \begin{array}{c} n \text{ even} \\ n \text{ odd} \end{array} \right\},$

(ii) $\displaystyle\int_{-\infty}^{\infty} e^{-x^2/2} H_n(x) dx = \left\{ \begin{array}{c} \sqrt{2\pi} n!/(n/2)! \\ 0 \end{array} \right\} \quad \text{for} \quad \left\{ \begin{array}{c} n \text{ even} \\ n \text{ odd} \end{array} \right\}.$

8 Show that

$$H_n(0) dx = \left\{ \begin{array}{c} 0 \\ (-1)^m \dfrac{(2m)!}{m!} \end{array} \right\} \quad \text{for} \quad \left\{ \begin{array}{c} n \text{ odd} \\ n = 2m \end{array} \right\}.$$

9 For positive integers k, m, and n, show that

$$\int_{-\infty}^{\infty} x^k e^{-x^2} H_m(x) H_{m+n}(x) dx$$
$$= \left\{ \begin{array}{c} 0 \\ \sqrt{\pi} 2^m (m+k)! \end{array} \right\} \quad \text{for} \quad \left\{ \begin{array}{c} n > k \\ n = k \end{array} \right\}.$$

10 Prove that

$$\int_{-\infty}^{\infty} e^{-a^2 x^2} H_{2n}(x) dx = \frac{(2n)!}{n!} \frac{\sqrt{\pi}}{a} \left[\frac{1 - a^2}{a^2}\right]^n,$$

Re $a^2 > 0$ and $n = 0, 1, 2, \ldots.$

11 Prove the expansions

(i) $e^{t^2}\cos 2xt = \sum_{n=0}^{\infty} \frac{(-1)^n H_{2n}(x)}{(2n)!} t^{2n}, \quad |t| < \infty,$

(ii) $e^{t^2}\sin 2xt = \sum_{n=0}^{\infty} \frac{(-1)^n H_{2n+1}(x)}{(2n+1)!} t^{2n+1}, \quad |t| < \infty.$

Note that these can be regarded as the generating functions for the even and the odd Hermite polynomials.

12 Show that for m integer the integral

$$\int_{-\infty}^{\infty} x^m e^{-x^2} H_n(x)dx = 0, \quad 0 \leq m \leq n-1.$$

13 The hypergeometric equation is given as

$$x(1-x)\frac{d^2y}{dx^2} + [\gamma - (\alpha+\beta+1)x]\frac{dy}{dx} - \alpha\beta y(x) = 0,$$

where α, β, and γ are arbitrary constants ($\gamma \neq$ integer and $\gamma \neq 0$).

(i) Show that it has the general solution

$$y(x) = C_0 F(\alpha,\beta,\gamma;x) + C_1 F(\alpha-\gamma+1,\beta-\gamma+1,2-\gamma;x),$$

valid for the region $|x| < 1$ and C_0 and C_1 are arbitrary integration constants, and the hypergeometric function is defined by

$$F(\alpha,\beta,\gamma;x) = \sum_{k=0}^{\infty} \frac{(\alpha)_k(\beta)_k}{(\gamma)_k}\frac{x^k}{k!}$$

with $(\alpha)_k = \alpha(\alpha+1)(\alpha+2)\cdots(\alpha+k-1)$.

(ii) If a regular series solution is required for the entire interval $[-1,1]$, the above series will not serve as the solution. What conditions do you have to impose on α, β to ensure a regular solution in this case?

(iii) Show that Legendre polynomials can be expressed as $P_l(x) = F(-l, l+1, 1; (1-x)/2)$.

14 Establish the following connections between the Hermite and the Laguerre polynomials:

(i) $L_n^{-1/2}(x) = (-1)^n \quad H_{2n}\left(\sqrt{x}\right)/2^{2n}n!,$

(ii) $L_n^{1/2}(x) = (-1)^n H_{2n+1}\left(\sqrt{x}\right)/2^{2n+1}n!\sqrt{x}.$

15 Derive the following recursion relations:

(i) $H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x),$

(ii) $H_n'(x) = 2nH_{n-1}(x).$

4

Gegenbauer and Chebyshev Polynomials

The sine and cosine functions play a central role in the study of oscillations and waves. They come from the solutions of the Helmholtz wave equation in Cartesian coordinates with the appropriate boundary conditions. The sine and cosine functions also form a basis for representing general waves and oscillations of various types, shapes, and sizes. On the other hand, solutions of the angular part of the Helmholtz equation in spherical polar coordinates are the spherical harmonics. Analogous to the oscillations of a piece of string, spherical harmonics correspond to the oscillations of a two-sphere, that is, the surface of a sphere in three dimensions. Spherical harmonics also form a complete set of orthonormal functions; hence they are very important in many theoretical and practical applications. For the oscillations of a three-sphere (hypersphere), along with the spherical harmonics, we also need the Gegenbauer polynomials. Gegenbauer polynomials are very useful in cosmology and quantum field theory in curved backgrounds. Both the spherical harmonics and the Gegenbauer polynomials are combinations of sines and cosines. Chebyshev polynomials form another complete and orthonormal set of functions, which are closely related to the Gegenbauer polynomials.

4.1 Wave Equation on a Hypersphere

Friedmann Robertson Walker models in cosmology, which are also called the **standard models**, are generally accepted as accurately describing the global properties of the universe like homogeneity, isotropy, and expansion. Among the standard models, closed universes correspond to the surface of a hypersphere (three-sphere), where the spacetime geometry is described by the line element

$$ds^2 = dt^2 - R(t)^2 \left[d\chi^2 + \sin^2\chi d\theta^2 + \sin^2\chi \sin^2\theta d\phi^2 \right] . \tag{4.1}$$

Here, t is the universal time and $R(t)$ is the time-dependent radius of the hypersphere. Angular coordinates have the ranges $\chi \in [0, \pi]$, $\theta \in [0, \pi]$, $\phi \in [0, 2\pi]$.

Mathematical Methods in Science and Engineering, Second Edition. Selçuk Ş. Bayın.

We now consider the **wave equation** for the **massless conformal scalar field** in a closed static universe, $R(t) = R_0$, also known as the **Einstein model**:

$$\boxed{\Box\Phi(t,\chi,\theta,\phi) + \frac{1}{R_0^2}\Phi(t,\chi,\theta,\phi) = 0.} \tag{4.2}$$

Here, $\Box$ stands for the **d'Alembert** or the **wave operator,** $\Box = g_{\mu\nu}\nabla^{\mu}\nabla^{\nu}$, where ∇^{μ} stands for the covariant derivative. Explicit evaluation of Eq. (4.2) is beyond the scope of this chapter; hence we suffice by saying that a **separable solution** of the form

$$\boxed{\Phi(t,\chi,\theta,\phi) = T(t)X(\chi)Y(\theta,\phi)} \tag{4.3}$$

reduces Eq. (4.2) to

$$\begin{aligned}&\left[\frac{1}{T(t)}\frac{d^2T(t)}{dt^2}\right] - \left[\frac{1}{R_0^2X(\chi)}\left(\frac{d^2X(\chi)}{d\chi^2} + \frac{2\cos\chi}{\sin\chi}\frac{dX(\chi)}{d\chi} - 1\right)\right] - \frac{1}{R_0^2\sin^2\chi}\\ &\times\left[\frac{1}{Y(\theta,\phi)}\left(\frac{\partial^2Y(\theta,\phi)}{\partial\theta^2} + \frac{\cos\theta}{\sin\theta}\frac{\partial Y(\theta,\phi)}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2Y(\theta,\phi)}{\partial\phi^2}\right)\right] = 0,\end{aligned} \tag{4.4}$$

where we have set $c = 1$.

Since t, χ, θ, ϕ are independent coordinates, this equation can be satisfied for all (t, χ, θ, ϕ) only when the expressions inside the square brackets are equal to constants. Introducing two **separation constants,** $-\omega^2$ and λ, we obtain the differential equations to be solved for $T(t)$, $X(\chi)$, and $Y(\theta,\phi)$, respectively, as

$$\boxed{\frac{1}{T(t)}\frac{d^2T(t)}{dt^2} = -\omega^2,} \tag{4.5}$$

$$\boxed{\frac{1}{Y(\theta,\phi)}\left(\frac{\partial^2Y(\theta,\phi)}{\partial\theta^2} + \frac{\cos\theta}{\sin\theta}\frac{\partial Y(\theta,\phi)}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2Y(\theta,\phi)}{\partial\phi^2}\right) = \lambda,} \tag{4.6}$$

$$\boxed{\begin{aligned}&\sin^2\chi\frac{d^2X(\chi)}{d\chi^2} + 2\sin\chi\cos\chi\frac{dX(\chi)}{d\chi} + \left(\omega^2 - \frac{1}{R_0^2}\right)R_0^2\sin^2\chi X(\chi)\\ &\quad = -\lambda X(\chi).\end{aligned}} \tag{4.7}$$

The two linearly independent solutions of Eq. (4.5) can be written immediately as $T(t) = e^{i\omega t}$ and $e^{-i\omega t}$, while the second Eq. (4.6) is nothing but the differential equation that the spherical harmonics, $Y_l^m(\theta,\phi)$, satisfy with λ and m given as

$$\lambda = -l(l+1), \quad l = 0,1,2,\ldots \quad \text{and} \quad m = 0,\pm1,\ldots,\pm l. \tag{4.8}$$

Before we try a series solution in the equation to be solved for $X(\chi)$ [Eq. (4.7)], we make the substitutions

$$\boxed{X(\chi) = C_0 \sin^l \chi C(\cos \chi), \quad x = \cos \chi, \quad x \in [-1, 1],} \tag{4.9}$$

to obtain the following differential equation for $C(x)$:

$$(1 - x^2)\frac{d^2C(x)}{dx^2} - (2l + 3)x\frac{dC(x)}{dx} + \left[-l(l + 2) + \left(\omega^2 - \frac{1}{R_0^2}\right)R_0^2\right] C(x) = 0. \tag{4.10}$$

The substitution in Eq. (4.9) is needed to ensure a two-term recursion relation with the **Frobenius method**. This equation has two **regular singular points** at the end points, $x = \pm 1$, hence we try a series solution of the form $C(x) = \sum_{k=0}^{\infty} a_k x^{k+\alpha}$ to write

$$\begin{aligned} &a_0\alpha(\alpha - 1)x^{\alpha-2} + a_1\alpha(\alpha + 1)x^{\alpha-1} + \sum_{k=0}^{\infty}\{a_{k+2}(k + \alpha + 2)(k + \alpha + 1) \\ &\quad - a_k[(k + \alpha)(k + \alpha - 1) + (2l + 3)(k + \alpha) - A]\}x^{k+\alpha} = 0, \end{aligned} \tag{4.11}$$

where $A = -l(l + 2) + (\omega^2 - \frac{1}{R_0^2})R_0^2$. Equation (4.11) cannot be satisfied for all x unless the coefficients of all the powers of x are zero, that is,

$$a_0\alpha(\alpha - 1) = 0, \quad a_0 \neq 0, \tag{4.12}$$

$$a_1\alpha(\alpha + 1) = 0, \tag{4.13}$$

$$a_{k+2} = a_k\left[\frac{(k + \alpha)(k + \alpha - 1) + (2l + 3)(k + \alpha) - A}{(k + \alpha + 2)(k + \alpha + 1)}\right], \quad k = 0, 1, 2, \ldots. \tag{4.14}$$

The **indicial equation** [Eq. (4.12)] has two roots as 0 and 1. Using the smaller root, $\alpha = 0$, we obtain the general solution as

$$\begin{aligned} C(x) = a_0&\left[1 - \frac{A}{2}x^2 - \left(\frac{2 + 2(2l + 3) - A}{3.4}\right)\frac{A}{2}x^4 + \cdots\right] \\ &+ a_1\left[x + \frac{(2l + 3) - A}{2.3}x^3 + \cdots\right]. \end{aligned} \tag{4.15}$$

Here, a_0 and a_1 are two integration constants and the **recursion relation** for the coefficients is given as

$$\boxed{a_{k+2} = a_k\left[\frac{k(k - 1) + (2l + 3)k - A}{(k + 2)(k + 1)}\right], \quad k = 0, 1, 2, \ldots.} \tag{4.16}$$

From the limit $a_{k+2}/a_k \to 1$ as $k \to \infty$, we see that both of these series diverge at the end points $x = \pm 1$ as $1/(1-x^2)$. To avoid the divergence at the end points, we terminate the series by restricting ωR_0 to integer values as

$$\omega_N = (N+1)/R_0, \quad N = 0, 1, 2, \dots . \tag{4.17}$$

Polynomial solutions obtained this way can be expressed in terms of the **Gegenbauer polynomials**.

Note that these frequencies mean that one can only fit integer multiples of full wavelengths around the circumference, $2\pi R_0$, of the universe, that is, $(1+N)\lambda_N = 2\pi R_0$, $N = 0, 1, 2, \dots$. Using the relation $\omega_N = 2\pi/\lambda_N$, we again obtain the frequencies of Eq. (4.17).

4.2 Gegenbauer Equation and Polynomials

In general, the **Gegenbauer equation** is written as

$$(1-x^2)\frac{d^2C_n^\lambda(x)}{dx^2} - (2\lambda+1)x\frac{dC_n^\lambda(x)}{dx} + n(n+2\lambda)C_n^\lambda(x) = 0. \tag{4.18}$$

For $\lambda = 1/2$, this equation reduces to the Legendre equation. For the integer values of n, its solutions reduce to the **Gegenbauer polynomials**:

$$C_n^\lambda(x) = \sum_{r=0}^{[n/2]} (-1)^r \frac{\Gamma(n-r+\lambda)}{\Gamma(\lambda)r!(n-2r)!}(2x)^{n-2r}. \tag{4.19}$$

4.2.1 Orthogonality and the Generating Function

Orthogonality relation of the Gegenbauer polynomials is given as

$$\int_{-1}^{1} (1-x^2)^{\lambda-\frac{1}{2}} C_n^\lambda(x) C_m^\lambda(x) dx = 2^{1-2\lambda} \frac{\pi\Gamma(n+2\lambda)}{(n+\lambda)\Gamma^2(\lambda)\Gamma(n+1)}\delta_{nm}. \tag{4.20}$$

Gegenbauer polynomials can also be defined by the following **generating function:**

$$\frac{1}{(1-2xt+t^2)^\lambda} = \sum_{n=0}^{\infty} C_n^\lambda(x)t^n, \quad |t| < 1, \quad |x| \le 1, \quad \lambda > -1/2. \tag{4.21}$$

We can now write the solution of Eq. (4.10) in terms of the Gegenbauer polynomials as $C(x) = C_{N-l}^{l+1}(x)$, thus obtaining the **complete solution** of the wave equation [Eq. (4.2)] as

$$\boxed{\Phi(t, \chi, \theta, \phi) = (c_1 e^{i\omega_N t} + c_2 e^{-i\omega_N t})(\sin^l \chi) C_{N-l}^{l+1}(\cos\chi) Y_l^m(\theta, \phi).} \tag{4.22}$$

4.2.2 Another Representation of the Solution

We now show that the function

$$\boxed{{}_1\Pi_l^N(\chi) = \sin^l \chi \frac{d^{l+1}(\cos N\chi)}{d(\cos\chi)^{l+1}}} \tag{4.23}$$

is another useful representation of the solution of the differential equation [Eq. (4.7)] for $X(\chi)$:

$$\sin^2\chi \frac{d^2X}{d\chi^2} + 2\sin\chi\cos\chi \frac{dX}{d\chi} + \left[\left(\omega^2 - \frac{1}{R_0^2}\right) R_0^2 \sin^2\chi - l(l+1)\right] X(\chi) = 0, \tag{4.24}$$

with $\omega = N/R_0, N = 1, 2, \ldots$. We first write Eq. (4.24) as

$$\frac{d}{d\chi}\left[\sin^2\chi \frac{dX}{d\chi}\right] + \left[\left(\omega^2 - \frac{1}{R_0^2}\right) R_0^2 \sin^2\chi - l(l+1)\right] X(\chi) = 0 \tag{4.25}$$

and then make the transformation $x = \cos\chi$ to obtain

$$\boxed{(1-x^2)^2 \frac{d^2X}{dx^2} - 3x(1-x^2)\frac{dX}{dx} + \left[(\omega^2 R_0^2 - 1)(1-x^2) - l(l+1)\right] X(x) = 0.} \tag{4.26}$$

First, substitute

$${}_1\Pi_l^N(\chi) = (1-x^2)^{l/2} \frac{d^{l+1}(\cos N\chi)}{dx^{l+1}} \tag{4.27}$$

into the above differential equation to write

$$(1-x^2)\frac{d^{l+3}(\cos N\chi)}{dx^{l+3}} - (2l+3)x\frac{d^{l+2}(\cos N\chi)}{dx^{l+2}} + \left[-l^2 - 2l - 1 + \omega^2 R_0^2\right] \frac{d^{l+1}(\cos N\chi)}{dx^{l+1}} = 0. \tag{4.28}$$

Now we need to show that $d^{l+1}(\cos N\chi)/dx^{l+1}$ satisfies the following second-order differential equation for $\omega = N/R_0$:

$$(1-x^2)\frac{d^2}{dx^2}\left[\frac{d^{l+1}(\cos N\chi)}{dx^{l+1}}\right] - (2l+3)x\frac{d}{dx}\left[\frac{d^{l+1}(\cos N\chi)}{dx^{l+1}}\right] + \left[-(l+1)^2 + \omega^2 R_0^2\right]\left[\frac{d^{l+1}(\cos N\chi)}{dx^{l+1}}\right] = 0. \tag{4.29}$$

We first show that the above equation is true for $l = 0$:

$$(1-x^2)\frac{d^3(\cos N\chi)}{dx^3} - 3x\frac{d^2(\cos N\chi)}{dx^2} + \left[-1 + \omega^2 R_0^2\right]\frac{d(\cos N\chi)}{dx} = 0. \tag{4.30}$$

Evaluating the derivatives explicitly gives $\omega = N/R_0$. Finally, the l-fold differentiation of Eq. (4.30) and the Leibnitz rule:

$$\frac{d^l(uv)}{dx^l} = \sum_{r=0}^{l}\binom{l}{r}\frac{d^r u}{dx^r}\frac{d^{l-r}v}{dx^{l-r}}, \tag{4.31}$$

gives the desired result. Note that N is not quantized yet, however, for finite solutions everywhere in the interval $x \in [-1,1]$, we restrict N to integer values, $N = 1, 2, \ldots$.

4.2.3 The Second Solution

The **second solution** of Eq. (4.24) can be written as

$$\boxed{{}_2\Pi_l^N(\chi) = \sin^l\chi\,\frac{d^{l+1}(\sin N\chi)}{d(\cos\chi)^{l+1}}.} \tag{4.32}$$

To prove that the above function is indeed a solution of Eq. (4.24), we use the same method used for ${}_1\Pi_l^N(\chi)$. Their **linear independence** can be established by showing that the **Wronskian**, which is defined by the determinant $W[u_1(x), u_2(x)] = u_1u_2' - u_2u_1'$, is different from zero. The **general solution** can now be given as the linear combination:

$$\boxed{X(\chi) = c_{01}\Pi_l^N(\chi) + c_{12}\Pi_l^N(\chi),} \tag{4.33}$$

where c_0 and c_1 are two integration constants. Since the second solution diverges at the end points, for finite solutions everywhere in the interval $\chi \in [0,\pi]$, or $x \in [-1,1]$, we set its coefficient in the general solution to zero.

4.2.4 Connection with the Gegenbauer Polynomials

To establish the connection of Eq. (4.23) with the Gegenbauer polynomials, we make use of the trigonometric expansion [3]:

$$\cos N\chi = \sum_{j=0}^{[N/2]} \frac{N(N-j-1)!(-1)^j 2^{N-(2j+1)}}{(N-2j)!j!} (\cos\chi)^{N-2j}, \tag{4.34}$$

which terminates when a coefficient is zero. Using the substitution $x = \cos\chi$, we can write

$$\frac{d^{l+1}(\cos N\chi)}{dx^{l+1}} = N \sum_{j=0}^{[(N-l-1)/2]} (-1)^j \frac{2^{N-(2j+1)}(N-j-1)!}{(N-2j-l-1)!j!} x^{N-2j-l-1}, \tag{4.35}$$

where $N = 1, 2, \ldots$ and where we have used the formula $\frac{d^m x^n}{dx^m} = \frac{n!}{(m-n)!} x^{m-n}$. Comparing this with the Gegenbauer polynomials [Eq. (4.19)]:

$$C_n^\lambda(x) = \sum_{r=0}^{[n/2]} (-1)^r \frac{\Gamma(n-r+\lambda)}{\Gamma(\lambda) r!(n-2r)!} (2x)^{n-2r}, \tag{4.36}$$

which satisfies the differential equation [Eq. (4.18)]:

$$(1-x^2)\frac{d^2 C_n^\lambda(x)}{dx^2} - (2\lambda+1)x\frac{dC_n^\lambda(x)}{dx} + n[n+2\lambda]C_n^\lambda(x) = 0, \tag{4.37}$$

we see that the function $d^{l+1}(\cos Nx)/dx^{l+1}$ is proportional to the Gegenbauer polynomial $C_{N-l-1}^{l+1}(x)$, $N = 1, 2, \ldots$. That is,

$$C_{N-l-1}^{l+1}(x) = \sum_{j=0}^{[(N-l-1)/2]} (-1)^j \frac{\Gamma(N-j)2^{N-2j-1-l}}{j!\Gamma(l+1)(N-2j-l-1)!} x^{N-2j-l-1} \tag{4.38}$$

$$= \sum_{j=0}^{[(N-l-1)/2]} (-1)^j \frac{(N-j-1)!2^{-l}2^{N-2j-1}}{j!l!(N-2j-l-1)!} x^{N-2j-l-1} \tag{4.39}$$

$$= \left(\frac{2^{-l}}{l!}\right) \sum_{j=0}^{[(N-l-1)/2]} (-1)^j \frac{2^{N-2j-1}(N-j-1)!}{j!(N-2j-l-1)!} x^{N-2j-l-1} \tag{4.40}$$

$$= \left(\frac{2^{-l}}{l!}\right) \frac{1}{N} \left[\frac{d^{l+1}(\cos N\chi)}{dx^{l+1}}\right]. \tag{4.41}$$

Hence, they both satisfy the same differential equation [Eq. (4.29)]. We can now write the solution of Eq. (4.24) as

$$\boxed{X(\chi) = c_0\, {}_1\Pi_l^N(\chi) = c_0 \sin^l\chi \frac{d^{l+1}(\cos N\chi)}{d(\cos\chi)^{l+1}},} \tag{4.42}$$

or as

$$\boxed{X(\chi) = C_0 \sin^l \chi C_{N-l-1}^{l+1}(\cos \chi).} \tag{4.43}$$

For finite solutions everywhere in the interval $\chi \in [0, \pi]$, we restrict N to integers, $N = 1, 2, \ldots$.

4.2.5 Evaluation of the Normalization Constant

Using the orthogonality condition of the Gegenbauer polynomials [Eq. (4.20)], we can write

$$\int_{-1}^{+1} (1 - x^2)^{l+1/2} [C_{N-l-1}^{l+1}(x)]^2 dx = \frac{\pi}{2^{2l+1} N (l!)^2} \frac{(N+l)!}{(N-l-1)!}. \tag{4.44}$$

We can also write the ratio

$$\frac{(N+l)!}{(N-l-1)!} = \frac{(N+l) \cdots N \cdots (N-l)(N-l-1)!}{(N-l-1)!} \tag{4.45}$$

$$= (N^2 - l^2) \cdots (N^2 - 1) N, \tag{4.46}$$

which gives

$$\int_{-1}^{+1} (1 - x^2)^{l+1/2} [C_{N-l-1}^{l+1}(x)]^2 \, dx = \frac{\pi (N^2 - l^2) \cdots (N^2 - 1)}{2^{2l+1} (l!)^2}. \tag{4.47}$$

This gives C_0 in Eq. (4.43) as

$$\boxed{C_0 = 2^{(2l+1)/2} l! [\pi (N^2 - l^2) \ldots (N^2 - 1)]^{-1/2}.} \tag{4.48}$$

We now use Eqs (4.35) and (4.38) to establish the relation

$$C_{N-l-1}^{l+1}(\cos \chi) = l! 2^l N \left[\frac{d^{l+1}(\cos N\chi)}{d(\cos \chi)^{l+1}} \right], \tag{4.49}$$

which yields c_0 in Eq. (4.42) as $c_0 = \left[\frac{\pi}{2} (N^2 - l^2) \cdots (N^2 - 1) N^2 \right]^{-1/2}$.

4.3 Chebyshev Equation and Polynomials

4.3.1 Chebyshev Polynomials of the First Kind

Polynomials defined as

$$\boxed{T_n(\cos \chi) = \cos(n\chi), \quad n = 0, 1, 2 \ldots} \tag{4.50}$$

are called the **Chebyshev polynomials** of the **first kind**. They satisfy the **Chebyshev equation:**

$$\boxed{(1-x^2)\frac{d^2T_n(x)}{dx^2}-x\frac{dT_n(x)}{dx}+n^2T_n(x)=0, \quad x=\cos\chi.} \tag{4.51}$$

4.3.2 Chebyshev and Gegenbauer Polynomials

The Chebyshev equation after $(l+1)$-fold differentiation yields

$$(1-x^2)\frac{d^{l+3}(\cos n\chi)}{dx^{l+3}}-(2l+3)x\frac{d^{l+2}(\cos n\chi)}{dx^{l+2}} + \left[-l^2-2l-1+n^2\right]\frac{d^{l+1}(\cos n\chi)}{dx^{l+1}}=0, \tag{4.52}$$

where $n=1,2,\ldots$. We now rearrange this as

$$\left\{(1-x^2)\frac{d^2}{dx^2}-(2l+3)x\frac{d}{dx}+[-l(l+2)+n^2-1]\right\}\left[\frac{d^{l+1}(\cos n\chi)}{dx^{l+1}}\right]=0, \tag{4.53}$$

$$\left\{(1-x^2)\frac{d^2}{dx^2}-[2(l+1)+1]x\frac{d}{dx}+(n-l-1)[(n-l-1)+2(l+1)]\right\} \times\left[\frac{d^{l+1}(\cos n\chi)}{dx^{l+1}}\right]=0 \tag{4.54}$$

and compare with Eq. (4.18) to obtain the following relation between the Gegenbauer and the **Chebyshev polynomials** of the **first kind**:

$$C_{n-l-1}^{l+1}(x)=\frac{d^{l+1}(\cos nx)}{dx^{l+1}}, \tag{4.55}$$

that is,

$$\boxed{C_{n-l-1}^{l+1}(x)=\frac{d^{l+1}T_n(x)}{dx^{l+1}}, \quad n=1,2,\ldots.} \tag{4.56}$$

4.3.3 Chebyshev Polynomials of the Second Kind

Chebyshev polynomials of the **second kind** are defined as

$$\boxed{U_n(x)=\sin(n\chi), \quad n=0,1,2\ldots,} \tag{4.57}$$

where $x=\cos\chi$. Chebyshev polynomials of the first and second kinds are linearly independent and they both satisfy the Chebyshev equation (4.51).

In terms of x, the Chebyshev polynomials are written as

$$T_n(x) = \sum_{r=0}^{[n/2]} (-1)^r \frac{n!}{(2r)!(n-2r)!}(1-x^2)^r x^{n-2r},$$
$$U_n(x) = \sum_{r=0}^{[(n-1)/2]} (-1)^r \frac{n!}{(2r+1)!(n-2r-1)!}(1-x^2)^{r+\frac{1}{2}} x^{n-2r-1}. \quad (4.58)$$

For some n values, the Chebyshev polynomials are given as follows:

Chebyshev polynomials of the first kind

$$T_0 = 1,$$
$$T_1(x) = x,$$
$$T_2(x) = 2x^2 - 1,$$
$$T_3(x) = 4x^3 - 3x,$$
$$T_4(x) = 8x^4 - 8x^2 + 1,$$
$$T_5(x) = 16x^5 - 20x^3 + 5x.$$

Chebyshev polynomials of the second kind

$$U_0 = 0,$$
$$U_1(x) = \sqrt{(1-x^2)},$$
$$U_2(x) = \sqrt{(1-x^2)}(2x),$$
$$U_3(x) = \sqrt{(1-x^2)}(4x^2 - 1),$$
$$U_4(x) = \sqrt{(1-x^2)}(8x^3 - 4x),$$
$$U_5(x) = \sqrt{(1-x^2)}(16x^4 - 12x^2 + 1).$$

4.3.4 Orthogonality and Generating Function

Generating functions of the Chebyshev polynomials are given as

$$\frac{1-t^2}{1-2tx+t^2} = T_0(x) + 2\sum_{n=1}^{\infty} T_n(x)t^n, \quad |t| < 1, \quad |x| \le 1,$$
$$\frac{\sqrt{1-x^2}}{1-2tx+t^2} = \sum_{n=0}^{\infty} U_{n+1}(x)t^n. \quad (4.59)$$

and their **orthogonality relations** are

$$\int_{-1}^{1} \frac{T_m(x)T_n(x)}{\sqrt{1-x^2}}dx = \begin{Bmatrix} 0 & m \neq n \\ \pi/2 & m = n \neq 0 \\ \pi & m = n = 0 \end{Bmatrix},$$

$$\int_{-1}^{1} \frac{U_m(x)U_n(x)}{\sqrt{1-x^2}}dx = \begin{Bmatrix} 0 & m \neq n \\ \pi/2 & m = n \neq 0 \\ 0 & m = n = 0 \end{Bmatrix}. \tag{4.60}$$

4.3.5 Another Definition

Sometimes the polynomials defined as

$$\begin{aligned} \overline{U}_0(x) &= 1, \\ \overline{U}_1(x) &= 2x, \\ \overline{U}_2(x) &= 4x^2 - 1, \\ \overline{U}_3(x) &= 8x^3 - 4x, \\ \overline{U}_4(x) &= 16x^4 - 12x^2 + 1, \end{aligned} \tag{4.61}$$

are also referred to as the **Chebyshev polynomials** of the **second kind**. They are related to $U_n(x)$ by the relation

$$\sqrt{1-x^2}\,\overline{U}_n(x) = U_{n+1}(x), \quad n = 0, 1, 2, \dots . \tag{4.62}$$

They satisfy the **differential equation**

$$(1-x^2)\frac{d^2\overline{U}_n(x)}{dx^2} - 3x\frac{d\overline{U}_n(x)}{dx} + n(n+2)\overline{U}_n(x) = 0 \tag{4.63}$$

and their **orthogonality relation** is given as

$$\int_{-1}^{1} dx\sqrt{1-x^2}\,\overline{U}_m(x)\overline{U}_n(x) = \frac{\pi}{2}\delta_{mn}. \tag{4.64}$$

Note that even though $\overline{U}_m(x)$ are polynomials, $U_m(x)$ are not. The **generating function** for $\overline{U}_m(x)$ is given as

$$\frac{1}{(1-2xt+t^2)} = \sum_{m=0}^{\infty} \overline{U}_m(x)t^m, \quad |t| < 1, \quad |x| < 1, \tag{4.65}$$

where $T_n(x)$ and $\overline{U}_n(x)$ satisfy the following **recursion relations:**

$$(1-x^2)T_n'(x) = -nxT_n(x) + nT_{n-1}(x), \tag{4.66}$$

$$(1-x^2)\overline{U}_n'(x) = -nx\overline{U}_n(x) + (n+1)\overline{U}_{n-1}(x). \tag{4.67}$$

Special values of the Chebyshev polynomials

$$\begin{aligned} T_n(1) &= 1, \\ T_n(-1) &= (-1)^n, \\ T_{2n}(0) &= (-1)^n, \\ T_{2n+1}(0) &= 0, \\ U_n(1) &= 0, \\ U_n(-1) &= 0, \\ U_{2n}(0) &= 0, \\ U_{2n+1}(0) &= (-1)^n. \end{aligned} \tag{4.68}$$

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Problems

1 By inspection, observe that the equation

$$\sin^2\chi \frac{d^2X(\chi)}{d\chi^2} + 2\sin\chi\cos\chi \frac{dX(\chi)}{d\chi} + \left(\omega^2 - \frac{1}{R_0^2}\right) R_0^2 \sin^2\chi X(\chi) = -\lambda X(\chi)$$

gives a three-term recursion relation and then drive the transformation $X(\chi) = C_0 \sin^l \chi C(\cos\chi)$, which gives a differential equation for $C(\cos\chi)$ with a two-term recursion relation.

2 Using the line element $ds^2 = c^2dt^2 - R(t)^2[d\chi^2 + \sin^2\chi d\theta^2 + \sin^2\chi \sin^2\theta d\phi^2]$, find the spatial volume of a closed universe. What is the circumference?

3 Show that the solutions of

$$(1-x^2)\frac{d^2C(x)}{dx^2}-(2l+3)x\frac{dC(x)}{dx}+\left[-l(l+2)+\left(\omega_N^2-\frac{1}{R_0^2}\right)R_0^2\right]C(x)=0$$

can be expressed in terms of the Gegenbauer polynomials as $C(x)=C_{N-l}^{l+1}(x)$, where $\omega_N=(N+1)/R_0$, $N=0,1,2,\ldots$.

4 Show the orthogonality relation of the Gegenbauer polynomials:

$$\int_{-1}^{1}(1-x^2)^{\lambda-\frac{1}{2}}C_n^{\lambda}(x)C_m^{\lambda}(x)dx=2^{1-2\lambda}\frac{\pi\Gamma(n+2\lambda)}{(n+\lambda)\Gamma^2(\lambda)\Gamma(n+1)}\delta_{nm}.$$

5 Show that the generating function

$$\frac{1}{(1-2xt+t^2)^{\lambda}}=\sum_{n=0}^{\infty}C_n^{\lambda}(x)t^n,\quad |t|<1,\quad |x|\le 1,\quad \lambda>-1/2$$

can be used to define the Gegenbauer polynomials.

6 Using the Frobenius method, find a series solution to the Chebyshev equation:

$$(1-x^2)\frac{d^2y(x)}{dx^2}-x\frac{dy(x)}{dx}+n^2y(x)=0,\quad x\in[-1,1].$$

For finite solutions in the entire interval $[-1,1]$, do you have to restrict n to integer values?

7 Show the following special values:

(i) $T_n(1)=1$, (v) $\overline{U}_n(1)=n+1$,
(ii) $T_n(-1)=(-1)^n$, (vi) $\overline{U}_n(-1)=(-1)^n(n+1)$,
(iii) $T_{2n}(0)=(-1)^n$, (vii) $\overline{U}_{2n}(0)=(-1)^n$,
(iv) $T_{2n+1}(0)=0$, (viii) $\overline{U}_{2n+1}(0)=0$.

8 Show that the following relations are true:
(i) $T_n(-x)=(-1)^nT_n(x)$,
(ii) $\overline{U}_n(-x)=(-1)^n\overline{U}_n(x)$.

9 Using the generating function, $1/(1-2xt+t^2)=\sum_{m=0}^{\infty}\overline{U}_m(x)t^m$, $|t|<1$, $|x|<1$, show that $\overline{U}_m(x)$ are defined as

$$\overline{U}_m(x)=\sum_{k=0}^{[m/2]}(-1)^k\frac{(m-k)!}{k!(m-2k)!}(2x)^{m-2k}.$$

10 Show that $T_n(x)$ and $U_n(x)$ satisfy the recursion relations
(i) $(1-x^2)T_n'(x) = -nxT_n(x) + nT_{n-1}(x)$,
(ii) $(1-x^2)U_n'(x) = -nxU_n(x) + nU_{n-1}(x)$.

11 Let $x = \cos\chi$ and find a series expansion of $C(x) = d^{l+1}(\cos N\chi)/d(\cos\chi)^{l+1}$ in terms of x. What happens when N is an integer.

12 Show that $y(x) = d^{l+1}(\cos N\chi)/dx^{l+1}$ satisfies the following second-order ordinary differential equation with $\omega^2 R_0^2 = N$:

$$(1-x^2)\frac{d^2y}{dx^2} - (2l+3)x\frac{dy}{dx} + [-(l+1)^2 + \omega^2 R_0^2]y(x) = 0, \quad x = \cos\chi.$$

13 Verify that the second solution:

$${}_2\Pi_l^N = (1-x^2)^{l/2}\frac{d^{l+1}(\sin N\chi)}{dx^{l+1}},$$

satisfies the following differential equation for $\omega^2 R_0^2 = N$ and $x = \cos\chi$:

$$(1-x^2)^2\frac{d^2X}{dx^2} - 3x(1-x^2)\frac{dX}{dx} + [(\omega^2 R_0^2 - 1)(1-x^2) - l(l+1)]X(x) = 0,$$

14 Show that

$${}_1\Pi_l^N = (1-x^2)^{l/2}\frac{d^{l+1}(\cos N\chi)}{dx^{l+1}},$$
$${}_2\Pi_l^N = (1-x^2)^{l/2}\frac{d^{l+1}(\sin N\chi)}{dx^{l+1}},$$

where $x = \cos\chi$, are linearly independent and examine their behavior at the end points of the interval $x \in [-1, 1]$. What restriction do you need to put on N for finite solutions everywhere.

15 Evaluate the normalization constants c_0 and C_0 in $X(\chi)$, where $X(\chi)$ is given as

$$X(\chi) = c_0\, {}_1\Pi_l^N(\chi) = c_0 \sin^l\chi \frac{d^{l+1}(\cos N\chi)}{d(\cos\chi)^{l+1}},$$

or as

$$X(\chi) = C_0 \sin^l\chi\, C_{N-l-1}^{l+1}(\cos\chi),$$

so that $\int_0^\pi |X(\chi)|^2 \sin^2\chi\, d\chi = 1$.

16 Using

$$C_n^\lambda(x) = \sum_{r=0}^{[n/2]} (-1)^r \frac{\Gamma(n-r+\lambda)}{\Gamma(\lambda) r!(n-2r)!} (2x)^{n-2r},$$

show that for $\lambda = 1/2$ Gegenbauer polynomials reduce to the Legendre polynomials, that is, $C_n^{1/2}(x) = P_n(x)$.

17 Prove the recursion relations
(i) $T_{n+1}(x) - 2xT_n(x) + T_{n-1}(x) = 0,$
(ii) $U_{n+1}(x) - 2xU_n(x) + U_{n-1}(x) = 0.$

18 Chebyshev polynomials $T_n(x)$ and $U_n(x)$ can be related to each other. Show the relations
(i) $(1-x^2)^{1/2} T_n(x) = U_{n+1}(x) - xU_n(x),$
(ii) $(1-x^2)^{1/2} U_n(x) = xT_n(x) - T_{n+1}(x).$

19 Obtain the Chebyshev expansion:

$$(1-x^2)^{1/2} = \frac{2}{\pi}\left[1 - 2\sum_{s=1}^{\infty} (4s^2-1)^{-1} T_{2s}(x)\right].$$

5

Bessel Functions

The important role that trigonometric and hyperbolic functions play in the study of oscillations is well known. The equation of motion of a uniform rigid rod of length $2l$ suspended from one end and oscillating freely in a plane is given as $I\ddot{\theta} = -mgl\sin\theta$, where I is the moment of inertia, m is the mass, g is the acceleration of gravity, and θ is the angular displacement of the rod from its equilibrium position. For small oscillations, using the approximation $\sin\theta \simeq \theta$, we obtain the general solution in terms of trigonometric functions as

$$\theta(t) = A\cos\omega_0 t + B\sin\omega_0 t, \quad \omega_0^2 = mgl/I. \tag{5.1}$$

Suppose the rod is oscillating inside a viscous fluid exerting a drag force proportional to $\dot{\theta}$ with the proportionality constant k as the drag coefficient. Now the equation of motion becomes $I\ddot{\theta} = -k\dot{\theta} - mgl\theta$. For fluids with low viscosity, oscillations die out exponentially but the general solution is still expressed in terms of trigonometric functions. However, for highly viscous fluids, where the inequality $(k/2I)^2 > \omega_0^2$ holds, one needs the hyperbolic functions to express the solution as

$$\theta(t) = e^{-(k/2I)t}\left[A\cosh q_0 t + B\sinh q_0 t\right], \quad q_0^2 = (k/2I)^2 - \omega_0^2. \tag{5.2}$$

Now consider small oscillations of a flexible chain with uniform density ρ_0, length l, and with loops very small compared to the length of the chain. The distance upwards from the free end of the chain is x and the displacement of the chain from its equilibrium position is $y(x,t)$ (Figure 5.1). For small oscillations, assuming the change in $y(x,t)$ with x is small: $\partial y/\partial x \ll 1$, we can write the y-component of the tension along the chain as $T_y(x) = \rho_0 gx(\partial y/\partial x)$. This gives the restoring force on a mass element of length Δx as

$$T_y(x+\Delta x) - T_y(x) = \frac{\partial}{\partial x}\left(\rho_0 gx\frac{\partial y}{\partial x}\right)\Delta x. \tag{5.3}$$

We can now write the equation of motion of a mass element of length Δx as

$$(\rho_0\Delta x)\frac{\partial^2 y(x,t)}{\partial t^2} = \frac{\partial}{\partial x}\left[\rho_0 gx\frac{\partial y(x,t)}{\partial x}\right]\Delta x, \tag{5.4}$$

Mathematical Methods in Science and Engineering, Second Edition. Selçuk Ş. Bayın.

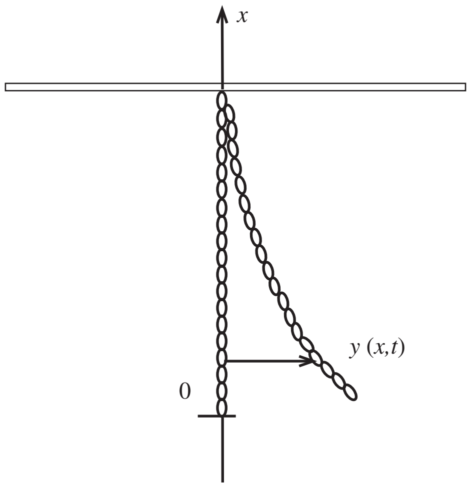

Figure 5.1 Flexible chain.

$$\frac{\partial^2 y(x,t)}{\partial t^2}\Delta x = g\frac{\partial}{\partial x}\left[x\frac{\partial y(x,t)}{\partial x}\right]\Delta x. \tag{5.5}$$

Since Δx is small but finite, we obtain the differential equation to be solved for $y(x,t)$ as

$$\boxed{\frac{\partial^2 y(x,t)}{\partial t^2} = g\frac{\partial}{\partial x}\left[x\frac{\partial y(x,t)}{\partial x}\right].} \tag{5.6}$$

Separating the variables as $y(x,t) = u(x)v(t)$, we write

$$\frac{\ddot{v}(t)}{v(t)} = \frac{g}{u(x)}\left[\frac{du}{dx} + x\frac{d^2u}{dx^2}\right] = -\omega^2, \tag{5.7}$$

where ω is the **separation constant**. The solution for $v(t)$ can be written immediately as

$$v(t) = c_0\cos(\omega t - \delta), \tag{5.8}$$

while $u(x)$ satisfies the differential equation

$$x\frac{d^2u}{dx^2} + \frac{du}{dx} + \frac{\omega^2}{g}u(x) = 0. \tag{5.9}$$

After defining a new independent variable, $z = 2\sqrt{x/g}$, the differential equation to be solved for $u(z)$ becomes

$$\boxed{\frac{d^2u}{dz^2} + \frac{1}{z}\frac{du}{dz} + \omega^2 u(z) = 0.} \tag{5.10}$$

To express the solutions of this equation, we need a new type of function called the **Bessel function**. This problem was first studied by Bernoulli, in 1732, however, he did not recognize the general nature of these functions. As we shall see, this equation is a special case of the **Bessel's equation**.

5.1 Bessel's Equation

If we write the **Laplace equation** in **cylindrical coordinates**:

$$\frac{\partial^2\Psi}{\partial\rho^2} + \frac{1}{\rho}\frac{\partial\Psi}{\partial\rho} + \frac{1}{\rho^2}\frac{\partial^2\Psi}{\partial\phi^2} + \frac{\partial^2\Psi}{\partial z^2} = 0, \tag{5.11}$$

and try a separable solution of the form $\Psi(\rho, \phi, z) = R(\rho)\Phi(\phi)Z(z)$, we obtain three ordinary differential equations to be solved for $R(\rho)$, $\Phi(\phi)$, and $Z(z)$:

$$\frac{d^2Z(z)}{dz^2} - k^2Z(z) = 0, \tag{5.12}$$

$$\frac{d^2\Phi(\phi)}{d\phi^2} + m^2\Phi(\phi) = 0, \tag{5.13}$$

$$\frac{d^2R(\rho)}{d\rho^2} + \frac{1}{\rho}\frac{dR(\rho)}{d\rho} + \left(k^2 - \frac{m^2}{\rho^2}\right)R(\rho) = 0. \tag{5.14}$$

Solutions of the first two equations can be written immediately as

$$Z(z) = \bar{c}_1e^{kz} + \bar{c}_2e^{-kz}, \tag{5.15}$$

$$\Phi(\phi) = c_1e^{im\phi} + c_2e^{-im\phi}. \tag{5.16}$$

The remaining Eq. (5.14) is known as the **Bessel equation**, which with the definitions $x = k\rho$ and $R(\rho) = J_m(x)$ can be written as

$$\boxed{J''_m(x) + \frac{1}{x}J'_m(x) + \left(1 - \frac{m^2}{x^2}\right)J_m(x) = 0.} \tag{5.17}$$

Solutions of this equation are called the **Bessel functions** of order m and they are shown as $J_m(x)$.

5.2 Bessel Functions

Series solution of the **Bessel's equation** is given as

$$\boxed{J_m(x) = \sum_{r=0}^{\infty} \frac{(-1)^r}{r!\Gamma(m+r+1)}\left(\frac{x}{2}\right)^{m+2r},} \tag{5.18}$$

which is called the **Bessel function** of the **first kind** of **order** m. A **second solution** can be written as

$$J_{-m}(x) = \sum_{r=0}^{\infty} \frac{(-1)^r}{r!\Gamma(-m+r+1)} \left(\frac{x}{2}\right)^{-m+2r}. \tag{5.19}$$

However, the second solution is independent of the first solution only for the noninteger values of m. For the integer values of m, the two solutions are related by

$$J_{-m}(x) = (-1)^m J_m(x). \tag{5.20}$$

When m takes integer values, the second and **linearly independent** solution can be taken as

$$N_m(x) = \frac{\cos m\pi J_m(x) - J_{-m}(x)}{\sin m\pi}, \tag{5.21}$$

which is called the **Neumann function**, or the **Bessel function** of the **second kind**. Note that $N_m(x)$ and $J_m(x)$ are linearly independent even for the integer values of m. Hence it is common practice to take $N_m(x)$ and $J_m(x)$ as the two linearly independent solutions for all m.

Other linearly independent solutions of Bessel's equation are given as the **Hankel functions**:

$$H_m^{(1)}(x) = J_m(x) + iN_m(x), \tag{5.22}$$

$$H_m^{(2)}(x) = J_m(x) - iN_m(x). \tag{5.23}$$

They are also called the **Bessel functions** of the **third kind**.

5.2.1 Asymptotic Forms

In the limit as $x \to 0$, Bessel function $J_m(x)$ is finite for $m \geq 0$ and behaves as

$$\lim_{x\to 0} J_m(x) \to \frac{1}{\Gamma(m+1)} \left(\frac{x}{2}\right)^m. \tag{5.24}$$

All the other functions diverge as

$$\lim_{x\to 0} N_m(x) \to \begin{cases} \frac{2}{\pi}\left[\ln\left(\frac{x}{2}\right) + \gamma\right], & m = 0, \\ -\frac{\Gamma(m)}{\pi}\left(\frac{2}{x}\right)^m, & m \neq 0, \end{cases} \tag{5.25}$$

where $\gamma = 0.5772\ldots$. In the limit as $x \to \infty$, functions $J_m(x), N_m(x), H_m^{(1)}(x)$, and $H_m^{(2)}(x)$ behave as

$$\boxed{J_m(x) \underset{x\to\infty}{\to} \sqrt{\frac{2}{\pi x}} \cos\left(x - \frac{m\pi}{2} - \frac{\pi}{4}\right),} \tag{5.26}$$

$$\boxed{N_m(x) \underset{x\to\infty}{\to} \sqrt{\frac{2}{\pi x}} \sin\left(x - \frac{m\pi}{2} - \frac{\pi}{4}\right),} \tag{5.27}$$

$$\boxed{H_m^{(1)}(x) \underset{x\to\infty}{\to} \sqrt{\frac{2}{\pi x}} \exp\left[i\left(x - \frac{m\pi}{2} - \frac{\pi}{4}\right)\right],} \tag{5.28}$$

$$\boxed{H_m^{(2)}(x) \underset{x\to\infty}{\to} \sqrt{\frac{2}{\pi x}} \exp\left[-i\left(x - \frac{m\pi}{2} - \frac{\pi}{4}\right)\right].} \tag{5.29}$$

Example 5.1 ***Bessel function*** $J_0(x)$
Show the following integral:

$$\int_0^{\pi/2} J_0(x\cos t)\cos t\, dt = \frac{\sin x}{x}. \tag{5.30}$$

Solution
Use the expansion

$$J_0(x\cos t) = \sum_{r=0}^{\infty} \frac{(-1)^r}{(r!)^2}\left(\frac{x\cos t}{2}\right)^{2r} \tag{5.31}$$

to obtain the desired result as

$$\int_0^{\pi/2} J_0(x\cos t)\cos t\, dt = \sum_{r=0}^{\infty} \int_0^{\pi/2} \frac{(-1)^r}{(r!)^2}\left(\frac{x\cos t}{2}\right)^{2r} \cos t\, dt \tag{5.32}$$

$$= \sum_{r=0}^{\infty} \frac{(-1)^r}{(r!)^2}\left(\frac{x}{2}\right)^{2r} \int_0^{\pi/2} (\cos t)^{2r+1}\, dt \tag{5.33}$$

$$= \sum_{r=0}^{\infty} \frac{(-1)^r}{(r!)^2} \left(\frac{x}{2}\right)^{2r} \frac{(2r)(2r-2)\dots 4.2}{(2r+1)(2r-1)\dots 3.1} \tag{5.34}$$

$$= \sum_{r=0}^{\infty} \frac{(-1)^r}{(r!)^2} \left(\frac{x}{2}\right)^{2r} \frac{2^r r! r!}{(2r+1)!} \tag{5.35}$$

$$= \frac{1}{x} \sum_{r=0}^{\infty} (-1)^r \frac{x^{2r+1}}{(2r+1)!} \tag{5.36}$$

$$= \frac{\sin x}{x}. \tag{5.37}$$

5.3 Modified Bessel Functions

If we take the argument of the Bessel functions $J_m(x)$ and $H_m^{(1)}(x)$ as imaginary, we obtain the **modified Bessel functions:**

$$\boxed{I_m(x) = \frac{J_m(ix)}{i^m},} \tag{5.38}$$

$$\boxed{K_m(x) = \frac{\pi i}{2}(i)^m H_m^{(1)}(ix).} \tag{5.39}$$

These functions are linearly independent solutions of the **differential equation**

$$\boxed{\frac{d^2R(x)}{dx^2} + \frac{1}{x}\frac{dR(x)}{dx} - \left(1 + \frac{m^2}{x^2}\right) R(x) = 0.} \tag{5.40}$$

Asymptotic forms of $I_m(x)$ and $K_m(x)$ as $x \to 0$ and $x \to \infty$ are given as (real $m \geq 0$)

$$\boxed{\lim_{x\to 0} I_m(x) \to \frac{x^m}{2^m \Gamma(m+1)},} \tag{5.41}$$

$$\boxed{\lim_{x\to 0} K_m(x) \to \begin{Bmatrix} -\left[\ln\left(\frac{x}{2}\right) + \gamma\right], & m = 0 \\ \frac{\Gamma(m)}{2}\left(\frac{2}{x}\right)^m, & m \neq 0 \end{Bmatrix},} \tag{5.42}$$

and

$$\boxed{\lim_{x\to\infty} I_m(x) \to \frac{1}{\sqrt{2\pi x}} e^x \left[1 + 0\left(\frac{1}{x}\right)\right],} \tag{5.43}$$

$$\lim_{x\to\infty} K_m(x) \to \sqrt{\frac{\pi}{2x}} e^{-x} \left[1 + 0\left(\frac{1}{x}\right)\right]. \tag{5.44}$$

5.4 Spherical Bessel Functions

Spherical Bessel functions, $j_l(x)$, $n_l(x)$, and $h_l^{(1,2)}(x)$, are defined as

$$\begin{aligned} j_l(x) &= \sqrt{\frac{\pi}{2x}} J_{l+\frac{1}{2}}(x), \\ n_l(x) &= \sqrt{\frac{\pi}{2x}} N_{l+\frac{1}{2}}(x), \\ h_l^{(1,2)}(x) &= \left(\frac{\pi}{2x}\right)^{1/2} \left[J_{l+\frac{1}{2}}(x) \pm i N_{l+\frac{1}{2}}(x)\right]. \end{aligned} \tag{5.45}$$

Bessel functions with **half integer indices**, $J_{l+\frac{1}{2}}(x)$ and $N_{l+\frac{1}{2}}(x)$, satisfy the differential equation

$$\frac{d^2y(x)}{dx^2} + \frac{1}{x}\frac{dy(x)}{dx} + \left[1 - \frac{(l+1/2)^2}{x^2}\right] y(x) = 0, \tag{5.46}$$

while the spherical Bessel functions, $j_l(x)$, $n_l(x)$, and $h_l^{(1,2)}(x)$, satisfy

$$\frac{d^2y(x)}{dx^2} + \frac{2}{x}\frac{dy(x)}{dx} + \left[1 - \frac{l(l+1)}{x^2}\right] y(x) = 0. \tag{5.47}$$

Spherical Bessel functions can also be defined as

$$j_l(x) = (-x)^l \left(\frac{1}{x}\frac{d}{dx}\right)^l \frac{\sin x}{x}, \tag{5.48}$$

$$n_l(x) = (-x)^l \left(\frac{1}{x}\frac{d}{dx}\right)^l \left(-\frac{\cos x}{x}\right). \tag{5.49}$$

Asymptotic forms of the spherical Bessel functions are given as

$$\begin{aligned}
j_l(x) &\to \frac{x^l}{(2l+1)!!}\left(1 - \frac{x^2}{2(2l+1)} + \cdots\right), \quad x \ll 1, \\
n_l(x) &\to -\frac{(2l-1)!!}{x^{l+1}}\left(1 - \frac{x^2}{2(1-2l)} + \cdots\right), \quad x \ll 1, \\
j_l(x) &= \frac{1}{x}\sin\left(x - \frac{l\pi}{x}\right), \quad x \gg 1, \\
n_l(x) &= -\frac{1}{x}\cos\left(x - \frac{l\pi}{x}\right), \quad x \gg 1,
\end{aligned} \tag{5.50}$$

where $(2l+1)!! = (2l+1)(2l-1)(2l-3)\dots 5 \cdot 3 \cdot 1$.

5.5 Properties of Bessel Functions

5.5.1 Generating Function

Bessel function, $J_n(x)$, can be defined by a **generating function**, $T(x,t)$, as

$$T(x,t) = \exp\left[\frac{1}{2}x\left(t - \frac{1}{t}\right)\right] = \sum_{n=-\infty}^{\infty} t^n J_n(x). \tag{5.51}$$

Example 5.2 ***Generating function***
Using the generating function definition [Eq. (5.51)], we can show that $J_n(x) = (-1)^n J_n(-x)$. We first write

$$\sum_{n=-\infty}^{\infty} J_n(-x)t^n = \exp\left\{\frac{1}{2}[-x(t-1/t)]\right\} \tag{5.52}$$

$$= e^{\frac{x}{2}[-t-1/(-t)]} \tag{5.53}$$

$$= \sum_{n=-\infty}^{\infty} J_n(x)(-t)^n \tag{5.54}$$

$$= \sum_{n=-\infty}^{\infty} (-1)^n J_n(x)t^n. \tag{5.55}$$

Comparing the equal powers of t, we obtain the desired result.

Example 5.3 ***Generating function***
To prove

$$J_n(x+y) = \sum_{r=-\infty}^{\infty} J_r(x) J_{n-r}(x), \tag{5.56}$$

we use the generating function [Eq. (5.51)] to write

$$e^{\frac{x}{2}(t-1/t)} e^{\frac{y}{2}(t-1/t)} = \sum_{n=-\infty}^{\infty} J_n(x+y) t^n. \tag{5.57}$$

Rewriting the left-hand side as

$$\left(\sum_{r=-\infty}^{\infty} J_r(x) t^r \right) \left(\sum_{s=-\infty}^{\infty} J_s(y) t^s \right) = \sum_{n=-\infty}^{\infty} J_n(x+y) t^n, \tag{5.58}$$

and calling $s = n - r$, we get

$$\sum_{n=-\infty}^{\infty} \left[\sum_{r=-\infty}^{\infty} J_r(x) J_{n-r}(y) \right] t^n = \sum_{n=-\infty}^{\infty} J_n(x+y) t^n, \tag{5.59}$$

which yields the desired result.

5.5.2 Integral Definitions

Bessel function $J_n(x)$ also has the following **integral definitions**:

$$\boxed{J_n(x) = \frac{1}{\pi} \int_0^{\pi} \cos[n\varphi - x \sin\varphi] d\varphi, \quad n = 0, 1, 2, \ldots,} \tag{5.60}$$

$$\boxed{J_n(x) = \frac{(x/2)^n}{\sqrt{\pi}\Gamma(n+1/2)} \int_{-1}^{1} (1-t^2)^{n-\frac{1}{2}} \cos xt \, dt, \quad n > -\frac{1}{2}.} \tag{5.61}$$

5.5.3 Recursion Relations of the Bessel Functions

Using the series definitions of the Bessel functions, we can obtain the following **recursion relations**:

$$\boxed{J_{m-1}(x) + J_{m+1}(x) = \frac{2m}{x} J_m(x),} \tag{5.62}$$

$$\boxed{J_{m-1}(x) - J_{m+1}(x) = 2J'_m(x).} \tag{5.63}$$

First by adding and then by subtracting these equations, we also obtain the following two relations:

$$\boxed{J_{m-1}(x) = \frac{m}{x}J_m(x) + J'_m(x),} \tag{5.64}$$

$$\boxed{J_{m+1}(x) = \frac{m}{x}J_m(x) - J'_m(x).} \tag{5.65}$$

Other Bessel functions, N_n, $H_n^{(1)}$, and $H_n^{(2)}$, satisfy the same recursion relations.

5.5.4 Orthogonality and Roots of Bessel Functions

From the asymptotic form [Eq. (5.26)] of the **Bessel function**, it is clear that it has **infinitely many roots**:

$$J_n(x_{nl}) = 0, \quad l = 1, 2, 3, \ldots \ . \tag{5.66}$$

Here, x_{nl} stands for the lth root of the nth-order Bessel function. When n takes integer values, the first three roots are given as

$$\begin{array}{llllll} n=0 & x_{0l} = 2.405 & 5.520 & 8.654 & \cdots, \\ n=1 & x_{1l} = 3.832 & 7.016 & 10.173 & \cdots, \\ n=2 & x_{2l} = 5.136 & 8.417 & 11.620 & \cdots. \end{array} \tag{5.67}$$

Higher-order roots are approximately given by the formula

$$x_{nl} \backsimeq l\pi + \left(n - \frac{1}{2}\right)\frac{\pi}{2}. \tag{5.68}$$

Orthogonality relation of the Bessel functions, in the interval $[0, a]$, is given as

$$\boxed{\int_0^a \rho J_n\left(x_{nl}\frac{\rho}{a}\right) J_n\left(x_{nl'}\frac{\rho}{a}\right) d\rho = \frac{a^2}{2}\left[J_{n+1}(x_{nl})\right]^2 \delta_{ll'}, \quad n \geq -1.} \tag{5.69}$$

Since Bessel functions also form a complete set, any sufficiently smooth function, $f(\rho)$, in the interval $\rho \in [0, a]$ can be expanded as

$$f(\rho) = \sum_{l=1}^{\infty} A_{nl} J_n\left(x_{nl}\frac{\rho}{a}\right), \quad n \geq -1, \tag{5.70}$$

where the expansion coefficients A_{nl} are found from

$$A_{nl} = \frac{2}{a^2 J_{n+1}^2(x_{nl})} \int_0^a \rho f(\rho) J_n\left(x_{nl}\frac{\rho}{a}\right) d\rho. \tag{5.71}$$

5.5.5 Boundary Conditions for the Bessel Functions

For the roots given in Eq. (5.67), we have used the **Dirichlet boundary condition**:

$$R(a) = 0. \tag{5.72}$$

In terms of the Bessel functions, this condition implies

$$J_n(ka) = 0 \tag{5.73}$$

and gives us the infinitely many roots [Eq. (5.67)] shown as x_{nl}. Now the functions

$$\left\{ J_n\left(x_{nl}\frac{\rho}{a}\right)\right\}, \quad n \geq 0, \tag{5.74}$$

form a **complete** and **orthogonal** set with respect to the index l. The same conclusion holds for the **Neumann boundary condition:**

$$\left.\frac{dR(\rho)}{d\rho}\right|_{\rho=a} = 0, \tag{5.75}$$

and the **general boundary condition**

$$\left[A_0\frac{dR(\rho)}{d\rho} + B_0R(\rho)\right]_{\rho=a} = 0. \tag{5.76}$$

In terms of the Bessel function, $J_n(kr)$, the Neumann and the general boundary conditions are written, respectively, as

$$k\left.\frac{dJ_n(x)}{dx}\right|_{x=ka} = 0 \tag{5.77}$$

and

$$\left[A_0J_n(x) + B_0k\frac{dJ_n(x)}{dx}\right]_{x=ka} = 0. \tag{5.78}$$

For the Neumann boundary condition [Eq. (5.77)], there exist infinitely many roots, which can be found from tables. However, for the general boundary condition, roots depend on the values that A_0 and B_0 take; thus each case must be handled separately by numerical analysis. From all three types of boundary conditions, we obtain a complete and orthogonal set as

$$\left\{ J_n\left(x_{nl}\frac{r}{a}\right)\right\}, \quad l = 1, 2, 3, \ldots. \tag{5.79}$$

Example 5.4 ***Flexible chain problem***
We now return to the flexible chain problem, where the equation of motion is written as [Eq. (5.10)]

$$\frac{d^2u}{dz^2} + \frac{1}{z}\frac{du}{dz} + \omega^2u = 0. \tag{5.80}$$

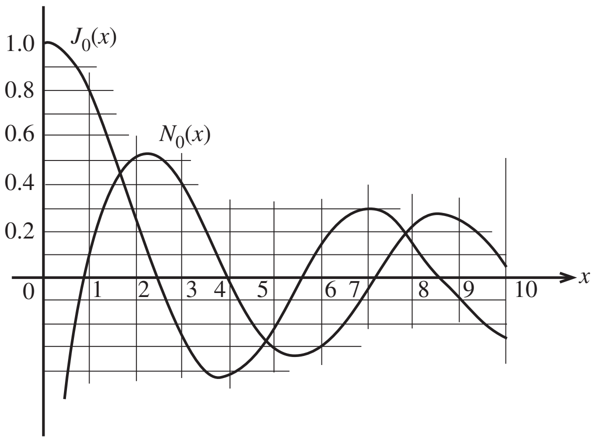

Figure 5.2 J_0 and N_0 functions.

The general solution of this equation is given as

$$u(z) = a_0 J_0(\omega z) + a_1 N_0(\omega z), \quad z = 2\sqrt{x/g}. \tag{5.81}$$

Since $N_0(\omega z)$ diverges at the origin, we choose a_1 as zero and obtain the displacement of the chain from its equilibrium position as (Figure 5.2)

$$y(x,t) = a_0 J_0(2\omega\sqrt{x/g})\cos(\omega t - \delta). \tag{5.82}$$

If we impose the condition

$$y(l,t) = J_0(2\omega_n\sqrt{l/g}) = 0,$$

we find the normal modes of the chain as

$$2\omega_n\sqrt{l/g} = 2.405,\ 5.520, \dots, \quad n = 1, 2, \dots. \tag{5.83}$$

If the shape of the chain at $t = 0$ is given as $f(x)$, we can write the solution as

$$y(x,t) = \sum_{n=1}^{\infty} A_n J_0(2\omega_n\sqrt{x/g})\cos(\omega_n t - \delta), \tag{5.84}$$

where the expansion coefficients are given as

$$A_n = \frac{2}{J_1^2(\omega_n)} \int_0^1 zf\left(\frac{g}{4}z^2\right) J_0(\omega_n z)dz.$$

Example 5.5 ***Tsunamis and wave motion in a channel***
The equation of motion for one-dimensional waves in a channel with breadth $b(x)$ and depth $h(x)$ is given as

$$\frac{\partial^2 \eta}{\partial t^2} = \frac{g}{b}\frac{\partial}{\partial x}\left(hb\frac{\partial \eta}{\partial x}\right), \tag{5.85}$$

where $\eta(x,t)$ is the displacement of the water surface from its equilibrium position and g is the acceleration of gravity. If the depth of the channel varies uniformly from the end of the channel, $x = 0$, to the mouth, $x = a$, as

$$h(x) = h_0 x/a, \tag{5.86}$$

we can try a separable solution of the form

$$\eta(x,t) = A(x)\cos(\omega t + \alpha), \tag{5.87}$$

to find the differential equation that $A(x)$ satisfies as

$$\frac{d}{dx}\left(x\frac{dA}{dx}\right) + kA = 0, \quad k = \omega^2 a/gh_0. \tag{5.88}$$

Solution that is finite at $x = 0$ can be obtained as

$$A(x) = A_0\left(1 - \frac{kx}{1^2} + \frac{k^2x^2}{1^2\cdot 2^2} - \cdots\right), \tag{5.89}$$

or as

$$A(x) = A_0 J_0(2k^{1/2}x^{1/2}). \tag{5.90}$$

After evaluating the constant A_0, we write the final solution as

$$\eta(x,t) = C\frac{J_0(2k^{1/2}x^{1/2})}{J_0(2k^{1/2}a^{1/2})}\cos(\omega t + \alpha). \tag{5.91}$$

With an appropriate normalization, a snapshot of this wave is shown in Figure 5.3. Note, how the amplitude increases and the wavelength decreases as shallow waters is reached. If hb is constant or at least a slow varying function of position, we can take it outside the brackets in Eq. (5.85), thus obtaining the wave velocity as $\sqrt{hg}$. This is characteristic of tsunamis, which are wave trains

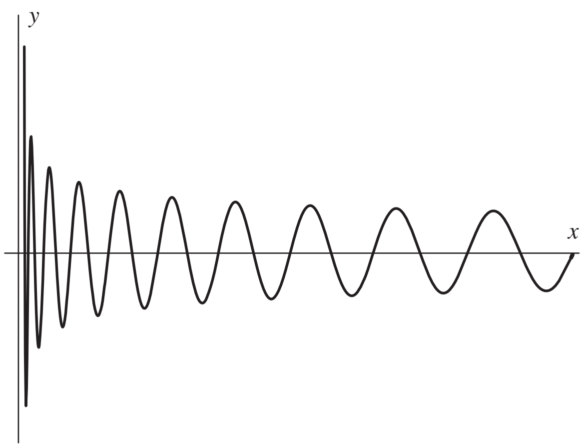

Figure 5.3 Channel waves.

caused by sudden displacement of large amounts of water by earthquakes, volcanoes, meteors, etc. Tsunamis have wavelengths in excess of 100 km and their period is around 1 h. In the Pacific Ocean, where typical water depth is 4000 m, tsunamis travel with velocities over 700 km/h. Since the energy loss of a wave is inversely proportional to its wavelength, tsunamis could travel transoceanic distances with little energy loss. Because of their huge wavelengths, they are imperceptible in deep waters; however, in reaching shallow waters, they compress and slow down. Thus to conserve energy, their amplitude increases to several or tens of meters in height as they reach the shore.

When both the breadth and the depth vary as

$$b(x) = b_0 x/a \quad \text{and} \quad h(x) = h_0 x/a, \tag{5.92}$$

respectively, the differential equation to be solved for $A(x)$ becomes

$$x\frac{d^2A}{dx^2} + 2\frac{dA}{dx} + kA = 0, \tag{5.93}$$

where

$$k = \omega^2 a/gh_0. \tag{5.94}$$

The solution is now obtained as

$$\eta(x,t) = A_0\left(1 - \frac{kx}{(1\cdot 2)} + \frac{k^2x^2}{(1\cdot 2)\cdot(2\cdot 4)} - \cdots\right)\cos(\omega t + \alpha), \tag{5.95}$$

which is

$$\eta(x,t) = A_0\frac{J_1(2k^{1/2}x^{1/2})}{k^{1/2}x^{1/2}}\cos(\omega t + \alpha). \tag{5.96}$$

5.5.6 Wronskian of Pairs of Solutions

The **Wronskian** of a pair of solutions of a second-order linear differential equation is defined by the determinant

$$W[u_1(x), u_2(x)] = \begin{vmatrix} u_1(x) & u_2(x) \\ u_1'(x) & u_2'(x) \end{vmatrix} = u_1u_2' - u_2u_1'. \tag{5.97}$$

The two solutions are linearly independent if and only if their Wronskian does not vanish identically. We now calculate the Wronskian of a pair of solutions of Bessel's equation:

$$u''(x) + \frac{1}{x}u'(x) + \left(1 - \frac{m^2}{x^2}\right)u(x) = 0, \tag{5.98}$$

thus obtaining a number of formulas that are very helpful in various calculations. For two solutions, u_1 and u_2, we write

$$\frac{d}{dx}(xu_1') + \left(1 - \frac{m^2}{x^2}\right) u_1(x) = 0, \tag{5.99}$$

$$\frac{d}{dx}(xu_2') + \left(1 - \frac{m^2}{x^2}\right) u_2(x) = 0. \tag{5.100}$$

We now multiply the second equation by u_1 and subtract the result from the first equation multiplied by u_2 to get

$$\frac{d}{dx}\left\{xW\left[u_1(x), u_2(x)\right]\right\} = 0. \tag{5.101}$$

This means

$$W\left[u_1(x), u_2(x)\right] = \frac{C}{x}, \tag{5.102}$$

where C is a constant independent of x but depends on the pair of functions whose Wronskian is calculated. For example,

$$\boxed{W\left[J_m(x), N_m(x)\right] = \frac{2}{\pi x},} \tag{5.103}$$

$$\boxed{W\left[J_m(x), H_m^{(2)}(x)\right] = -\frac{2i}{\pi x},} \tag{5.104}$$

$$\boxed{W\left[H_m^{(1)}(x), H_m^{(2)}(x)\right] = -\frac{4i}{\pi x}.} \tag{5.105}$$

Since C is independent of x, it can be calculated using the asymptotic forms of these functions in the limit $x \to 0$ as

$$C = \lim_{x\to 0} xW\left[u_1(x), u_2(x)\right]. \tag{5.106}$$

5.6 Transformations of Bessel Functions

Sometimes we encounter differential equations, solutions of which can be written in terms of Bessel functions. For example, consider the function

$$\boxed{y(x; \alpha, \beta, \gamma) = x^\alpha J_n(\beta x^\gamma),} \tag{5.107}$$

where α, β, and γ are three constant parameters. To find the differential equation that $y(x; \alpha, \beta, \gamma)$ satisfies, we substitute $g = y/x^\alpha$, $w = \beta x^\gamma$, to write

$g(w) = J_n(w)$. Hence, $g(w)$ satisfies Bessel's equation [Eq. (5.17)]:

$$w^2 \frac{d^2 g}{dw^2} + w \frac{dg}{dw} + (w^2 - n^2) g(w) = 0, \tag{5.108}$$

which can also be written as

$$w \frac{d}{dw} \left(w \frac{dg}{dw} \right) + (w^2 - n^2) g(w) = 0. \tag{5.109}$$

We now write

$$w \frac{dg}{dw} = w \frac{dg/dx}{dw/dx} = \frac{x}{\gamma} \frac{dg}{dx}, \tag{5.110}$$

hence the first term in Eq. (5.109) becomes

$$w \frac{d}{dw} \left(w \frac{dg}{dw} \right) = \frac{1}{\gamma^2} x \frac{d}{dx} \left(x \frac{dg}{dx} \right). \tag{5.111}$$

Using $g = y/x^\alpha$ we can also write

$$x \frac{dg}{dx} = \frac{y'}{x^{\alpha-1}} - \frac{\alpha y}{x^\alpha}, \tag{5.112}$$

which leads to

$$\begin{aligned} x \frac{d}{dx} \left(x \frac{dg}{dx} \right) &= x \frac{d}{dx} \left(\left[\frac{y'}{x^{\alpha-1}} - \frac{\alpha y}{x^\alpha} \right] \right) \\ &= \frac{y''}{x^{\alpha-2}} - \frac{(2\alpha - 1) y'}{x^{\alpha-1}} + \frac{\alpha^2 y}{x^\alpha}. \end{aligned} \tag{5.113}$$

Using Eqs (5.111) and (5.113) in Eq. (5.109), we obtain the differential equation that $y(x; \alpha, \beta, \gamma)$ satisfies as

$$\boxed{\frac{d^2 y}{dx^2} - \left(\frac{2\alpha - 1}{x} \right) \frac{dy}{dx} + \left(\beta^2 \gamma^2 x^{2\gamma-2} + \frac{\alpha^2 - n^2 \gamma^2}{x^2} \right) y(x) = 0.} \tag{5.114}$$

The general solution of Eq. (5.114) can be written as

$$\boxed{y(x) = x^\alpha \left[C_0 J_n(\beta x^\gamma) + C_1 N_n(\beta x^\gamma) \right].} \tag{5.115}$$

5.6.1 Critical Length of a Rod

When a thin uniform vertical rod is clamped at one end, its vertical position is stable granted that its length is less than a critical length. When the rod has the critical length, the vertical position is only a neutral equilibrium position. That is, the rod stays in the displaced position after it has been displaced slightly [3]. Let the rod be in equilibrium when deviating slightly from the vertical position (Figure 5.4). Let l be the length of the rod, a be the radius of its cross section,

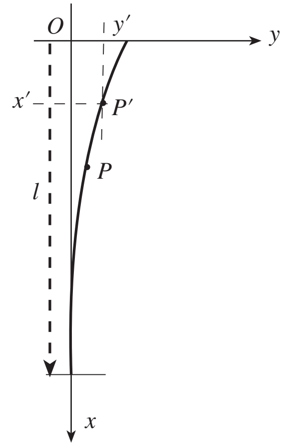

Figure 5.4 Bending of a rod.

and ρ_0 be the uniform density. Let P be an arbitrary point on the rod and P' be a point above it (Figure 5.4). We now consider the part of the rod in equilibrium above the point P. If we take a mass element, $\rho_0\, dx'$, at P', the torque acting on it due to the weight of the upper part of the rod will be will be the integral

$$\int_0^x \rho_0 g(y' - y)dx, \tag{5.116}$$

where g is the acceleration of gravity. This will be balanced by the torque from the elastic forces acting on the rod. From the theory of elasticity, this torque is equal to

$$EI\frac{d^2y}{dx^2}, \tag{5.117}$$

where E is Young's modulus and we take $I = \frac{1}{4}\pi a^2$. Equating the two torques gives

$$EI\frac{d^2y}{dx^2} = \int_0^x \rho_0 g(y'(x') - y(x))dx'. \tag{5.118}$$

Using the formula

$$\frac{d}{dx}\int_{A(x)}^{B(x)} F(x,\xi)d\xi = \int_{A(x)}^{B(x)} \frac{\partial F(x,\xi)}{\partial x}d\xi + F(x,B(x))\frac{dB(x)}{dx} - F(x,A(x))\frac{dA(x)}{dx}, \tag{5.119}$$

we differentiate Eq. (5.118) with respect to x:

$$EI\frac{d^3y}{dx^3} = -\rho_0 gx\frac{dy}{dx}, \tag{5.120}$$

and rewrite to obtain

$$\frac{d^3y}{dx^3} + k^2\frac{dy}{dx} = 0, \quad k^2 = \frac{\rho_0 g}{EI}. \tag{5.121}$$

Comparing with Eq. (5.114), we see that the solution for $\frac{dy}{dx}$ can be written in terms of the Bessel functions as

$$\frac{dy}{dx} = \sqrt{x}\left(C_0 J_{-1/3}\left(\frac{2k}{3}x^{2/3}\right) + C_1 J_{1/3}\left(\frac{2k}{3}x^{2/3}\right)\right). \tag{5.122}$$

For the desired solution, we have to satisfy the following boundary conditions:

(i) Since there is no torque at the top, where $x = 0$, we need to have

$$\left(\frac{d^2y}{dx^2}\right)_{x=0} = 0. \tag{5.123}$$

(ii) At the bottom, where the rod is fixed and vertical, we need to satisfy

$$\left(\frac{dy}{dx}\right)_{x=l} = 0. \tag{5.124}$$

To satisfy the first boundary condition, we set $C_1 = 0$, thus obtaining

$$\frac{dy}{dx} = C_0\sqrt{x}J_{-1/3}\left(\frac{2k}{3}x^{2/3}\right). \tag{5.125}$$

The second condition can be satisfied with $C_0 = 0$, which is the trivial solution. For a nontrivial solution, $C_0 \neq 0$, we set

$$J_{-1/3}\left(\frac{2k}{3}l^{2/3}\right) = 0 \tag{5.126}$$

and take the smallest root as the physical solution:

$$\frac{2k}{3}l^{3/2} = 1.8663. \tag{5.127}$$

For a steel rod of radius 0.15 cm, $E = 84{,}000$ tons/cm^2 and density 7.9 g/cm^3, we find $l \cong 1.15$ m.

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Problems

1 Drive the following recursion relations:

(i) $J_{m-1}(x) + J_{m+1}(x) = \dfrac{2m}{x} J_m(x), \quad m = 1, 2, \ldots,$

(ii) $J_{m-1}(x) - J_{m+1}(x) = 2J'_m(x), \quad m = 1, 2, \ldots.$

Use the first equation to express a Bessel function of arbitrary order ($m = 0, 1, 2, \ldots$) in terms of J_0 and J_1. Show that for $m = 0$, the second equation is replaced by $J'_0(x) = -J_1(x)$.

2 Write the wave equation, $\nabla^2 \Psi(\vec{r}, t) - \frac{1}{c^2} \frac{\partial^2}{\partial t^2} \Psi(\vec{r}, t) = 0$, in spherical polar coordinates. Using the method of separation of variables, show that the solutions for the radial part are given in terms of the spherical Bessel functions.

3 Use the result in Problem 2 to find the solutions for a spherically split antenna. On the surface, $r = a$, take the solution as

$$\Psi(\vec{r}, t)|_{r=a} = \begin{cases} V_0 e^{-iw_0 t}, & 0 < \theta < \pi/2, \\ -V_0 e^{-iw_0 t}, & \frac{\pi}{2} < \theta < \pi, \end{cases}$$

and assume that in the limit as $r \to \infty$ solution behaves as

$$\psi \approx \frac{1}{r} e^{i(k_0 r - \omega_0 t)}, \quad k = k_0 = \omega_0 / c.$$

4 Solve the wave equation

$$\vec{\nabla}^2 \Psi - \frac{1}{v^2} \frac{\partial^2 \Psi}{\partial t^2} = 0, \quad k = \frac{\omega}{c}.$$

for the oscillations of a circular membrane with radius a and clamped at the boundary. What boundary conditions did you use? What are the lowest three modes?

5 Verify the following Wronskians:

(i) $W\left[J_m(x), N_m(x)\right] = \dfrac{2}{\pi x},$

(ii) $W\left[J_m(x), H_m^{(2)}(x)\right] = -\dfrac{2i}{\pi x},$

(iii) $W\left[H_m^{(1)}(x), H_m^{(2)}(x)\right] = -\dfrac{4i}{\pi x}.$

6 Find the constant C in the Wronskian

$$W\left[I_m(x), K_m(x)\right] = \frac{C}{x}.$$

7 Show that the stationary distribution of temperature, $T(\rho, z)$, in a cylinder of length l and radius a with one end held at temperature T_0 while the rest of the cylinder is held at zero is given as

$$T(\rho, z) = 2T_0 \sum_{n=1}^{\infty} \frac{J_0\left(x_n \frac{\rho}{a}\right) \sinh\left(x_n \frac{l-z}{a}\right)}{x_n J_1(x_n) \sinh\left(x_n \frac{l}{a}\right)}.$$

Hint: Use cylindrical coordinates and solve the Laplace equation,

$$\vec{\nabla}^2 T(\rho, z) = 0,$$

by the method of separation of variables.

8 Consider the cooling of an infinitely long cylinder heated to an initial temperature $f(\rho)$. Solve the heat transfer equation:

$$c\rho_0 \frac{\partial T(\rho, t)}{\partial t} = k\vec{\nabla}^2 T(\rho, t)$$

with the boundary condition

$$\left.\frac{\partial T}{\partial \rho} + hT\right|_{\rho=a} = 0$$

and the initial condition

$$T(\rho, 0) = f(\rho) \ \text{(finite)}.$$

$T(\rho, t)$ is the temperature distribution in the cylinder and the physical parameters of the problem are defined as

k – thermal conductivity
c – heat capacity
ρ_0 – density
λ – emissivity

and $h = \lambda/k$.
Hint: Use the method of separation of variables and show that the solution can be expressed as

$$T(\rho, t) = \sum_{n=1}^{\infty} C_n J_0\left(x_n \frac{\rho}{a}\right) e^{-x_n^2 t/a^2 b}, \quad b = c\rho_0/k,$$

then find C_n so that the initial condition

$$T(\rho, 0) = f(\rho)$$

is satisfied. Where does x_n come from?

6

Hypergeometric Functions

Hypergeometric function, $F(a, b, c; x)$, is a special function defined by the hypergeometric series. It is the solution of a linear second-order ordinary differential equation called the **hypergeometric equation**:

$$\boxed{x(1-x)\frac{d^2y(x)}{dx^2} + [c-(a+b+1)x]\frac{dy(x)}{dx} - aby(x) = 0.} \tag{6.1}$$

Majority of the second-order ordinary linear differential equations encountered in science and engineering can be expressed in terms of the three parameters (a, b, c) of the hypergeometric equation and its transformations.

6.1 Hypergeometric Series

The hypergeometric equation has three **regular singular points** at $x = 0, 1$ and ∞; hence we can find a series solution about the origin using the **Frobenius method**. Substituting the series

$$y = \sum_{r=0}^{\infty} a_r x^{s+r}, \quad a_0 \neq 0, \tag{6.2}$$

into Eq. (6.1) gives

$$x(1-x)\sum_{r=0}^{\infty} a_r(s+r)(s+r-1)x^{s+r-2}$$
$$+ \{c-(a+b+1)x\}\sum_{r=0}^{\infty} a_r(s+r)x^{s+r-1} - ab\sum_{r=0}^{\infty} a_r x^{s+r} = 0, \tag{6.3}$$

Mathematical Methods in Science and Engineering, Second Edition. Selçuk Ş. Bayın.

which we write as

$$\sum_{r=0}^{\infty} a_r(s+r)(s+r-1)x^{s+r-1} - \sum_{r=0}^{\infty} a_r(s+r)(s+r-1)x^{s+r} \tag{6.4}$$
$$+ c\sum_{r=0}^{\infty} a_r(s+r)x^{s+r-1} - (a+b+1)\sum_{r=0}^{\infty} a_r(s+r)x^{s+r} - ab\sum_{r=0}^{\infty} a_r x^{s+r} = 0.$$

After rearranging, we obtain

$$\sum_{r=0}^{\infty}[(s+r)(s+r-1) + c(s+r)]a_r x^{s+r-1} \tag{6.5}$$
$$-\sum_{r=1}^{\infty}[(s+r-1)(s+r-2) + (a+b+1)(s+r-1) + ab]a_{r-1}x^{s+r-1} = 0.$$

Writing the first term explicitly:

$$[s(s-1) + sc]a_0 x^{s-1} + \sum_{r=1}^{\infty}\{[(s+r)(s+r-1) + c(s+r)]a_r$$
$$- a_{r-1}[(s+r-1)(s+r-2) + ab + (a+b+1)(s+r-1)]\}x^{s+r-1} = 0, \tag{6.6}$$

and setting the coefficients of all the powers of x to zero, we obtain the **indicial equation:**

$$[s(s-1) + sc]a_0 = 0, \quad a_0 \neq 0, \tag{6.7}$$

and the recursion relation:

$$a_r = \frac{(s+r-1+a)(s+r-1+b)}{(s+r)(s+r-1+c)}a_{r-1}, \quad r \geq 1. \tag{6.8}$$

Roots of the indicial equation are $s = 0$ and $s = 1 - c$. Starting with the first root, $s = 0$, we write the recursion relation as

$$a_r = \frac{(r-1+a)(r-1+b)}{(r-1+c)r}a_{r-1}, \quad r \geq 1, \tag{6.9}$$

and obtain the following coefficients for the series:

$$a_1 = \frac{ab}{c}a_0,$$
$$a_2 = \frac{(a+1)(b+1)}{(c+1)2}a_{1,}$$
$$a_3 = \frac{(a+2)(b+2)}{(c+2)3}a_2,$$
$$a_4 = \frac{(a+3)(b+3)}{(c+3)4}a_3,$$
$$\vdots$$

Writing the general term:

$$a_k = a_0 \frac{a(a+1)(a+2)\cdots(a+k-1)b(b+1)\cdots(b+k-1)}{c(c+1)\cdots(c+k-1)1\cdot 2\cdot 3\cdots k}, \tag{6.10}$$

we obtain the **series solution** as

$$y_1(x) = a_0\left[1 + \frac{ab}{c}\frac{x}{1!} + \frac{a(a+1)b(b+1)}{c(c+1)}\frac{x^2}{2!} + \cdots\right], \tag{6.11}$$

$$\boxed{y_1(x) = a_0\frac{\Gamma(c)}{\Gamma(a)\Gamma(b)}\sum_{k=0}^{\infty}\frac{\Gamma(a+k)\Gamma(b+k)}{\Gamma(c+k)}\frac{x^k}{k!}, \quad c \neq 0, -1, -2, \ldots\ .} \tag{6.12}$$

Similarly, for the other root, $s = 1 - c$, the recursion relation becomes

$$a_r = a_{r-1}\frac{(r+a-c)(r+b-c)}{r(1-c+r)}, \quad r \geq 1, \tag{6.13}$$

which gives the following coefficients for the second series:

$$\begin{aligned}
a_1 &= a_0\frac{(a-c+1)(b-c+1)}{(2-c)},\\
a_2 &= a_1\frac{(a-c+2)(b-c+2)}{2(3-c)},\\
a_3 &= a_2\frac{(a-c+3)(b-c+3)}{3(4-c)},\\
&\vdots
\end{aligned}$$

Writing the general term:

$$a_k = a_0\left[\frac{(a-c+1)(a-c+2)\cdots(a-c+k)(b-c+1)\cdots(b-c+k)}{(2-c)(3-c)\cdots(k+1-c)k!}\right], \tag{6.14}$$

we obtain the **second series solution** as

$$y_2(x) = a_0 x^{1-c}\sum_{k=0}^{\infty} a_k x^k, \tag{6.15}$$

$$\boxed{y_2(x) = a_0 x^{1-c}\left[1 + \frac{(a+1-c)(1+b-c)}{(2-c)}\frac{x}{1!} + \cdots\right], \quad c \neq 2, 3, 4, \ldots.} \tag{6.16}$$

If we set a_0 to 1 in the first series solution [Eq. (6.12)], then $y_1(x)$ becomes the **hypergeometric function** (or series):

$$\boxed{y_1(x) = F(a, b, c; x).} \tag{6.17}$$

The hypergeometric function is convergent in the interval $|x| < 1$. For convergence at the end point $x = 1$ one needs $c > a + b$, and for convergence at $x = -1$ one needs $c > a + b - 1$. The **second solution**, $y_2(x)$, can be expressed in term of the hypergeometric function as

$$\boxed{y_2(x) = x^{1-c}F(a - c + 1, b - c + 1, 2 - c; x), \quad c \neq 2, 3, 4, \dots .} \tag{6.18}$$

The **general solution** of the hypergeometric equation is now written as

$$\boxed{y(x) = AF(a, b, c; x) + Bx^{1-c}F(a - c + 1, b - c + 1, 2 - c; x).} \tag{6.19}$$

Sometimes the hypergeometric function, $F(a, b, c; x)$, is also written as

$${}_2F_1(a, b, c; x). \tag{6.20}$$

One can also find series solutions about the regular singular point $x = 1$ as

$$\boxed{y_3(x) = F(a, b, a + b + 1 - c; 1 - x),} \tag{6.21}$$

$$\boxed{y_4(x) = (1 - x)^{c-a-b}F(c - a, c - b, c - a - b + 1; 1 - x).} \tag{6.22}$$

The interval of convergence of these series is $0 < x < 2$. Series solutions appropriate for the singular point at infinity are given as

$$\boxed{y_5(x) = (-x)^{-a}F(a, a - c + 1, a - b + 1; x^{-1}),} \tag{6.23}$$

$$\boxed{y_6(x) = (-x)^{-b}F(b - c + 1, b, b - a + 1; x^{-1}),} \tag{6.24}$$

which converge for $|x| > 1$.

These constitute the six solutions found by Kummer [1, 2]. Since the hypergeometric equation can only have two linearly independent solutions, any three of the solutions, $y_1, \dots, y_6$, are connected by linear relations with constant coefficients [2]. For example,

$$y_1(x) = \frac{\Gamma(c)\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)}y_3(x) + \frac{\Gamma(c)\Gamma(a+b-c)}{\Gamma(a)\Gamma(b)}y_4(x) \tag{6.25}$$

$$= \frac{\Gamma(c)\Gamma(b-a)}{\Gamma(c-a)\Gamma(b)}y_5(x) + \frac{\Gamma(c)\Gamma(a-b)}{\Gamma(c-b)\Gamma(a)}y_6(x). \tag{6.26}$$

The **basic integral representation** of the hypergeometric function is:

$$F(a, b, c; x) = \frac{\Gamma(c)}{\Gamma(b)\Gamma(c-b)} \int_0^1 \frac{t^{b-1}(1-t)^{c-b-1}dt}{(1-tx)^a}, \quad \mathrm{Re}\, c > \mathrm{Re}\, b > 0. \tag{6.27}$$

This integral, which can be proven by expanding $(1 - tx)^{-a}$ in binomial series and then integrating term by term, transforms into an integral of the same type by the **Euler's hypergeometric transformations** [2]:

$$\begin{aligned} t &\to t, \\ t &\to 1-t, \\ t &\to (1-t)/(1-tx), \\ t &\to t/(1-x+tx). \end{aligned} \tag{6.28}$$

Applications of the four Euler transformations to the six Kummer solutions give all the possible 24 forms of the solutions of the hypergeometric equation. These solutions and a list of 20 relations among them can be found in Erdelyi *et al.* [2].

6.2 Hypergeometric Representations of Special Functions

Majority of the special functions can be represented in terms of hypergeometric functions. If we change the independent variable in Eq. (6.1) to

$$x = \frac{(1-\xi)}{2}, \tag{6.29}$$

the hypergeometric equation becomes

$$(1-\xi^2)\frac{d^2y}{d\xi^2} + [(a+b+1-2c) - (a+b+1)\xi]\frac{dy}{d\xi} - aby = 0. \tag{6.30}$$

Choosing the parameters a, b, and c as

$$a = -\nu, \ b = \nu + 1, \ c = 1, \tag{6.31}$$

Eq. (6.30) becomes

$$(1-\xi^2)\frac{d^2y}{d\xi^2} - 2\xi\frac{dy}{d\xi} + \nu(\nu+1)y = 0. \tag{6.32}$$

This is nothing but the **Legendre equation**, whose finite solutions are given as the Legendre polynomials:

$$y_\nu(\xi) = P_\nu(\xi). \tag{6.33}$$

Hence, the **Legendre polynomials** can be expressed in terms of the hypergeometric functions as

$$\boxed{P_\nu(\xi) = F\left(-\nu, \nu+1, 1; \frac{1-\xi}{2}\right), \quad \nu = 0, 1, 2, \ldots .} \tag{6.34}$$

Similarly, we can write the **associated Legendre polynomials** as

$$\boxed{P_n^m(x) = \frac{(n+m)!}{(n-m)!}\frac{(1-x^2)^{m/2}}{2^m m!}F\left(m-n, m+n+1, m+1; \frac{1-x}{2}\right)} \tag{6.35}$$

and the **Gegenbauer polynomials** as

$$\boxed{C_n^\lambda(x) = \frac{\Gamma(n+2\lambda)}{n!\Gamma(2\lambda)}F\left(-n, n+2\lambda, \lambda+\frac{1}{2}; \frac{1-x}{2}\right).} \tag{6.36}$$

The main reason for our interest in hypergeometric functions is that the solutions of so many of the second-order ordinary linear differential equations encountered in science and engineering can be expressed in terms of $F(a, b, c; x)$.

6.3 Confluent Hypergeometric Equation

Hypergeometric equation:

$$z(1-z)\frac{d^2y(z)}{dz^2} + [c - (a+b+1)z]\frac{dy(z)}{dz} - aby(z) = 0 \tag{6.37}$$

has three regular singular points at $z = 0, 1$, and ∞. By setting $z = x/b$ and taking the limit as $b \to \infty$ we can merge the singularities at b and infinity. This gives us the **confluent hypergeometric equation**:

$$\boxed{x\frac{d^2y}{dx^2} + (c-x)\frac{dy}{dx} - ay = 0,} \tag{6.38}$$

whose solutions are the **confluent hypergeometric functions** $M(a, c; x)$. The confluent hypergeometric equation has a regular singular point at $x = 0$ and an essential singularity at infinity. Bessel functions, $J_n(x)$, and the Laguerre polynomials, $L_n(x)$, can be written in terms of the solutions of the confluent hypergeometric equation, respectively, as

$$J_n(x) = \frac{e^{-ix}}{n!}\left(\frac{x}{2}\right)^n M\left(n + \frac{1}{2}, 2n + 1; 2ix\right), \tag{6.39}$$

$$L_n(x) = M(-n, 1; x). \tag{6.40}$$

Linearly independent solutions of Eq. (6.38) are given as

$$y_1(x) = M(a, c, x) = 1 + \frac{a}{c}\frac{x}{1!} + \frac{a(a+1)}{c(c+1)}\frac{x^2}{2!} + \frac{a(a+1)(a+2)}{c(c+1)(c+2)}\frac{x^3}{3!} + \cdots,$$
$$c \neq 0, -1, -2, \ldots \tag{6.41}$$

and

$$y_2(x) = x^{1-c}M(a + 1 - c, 2 - c; x), \quad c \neq 2, 3, 4, \ldots. \tag{6.42}$$

The basic **integral representation** of the confluent hypergeometric functions, which are also shown as

$${}_1F_1(a, c; x), \tag{6.43}$$

can be given as

$$\boxed{M(a, c; x) = \frac{\Gamma(c)}{\Gamma(a)\Gamma(c-a)}\int_0^1 dt\, e^{xt} t^{a-1}(1-t)^{c-a-1}, \quad \mathrm{Re}\, c > \mathrm{Re}\, a > 0.} \tag{6.44}$$

6.4 Pochhammer Symbol and Hypergeometric Functions

Using the **Pochhammer symbol**:

$$(\alpha)_r = \alpha(\alpha + 1)\cdots(\alpha + r - 1), \tag{6.45}$$

$$(\alpha)_r = \frac{\Gamma(\alpha + r)}{\Gamma(\alpha)}, \tag{6.46}$$

where r is a positive integer and $(\alpha)_0 = 1$, we can write the **hypergeometric function** [Eq. (6.12)] as

$$F(a, b, c; x) = \sum_{r=0}^{\infty} \frac{(a)_r (b)_r}{(c)_r} \frac{x^r}{r!}. \tag{6.47}$$

We have mentioned that the **hypergeometric functions** are also written as ${}_2F_1(a, b, c; x)$. This follows from the general definition:

$$ {}_mF_n(a_1, a_2, \ldots, a_m, b_1, b_2, \ldots, b_n; x) = \sum_{r=0}^{\infty} \frac{(a_1)_r \cdots (a_m)_r}{(b_1)_r \cdots (b_n)_r} \frac{x^r}{r!}, \tag{6.48}$$

where $m = 2,\ n = 1$ and the $m = 1,\ n = 1$ cases correspond to the **hypergeometric** and the **confluent hypergeometric** functions, respectively. The $m = 0,\ n = 1$ case is also called the **hypergeometric limit function** ${}_0F_1(-, b; x)$. Hypergeometric function ${}_2F_1(a, b, c; x)$ satisfies the **hypergeometric equation** [Eq. (6.1)]:

$$x(1 - x)y'' + [c - (a + b + 1)x]y' - aby(x) = 0. \tag{6.49}$$

Many of the special functions of physics and engineering can be written in terms of the hypergeometric function:

$$\begin{aligned}
P_l(x) &= {}_2F_1\left(-l, l + 1, 1; \frac{1 - x}{2}\right), \\
P_l^m(x) &= \frac{(l + m)!}{(l - m)!} \frac{(1 - x^2)^{m/2}}{2^m m!}\, {}_2F_1\left(m - l, m + l + 1, m + 1; \frac{1 - x}{2}\right), \\
C_n^\lambda(x) &= \frac{\Gamma(n + 2\lambda)}{n!\Gamma(2\lambda)}\, {}_2F_1\left(-n, n + 2\lambda, \lambda + \frac{1}{2}; \frac{1 - x}{2}\right), \\
U_n(x) &= n\sqrt{1 - x^2}\, {}_2F_1\left(-n + 1, n + 1, \frac{3}{2}; \frac{1 - x}{2}\right), \\
T_n(x) &= {}_2F_1\left(-n, n, \frac{1}{2}; \frac{1 - x}{2}\right).
\end{aligned} \tag{6.50}$$

The **confluent hypergeometric function**, $M(a, c; x)$, which is also written as ${}_1F_1(a, c; x)$, satisfies

$$xy'' + (c - x)y' - ay(x) = 0. \tag{6.51}$$

In terms of the Pochhammer symbols ${}_1F_1(a, c; x)$ is given as

$$\boxed{{}_1F_1(a, c; x) = \sum_{r=0}^{\infty} \frac{(a)_r}{(c)_r} \frac{x^r}{r!}.} \tag{6.52}$$

Some of the special functions, which could be expressed in terms of the confluent hypergeometric function, are given below:

$$\begin{aligned} J_n(x) &= \frac{e^{-ix}}{n!}\left(\frac{x}{2}\right)^n {}_1F_1\left(n + \frac{1}{2}, 2n + 1; 2ix\right), \\ H_{2n}(x) &= (-1)^n \frac{(2n)!}{n!}\ {}_1F_1\left(-n, \frac{1}{2}; x^2\right), \\ H_{2n+1}(x) &= (-1)^n \frac{2(2n+1)!x}{n!}\ {}_1F_1\left(-n, \frac{3}{2}; x^2\right), \\ L_n(x) &= {}_1F_1(-n, 1; x), \\ L_n^k(x) &= \frac{\Gamma(n+k+1)}{n!\Gamma(k+1)}\ {}_1F_1(-n, k+1; x). \end{aligned} \tag{6.53}$$

To prove these relations we can write the series expressions for the hypergeometric function and then compare with the series representation of the corresponding function. For example, consider

$$P_l(x) = {}_2F_1\left(-l, l+1, 1; \frac{1-x}{2}\right). \tag{6.54}$$

We write the hypergeometric function as

$${}_2F_1\left(-l, l+1, 1; \frac{1-x}{2}\right) = \sum_{r=0}^{\infty} \frac{(-l)_r (l+1)_r}{(1)_r} \frac{[(1-x)/2]^r}{r!}. \tag{6.55}$$

Using

$$(-l)_r = \begin{cases} (-1)^r \dfrac{l!}{(l-r)!}, & r \le l, \\ 0, & r \ge (l+1), \end{cases} \tag{6.56}$$

and

$$(l+1)_r = \frac{(l+r)!}{l!}, \quad (1)_r = r!\ , \tag{6.57}$$

we obtain

$${}_2F_1\left(-l, l+1, 1; \frac{1-x}{2}\right) = \sum_{r=0}^{\infty} \frac{(l+r)!}{2^r (l-r)!(r!)^2} (x-1)^r. \tag{6.58}$$

To obtain the desired result, we need the Taylor series expansion of $P_l(x)$ around $x = 1$ as

$$P_l(x) = \sum_{r=0}^{\infty} P_l^{(r)}(1)\frac{(x-1)^r}{r!}, \tag{6.59}$$

where $P_l^{(r)}(1)$ stands for the rth derivative of $P_l(x)$ evaluated at $x = 1$. Using the Rodriguez formula of $P_l(x)$:

$$P_l(x) = \frac{1}{2^l l!}\frac{d^l}{dx^l}(x^2-1)^l, \tag{6.60}$$

we can evaluate these derivatives as

$$P_l^{(r)}(1) = \begin{cases} \dfrac{1}{2^r r!}\dfrac{(r+l)!}{(l-r)!}, & l \geq r, \\ 0, & l < r, \end{cases} \tag{6.61}$$

which when substituted into Eq. (6.59) and compared with Eq. (6.58) yields the desired result. Of course, we can also use the method in Section 6.2. That is, by making an appropriate transformation of the independent variable in the hypergeometric equation and then by comparing the result with the equation at hand to find the parameters.

Pochhammer symbols are very useful in manipulations with hypergeometric functions. For example, to prove the **integral representation** of the hypergeometric function [Eq. (6.27)], we start with the basic series definition [Eq. (6.47)] and write

$$_2F_1(a,b,c;x) = \sum_{r=0}^{\infty} \frac{(a)_r(b)_r}{(c)_r}\frac{x^r}{r!} \tag{6.62}$$

$$= \sum_{r=0}^{\infty} \frac{\Gamma(a+r)\Gamma(b+r)\Gamma(c)}{\Gamma(a)\Gamma(b)\Gamma(c+r)}\frac{x^r}{r!}. \tag{6.63}$$

Using the following relation between the beta and the gamma functions:

$$B(p,q) = \frac{\Gamma(p)\Gamma(q)}{\Gamma(p+q)}, \tag{6.64}$$

we write this as

$$_2F_1(a,b,c;x) = \frac{\Gamma(c)}{\Gamma(a)\Gamma(b)\Gamma(c-b)}\sum_{r=0}^{\infty}\Gamma(a+r)\left[\frac{\Gamma(c-b)\Gamma(b+r)}{\Gamma(c+r)}\right]\frac{x^r}{r!} \tag{6.65}$$

$$= \frac{\Gamma(c)}{\Gamma(a)\Gamma(b)\Gamma(c-b)}\sum_{r=0}^{\infty}\Gamma(a+r)B(b+r,c-b)\frac{x^r}{r!}. \tag{6.66}$$

We now use the integral definition of the beta function:

$$B(p,q) = \int_0^1 t^{p-1}(1-t)^{q-1}dt, \quad p > 0, \quad q > 0, \tag{6.67}$$

to write

$${}_2F_1(a,b,c;x) = \frac{\Gamma(c)}{\Gamma(a)\Gamma(b)\Gamma(c-b)} \sum_{r=0}^{\infty} \Gamma(a+r) \int_0^1 t^{b+r-1}(1-t)^{c-b-1}dt \frac{x^r}{r!}. \tag{6.68}$$

Finally, rearranging and using the binomial expansion:

$$(1-xt)^{-a} = \sum_{r=0}^{\infty} \frac{\Gamma(a+r)}{\Gamma(a)} \frac{(xt)^r}{r!}, \tag{6.69}$$

we obtain the desired result:

$${}_2F_1(a,b,c;x) = \frac{\Gamma(c)}{\Gamma(b)\Gamma(c-b)} \int_0^1 \frac{t^{b-1}(1-t)^{c-b-1}dt}{(1-tx)^a}, \quad \operatorname{Re} c > \operatorname{Re} b > 0. \tag{6.70}$$

6.5 Reduction of Parameters

Pochhammer notation is also very useful in getting rid of a parameter in the numerator or the denominator of the hypergeometric function. For example, in the confluent hypergeometric series:

$${}_1F_1(a,b;x) = \sum_{k=0}^{\infty} \frac{(a)_k}{(b)_k} \frac{x^k}{k!}, \tag{6.71}$$

$$(a)_k = a(a+1)\cdots(a+k-1), \quad a \neq 0,\ (a)_0 = 1, \tag{6.72}$$

note that

$$\frac{(a)_k}{a^k} = \frac{a}{a}\frac{(a+1)}{a}\cdots\frac{(a+k-1)}{a} \tag{6.73}$$

$$= 1\left(1+\frac{1}{a}\right)\left(1+\frac{2}{a}\right)\cdots\left(1+\frac{k-1}{a}\right), \tag{6.74}$$

thus, for finite k, we have the limit

$$\lim_{a\to\infty} \frac{(a)_k}{a^k} \to 1. \tag{6.75}$$

Similarly,

$$\lim_{b\to\infty} \frac{b^k}{(b)_k} \to 1. \tag{6.76}$$

Using these limits, we can write

$$\lim_{a\to\infty} {}_1F_1\left(a, b; \frac{x}{a}\right) = {}_0F_1(-, b; x). \tag{6.77}$$

Using this procedure, we can write the binomial function as

$$\lim_{b\to\infty} {}_1F_0(a, b; bz) = {}_1F_0(a, -; x) = (1-x)^{-a}, \quad |x| < 1. \tag{6.78}$$

We can also write the exponential function as

$$\lim_{b\to\infty} {}_0F_1(-, b; bx) = {}_0F_0(-, -; x) = e^x, \tag{6.79}$$

$$\lim_{a\to\infty} {}_1F_0\left(a, -; \frac{x}{a}\right) = {}_0F_0(-, -; x) = e^x. \tag{6.80}$$

Example 6.1 ***Confluent hypergeometric series***
Using the fact that confluent hypergeometric series is convergent for all x, which can be verified by standard methods, find the solutions of

$$x^2y'' + \left\{-\frac{x^2}{4} + kx + \frac{1}{4} - m^2\right\} y(x) = 0 \tag{6.81}$$

for the interval $x \in [0, \infty)$.

Solution
First obtain the transformation,

$$y(x) = x^{\left(\frac{1}{2}-m\right)} e^{-x/2} w(x), \tag{6.82}$$

which reduces the above differential equation into a differential equation with a two-term recursion relation and then find the solution for $w(x)$ in terms of the hypergeometric functions.

Example 6.2 ***Hypergeometric series***
Show that the transformation $t \to 1-t$ transforms the basic integral representation of the hypergeometric function [Eq. (6.27)]:

$$ {}_2F_1(a, b, c; x) = \frac{\Gamma(c)}{\Gamma(b)\Gamma(c-b)} \int_0^1 \frac{t^{b-1}(1-t)^{c-b-1}dt}{(1-tx)^a}, \quad \text{Re}\, c > \text{Re}\, b > 0, \tag{6.83}$$

into an integral of the same form and then prove

$$ {}_2F_1(a, b, c; x) = (1-x)^{-a}\, {}_2F_1\left(a, c-b, c; \frac{x}{x-1}\right). \tag{6.84}$$

Solution
Substituting $t \to 1-t$ in the integral definition [Eq. (6.83)]:

$$ {}_2F_1(a, b, c; x) = \frac{\Gamma(c)}{\Gamma(b)\Gamma(c-b)} \int_0^1 \frac{(1-t)^{b-1}t^{c-b-1}\, dt}{(1-(1-t)x)^a}, \tag{6.85}$$

and rearranging terms yields the desired result [Eq. (6.84)]:

$$ {}_2F_1(a,b,c;x) = \frac{\Gamma(c)}{\Gamma(b)\Gamma(c-b)} \int_0^1 (1-t)^{b-1} t^{c-b-1} (1-x)^{-a} \left(1 - \frac{xt}{x-1}\right)^{-a} dt \tag{6.86} $$

$$ = (1-x)^{-a} \frac{\Gamma(c)}{\Gamma(b)\Gamma(c-b)} \int_0^1 (1-t)^{b-1} t^{c-b-1} \quad \left(1 - \frac{xt}{x-1}\right)^{-a} dt \tag{6.87} $$

$$ = (1-x)^{-a} \ {}_2F_1\left(a, c-b, c; \frac{x}{x-1}\right). \tag{6.88} $$

Bibliography

1 Abramowitz, M. and Stegun, I.A. (eds) (1965) *Handbook of Mathematical Functions with Formulas Graphs and Mathematical Tables*, Dover Publications.

2 Erdelyi, A., Oberhettinger, M.W., and Tricomi, F.G. (1981) *Higher Transcendental Functions*, vol. **I**, Krieger, New York.

Problems

1 Show that the Hermite polynomials can be expressed as

(i) $H_{2n}(x) = (-1)^n \frac{(2n)!}{n!} M\left(-n, \frac{1}{2}; x^2\right)$,

(ii) $H_{2n+1}(x) = (-1)^n \frac{2(2n+1)!}{n!} xM\left(-n, \frac{3}{2}; x^2\right)$.

2 Show that associated Legendre polynomials can be written as

$$ P_n^m(x) = \frac{(n+m)!}{(n-m)!} \frac{(1-x^2)^{m/2}}{2^m m!} F\left(m-n, m+n+1, m+1; \frac{1-x}{2}\right). $$

3 Derive the Kummer formula

$$ M(a,c,x) = e^x M(c-a, c; -x). $$

4 Show that the associated Laguerre polynomials can be written as

$$ L_n^k(x) = \frac{(n+k)!}{n!k!} M(-n, k+1; x). $$

5 Show that the modified Bessel functions can be expressed as

$$I_n(x) = \frac{e^{-x}}{n!}\left(\frac{x}{2}\right)^n M\left(n+\frac{1}{2}, 2n+1; 2x\right).$$

6 Write the Chebyshev polynomials in terms of the hypergeometric functions.

7 Show that Gegenbauer polynomials can be expressed as

$$C_n^\lambda(x) = \frac{\Gamma(n+2\lambda)}{n!\Gamma(2\lambda)} F\left(-n, n+2\lambda, \lambda+\frac{1}{2}; \frac{1-x}{2}\right).$$

8 Express the solutions of

$$t(1-t^2)\frac{d^2y}{dt^2} + 2\left[\gamma - \frac{1}{2} - \left(\alpha+\beta+\frac{1}{2}\right)t^2\right]\frac{dy}{dt} - 4\alpha\beta t y(t) = 0$$

in terms of the hypergeometric functions.
Hint: Try the substitution $x = t^2$.

9 Show the following relations:

(i) $(1-x)^{-\alpha} = F(\alpha, \beta, \beta; x)$, (ii) $\ln(1-x) = -xF(1,1,2;x)$,

(iii) $\sin^{-1}x = xF\left(\frac{1}{2}, \frac{1}{2}, \frac{3}{2}; x^2\right)$, (iv) $e^x = M(\alpha, \alpha; x)$.

10 Derive the following integral representation of the confluent hypergeometric function:

$$M(a, c; x) = \frac{\Gamma(c)}{\Gamma(a)\Gamma(c-a)}\int_0^1 dt\, e^{xt} t^{a-1}(1-t)^{c-a-1}, \quad \operatorname{Re} c > \operatorname{Re} a > 0.$$

11 Using the integral definition of the hypergeometric function:

$$F(a, b, c; x) = \frac{\Gamma(c)}{\Gamma(b)\Gamma(c-b)}\int_0^1 \frac{t^{b-1}(1-t)^{c-b-1}dt}{(1-tx)^a}, \quad \operatorname{Re} c > \operatorname{Re} b > 0,$$

show that

$${}_2F_1(a, b, c; 1) = \frac{\Gamma(c)\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)}.$$

Hint: Use the relation between the beta and the gamma functions: $B(p, q) = \Gamma(p)\Gamma(q)/\Gamma(p+q)$, and the integral definition of the beta function:

$$B(p, q) = \int_0^1 t^{p-1}(1-t)^{q-1}dt, \quad p > 0, \quad q > 0.$$

12 Using the Pochhammer symbols show

$$\lim_{q\to 1} {}_0F_1\left(-, \frac{1}{q-1}; -\frac{z}{q-1}\right) = e^{-x},$$

and

$$\lim_{q\to 1} {}_1F_0\left(\frac{1}{q-1}, -; -(q-1)x\right) = \lim_{q\to 1} [1+(q-1)x]^{-1/(q-1)} = e^{-x}.$$

A result, which plays an important role in **Tsallis thermodynamics**.

7

Sturm–Liouville Theory

Majority of the frequently encountered partial differential equations in physics and engineering can be solved by the method of separation of variables. This method helps us to reduce a second-order partial differential equation into a set of ordinary differential equations with some new parameters called the separation constants. We have seen that solutions of these equations with the appropriate boundary conditions have properties reminiscent of an eigenvalue problem. In this chapter, we study these properties systematically in terms of the Sturm–Liouville theory.

7.1 Self-Adjoint Differential Operators

We define a second-order **linear differential operator** $£$ as

$$\boxed{£ = P_0(x)\frac{d^2}{dx^2} + P_1(x)\frac{d}{dx} + P_2(x), \qquad x \in [a,b],} \tag{7.1}$$

where $P_i(x)$, $i = 0, 1, 2$, are real functions with the first $(2-i)$ derivatives continuous. In addition, in the open interval (a, b), $P_0(x)$ does not vanish even though it could have zeroes at the end points. We now define the **adjoint operator** $\overline{£}$ as

$$\boxed{\overline{£}u(x) = \frac{d^2}{dx^2}[P_0(x)u(x)] - \frac{d}{dx}[P_1(x)u(x)] + P_2(x)u(x),} \tag{7.2}$$

$$\overline{£}u(x) = \left[P_0\frac{d^2}{dx^2} + (2P_0' - P_1)\frac{d}{dx} + P_0''(x) - P_1'(x) + P_2(x)\right] u(x). \tag{7.3}$$

The **sufficient** and **necessary** condition for an operator, $£$, to be **self-adjoint**, that is, $£ = \overline{£}$ is now found as

$$\boxed{P_0'(x) = P_1(x).} \tag{7.4}$$

Mathematical Methods in Science and Engineering, Second Edition. Selçuk Ş. Bayın.

A **self-adjoint operator** can also be written in the form

$$\boxed{\bar{\pounds}u(x) = \pounds u(x) = \frac{d}{dx}\left[p(x)\frac{du(x)}{dx}\right] + q(x)u(x),} \tag{7.5}$$

where $p(x) = P_0(x)$, $q(x) = P_2(x)$. This is also called the **first canonical form**. An operator that is not self-adjoint can always be made self-adjoint by multiplying with

$$\boxed{\frac{1}{P_0(x)}\exp\left[\int^x \frac{P_1(x)}{P_0(x)}dx\right].} \tag{7.6}$$

Among the equations we have seen, the Legendre equation is self-adjoint, whereas the Hermite and the Laguerre equations are not.

7.2 Sturm–Liouville Systems

The operator, £, defined in Eq. (7.5) is called the **Sturm–Liouville operator**. Using this operator, we can define a differential equation:

$$\boxed{\pounds u(x) = -\lambda\omega(x)\, u(x),} \tag{7.7}$$

which is called the **Sturm–Liouville equation**. This equation defines an eigenvalue problem for the operator £ with the eigenvalue $-\lambda$ and the eigenfunction $u(x)$. The weight function, $\omega(x)$, satisfies the condition $\omega(x) > 0$, except for a finite number of isolated points, where it could have zeroes.

A differential equation alone cannot be a complete description of a physical problem. Therefore, one also needs the boundary conditions to determine the integration constants. We now supplement the above differential equation with the following **boundary conditions**:

$$v(x)p(x)u'(x)|_{x=a} = 0, \tag{7.8}$$

$$v(x)p(x)u'(x)|_{x=b} = 0, \tag{7.9}$$

where $u(x)$ and $v(x)$ are any two solutions of Eq. (7.7) with the same or different λ values. Now the differential equation [Eq. (7.7)] plus the boundary conditions [Eqs. (7.8) and (7.9)] is called a **Sturm–Liouville system**. However, we could also work with something less restrictive as

$$\boxed{v(x)p(x)u'(x)|_{x=a} = v(x)p(x)u'(x)|_{x=b},} \tag{7.10}$$

which in general corresponds to one of the following cases:

1. Cases where the solutions, $u(x)$ and $v(x)$, are zero at the end points; $x = a$ and $x = b$. Such conditions are called the (homogeneous) **Dirichlet conditions.** Boundary conditions for the vibrations of a string fixed at both ends are of this type.
2. Cases where the derivatives, $u'(x)$ and $v'(x)$, are zero at the end points; $x = a$ and $x = b$. Acoustic wave problems require this type of boundary conditions. They are called the (homogeneous) **Neumann conditions.**
3. Cases where

   $$[u(x) + \alpha u'(x)]_{x=a} = 0 \tag{7.11}$$

   and

   $$[v(x) + \beta v'(x)]_{x=b} = 0, \tag{7.12}$$

   where α and β are constants independent of the eigenvalues. An example for this type of boundary conditions, which are called **general unmixed**, is the vibrations of a string with elastic connections.
4. Cases where one type of boundary conditions is satisfied at $x = a$ and another type at $x = b$.

A common property of all these conditions is that the value of $u'(x)$ and the value of $u(x)$ at the end point a are independent of their values at the other end point b; hence they are called **unmixed boundary conditions**. Depending on the problem, it is also possible to impose more complicated boundary conditions.

Even though the operator $\pounds$ is real, solutions of Eq. (7.7) could involve complex functions; thus we write Eq. (7.10) as

$$\boxed{v^* p u' |_{x=a} = v^* p u' |_{x=b}} \tag{7.13}$$

along with its complex conjugate:

$$v p u'^* |_{x=a} = v p u'^* |_{x=b}. \tag{7.14}$$

Since all the eigenfunctions satisfy the same boundary conditions, we can interchange u and v to write

$$\boxed{v'^* p u |_{x=a} = v'^* p u |_{x=b}.} \tag{7.15}$$

7.3 Hermitian Operators

We now show that the self-adjoint operator $\pounds$ and the differential equation

$$\boxed{\pounds u(x) + \lambda \omega(x) u(x) = 0,} \tag{7.16}$$

along with the boundary conditions [Eqs. (7.13) and (7.15)] have an interesting property. We first multiply $£u(x)$ from the left with v^* and integrate over $[a, b]$:

$$\int_a^b v^* £u dx = \int_a^b v^*(pu')' dx + \int_a^b v^* qu dx. \tag{7.17}$$

Integrating the first term on the right-hand side by parts gives

$$\int_a^b v^*(pu')' dx = v^* pu' |_a^b - \int_a^b (v^{*'} p) u' dx. \tag{7.18}$$

Using the boundary condition (7.13), the integrated term is zero. Integrating the second term in Eq. (7.18) by parts again and using the boundary condition (7.15), we see that the integrated term is again zero, thus obtaining

$$\int_a^b v^*(pu')' dx = \int_a^b u(pv^{*'})' dx. \tag{7.19}$$

Substituting this result in Eq. (7.17), we obtain

$$\boxed{\int_a^b v^* £u dx = \int_a^b u £v^* dx.} \tag{7.20}$$

Operators that satisfy this relation are called **Hermitian** with respect to the functions u and v satisfying the boundary conditions in Eqs. (7.13) and (7.15). In other words, hermiticity of an operator is closely tied to the boundary conditions imposed.

7.4 Properties of Hermitian Operators

Hermitian operators have the following very useful properties:

1. Eigenvalues are real.
2. Eigenfunctions are orthogonal with respect to a weight function $w(x)$.
3. Eigenfunctions form a complete set.

7.4.1 Real Eigenvalues

Let us write the eigenvalue equations for the eigenvalues λ_i and λ_j as

$$£u_i + \lambda_i \omega(x) u_i = 0, \tag{7.21}$$

$$£u_j + \lambda_j \omega(x) u_j = 0. \tag{7.22}$$

In these equations even though the $£$ operator and the weight function $\omega(x)$ are real, the eigenfunctions and the eigenvalues could be complex. Taking the complex conjugate of Eq. (7.22), we write

$$£u_j^* + \lambda_j^* w(x) u_j^* = 0. \tag{7.23}$$

We multiply Eq. (7.21) by u_j^* and Eq. (7.23) by u_i and subtract to get

$$u_j^* £ u_i - u_i £ u_j^* = (\lambda_j^* - \lambda_i)\omega(x)u_i u_j^*. \tag{7.24}$$

We now integrate both sides:

$$\int_a^b u_j^* £ u_i dx - \int_a^b u_i £ u_j^* dx = (\lambda_j^* - \lambda_i) \int_a^b u_i u_j^* \omega(x) dx. \tag{7.25}$$

For **Hermitian operators**, the left-hand side of the above equation is zero, thus we obtain

$$(\lambda_j^* - \lambda_i) \int_a^b u_i u_j^* \omega(x) dx = 0. \tag{7.26}$$

Since $\omega(x) \neq 0$, except for a finite number of isolated points, for $i = j$, we conclude that

$$\lambda_i^* = \lambda_i. \tag{7.27}$$

That is, the eigenvalues of Hermitian operators are real. In quantum mechanics, eigenvalues correspond to precisely measured quantities; thus observables like energy and momentum are represented by Hermitian operators.

7.4.2 Orthogonality of Eigenfunctions

When $i \neq j$ and when the eigenfunctions are distinct, $\lambda_i \neq \lambda_j$, Eq. (7.26) gives

$$\int_a^b u_i(x) u_j^*(x) \omega(x) dx = 0, \qquad i \neq j. \tag{7.28}$$

We say that the eigenfunctions are orthogonal with respect to the weight function $\omega(x)$ in the interval $[a, b]$. In the case of degenerate eigenvalues, that is, when two different eigenfunctions have the same eigenvalue, $i \neq j$ but $\lambda_i = \lambda_j$, then the integral $\int_a^b u_i u_j^* \omega dx$ does not have to vanish. However, in such cases we can always use the **Gram–Schmidt orthogonalization** method to choose the eigenfunctions as orthogonal. In summary, in any case, we can normalize the eigenfunctions to define an **orthonormal set** with respect to the **weight function** $w(x)$ as

$$\boxed{\int_a^b u_i(x) u_j^*(x) \omega(x) dx = \delta_{ij}.} \tag{7.29}$$

7.4.3 Completeness and the Expansion Theorem

Proof of **completeness** of the set of eigenfunctions is rather technical and can be found in Courant and Hilbert [3]. What is important in most applications is that any sufficiently well-behaved and at least piecewise continuous function can be expressed as an infinite series in terms of the set $\{u_m(x)\}$ as

$$F(x) = \sum_{m=0}^{\infty} a_m u_m(x). \tag{7.30}$$

For a Sturm–Liouville system, using variational analysis, it can be shown that the limit

$$\boxed{\lim_{N\to\infty} \int_a^b \left[F(x) - \sum_{m=0}^{N} a_m u_m(x)\right]^2 \omega(x)dx \to 0} \tag{7.31}$$

is true [4, p. 338]. This means that in the interval $[a, b]$, the series $\sum_{m=0}^{\infty} a_m u_m(x)$ converges to $F(x)$ in the mean. However, convergence in the mean does not imply uniform or pointwise convergence, which requires

$$\boxed{\lim_{N\to\infty} \sum_{m=0}^{N} a_m u_m(x) \to F(x).} \tag{7.32}$$

For most practical situations, convergence in the mean accompanies uniform convergence and is sufficient. Note that uniform convergence also implies pointwise convergence but not vice versa. We conclude this section by stating a theorem from Courant and Hilbert [3, p. 427, vol. I].

The expansion theorem: Any piecewise continuous function defined in the fundamental interval $[a, b]$ with a square integrable first derivative, that is, sufficiently smooth, could be expanded in an eigenfunction series:

$$F(x) = \sum_{m=0}^{\infty} a_m u_m(x), \tag{7.33}$$

which converges absolutely and uniformly in all subintervals free of points of discontinuity. At the points of discontinuity, this series represents, as in the Fourier series, the arithmetic mean of the right- and the left-hand limits.

In this theorem, the function $F(x)$ does not have to satisfy the boundary conditions. This theorem also implies convergence in the mean and pointwise convergence. The derivative is square integrable means that the integral of the square of the derivative is finite for all the subintervals of the fundamental domain $[a, b]$ in which the function is continuous.

7.5 Generalized Fourier Series

Series expansion of a sufficiently smooth $F(x)$ in terms of the set $\{u_m(x)\}$ can now be written as

$$\boxed{F(x) = \sum_{m=0}^{\infty} a_m u_m(x),} \tag{7.34}$$

which is called the **generalized Fourier series** of $F(x)$. Expansion coefficients, a_m, are found by using the orthogonality relation of $\{u_m(x)\}$ as

$$\int_a^b F(x)u_m^*(x)\omega(x)dx = \int_a^b \sum_n a_n u_n(x)u_m^*(x)\omega(x)dx \tag{7.35}$$

$$= \sum_n a_n \left[\int_a^b u_n(x)u_m^*(x)\omega(x)dx\right] \tag{7.36}$$

$$= \sum_n a_n \delta_{nm}, \tag{7.37}$$

thus

$$\boxed{a_m = \int_a^b F(x)u_m^*(x)\omega(x)dx.} \tag{7.38}$$

Substituting a_m in Eq. (7.34) we get

$$F(x) = \sum_{m=0}^{\infty} \int_a^b F(x')u_m^*(x')\omega(x')u_m(x)dx' \tag{7.39}$$

$$= \int_a^b F(x')\left[\sum_{m=0}^{\infty} u_m^*(x')\omega(x')u_m(x)\right] dx'. \tag{7.40}$$

Using the basic definition of the **Dirac-delta function**:

$$g(x) = \int g(x')\delta(x - x')dx', \tag{7.41}$$

we can give a formal expression of the **completeness** of the set $\{\phi_m(x)\}$ as

$$\boxed{\sum_{m=0}^{\infty} u_m^*(x')\omega(x')u_m(x) = \delta(x - x').} \tag{7.42}$$

It is needless to say that this is not a proof of completeness.

7.6 Trigonometric Fourier Series

The trigonometric Fourier series are defined with respect to the eigenvalue problem:

$$\frac{d^2y}{dx^2} + n^2y(x) = 0, \tag{7.43}$$

where the operator, £, is given as

$$£ = d^2/dx^2. \tag{7.44}$$

This could correspond to a vibrating string. Using the periodic boundary conditions:

$$u(a) = u(b), \qquad v(a) = v(b), \tag{7.45}$$

we find the eigenfunctions as

$$\begin{aligned} u_n &= \cos nx, \qquad n = 0, 1, 2, \dots, \\ v_m &= \sin mx, \qquad m = 1, 2, \dots. \end{aligned} \tag{7.46}$$

Orthogonality of the eigenfunctions is expressed as

$$\int_{x_0}^{x_0+2\pi} \sin mx \sin nx dx = A_n \delta_{nm}, \tag{7.47}$$

$$\int_{x_0}^{x_0+2\pi} \cos mx \cos nx dx = B_n \delta_{nm}, \tag{7.48}$$

$$\int_{x_0}^{x_0+2\pi} \sin mx \cos nx dx = 0, \tag{7.49}$$

where

$$A_n = \begin{cases} \pi & n \neq 0, \\ 0 & n = 0, \end{cases} \tag{7.50}$$

$$B_n = \begin{cases} \pi & n \neq 0, \\ 2\pi & n = 0. \end{cases} \tag{7.51}$$

Now the trigonometric Fourier series of any sufficiently well-behaved function becomes

$$f(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty} [a_n \cos nx + b_n \sin nx], \tag{7.52}$$

where the expansion coefficients are given as

$$a_n = \frac{1}{\pi} \int_{-\pi}^{\pi} f(t) \cos nt dt, \qquad n = 0, 1, 2, \dots, \tag{7.53}$$

and

$$b_n = \frac{1}{\pi}\int_{-\pi}^{\pi} f(t)\sin nt dt, \qquad n = 1, 2, \ldots. \tag{7.54}$$

Example 7.1 ***Trigonometric Fourier series***
The trigonometric Fourier series of a **square wave:**

$$f(x) = \begin{cases} +\frac{d}{2}, & 0 < x < \pi, \\ -\frac{d}{2}, & -\pi < x < 0, \end{cases} \tag{7.55}$$

can now be written as

$$f(x) = \frac{2d}{\pi}\sum_{n=0}^{\infty}\frac{\sin(2n+1)x}{(2n+1)}, \tag{7.56}$$

where we have substituted the coefficients

$$a_n = 0, \tag{7.57}$$

$$b_n = \frac{d}{n\pi}(1 - \cos n\pi) = \begin{cases} 0, & n = \text{even}, \\ \frac{2d}{n\pi}, & n = \text{odd}. \end{cases} \tag{7.58}$$

7.7 Hermitian Operators in Quantum Mechanics

In quantum mechanics, the state of a system is completely described by a complex valued function, $\Psi(x)$, in terms of the real variable x. Observable quantities are represented by differential operators acting on the wave function. These operators are not necessarily second-order and are usually obtained from their classical expressions by replacing position, momentum, and energy with their operator counterparts:

$$\begin{aligned} \vec{x} &\to \vec{x}, \\ \vec{p} &\to -i\hbar\vec{\nabla}, \\ E &\to i\hbar\frac{\partial}{\partial t}. \end{aligned} \tag{7.59}$$

For example, the angular momentum operator, $\vec{\mathbf{L}}$, is obtained from its classical expression, $\vec{L} = \vec{r} \times \vec{p}$, as

$$\vec{\mathbf{L}} = -i\hbar(\vec{r} \times \vec{\nabla}). \tag{7.60}$$

Similarly, the Hamiltonian operator, **H**, is obtained from its classical expression, $H = p^2/2m + V(x)$, as

$$\mathbf{H} = -\frac{1}{2m}\vec{\nabla}^2 + V(x). \tag{7.61}$$

The observable value of a physical property is given by the expectation value of the corresponding operator, £, as $\langle £ \rangle = \int \Psi^* \boldsymbol{£} \Psi dx$. Because $\langle £ \rangle$ corresponds to a measurable quantity, it has to be real; hence observable properties in quantum mechanics are represented by Hermitian operators.

For the real Sturm–Liouville operators, hermiticity [Eq. (7.20)] was defined with respect to the eigenfunctions, u and v, which satisfy the boundary conditions in Eqs. (7.13) and (7.15). To accommodate complex operators in quantum mechanics, we modify this definition as

$$\boxed{\int \Psi_1^* \boldsymbol{£} \Psi_2 dx = \int (\boldsymbol{£}\Psi_1)^* \Psi_2 dx,} \tag{7.62}$$

where Ψ_1 and Ψ_2 do not have to be the eigenfunctions of the operator $\boldsymbol{£}$. The fact that Hermitian operators have real expectation values can be seen from

$$\langle £ \rangle = \int \Psi^* \boldsymbol{£} \Psi dx \tag{7.63}$$

$$= \int (£\boldsymbol{\Psi})^* \Psi dx \tag{7.64}$$

$$= \langle \boldsymbol{£} \rangle^*. \tag{7.65}$$

A Hermitian Sturm–Liouville operator must be second-order. However, in quantum mechanics, the order of the Hermitian operators is not restricted. Remember that the momentum operator is first order, but it is Hermitian because of the presence of i in its definition:

$$\langle p \rangle = \int_{-\infty}^{\infty} \Psi^* \left(-i\hbar\frac{\partial}{\partial x}\right) \Psi dx \tag{7.66}$$

$$= \int_{-\infty}^{\infty} \left(-i\hbar\frac{\partial}{\partial x}\Psi\right)^* \Psi dx \tag{7.67}$$

$$= i\hbar \Psi^* \Psi|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \Psi^* \left(i\hbar\frac{\partial}{\partial x}\right) \Psi dx \tag{7.68}$$

$$= \int_{-\infty}^{\infty} \Psi^* \left(-i\hbar\frac{\partial}{\partial x}\right) \Psi dx. \tag{7.69}$$

In proving that the momentum operator is Hermitian, we have also imposed the boundary condition that Ψ is sufficiently smooth and vanishes at large distances.

A general boundary condition that all wave functions must satisfy is that they have to be square integrable, and thus normalizable. Space of all square integrable functions actually forms an infinite dimensional vector space called L_2 or the **Hilbert space**. Functions in this space can be expanded as generalized Fourier series in terms of the complete and orthonormal set of eigenfunctions, $\{u_m(x)\}$, of a Hermitian operator. Eigenfunctions satisfy the eigenvalue equation

$$\pounds u_m(x) = \lambda_m u_m(x), \tag{7.70}$$

where λ_m represents the eigenvalues. In other words, $\{u_m(x)\}$ spans the infinite dimensional vector space of square integrable functions. The inner product, which is the analog of the dot product in Hilbert space, is defined as

$$(\Psi_1, \Psi_2) = \int \Psi_1^*(x)\Psi_2(x)dx. \tag{7.71}$$

The inner product has the following properties:

$$(\Psi_1, \alpha\Psi_2) = \alpha(\Psi_1, \Psi_2), \tag{7.72}$$

$$(\alpha\Psi_1, \Psi_2) = \alpha^*(\Psi_1, \Psi_2), \tag{7.73}$$

$$(\Psi_1, \Psi_2)^* = (\Psi_2, \Psi_1), \tag{7.74}$$

$$(\Psi_1 + \Psi_2, \Psi_3) = (\Psi_1, \Psi_3) + (\Psi_2, \Psi_3), \tag{7.75}$$

where α is a complex number. The inner product also satisfies the **triangle inequality:**

$$|\Psi_1 + \Psi_2| \leq |\Psi_1| + |\Psi_2| \tag{7.76}$$

and the **Schwartz inequality:**

$$|\Psi_1||\Psi_2| \geq |(\Psi_1, \Psi_2)|. \tag{7.77}$$

An important consequence of the Schwartz inequality is that the convergence of (Ψ_1, Ψ_2) follows from the convergence of (Ψ_1, Ψ_1) and (Ψ_2, Ψ_2).

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Problems

1 Show that the Laguerre equation,

$$x\frac{d^2y}{dx^2} + (1-x)\frac{dy}{dx} + ny = 0,$$

can be brought into the self-adjoint form by multiplying it with e^{-x} .

2 Write the Chebyshev equation:

$$(1-x^2)T_n''(x) - xT_n'(x) + n^2T_n(x) = 0,$$

in the self-adjoint form.

3 Find the weight function for the associated Laguerre equation:

$$x\frac{d^2y}{dx^2} + (k+1-x)\frac{dy}{dx} + ny = 0.$$

4 A function $y(x)$ is to be a finite solution of the differential equation

$$x(1-x)\frac{d^2y}{dx^2} + \left(\frac{3}{2} - 2x\right)\frac{dy}{dx} + \left[\lambda - \frac{(2+5x-x^2)}{4x(1-x)}\right]y(x) = 0,$$

in the entire interval $x \in [0,1]$.

(i) Show that this condition can only be satisfied for certain values of λ and write the solutions explicitly for the lowest three values of λ.
(ii) Find the weight function $w(x)$.
(iii) Show that the solution set $\{y_\lambda(x)\}$ is orthogonal with respect to the $w(x)$ found above.

5 Show that the Legendre equation can be written as

$$\frac{d}{dx}\left[(1-x^2)P_l'\right] + l(l+1)P_l = 0.$$

6 For following the Sturm–Liouville equation:

$$\frac{d^2y}{dx^2} + \lambda y = 0,$$

using the boundary conditions:

$$y(0) = 0, \quad y(\pi) - y'(\pi) = 0,$$

find the eigenvalues and the eigenfunctions.

7 Find the eigenvalues and the eigenfunctions of the Sturm–Liouville system

$$\frac{d}{dx}\left[(x^2+1)\frac{dy}{dx}\right] + \frac{\lambda}{x^2+1}y = 0, \quad y(0) = 0, \quad y(1) = 0.$$

Hint: Try the substitution $x = \tan t$.

8 Show that the Hermite equation can be written as

$$\frac{d}{dx}[e^{-x^2}H_n'] + 2ne^{-x^2}H_n = 0.$$

9 Given the Sturm–Liouville equation

$$\frac{d}{dx}\left[p(x)\frac{d}{dx}y(x)\right] + \lambda_n w(x)y(x) = 0.$$

If $y_n(x)$ and $y_m(x)$ are two orthogonal solutions and satisfy the appropriate boundary conditions, then show that $y_n'(x)$ and $y_m'(x)$ are orthogonal with the weight function $p(x)$.

10 Show that the Bessel equation can be written in the self-adjoint form as

$$\frac{d}{dx}[xJ_n'] + \left(x - \frac{n^2}{x}\right)J_n = 0.$$

11 Find the trigonometric Fourier expansion of

$$f(x) = \begin{cases} \pi, & -\pi \le x < 0, \\ x, & 0 < x \le \pi. \end{cases}$$

12 Show that the angular momentum operator,

$$\vec{\mathbf{L}} = -i\hbar(\vec{r} \times \vec{\nabla}),$$

and $\vec{\mathbf{L}}^2$ are Hermitian.

13 (i) Write the operators $\vec{\mathbf{L}}^2$ and L_z in spherical polar coordinates and show that they have the same eigenfunctions.
(ii) What are their eigenvalues?
(iii) Write the L_x and L_y operators in spherical polar coordinates.

14 For a Sturm–Liouville operator:

$$£ = \frac{d}{dx}\left[p(x)\frac{d}{dx}\right] + q(x),$$

let $u(x)$ be a nontrivial solution satisfying $\pounds u = 0$ with the boundary condition at $x = a$, and let $v(x)$ be another nontrivial solution satisfying $\pounds v = 0$ with the boundary condition at $x = b$. Show that the Wronskian is given as

$$W[u, v] = \begin{vmatrix} u & v \\ u' & v' \end{vmatrix} = uv' - vu' = \frac{A(\text{constant})}{p(x)}.$$

15 For the inner product defined as

$$(\Psi_1, \Psi_2) = \int \Psi_1^*(x)\Psi_2(x)dx,$$

prove the following properties, where α is a complex number:

$$\begin{aligned} (\Psi_1, \alpha\Psi_2) &= \alpha(\Psi_1, \Psi_2), \\ (\alpha\Psi_1, \Psi_2) &= \alpha^*(\Psi_1, \Psi_2), \\ (\Psi_1, \Psi_2)^* &= (\Psi_2, \Psi_1), \\ (\Psi_1 + \Psi_2, \Psi_3) &= (\Psi_1, \Psi_3) + (\Psi_2, \Psi_3). \end{aligned}$$

16 (i) Prove the triangle inequality:

$$|\Psi_1 + \Psi_2| \leq |\Psi_1| + |\Psi_2|.$$

(ii) Prove the Schwartz inequality:

$$|\Psi_1||\Psi_2| \geq |(\Psi_1, \Psi_2)|.$$

17 Show that the differential equation

$$y'' + p_1(x)y' + [p_2(x) + \lambda r(x)]y(x) = 0$$

can be put into self-adjoint form as

$$\frac{d}{dx}\left[e^{[\int^x p_1(x)dx]}\frac{dy(x)}{dx}\right] + p_2(x)e^{[\int^x p_1(x)dx]}y(x) + \lambda r(x)e^{[\int^x p_1(x)dx]}y(x) = 0.$$

8

Factorization Method

Factorization method is an elegant way to solve Sturm–Liouville systems. It basically allows us to replace a Sturm–Liouville equation, a second-order linear differential equation, with a pair of first-order differential equations. For a large class of problems the method immediately yields the eigenvalues and allows us to write the ladder operators for the problem. These operators are then used to construct the eigenfunctions from a base function. Once the base function is normalized, the manufactured eigenfunctions are also normalized and satisfy the same boundary conditions as the base function. We first introduce the method of factorization and its basic features in terms of five theorems. Next, we show how the eigenvalues and the eigenfunctions are obtained and introduce six basic types of factorization. In fact, factorization of a given second-order differential equation is reduced to identifying the type it belongs to. To demonstrate the usage of the method, we discuss the associated Legendre equation and the spherical harmonics in detail. We also discuss the radial part of the Schrödinger equation for the hydrogen-like atoms. The Gegenbauer polynomials, symmetric top, Bessel functions, and the harmonic oscillator problem are the other examples we discuss in terms of the factorization method. Further details and an extensive table of differential equations that can be solved by this technique is given by Infeld and Hull [3], where this method was introduced for the first time.

8.1 Another Form for the Sturm–Liouville Equation

The **Sturm–Liouville equation** is usually written in the **first canonical form** as

$$\boxed{\frac{d}{dx}\left[p(x)\frac{d\Psi(x)}{dx}\right] + q(x)\Psi(x) + \lambda w(x)\Psi(x) = 0, \quad x \in [\alpha, \beta],} \tag{8.1}$$

Mathematical Methods in Science and Engineering, Second Edition. Selçuk Ş. Bayın.

where $p(x)$ is different from zero in the open interval (α, β); however, it could have zeroes at the end points of the interval. We also impose the **boundary conditions**

$$\boxed{\Psi^* p \Phi' \mid_{x=\alpha} = \Psi^* p \Phi' \mid_{x=\beta},} \tag{8.2}$$

$$\boxed{\Psi'^* p \Phi \mid_{x=\alpha} = \Psi'^* p \Phi \mid_{x=\beta},} \tag{8.3}$$

where Φ and Ψ are any two solutions corresponding to the same or different eigenvalue. Solutions also satisfy the **orthogonality relation:**

$$\boxed{\int_\alpha^\beta dx w(x) \Psi_{\lambda_l}^*(x) \Psi_{\lambda_{l'}}(x) = 0, \quad \lambda_{l'} \neq \lambda_l.} \tag{8.4}$$

If $p(x)$ and $w(x)$ are never negative and $w(x)/p(x)$ exists everywhere in (α, β), using the transformations

$$y(z) = \Psi(x) \left[w(x) p(x) \right]^{1/4} \tag{8.5}$$

and

$$dz = dx \left[\frac{w(x)}{p(x)} \right]^{1/2}, \tag{8.6}$$

we can cast the Sturm–Liouville equation into another form, also known as the **second canonical form:**

$$\boxed{\frac{d^2 y_\lambda^m(z)}{dz^2} + \{\lambda + r(z, m)\} y_\lambda^m(z) = 0,} \tag{8.7}$$

where

$$r(z, m) = \frac{q}{w} + \frac{3}{16} \left[\frac{1}{w} \frac{dw}{dz} + \frac{1}{p} \frac{dp}{dz} \right]^2 - \frac{1}{4} \left[\frac{2}{pw} \frac{dp}{dz} \frac{dw}{dz} + \frac{1}{w} \frac{d^2 w}{dz^2} + \frac{1}{p} \frac{d^2 p}{dz^2} \right]. \tag{8.8}$$

Here, m and λ are two constant parameters that usually enter into our equations through the process of separation of variables. Their values are restricted by the boundary conditions and in most cases take discrete (real) values like

$$\lambda_0, \lambda_1, \lambda_2, \ldots, \lambda_l, \ldots \tag{8.9}$$

and

$$m = m_0, m_0 + 1, m_0 + 2, \ldots. \tag{8.10}$$

However, we could take $m_0 = 0$ without any loss of generality. The **orthogonality relation** is now given as

$$\boxed{\int_a^b dz y_{\lambda_{l'}}^{*m}(z) y_{\lambda_l}^m(z) = 0, \quad \lambda_{l'} \neq \lambda_l.} \tag{8.11}$$

8.2 Method of Factorization

We can write Eq. (8.7) in operator form:

$$\boxed{\pounds(z,m) y_{\lambda_l}^m(z) = -\lambda_l y_{\lambda_l}^m(z),} \tag{8.12}$$

where

$$\pounds(z,m) = \frac{d^2}{dz^2} + r(z,m). \tag{8.13}$$

We now define two **operators** $O_+(z,m)$ and $O_-(z,m)$ as

$$O_\pm(z,m) = \pm\frac{d}{dz} - k(z,m) \tag{8.14}$$

so that

$$\boxed{\pounds(z,m) = O_+(z,m)O_-(z,m).} \tag{8.15}$$

We say Eq. (8.7) is **factorized** if we could replace it by one of the following equations:

$$\boxed{O_+(z,m)O_-(z,m)y_{\lambda_l}^m(z) = [\lambda - \mu(m)]y_{\lambda_l}^m(z)} \tag{8.16}$$

or

$$\boxed{O_-(z,m+1)O_+(z,m+1)y_{\lambda_l}^m(z) = [\lambda - \mu(m+1)]y_{\lambda_l}^m(z).} \tag{8.17}$$

Substituting the definitions of $O_+(z,m)$ and $O_-(z,m)$ into Eqs. (8.16) and (8.17), we obtain two equations that $k(z,m)$ and $\mu(m)$ should satisfy simultaneously as

$$-\frac{dk(z,m)}{dz} + k^2(z,m) = -r(z,m) - \mu(m), \tag{8.18}$$

$$\frac{dk(z,m+1)}{dz} + k^2(z,m+1) = -r(z,m) - \mu(m+1). \tag{8.19}$$

8.3 Theory of Factorization and the Ladder Operators

We now summarize the **fundamental ideas** of the factorization method in terms of **five basic theorems**. The first theorem basically tells us how to generate the solutions with different m given $y^m_{\lambda_l}(z)$.

Theorem 8.1 If $y^m_{\lambda_l}(z)$ is a solution of Eq. (8.12) corresponding to the eigenvalues λ and m, then

$$O_+(z, m+1)y^m_{\lambda_l}(z) = y^{m+1}_{\lambda_l}(z), \tag{8.20}$$

$$O_-(z, m)y^m_{\lambda_l}(z) = y^{m-1}_{\lambda_l}(z) \tag{8.21}$$

are also solutions corresponding to the same λ but different m as indicated.

Proof: Multiply Eq. (8.17) by $O_+(m+1)$:

$$\begin{aligned} &O_+(z, m+1)[O_-(z, m+1)O_+(z, m+1)y^m_{\lambda_l}(z)] \\ &\quad = O_+(z, m+1)[\lambda - \mu(m+1)]y^m_{\lambda_l}(z). \end{aligned} \tag{8.22}$$

This can be written as

$$\begin{aligned} &O_+(z, m+1)O_-(z, m+1)[O_+(z, m+1)y^m_{\lambda_l}(z)] \\ &\quad = [\lambda - \mu(m+1)][O_+(z, m+1)y^m_{\lambda_l}(z)]. \end{aligned} \tag{8.23}$$

We now let $m \to m+1$ in Eq. (8.16) to write

$$O_+(z, m+1)O_-(z, m+1)y^{m+1}_{\lambda_l}(z) = [\lambda - \mu(m+1)]y^{m+1}_{\lambda_l}(z) \tag{8.24}$$

and compare this with Eq. (8.23) to get Eq. (8.20). Thus, the theorem is proven. Proof of Eq. (8.21) is accomplished by multiplying Eq. (8.16) with $O_-(z, m)$ and by comparing it with the equation obtained by letting $m \to m-1$ in Eq. (8.17).

This theorem says that if we know the solution $y^m_{\lambda_l}(z)$, we can use $O_+(z, m+1)$ to generate the solutions corresponding to the eigenvalues

$$(m+1), (m+2), (m+3), \dots . \tag{8.25}$$

Similarly, $O_-(z, m)$ can be used to generate the solutions with the eigenvalues

$$\dots, (m-3), (m-2), (m-1). \tag{8.26}$$

$O_\pm(z, m)$ are also called the **step-up/-down** or **ladder** operators.

Theorem 8.2 If $y_1(z)$ and $y_2(z)$ are two solutions satisfying the boundary condition

$$y_1^* y_2|_b = y_1^* y_2|_a, \tag{8.27}$$

then

$$\int_a^b dz y_1^*(z)[O_-(z,m)y_2(z)] = \int_a^b dz y_2(z)[O_+(z,m)y_1(z)]^*. \tag{8.28}$$

We say that O_- and O_+ are **Hermitian**, that is, $O_- = O_+^\dagger$ with respect to $y_1(z)$ and $y_2(z)$. Note that the boundary condition [Eq. (8.27)] needed for the factorization method is more restrictive than the boundary conditions [Eqs. (8.2) and (8.3)] used for the solutions of the Sturm–Liouville problem. Condition in Eq. (8.27) includes the periodic boundary conditions as well as the cases where the solutions vanish at the end points.

Proof: Proof can easily be accomplished by using the definition of the ladder operators and integration by parts:

$$\int_a^b dz y_1^*(z)[O_-(z,m)y_2(z)] = \int_a^b dz y_1^*(z)\left[\left(-\frac{d}{dz} - k(z,m)\right) y_2(z)\right] \tag{8.29}$$

$$= -\int_a^b dz y_1^*(z)\frac{dy_2(z)}{dz} - \int_a^b dz y_1^*(z)k(z,m)y_2(z) \tag{8.30}$$

$$= -y_1^* y_2|_a^b + \int_a^b dz y_2 \frac{dy_1^*}{dz} - \int_a^b dz y_1^* k(z,m)y_2. \tag{8.31}$$

Finally, using the boundary condition [Eq. (8.27)], we write this as

$$\int_a^b dz y_1^*(z)[O_-(z,m)y_2(z)] = \int_a^b dz y_2(z)\left[\left(\frac{d}{dz} - k(z,m)\right) y_1(z)\right]^* \tag{8.32}$$

$$= \int_a^b dz y_2(z)[O_+(z,m)y_1(z)]^*. \tag{8.33}$$

Theorem 8.3 If

$$\int_a^b dz\left[y_{\lambda_l}^m(z)\right]^2 \tag{8.34}$$

exists and if $\mu(m)$ is an increasing function of m ($m > 0$), then

$$\int_a^b dz\left[O_+(z,m+1)y_{\lambda_l}^m(z)\right]^2 \tag{8.35}$$

also exists. If $\mu(m)$ is a decreasing function of m ($m > 0$), then

$$\int_a^b dz\left[O_-(z,m)y_{\lambda_l}^m(z)\right]^2 \tag{8.36}$$

also exists. $O_+(z, m+1)y^m_{\lambda_l}(z)$ and $O_-(z, m)y^m_{\lambda_l}(z)$ also satisfy the same boundary condition as $y^m_{\lambda_l}(z)$.

Proof: We take $y_2 = y^m_{\lambda_l}(z)$ and $y_1 = y^{m-1}_{\lambda_l}(z)$ in Theorem 8.2 to write

$$\int_a^b dz y^{*m-1}_{\lambda_l}(z)[O_-(z, m)y^m_{\lambda_l}(z)] = \int_a^b dz y^m_{\lambda_l}(z)[O_+(z, m)y^{m-1}_{\lambda_l}(z)]^*. \quad (8.37)$$

Solution $O_-(z, m)y^m_{\lambda_l}(z)$ in Eq. (8.21) is equal to $y^{m-1}_{\lambda_l}(z)$ only up to a constant factor. Similarly, $O_+(z, m)y^{m-1}_{\lambda_l}(z)$ is only equal to $y^m_{\lambda_l}(z)$ up to another constant factor. Thus, we can write

$$\int_a^b dz y^m_{\lambda_l}(z)y^m_{\lambda_l}(z)^* = C(l, m)\int_a^b dz y^{*m-1}_{\lambda_l}(z)y^{m-1}_{\lambda_l}(z), \quad (8.38)$$

$$\int_a^b dz[y^m_{\lambda_l}(z)]^2 = C(l, m)\int_a^b dz[y^{m-1}_{\lambda_l}(z)]^2, \quad (8.39)$$

where $C(l, m)$ is a constant independent of z but dependent on l and m. We are interested in differential equations, the coefficients of which may have singularities only at the end points of our interval. Square integrability of a solution actually depends on the behavior of the solution near the end points. Thus, it is a boundary condition. Hence, for a given square integrable eigenfunction $y^m_{\lambda_l}(z)$, the manufactured eigenfunction $y^{m-1}_{\lambda_l}(z)$ is also square integrable as long as $C(l, m)$ is different from zero. Because we have used Theorem 8.2, $y^{m-1}_{\lambda_l}(z)$ also satisfies the same boundary condition as $y^m_{\lambda_l}(z)$. A parallel argument is given for $y^{m+1}_{\lambda_l}(z)$. In conclusion, if $y^m_{\lambda_l}(z)$ is a square integrable function satisfying the boundary condition [Eq. (8.27)], then all other eigenfunctions manufactured from it by the ladder operators $O_\pm(z, m)$ are square integrable and satisfy the same boundary condition. For a complete proof $C(l, m)$ must be studied separately for each factorization type. For our purposes, it is sufficient to say that $C(l, m)$ is different from zero for all physically meaningful cases.

Theorem 8.4 If $\mu(m)$ is an increasing function and $m > 0$, then there exists a maximum value for m, say $m_{\max} = l$, and λ is given as $\lambda = \mu(l+1)$. If $\mu(m)$ is a decreasing function and $m > 0$, then there exists a minimum value for m, say $m_{\min} = l'$, and λ is $\lambda = \mu(l')$.

Proof: Assume that we have some function $y^m_{\lambda_l}(z)$, where $m > 0$, which satisfies the boundary condition [Eq. (8.27)]. We can then write

$$\int_a^b dz[y^{m+1}_{\lambda_l}(z)]^2 = \int_a^b dz[O_+(z, m+1)y^m_{\lambda_l}(z)][O_+(z, m+1)y^m_{\lambda_l}(z)]^* \quad (8.40)$$

$$= \int_a^b dz y_{\lambda_l}^{*m}(z)[O_-(z, m+1)O_+(z, m+1)y_{\lambda_l}^m(z)] \quad (8.41)$$

$$= [\lambda - \mu(m+1)] \int_a^b dz[y_{\lambda_l}^m(z)]^2, \quad (8.42)$$

where we have first used Eq. (8.28) and then Eq. (8.17). Continuing this process k times we get

$$\int_a^b dz[y_{\lambda_l}^{m+k}(z)]^2 = [\lambda - \mu(m+k)] \cdots [\lambda - \mu(m+2)][\lambda - \mu(m+1)] \times \int_a^b dz[y_{\lambda_l}^m(z)]^2. \quad (8.43)$$

If $\mu(m)$ is an increasing function of m, eventually we are going to reach a value of m, say $m_{\max} = l$, that leads us to the contradiction

$$\int_a^b dz[y_{\lambda_l}^{l+1}(z)]^2 < 0, \quad (8.44)$$

unless $y_{\lambda_l}^{l+1}(z) = 0$, that is,

$$O_+(z, l+1)y_{\lambda_l}^l(z) = 0. \quad (8.45)$$

Since $\int_a^b dz[y_{\lambda_l}^l(z)]^2 \neq 0$, using Eq. (8.42) with $m = l$, we determine λ as

$$\lambda = \lambda_l = \mu(l+1). \quad (8.46)$$

Similarly, it could be shown that if $\mu(m)$ is a decreasing function of m, then there exists a minimum value of m, say $m_{\min} = l$, such that

$$O_-(z, l)y_{\lambda_l}^l(z) = 0. \quad (8.47)$$

λ in this case is determined as

$$\lambda = \lambda_l = \mu(l). \quad (8.48)$$

Cases for $m < 0$ are also shown in Figure 8.1.

We have mentioned that the square integrability of the solutions is itself a boundary condition, which is usually related to the symmetries of the problem. For example, in the case of the associated Legendre equation the end points of our interval correspond to the north and south poles of a sphere. For a spherically symmetric problem, location of the poles is arbitrary. Hence useful solutions should be finite everywhere on a sphere. In the Frobenius method this forces us to restrict λ to certain integer values (Chapter 1). In the factorization method we also have to restrict λ, this time through Eq. (8.42) to ensure the square integrability of the solutions for a given $\mu(m)$.

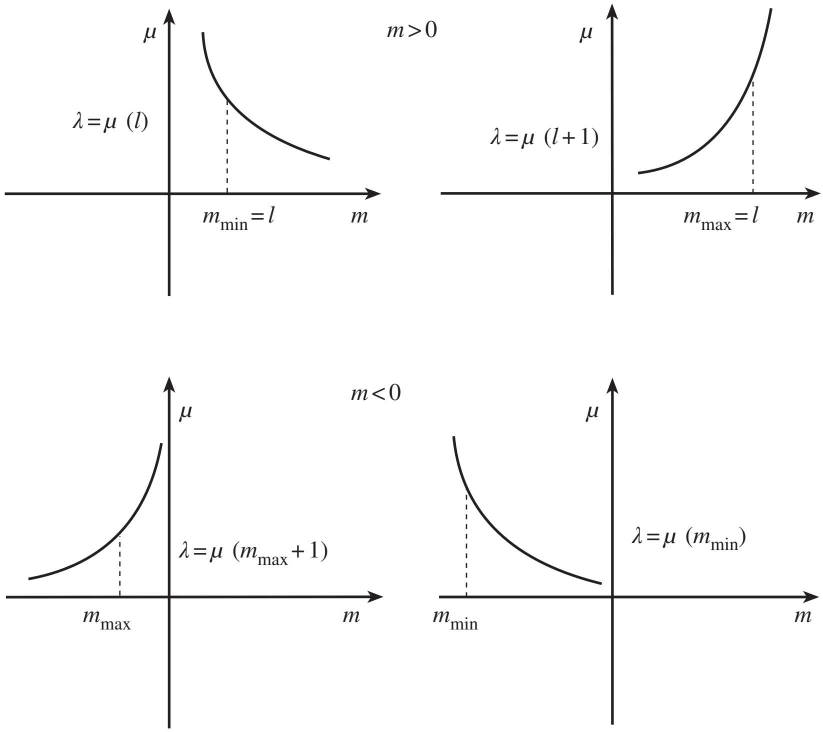

Figure 8.1 Different cases for $\mu(m)$.

Theorem 8.5 When Theorem 8.3 holds, we can arrange the ladder operators to preserve not just the square integrability but also the normalization of the eigenfunctions. When $\mu(m)$ is an increasing function of m, we can define new normalized ladder operators:

$$\pounds_{\pm}(z,l,m) = \left[\mu(l+1) - \mu(m)\right]^{-1/2} O_{\pm}(z,m), \tag{8.49}$$

which ensures us the normalization of the manufactured solutions.

When $\mu(m)$ is a decreasing function, normalized ladder operators are defined as

$$\pounds_{\pm}(z,l,m) = \left[\mu(l) - \mu(m)\right]^{-1/2} O_{\pm}(z,m). \tag{8.50}$$

Proof: Using Eq. (8.42) we write

$$\int_a^b \left[y_{\lambda_l}^{m+1}(z)\right]^2 dz = [\lambda - \mu(m+1)] \int_a^b \left[y_{\lambda_l}^{m}(z)\right]^2 dz, \tag{8.51}$$

$$\int_a^b \frac{\left[y_{\lambda_l}^{m+1}(z)\right]^2}{[\lambda - \mu(m+1)]} dz = \int_a^b \left[y_{\lambda_l}^{m}(z)\right]^2 dz. \tag{8.52}$$

Since

$$y_{\lambda_l}^{m+1}(z) = O_+(z, m+1) y_{\lambda_l}^{m}(z), \tag{8.53}$$

we write

$$\int_a^b \left[\frac{O_+(z, m+1)}{[\lambda - \mu(m+1)]^{1/2}} y_{\lambda_l}^{m}(z) \right]^2 dz = \int_a^b [y_{\lambda_l}^{m}(z)]^2 dz. \tag{8.54}$$

Define a new operator $£_+(z, l, m)$; then Eq. (8.54) becomes

$$\int_a^b \left[£_+(z, l, m+1) y_{\lambda_l}^{m}(z) \right]^2 dz = \int_a^b \left[y_{\lambda_l}^{m}(z) \right]^2 dz. \tag{8.55}$$

Thus, if $y_{\lambda_l}^{m}(z)$ is normalized, then the eigenfunction manufactured from $y_{\lambda_l}^{m}(z)$ by the operator $£_+$ is also normalized. Similarly, one could show that

$$\int_a^b \left[\frac{O_-(z, l, m)}{[\lambda - \mu(m)]^{1/2}} y_{\lambda_l}^{m}(z) \right]^2 dz = \int_a^b [£_-(z, l, m) y_{\lambda_l}^{m}(z)]^2 dz \tag{8.56}$$

$$= \int_a^b [y_{\lambda_l}^{m-1}(z)]^2 dz = \int_a^b [y_{\lambda_l}^{m}(z)]^2 dz. \tag{8.57}$$

In conclusion, once $y_{\lambda_l}^{m}(z)$ is normalized, the manufactured eigenfunctions

$$y_{\lambda_l}^{m+1}(z) = £_+(z, l, m+1) y_{\lambda_l}^{m}(z), \tag{8.58}$$

$$y_{\lambda_l}^{m-1}(z) = £_-(z, l, m) y_{\lambda_l}^{m}(z) \tag{8.59}$$

are also normalized. Depending on the functional forms of $\mu(m)$, $£_\pm(z, l, m)$ are given in Eqs. (8.49) and (8.50).

8.4 Solutions via the Factorization Method

We can now manufacture the eigenvalues and the eigenfunctions of an equation once it is factored, that is, once the $k(z, m)$ and the $\mu(m)$ functions corresponding to a given $r(z, m)$ are known. For $m > 0$, depending on whether $\mu(m)$ is an increasing or a decreasing function, there are two cases.

8.4.1 Case I ($m > 0$ and $\mu(m)$ is an increasing function)

In this case, from Theorem 8.4 there is a maximum value for m,

$$m = 0, 1, 2, \ldots, l, \tag{8.60}$$

and the eigenvalues λ_l are given as

$$\lambda = \lambda_l = \mu(l+1). \tag{8.61}$$

Since there is no eigenstate with $m > l$, we can write

$$O_+(z, l+1)y_l^l(z) = 0. \tag{8.62}$$

Thus, we obtain the differential equation

$$\left\{ \frac{d}{dz} - k(z, l+1) \right\} y_l^l(z) = 0. \tag{8.63}$$

Note that we have written $y_{\lambda_l}^l(z) = y_l^l(z)$. Integrating Eq. (8.63) we get

$$\frac{dy_l^l}{y_l^l} = k(z, l+1)dz, \tag{8.64}$$

$$\ln y_l^l(z) = \int^z k(z, l+1)dz, \tag{8.65}$$

or

$$y_l^l(z) = C \exp\left\{ \int^z k(z, l+1)dz \right\}. \tag{8.66}$$

Here, C is a constant to be determined from the normalization condition $\int_a^b dz[y_l^l(z)]^2 = 1$. For a given l, once $y_l^{m=l}(z)$ is found, all the other normalized eigenfunctions with $m = l, l-1, l-2, \ldots, 2, 1, 0$, can be constructed by repeated applications of the step-down operator $£_-(z, l, m)$ as

$$y_l^{m-1}(z) = [\mu(l+1) - \mu(m)]^{-1/2} O_-(z, m) y_l^m(z) \tag{8.67}$$

$$= £_-(z, l, m) y_l^m(z). \tag{8.68}$$

8.4.2 Case II ($m > 0$ and $\mu(m)$ is a decreasing function)

In this case, from Theorem 8.4 there is a minimum value for m, where

$$m = l, l+1, l+2, \ldots. \tag{8.69}$$

For this case, we can write

$$O_-(z, l)y_l^l(z) = 0, \tag{8.70}$$

$$\left\{ -\frac{d}{dz} - k(z, l) \right\} y_l^l(z) = 0. \tag{8.71}$$

Thus,

$$y_l^{m=l}(z) = C \exp\left\{ -\int^z k(z, l)dz \right\}, \tag{8.72}$$

where C is determined from the normalization condition $\int_a^b dz[y_l^l(z)]^2 = 1$. Now all the other normalized eigenfunctions for $m = l, l+1, l+2, \ldots$ are obtained from $y_l^l(z)$ by repeated applications of the formula

$$y_l^{m+1}(z) = [\mu(l) - \mu(m+1)]^{-1/2} O_+(z, m+1) y_l^m(z) \tag{8.73}$$

$$= £_+(z, l, m) y_l^m(z). \tag{8.74}$$

Cases with $m < 0$ are handled similarly. In Section 8.6, we see how such a case is treated with spherical harmonics.

8.5 Technique and the Categories of Factorization

In Section 8.2, we saw that in order to accomplish factorization we need to determine the two functions $k(z, m)$ and $\mu(m)$, which satisfy the following two equations:

$$\frac{dk(z, m+1)}{dz} + k^2(z, m+1) = -r(z, m) - \mu(m+1), \tag{8.75}$$

$$-\frac{dk(z, m)}{dz} + k^2(z, m) = -r(z, m) - \mu(m). \tag{8.76}$$

Here, $r(z, m)$ is known from the equation for which the factorization is sought, that is, from

$$\left[\frac{d^2}{dz^2} + r(z, m)\right] y^m_{\lambda_l}(z) = -\lambda_l y^m_{\lambda_l}(z). \tag{8.77}$$

However, following Infeld and Hull [3] we subtract Eq. (8.76) from Eq. (8.75) to obtain the difference equation:

$$-k^2(z, m) + k^2(z, m+1) + \frac{dk(z, m)}{dz} + \frac{dk(z, m+1)}{dz} = \mu(m) - \mu(m+1). \tag{8.78}$$

This is the necessary equation that $k(z, m)$ and $\mu(m)$ should satisfy. This is also a sufficient condition, because $k(z, m)$ and $\mu(m)$ satisfying this equation give a unique $r(z, m)$ from Eq. (8.75) or (8.76). We now categorize all possible forms of $k(z, m)$ and $\mu(m)$ that satisfy Eq. (8.78).

8.5.1 Possible Forms for $k(z, m)$

8.5.1.1 Positive powers of m

We first consider $k(z, m)$ with the m dependence given as

$$k(z, m) = k_0(z) + mk_1(z). \tag{8.79}$$

To find $\mu(m)$ we write Eq. (8.78) for successive values of m as (we suppress the z dependence of $k(z, m)$)

$$\begin{aligned}
k^2(m) - k^2(m-1) + k'(m) + k'(m-1) &= \mu(m-1) - \mu(m),\\
k^2(m-1) - k^2(m-2) + k'(m-1) + k'(m-2) &= \mu(m-2) - \mu(m-1),\\
k^2(m-2) - k^2(m-3) + k'(m-2) + k'(m-3) &= \mu(m-3) - \mu(m-2),\\
&\vdots\\
k^2(1) - k^2(0) + k'(1) + k'(0) &= \mu(0) - \mu(1).
\end{aligned}$$

Addition of these equations gives

$$k^2(m) - k^2(0) + 2mk_0' + k_1' \left[\sum_{m'=1}^{m} m' + \sum_{m'=0}^{m-1} m' \right] = \mu(0) - \mu(m), \tag{8.80}$$

where we have used $k'(z,m) = k_0'(z) + mk_1'(z)$. Also using

$$\sum_{m'=1}^{m} m' + \sum_{m'=0}^{m-1} m' = \frac{m(m+1)}{2} + \frac{m(m-1)}{2} \tag{8.81}$$

$$= m^2, \tag{8.82}$$

and since from Eq. (8.79) we can write

$$k^2(m) - k^2(0) = [k_0 + mk_1]^2 - k_0^2, \tag{8.83}$$

we finally obtain

$$\mu(m) - \mu(0) = -m^2(k_1^2 + k_1') - 2m(k_0 k_1 + k_0'). \tag{8.84}$$

Since $\mu(m)$ is only a function of m, this could only be satisfied if the coefficients of m are constants:

$$k_1^2 + k_1' = \text{const.} = -a^2, \tag{8.85}$$

$$k_0 k_1 + k_0' = \text{const.} = -a^2 c \quad \text{if } a \neq 0, \tag{8.86}$$

$$k_0 k_1 + k_0' = \text{const.} = b \quad \text{if } a = 0. \tag{8.87}$$

This determines $\mu(m)$ as

$$\mu(m) = \mu(0) + a^2(m^2 + 2mc) \quad \text{for } a \neq 0, \tag{8.88}$$

$$\mu(m) = \mu(0) - 2mb \quad \text{for } a = 0. \tag{8.89}$$

In these equations, we could take $\mu(0) = 0$ without any loss of generality.

Using these results, we now obtain the following categories:

(A) For $a \neq 0$, Eq. (8.85) gives

$$\frac{dk_1}{k_1^2 + a^2} = -dz, \tag{8.90}$$

$$k_1 = a \cot a(z + p). \tag{8.91}$$

Substituting this into Eq. (8.86) and integrating gives

$$k_0(z) = ca \cot a(z+p) + \frac{d}{\sin a(z+p)}, \tag{8.92}$$

where p and d are integration constants.

With these k_0 and k_1 functions in Eq. (8.79) and the $\mu(m)$ given in Eq. (8.88), we obtain $r(z,m)$ from Eq. (8.75) or (8.76) as

$$r(z,m) = -\frac{a^2(m+c)(m+c+1) + d^2 + 2ad(m+c+\frac{1}{2})\cos a(z+p)}{\sin^2 a(z+p)}. \tag{8.93}$$

We now obtain our first factorization type as

$$k(z,m) = (m+c)a\cot a(z+p) + \frac{d}{\sin a(z+p)}, \tag{8.94}$$

$$\mu(m) = a^2(m+c)^2, \text{we set } \mu(0) = a^2c^2. \tag{8.95}$$

(B)

$$k_1 = \text{const.} = ia, \tag{8.96}$$

$$k_0 = ica + de^{-iaz}. \tag{8.97}$$

For this type, after writing a instead of ia and adding $-a^2c^2$ to $\mu(m)$, we get

$$r(z,m) = -d^2e^{2az} + 2ad\left(m + c + \frac{1}{2}\right)e^{az}, \tag{8.98}$$

$$k(z,m) = de^{az} - m - c, \tag{8.99}$$

$$\mu(m) = -a^2(m+c)^2. \tag{8.100}$$

(C)

$$k_1 = \frac{1}{z}, \quad a = 0, \tag{8.101}$$

$$k_0 = \frac{b}{2}z + \frac{d}{z}. \tag{8.102}$$

After writing c for d and adding $b/2$ to $\mu(m)$ we obtain

$$r(z,m) = -\frac{(m+c)(m+c+1)}{z^2} - \frac{b^2z^2}{4} + b(m-c), \tag{8.103}$$

$$k(z,m) = (m+c)/z + bz/2, \tag{8.104}$$

$$\mu(m) = -2bm + b/2. \tag{8.105}$$

(D)

$$k_1 = 0, \quad a = 0, \tag{8.106}$$

$$k_0 = bz + d. \tag{8.107}$$

In this case, the operators O_+ and O_- are independent of m. The functions $r(z,m)$, $k(z,m)$, and $\mu(m)$ are now given as

$$r(z,m) = -(bz+d)^2 + b(2m+1), \tag{8.108}$$

$$k(z,m) = bz + d, \tag{8.109}$$

$$\mu(m) = -2bm. \tag{8.110}$$

We can also try higher positive powers of m in $k(z,m)$ as

$$k(z,m) = k_0(z) + mk_1(z) + m^2k_2(z) + \cdots. \tag{8.111}$$

However, no new categories result (see Problems 5 and 6). Also note that the types B, C, and D can be viewed as the limiting forms of type A.

8.5.1.2 Negative powers of *m*

We now try negative powers of m as

$$k(z,m) = \frac{k_{-1}(z)}{m} + k_0(z) + k_1(z)m. \tag{8.112}$$

We again write Eq. (8.78) for successive values of m as

$$\begin{gathered}
k^2(m) - k^2(m-1) + k'(m) + k'(m-1) = \mu(m-1) - \mu(m),\\
k^2(m-1) - k^2(m-2) + k'(m-1) + k'(m-2) = \mu(m-2) - \mu(m-1),\\
k^2(m-2) - k^2(m-3) + k'(m-2) + k'(m-3) = \mu(m-3) - \mu(m-2),\\
\vdots\\
k^2(2) - k^2(1) + k'(2) + k'(1) = \mu(1) - \mu(2),
\end{gathered}$$

where we have suppressed the z dependence of $k(z,m)$. Adding these equations and using

$$k'(z,m) = \frac{k'_{-1}(z)}{m} + k'_0(z) + k'_1(z)m, \tag{8.113}$$

give

$$\begin{aligned}
&k^2(m) - k^2(1) + k'_{-1}\left[\sum_{m'=2}^{m}\frac{1}{m'} + \sum_{m'=1}^{m-1}\frac{1}{m'}\right] + k'_0[2m-2]\\
&\quad + k'_1\left[\sum_{m'=2}^{m} m' + \sum_{m'=1}^{m-1} m'\right] = \mu(1) - \mu(m).
\end{aligned} \tag{8.114}$$

Since the series

$$\left[\sum_{m'=2}^{m}\frac{1}{m'} + \sum_{m'=1}^{m-1}\frac{1}{m'}\right], \tag{8.115}$$

which is the coefficient of k'_{-1}, contains a logarithmic dependence on m, we set k_{-1} to a constant:

$$k_{-1} = q \neq 0. \tag{8.116}$$

Also using

$$\sum_{m'=2}^{m} m' + \sum_{m'=1}^{m-1} m' = m^2 - 1 \tag{8.117}$$

and Eq. (8.112) we write

$$k^2(m) - k^2(1) = \frac{k_{-1}^2}{m^2} + k_1^2 m^2 + \frac{2k_{-1}k_0}{m} + 2k_0k_1 m - k_{-1}^2 - k_1^2 - 2k_{-1}k_0 - 2k_0k_1. \tag{8.118}$$

Now Eq. (8.114) becomes

$$\frac{k_{-1}^2}{m^2} + k_1^2 m^2 + \frac{2k_{-1}k_0}{m} + 2k_0 k_1 m - k_{-1}^2 - k_1^2 - 2k_{-1}k_0 - 2k_0 k_1 \\ + k_0'[2m-2] + k_1'[m^2-1] = \mu(1) - \mu(m). \tag{8.119}$$

After some simplification and setting $\mu(1) = 0$, which we can do without any loss of generality, Eq. (8.119) gives

$$\frac{k_{-1}^2}{m^2} + \frac{2k_0 k_{-1}}{m} + m(2k_0k_1 + 2k_0') + m^2(k_1^2 + k_1') \\ + \left[-(k_1^2 + k_1') - k_{-1}^2 - 2k_0' - 2(k_1 + k_{-1})k_0\right] = -\mu(m). \tag{8.120}$$

We now have two new categories corresponding to the cases $a \neq 0$ and $a = 0$ with

$$k_{-1} = q, \tag{8.121}$$

$$k_0 = 0, \tag{8.122}$$

$$k_1^2 + k_1' = -a^2. \tag{8.123}$$

(E)

$$k_1 = a \cot a(z+p),\ k_0 = 0,\ k_{-1} = q \quad \text{for } a \neq 0. \tag{8.124}$$

$r(z,m)$, $k(z,m)$, and $\mu(m)$ are now given as

$$r(z,m) = -\frac{m(m+1)a^2}{\sin^2 a(z+p)} - 2aq \cot a(z+p), \tag{8.125}$$

$$k(z,m) = ma \cot a(z+p) + q/m, \tag{8.126}$$

$$\mu(m) = a^2 m^2 - q^2/m^2. \tag{8.127}$$

(F) Our final category is obtained for $a = 0$ as

$$k_1 = 1/z,\ k_0 = 0,\ k_{-1} = q, \tag{8.128}$$

where

$$r(z,m) = -2q/z - m(m+1)/z^2, \tag{8.129}$$

$$k(z,m) = m/z + q/m, \tag{8.130}$$

$$\mu(m) = -q^2/m^2. \tag{8.131}$$

Further generalization of these cases by considering higher negative powers of m leads to no new categories as long as we have a finite number of terms with negative powers in $k(z,m)$. Type F can also be viewed as the limiting form of type E with $a \to 0$. Entries in the table of factorizations given by Infeld and Hull [3] can be used, with our notation with the replacements $x \to z$ and $L(m) = \mu(m)$.

8.6 Associated Legendre Equation (Type A)

The **Legendre equation** is given as

$$\boxed{\frac{d^2\Theta(\theta)}{d\theta^2} + \cot\theta \frac{d\Theta(\theta)}{d\theta} + \left[\lambda_l - \frac{m^2}{\sin^2\theta}\right]\Theta(\theta) = 0,} \tag{8.132}$$

where $\theta \in [0, \pi]$ and $m = 0, \pm 1, \pm 2, \ldots$. We can put this into the first canonical form by the substitutions $x = \cos\theta$ and $\Theta(\theta) = P(x)$ as

$$\left(1 - x^2\right) \frac{d^2P(x)}{dx^2} - 2x\frac{dP(x)}{dx} + \left[\lambda_l - \frac{m^2}{(1 - x^2)}\right]P(x) = 0, \tag{8.133}$$

$$\frac{d}{dx}\left[\left(1 - x^2\right) \frac{dP(x)}{dx}\right] + \left[\lambda_l - \frac{m^2}{(1 - x^2)}\right]P(x) = 0, \quad x \in [-1, 1]. \tag{8.134}$$

We now make the following substitutions:

$$w(x) = 1,\ p(x) = \left(1 - x^2\right),\ dz = dx/\left(1 - x^2\right)^{1/2},\ y(x) = P(x)(1 - x^2)^{1/4}, \tag{8.135}$$

which in terms of θ means:

$$w(x) = 1,\ p(x) = \sin^2\theta,\ dz = -d\theta,\ y(\theta) = P\big(\cos\theta\big)\ \sin^{1/2}\theta, \tag{8.136}$$

and thus leads us to the **second canonical** form:

$$\boxed{\frac{d^2y(\theta)}{d\theta^2} + \left[\left(\lambda_l + \frac{1}{4}\right) - \frac{\left(m^2 - \frac{1}{4}\right)}{\sin^2\theta}\right]y(\theta) = 0.} \tag{8.137}$$

If we call

$$\lambda = \left(\lambda_l + \frac{1}{4}\right) \tag{8.138}$$

and compare with

$$\frac{d^2y_\lambda^m(z)}{dz^2} + \{\lambda + r(z, m)\}y_\lambda^m(z) = 0, \tag{8.139}$$

we obtain

$$r(z, m) = \frac{\left(m^2 - \frac{1}{4}\right)}{\sin^2 z}. \tag{8.140}$$

This is exactly type A with the coefficients read from Eq. (8.93) as

$$a = 1,\ c = -1/2,\ d = 0,\ p = 0,\ z = \theta. \tag{8.141}$$

Thus, from Eqs. (8.94) and (8.95), we obtain the factorization of the associated Legendre equation as

$$k(z,m) = \left(m - \frac{1}{2}\right)\cot\theta, \tag{8.142}$$

$$\mu(m) = \left(m - \frac{1}{2}\right)^2. \tag{8.143}$$

For convenience, we have taken $\mu(0) = a^2c^2$ rather than zero in Eq. (8.95).

8.6.1 Determining the Eigenvalues, λ_l

For $m > 0$,

$$\mu(m) = \left(m - \frac{1}{2}\right)^2. \tag{8.144}$$

Thus, $\mu(m)$ is an increasing function of m and from Theorem 8.4, we know that there exists a maximum value for m, say $m_{\max} = l$. This determines λ as

$$\lambda = \mu(l+1) \tag{8.145}$$

$$= \left(l + \frac{1}{2}\right)^2. \tag{8.146}$$

On the other hand, for $m < 0$ we could write

$$\mu(m) = \left(|m| + \frac{1}{2}\right)^2. \tag{8.147}$$

Again from the conclusions of Theorem 8.4, there exists a minimum value, $m_{\min}$, thus determining λ as

$$\lambda = m_{\min} \tag{8.148}$$

$$= \left(|m_{\min}| + \frac{1}{2}\right)^2. \tag{8.149}$$

To find $m_{\min}$ we equate the two expressions [Eqs. (8.146) and (8.149)] for λ to obtain

$$\left(l + \frac{1}{2}\right)^2 = \left(|m_{\min}| + \frac{1}{2}\right)^2, \tag{8.150}$$

$$|m_{\min}| = l, \tag{8.151}$$

$$m_{\min} = -l. \tag{8.152}$$

Since m changes by integer amounts, we could write

$$m_{\min} = m_{\max} - \text{integer}, \tag{8.153}$$

$$-l = l - \text{integer}, \tag{8.154}$$

$$2l = \text{integer}. \tag{8.155}$$

This equation says that l could only take integer values $l = 0, 1, 2, \ldots$. We can now write the eigenvalues λ_l as

$$\lambda_l + \frac{1}{4} = \lambda \tag{8.156}$$

$$= \left(l + \frac{1}{2}\right)^2 \tag{8.157}$$

$$= l^2 + l + \frac{1}{4}, \tag{8.158}$$

$$\lambda_l = l(l+1). \tag{8.159}$$

Note that Eq. (8.155) also has the solution $l = \text{integer}/2$. We will elaborate this case in Chapter 10 in Problem 11.

8.6.2 Construction of the Eigenfunctions

Since $m_{\max} = l$, there are no states with $m > l$. Thus,

$$O_+(z, l+1)y^l_{\lambda_l}(z) = 0, \tag{8.160}$$

$$\left\{\frac{d}{dz} - k(z, l+1)\right\} y^l_{\lambda_l}(z) = 0. \tag{8.161}$$

This gives

$$\ln y^l_{\lambda_l}(z) - \ln N = \int^z k(z', l+1)dz' \tag{8.162}$$

$$= \left(l + \frac{1}{2}\right) \int \cot\theta d\theta \tag{8.163}$$

$$= \left(l + \frac{1}{2}\right) \ln(\sin\theta) \tag{8.164}$$

$$= \ln\,(\sin\theta)^{\left(l+\frac{1}{2}\right)}. \tag{8.165}$$

Hence, the state with $m_{\max} = l$ is determined as

$$y^l_{\lambda_l}(\theta) = N(\sin\theta)^{\left(l+\frac{1}{2}\right)}. \tag{8.166}$$

N is a normalization constant to be determined from

$$\int_0^\pi [y^l_{\lambda_l}(\theta)]^2 d\theta = 1, \tag{8.167}$$

$$N^2 \int_0^\pi (\sin\theta)^{2l+1} d\theta = 1, \tag{8.168}$$

which gives

$$N = (-1)^l \left[\frac{(2l+1)!}{2^{2l+1} l!^2}\right]^{1/2}. \tag{8.169}$$

The factor of $(-1)^l$, which is called the **Condon–Shortley phase**, is introduced for convenience. Thus, the normalized eigenfunction corresponding to $m_{\max} = l$ is

$$y^l_{\lambda_l}(\theta) = (-1)^l \left[\frac{(2l+1)!}{2^{2l+1} l!^2}\right]^{1/2} (\sin\theta)^{\left(l+\frac{1}{2}\right)}. \tag{8.170}$$

Using this eigenfunction (eigenstate), we can construct the remaining eigenstates by using the normalized ladder operators [Eqs. (8.49) and (8.50)]. For moving down the ladder we use

$$£_-(\theta, m) = \frac{O_-(\theta, m)}{\sqrt{\mu(l+1) - \mu(m)}} \tag{8.171}$$

$$= \frac{1}{\sqrt{\left(l+\frac{1}{2}\right)^2 - \left(m-\frac{1}{2}\right)^2}} \left[-\frac{d}{d\theta} - \left(m - \frac{1}{2}\right)\cot\theta\right] \tag{8.172}$$

$$= \frac{1}{\sqrt{(l+m)(l-m+1)}} \left[-\frac{d}{d\theta} - \left(m - \frac{1}{2}\right)\cot\theta\right] \tag{8.173}$$

and for moving up the ladder

$$£_+(\theta, m+1) = \frac{O_+(\theta, m+1)}{\sqrt{\mu(l+1) - \mu(m+1)}} \tag{8.174}$$

$$= \frac{1}{\sqrt{\left(l+\frac{1}{2}\right)^2 - \left(m+\frac{1}{2}\right)^2}} \left[\frac{d}{d\theta} - \left(m + \frac{1}{2}\right)\cot\theta\right] \tag{8.175}$$

$$= \frac{1}{\sqrt{(l-m)(l+m+1)}} \left[\frac{d}{d\theta} - \left(m + \frac{1}{2}\right)\cot\theta\right]. \tag{8.176}$$

Needless to say, the eigenfunctions generated by the operators $£_\pm$ are also normalized (Theorem 8.5).

Now the **normalized** associated Legendre polynomials are related to $y^l_{\lambda_l}(\theta)$ by

$$P^m_l(\cos\theta) = \frac{y^m_{\lambda_l}(\theta)}{\sqrt{\sin\theta}}. \tag{8.177}$$

8.6.3 Ladder Operators for *m*

Spherical harmonics are defined as

$$Y^m_l(\theta, \phi) = P^m_l(\cos\theta)\frac{e^{im\phi}}{\sqrt{2\pi}}. \tag{8.178}$$

Using Eq. (8.177), we write

$$Y_l^m(\theta,\phi) = \frac{y_{\lambda_l}^m(\theta)}{\sqrt{\sin\theta}}\frac{e^{im\phi}}{\sqrt{2\pi}}. \tag{8.179}$$

Using

$$y_{\lambda_l}^{m-1}(\theta) = \pounds\_(\theta,m)y_{\lambda_l}^m(\theta) \tag{8.180}$$

and Eq. (8.171) we could also write

$$\sqrt{\sin\theta}P_l^{m-1}(\theta)\frac{e^{i(m-1)\phi}}{\sqrt{2\pi}} = e^{-i\phi}\pounds\_(\theta,m)\left[\sqrt{\sin\theta}P_l^m(\theta)\frac{e^{im\phi}}{\sqrt{2\pi}}\right] \tag{8.181}$$

$$= \frac{e^{-i\phi}\left[-\frac{d}{d\theta}-\left(m-\frac{1}{2}\right)\cot\theta\right]\left[\sqrt{\sin\theta}P_l^m(\theta)\frac{e^{im\phi}}{\sqrt{2\pi}}\right]}{\sqrt{(l+m)(l-m+1)}} \tag{8.182}$$

$$= \frac{e^{-i\phi}\frac{e^{im\phi}}{\sqrt{2\pi}}\left[-\frac{d\sqrt{\sin\theta}P_l^m(\theta)}{d\theta}-\left(m-\frac{1}{2}\right)\cot\theta\sqrt{\sin\theta}P_l^m(\theta)\right]}{\sqrt{(l+m)(l-m+1)}} \tag{8.183}$$

$$= \frac{\sqrt{\sin\theta}e^{-i\phi}\frac{e^{im\phi}}{\sqrt{2\pi}}\left[-\frac{d}{d\theta}-m\cot\theta\right]P_l^m(\theta)}{\sqrt{(l+m)(l-m+1)}} \tag{8.184}$$

$$= \frac{\sqrt{\sin\theta}e^{-i\phi}}{\sqrt{(l+m)(l-m+1)}}\left[-\frac{d}{d\theta}-m\cot\theta\right]\left(P_l^m(\theta)\frac{e^{im\phi}}{\sqrt{2\pi}}\right). \tag{8.185}$$

Cancelling $\sqrt{\sin\theta}$ on both sides and noting that

$$\frac{\partial Y_l^m(\theta,\phi)}{\partial\phi} = imP_l^m(\theta)\frac{e^{im\phi}}{\sqrt{2\pi}}, \tag{8.186}$$

and using Eq. (8.179), we finally write

$$\boxed{Y_l^{m-1}(\theta,\phi) = \frac{e^{-i\phi}}{\sqrt{(l+m)(l-m+1)}}\left[-\frac{\partial}{\partial\theta}+i\cot\theta\frac{\partial}{\partial\phi}\right]Y_l^m(\theta,\phi).} \tag{8.187}$$

Similarly,

$$\boxed{Y_l^{m+1}(\theta,\phi) = \frac{e^{i\phi}}{\sqrt{(l-m)(l+m+1)}}\left[\frac{\partial}{\partial\theta}+i\cot\theta\frac{\partial}{\partial\phi}\right]Y_l^m(\theta,\phi).} \tag{8.188}$$

We now define the ladder operators L_+ and L_- for the m index of the spherical harmonics as

$$\boxed{L_- = e^{-i\phi}\left[-\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\phi}\right],} \tag{8.189}$$

$$\boxed{L_+ = e^{i\phi}\left[+\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\phi}\right],} \tag{8.190}$$

thus

$$Y_l^{m-1}(\theta,\phi) = \frac{L_- Y_l^m(\theta,\phi)}{\sqrt{(l+m)(l-m+1)}}, \tag{8.191}$$

$$Y_l^{m+1}(\theta,\phi) = \frac{L_+ Y_l^m(\theta,\phi)}{\sqrt{(l-m)(l+m+1)}}. \tag{8.192}$$

We can now construct the spherical harmonics from the eigenstate:

$$Y_l^0(\theta,\phi) = \sqrt{\frac{2l+1}{2}}P_l(\cos\theta)\frac{1}{\sqrt{2\pi}}, \tag{8.193}$$

by successive operations of the ladder operators as

$$\boxed{Y_l^m(\theta,\phi) = \sqrt{\frac{2l+1}{2}\frac{(l-m)!}{(l+1)!}\frac{1}{2\pi}}[L_+]^m P_l(\cos\theta),} \tag{8.194}$$

$$\boxed{Y_l^{-m}(\theta,\phi) = \sqrt{\frac{2l+1}{2}\frac{(l-m)!}{(l+1)!}\frac{1}{2\pi}}[L_-]^m P_l(\cos\theta).} \tag{8.195}$$

Note that $P_l^{m=0}(\cos\theta) = P_l(\cos\theta)$ is the Legendre polynomial and $[L_-]^* = -[L_+]$, and

$$Y_l^{*m}(\theta,\phi) = (-1)^m Y_l^{-m}(\theta,\phi). \tag{8.196}$$

8.6.4 Interpretation of the L_+ and L_- Operators

In quantum mechanics, the angular momentum operator (we set $\hbar = 1$) is given as $\vec{L} = -i\vec{r}\times\vec{\nabla}$. We write this in spherical polar coordinates:

$$\vec{L} = -i\begin{pmatrix} \widehat{\mathbf{e}}_r & \widehat{\mathbf{e}}_\theta & \widehat{\mathbf{e}}_\phi \\ r & 0 & 0 \\ \frac{\partial}{\partial r} & \frac{1}{r}\frac{\partial}{\partial\theta} & \frac{1}{r\sin\theta}\frac{\partial}{\partial\phi} \end{pmatrix} \tag{8.197}$$

$$= -i\left[-\widehat{\mathbf{e}}_\theta\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\phi}\right) + \widehat{\mathbf{e}}_\phi\left(\frac{\partial}{\partial\theta}\right)\right]. \tag{8.198}$$

The basis vectors, $\widehat{\mathbf{e}}_\theta$ and $\widehat{\mathbf{e}}_\phi$, in spherical polar coordinates are written in terms of the basis vectors $(\widehat{\mathbf{e}}_x, \widehat{\mathbf{e}}_y, \widehat{\mathbf{e}}_z)$ of the Cartesian coordinates as

$$\widehat{\mathbf{e}}_\theta = (\cos\theta\cos\phi)\widehat{\mathbf{e}}_x + (\cos\theta\sin\phi)\widehat{\mathbf{e}}_y - (\sin\theta)\widehat{\mathbf{e}}_z, \tag{8.199}$$

$$\widehat{\mathbf{e}}_\phi = -(\sin\theta)\widehat{\mathbf{e}}_x + (\cos\phi)\widehat{\mathbf{e}}_y. \tag{8.200}$$

Thus, the angular momentum operator in Cartesian coordinates becomes

$$\vec{L} = L_x\widehat{\mathbf{e}}_x + L_y\widehat{\mathbf{e}}_y + L_z\widehat{\mathbf{e}}_z \tag{8.201}$$

$$= \widehat{\mathbf{e}}_x\left(i\cot\theta\cos\phi\frac{\partial}{\partial\phi} + i\sin\phi\frac{\partial}{\partial\theta}\right) + \widehat{\mathbf{e}}_y\left(i\cot\theta\sin\phi\frac{\partial}{\partial\phi} - i\cos\phi\frac{\partial}{\partial\theta}\right) \tag{8.202}$$

$$+ \widehat{\mathbf{e}}_z\left(-i\frac{\partial}{\partial\phi}\right).$$

It is now clearly seen that

$$L_+ = L_x + iL_y, \tag{8.203}$$

$$L_- = L_x - iL_y, \tag{8.204}$$

and

$$L_z = -i\frac{\partial}{\partial\phi}. \tag{8.205}$$

Also note that

$$\vec{L}^2 = L_x^2 + L_y^2 + L_z^2 \tag{8.206}$$

$$= \frac{1}{2}(L_+L_- + L_-L_+) + L_z^2 \tag{8.207}$$

$$= -\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left[\sin\theta\frac{\partial}{\partial\theta}\right] + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]. \tag{8.208}$$

From the definition of L_z, it is seen that

$$L_zY_l^m = mY_l^m, \quad m = -l, \dots, 0, \dots, l. \tag{8.209}$$

Also using the L_+ and L_- operators defined in Eqs. (8.189) and (8.190) and Eqs. (8.191) and (8.192), we can write

$$\vec{L}^2 Y_l^m = \frac{1}{2}(L_+L_- + L_-L_+)Y_l^m + L_z^2Y_l^m \tag{8.210}$$

$$= l(l+1)Y_l^m, \quad l = 0, 1, 2, 3 \dots. \tag{8.211}$$

Thus, Y_l^m are the simultaneous eigenfunctions of the $\vec{L}^2$ and the L_z operators. To understand the physical meaning of the angular momentum operators, consider a scalar function, $\Psi(r, \theta, \phi)$, which may represent some physical system or could be a wave function. We now operate on this function with an operator R, the effect of which is to rotate a physical system by α counterclockwise about the z-axis. $R\Psi(r, \theta, \phi)$ is now a new function representing the physical system after it has been rotated. This is equivalent to replacing ϕ by $\phi + \alpha$ in $\Psi(r, \theta, \phi)$. After making a Taylor series expansion about $\alpha = 0$, we get

$$R\Psi(r, \theta, \phi) = \Psi(r, \theta, \phi') = \Psi(r, \theta, \phi + \alpha) \tag{8.212}$$

$$= \Psi(r, \theta, \phi) + \left.\frac{\partial\Psi}{\partial\alpha}\right|_{\alpha=0} \alpha + \frac{1}{2!}\left.\frac{\partial^2\Psi}{\partial\alpha^2}\right|_{\alpha=0} \alpha^2 + \cdots + \frac{1}{n!}\left.\frac{\partial^n\Psi}{\partial\alpha^n}\right|_{\alpha=0} \alpha^n \dots . \tag{8.213}$$

In terms of the coordinate system (r, θ, ϕ), this corresponds to a rotation about the z-axis by $-\alpha$. Thus, with the replacement $d\alpha \to -d\phi$, we get

$$R\Psi(r, \theta, \phi)$$
$$= \Psi(r, \theta, \phi) - \left.\frac{\partial\Psi}{\partial\phi}\right|_{\alpha=0} \alpha + \frac{1}{2!}\left.\frac{\partial^2\Psi}{\partial\phi^2}\right|_{\alpha=0} \alpha^2 + \cdots + \frac{(-1)^n}{n!}\left.\frac{\partial^n\Psi}{\partial\phi^n}\right|_{\alpha=0} \alpha^n \dots \tag{8.214}$$

$$= \left[1 - \left.\frac{\partial}{\partial\phi}\right|_{\alpha=0} \alpha + \frac{1}{2!}\left.\frac{\partial^2}{\partial\phi^2}\right|_{\alpha=0} \alpha^2 + \cdots + \frac{(-1)^n}{n!}\left.\frac{\partial^n}{\partial\phi^n}\right|_{\alpha=0} \alpha^n \cdots\right] \Psi(r, \theta, \phi) \tag{8.215}$$

$$= \left[\exp\left(-\alpha\frac{\partial}{\partial\phi}\right)\right] \Psi(r, \theta, \phi) = [\exp(-i\alpha L_z)]\Psi(r, \theta, \phi). \tag{8.216}$$

For a rotation about an arbitrary axis along the unit vector $\hat{\mathbf{n}}$ this becomes

$$R\Psi(r, \theta, \phi) = [\exp(-i\alpha\overrightarrow{L} \cdot \hat{\mathbf{n}})]\Psi(r, \theta, \phi). \tag{8.217}$$

Thus, the angular momentum operator $\overrightarrow{L}$ is related to the rotation operator R by

$$\boxed{R = \exp(-i\alpha\overrightarrow{L} \cdot \hat{\mathbf{n}}).} \tag{8.218}$$

8.6.5 Ladder Operators for *l*

We now write $\lambda_l = l(l + 1)$ and $-m^2 = \lambda$ in Eq. (8.132) to obtain

$$\frac{d^2\Theta(\theta)}{d\theta^2} + \cot\theta\frac{d\Theta(\theta)}{d\theta} + \left[l(l+1) + \frac{\lambda}{\sin^2\theta}\right]\Theta(\theta) = 0. \tag{8.219}$$

We can put this equation into the **second canonical form** by the transformation

$$z = \ln\left(\tan\frac{\theta}{2}\right), \ \Theta(\theta) = V(z), \ z \in [-\infty, \infty], \tag{8.220}$$

as

$$\boxed{\frac{d^2V(z)}{dz^2} + \left[\lambda + \frac{l(l+1)}{\cosh^2\theta}\right] V(z) = 0.} \tag{8.221}$$

Because the roles of l and m are interchanged, we can vary l for fixed m. Comparing Eq. (8.221) with

$$\frac{d^2V(z)}{dz^2} + [\lambda + r(z,l)]V(z) = 0 \tag{8.222}$$

and Eq. (8.93), we see that this is of type A with

$$a = i, \ c = 0, \ p = i\pi/2, \text{ and } d = 0. \tag{8.223}$$

Its factorization is, therefore, obtained as

$$O_+(z,l)O_-(z,l)V_l^{\lambda_m}(z) = [\lambda_m - \mu(l)]V_l^{\lambda_m}(z) \tag{8.224}$$

with

$$k(z,l) = l \tanh z, \tag{8.225}$$

$$\mu(l) = -l^2. \tag{8.226}$$

Thus, the **ladder operators** are

$$\boxed{O_\pm(z,l) = \pm\frac{d}{dz} - l\tanh z.} \tag{8.227}$$

Because $\mu(l)$ is a decreasing function, from Theorem 8.4 we obtain the top of the ladder for some minimum value of l, say m, thus $\lambda = -m^2$. We can now write

$$O_+(z,l)O_-(z,l)V_l^{\lambda_m}(z) = [-m^2 + l^2]V_l^{\lambda_m}(z), \tag{8.228}$$

$$O_-(z,l+1)O_+(z,l+1)V_l^{\lambda_m}(z) = [-m^2 + (l+1)^2]V_l^{\lambda_m}(z). \tag{8.229}$$

Using

$$\int_{-\infty}^{+\infty} [V_{l-1}^{\lambda_m}(z)]^2 dz = \int_{-\infty}^{+\infty} [O_-(z,l)V_l^{\lambda_m}(z)]^2 dz \tag{8.230}$$

$$= \int_{-\infty}^{+\infty} V_l^{\lambda_m}(z)[O_+(z,l)O_-(z,l)V_l^{\lambda_m}(z)]dz \tag{8.231}$$

$$= [-m^2 + l^2]\int_{-\infty}^{+\infty} \left[V_l^{\lambda_m}(z)\right]^2 dz, \tag{8.232}$$

we again see that $l_{\min} = m$, so that

$$O_-(z,l)V_m^{\lambda_m}(z) = 0. \tag{8.233}$$

Because we do not have a state lower than $l = m$, using the definition of $O_-(z, l)$, we can use Eq. (8.71) to find $V_l^{\lambda_l}(z)$ as

$$\left[-\frac{d}{dz} - m\tanh z\right] V_m^{\lambda_m}(z) = 0, \tag{8.234}$$

$$\int \frac{dV_m^{\lambda_m}(z)}{V_m^{\lambda_m}(z)} = -m \int \frac{\sinh z}{\cosh z} dz, \tag{8.235}$$

$$V_m^{\lambda_m}(z) = N' \frac{1}{\cosh^m z}, \tag{8.236}$$

where N' is a normalization constant in the z-space. Using the transformation given in Eq. (8.220) and, since $l = m$, we write $V_m^{\lambda_m}(z)$ as

$$V_m^m(\theta) = V_l^l(\theta) = N \sin^l \theta. \tag{8.237}$$

From Eqs. (8.177) and (8.166), we note that for $m = l$

$$y_l^l(\theta) = \sqrt{\sin\theta} P_l^l \propto (\sin\theta)^{(l+\frac{1}{2})}, \tag{8.238}$$

$$V_l^l(\theta) \propto y_l^l(\theta)/\sqrt{\sin\theta}. \tag{8.239}$$

Thus, for general m

$$V_l^m(\theta) = C_{lm} \frac{y_l^m(\theta)}{\sqrt{\sin\theta}}, \tag{8.240}$$

where C_{lm} is needed to ensure normalization in θ-space. Using Eq. (8.50) of Theorem 8.5 and Eq. (8.20), we now find the step-up operator for the l index as

$$V_{l+1}^m(\theta) = \frac{1}{\sqrt{(l+1)^2 - m^2}} \left\{\frac{d}{dz} - (l+1)\tanh z\right\} V_l^m(\theta), \tag{8.241}$$

$$C_{l+1,m} \frac{y_{l+1}^m(\theta)}{\sqrt{\sin\theta}} = \frac{C_{lm}}{\sqrt{(l+1)^2 - m^2}} \left\{\frac{d}{dz} - (l+1)\tanh z\right\} \frac{y_l^m(\theta)}{\sqrt{\sin\theta}}. \tag{8.242}$$

Taking tanh of both sides in Eq. (8.220), we write

$$\tanh z = -\cos\theta, \tag{8.243}$$

$$\frac{d}{dz} = \sin\theta \frac{d}{d\theta} \tag{8.244}$$

and obtain

$$y_{l+1}^m(\theta) C_{l+1,m} = \frac{C_{lm}}{\sqrt{(l+1+m)(l+1-m)}} \left\{\sin\theta \frac{d}{d\theta} + \left(l + \frac{1}{2}\right)\cos\theta\right\} y_l^m(\theta), \tag{8.245}$$

Similarly for the step-down operator, we find

$$y_{l-1}^{m}(\theta)C_{l-1,m} = \frac{C_{lm}}{\sqrt{(l-m)(l+m)}}\left\{-\sin\theta\frac{d}{d\theta}+\left(l+\frac{1}{2}\right)\cos\theta\right\}y_l^m(\theta). \tag{8.246}$$

Using our previous results [Eqs. (8.171) and (8.174)], ladder operators for the m index in $y_l^m(\theta)$ can be written as

$$y_l^{m+1}(\theta) = \frac{1}{\sqrt{(l-m)(l+m+1)}}\times\left\{\frac{d}{d\theta}-\left(m+\frac{1}{2}\right)\cot\theta\right\}y_l^m(\theta), \tag{8.247}$$

$$y_l^{m-1}(\theta) = \frac{1}{\sqrt{(l+m)(l-m+1)}}\times\left\{-\frac{d}{d\theta}-\left(m-\frac{1}{2}\right)\cot\theta\right\}y_l^m(\theta). \tag{8.248}$$

To evaluate the normalization constant in θ-space, first we show that the ratio $C_{lm}/C_{l+1,m}$ is independent of m. Starting with the state (l,m) we can reach $(l+1,m+1)$ in two ways.

Path I. $(l,m)\to(l,m+\mathbf{1})\to(l+\mathbf{1},m+\mathbf{1})$: For this path, using Eqs. (8.245) and (8.247) we write

$$y_{l+1}^{m+1}(\theta)\frac{C_{l+1,m+1}}{C_{l,m+1}} = \frac{\left\{\sin\theta\frac{d}{d\theta}+\left(l+\frac{1}{2}\right)\cos\theta\right\}\left\{\frac{d}{d\theta}-\left(m+\frac{1}{2}\right)\cot\theta\right\}y_l^m(\theta)}{\sqrt{(l-m)^2(l+m+1)(l+m+2)}}. \tag{8.249}$$

The numerator on the right-hand side is

$$\left\{\left[\sin\theta\frac{d^2y_l^m}{d\theta^2}\right]+(l-m)\cos\theta\frac{dy_l^m}{d\theta}+\frac{m+\frac{1}{2}}{\sin\theta}\left[1-\left(l+\frac{1}{2}\right)\cos^2\theta\right]y_l^m\right\}. \tag{8.250}$$

Using Eq. (8.137) with $\lambda_l = l(l+1)$ and simplifying, we obtain

$$y_{l+1}^{m+1}(\theta) = \frac{C_{l,m+1}}{C_{l+1,m+1}}\frac{1}{(l-m)}\frac{(l-m)}{\sqrt{(l+m+1)(l+m+2)}} \times\left\{\cos\theta\frac{d}{d\theta}-\frac{m+\frac{1}{2}}{\sin\theta}-\left(l+\frac{1}{2}\right)\sin\theta\right\}y_l^m(\theta). \tag{8.251}$$

Path II. $(l, m) \to (l + \mathbf{1}, m) \to (l + \mathbf{1}, m + \mathbf{1})$: Following the same procedure as in the first path, we obtain

$$y_{l+1}^{m+1}(\theta) = \frac{C_{l,m}}{C_{l+1,m}} \frac{1}{(l+1-m)} \frac{(l+1-m)}{\sqrt{(l+m+1)(l+m+2)}} \times \left\{ \cos\theta \frac{d}{d\theta} - \frac{m+\frac{1}{2}}{\sin\theta} - \left(l + \frac{1}{2}\right) \sin\theta \right\} y_l^m(\theta). \tag{8.252}$$

Thus, we obtain

$$\frac{C_{l,m+1}}{C_{l+1,m+1}} = \frac{C_{l,m}}{C_{l+1,m}}, \tag{8.253}$$

which means that $C_{l,m}/C_{l+1,m}$ is independent of m. Using this result, we can now evaluate $C_{lm}/C_{l+1,m}$. First using Eq. (8.170), we write

$$y_{l+1}^{l}(\theta) = \frac{C_{ll}}{C_{l+1,l}} \left\{ \sin\theta \frac{d}{d\theta} + \left(l + \frac{1}{2}\right) \cos\theta \right\} \frac{\sin^{l+1/2}\theta}{\sqrt{2l+1}} (-1)^l \sqrt{\frac{1 \cdot 3 \cdot 5 \cdots (2l+1)}{2[2 \cdot 4 \cdot 6 \cdots (2l)]}} \tag{8.254}$$

$$= \frac{C_{ll}}{C_{l+1,l}} \sin^{l+1/2}\theta \cos\theta \sqrt{2l+1} (-1)^l \sqrt{\frac{1 \cdot 3 \cdot 5 \cdots (2l+1)}{2[2 \cdot 4 \cdot 6 \cdots (2l)]}}. \tag{8.255}$$

Using Eqs. (8.170) and (8.171), we can also write

$$y_{l+1}^{l}(\theta) = £\_(\theta, l+1) y_{l+1}^{l+1}(\theta) \tag{8.256}$$

$$= £\_(\theta, l+1) \left[\sin^{l+3/2}\theta (-1)^{l+1} \sqrt{\frac{1 \cdot 3 \cdot 5 \cdots (2l+3)}{2[2 \cdot 4 \cdot 6 \cdots 2(l+1)]}} \right] \tag{8.257}$$

$$= \sqrt{(2l+3)} (-1)^l \sqrt{\frac{1 \cdot 3 \cdot 5 \cdots (2l+1)}{2[2 \cdot 4 \cdot 6 \cdots (2l)]}} \sin^{l+1/2}\theta \cos\theta. \tag{8.258}$$

Comparing these we get

$$\frac{C_{ll}}{C_{l+1,l}} = \frac{C_{lm}}{C_{l+1,m}} = \sqrt{\frac{2l+3}{2l+1}}. \tag{8.259}$$

8.6.6 Complete Set of Ladder Operators

Finally, using

$$Y_l^m(\theta, \phi) = \frac{y_l^m(\theta)}{\sqrt{\sin\theta}} \frac{e^{im\phi}}{\sqrt{2\pi}}, \tag{8.260}$$

we write the complete set of normalized ladder operators of the spherical harmonics for the indices l and m as

$$Y_{l+1}^{m}(\theta,\phi) = \sqrt{\frac{(2l+3)}{(2l+1)(l+1+m)(l+1-m)}} \times \left\{ \sin\theta \frac{\partial}{\partial\theta} + (l+1)\cos\theta \right\} Y_l^m(\theta,\phi), \tag{8.261}$$

$$Y_{l-1}^{m}(\theta,\phi) = \sqrt{\frac{(2l-1)}{(2l+1)(l-m)(l+m)}} \times \left\{ -\sin\theta \frac{\partial}{\partial\theta} + l\cos\theta \right\} Y_l^m(\theta,\phi). \tag{8.262}$$

and

$$Y_l^{m-1}(\theta,\phi) = \frac{e^{-i\phi}\left[-\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\phi}\right]}{\sqrt{(l+m)(l-m+1)}} Y_l^m(\theta,\phi), \tag{8.263}$$

$$Y_l^{m+1}(\theta,\phi) = \frac{e^{+i\phi}\left[\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\phi}\right]}{\sqrt{(l-m)(l+m+1)}} Y_l^m(\theta,\phi). \tag{8.264}$$

Adding Eqs. (8.261) and (8.262), we also obtain a useful relation

$$\cos\theta Y_l^m(\theta,\phi) = \sqrt{\frac{(l+1+m)(l+1-m)}{(2l+1)(2l+3)}} Y_{l+1}^m(\theta,\phi) + \sqrt{\frac{(l-m)(l+m)}{(2l+1)(2l-1)}} Y_{l-1}^m(\theta,\phi). \tag{8.265}$$

8.7 Schrödinger Equation and Single-Electron Atom (Type F)

The radial part of the Schrödinger equation for a single-electron atom is given as

$$\frac{d}{dr}\left(r^2 \frac{dR_l(r)}{dr}\right) + r^2 k^2(r) R_l(r) - l(l+1)R_l(r) = 0, \tag{8.266}$$

where

$$k^2(r) = \frac{2m}{\hbar^2}\left[E + \frac{Ze^2}{r}\right], \tag{8.267}$$

Z is the atomic number, and e is the electron's charge. Because the electrons in an atom are bounded, their energy values should satisfy $E < 0$. In this equation, if we change the dependent variable as $R_l(r) = u_{E,l}(r)/r$, the differential equation to be solved for $u_{E,l}(r)$ becomes

$$-\frac{\hbar^2}{2m}\frac{d^2u_{E,l}}{dr^2} + \left[\frac{\hbar^2 l(l+1)}{2mr^2} - \frac{Ze^2}{r}\right]u_{E,l}(r) = Eu_{E,l}(r). \tag{8.268}$$

We have seen in Chapter 2 that the conventional method allows us to express the solutions of this equation in terms of the Laguerre polynomials. To solve this problem with the factorization method we first write Eq. (8.268) as

$$\frac{d^2u_{E,l}}{d\left(r/\frac{\hbar^2}{mZe^2}\right)^2} + \left[\frac{2}{\left(r/\frac{\hbar^2}{mZe^2}\right)} - \frac{l(l+1)}{\left(r/\frac{\hbar^2}{mZe^2}\right)^2}\right]u_{E,l}(r) + \left(\frac{2\hbar^2E}{mZ^2e^4}\right)u_{E,l}(r) = 0. \tag{8.269}$$

Taking the unit of length as $\hbar^2/mZe^2$ and defining $\lambda = 2\hbar^2E/mZ^2e^4$, Eq. (8.269) becomes

$$\frac{d^2u_\lambda^l}{dr^2} + \left[\lambda + \left(\frac{2}{r} - \frac{l(l+1)}{r^2}\right)\right]u_\lambda^l = 0. \tag{8.270}$$

This is Type F with

$$q = -1 \text{ and } m = l.$$

Thus, we determine $k(r,l)$ and $\mu(l)$ as

$$k(r,l) = \frac{l}{r} - \frac{1}{l}, \tag{8.271}$$

$$\mu(l) = -\frac{1}{l^2}. \tag{8.272}$$

Because $\mu(l)$ is an increasing function, we have $l_{\max}$, say n'; thus, we obtain λ as

$$\lambda = -\frac{1}{(n'+1)^2}, \quad n' = 0,1,2,3,\ldots \tag{8.273}$$

$$= -\frac{1}{n^2}, \quad n = 1,2,3,\ldots. \tag{8.274}$$

Note that $l \le n = 1,2,3,\ldots$. We also have

$$u_n^{l=n} = (2/n)^{n+1/2}[(2n)!]^{-1/2}r^n \exp\left(-\frac{r}{n}\right), \tag{8.275}$$

where

$$u_n^{l-1} = [\pounds_-(r,l)]u_n^n, \tag{8.276}$$

$$u_n^{l+1} = [\pounds_+(r,l+1)]u_n^n. \tag{8.277}$$

The normalized ladder operators are defined by Eq. (8.49) as

$$\pounds_\pm(r,l) = \left[-\frac{1}{n^2} + \frac{1}{l^2}\right]^{-1/2}\left\{\pm\frac{d}{dr} - \frac{l}{r} + \frac{1}{l}\right\}. \tag{8.278}$$

Using (8.274), the energy levels are obtained as

$$E_n = -\frac{mZ^2e^4}{2\hbar^2 n^2}, \quad n = 1, 2, 3, \dots, \tag{8.279}$$

which are the quantized **Bohr energy levels**.

8.8 Gegenbauer Functions (Type A)

The Gegenbauer equation is in general given as

$$(1-x^2)\frac{d^2C_n^{\lambda'}(x)}{dx^2} - (2\lambda'+1)x\frac{dC_n^{\lambda'}(x)}{dx} + n(n+2\lambda')C_n^{\lambda'}(x) = 0. \tag{8.280}$$

For $\lambda = 1/2$, this equation reduces to the Legendre equation. For integer values of n its solutions reduce to the Gegenbauer or the Legendre polynomials:

$$C_n^{\lambda'}(x) = \sum_{r=0}^{[n/2]} (-1)^r \frac{\Gamma(n-r+\lambda')}{\Gamma(\lambda')r!(n-2r)!}(2x)^{n-2r}. \tag{8.281}$$

In the study of surface oscillations of a hypersphere one encounters the equation

$$(1-x^2)\frac{d^2U_\lambda^m(x)}{dx^2} - (2m+3)x\frac{dU_\lambda^m(x)}{dx} + \lambda U_\lambda^m(x) = 0, \tag{8.282}$$

solutions of which could be expressed in terms of the Gegenbauer polynomials as

$$U_\lambda^m(x) = C_{l-m}^{m+1}(x), \tag{8.283}$$

where $\lambda = (l-m)(l+m+2)$. Using

$$x = -\cos\theta, \tag{8.284}$$

$$U_\lambda^m(x) = Z_\lambda^m(\theta)(\sin\theta)^{-m-1}, \tag{8.285}$$

we can put Eq. (8.282) into the second canonical form as

$$\frac{d^2Z_\lambda^m(\theta)}{d\theta^2} + \left[-\frac{m(m+1)}{\sin^2\theta} + (\lambda + (m+1)^2)\right] Z_\lambda^m(\theta) = 0. \tag{8.286}$$

On the introduction of $\lambda'' = \lambda + (m+1)^2$ and comparing with Eq. (8.93), this is of type A with

$$c = p = d = 0,\ a = 1,\ z = \theta, \tag{8.287}$$

thus, its factorization is obtained as

$$k(\theta, m) = m\cot\theta, \tag{8.288}$$

$$\mu(m) = m^2. \tag{8.289}$$

The solutions are found by using

$$Z_\lambda^{m=l}(\theta) = \pi^{-1/4}\left[\frac{\Gamma(l+2)}{\Gamma(l+3/2)}\right]^{1/2} \sin^{l+1}\theta \tag{8.290}$$

and the formula

$$Z_l^{m-1} = [(l+1)^2 - m^2)]^{-1/2}\left\{-\frac{d}{d\theta} - m\cot\theta\right\} Z_l^m. \tag{8.291}$$

Note that Z_l^m is the eigenfunction corresponding to the eigenvalue

$$\lambda'' = (l+1)^2, \quad l - m = 0, 1, 2, \ldots, \tag{8.292}$$

that is, to

$$\lambda = (l+1)^2 - (m+1)^2 \tag{8.293}$$

$$= (l-m)(l+m+2). \tag{8.294}$$

8.9 Symmetric Top (Type A)

The wave equation for a symmetric top is encountered in the study of simple molecules. If we separate the wave function as

$$U = \Theta(\theta)\exp(i\kappa\phi)\exp(im\psi), \tag{8.295}$$

where θ, ϕ, and ψ are the Euler angles and κ and m are integers, $\Theta(\theta)$ satisfies the second-order ordinary differential equation

$$\frac{d^2\Theta(\theta)}{d\theta^2} + \cot\theta\frac{d\Theta(\theta)}{d\theta} - \frac{(m-\kappa\cos\theta)^2}{\sin^2\theta}\Theta(\theta) + \sigma\Theta(\theta) = 0, \tag{8.296}$$

where

$$\sigma = \frac{8\pi^2 AW}{h^2} - \frac{A\kappa^2}{C}. \tag{8.297}$$

A, W, C, and h are the other constants that come from the physics of the problem. With the substitution $Y = \Theta(\theta)\sin^{1/2}\theta$, Eq. (8.296) becomes

$$\frac{d^2Y}{d\theta^2} - \left[\frac{(m-1/2)(m+1/2) + \kappa^2 - 2m\kappa\cos\theta}{\sin^2\theta}\right] Y + (\sigma + \kappa^2 + 1/4)Y = 0. \tag{8.298}$$

This equation is of type A, and we identify the parameters in Eq. (8.93) as

$$a = 1,\ c = -1/2, \quad d = -\kappa, \quad p = 0.$$

The factorization is now given by

$$k(\theta, m) = (m - 1/2)\cot\theta - \kappa/\sin\theta, \tag{8.299}$$

$$\mu(m) = (m - 1/2)^2. \tag{8.300}$$

Eigenfunctions can be obtained from

$$Y_{J\kappa}^{J} = \left[\frac{\Gamma(2J+2)}{\Gamma(J-\kappa+1)\Gamma(J+\kappa+1)}\right]^{1/2} \sin^{J-\kappa+1/2}\frac{\theta}{2}\cos^{J+\kappa+1/2}\frac{\theta}{2} \tag{8.301}$$

by using

$$Y_{J\kappa}^{m-1} = \left[\left(J+\frac{1}{2}\right)^2 - \left(m-\frac{1}{2}\right)^2\right]^{-1/2} \left\{-\frac{d}{d\theta} - (m-1/2)\cot\theta + \frac{\kappa}{\sin\theta}\right\} Y_{J\kappa}^{m}. \tag{8.302}$$

The corresponding eigenvalues are

$$\sigma + \kappa + 1/4 = (J+1/2)^2, \tag{8.303}$$

$$J - |m| \text{ and } J - |\kappa| = 0, 1, 2, \ldots, \tag{8.304}$$

so that

$$W = \frac{J(J+1)h^2}{8\pi^2 A} + \left(\frac{1}{C} - \frac{1}{A}\right)\frac{\kappa^2 h^2}{8\pi^2}. \tag{8.305}$$

8.10 Bessel Functions (Type C)

Bessel's equation:

$$x^2 J_m''(x) + xJ_m'(x) + (\lambda x^2 - m^2)J_m(x) = 0, \tag{8.306}$$

multiplied by $1/x$, gives the first canonical form as

$$\frac{d}{dx}\left[x\frac{dJ_m(x)}{dx}\right] + \left(\lambda x - \frac{m^2}{x}\right)J_m(x) = 0, \tag{8.307}$$

where $p(x) = x$ and $w(x) = x$. A second transformation:

$$\frac{dz}{dx} = \sqrt{\frac{w}{p}} = 1, \tag{8.308}$$

$$J_m = \frac{\Psi}{[wp]^{1/4}} = \frac{\Psi}{\sqrt{x}}, \tag{8.309}$$

gives us the second canonical form:

$$\frac{d^2\Psi}{dx^2} + \left[\lambda - \frac{(m^2 - 1/4)}{x^2}\right]\Psi = 0. \tag{8.310}$$

This is type C, and its factorization is given as

$$k(x,m) = \frac{\left(m - \frac{1}{2}\right)}{x}, \tag{8.311}$$

$$\mu(m) = 0. \tag{8.312}$$

Because $\mu(m)$ is neither a decreasing nor an increasing function of m, we have no limit, upper or lower, to the ladder. We have only the recursion relations

$$\Psi_{m+1} = \frac{1}{\sqrt{x}}\left\{\frac{d}{dx} - \frac{(m+1/2)}{x}\right\}\Psi_m, \tag{8.313}$$

$$\Psi_{m-1} = \frac{1}{\sqrt{x}}\left\{-\frac{d}{dx} - \frac{(m-1/2)}{x}\right\}\Psi_m, \tag{8.314}$$

where

$$\Psi_m = x^{1/2}J_m(\lambda^{1/2}x). \tag{8.315}$$

8.11 Harmonic Oscillator (Type D)

The Schrödinger equation for the harmonic oscillator is written as

$$\frac{d^2\Psi}{d\xi^2} - \xi^2\Psi + \lambda\Psi = 0, \tag{8.316}$$

where the physical variables, ξ and λ, are given as $\xi = (\hbar/\mu\omega)^{1/2}x$, $\lambda = 2E/\hbar\omega$. This equation can be written in either of the two forms (see Problem 14)

$$O_-O_+\Psi_\lambda = (\lambda+1)\Psi_\lambda, \tag{8.317}$$

$$O_+O_-\Psi_\lambda = (\lambda-1)\Psi_\lambda, \tag{8.318}$$

and where

$$O_\pm = \pm\frac{d}{d\xi} - \xi \quad . \tag{8.319}$$

Operating on Eq. (8.317) with O_+ and on Eq. (8.318) with O_- we obtain the analog of Theorem 8.1 as

$$\Psi_{\lambda+2} \propto O_+\Psi_\lambda, \tag{8.320}$$

$$\Psi_{\lambda-2} \propto O_-\Psi_\lambda. \tag{8.321}$$

Moreover, corresponding to Theorem 8.4, we find that we cannot lower the eigenvalue λ indefinitely. Thus, we have a bottom of the ladder as

$$\lambda = 2n+1, \quad n = 0,1,2,\dots. \tag{8.322}$$

Hence, the ground state must satisfy

$$O_-\Psi_0 = 0, \tag{8.323}$$

which determines Ψ_0 as

$$\Psi_0 = \pi^{-1/4}\exp(-\xi^2/2). \tag{8.324}$$

Now the other eigenfunctions can be obtained from

$$\Psi_{n+1} = [2n+2]^{-1/2} O_+ \Psi_n, \tag{8.325}$$

$$\Psi_{n-1} = [2n]^{-1/2} O_- \Psi_n. \tag{8.326}$$

8.12 Differential Equation for the Rotation Matrix

We now consider the following differential equation that the rotation matrix, $d^l_{mm'}(\beta)$, satisfies:

$$\left\{ \frac{d^2}{d\beta^2} + \cot\beta \frac{d}{d\beta} + \left[l(l+1) - \left(\frac{m^2 + m'^2 - 2mm'\cos\beta}{\sin^2\beta} \right) \right] \right\} d^l_{m'm}(\beta) = 0. \tag{8.327}$$

A detailed discussion of the rotation matrix will be presented in Chapter 10; however, here we look at it entirely from the point of view of the factorization method as a second-order differential equation.

8.12.1 Step-Up/Down Operators for *m*

Considering m as a parameter, we now find the normalized step-up and step-down operators, $£_+(m+1)$ and $£_-(m)$, that change the index m while keeping the index m' fixed. We first put the above differential equation into **first canonical form**:

$$\frac{d}{dx}\left[p(x) \frac{du(x)}{dx} \right] + q(x)u(x) = -\lambda w(x)u(x), \tag{8.328}$$

as

$$\frac{d}{d\beta}\left[\sin\beta \frac{d}{d\beta} d^l_{m'm}(\beta) \right] - \left(\frac{m^2 + m'^2 - 2mm'\cos\beta}{\sin\beta} \right) d^l_{m'm}(\beta)$$
$$= -l(l+1)\sin\beta\, d^l_{m'm}(\beta), \tag{8.329}$$

where

$$\lambda = l(l+1), \tag{8.330}$$

$$p(\beta) = \sin\beta, \tag{8.331}$$

$$q(\beta) = -\frac{m^2 + m'^2 - 2mm'\cos\beta}{\sin\beta}, \tag{8.332}$$

$$w(\beta) = \sin\beta. \tag{8.333}$$

Making the substitutions [Eqs. (8.5) and (8.6)]:

$$d^l_{m'm}(\beta) = \frac{y(\lambda_l, m', m, \beta)}{\sqrt{\sin\beta}}, \; dz = d\beta, \tag{8.334}$$

we obtain the **second canonical form** [Eq. (8.7)]:

$$\frac{d^2y}{d\beta^2} + [\lambda_l + r(z,m)]y(z) = 0, \tag{8.335}$$

where

$$\lambda_l = l(l+1) + \frac{1}{4}, \tag{8.336}$$

$$r(z,m) = -\frac{m^2 + m'^2 - 2mm'\cos\beta - \frac{1}{4}}{\sin^2\beta}. \tag{8.337}$$

Comparing $r(z,m)$ with Eq. (8.93), this is type A in Section 8.5. We determine the coefficients in Eq. (8.93) and write $k(\beta,m)$ and $\mu(m)$ as

$$k(\beta,m) = (m-1/2)\cot\beta - \frac{m'}{\sin\beta}, \tag{8.338}$$

$$\mu(m) = (m-1/2)^2. \tag{8.339}$$

Now the ladder operators [Eq. (8.14)] become

$$O_{\pm}(m) = \pm\frac{d}{d\beta} - k(\beta,m) \tag{8.340}$$

$$= \pm\frac{d}{d\beta} - \left(m - \frac{1}{2}\right)\cot\beta + \frac{m'}{\sin\beta}. \tag{8.341}$$

Using $\mu(m)$:

$$\mu(m) = \left(m - \frac{1}{2}\right)^2, \tag{8.342}$$

and Theorem 8.1, we can show that $|m| \leq l$. We now construct the eigenfunctions starting from the top of the ladder, $m = l$, and write

$$O_+(l+1)y(\lambda_l, m', l, \beta) = 0, \tag{8.343}$$

$$\left(+\frac{d}{d\beta} - \left(l + \frac{1}{2}\right)\cot\beta + \frac{m'}{\sin\beta}\right) y(\lambda_l, m', l, \beta) = 0. \tag{8.344}$$

Integrating Eq. (8.344) gives

$$y(\lambda_l, m', l, \beta) = \sin^{l+1/2}\beta\,\tan^{-m'}(\beta/2). \tag{8.345}$$

Using Eq. (8.334), we obtain

$$d^l_{m'l} = \sin^l\beta\,\tan^{-m'}(\beta/2). \tag{8.346}$$

8.12.2 Step-Up/Down Operators for *m′*

Keeping m as fixed and treating m' as a parameter, we follow similar steps to determine that this is still a type A problem (Section 8.5). We first find $k(\beta, m')$ and $\mu(m')$ to write the ladder operators, and then show that m' satisfies $|m'| \leq l$.

Note that $r(z, m, m', \beta)$ is symmetric in m and m'. From the definition of $d^l_{m'm}(\beta)$ [Eq. (10.295)]:

$$d^l_{m'm}(\beta) = \iint d\Omega Y^*_{lm'}(\theta,\phi) e^{-i\beta L_y} Y_{lm}(\theta,\phi), \tag{8.347}$$

it is seen that the $d^l_{m'm}(\beta)$ are the elements of unitary matrices, furthermore, they are real; hence,

$$d^l_{m'm}(\beta) = d^l_{mm'}(-\beta) \tag{8.348}$$

is true (Problem 16). In order to satisfy this relation, we introduce a factor of -1 into the definition of the ladder operators $O_\pm(m')$ as

$$O_\pm(m') = -\left[\pm\frac{d}{d\beta} - K(\beta, m')\right] \tag{8.349}$$

$$= -\left[\pm\frac{d}{d\beta} - \left(m' - \frac{1}{2}\right)\cot\beta + \frac{m}{\sin\beta}\right]. \tag{8.350}$$

Using [Eq. (8.345)]

$$y(l, m', m = l, \beta) = \sin^{l+1/2}\beta \tan^{-m'}(\beta/2) \tag{8.351}$$

in the definition

$$d^l_{m'm}(\beta) = \frac{y(l, m, m', \beta)}{\sqrt{\sin\beta}}, \tag{8.352}$$

we can write

$$d^l_{ll}(\beta) = (1 + \cos\beta)^l. \tag{8.353}$$

8.12.3 Normalized Functions with $m = m' = l$

Using the weight function [Eq. (8.333)], $w(\beta)$, we evaluate the normalization constant for $m = m' = l$ as

$$\int_0^\pi w(\beta)[d^l_{ll}(\beta)]^2 d\beta = \frac{2^{2l+1}}{2l+1}, \tag{8.354}$$

which allows us to write the normalized $d^l_{ll}(\beta)$ as

$$d^l_{ll}(\beta) = \left(\frac{2l+1}{2^{2l+1}}\right)^{1/2}(1 + \cos\beta)^l. \tag{8.355}$$

8.12.4 Full Matrix for $l = 2$

To construct the full matrix $d^2_{m'm}(\beta)$, we use the eigenfunctions

$$d^l_{m'l}(\beta) = C^l_{m'l}\, \sin^l\,\beta\, \tan^{-m'}\left(\frac{\beta}{2}\right), \tag{8.356}$$

where $C^l_{m'l}$ are the normalization constants and write

$$d^2_{m'2}(\beta) = C^2_{m'2}\ \sin^2\ \beta\ \tan^{-m'}\left(\frac{\beta}{2}\right). \tag{8.357}$$

Hence, the components of $d^2_{m'2}(\beta)$ are obtained as

$$\begin{aligned}
d^2_{22}(\beta) &= \left(\frac{5}{2}\right)^{1/2}\left(\frac{1+\cos\beta}{2}\right)^2,\\
d^2_{12}(\beta) &= -\left(\frac{5}{2}\right)^{1/2}\frac{\sin\beta}{2}(1+\cos\beta),\\
d^2_{02}(\beta) &= \left(\frac{15}{16}\right)^{1/2}\sin^2\beta,\\
d^2_{-1,2}(\beta) &= -\left(\frac{5}{2}\right)^{1/2}\frac{\sin\beta}{2}(1-\cos\beta),\\
d^2_{-2,2}(\beta) &= \left(\frac{5}{2}\right)^{1/2}\left(\frac{1-\cos\beta}{2}\right)^2.
\end{aligned} \tag{8.358}$$

As the reader can check, we can also generate these functions by acting on the normalized $d^2_{22}(\beta)$ with the normalized ladder operator $£_-(m')$, which acts on m' and lowers it by one while keeping m fixed. Equation (8.358) gives only the first column of the 5×5 matrix, $d^2_{m'm}(\beta)$, where $m=2$ and m' takes the values $2, 1, 0, -1, -2$. For the remaining columns, we use the normalized ladder operator:

$$£_-(m) = \frac{-\frac{d}{d\beta} - \left(m-\frac{1}{2}\right)\cot\beta + \frac{m'}{\sin\beta}}{\sqrt{(l+m)(l-m+1)}}, \tag{8.359}$$

which keeps m' fixed and lowers m by one as

$$£_-(m)\ y(\lambda, m', m, \beta) = y(\lambda, m', m-1, \beta). \tag{8.360}$$

Similarly, we can write the other normalized ladder operator $£_+(m)$.

We now use

$$\sqrt{\sin\beta}\, d^l_{m'm} = y(\lambda, m', m, \beta) \tag{8.361}$$

in Eqs. (8.359) and (8.360) to obtain

$$d^l_{m',m-1} = \frac{1}{\sqrt{(l+m)(l-m+1)}}\left[-\frac{d}{d\beta} - m\cot\beta + \frac{m'}{\sin\beta}\right] d^l_{m'm}. \tag{8.362}$$

In conjunction with the normalized eigenfunctions [Eq. (8.358)], each of which is the top of the ladder for the corresponding row, we use this formula to generate the remaining 20 elements of the $d^l_{m'm}$ matrix.

Note: You can use the symmetry relation in Eq. (8.348) to check your algebra. Also show the relation (Problem 17)

$$d^l_{m'm}(\beta) = (-1)^{m'-m} d^l_{mm'}(\beta). \tag{8.363}$$

8.12.5 Step-Up/Down Operators for *l*

To find the step-up/-down operators that shift the index l for fixed m and m' that give the **normalized** functions $d^l_{mm'}(\beta)$, we transform the differential equation for $d^l_{mm'}(\beta)$ into an appropriate form. We start with the equation that $d^l_{m'm}(\beta)$ satisfies:

$$\left\{\frac{d^2}{d\beta^2} + \cot\beta\frac{d}{d\beta} + \left[l(l+1) - \frac{m^2 + m'^2 - 2mm'\cos\beta}{\sin^2\beta}\right]\right\} d^l_{m'm}(\beta) = 0, \tag{8.364}$$

and substitute

$$z = \ln(\tan\beta/2), \tag{8.365}$$

$$d^l_{m'm}(\beta) = K^l_{m'm}(z), \tag{8.366}$$

to obtain

$$\frac{d^2K^l_{m'm}}{dz^2} + \left[-(m^2 + m'^2) + \frac{l(l+1)}{\cosh^2 z} - 2mm'\tanh z\right] K^l_{m'm}(z) = 0, \tag{8.367}$$

which is in **second canonical form**. We now proceed similar to the previous case. Comparing with type E in Section 8.5, we obtain

$$O_\pm(l) = \pm\frac{d}{dz} - \left(l\tanh z + \frac{mm'}{l}\right). \tag{8.368}$$

The normalized ladder operators, $\pounds_\pm(l)$ for the **normalized** eigenfunctions become

$$d^{l-1}_{m'm}(\beta) = \left[\frac{l\sqrt{(2l-1)/(2l+1)}}{\sqrt{[l^2 - m^2][l^2 - m'^2]}}\right]\left[-\sin\beta\frac{d}{d\beta} + l\cos\beta - \frac{m'm}{l}\right] d^l_{m'm}(\beta) \tag{8.369}$$

and

$$d^{l+1}_{m'm}(\beta) = \left[\frac{(l+1)\sqrt{(2l+3)/(2l+1)}}{\sqrt{[(l+1)^2 - m^2][(l+1)^2 - m'^2]}}\right] \times \left[\sin\beta\frac{d}{d\beta} + (l+1)\cos\beta - \frac{m'm}{(l+1)}\right] d^l_{m'm}(\beta). \tag{8.370}$$

For a recursion relation, we simply add the above expressions.

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Problems

1 Starting from the first canonical form of the Sturm–Liouville equation:

$$\frac{d}{dx}\left[p(x)\frac{d\Psi(x)}{dx}\right] + q(x)\Psi(x) + \lambda w(x)\Psi(x) = 0, \quad x \in [a, b],$$

derive the second canonical form:

$$\frac{d^2 y_\lambda^m(z)}{dz^2} + \{\lambda + r(z, m)\}y_\lambda^m(z) = 0,$$

where

$$r(z, m) = \frac{q}{w} + \frac{3}{16}\left[\frac{1}{w}\frac{dw}{dz} + \frac{1}{p}\frac{dp}{dz}\right]^2 - \frac{1}{4}\left[\frac{2}{pw}\frac{dp}{dz}\frac{dw}{dz} + \frac{1}{w}\frac{d^2w}{dz^2} + \frac{1}{p}\frac{d^2p}{dz^2}\right],$$

by using the transformations $y(z) = \Psi(x)[w(x)p(x)]^{1/4}$ and $dz = dx\left[\frac{w(x)}{p(x)}\right]^{1/2}$.

2 Derive the normalization constants in

$$Y_l^m(\theta, \phi) = \sqrt{\frac{2l+1}{2}\frac{(l-m)!}{(l+1)!}\frac{1}{2\pi}}[L_+]^m P_l(\cos\theta)$$

and

$$Y_l^{-m}(\theta, \phi) = \sqrt{\frac{2l+1}{2}\frac{(l-m)!}{(l+1)!}\frac{1}{2\pi}}[L_-]^m P_l(\cos\theta).$$

3 Derive the normalization constant in

$$y_l^{\lambda_l}(\theta) = (-1)^l\left[\frac{(2l+1)!}{2^{2l+1}l!^2}\right]^{1/2}(\sin\theta)^{\left(l+\frac{1}{2}\right)}.$$

4 Derive Eq. (8.221), which is given as

$$\frac{d^2V(z)}{dz^2} + \left[\lambda + \frac{l(l+1)}{\cosh^2\theta}\right] V(z) = 0.$$

5 The general solution of the differential equation

$$\frac{d^2y}{dx^2} + \lambda y = 0$$

is given as the linear combination

$$y(x) = C_0 \sin\sqrt{\lambda}x + C_1 \cos\sqrt{\lambda}x.$$

Show that factorization of this equation leads to the trivial result with

$$k(x,m) = 0,\ \ \mu(m) = 0,$$

and the corresponding ladder operators just produce other linear combinations of $\sin\sqrt{\lambda}x$ and $\cos\sqrt{\lambda}x$.

6 Show that taking

$$k(z,m) = k_0(z) + k_1(z)m + k_2(z)m^2$$

does not lead to any new categories, except the trivial solution given in Problem 5. A similar argument works for higher powers of m.

7 Show that as long as we admit a finite number of negative powers of m in $k(z,m)$, no new factorization types appear.

8 Show that

$$\mu(m) + m^2(k_1^2 + k_1') + 2m(k_0k_1 + k_0')$$

is a periodic function of m with the period 1.
Use this result to verify

$$\mu(m) - \mu(0) = -m^2(k_1^2 + k_1') - 2m(k_0k_1 + k_0').$$

9 Derive the step-down operator in

$$y_m^{l-1}(\theta)C_{l-1,m} = \frac{C_{lm}}{\sqrt{(l-m)(l+m)}}\left\{-\sin\theta\frac{d}{d\theta} + \left(l+\frac{1}{2}\right)\cos\theta\right\} y_m^l(\theta).$$

10 Follow the same procedure used in Path I in Section 8.6.5 to derive the equation

$$y_{l+1}^{m+1}(\theta) = \frac{C_{l,m}}{C_{l+1,m}}\frac{1}{(l+1-m)}\frac{(l+1-m)}{\sqrt{(l+m+1)(l+m+2)}}$$
$$\times\left\{\cos\theta\frac{d}{d\theta} - \frac{m+\frac{1}{2}}{\sin\theta} - \left(l+\frac{1}{2}\right)\sin\theta\right\} y_l^m(\theta).$$

11 Use the factorization method to show that the spherical Hankel functions of the first kind:

$$h_l^{(1)} = j_l + i n_l,$$

can be expressed as

$$h_l^{(1)}(x) = (-1)^l x^l \left[\frac{1}{x}\frac{d}{dx}\right]^l h_0^{(1)}(x)$$
$$= (-1)^l x^l \left[\frac{1}{x}\frac{d}{dx}\right]^l \left(\frac{-ie^{ix}}{x}\right).$$

Hint: Introduce $u_l(x) = y_l(x)/x^{l+1}$ in

$$y_l'' + \left[1 - \frac{l(l+1)}{x^2}\right] y_l = 0.$$

12 Using the factorization method, find a recursion relation relating the normalized eigenfunctions $y(n, l, r)$ of the differential equation

$$\frac{d^2y}{dr^2} + \left[\frac{2}{r} - \frac{l(l+1)}{r^2}\right] y - \frac{1}{n^2} y = 0$$

to the eigenfunctions with $l \pm 1$.
Hint: First show that $l = n-1, n-2, \dots, l =$ integer and the normalization is $\int_0^\infty y^2(n, l, r)dr = 1$.

13 The harmonic oscillator equation

$$\frac{d^2\Psi}{dx^2} + (\varepsilon - x^2)\Psi(x) = 0$$

is a rather special case of the factorization method because the operators $O_\pm$ are independent of any parameter.

(i) Show that the above equation factorizes as

$$O_+ = \frac{d}{dx} - x,$$
$$O_- = -\frac{d}{dx} - x.$$

(ii) In particular, show that if $\Psi_\varepsilon(x)$ is a solution for the energy eigenvalue ε, then

$$O_+ \Psi_\varepsilon(x)$$

is a solution for $\varepsilon + 2$, while

$$O_- \Psi_\varepsilon(x)$$

is a solution for $\varepsilon - 2$.

(iii) Show that ε has a minimum

$$\varepsilon_{\min} = 1,$$

with

$$\varepsilon_n = 2n + 1, \quad n = 0, 1, 2, \ldots$$

and show that the $\varepsilon < 0$ eigenvalues are not allowed.

(iv) Using the factorization technique, find the eigenfunction corresponding to $\varepsilon_{\min}$ and then use it to express all the remaining eigenfunctions.

Hint: Use the identity

$$\left[\frac{d}{dx} - x\right]\Phi(x) = e^{x^2/2}\frac{d}{dx}\left(e^{-\frac{x^2}{2}}\Phi(x)\right).$$

14 Show that the standard method for the harmonic oscillator problem leads to a single ladder with each function on the ladder corresponding to a different eigenvalue λ. This follows from the fact that $r(z, m)$ is independent of m. The factorization we have introduced in Section 8.11 is simpler, and in fact the method of factorization originated from this treatment of the problem.

15 The spherical Bessel functions, $j_l(x)$, are related to the solutions of

$$\frac{d^2y_l}{dx^2} + \left[1 - \frac{l(l+1)}{x^2}\right]y_l(x) = 0,$$

(regular at $x = 0$) by

$$j_l(x) = \frac{y_l(x)}{x}.$$

Using the factorization technique, derive recursion formulae

(i) relating $j_l(x)$ to $j_{l+1}(x)$ and $j_{l-1}(x)$,

(ii) relating $j_l'(x)$ to $j_{l+1}(x)$ and $j_{l-1}(x)$.

16 Show that the relation in Eq. (8.348):

$$d^l_{m'm}(\beta) = d^l_{mm'}(-\beta),$$

is true.

17 Use the symmetry relation in Eq. (8.348) to check your algebra in Section 8.12.4. Also show the relation in Eq. (8.363):

$$d^l_{m'm}(\beta) = (-1)^{m'-m}d^l_{mm'}(\beta).$$

18 Complete the details of the derivation that lead to Eqs. (8.369) and (8.370).

9

Coordinates and Tensors

Using a coordinate system is probably the fastest way to introduce mathematics into the study of nature. A coordinate system in tune with the symmetries of the physical system at hand, not only simplifies the algebra but also makes the interpretation of the solution easier. Once a coordinate system is defined, physical processes can be studied in terms of operations among mathematical symbols like scalars, vectors, tensors, etc. that represents the physical properties of the system. Regularities and symmetries among the physical phenomena can now be expressed in terms of mathematical expressions as laws of nature. Naturally, the true laws of nature should not depend on what coordinate system is being used. Therefore, it should be possible to express the laws of nature in coordinate independent formalism. In this regard, tensor equations, which preserve their form under general coordinate transformations, have proven to be very useful. In this chapter, we start with the Cartesian coordinates and their transformations. We also introduce Cartesian tensors and their application to the theory of elasticity. We then generalize our discussion to generalized coordinates and general tensors. Curvature, parallel transport, geodesics are other interesting topics discussed in this chapter. The next stop in our discussion is coordinate systems in Minkowski spacetime and their transformation properties. We also introduce four-tensors in spacetime and discuss covariance of laws of nature. We finally discuss Maxwell's equations and their transformation properties.

9.1 Cartesian Coordinates

In three-dimensional Euclidean space, a Cartesian coordinate system can be constructed by choosing three mutually orthogonal straight lines. A point, **P**, can be defined either by giving its coordinates (x_1, x_2, x_3) or by using the **position vector** $\overrightarrow{r} = (x_1, x_2, x_3)$:

$$\overrightarrow{r} = x_1\widehat{\mathbf{e}}_1 + x_2\widehat{\mathbf{e}}_2 + x_3\widehat{\mathbf{e}}_3, \tag{9.1}$$

Mathematical Methods in Science and Engineering, Second Edition. Selçuk Ş. Bayın.

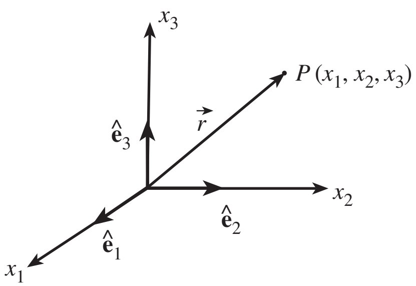

Figure 9.1 Cartesian coordinate system.

where $\hat{\mathbf{e}}_i$ are the **unit basis vectors** along the coordinate axis (Figure 9.1). Similarly, an arbitrary vector, $\vec{a}$, in Euclidean space can be defined in terms of its coordinates (a_1, a_2, a_3) as

$$\boxed{\vec{a} = a_1\hat{\mathbf{e}}_1 + a_2\hat{\mathbf{e}}_2 + a_3\hat{\mathbf{e}}_3,} \tag{9.2}$$

where the **magnitude**, a or $|\vec{a}|$, is given as

$$\boxed{a = |\vec{a}| = \sqrt{a_1^2 + a_2^2 + a_3^2}.} \tag{9.3}$$

9.1.1 Algebra of Vectors

i) **Multiplication** of a vector with a constant, c, is done by multiplying each component with that constant:

$$\boxed{c\vec{a} = (ca_1, ca_2, ca_3).} \tag{9.4}$$

ii) **Addition** or **subtraction** of vectors is done by adding or subtracting the corresponding components:

$$\boxed{\vec{a} \pm \vec{b} = (a_1 \pm b_1, a_2 \pm b_2, a_3 \pm b_3).} \tag{9.5}$$

iii) **Vector multiplication:**

a) The **dot product** or the **scalar product** of two vectors, $\vec{a}$ and $\vec{b}$, is a scalar defined as

$$\boxed{(a, b) = \vec{a} \cdot \vec{b} = ab\cos\theta_{ab},} \tag{9.6}$$

or as

$$\boxed{(a, b) = a_1b_1 + a_2b_2 + a_3b_3,} \tag{9.7}$$

where θ_{ab} is the angle between the two vectors (Figure 9.2).

b) The **cross product** or the **vector product**, $\vec{a} \times \vec{b}$, of two vectors is another vector defined as

$$\boxed{\vec{a} \times \vec{b} = (a_2b_3 - a_3b_2)\hat{\mathbf{e}}_1 + (a_3b_1 - a_1b_3)\hat{\mathbf{e}}_2 + (a_1b_2 - a_2b_1)\hat{\mathbf{e}}_3.} \tag{9.8}$$

Using the **permutation symbol**, we can write the components of a vector product as

$$\boxed{\left(\vec{a} \times \vec{b}\right)_i = \sum\nolimits_{j,k=1}^{3} \epsilon_{ijk} a_j b_k,} \tag{9.9}$$

where the permutation symbol takes the values

$$\boxed{\epsilon_{ijk} = \begin{cases} +1 & \text{for cyclic permutations,} \\ 0 & \text{when any two indices are equal,} \\ -1 & \text{for anticyclic permutations.} \end{cases}} \tag{9.10}$$

The **magnitude** of a vector product is given as

$$\boxed{\left|\vec{a} \times \vec{b}\right| = ab \sin\theta_{ab},} \tag{9.11}$$

where the direction is conveniently found by the right-hand rule (Figure 9.2).

9.1.2 Differentiation of Vectors

In Cartesian coordinates, motion of a particle is described by giving its position as a function of time (Figure 9.3):

$$\vec{r}(t) = (x_1(t), x_2(t), x_3(t)). \tag{9.12}$$

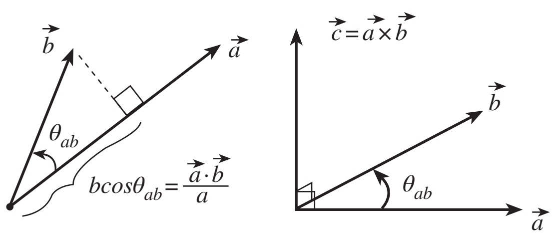

Figure 9.2 Scalar and vector products.

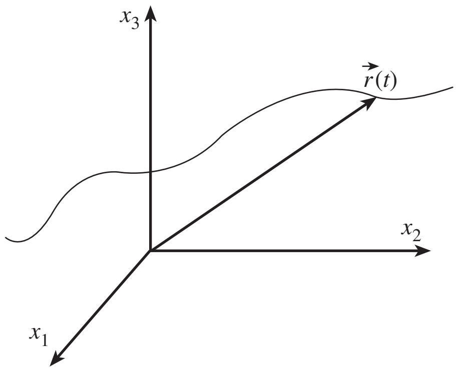

Figure 9.3 Motion in Cartesian coordinates.

Velocity, $\vec{v}$, and acceleration, $\vec{a}$, are now defined as the derivatives

$$\begin{aligned}\vec{v} &= \frac{d\vec{r}}{dt} = \lim_{\Delta t \to 0} \frac{\vec{r}(t+\Delta t) - \vec{r}(t)}{\Delta t} \\ &= \frac{dx_1}{dt}\hat{\mathbf{e}}_1 + \frac{dx_2}{dt}\hat{\mathbf{e}}_2 + \frac{dx_3}{dt}\hat{\mathbf{e}}_3,\end{aligned} \tag{9.13}$$

and

$$\begin{aligned}\vec{a} &= \frac{d\vec{v}}{dt} = \lim_{\Delta t \to 0} \frac{\vec{v}(t+\Delta t) - \vec{v}(t)}{\Delta t} \\ &= \frac{dv_1}{dt}\hat{\mathbf{e}}_1 + \frac{dv_2}{dt}\hat{\mathbf{e}}_2 + \frac{dv_3}{dt}\hat{\mathbf{e}}_3.\end{aligned} \tag{9.14}$$

Similarly, the derivative of a general vector, $\vec{A}$, with respect to a parameter, t, is defined as

$$\frac{d\vec{A}}{dt} = \lim_{\Delta t \to 0} \frac{\vec{A}(t+\Delta t) - \vec{A}(t)}{\Delta t}, \tag{9.15}$$

thus

$$\boxed{\frac{d\vec{A}}{dt} = \frac{dA_1}{dt}\hat{\mathbf{e}}_1 + \frac{dA_2}{dt}\hat{\mathbf{e}}_2 + \frac{dA_3}{dt}\hat{\mathbf{e}}_3.} \tag{9.16}$$

Generalization of these equations to n dimensions is obvious.

9.2 Orthogonal Transformations

There are many ways to choose the orientation of the Cartesian axes. Symmetries of the physical system often make certain orientations more advantageous than the others. In general, we need a dictionary to translate the coordinates

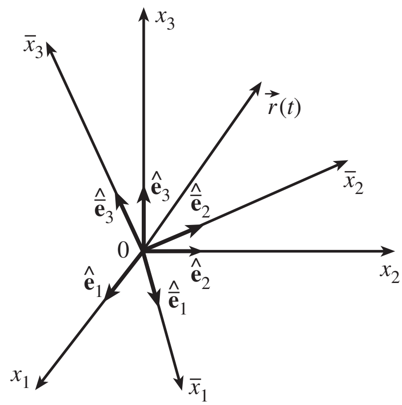

Figure 9.4 Unit basis vectors.

assigned in one Cartesian system to another. A connection between the components of the position vector, $\overrightarrow{r}$, assigned by two sets of Cartesian axes with a common origin (Figure 9.4),

$$\overrightarrow{r} = x_1\hat{\mathbf{e}}_1 + x_2\hat{\mathbf{e}}_2 + x_3\hat{\mathbf{e}}_3, \tag{9.17}$$

$$\overrightarrow{r} = \bar{x}_1\hat{\bar{\mathbf{e}}}_1 + \bar{x}_2\hat{\bar{\mathbf{e}}}_2 + \bar{x}_3\hat{\bar{\mathbf{e}}}_3, \tag{9.18}$$

can be obtained as

$$\begin{aligned}
\bar{x}_1 &= (\hat{\bar{\mathbf{e}}}_1 \cdot \overrightarrow{r}) = x_1(\hat{\bar{\mathbf{e}}}_1 \cdot \hat{\mathbf{e}}_1) + x_2(\hat{\bar{\mathbf{e}}}_1 \cdot \hat{\mathbf{e}}_2) + x_3(\hat{\bar{\mathbf{e}}}_1 \cdot \hat{\mathbf{e}}_3),\\
\bar{x}_2 &= (\hat{\bar{\mathbf{e}}}_2 \cdot \overrightarrow{r}) = x_1(\hat{\bar{\mathbf{e}}}_2 \cdot \hat{\mathbf{e}}_1) + x_2(\hat{\bar{\mathbf{e}}}_2 \cdot \hat{\mathbf{e}}_2) + x_3(\hat{\bar{\mathbf{e}}}_2 \cdot \hat{\mathbf{e}}_3),\\
\bar{x}_3 &= (\hat{\bar{\mathbf{e}}}_3 \cdot \overrightarrow{r}) = x_1(\hat{\bar{\mathbf{e}}}_3 \cdot \hat{\mathbf{e}}_1) + x_2(\hat{\bar{\mathbf{e}}}_3 \cdot \hat{\mathbf{e}}_2) + x_3(\hat{\bar{\mathbf{e}}}_3 \cdot \hat{\mathbf{e}}_3),
\end{aligned} \tag{9.19}$$

which can also be written as

$$\boxed{\begin{aligned}
\bar{x}_1 &= (\cos\theta_{11})\,x_1 + (\cos\theta_{12})x_2 + (\cos\theta_{13})x_3,\\
\bar{x}_2 &= (\cos\theta_{21})\,x_1 + (\cos\theta_{22})x_2 + (\cos\theta_{23})x_3,\\
\bar{x}_3 &= (\cos\theta_{31})\,x_1 + (\cos\theta_{32})x_2 + (\cos\theta_{33})x_3.
\end{aligned}} \tag{9.20}$$

In these equations, $\cos\theta_{ij}$ are called the **direction cosines** defined as

$$\boxed{\cos\theta_{ij} = \hat{\bar{\mathbf{e}}}_i \cdot \hat{\mathbf{e}}_j.} \tag{9.21}$$

Note that the first unit basis vector is always taken as the barred system, that is,

$$\cos\theta_{ji} = \hat{\bar{\mathbf{e}}}_j \cdot \hat{\mathbf{e}}_i. \tag{9.22}$$

The **transformation equations** obtained for the position vector are also true for an arbitrary vector, $\overrightarrow{a}$, as

$$\boxed{\begin{aligned}\bar{a}_1 &= (\cos\theta_{11})\,a_1 + (\cos\theta_{12})a_2 + (\cos\theta_{13})a_3,\\ \bar{a}_2 &= (\cos\theta_{21})\,a_1 + (\cos\theta_{22})a_2 + (\cos\theta_{23})a_3,\\ \bar{a}_3 &= (\cos\theta_{31})\,a_1 + (\cos\theta_{32})a_2 + (\cos\theta_{33})a_3.\end{aligned}} \tag{9.23}$$

The transformation equations given in Eq. (9.23) are the special case of **general linear transformation**, which can be written as

$$\begin{aligned}\bar{x}_1 &= a_{11}x_1 + a_{12}x_2 + a_{13}x_3,\\ \bar{x}_2 &= a_{21}x_1 + a_{22}x_2 + a_{23}x_3,\\ \bar{x}_3 &= a_{31}x_1 + a_{32}x_2 + a_{33}x_3,\end{aligned} \tag{9.24}$$

where a_{ij} are constants independent of $\overrightarrow{r}$ and $\overrightarrow{\bar{r}}$. Using the **Einstein summation convention**, Eq. (9.24) can also be written as

$$\bar{x}_i = a_{ij}x_j, \tag{9.25}$$

where summation over the repeated indices, which are also called the **dummy indices,** is implied. In other words, Eq. (9.25) means

$$\bar{x}_i = a_{ij}x_j \tag{9.26}$$

$$= \sum_{j=1}^{3} a_{ij}x_j. \tag{9.27}$$

In Eq. (9.26), the **free index**, i, can take the values $1, 2, 3$. Unless otherwise stated, we will use the Einstein summation convention. Magnitude of $\overrightarrow{r}$ in this notation is shown as $r = \sqrt{x_i x_i}$.

Using matrix notation [1], transformation equations (9.24) can also be written as

$$\boxed{\bar{\mathbf{r}} = \mathbf{A}\mathbf{r},} \tag{9.28}$$

where $\mathbf{r}$ and $\bar{\mathbf{r}}$ are represented by the **column matrices**:

$$\mathbf{r} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}, \quad \bar{\mathbf{r}} = \begin{bmatrix} \bar{x}_1 \\ \bar{x}_2 \\ \bar{x}_3 \end{bmatrix}, \tag{9.29}$$

and the **transformation matrix**, **A**, is represented by the **square matrix**

$$\mathbf{A} = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}. \tag{9.30}$$

We use both boldface letter **r** and $\overrightarrow{r}$ to denote a vector. Generalization of these formulas to n dimensions is again obvious. The **transpose** of a matrix is obtained by interchanging its rows and columns. For example, the transpose of **r** is a **row matrix**:

$$\widetilde{\mathbf{r}} = \begin{bmatrix} x_1 & x_2 & x_3 \end{bmatrix} \tag{9.31}$$

and the transpose of **A** is written as

$$\widetilde{\mathbf{A}} = \begin{bmatrix} a_{11} & a_{21} & a_{31} \\ a_{12} & a_{22} & a_{32} \\ a_{13} & a_{23} & a_{33} \end{bmatrix}. \tag{9.32}$$

We can now write the square of the magnitude of **r** as

$$\begin{aligned} r^2 &= \widetilde{\mathbf{r}}\mathbf{r} = \begin{bmatrix} x_1 & x_2 & x_3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \\ &= x_1^2 + x_2^2 + x_3^2. \end{aligned} \tag{9.33}$$

The magnitude squared of $\bar{\mathbf{r}}$ is now given as

$$\widetilde{\bar{\mathbf{r}}}\,\bar{\mathbf{r}} = \widetilde{\mathbf{r}}\left(\widetilde{\mathbf{A}}\mathbf{A}\right)\mathbf{r}, \tag{9.34}$$

where we have used the matrix property

$$\widetilde{\mathbf{AB}} = \widetilde{\mathbf{B}}\widetilde{\mathbf{A}}. \tag{9.35}$$

From Eq. (9.34), it is seen that linear transformations that preserve the length of a vector must satisfy the condition

$$\boxed{\widetilde{\mathbf{A}}\mathbf{A} = \mathbf{I},} \tag{9.36}$$

where **I** is the **identity matrix**:

$$\boxed{\mathbf{I} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}.} \tag{9.37}$$

Such transformations are called **orthogonal transformations**. In terms of components, the **orthogonality condition** [Eq. (9.36)] can be written as

$$\boxed{[\widetilde{\mathbf{A}}]_{ik}[\mathbf{A}]_{kj} = a_{ki}a_{kj} = \delta_{ij}.} \tag{9.38}$$

Taking the determinant of the orthogonality relation, we see that the determinant of transformations that preserve the length of a vector satisfies

$$[\det \mathbf{A}]^2 = 1, \tag{9.39}$$

thus

$$\boxed{\det \mathbf{A} = \pm 1.} \tag{9.40}$$

Orthogonal transformations are basically transformations among Cartesian coordinates without a scale change. Transformations with $\det \mathbf{A} = 1$ are called **proper transformations**. They are composed of rotations and translations. Transformations with $\det \mathbf{A} = -1$ are called **improper transformations**, which involve reflections.

9.2.1 Rotations About Cartesian Axes

For rotations about the x_3-axis, the rotation matrix takes the form

$$\mathbf{R}_3 = \begin{bmatrix} a_{11} & a_{12} & 0 \\ a_{21} & a_{22} & 0 \\ 0 & 0 & 1 \end{bmatrix}. \tag{9.41}$$

Using the direction cosines [Eqs. (9.20) and (9.21)], we can write $R_3(\theta)$ for counterclockwise rotations as (Figure 9.5)

$$\mathbf{R}_3(\theta) = \begin{bmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{bmatrix}. \tag{9.42}$$

Similarly, the rotation matrices corresponding to counterclockwise rotations about the x_1- and x_2-axis can be written, respectively, as

$$\mathbf{R}_1(\phi) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\phi & \sin\phi \\ 0 & -\sin\phi & \cos\phi \end{bmatrix}, \quad \mathbf{R}_2(\psi) = \begin{bmatrix} \cos\psi & 0 & -\sin\psi \\ 0 & 1 & 0 \\ \sin\psi & 0 & \cos\psi \end{bmatrix}. \tag{9.43}$$

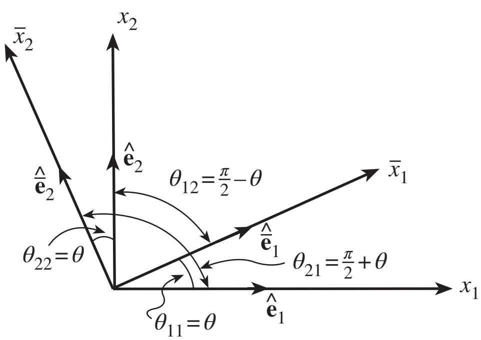

Figure 9.5 Angles for the direction cosines in $R_3(\theta)$.

9.2.2 Formal Properties of the Rotation Matrix

(i) Two sequentially performed rotations, **A** and **B**, are equivalent to another rotation, **C**, as

$$\boxed{\mathbf{C} = \mathbf{AB}.} \tag{9.44}$$

(ii) Because matrix multiplications do not commute, the order of rotations is important, that is, in general

$$\boxed{\mathbf{AB} \neq \mathbf{BA}.} \tag{9.45}$$

However, the **associative law** holds between any three rotations $\mathbf{A}, \mathbf{B}$, and $\mathbf{C}$:

$$\boxed{\mathbf{A}(\mathbf{BC}) = (\mathbf{AB})\mathbf{C}.} \tag{9.46}$$

(iii) The **inverse** transformation matrix $\mathbf{A}^{-1}$ exists, and from the orthogonality relation [Eq. (19.36)], it is equal to the **transpose** of **A**, that is,

$$\boxed{\mathbf{A}^{-1} = \widetilde{\mathbf{A}}.} \tag{9.47}$$

Thus for **orthogonal transformations**, we can write

$$\boxed{\widetilde{\mathbf{A}}\mathbf{A} = \mathbf{A}\widetilde{\mathbf{A}} = \mathbf{I}.} \tag{9.48}$$

9.2.3 Euler Angles and Arbitrary Rotations

The most general rotation matrix has nine components [Eq. (9.30)]. However, the orthogonality relation, $\mathbf{A}\widetilde{\mathbf{A}} = \mathbf{I}$, written explicitly as

$$\begin{aligned}
a_{11}^2 + a_{12}^2 + a_{13}^2 &= 1, \\
a_{22}^2 + a_{21}^2 + a_{23}^2 &= 1, \\
a_{33}^2 + a_{31}^2 + a_{32}^2 &= 1, \\
a_{11}a_{21} + a_{12}a_{22} + a_{13}a_{23} &= 0, \\
a_{11}a_{31} + a_{12}a_{32} + a_{13}a_{33} &= 0, \\
a_{21}a_{31} + a_{22}a_{32} + a_{23}a_{33} &= 0,
\end{aligned} \tag{9.49}$$

gives six relations among these components. Hence, only three of them can be independent. In the study of rotating systems, to describe the orientation of a system, it is important to define a set of three independent parameters. There are a number of choices. The most common and useful are the three

Euler angles. They correspond to three successive rotations about the Cartesian axes so that the final orientation of the system is obtained. The convention we follow is the most widely used one in applied mechanics, in celestial mechanics, and frequently, in molecular and solid-state physics. For different conventions, we refer the reader to Goldstein *et al.* [4].

The sequence starts with a counterclockwise rotation by ϕ about the x_3-axis of the initial state of the system as

$$\boxed{\mathbf{B}(\phi)\colon\ (x_1, x_2, x_3) \to (x'_1, x'_2, x'_3).} \tag{9.50}$$

This is followed by a counterclockwise rotation by θ about the x'_1 of the intermediate axis as

$$\boxed{\mathbf{C}(\theta)\colon\ (x'_1, x'_2, x'_3) \to (x''_1, x''_2, x''_3).} \tag{9.51}$$

Finally, the desired orientation is achieved by a counterclockwise rotation about the x''_3-axis by ψ as

$$\boxed{\mathbf{D}(\psi)\colon\ (x''_1, x''_2, x''_3) \to (\bar{x}_1, \bar{x}_2, \bar{x}_3).} \tag{9.52}$$

Here, $\mathbf{A}(\phi)$, $\mathbf{B}(\theta)$, and $\mathbf{C}(\psi)$ are the rotation matrices for the corresponding transformations, which are given as

$$\mathbf{B}(\phi) = \begin{bmatrix} \cos\phi & \sin\phi & 0 \\ -\sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{bmatrix}, \tag{9.53}$$

$$\mathbf{C}(\phi) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & \sin\theta \\ 0 & -\sin\theta & \cos\theta \end{bmatrix}, \tag{9.54}$$

$$\mathbf{D}(\psi) = \begin{bmatrix} \cos\psi & \sin\psi & 0 \\ -\sin\psi & \cos\psi & 0 \\ 0 & 0 & 1 \end{bmatrix}. \tag{9.55}$$

In terms of the individual rotation matrices, the complete transformation matrix, $\mathbf{A}$, can be written as the product $\mathbf{A} = \mathbf{DCB}$, thus

$$\mathbf{A} = \begin{bmatrix} \cos\psi\cos\phi - \cos\theta\sin\phi\sin\psi & \cos\psi\sin\phi + \cos\theta\cos\phi\sin\psi & \sin\psi\sin\theta \\ -\sin\psi\cos\phi - \cos\theta\sin\phi\cos\psi & -\sin\psi\sin\phi + \cos\theta\cos\phi\cos\psi & \cos\psi\sin\theta \\ \sin\theta\sin\phi & -\sin\theta\cos\phi & \cos\theta \end{bmatrix}. \tag{9.56}$$

The inverse of **A** is $\mathbf{A}^{-1} = \widetilde{\mathbf{A}}$. We can also consider the elements of the rotation matrix as a function of some single parameter, t, and write

$$\phi = \omega_\phi t, \quad \omega = \omega_\theta t, \quad \psi = \omega_\psi t. \tag{9.57}$$

If t is taken as time, ω can be interpreted as the constant angular velocity about the axis of rotation.

In general, the rotation matrix can be written as

$$\mathbf{A}(t) = \begin{bmatrix} a_{11}(t) & a_{12}(t) & a_{13}(t) \\ a_{21}(t) & a_{22}(t) & a_{23}(t) \\ a_{31}(t) & a_{32}(t) & a_{33}(t) \end{bmatrix}. \tag{9.58}$$

Using trigonometric identities, it can be shown that

$$\boxed{\mathbf{A}(t_2 + t_1) = \mathbf{A}(t_2)\mathbf{A}(t_1).} \tag{9.59}$$

Differentiating with respect to t_2 and putting $t_2 = 0$ and $t_1 = t$, we obtain a result that will be useful shortly as

$$\boxed{\mathbf{A}'(t) = \mathbf{A}'(0)\mathbf{A}(t).} \tag{9.60}$$

9.2.4 Active and Passive Interpretations of Rotations

It is possible to view the rotation matrix, **A**, in

$$\bar{\mathbf{r}} = \mathbf{A}\mathbf{r} \tag{9.61}$$

as an operator acting on **r** and rotating it in the opposite direction (clockwise), while keeping the coordinate axes fixed (Figure 9.6b).

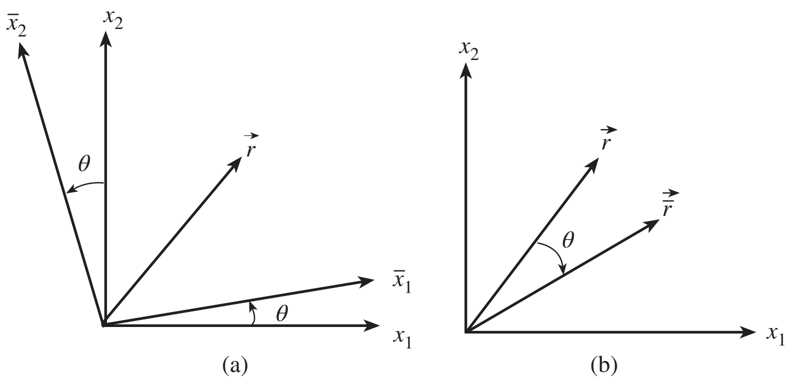

Figure 9.6 Passive and active views of the rotation matrix.

This is called the **active view**. The case where $\mathbf{r}$ is fixed but the coordinate axes are rotated counterclockwise is called the **passive view** (Figure 9.6a). In principle, both the active and passive views lead to the same result. However, as in quantum mechanics, sometimes the active view may offer some advantages in studying the symmetries of a physical system.

In the case of the active view, we also need to know how an operator, $\mathbf{A}$, transforms under coordinate transformations. Considering a transformation represented by the matrix $\mathbf{B}$, we multiply both sides of Eq. (9.61) by $\mathbf{B}$ to write

$$\mathbf{B}\bar{\mathbf{r}} = \mathbf{BAr}. \tag{9.62}$$

Using $\mathbf{BB}^{-1} = \mathbf{B}^{-1}\mathbf{B} = \mathbf{I}$, we now write Eq. (9.62) as

$$\mathbf{B}\bar{\mathbf{r}} = \mathbf{BAB}^{-1}\mathbf{Br}, \tag{9.63}$$

$$\bar{\mathbf{r}}' = \mathbf{A}'\mathbf{r}'. \tag{9.64}$$

In the new coordinate system, $\bar{\mathbf{r}}$ and $\mathbf{r}$ are related by $\bar{\mathbf{r}}' = \mathbf{B}\bar{\mathbf{r}}$ and $\mathbf{r}' = \mathbf{Br}$. Thus the operator $\mathbf{A}'$ becomes

$$\boxed{\mathbf{A}' = \mathbf{BAB}^{-1}.} \tag{9.65}$$

This is called **similarity transformation**. If $\mathbf{B}$ is an **orthogonal transformation**, we then write

$$\boxed{\mathbf{A}' = \mathbf{BA}\widetilde{\mathbf{B}}.} \tag{9.66}$$

In terms of components, this can also be written as

$$a'_{ij} = b_{ik}a_{kl}b_{jl}. \tag{9.67}$$

9.2.5 Infinitesimal Transformations

A proper orthogonal transformation depending on a single continuous parameter t can be shown as

$$\mathbf{r}(t) = \mathbf{A}(t)\mathbf{r}(0). \tag{9.68}$$

Differentiating and using Eq. (9.60), we obtain

$$\frac{d\mathbf{r}(t)}{dt} = \mathbf{A}'(t)\mathbf{r}(0) \tag{9.69}$$

$$= \mathbf{A}'(0)\mathbf{A}(t)\mathbf{r}(0) \tag{9.70}$$

$$= \mathbf{Xr}(t), \tag{9.71}$$

where

$$\boxed{\mathbf{X} = \mathbf{A}'(0).} \tag{9.72}$$

Differentiating Eq. (9.71), we can now obtain the higher-order derivatives as

$$\begin{aligned}\frac{d^2\mathbf{r}(t)}{dt^2} &= \mathbf{X}^2\mathbf{r}(t),\\ \frac{d^3\mathbf{r}(t)}{dt^3} &= \mathbf{X}^3\mathbf{r}(t),\\ &\vdots\end{aligned} \tag{9.73}$$

Using these in the **Taylor series** expansion of $\mathbf{r}(t)$ about $t = 0$, we write

$$\mathbf{r}(t) = \mathbf{r}(0) + \frac{d\mathbf{r}(0)}{dt}t + \frac{1}{2!}\frac{d^2\mathbf{r}(0)}{dt^2}t^2 + \cdots, \tag{9.74}$$

thus obtaining

$$\mathbf{r}(t) = \left(\mathbf{I} + \mathbf{X}t + \frac{1}{2!}\mathbf{X}^2t^2 + \cdots\right)\mathbf{r}(0). \tag{9.75}$$

This series converges, yielding

$$\boxed{\mathbf{r}(t) = \exp(\mathbf{X}t)\mathbf{r}(0).} \tag{9.76}$$

This is called the **exponential form** of the transformation matrix. For infinitesimal transformations, t is small; hence, we can write

$$\mathbf{r}(t) \simeq (\mathbf{I} + \mathbf{X}t)\mathbf{r}(0), \tag{9.77}$$

$$\mathbf{r}(t) - \mathbf{r}(0) \simeq \mathbf{X}t\mathbf{r}(0), \tag{9.78}$$

$$\delta\mathbf{r} \simeq \mathbf{X}t\mathbf{r}(0), \tag{9.79}$$

where $\mathbf{X}$ is called the **generator** of the infinitesimal transformation.

Using the definition of $\mathbf{X}$ in Eq. (9.72) and the rotation matrices [Eqs. (9.42) and (9.43)], we can write the generators as

$$\boxed{\mathbf{X}_1 = \begin{bmatrix}0 & 0 & 0\\ 0 & 0 & 1\\ 0 & -1 & 0\end{bmatrix},\quad \mathbf{X}_2 = \begin{bmatrix}0 & 0 & -1\\ 0 & 0 & 0\\ 1 & 0 & 0\end{bmatrix},\quad \mathbf{X}_3 = \begin{bmatrix}0 & 1 & 0\\ -1 & 0 & 0\\ 0 & 0 & 0\end{bmatrix}.} \tag{9.80}$$

An arbitrary infinitesimal rotation by the amounts t_1, t_2, and t_3 about their respective axes can be written as

$$\mathbf{r} = (\mathbf{I} + \mathbf{X}_3t_3)(\mathbf{I} + \mathbf{X}_2t_2)(\mathbf{I} + \mathbf{X}_1t_1)\mathbf{r}(0) \tag{9.81}$$

$$= (\mathbf{I} + \mathbf{X}_3t_3 + \mathbf{X}_2t_2 + \mathbf{X}_1t_1)\mathbf{r}(0). \tag{9.82}$$

Defining the vector

$$\mathbf{X} = \mathbf{X}_1\hat{\mathbf{e}}_1 + \mathbf{X}_2\hat{\mathbf{e}}_2 + \mathbf{X}_3\hat{\mathbf{e}}_3 \tag{9.83}$$

$$= (\mathbf{X}_1, \mathbf{X}_2, \mathbf{X}_3) \tag{9.84}$$

and the unit vector

$$\hat{\mathbf{n}} = \frac{1}{\sqrt{t_1^2 + t_2^2 + t_3^2}} \begin{bmatrix} t_1 \\ t_2 \\ t_3 \end{bmatrix}, \tag{9.85}$$

we can write Eq. (9.82) as

$$\boxed{\mathbf{r}(t) = (\mathbf{I} + \mathbf{X} \cdot \hat{\mathbf{n}}t)\mathbf{r}(0),} \tag{9.86}$$

where $t = \sqrt{t_1^2 + t_2^2 + t_3^2}$. This is an **infinitesimal rotation** about an axis in the direction $\hat{\mathbf{n}}$ by the amount t. For **finite rotations**, we write

$$\boxed{\mathbf{r}(t) = e^{\mathbf{X} \cdot \hat{\mathbf{n}}t}\mathbf{r}(0).} \tag{9.87}$$

9.2.6 Infinitesimal Transformations Commute

Two successive infinitesimal transformations by the amounts t_1 and t_2 can be written as

$$\mathbf{r} = (\mathbf{I} + \mathbf{X}_2 t_2)(\mathbf{I} + \mathbf{X}_1 t_1)\mathbf{r}(0) \tag{9.88}$$

$$= [\mathbf{I} + (t_1\mathbf{X}_1 + t_2\mathbf{X}_2)]\mathbf{r}(0). \tag{9.89}$$

Because matrices commute with respect to addition and subtraction, infinitesimal transformations also commute, that is,

$$\mathbf{r} = [\mathbf{I} + (t_2\mathbf{X}_2 + t_1\mathbf{X}_1)]\ \mathbf{r}(0) \tag{9.90}$$

$$= (\mathbf{I} + \mathbf{X}_1 t_1)(\mathbf{I} + \mathbf{X}_2 t_2)\mathbf{r}(0). \tag{9.91}$$

For finite rotations, this is clearly not true. Using Eq. (9.43), we can write the rotation matrix for a rotation about the x_2-axis followed by a rotation about the x_1-axis as

$$\mathbf{R}_1\mathbf{R}_2 = \begin{bmatrix} \cos\psi & 0 & -\sin\psi \\ \sin\phi\sin\psi & \cos\phi & \sin\phi\cos\psi \\ \cos\phi\sin\psi & -\sin\phi & \cos\phi\cos\psi \end{bmatrix}. \tag{9.92}$$

Reversing the order, we get

$$\mathbf{R}_2\mathbf{R}_1 = \begin{bmatrix} \cos\psi & \sin\psi\sin\phi & -\sin\psi\cos\phi \\ 0 & \cos\phi & \sin\phi \\ \sin\psi & -\cos\psi\sin\phi & \cos\psi\cos\phi \end{bmatrix}. \tag{9.93}$$

It is clear that for finite rotations, these two matrices are not equal:

$$\mathbf{R}_1\mathbf{R}_2 \neq \mathbf{R}_2\mathbf{R}_1. \tag{9.94}$$

However, for small rotations by the amounts $\delta\psi$ and $\delta\phi$, we can use the approximations

$$\sin\delta\psi \simeq \delta\psi, \quad \sin\delta\phi \simeq \delta\phi, \tag{9.95}$$

$$\cos\delta\psi \simeq 1, \quad \cos\delta\phi \simeq 1, \tag{9.96}$$

to find

$$\mathbf{R}_1\mathbf{R}_2 = \begin{bmatrix} 1 & 0 & -\delta\psi \\ \delta\psi & 1 & \delta\phi \\ \delta\psi & -\delta\phi & 1 \end{bmatrix} = \mathbf{R}_2\mathbf{R}_1. \tag{9.97}$$

Note that in terms of the generators [Eq. (9.80)], we can also write this as

$$\mathbf{R}_1\mathbf{R}_2 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} + \delta\psi \begin{bmatrix} 0 & 0 & -1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix} + \delta\phi \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{bmatrix} \tag{9.98}$$

$$= \mathbf{I} + \delta\psi\mathbf{X}_1 + \delta\phi\mathbf{X}_2 \tag{9.99}$$

$$= \mathbf{I} + \delta\phi\mathbf{X}_2 + \delta\psi\mathbf{X}_1 \tag{9.100}$$

$$= \mathbf{R}_2\mathbf{R}_1, \tag{9.101}$$

which again proves that infinitesimal rotations commute.

9.3 Cartesian Tensors

Certain physical properties like temperature and mass can be described completely by giving a single number. They are called **scalars**. Under orthogonal transformations, scalars preserve their value. Distance, speed, and charge are other examples of scalars. On the other hand, **vectors** in three dimensions require three numbers for a complete description, that is, their components (a_1, a_2, a_3). Under orthogonal transformations, we have seen that vectors transform as $a'_i = A_{ij}a_j$.

There are also physical properties that in three dimensions require nine components for a complete description. For example, stresses in a solid have nine components that can be conveniently represented as a 3×3 matrix:

$$t_{ij} = \begin{bmatrix} t_{11} & t_{12} & t_{13} \\ t_{21} & t_{22} & t_{23} \\ t_{31} & t_{32} & t_{33} \end{bmatrix}. \tag{9.102}$$

Components of the stress tensor, t_{ij}, correspond to the forces acting on a unit area element, where t_{ij} is the ith component of the force acting on the unit area element when the normal is pointing along the jth axis. Under orthogonal transformations, stresses transform as $t'_{ij} = A_{ik}A_{jl}t_{kl}$. Stresses, vectors, and scalars are special cases of a more general type of objects called **tensors**.

In general, **Cartesian tensors** are defined in terms of their transformation properties under **orthogonal transformations** as

$$\boxed{T_{ijk\dots} = A_{ii'}A_{jj'}A_{kk'}\dots T_{i'j'k'\dots}.} \tag{9.103}$$

All indices take the values $1, 2, 3, \dots, n$, where n is the dimension of space. An important property of tensors is their **rank**, which is equal to the number of **free indices**. In this regard, scalars are tensors of zeroth-rank, vectors are tensors of first-rank, and stress tensor is a second-rank tensor.

9.3.1 Operations with Cartesian Tensors

For operations with Cartesian tensors, the following rules apply:

(i) **Multiplication** with aconstant is accomplished by multiplying each component of the tensor with that constant.

(ii) **Addition or subtraction** of tensors of equal rank can be done by adding or subtracting the corresponding tensors term by term.

(iii) **Rank** of a composite tensor is equal to the number of its free indices. For example, $A_{ikj}B_{jlm}$ is a fourth-rank tensor, since there is summation over the index j. Similarly, $A_{ijk}B_{ijk}$ is a scalar, and $A_{ijkl}B_{jkl}$ is a vector.

(iv) We can obtain a lower-rank tensor by **contracting**, in other words, by summing over some of the indices of a tensor or by contracting the indices of a tensor with another tensor:

$$\begin{aligned} A_{ij} &= A_{ikkj}, \\ A_{ijk} &= D_{ijklm}B_{lm}, \\ A_{ij} &= C_{ijk}D_k. \end{aligned} \tag{9.104}$$

For a second-rank tensor, by contracting the two indices, we obtain a scalar called the **trace**:

$$A = A_{ii} = A_{11} + A_{22} + A_{33} + \cdots + A_{nn}. \tag{9.105}$$

(v) In a tensor equation, **rank** of both sides must match, that is,

$$A_{ij\dots n} = B_{ij\dots n}. \tag{9.106}$$

(vi) We have seen that tensors are defined with respect to their transformation properties. For example, from two vectors, a_i and b_j, we can form a second-rank tensor t_{ij} as $t_{ij} = a_ib_j$. This is also called the **outer product** of two vectors. The fact that t_{ij} is a second-rank tensor can easily be verified by checking its transformation properties under orthogonal transformations.

9.3.2 Tensor Densities or Pseudotensors

Let us now consider the **Kronecker delta**, which is defined in all coordinates as

$$\boxed{\delta_{ij} = \begin{cases} 1, & \text{for } i = j, \\ 0, & \text{for } i \neq j. \end{cases}} \tag{9.107}$$

To see that it is a second-rank tensor, we check how it transforms under orthogonal transformations, that is,

$$\delta'_{ij} = a_{ik}a_{jl}\delta_{kl} \tag{9.108}$$

$$= a_{ik}a_{jk}. \tag{9.109}$$

From the orthogonality relation [Eq. (9.48)], this gives $\delta'_{ij} = \delta_{ij}$. Hence the Kronecker delta is a second-rank tensor.

Let us now investigate the tensor property of the **permutation symbol** or the **Levi-Civita symbol**. It is defined in all coordinates as

$$\boxed{\epsilon_{ijk} = \begin{cases} +1 & \text{for cyclic permutations,} \\ 0 & \text{when any two indices are equal,} \\ -1 & \text{for anticyclic permutations.} \end{cases}} \tag{9.110}$$

For ϵ_{ijk} to be a third-rank tensor, it must transform as

$$\epsilon'_{ijk} = a_{il}a_{jm}a_{kn}\epsilon_{lmn} \tag{9.111}$$

$$= \epsilon_{ijk}. \tag{9.112}$$

However, using the definition of a determinant, one can show that the right-hand side is

$$\epsilon'_{ijk} = \epsilon_{ijk} \det a, \tag{9.113}$$

thus if we admit improper transformations where $\det a = -1$, ϵ_{ijk} is not a tensor. A tensor that transforms according to the law

$$\boxed{T'_{ijk\ldots} = a_{il}a_{jm}a_{kn} \cdots T_{lmn\ldots} \det a} \tag{9.114}$$

is called a **pseudotensor** or a **tensor density**.

The **cross product** of two vectors, $\vec{c} = \vec{a} \times \vec{b}$, which in terms of coordinates can be written as $c_i = \epsilon_{ijk}a_jb_k$, is a **pseudovector**, whereas the **triple product**:

$$\boxed{\vec{c} \cdot (\vec{a} \times \vec{b}) = \epsilon_{ijk}c_i \ a_jb_k,} \tag{9.115}$$

is a **pseudoscalar**.

9.4 Cartesian Tensors and the Theory of Elasticity

We now elaborate the basic features of Cartesian tensors through their application to the theory of elasticity.

9.4.1 Strain Tensor

All bodies deform under stress, where every point, $\overrightarrow{r}$, of the undeformed body is translated into another point, $\overrightarrow{r}'$, of the deformed body (Figure 9.7):

$$\overrightarrow{r}' = \overrightarrow{r} + \overrightarrow{\eta}(\overrightarrow{r}). \tag{9.116}$$

We can also write

$$x_i' = x_i + \eta_i, \quad i = 1, 2, 3. \tag{9.117}$$

The distance between two infinitesimally close points is given as

$$d\overrightarrow{r}^2 = (dx_1^2 + dx_2^2 + dx_3^2)^{1/2}, \tag{9.118}$$

which after deformation becomes

$$d\overrightarrow{r}'^2 = (dx_1'^2 + dx_2'^2 + dx_3'^2)^{1/2}. \tag{9.119}$$

Using Eq. (9.117), we can write

$$dx_i' = dx_i + d\eta_i \tag{9.120}$$

$$= dx_i + \sum_{k=1}^{3} \frac{\partial \eta_i}{\partial x_k} dx_k. \tag{9.121}$$

Adopting the **Einstein summation convention**, where repeated indices are summed over, we can ignore the summation sign in Eq. (9.121):

$$dx_i' = x_i + \frac{\partial \eta_i}{\partial x_k} dx_k, \tag{9.122}$$

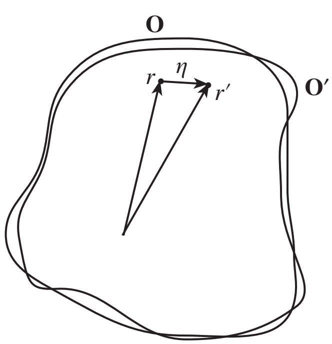

Figure 9.7 In a general deformation, every point is displaced.

which allows us to write the distance between two infinitesimally close points after deformation as

$$\overrightarrow{dr}'^2 = dx_i'dx_i' = \left(dx_i + \frac{\partial \eta_i}{\partial x_k}dx_k\right)\left(dx_i + \frac{\partial \eta_i}{\partial x_l}dx_l\right) \tag{9.123}$$

$$= dx_idx_i + \frac{\partial \eta_i}{\partial x_l}dx_idx_l + \frac{\partial \eta_i}{\partial x_k}dx_idx_k + \frac{\partial \eta_i}{\partial x_k}\frac{\partial \eta_i}{\partial x_l}dx_kdx_l. \tag{9.124}$$

This can also be written as

$$\overrightarrow{dr}'^2 = \overrightarrow{dr}^2 + 2e_{kl}dx_kdx_l, \tag{9.125}$$

where

$$e_{kl} = \frac{1}{2}\left(\frac{\partial \eta_k}{\partial x_l} + \frac{\partial \eta_l}{\partial x_k} + \frac{\partial \eta_i}{\partial x_k}\frac{\partial \eta_i}{\partial x_l}\right). \tag{9.126}$$

For small deformations, $\eta_i \ll x_i$, we can ignore the second-order terms to define the **strain tensor** as

$$\boxed{e_{kl} = \frac{1}{2}\left(\frac{\partial \eta_k}{\partial x_l} + \frac{\partial \eta_l}{\partial x_k}\right),} \tag{9.127}$$

which is a second-rank symmetric tensor, $e_{kl} = e_{lk}$.

9.4.2 Stress Tensor

Let $\overrightarrow{F}$ be the force per unit volume and $\overrightarrow{F}dV$ be the force acting on an infinitesimal portion of the body, which when integrated over a given volume, $\int_V \overrightarrow{F}dV$, gives the total force acting on that volume of the body. We now assume that the force $\overrightarrow{F}$ can be written as the divergence of a second-rank tensor, σ_{ik}, as

$$F_i = \frac{\partial \sigma_{ik}}{\partial x_k}. \tag{9.128}$$

Using the divergence theorem, we can write the ith component of the **force** as

$$\boxed{\int_V F_i dV = \int_V \frac{\partial \sigma_{ik}}{\partial x_k}dV = \oint_S \sigma_{ik}ds_k,} \tag{9.129}$$

where S is a surface that encloses the volume V and such that the area element, $\overrightarrow{ds}$, is oriented in the direction of the outward normal to S. The second-rank tensor, σ_{ik}, is called the **stress tensor**. In the above equation, $\sigma_{ik}ds_k$ gives the ith component of the force acting on the surface element when the normal to the surface points in the kth direction. In other words, σ_{ik} is the ith component of the force acting on a unit test area when the normal points in the kth direction.

We now write the **torque**, M_{ik}, acting on a volume V of the body due to $\overrightarrow{F}$ as the integral

$$M_{ik} = \int_V m_{ik} dV = \int_V \left(\frac{\partial \sigma_{il}}{\partial x_l} x_k - \frac{\partial \sigma_{kl}}{\partial x_l} x_i \right) dV, \tag{9.130}$$

where the torque per unit volume, m_{ik}, is defined as

$$m_{ik} = F_i x_k - F_k x_i = \left(\frac{\partial \sigma_{il}}{\partial x_l} x_k - \frac{\partial \sigma_{kl}}{\partial x_l} x_i \right). \tag{9.131}$$

We can also write M_{ik} as

$$M_{ik} = \int_V \frac{\partial(\sigma_{il} x_k - \sigma_{kl} x_i)}{\partial x_l} dV - \int \left(\sigma_{il} \frac{\partial x_k}{\partial x_l} - \sigma_{kl} \frac{\partial x_i}{\partial x_l} \right) dV, \tag{9.132}$$

which after using the partial derivatives:

$$\frac{\partial x_k}{\partial x_l} = \delta_{kl}, \; \frac{\partial x_i}{\partial x_l} = \delta_{il}, \tag{9.133}$$

and the divergence theorem for the first integral, yields

$$M_{ik} = \oint_S (\sigma_{il} x_k - \sigma_{kl} x_i) ds_l + \int_V (\sigma_{ki} - \sigma_{ik}) dV. \tag{9.134}$$

Assuming that the stress tensor is symmetric, we now obtain M_{ij} as

$$M_{ik} = \int_V m_{ij} dV, \tag{9.135}$$

$$\boxed{M_{ik} = \oint_S (\sigma_{il} x_k - \sigma_{kl} x_i) ds_l.} \tag{9.136}$$

9.4.3 Thermodynamics and Deformations

Under external stresses all bodies deform. However, for sufficiently small strains, when the stresses are removed they all return to their original shapes. Such deformations are called **elastic**. When a body is strained beyond its elastic domain, there is always some residual deformation left when the stresses are removed, which is called **plastic** deformation.

In practice, we are interested in the **stress–strain relation**. To find such a relation, we confine ourselves to the elastic domain. Furthermore, we assume that the deformation is performed sufficiently slowly, so that the entire process is reversible. Hence we can write the first law of thermodynamics as

$$dU = T\,dS - dW,$$

where the infinitesimal work done, dW, for infinitesimal deformations can be written as

$$dW = \left(\frac{\partial \sigma_{ik}}{\partial x_k}\right) \delta\eta_i dV. \tag{9.137}$$

For a finite deformation, we integrate over the region of interest:

$$\int_V dW = \int_V \left(\frac{\partial \sigma_{ik}}{\partial x_k}\right) \delta\eta_i dV, \tag{9.138}$$

which after integration by parts becomes

$$\int_V dW = \oint_S \sigma_{ik}\delta\eta_i ds_k - \int_V \sigma_{ik}\frac{\partial(\delta\eta_i)}{\partial x_k} dV. \tag{9.139}$$

We let the surface, S, be at infinity. Assuming that there are no stresses on the body at infinity, the surface term in the above integral vanishes. In addition using the symmetry of the strain tensor, we can write

$$\int_V dW = -\frac{1}{2}\int_V \sigma_{ik}\left(\frac{\partial(\delta\eta_i)}{\partial x_k} + \frac{\partial(\delta\eta_k)}{\partial x_i}\right) dV \tag{9.140}$$

$$= -\frac{1}{2}\int_V \sigma_{ik}\delta\left(\frac{\partial\eta_i}{\partial x_k} + \frac{\partial\eta_k}{\partial x_i}\right) dV \tag{9.141}$$

$$= -\int_V \sigma_{ik}\delta e_{ik} dV. \tag{9.142}$$

In other words, the work done per unit volume, w, is

$$w = -\sigma_{ik}\delta e_{ik}. \tag{9.143}$$

From now on, we consider all thermodynamic quantities like the entropy, s, work, w, internal energy, u, etc. in terms of their values per unit volume of the undeformed body and denote them with lower case letters. Now the **first law of thermodynamics** becomes

$$\boxed{du(s, e_{ik}) = T\,ds + \sigma_{ik} de_{ik},} \tag{9.144}$$

where the scalar function $u(s, e_{ik})$ is called the **thermodynamic potential**. The **Helmholtz free energy**, $f(T, e_{ik})$, is defined as

$$f(T, e_{ik}) = u - Ts, \tag{9.145}$$

which allows us to write the differential

$$df = -sdT + \sigma_{ik} de_{ik}. \tag{9.146}$$

Similarly, we write the **Gibbs free** energy, $g(T, \sigma_{ik})$, as

$$g(T, \sigma_{ik}) = u - Ts - \sigma_{ik}e_{ik} \tag{9.147}$$

$$= f - \sigma_{ik}e_{ik}, \tag{9.148}$$

which gives the differential

$$dg = -sdT - e_{ik}d\sigma_{ik}. \tag{9.149}$$

We can now obtain the **stress tensor** using the partial derivative

$$\boxed{\sigma_{ik} = \left(\frac{\partial u(s, e_{ik})}{\partial e_{ik}}\right)_s,} \tag{9.150}$$

or,

$$\boxed{\sigma_{ik} = \left(\frac{\partial f(T, e_{ik})}{\partial e_{ik}}\right)_T.} \tag{9.151}$$

Similarly, the **strain tensor** can be obtained as

$$\boxed{e_{ik} = -\left(\frac{\partial g(T, \sigma_{ik})}{\partial \sigma_{ik}}\right)_T.} \tag{9.152}$$

In these expressions, the subscripts outside the parentheses indicate the variables held constant.

9.4.4 Connection between Shear and Strain

Pure shear is a deformation that preserves the volume but alters the shape of the body. Since the fractional change in volume is

$$\frac{\Delta V}{V} = tr(e_{ij}) = e_{ii}, \tag{9.153}$$

for pure shear the strain tensor is traceless. In hydrostatic compression, bodies suffer equal compression in all directions, hence the corresponding strain tensor is proportional to the identity tensor, $e_{ik} \propto \delta_{ik}$, and the stress tensor is given as $\sigma_{ik} = -P\delta_{ik}$, where P is the **hydrostatic pressure**. A **general deformation** can be written as the sum of pure shear and hydrostatic compression as

$$\boxed{e_{ik} = \left(e_{ik} - \frac{1}{3}\delta_{ik}e_{ll}\right) + \frac{1}{3}\delta_{ik}e_{ll}.} \tag{9.154}$$

Note that the first term on the right-hand side is traceless, hence represents pure shear while the second term corresponds to hydrostatic compression.

We consider isotropic bodies deformed at **constant temperature**, thus eliminating the contribution due to thermal expansion. To obtain a relation between the shear and the stress tensors, we first need to find the Helmholtz free energy,

$f(T, e_{ik})$, and then expand it in powers of e_{ik} about the undeformed state of the body, that is, $e_{ik} = 0$. Since when the body is undeformed the stresses vanish:

$$\sigma_{ik}\big|_{e_{ik}=0} = \left(\frac{\partial f(T, e_{ik})}{\partial e_{ik}}\right)_T\Bigg|_{e_{ik}=0} = 0, \tag{9.155}$$

there is no linear term in the expansion of $f(T, e_{ik})$. In addition, since $f(T, e_{ik})$ is a scalar function, the most general expression for $f(T, e_{ik})$ valid up to second-order can be written as

$$f(T, e_{ik}) = \frac{1}{2}\lambda(e_{ii})^2 + \mu(e_{ik})^2, \tag{9.156}$$

where λ and μ are called the **Lamé coefficients** and e_{ii}^2 and $e_{ij}^2 = e_{ik}e_{ki}$ are the only second-order scalars composed of the strain tensor. We now write the differential of $f(T, e_{ik})$ as

$$df = \lambda e_{ii} de_{ii} + 2\mu e_{ik} de_{ik} \tag{9.157}$$

and substitute $de_{ii} = \delta_{ik} de_{ik}$ to get

$$df = \lambda e_{ii}\delta_{ik} de_{ik} + 2\mu e_{ik} de_{ik} \tag{9.158}$$

$$= \left(\lambda e_{ii}\delta_{ik} + 2\mu e_{ik}\right) de_{ik}. \tag{9.159}$$

This gives the partial derivative

$$\left(\frac{\partial f(T, e_{ik})}{\partial e_{ik}}\right)_T = \lambda e_{ii}\delta_{ik} + 2\mu e_{ik}, \tag{9.160}$$

which is also equal to the **stress tensor** [Eq. (9.151)]:

$$\boxed{\sigma_{ik} = \lambda e_{ii}\delta_{ik} + 2\mu e_{ik}.} \tag{9.161}$$

We can also obtain a formula that expresses the strain tensor in terms of the stress tensor. Using Eq. (9.161), we first write the following relation between the traces:

$$\sigma_{ii} = 3\lambda e_{ii} + 2\mu e_{ii} \tag{9.162}$$

$$= (3\lambda + 2\mu)e_{ii}, \tag{9.163}$$

which when substituted back into Eq. (9.161) gives

$$\sigma_{ik} = \lambda\frac{\sigma_{ii}}{(3\lambda + 2\mu)}\delta_{ik} + 2\mu e_{ik} \tag{9.164}$$

and then yields the desired expression as

$$\boxed{e_{ik} = \frac{1}{2\mu}\sigma_{ik} - \frac{\lambda\sigma_{ii}}{2\mu(3\lambda + 2\mu)}\delta_{ik}.} \tag{9.165}$$

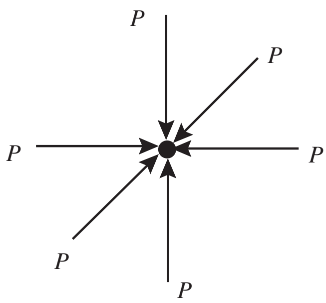

Figure 9.8 Hydrostatic compression.

By considering specific deformations, it is possible to relate the **Lamé coefficients** to the directly measurable quantities like the **bulk modulus**, K, **shear modulus**, G, **Young's modulus**, Y, etc. For example, the bulk modulus is defined as (Figure 9.8)

$$P = -K\frac{\Delta V}{V}, \tag{9.166}$$

where P is the hydrostatic pressure and $\frac{\Delta V}{V}$ is the fractional change in volume. Using

$$\frac{\Delta V}{V} = e_{ii} \text{ and } \sigma_{ii} = -3P, \tag{9.167}$$

which follows from the stress tensor for hydrostatic compressions:

$$\sigma_{ik} = -P\delta_{ik}, \tag{9.168}$$

we can write [Eq. (9.163)]

$$-3P = (3\lambda + 2\mu)\frac{\Delta V}{V}, \tag{9.169}$$

$$P = -\left(\lambda + \frac{2}{3}\mu\right)\frac{\Delta V}{V}, \tag{9.170}$$

thus obtaining the relation

$$\boxed{K = \left(\lambda + \frac{2}{3}\mu\right).} \tag{9.171}$$

We now consider a long bar of length L with the cross-sectional area A pulled longitudinally with the force (Figure 9.9)

$$T = \sigma_{33}A. \tag{9.172}$$

Note that σ_{33} is the only non-zero component of the stress tensor and the **Young's modulus** is defined as

$$\sigma_{33} = Y\frac{\Delta L}{L}. \tag{9.173}$$

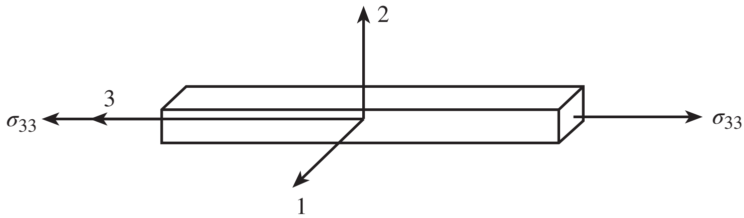

Figure 9.9 Longitudinally stretched bar.

As the bar stretches along the longitudinal direction, it gets thinner along the transverse directions by the relation

$$\begin{pmatrix} \Delta x_1/x_1 \\ \text{or} \\ \Delta x_2/x_2 \end{pmatrix} = -\sigma \frac{\Delta L}{L}, \tag{9.174}$$

where σ is called the **Poisson's ratio**. We now write the displacements as

$$\eta_1 = x_1 \left(-\sigma \frac{\Delta L}{L}\right), \tag{9.175}$$

$$\eta_2 = x_2 \left(-\sigma \frac{\Delta L}{L}\right), \tag{9.176}$$

$$\eta_3 = x_3 \left(\frac{\Delta L}{L}\right), \tag{9.177}$$

which yields the nonzero components of the strain tensor as

$$e_{11} = e_{22} = -\sigma \frac{\Delta L}{L} \tag{9.178}$$

$$= -\sigma e_{33}, \tag{9.179}$$

$$e_{33} = \frac{\Delta L}{L}. \tag{9.180}$$

Using Eq. (9.161) for σ_{33}:

$$\sigma_{33} = \lambda e_{kk} + 2\mu e_{33}, \tag{9.181}$$

we obtain the relation

$$\boxed{Y = (-2\sigma + 1)\lambda + 2\mu.} \tag{9.182}$$

Similarly, using $\sigma_{11} = \sigma_{22} = 0$, Eq. (9.161) gives another relation as

$$\boxed{0 = (-2\sigma + 1)\lambda + 2\mu(-\sigma).} \tag{9.183}$$

We now consider a metal plate sheared as shown in Figure 9.10a, where the deformations are given as

$$\eta_1 = \frac{\theta}{2} x_2, \quad \eta_2 = \frac{\theta}{2} x_1, \quad \eta_3 = 0. \tag{9.184}$$

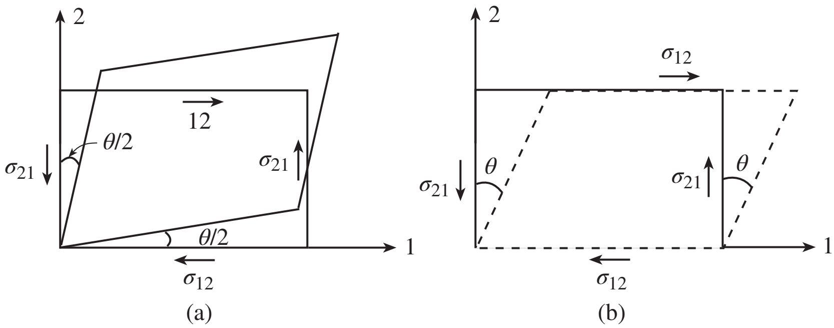

Figure 9.10 Pure shear.

In this case, the only nonvanishing components of the strain tensor [Eq. (9.127)] are

$$e_{12} = e_{21} = \theta/2. \tag{9.185}$$

Inserting these into Eq. (9.161), we obtain

$$\sigma_{12} = \mu\left(\frac{\theta}{2} + \frac{\theta}{2}\right) = \mu\theta. \tag{9.186}$$

In engineering shear modulus, G, is defined in terms of the total angle of deformation (Figure 9.10b) as $\sigma_{12} = G\theta$, hence $\mu = G$. Using Eqs. (9.171), (9.182), and (9.183), we can express the **Lamé coefficients**, λ and μ, and the **Poisson's ratio**, σ, in terms of the **Bulk modulus**, K, **Young's modulus**, Y, and the **shear modulus**, G, which are experimentally easy to measure.

9.4.5 Hook's Law

We can also obtain the relation between the stress and the strain tensors [Eq. (9.161)] by writing the **Hook's law** in **covariant form** as

$$\boxed{\sigma_{ij} = E_{ijkl}e_{kl},} \tag{9.187}$$

where E_{ijkl} is a **fourth-rank** tensor called the **elasticity tensor**. It obeys the following symmetry properties:

$$E_{ijkl} = E_{klij} = E_{jikl} = E_{ijlk}. \tag{9.188}$$

For an isotropic body, the most general tensor with the required symmetries can be written as

$$\boxed{E_{ijkl} = \lambda\delta_{ij}\delta_{kl} + \mu(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}),} \tag{9.189}$$

where λ and μ are the Lamé coefficients. Substituting Eq. (9.189) into (9.187) gives

$$\sigma_{ij} = \lambda\delta_{ij}e_{kk} + 2\mu e_{ij}, \tag{9.190}$$

which is Eq. (9.161).

9.5 Generalized Coordinates and General Tensors

So far we have confined our discussion to Cartesian tensors, which are defined with respect to their transformation properties under orthogonal transformations. However, the presence of symmetries in the physical system often makes other coordinate systems more practical. For example, in central force problems, it is advantageous to work with the spherical polar coordinates, which reflect the spherical symmetry of the system best. For axially symmetric problems, use of the cylindrical coordinates simplifies equations significantly. Usually, symmetries indicate which coordinate system to use. However, in less obvious cases, finding the symmetries of a given system and their generators can help us to construct the most advantageous coordinate system. We now extend our discussion of Cartesian coordinates and Cartesian tensors to generalized coordinates and general tensors. These definitions can also be used for defining tensors in spacetime and also for tensors in curved spaces.

A **general coordinate transformation** can be defined as

$$\overline{x}^i = \overline{x}^i(x^1, x^2, \dots, x^n), \quad i = 1, \dots, n. \tag{9.191}$$

In short, we write this as

$$\boxed{\overline{x}^i = \overline{x}^i(x^k).} \tag{9.192}$$

The **inverse transformation** is defined as

$$\boxed{x^k = x^k\left(\overline{x}^i\right),} \tag{9.193}$$

where the indices take the values $i, k = 1, \dots, n$. For reasons to become clear later, we have written all the indices as superscripts. Differentiating Eq. (9.192), we can write the transformation law for infinitesimal displacements as

$$d\overline{x}^i = \sum_{k=1}^{n} \left[\frac{\partial \overline{x}^i}{\partial x^k}\right] dx^k. \tag{9.194}$$

We now consider a scalar function, $\phi(x^i)$, and differentiate with respect to $\overline{x}^i$ to write

$$\frac{\partial \phi}{\partial \overline{x}^i} = \sum_{k=1}^{n} \left[\frac{\partial x^k}{\partial \overline{x}^i}\right] \frac{\partial \phi}{\partial x^k}. \tag{9.195}$$

Until we reestablish the Einstein summation convention for general tensors, we write the summation signs explicitly.

9.5.1 Contravariant and Covariant Components

Using the transformation properties of the infinitesimal displacements and the gradient of a scalar function, we now define contravariant and covariant components. A **contravariant component** is defined with respect to the transformation rule

$$\boxed{\overline{a}^i = \sum_{k=1}^{n} \left[\frac{\partial \overline{x}^i}{\partial x^k}\right] a^k,} \tag{9.196}$$

where the **inverse** transformation is defined as

$$\boxed{a^k = \sum_{i=1}^{n} \left[\frac{\partial x^k}{\partial \overline{x}^i}\right] \overline{a}^i.} \tag{9.197}$$

We also define a **covariant component** according to the transformation rule

$$\boxed{\overline{a}_i = \sum_{k=1}^{n} \left[\frac{\partial x^k}{\partial \overline{x}^i}\right] a_k,} \tag{9.198}$$

where the components are now shown as subscripts. The **inverse** transformation is written as

$$\boxed{a_k = \sum_{i=1}^{n} \left[\frac{\partial \overline{x}^i}{\partial x^k}\right] \overline{a}_i.} \tag{9.199}$$

A second-rank tensor can be contravariant, covariant, or with mixed indices with the following transformation properties:

$$\overline{T}^{ij} = \sum_{k=1}^{n}\sum_{l=1}^{n} \left[\frac{\partial \overline{x}^i}{\partial x^k}\frac{\partial \overline{x}^j}{\partial x^l}\right] T^{kl}, \tag{9.200}$$

$$\overline{T}_{ij} = \sum_{k=1}^{n}\sum_{l=1}^{n} \left[\frac{\partial x^k}{\partial \overline{x}^i}\frac{\partial x^l}{\partial \overline{x}^j}\right] T_{kl}, \tag{9.201}$$

$$\overline{T}^i_j = \sum_{k=1}^{n}\sum_{l=1}^{n} \left[\frac{\partial \overline{x}^i}{\partial x^k}\frac{\partial x^l}{\partial \overline{x}^j}\right] T^k_l. \tag{9.202}$$

Similarly, a **general tensor** can be defined with mixed indices as

$$\overline{T}^{i_1 i_2 \cdots}_{j_1 j_2 \cdots} = \sum_{k_1=1}^{n}\sum_{k_2=1}^{n}\cdots\sum_{l_1=1}^{n}\sum_{l_2=1}^{n}\cdots\left[\frac{\partial \overline{x}^{i_1}}{\partial x^{k_1}}\frac{\partial \overline{x}^{i_2}}{\partial x^{k_2}}\cdots\frac{\partial x^{l_1}}{\partial \overline{x}^{j_1}}\frac{\partial x^{l_2}}{\partial \overline{x}^{j_2}}\cdots\right] T^{k_1 k_2 \cdots}_{l_1 l_2 \cdots}. \tag{9.203}$$

Using Eqs. (9.199) and (9.198), we write

$$a_k = \sum_{i=1}^{n}\left[\frac{\partial \overline{x}^i}{\partial x^k}\right]\overline{a}_i \tag{9.204}$$

$$= \sum_{k'=1}^{n}\left[\sum_{i=1}^{n}\frac{\partial \overline{x}^i}{\partial x^k}\frac{\partial x^{k'}}{\partial \overline{x}^i}\right] a_{k'} \tag{9.205}$$

$$= \sum_{k'=1}^{n}\delta^{k'}_k a_{k'} \tag{9.206}$$

$$= a_k, \tag{9.207}$$

where $\delta^{k'}_k$ is the **Kronecker delta**, which is a second-rank tensor with the transformation property

$$\overline{\delta}^i_j = \sum_{k=1}^{n}\sum_{l=1}^{n}\left[\frac{\partial \overline{x}^i}{\partial x^k}\frac{\partial x^l}{\partial \overline{x}^j}\right]\delta^k_l = \delta^i_j. \tag{9.208}$$

It is the only second-rank tensor with this property.

9.5.2 Metric Tensor and the Line Element

Let us now see how the distance between two infinitesimally close points transforms under general coordinate transformations. We take our unbarred coordinate system as the Cartesian coordinates; hence, the line element that gives the square of the distance between two infinitesimally close points is

$$ds^2 = \sum_{k=1}^{n} dx^k dx^k. \tag{9.209}$$

Because distance is a scalar, its value does not change under general coordinate transformations, $d\overline{s}^2 = ds^2$, hence we can write

$$ds^2 = \sum_{k=1}^{n}\left[\sum_{i=1}^{n}\frac{\partial x^k}{\partial \overline{x}^i}d\overline{x}^i\right]\left[\sum_{j=1}^{n}\frac{\partial x^k}{\partial \overline{x}^j}d\overline{x}^j\right], \tag{9.210}$$

$$d\overline{s}^2 = \sum_{i=1}^{n}\sum_{j=1}^{n}\left[\sum_{k=1}^{n}\frac{\partial x^k}{\partial \overline{x}^i}\frac{\partial x^k}{\partial \overline{x}^j}\right]d\overline{x}^i d\overline{x}^j, \tag{9.211}$$

$$\boxed{d\bar{s}^2 = \sum_{i=1}^{n}\sum_{j=1}^{n} g_{ij} d\bar{x}^i d\bar{x}^j,} \tag{9.212}$$

where the symmetric second-rank tensor, g_{ij}, is called the **metric tensor** or the **fundamental tensor**:

$$\boxed{g_{ij} = \sum_{k=1}^{n} \frac{\partial x^k}{\partial \bar{x}^i}\frac{\partial x^k}{\partial \bar{x}^j}.} \tag{9.213}$$

The metric tensor is the singly most important tensor in the study of curved spaces and spacetimes. If we write the line element [Eq. (9.209)] in Cartesian coordinates as $ds^2 = \sum_{i=1}^{n}\sum_{j=1}^{n} \delta_{ij} dx^i dx^j$, we see that the metric tensor is the identity matrix $g_{ij} = \mathbf{I} = \delta_{ij}$.

Given an arbitrary contravariant vector u^i, let us see how

$$\left[\sum_{j=1}^{n} g_{ij} u^j\right] \tag{9.214}$$

transforms. We first write $\sum_{j=1}^{n}\left[\bar{g}_{ij}\bar{u}^j\right]$ as

$$\sum_{j=1}^{n}\left[\bar{g}_{ij}\bar{u}^j\right] = \sum_{j=1}^{n}\left[\sum_{k=1}^{n}\sum_{l=1}^{n}\frac{\partial x^k}{\partial \bar{x}^i}\frac{\partial x^l}{\partial \bar{x}^j} g_{kl}\right]\left[\sum_{m=1}^{n}\frac{\partial \bar{x}^j}{\partial x^m} u^m\right] \tag{9.215}$$

$$= \sum_{m=1}^{n}\sum_{k=1}^{n}\sum_{l=1}^{n}\left[\frac{\partial x^k}{\partial \bar{x}^i}\left(\sum_{j=1}^{n}\frac{\partial x^l}{\partial \bar{x}^j}\frac{\partial \bar{x}^j}{\partial x^m}\right)\right] g_{kl} u^m \tag{9.216}$$

$$= \sum_{m=1}^{n}\sum_{k=1}^{n}\sum_{l=1}^{n}\left[\frac{\partial x^k}{\partial \bar{x}^i}\delta^l_m\right] g_{kl} u^m \tag{9.217}$$

$$= \sum_{k=1}^{n}\left[\frac{\partial x^k}{\partial \bar{x}^i}\right]\left[\sum_{m=1}^{n} g_{km} u^m\right]. \tag{9.218}$$

Comparing with Eq. (9.198), we see that the expression

$$\left[\sum_{m=1}^{n} g_{km} u^m\right] \tag{9.219}$$

transforms like a covariant vector; thus we define the **covariant components** of u^i as

$$\boxed{u_i = \sum_{j=1}^{n} g_{ij} u^j.} \tag{9.220}$$

Similarly, we can define the metric tensor [Eq. (9.213)] with **contravariant components** as

$$g^{kl} = \sum_{i=1}^{n} \left[\frac{\partial \overline{x}^k}{\partial x^i} \frac{\partial \overline{x}^l}{\partial x^i} \right], \tag{9.221}$$

where

$$\sum_{k=1}^{n} g_{kl} g^{kl'} = \sum_{k=1}^{n} \left[\sum_{i=1}^{n} \frac{\partial x^i}{\partial \overline{x}^k} \frac{\partial x^i}{\partial \overline{x}^l} \right] \left[\sum_{i'=1}^{n} \frac{\partial \overline{x}^k}{\partial x^{i'}} \frac{\partial \overline{x}^{l'}}{\partial x^{i'}} \right] \tag{9.222}$$

$$= \sum_{i=1}^{n} \sum_{i'=1}^{n} \left[\sum_{k=1}^{n} \frac{\partial x^i}{\partial \overline{x}^k} \frac{\partial \overline{x}^k}{\partial x^{i'}} \right] \left[\frac{\partial x^i}{\partial \overline{x}^l} \frac{\partial \overline{x}^{l'}}{\partial x^{i'}} \right] \tag{9.223}$$

$$= \sum_{i=1}^{n} \sum_{i'=1}^{n} \delta^i_{i'} \left[\frac{\partial x^i}{\partial \overline{x}^l} \frac{\partial \overline{x}^{l'}}{\partial x^{i'}} \right] \tag{9.224}$$

$$= \sum_{i=1}^{n} \left[\frac{\partial x^i}{\partial \overline{x}^l} \frac{\partial \overline{x}^{l'}}{\partial x^i} \right] \tag{9.225}$$

$$= \delta^{l'}_l . \tag{9.226}$$

Using the symmetry of the metric tensor, we can write

$$\sum_{k=1}^{n} g_{lk} g^{kl'} = g^{l'}_l = \delta^{l'}_l . \tag{9.227}$$

We see that the **metric tensor** can be used to **lower** and **raise indices** of a given tensor. Thus a given vector, $\overrightarrow{u}$, can be expressed in terms of either its covariant or its contravariant components. In general, the two types of components are different, and they are related by

$$u_i = \sum_{j=1}^{n} g_{ij} u^j, \tag{9.228}$$

$$u^i = \sum_{j=1}^{n} g^{ij} u_j. \tag{9.229}$$

For the Cartesian coordinates, the metric tensor is the Kronecker delta; thus we can write

$$g_{ij} = \delta_{ij} = \delta^j_i = \delta^i_j = \delta^{ij} = g^{ij}. \tag{9.230}$$

Hence, both the covariant and the contravariant components are equal in Cartesian coordinates, there is no need for distinction between them.

Contravariant components of the metric tensor are also given as [1, 3]

$$g^{ij} = \frac{\triangle^{ji}}{g}, \tag{9.231}$$

where

$$\triangle^{ji} = \text{cofactor}[\, g_{ji}] \ \text{ and } \ g = \det g_{ij}. \tag{9.232}$$

9.5.3 Geometric Interpretation of Components

Covariant and contravariant indices can be geometrically interpreted in terms of **oblique axis**. A vector $\vec{a}$ in the coordinate system shown in Figure 9.11 can be written as

$$\vec{a} = a^1\hat{\mathbf{e}}_1 + a^2\hat{\mathbf{e}}_2, \tag{9.233}$$

where $\hat{\mathbf{e}}_i$ are the unit basis vectors along the coordinate axes. As seen, the contravariant components are found by drawing parallel lines to the coordinate axes. However, we can also define components by dropping perpendiculars to the coordinate axes as

$$a_i = \vec{a} \cdot \hat{\mathbf{e}}_i, \ \ i = 1, 2. \tag{9.234}$$

The scalar product of two vectors is given as

$$\vec{a} \cdot \vec{b} = (a^1\hat{\mathbf{e}}_1 + a^2\hat{\mathbf{e}}_2) \cdot (b^1\hat{\mathbf{e}}_1 + b^2\hat{\mathbf{e}}_2) \tag{9.235}$$

$$= a^1b^1(\hat{\mathbf{e}}_1 \cdot \hat{\mathbf{e}}_1) + a^1b^2(\hat{\mathbf{e}}_1 \cdot \hat{\mathbf{e}}_2) + a^2b^1(\hat{\mathbf{e}}_2 \cdot \hat{\mathbf{e}}_1) + a^2b^2(\hat{\mathbf{e}}_2 \cdot \hat{\mathbf{e}}_2). \tag{9.236}$$

Defining a symmetric matrix

$$g_{ij} = \hat{\mathbf{e}}_i \cdot \hat{\mathbf{e}}_j, \ \ i, j = 1, 2, \tag{9.237}$$

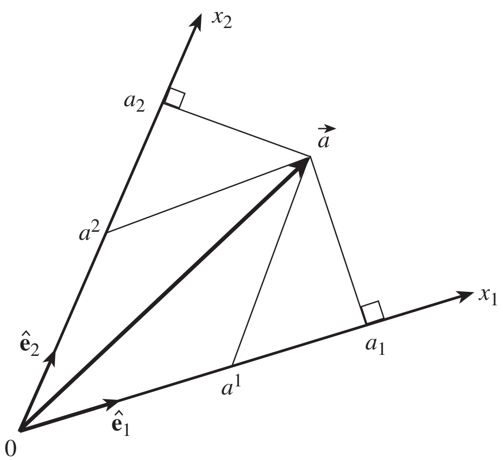

Figure 9.11 Covariant and contravariant components.

we can write Eq. (9.236) as

$$\vec{a} \cdot \vec{b} = \sum_{i=1}^{2} \sum_{j=1}^{2} g_{ij} a^i b^j. \tag{9.238}$$

We can also write

$$\vec{a} \cdot \vec{b} = \vec{a} \cdot (b^1 \hat{\mathbf{e}}_1 + b^2 \hat{\mathbf{e}}_2) \tag{9.239}$$

$$= b^1 (\vec{a} \cdot \hat{\mathbf{e}}_1) + b^2 (\vec{a} \cdot \hat{\mathbf{e}}_2) \tag{9.240}$$

$$= b^1 a_1 + b^2 a_2 = \sum_{i=1}^{2} b^i a_i = \sum_{i=1}^{2} a^i b_i. \tag{9.241}$$

All these remind us tensors. To prove that $\vec{a} \cdot \vec{b}$ is a tensor equation, we have to prove that it has the same form in another coordinate system. It is clear that in another coordinate system with the basis vectors $\hat{\mathbf{e}}'_1$ and $\hat{\mathbf{e}}'_2$, $\vec{a} \cdot \vec{b}$ will have the same form as

$$\vec{a} \cdot \vec{b} = \sum_{k=1}^{2} \sum_{l=1}^{2} g'_{kl} a'^k b'^l = \sum_{i=1}^{2} \sum_{j=1}^{2} g_{ij} a^i b^j, \tag{9.242}$$

where $g'_{kl} = \hat{\mathbf{e}}'_k \cdot \hat{\mathbf{e}}'_l$, thus proving its tensor character. Because $\vec{a}$ and $\vec{b}$ are arbitrary vectors, we can take them as the infinitesimal displacement vector as $a^i = b^i = dx^i$, thus

$$ds^2 = \sum_{i=1}^{2} \sum_{j=1}^{2} g_{ij} dx^i dx^j \tag{9.243}$$

gives the line element with the metric

$$g_{ij} = \hat{\mathbf{e}}_i \cdot \hat{\mathbf{e}}_j, \quad i, j = 1, 2. \tag{9.244}$$

Hence a^i and a_i are indeed the contravariant and the covariant components of an arbitrary vector, and the difference between the covariant and the contravariant components is real.

In curved spaces dx^i corresponds to the coordinate increments on the surface. The metric tensor g_{ij} can now be interpreted as the product $\hat{\mathbf{e}}_i \cdot \hat{\mathbf{e}}_j$ of the unit tangent vectors along the coordinate axis.

9.5.4 Interpretation of the Metric Tensor

In classical physics, space is an endless continuum, where everything in the universe exists. In other words, space is the *arena* in which all processes take place. We use coordinate systems to assign numbers called coordinates to every point in space, which in turn allow us to study physical processes in terms of separations and directions. Obviously, there are infinitely many possibilities for the coordinate system that one can use. In this regard, tensors, defined in terms of their transformation properties under general coordinate transformations, have proven to be very useful in physics. Since the **metric tensor** contains crucial information regarding the intrinsic properties of the physical space, it plays a fundamental role in physics. However, this information is not always easily revealed by the metric tensor.

Let us consider a two-dimensional universe with two-dimensional *intelligent* bugs living in it. A group of bugs in this universe use a coordinate system that allows them to write the line element as (Figure 9.12)

$$ds^2 = dx^2 + dy^2, \quad x, y \in (-\infty, \infty), \tag{9.245}$$

while the others prefer to work with a different coordinate system and express the line element as

$$ds^2 = dr^2 + r^2 d\theta^2, \; r \in [0, \infty), \quad \theta \in [0, 2\pi]. \tag{9.246}$$

In the first coordinate system, the metric tensor is obviously the identity tensor:

$$g_{ij} = \mathbf{I} = \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix}, \tag{9.247}$$

while in the second coordinate system, it is a function of position:

$$g_{ij} = \begin{pmatrix} 1 & 0 \\ 0 & r^2 \end{pmatrix}. \tag{9.248}$$

A path connecting two points in space can be written in the first coordinate system as $y = y(x)$, while in the second coordinate system it will be expressed as $r = r(\theta)$. Since the **path length**, $l = \int_1^2 ds$, is a scalar, its value does not depend on the coordinate system used. Since l is basically the length that the

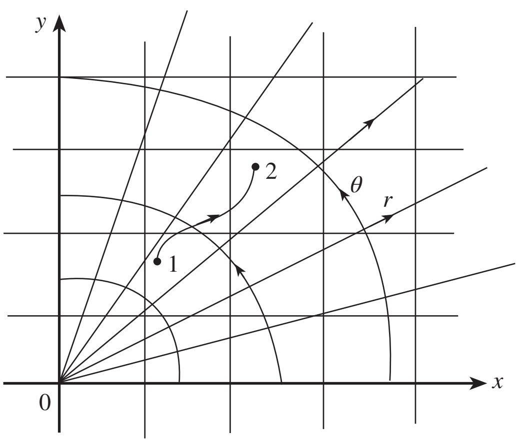

Figure 9.12 Cartesian and plane polar coordinates.

bugs will measure by laying their rulers end to end along the path, it is also called the **proper length**. Since one can also calculate l, the first group of bugs [Eq. (9.245)] will use the formula

$$l = \int_1^2 ds = \int_1^2 dx\sqrt{1 + \left(\frac{dy}{dx}\right)^2}, \tag{9.249}$$

while the second group of bugs [Eq. (9.246)] will use

$$l = \int_1^2 ds = \int_1^2 d\theta\sqrt{r^2 + \left(\frac{dr}{d\theta}\right)^2}. \tag{9.250}$$

A group of bugs immediately set out to investigate the properties of their space by taking direct measurements using rulers and protractors. They draw circles of various sizes at various locations in their universe and measure their circumference to radius ratios. Operationally, this is a well-defined procedure; first, they pick a point and connect all points equidistant from that point and then measure the (proper) circumference by laying their rulers end to end along the periphery. To measure the (proper) radius, they lay their rulers from the center onwards along one of the axes. Their measurements turn out to be in perfect agreement with their calculations. For the first group of bugs using the first coordinate system [Eq. (9.245)], equation of a circle is given by

$$x^2 + y^2 = r_0^2,\ r_0 = \text{radius}. \tag{9.251}$$

For the second group using Eq. (9.246), a circle is simply written as $r = r_0$. In the first coordinate system, the circumference is calculated as

$$c = \int ds_{(x^2+y^2=r_0^2)} = \int dx\sqrt{1 + \left(\frac{dy}{dx}\right)^2} \tag{9.252}$$

$$= 4\int_0^{r_0} \frac{dx}{\left(1 - \frac{x^2}{r_0^2}\right)^{1/2}} = 2\pi r_0, \tag{9.253}$$

while in the second coordinate system, the circumference is found as

$$c = \int ds_{(r=r_0)} = \int d\theta\sqrt{r^2 + \left(\frac{dr}{d\theta}\right)^2} \tag{9.254}$$

$$= r_0\int_0^{2\pi} d\theta = 2\pi r_0. \tag{9.255}$$

On the other hand, in the first coordinate system, the radius is calculated as

$$\text{radius} = \int ds_{(y=0)} = \int_0^{r_0} dx\sqrt{1+\frac{dy}{dx}} \tag{9.256}$$

$$= \int_0^{r_0} dx = r_0, \tag{9.257}$$

while in the second coordinate system, it is found as

$$\text{radius} = \int ds_{(\theta=\theta_0)} = \int_0^{r_0} dr\sqrt{1+r^2\frac{d\theta}{dr}} \tag{9.258}$$

$$= \int_0^{r_0} dr = r_0. \tag{9.259}$$

In conclusion, no matter how large or small circles the bugs draw and regardless of the location of these circles, they always find the same number for the circumference to radius ratio, c/r_0, which is twice a mysterious number they called π. Furthermore, when they draw triangles of various sizes and orientations, regardless of the location of these triangles, they always find the sum of the interior angles equal to the same mysterious number π. Being intelligent creatures capable of abstract thought, these bugs immediately notice that they are living in a flat universe. In fact, the first metric is nothing but the Pythagoras' theorem in Cartesian coordinates, while the second metric is the same metric written in plane polar coordinates. The two coordinate systems are related by the transformation equations

$$x = r\cos\theta, \tag{9.260}$$

$$y = r\sin\theta. \tag{9.261}$$

In fact, these conclusions would remain intact even if they had used another coordinate system. Such as the following somewhat *strange* looking coordinate system (η, ξ):

$$ds^2 = (\eta^2+\xi^2)(d\eta^2+d\xi^2), \tag{9.262}$$

$$g_{ij} = \begin{pmatrix} \eta^2+\xi^2 & 0 \\ 0 & \eta^2+\xi^2 \end{pmatrix}, \tag{9.263}$$

where the two metrics [Eqs. (9.263) and (9.247)] are related by the coordinate transformation $x = \eta\xi$, $y = (1/2)(\eta^2 - \xi^2)$.

Now consider another two-dimensional universe, where this time the line element is given as

$$ds^2 = \frac{dr^2}{\left(1-\frac{r^2}{R^2}\right)} + r^2 d\phi^2, \quad r \in [0, R], \quad \phi \in [0, 2\pi]. \tag{9.264}$$

A circle in this universe is defined by

$$r = r_0. \tag{9.265}$$

The proper radius, r_p, and the proper circumference, c_p, that the bugs will measure in this universe are calculated, respectively, as

$$r_p = \int ds_{(\phi=\phi_0)} = \int_0^{r_0} \frac{dr}{\left(1-\frac{r^2}{R^2}\right)^{1/2}} = R\sin^{-1}(r_0/R). \tag{9.266}$$

$$c_p = \int ds_{(r=r_0)} = r_0 \int_0^{2\pi} d\phi = 2\pi r_0, \tag{9.267}$$

thus yielding the ratio

$$\frac{c_p}{r_p} = \frac{2\pi r_0}{R\sin^{-1}(r_0/R)}. \tag{9.268}$$

Clearly, this ratio depends on the size of the circle and only in the limit as the radius of the circle goes to zero, $r_0 \to 0$, or as $R \to \infty$, goes to 2π. Expansion of c_p/r_p in powers of r_0/R,

$$\frac{c_p}{r_p} = 2\pi\left[1 - \frac{1}{6}\left(\frac{r_0}{R}\right)^2 + \cdots\right] \tag{9.269}$$

shows that in general these bugs will measure a c_p/r_p ratio smaller than 2π.

To the bugs, this looks rather strange and they argue that there must be a force field that effects the rulers to give this $c_p/r_p < 2\pi$ ratio. In fact, one of the bugs uses the transformation

$$r = \frac{\rho}{(1+\rho^2/4R^2)} \tag{9.270}$$

to write the line element [Eq. (9.264)] as

$$ds^2 = \frac{1}{(1+\rho^2/4R^2)^2}[d\rho^2 + \rho^2 d\phi^2], \tag{9.271}$$

which demonstrates that the proper lengths, hence the rulers, in their universe are indeed shortened by the factor $1/(1+\rho^2/4R^2)$ with respect to a flat universe. They even develop a field theory, where there is a force field that shortens the rulers by the factor $1/(1+\rho^2/4R^2)$. Like the electric field, which effects only electrically charged objects, this field may also effect only certain types of matter possessing a new type of charge. To check this, they repeat their measurements with different rulers made from all kinds of different materials they could find. No matter how hard they try and how precise their measurements are made, to their surprise, they always find the same circumference to radius ratio [Eq. (9.268)]. Whatever this field is, apparently it is effecting everything precisely the same way. In other words, it is a universal force field. This fact continues to intrigue them, but not knowing what to do with it, they continue with the force field concept, which after all appears to work fine in terms of their existing data.

Then comes a brilliant scientist and says that all these years they have been mesmerized by the beauty and the simplicity of the geometry on flat space, but the measurements they have been getting actually could indicate that they may be living on the surface of a sphere in a hyperspace with three dimensions. Then the brilliant bug shows them that the transformation

$$\frac{r}{R} = \sin\theta \tag{9.272}$$

transforms their line element [Eq. (9.264)] into the form

$$ds^2 = R^2 d\theta^2 + R^2 \sin^2 \theta d\phi^2, \tag{9.273}$$

which when compared with the line element in three-dimensional space in spherical coordinates:

$$ds^2 = dr^2 + r^2 d\theta^2 + r^2 \sin^2 \theta d\phi^2, \tag{9.274}$$

corresponds to the line element on the surface of a sphere with radius $r = R$ (Figure 9.13).

In summary, these bugs do not need a force field to explain their observations. All they have to do is to accept that they are living on the two-dimensional surface of a sphere in three dimensions. Since the geometry of space is something experimentally detectable, the fact that they have been getting the same geometry regardless of the internal structure of their measuring instruments: rulers, protractors, etc., indicates that this new geometry is universal. That is, it is the geometry of the physical space that everything exists in.

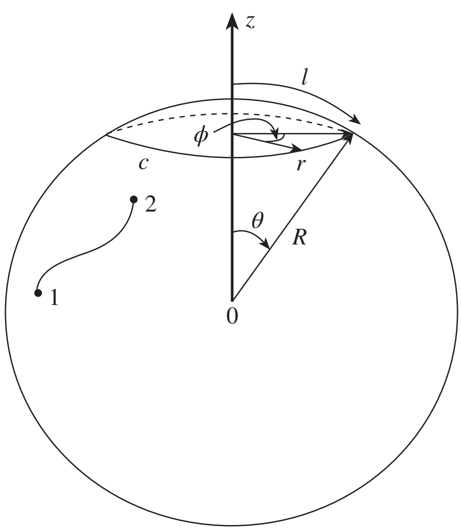

Figure 9.13 Bugs living on a sphere.

There is actually another possible geometry for the two-dimensional bugs, where the line element is this time given as

$$ds^2 = \frac{dr^2}{\left(1 + \frac{r^2}{R^2}\right)} + r^2 d\phi^2, \quad r \in [0, \infty], \quad \phi \in [0, 2\pi]. \tag{9.275}$$

In this case, the ratio of the circumference to the radius of a circle is greater than 2π:

$$\frac{c_p}{r_p} = \frac{2\pi r_0}{R \sinh^{-1}(r_0/R)} = 2\pi \left[1 + \frac{1}{6}\left(\frac{r_0}{R}\right)^2 + \cdots\right], \tag{9.276}$$

and the interior angles of triangles are less than π. Such surfaces can be visualized as the surface of a saddle (Figure 9.14). These are the three basic geometries for the surfaces in three dimensions. Of course, in general, the surfaces could be something rather arbitrary with lots of bumps and dimples like the surface of an orange or an apple.

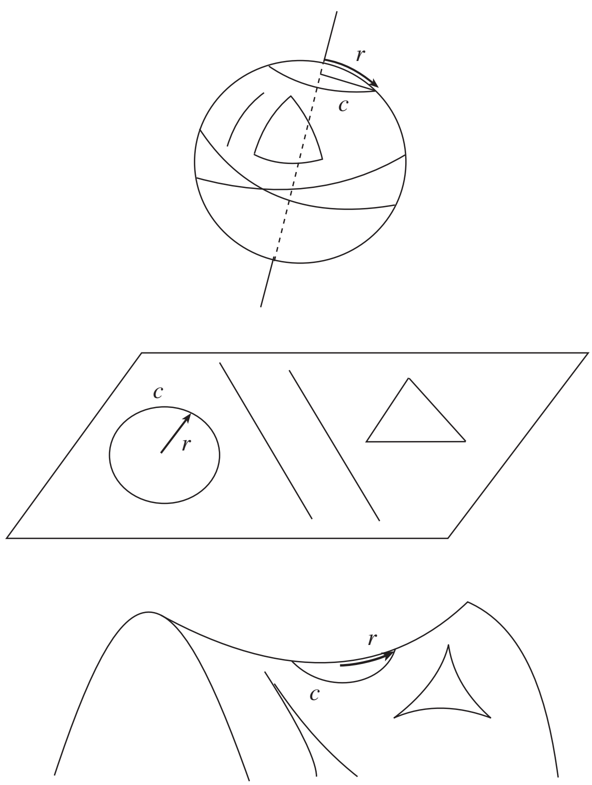

Figure 9.14 Geometry is an experimental science.

9.6 Operations with General Tensors

9.6.1 Einstein Summation Convention

Algebraic operations like addition, subtraction, and multiplication are accomplished the same way as in Cartesian tensors. For general tensors, the Einstein summation convention, which implies summation over repeated indices, is used by writing one of the indices as covariant and the other as contravariant. For example, the line element can be written in any one of the following forms:

$$ds^2 = g_{ij}dx^i dx^j = dx_j dx^j = dx^i dx_i \tag{9.277}$$

$$= g^{ij}dx_i dx_j = dx^j dx_j = dx_i dx^i. \tag{9.278}$$

From now on, unless otherwise stated, we use this version of the Einstein summation convention.

9.6.2 Contraction of Indices

We can lower the rank of a tensor by contracting some of its indices as

$$E^{ij} = T^{ijk}_{\ \ \ k}, \tag{9.279}$$

$$C^i = D^{ijk}_{\ \ jk}. \tag{9.280}$$

We can also lower the rank of a tensor by contracting it with another tensor:

$$F^{ij} = D^{ijk}E_k, \tag{9.281}$$

$$A = B^i C_i. \tag{9.282}$$

9.6.3 Multiplication of Tensors

We can obtain tensors of higher rank by multiplying two lower-rank tensors:

$$C_{ijk} = A_{ij}D_k, \tag{9.283}$$

$$T_{ij} = A_i B_j, \tag{9.284}$$

$$F^{lm}_{ij} = B_i C^l D^m_j. \tag{9.285}$$

This is also called the **outer product**.

9.6.4 The Quotient Theorem

A very useful theorem in tensor operations is the quotient theorem. Suppose $T^{i_1\dots i_n}_{j_1\dots j_m}$ is a given **matrix** and $A^{j_l\dots j_m}_{i_k\dots i_n}$ is an arbitrary **tensor**. Suppose that it is also known that

$$S^{i_1\dots i_{k-1}}_{j_1\dots j_{l-1}} = T^{i_1\dots i_{k-1}i_k\dots i_n}_{j_1\dots j_{l-1}j_l\dots j_m} A^{j_l\dots j_m}_{i_k\dots i_n} \tag{9.286}$$

is a tensor. Then, by the quotient theorem,

$$T^{i_1 \dots i_n}_{j_1 \dots j_m} \tag{9.287}$$

is also a tensor. This could be easily checked by using the transformation properties of tensors.

9.6.5 Equality of Tensors

Two tensors are equal, if and only if all their corresponding components are equal. For example, two third-rank tensors, **A** and **B**, are equal if and only if

$$A^{ij}_k = B^{ij}_k, \text{ for all } i, j, \text{ and } k. \tag{9.288}$$

As a consequence of this, a tensor is not zero unless all of its components vanish.

9.6.6 Tensor Densities

A tensor density of **weight** w transforms according to the law

$$\boxed{\overline{T}^{i_1 i_2 \dots}_{j_1 j_2 \dots} = \left[\frac{\partial \overline{x}^{i_1}}{\partial x^{k_1}} \frac{\partial \overline{x}^{i_2}}{\partial x^{k_2}} \cdots \frac{\partial x^{l_1}}{\partial \overline{x}^{j_1}} \frac{\partial x^{l_2}}{\partial \overline{x}^{j_2}} \cdots\right] T^{k_1 k_2 \dots}_{l_1 l_2 \dots} \left|\frac{\partial x}{\partial \overline{x}}\right|^w} \tag{9.289}$$

where $\left|\frac{\partial x}{\partial \overline{x}}\right|$ is the **Jacobian** of the transformation, that is,

$$\boxed{\left|\frac{\partial x}{\partial \overline{x}}\right| = \det \begin{bmatrix} \frac{\partial x^1}{\partial \overline{x}^1} & \frac{\partial x^1}{\partial \overline{x}^2} & \dots & \frac{\partial x^1}{\partial \overline{x}^n} \\ \frac{\partial x^2}{\partial \overline{x}^1} & \dots & \dots & \dots \\ \vdots & \vdots & \vdots & \vdots \\ \dots & \dots & \dots & \frac{\partial x^n}{\partial \overline{x}^n} \end{bmatrix}.} \tag{9.290}$$

The **permutation symbol** ϵ_{ijk} is a third-rank tensor density of weight -1. The **volume element**,

$$d^n x = dx^1 dx^2 \dots dx^n, \tag{9.291}$$

transforms as

$$\boxed{d^n \overline{x} = d^n x \left|\frac{\partial x}{\partial \overline{x}}\right|^{-1},} \tag{9.292}$$

hence it is a scalar density of weight -1.

The **metric tensor** is a second-rank tensor that transforms as

$$\overline{g}_{ij} = \frac{\partial x^k}{\partial \overline{x}^i}\frac{\partial x^l}{\partial \overline{x}^j} g_{kl}. \tag{9.293}$$

Using matrix multiplication, determinant of the metric tensor transforms as

$$\overline{g} = g\left|\frac{\partial x}{\partial \overline{x}}\right|^2, \quad \text{or} \quad \sqrt{|\overline{g}|} = \sqrt{|g|}\left|\frac{\partial x}{\partial \overline{x}}\right|. \tag{9.294}$$

In the last equation, we have used absolute values in anticipation of applications to relativity, where the metric has signature $(- + ++)$ or $(+ - --)$. From Eqs. (9.292) and (9.294), it is seen that $\sqrt{|g|}d^n x$ is a scalar:

$$\sqrt{|\overline{g}|}d^n\overline{x} = \sqrt{|g|}d^n x. \tag{9.295}$$

9.6.7 Differentiation of Tensors

We start by taking the **derivative** of the transform of a **covariant vector**, $\overline{u}_i = \frac{\partial x^j}{\partial \overline{x}^i}u_j$, as

$$\frac{\partial \overline{u}_i}{\partial \overline{x}^k} = \frac{\partial^2 x^j}{\partial \overline{x}^k \partial \overline{x}^i}u_j + \frac{\partial x^j}{\partial \overline{x}^i}\left[\frac{\partial u_j}{\partial x^l}\frac{\partial x^l}{\partial \overline{x}^k}\right]. \tag{9.296}$$

If we write this as

$$\frac{\partial \overline{u}_i}{\partial \overline{x}^k} = \frac{\partial^2 x^j}{\partial \overline{x}^i \partial \overline{x}^k}u_j + \frac{\partial x^j}{\partial \overline{x}^i}\frac{\partial x^l}{\partial \overline{x}^k}\frac{\partial u_j}{\partial x^l} \tag{9.297}$$

and if the first term on the right-hand side was absent, then the derivative of u_j would simply be a second-rank tensor. Rearranging this equation as

$$\frac{\partial \overline{u}_i}{\partial \overline{x}^k} = \frac{\partial}{\partial \overline{x}^i}\left[\frac{\partial x^j}{\partial \overline{x}^k}\right]u_j + \frac{\partial x^j}{\partial \overline{x}^i}\frac{\partial x^l}{\partial \overline{x}^k}\frac{\partial u_j}{\partial x^l} \tag{9.298}$$

$$= \frac{\partial [a^j_k]}{\partial \overline{x}^i} \quad u_j + \frac{\partial x^j}{\partial \overline{x}^i}\frac{\partial x^l}{\partial \overline{x}^k}\frac{\partial u_j}{\partial x^l}, \tag{9.299}$$

we see that the problem is due to the fact that in general the transformation matrix, $[a^j_k]$, changes with position. For transformations between the Cartesian coordinates, the transformation matrix is independent of coordinates; thus this problem does not arise. However, we can still define a covariant derivative that transforms like a tensor.

We first consider the metric tensor, which transforms as

$$\overline{g}_{ij} = \frac{\partial x^k}{\partial \overline{x}^i}\frac{\partial x^l}{\partial \overline{x}^j} g_{kl}, \tag{9.300}$$

and differentiate it with respect to $\overline{x}^m$:

$$\frac{\partial \overline{g}_{ij}}{\partial \overline{x}^m} = \frac{\partial^2 x^k}{\partial \overline{x}^i \partial \overline{x}^m} \frac{\partial x^l}{\partial \overline{x}^j} g_{kl} + \frac{\partial x^k}{\partial \overline{x}^i} \frac{\partial^2 x^l}{\partial \overline{x}^j \partial \overline{x}^m} g_{kl} + \frac{\partial x^k}{\partial \overline{x}^i} \frac{\partial x^l}{\partial \overline{x}^j} \frac{\partial x^n}{\partial \overline{x}^m} \frac{\partial g_{kl}}{\partial x^n}. \tag{9.301}$$

Permuting the indices, $(ijm) \to (mij) \to (jmi)$, we obtain two more equations:

$$\frac{\partial \overline{g}_{mi}}{\partial \overline{x}^j} = \frac{\partial^2 x^k}{\partial \overline{x}^m \partial \overline{x}^j} \frac{\partial x^l}{\partial \overline{x}^i} g_{kl} + \frac{\partial x^k}{\partial \overline{x}^m} \frac{\partial^2 x^l}{\partial \overline{x}^i \partial \overline{x}^j} g_{kl} + \frac{\partial x^k}{\partial \overline{x}^m} \frac{\partial x^l}{\partial \overline{x}^i} \frac{\partial x^n}{\partial \overline{x}^j} \frac{\partial g_{kl}}{\partial x^n}, \tag{9.302}$$

$$\frac{\partial \overline{g}_{jm}}{\partial \overline{x}^i} = \frac{\partial^2 x^k}{\partial \overline{x}^j \partial \overline{x}^i} \frac{\partial x^l}{\partial \overline{x}^m} g_{kl} + \frac{\partial x^k}{\partial \overline{x}^j} \frac{\partial^2 x^l}{\partial \overline{x}^m \partial \overline{x}^i} g_{kl} + \frac{\partial x^k}{\partial \overline{x}^j} \frac{\partial x^l}{\partial \overline{x}^m} \frac{\partial x^n}{\partial \overline{x}^i} \frac{\partial g_{kl}}{\partial x^n}. \tag{9.303}$$

Adding the first two equations and subtracting the last one from the result and after some rearrangement of indices, we obtain

$$\frac{1}{2}\left[\frac{\partial \overline{g}_{ik}}{\partial \overline{x}^j} + \frac{\partial \overline{g}_{jk}}{\partial \overline{x}^i} - \frac{\partial \overline{g}_{ij}}{\partial \overline{x}^k}\right] = \frac{\partial x^l}{\partial \overline{x}^i} \frac{\partial x^m}{\partial \overline{x}^j} \frac{\partial x^n}{\partial \overline{x}^k} \frac{1}{2}\left[\frac{\partial g_{\ln}}{\partial x^m} + \frac{\partial g_{mn}}{\partial x^l} - \frac{\partial g_{lm}}{\partial x^n}\right] + g_{lm} \frac{\partial x^l}{\partial \overline{x}^k} \frac{\partial^2 x^m}{\partial \overline{x}^i \partial \overline{x}^j}. \tag{9.304}$$

Defining **Christoffel symbols** of the **first kind** as

$$[ij,k] = \frac{1}{2}\left[\frac{\partial g_{ik}}{\partial x^j} + \frac{\partial g_{jk}}{\partial x^i} - \frac{\partial g_{ij}}{\partial x^k}\right], \tag{9.305}$$

we write Eq. (9.304) as

$$\overline{[ij,k]} = \frac{\partial x^l}{\partial \overline{x}^i} \frac{\partial x^m}{\partial \overline{x}^j} \frac{\partial x^n}{\partial \overline{x}^k} [lm,n] + g_{lm} \frac{\partial x^l}{\partial \overline{x}^k} \frac{\partial^2 x^m}{\partial \overline{x}^i \partial \overline{x}^j}, \tag{9.306}$$

where

$$\overline{[ij,k]} = \frac{1}{2}\left[\frac{\partial \overline{g}_{ik}}{\partial \overline{x}^j} + \frac{\partial \overline{g}_{jk}}{\partial \overline{x}^i} - \frac{\partial \overline{g}_{ij}}{\partial \overline{x}^k}\right]. \tag{9.307}$$

We can easily solve this equation for the second derivative to obtain

$$\frac{\partial^2 x^h}{\partial \overline{x}^i \partial \overline{x}^j} = \frac{\partial x^h}{\partial \overline{x}^p} \overline{\left\{ \begin{matrix} p \\ ij \end{matrix} \right\}} - \frac{\partial x^l}{\partial \overline{x}^i} \frac{\partial x^m}{\partial \overline{x}^j} \left\{ \begin{matrix} h \\ lm \end{matrix} \right\}, \tag{9.308}$$

where we have defined the **Christoffel symbols** of the **second kind** as

$$\left\{ \begin{matrix} i \\ jk \end{matrix} \right\} = g^{il}[jk,l]. \tag{9.309}$$

Substituting Eq. (9.308) in Eq. (9.297), we get

$$\frac{\partial \overline{u}_i}{\partial \overline{x}^k} = \frac{\partial x^j}{\partial \overline{x}^l}\overline{\left\{\begin{matrix} l \\ ik \end{matrix}\right\}}u_j - \frac{\partial x^l}{\partial \overline{x}^i}\frac{\partial x^m}{\partial \overline{x}^k}\left\{\begin{matrix} j \\ lm \end{matrix}\right\}u_j + \frac{\partial x^j}{\partial \overline{x}^i}\frac{\partial x^l}{\partial \overline{x}^k}\frac{\partial u_j}{\partial x^l}. \tag{9.310}$$

Rearranging, and using the symmetry property of the Christoffel symbol of the second kind:

$$\left\{\begin{matrix} i \\ jk \end{matrix}\right\} = \left\{\begin{matrix} i \\ kj \end{matrix}\right\}, \tag{9.311}$$

this becomes

$$\frac{\partial \overline{u}_i}{\partial \overline{x}^k} - \overline{\left\{\begin{matrix} l \\ ik \end{matrix}\right\}}\left[\frac{\partial x^j}{\partial \overline{x}^l}u_j\right] = \frac{\partial x^j}{\partial \overline{x}^i}\frac{\partial x^l}{\partial \overline{x}^k}\left[\frac{\partial u_j}{\partial x^l} - \left\{\begin{matrix} m \\ jl \end{matrix}\right\}u_m\right], \tag{9.312}$$

$$\left[\frac{\partial \overline{u}_i}{\partial \overline{x}^k} - \overline{\left\{\begin{matrix} l \\ ik \end{matrix}\right\}}\overline{u}_l\right] = \frac{\partial x^j}{\partial \overline{x}^i}\frac{\partial x^l}{\partial \overline{x}^k}\left[\frac{\partial u_j}{\partial x^l} - \left\{\begin{matrix} m \\ jl \end{matrix}\right\}u_m\right]. \tag{9.313}$$

The above equation shows that

$$\left[\frac{\partial u_j}{\partial x^l} - \left\{\begin{matrix} m \\ jl \end{matrix}\right\}u_m\right]$$

transforms like a covariant second-rank tensor. Thus we define the **covariant derivative** of a **covariant vector**, u_i, as

$$\boxed{u_{i;j} = \frac{\partial u_i}{\partial x^j} - \left\{\begin{matrix} k \\ ij \end{matrix}\right\}u_k.} \tag{9.314}$$

Similarly, the **covariant derivative** of a **contravariant vector** is defined as

$$\boxed{u^i_{;j} = \frac{\partial u^i}{\partial x^j} + \left\{\begin{matrix} i \\ jk \end{matrix}\right\}u^k.} \tag{9.315}$$

The covariant derivative is also shown as ∂_i, that is, $\partial_j u_i = u_{i;j}$. The covariant derivative of a higher-rank tensor is obtained by treating each index at a time as

$$T^{i_1 i_2 \cdots}_{j_1 j_2 \cdots ;\, k} = \frac{\partial T^{i_1 i_2 \cdots}_{j_1 j_2 \cdots}}{\partial x^k} + \left\{\begin{matrix} i_1 \\ kl \end{matrix}\right\}T^{l i_2 \cdots}_{j_1 j_2 \cdots} + \cdots - \left\{\begin{matrix} m \\ kj_1 \end{matrix}\right\}T^{i_1 i_2 \cdots}_{m j_2 \cdots} - \cdots . \tag{9.316}$$

Covariant derivatives obey the same **distribution rules** as ordinary derivatives:

$$\boxed{(AB)_{;i} = A_{;i}B + AB_{;i},} \tag{9.317}$$

$$\boxed{(aA + bB)_{;i} = aA_{;i} + bB_{;i},} \tag{9.318}$$

where A and B are tensors of arbitrary rank and a and b are scalars.

9.6.8 Some Covariant Derivatives

In the following, we also show equivalent ways of writing certain operations.

1. We can write the **covariant derivative** or the **gradient** of a scalar function, Ψ, as an ordinary derivative:

$$\boxed{\vec{\nabla}\Psi = \Psi_{;j} = \partial_j \Psi = \frac{\partial \Psi}{\partial x^j}.} \tag{9.319}$$

   This is also the covariant component of the gradient

$$\left(\vec{\nabla}\Psi\right)_i. \tag{9.320}$$

2. Using the symmetry of Christoffel symbols, **curl** of a vector field, $\vec{v}$, can be defined as the second-rank tensor

$$\left(\vec{\nabla}\times\vec{v}\right)_{ij} = \partial_j v_i - \partial_i v_j = v_{i;j} - v_{j;i}, \tag{9.321}$$

$$\boxed{\left(\vec{\nabla}\times\vec{v}\right)_{ij} = \frac{\partial v_i}{\partial x^j} - \frac{\partial v_j}{\partial x^i}.} \tag{9.322}$$

   Note that because we have used the symmetry of the Christoffel symbols, the curl operation can only be performed on the covariant components of a vector.
3. The covariant derivative of the metric tensor is zero:

$$\boxed{\partial_k g_{ij} = g_{ij;k} = 0,} \tag{9.323}$$

   where with Eq. (9.316) and the definition of Christoffel symbols the proof is straightforward.
4. A frequently used property of the Christoffel symbol of the second kind is

$$\boxed{\left\{ \begin{matrix} i \\ ik \end{matrix} \right\} = \frac{1}{2} g^{il} \frac{\partial g_{il}}{\partial x^k} = \frac{\partial (\ln \sqrt{|g|})}{\partial x^k}.} \tag{9.324}$$

   In the derivation, we use the result:

$$\frac{\partial g}{\partial x^k} = g g^{il} \frac{\partial g_{il}}{\partial x^k}, \tag{9.325}$$

   from the theory of matrices, where $g = \det g_{ij}$.
5. We can now define **covariant divergence** as

$$\vec{\nabla}\cdot\vec{v} = \partial_i v^i = v^i_{;i} = \frac{\partial v^i}{\partial x^i} + \left\{ \begin{matrix} i \\ ik \end{matrix} \right\} v^k, \tag{9.326}$$

$$\boxed{\vec{\nabla}\cdot\vec{v} = \frac{1}{|g|^{1/2}}\frac{\partial}{\partial x^k}[|g|^{1/2}v^k].} \tag{9.327}$$

If v^i is a tensor density of weight $+1$, divergence becomes

$$\vec{\nabla}\cdot\vec{v} = v^i_{;i} \ (= \partial_i v^i), \tag{9.328}$$

which is again a scalar density of weight $+1$.

6. Using Eq. (9.320), we write the contravariant component of the gradient of a scalar function as

$$\left(\vec{\nabla}\Psi\right)^i = g^{ij}\Psi_{;j} = g^{ij}\frac{\partial\Psi}{\partial x^j}. \tag{9.329}$$

We can now define the **Laplacian**, $\vec{\nabla}^2\Psi$, as a scalar field:

$$\boxed{\vec{\nabla}\cdot(\vec{\nabla}\Psi) = (\vec{\nabla}\Psi)^i_{;i} = \partial_i\partial^i\Psi = \frac{1}{|g|^{1/2}}\frac{\partial}{\partial x^i}\left[|g|^{1/2}g^{ik}\frac{\partial\Psi}{\partial x^k}\right].} \tag{9.330}$$

9.6.9 Riemann Curvature Tensor

Let us take the covariant derivative of v_i twice. The difference, $v_{i;jk} - v_{i;kj}$, can be written as

$$\boxed{v_{i;jk} - v_{i;kj} = R^l_{ijk}v_l,} \tag{9.331}$$

where R^l_{ijk} is the fourth-rank **Riemann curvature tensor**, which plays a central role in the structure of Riemann spaces:

$$\boxed{R^l_{ijk} = \begin{Bmatrix} l \\ mj \end{Bmatrix}\begin{Bmatrix} m \\ ik \end{Bmatrix} - \begin{Bmatrix} l \\ mk \end{Bmatrix}\begin{Bmatrix} m \\ ij \end{Bmatrix} + \frac{\partial}{\partial x^j}\begin{Bmatrix} l \\ ik \end{Bmatrix} - \frac{\partial}{\partial x^k}\begin{Bmatrix} l \\ ij \end{Bmatrix}.} \tag{9.332}$$

The Riemann curvature tensor satisfies the following symmetry properties:

$$R_{ijkl} = -R_{ijlk}, \tag{9.333}$$

$$R_{ijkl} = -R_{jikl}, \tag{9.334}$$

$$R_{ijkl} = R_{klij}. \tag{9.335}$$

The significance of the Riemann curvature tensor is that all of its components **vanish** only in **flat space**, that is, we cannot find a coordinate system where $R_{ijkl} = 0$ unless the space is truly flat.

An important scalar in Riemann spaces is the **Riemann curvature scalar**, which is obtained from R_{ijkl} by contracting its indices as

$$\boxed{R = g^{jl}g^{ik}R_{ijkl} = g^{jl}R^{k}{}_{jkl} = R^{k\ j}{}_{jk}\ .} \tag{9.336}$$

Note that $R_{ijkl} = 0$ implies $R = 0$, but not vice versa.

9.7 Curvature

We have seen that from the appearance of a metric tensor one cannot tell whether the underlying space is curved or not. A complicated looking metric with all or some of its components depending on position may very well be due to an unusual choice of coordinates. Still, the metric tensor possesses all the necessary information regarding the intrinsic properties of the underlying space. **Intrinsic curvature** is defined entirely in terms of measurements that can be carried out in the space itself and not on how the space is embedded in a higher dimension. Our task is now to find a way to extract this information from the metric tensor. Furthermore, we would like to find a way that works not just for two-dimensional surfaces, but also for surfaces with any number of dimensions and for any shape. In other words, we need a criteria more sophisticated than just the circumference to radius ratio of a circle.

Let the intelligent bugs living on the two-dimensional surface of a sphere, transport a small vector over a closed path always pointing in the same direction so that it remains parallel to itself. This is called **parallel transport**. When the vector comes back to its starting point, it will be seen that the vector has turned a certain angle ϑ (Figure 9.15). This angle, which is zero in flat space, for a sufficiently small area enclosed by the path, δA, is proportional to the area:

$$\delta\vartheta = K\delta A. \tag{9.337}$$

The proportionality constant, K, is called the **Gaussian curvature**. For a sphere, $K = 1/R^2$. In fact, for a triangular path, this angle is precisely the excess over π for the sum of the interior angles of the triangle. For a flat space, we can take R as infinity, thus obtaining $K = 0$. For the saddle like surface in Figure 9.14, the Gaussian curvature is negative: $K = -1/R^2$. Gaussian curvature can be defined locally in terms of the radii of curvature in two perpendicular planes as $K = 1/R_1R_2$, where for a sphere $R_1 = R_2 = R$, hence $K = 1/R^2$. For a cylinder, $K = 0$, since $R_1 = R$ and $R_2 = \infty$.

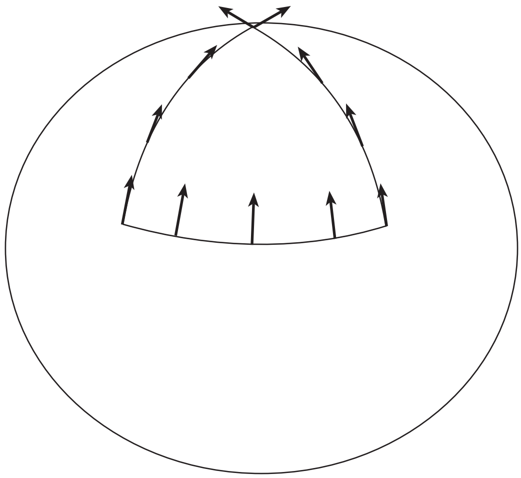

Figure 9.15 Parallel transport.

The general description of curvature in many-dimensional surfaces is still based on parallel transport over closed paths. However, this time $\delta\vartheta$ will also depend on the orientation of the path. The fact that the parallel transported vectors over closed paths in general do not coincide with themselves is due to the fact that the covariant derivatives with respect to j and k in $v_{i;jk}$ do not commute, $v_{i;jk} \neq v_{i;kj}$, unless the space is flat. We have mentioned that the difference between $v_{i;jk}$ and $v_{i;kj}$ is given in terms of a fourth-rank tensor, R^l_{ijk}, called the **Riemann curvature tensor**, or in short, the **curvature tensor** [Eqs. (9.331) and (9.332)]:

$$v_{i;jk} - v_{i;kj} = R^l_{ijk} v_l, \tag{9.338}$$

$$R^l_{ijk} = \begin{Bmatrix} l \\ mj \end{Bmatrix}\begin{Bmatrix} m \\ ik \end{Bmatrix} - \begin{Bmatrix} l \\ mk \end{Bmatrix}\begin{Bmatrix} m \\ ij \end{Bmatrix} + \frac{\partial}{\partial x^j}\begin{Bmatrix} l \\ ik \end{Bmatrix} - \frac{\partial}{\partial x^k}\begin{Bmatrix} l \\ ij \end{Bmatrix}. \tag{9.339}$$

To understand the properties of the curvature tensor, we now discuss parallel transport in detail.

9.7.1 Parallel Transport

Covariant differentiation [Eq. (9.315)] over the entire space is defined as

$$v^i_{;j} = \frac{\partial v^i}{\partial x^j} + \begin{Bmatrix} i \\ jk \end{Bmatrix} v^k, \tag{9.340}$$

where the Chrisfoffel symbols of the second kind are defined as [Eq. (9.309)]

$$\begin{Bmatrix} i \\ jk \end{Bmatrix} = \frac{g^{il}}{2}\left(\frac{\partial g_{jl}}{\partial x^k} + \frac{\partial g_{kl}}{\partial x^j} - \frac{\partial g_{jk}}{\partial x^l}\right). \tag{9.341}$$

However, we are frequently interested in covariant differentiation along a path parametrized as $x^i(\tau)$. Along $x^i(\tau)$, we can also parametrize a vector in terms of τ as $v^i(\tau)$. Now the covariant derivative of v^i over the path $x^i(\tau)$ becomes

$$\frac{Dv^i}{D\tau} = v^i_{;j}\frac{dx^j}{d\tau} = \frac{\partial v^i}{\partial x^j}\frac{dx^j}{d\tau} + \left\{ \begin{matrix} i \\ jk \end{matrix} \right\} \frac{dx^j}{d\tau}v^k, \tag{9.342}$$

$$\boxed{\frac{Dv^i}{D\tau} = \frac{dv^i}{d\tau} + \left\{ \begin{matrix} i \\ jk \end{matrix} \right\} \frac{dx^j}{d\tau}v^k.} \tag{9.343}$$

Note that $\frac{Dv^i}{D\tau}$ is a covariant expression, hence valid in all coordinate systems. A vector parallel transported along a curve satisfies

$$\frac{Dv^i}{D\tau} = 0, \tag{9.344}$$

that is,

$$\frac{dv^i}{d\tau} = -\left\{ \begin{matrix} i \\ jk \end{matrix} \right\} \frac{dx^j}{d\tau}v^k. \tag{9.345}$$

For a covariant vector, the parallel transport equation becomes

$$\frac{dv_i}{d\tau} = \left\{ \begin{matrix} k \\ ij \end{matrix} \right\} \frac{dx^j}{d\tau}v_k. \tag{9.346}$$

Parallel transport is what comes closest to a constant vector along a curve in curved space (Figure 9.15).

9.7.2 Round Trips via Parallel Transport

We have obtained the formula [Eq. (9.346)] that tells us how a vector changes when parallel transported along a curve. We now apply this result to see whether a given vector returns to its initial state when parallel transported along a small but closed path. If the curve is sufficiently small, we can expand the Christoffel symbols:

$$\Gamma^k_{ij}(x) = \left\{ \begin{matrix} k \\ ij \end{matrix} \right\}, \tag{9.347}$$

and the vector v_i around some point $X = x(\tau_0)$ as

$$\Gamma^k_{ij}(x) = \Gamma^k_{ij}(X) + (x^l(\tau) - X^l)\frac{\partial}{\partial X^l}\Gamma^k_{ij}(X) + \cdots, \tag{9.348}$$

$$v_i(\tau) = v_i(\tau_0) + \Gamma^k_{ij}(X)(x^j(\tau) - X^j)v_k(\tau_0) + \cdots, \tag{9.349}$$

where we have used Eq. (9.346) to first order in $(x^j(\tau) - X^j)$ to write Eq. (9.349). Substituting Eqs. (9.348) and (9.349) into Eq. (9.346) and only keeping terms of up to second-order, we get

$$v_i(\tau) \simeq v_i(\tau_0) + \int_{\tau_0}^{\tau} \left[\Gamma^k_{ij}(X) + (x^l(\tau) - X^l)\frac{\partial}{\partial X^l}\Gamma^k_{ij}(X) + \cdots\right] \times [v_k(\tau_0) + v_m(\tau_0)\Gamma^m_{kl}(X)(x^l(\tau) - X^l) + \cdots]\frac{dx^j(\tau)}{d\tau}d\tau. \tag{9.350}$$

We could simplify this further to write

$$v_i(\tau) \simeq v_i(\tau_0) + \Gamma^k_{ij}(X)v_k(\tau_0)\int_{\tau_0}^{\tau}\frac{dx^j(\tau)}{d\tau}d\tau + \left[\frac{\partial}{\partial X^l}\Gamma^m_{ij}(X) + \Gamma^k_{ij}(X)\Gamma^m_{kl}(X)\right]v_m(\tau_0)\int_{\tau_0}^{\tau}(x^l(\tau) - X^l)\frac{dx^j}{d\tau}d\tau. \tag{9.351}$$

Since for a closed path x^i returns to its initial value X^i for some τ_1:

$$\int_{\tau_0}^{\tau_1}\frac{dx^j}{d\tau}d\tau = 0. \tag{9.352}$$

This gives the change in value, Δv_i, of the vector v_i when parallel transported over a sufficiently small closed path as

$$\Delta v_i = \left[\frac{\partial}{\partial X^l}\Gamma^m_{ij}(X) + \Gamma^k_{ij}(X)\Gamma^m_{kl}(X)\right]v_m(\tau_0)\int_{\tau_0}^{\tau_1}x^l(\tau)\frac{dx^j}{d\tau}d\tau, \tag{9.353}$$

or as

$$\Delta v_i = \left[\frac{\partial}{\partial X^l}\Gamma^m_{ij}(X) + \Gamma^k_{ij}(X)\Gamma^m_{kl}(X)\right]v_m(\tau_0)\oint x^l(\tau)dx^j. \tag{9.354}$$

The integral, $\oint x^l(\tau)dx^j$, is in general nonzero and antisymmetric:

$$\oint x^l(\tau)dx^j = \int_{\tau_0}^{\tau_1}\frac{d(x^lx^j)}{d\tau}d\tau - \int_{\tau_0}^{\tau_1}x^j\frac{dx^l}{d\tau}d\tau \tag{9.355}$$

$$= -\oint x^j(\tau)dx^l, \tag{9.356}$$

hence, we can also write Δv_i as

$$\Delta v_i = \left[\frac{\partial}{\partial X^j}\Gamma^m_{il}(X) + \Gamma^k_{il}(X)\Gamma^m_{kj}(X)\right]v_m(\tau_0)\oint x^j(\tau)dx^l \tag{9.357}$$

$$= -\left[\frac{\partial}{\partial X^j}\Gamma^m_{il}(X) + \Gamma^k_{il}(X)\Gamma^m_{kj}(X)\right]v_m(\tau_0)\oint x^l(\tau)dx^j. \tag{9.358}$$

Adding Eqs. (9.354) and (9.358), we write

$$2\Delta v_i = \left[\frac{\partial}{\partial X^l}\Gamma^m_{ij}(X) - \frac{\partial}{\partial X^j}\Gamma^m_{il}(X) + \Gamma^k_{ij}(X)\Gamma^m_{kl}(X) - \Gamma^k_{il}(X)\Gamma^m_{kj}(X)\right] \times v_m(\tau_0)\oint x^l(\tau)dx^j. \tag{9.359}$$

The quantity inside the square brackets is nothing but R^m_{ilj}, that is, the curvature tensor, hence

$$\boxed{\Delta v_i = \frac{1}{2} R^m_{ilj} v_m(\tau_0) \oint x^l(\tau) dx^j.} \tag{9.360}$$

This result indicates that a vector, v_i, parallel transported over a small closed path does not return to its initial value unless R^m_{ilj} vanishes at X. If we take our closed path as a small parallelogram with the sides $\Delta_1 x^i$ and $\Delta_2 x^j$, then $\oint x^l(\tau)dx^j$ are the components of the area of the parallelogram (Figure 9.16):

$$\oint x^l(\tau) dx^j = \Delta_1 x^l \Delta_2 x^j - \Delta_1 x^j \Delta_2 x^l. \tag{9.361}$$

For a finite closed path C enclosing an area A, we can subdivide A into small cells each bounded by c_N. The change in v_i when parallel transported around C can then be written as the sum

$$\Delta v_i = \sum_N \Delta_N v_i. \tag{9.362}$$

This follows from the fact that the change in v_i around the neighboring cells are cancelled, thus leaving only the outermost cell boundaries making up the path C.

9.7.3 Algebraic Properties of the Curvature Tensor

To reveal the algebraic properties of the curvature tensor, we write it as $R_{ijkl} = g_{im} R^m_{jkl}$. Using Eq. (9.332), this can be written as

$$R_{ijkl} = \frac{1}{2}\left[\frac{\partial^2 g_{jk}}{\partial x^l \partial x^i} - \frac{\partial^2 g_{ik}}{\partial x^l \partial x^j} + \frac{\partial^2 g_{il}}{\partial x^k \partial x^j} - \frac{\partial^2 g_{jl}}{\partial x^k \partial x^i}\right] + g_{nm}[\Gamma^n_{li}\Gamma^m_{jk} - \Gamma^n_{ki}\Gamma^m_{jl}]. \tag{9.363}$$

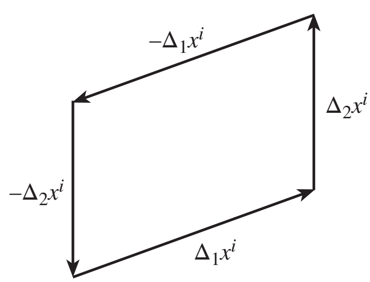

Figure 9.16 Parallelogram.

From this equation, the following properties are evident:

(i) **Symmetry**:

$$R_{ijkl} = R_{klij}. \tag{9.364}$$

(ii) **Antisymmetry**:

$$R_{ijkl} = -R_{jikl} = -R_{ijlk} = R_{jilk}. \tag{9.365}$$

(iii) **Cyclicity**:

$$R_{ijkl} + R_{iljk} + R_{iklj} = 0. \tag{9.366}$$

There is one more symmetry called the **Bianchi identity**, which is not obvious but could be shown by direct substitution:

(iv) **Bianchi identity**:

$$R_{ijkl;m} + R_{ijmk;l} + R_{ijlm;k} = 0. \tag{9.367}$$

9.7.4 Contractions of the Curvature Tensor

Using the symmetry property, we can contract the first and the third indices to get a very important symmetric second-rank tensor called the **Ricci tensor**:

$$\boxed{g^{ik}R_{ijkl} = R_{jl},} \tag{9.368}$$

where $R_{jl} = R_{lj}$. The antisymmetry property of the curvature tensor indicates that this is the only second-rank tensor that can be constructed by contracting the indices of the curvature tensor. Contracting the first and the third, and then the second and the fourth indices of the curvature tensor gives us the only scalar, R, the **Riemann curvature scalar**, that can be constructed from the curvature tensor as

$$\boxed{g^{jl}g^{ik}R_{ijkl} = g^{jl}R_{jl} = R^j_j = R.} \tag{9.369}$$

Finally, contracting the Bianchi identity gives

$$g^{ik}R_{ijkl;m} + g^{ik}R_{ijmk;l} + g^{ik}R_{ijlm;k} = 0, \tag{9.370}$$

$$R_{jl;m} - R_{jm;l} + R^k_{jlm;k} = 0. \tag{9.371}$$

Contracting once more yields

$$R_{;m} - R^j_{m;j} - R^k_{m;k} = 0, \tag{9.372}$$

$$\left(R^j_m - \frac{1}{2}R\delta^j_m\right)_{;j} = 0, \tag{9.373}$$

which can also be written as

$$\boxed{\left(R^{ij} - \frac{1}{2}Rg^{ij}\right)_{;j} = 0.} \tag{9.374}$$

9.7.5 Curvature in *n* Dimensions

The **curvature tensor**, R_{ijkl}, in n dimensions has n^4 **components**. In four dimensions it has 256, in three dimensions 81, and in two dimensions 16 components. However, due to its large number of symmetries expressed in Eqs. (9.364)–(9.367), it has only

$$\boxed{C_n = \frac{1}{12}N^2(N^2 - 1)} \tag{9.375}$$

independent components. In four dimensions, this gives the number of independent components as 20, in three dimensions as 6, and in two dimensions as 1.

In one dimension, the curvature tensor has only one component, R_{1111}, which due to Eq. (9.366) or (9.367) is always zero. In other words, in one dimension, we cannot have intrinsic curvature. It sounds odd that a curved wire has zero curvature. However, curvature tensor reflects the inner properties of the space and not how it is embedded or viewed from a higher dimension. Indeed, in one dimension, we can always transform the line element, $ds^2 = g_{11}(x)dx^2$, everywhere into the form $ds^2 = dx'^2$, via the coordinate transformation

$$x' = \int \sqrt{g_{11}}dx. \tag{9.376}$$

Another way to see this is that we can always straighten a bent wire without cutting it.

In two dimensions, R_{ijkl} has only one independent component, which can be taken as R_{1212}. Using Eqs. (9.363)–(9.367), we can write all the components of R_{ijkl} as

$$\boxed{\begin{aligned} R_{1212} &= -R_{2112} = -R_{1221} = R_{2121}, \\ R_{1111} &= R_{1112} = R_{1121} = R_{1122} = 0, \\ R_{1211} &= R_{1222} = R_{2111} = R_{2122} = 0, \\ R_{2211} &= R_{2212} = R_{2221} = R_{2222} = 0. \end{aligned}} \tag{9.377}$$

These can be conveniently expressed as

$$R_{ijkl} = (g_{ik}g_{jl} - g_{il}g_{jk})\frac{R_{1212}}{g}, \tag{9.378}$$

where g is the determinant $g = (g_{11}g_{22} - g_{12}^2)$. If we contract i and k in R_{ijkl}, we get

$$R_{jl} = g_{jl}\frac{R_{1212}}{g}. \tag{9.379}$$

Contracting j and l in R_{jl} gives the **Riemann curvature scalar**

$$R = \frac{2R_{1212}}{g}. \tag{9.380}$$

We can now write the curvature tensor as

$$\boxed{R_{ijkl} = \frac{R}{2}(g_{ik}g_{jl} - g_{il}g_{jk}).} \tag{9.381}$$

The **Gaussian curvature**, K, introduced in Eq. (9.337) is related to the Riemann curvature scalar R as

$$K = \frac{R}{2} = \frac{R_{1212}}{g}, \tag{9.382}$$

which for a sphere of radius a becomes $K = 1/a^2$.

Example 9.1 ***Laplacian as a scalar field***
We consider the line element

$$ds^2 = dr^2 + r^2 d\theta^2 + r^2 \sin^2\theta d\phi^2, \tag{9.383}$$

where

$$x^1 = r, \quad x^2 = \theta, \quad x^3 = \phi \tag{9.384}$$

and

$$g_{11} = 1, \; g_{22} = r^2, \; g_{33} = r^2 \sin^2\theta. \tag{9.385}$$

Contravariant components g^{ij} are:

$$g^{11} = 1, \quad g^{22} = \frac{1}{r^2}, \quad g^{33} = \frac{1}{r^2\sin^2\theta}. \tag{9.386}$$

Using Eq. (9.330) and $g = r^4 \sin^2\theta$, we can write the Laplacian as

$$\partial_i \partial^i \Psi = \frac{1}{|g|^{1/2}} \frac{\partial}{\partial x^i} \left[|g|^{1/2} g^{ik} \frac{\partial \Psi}{\partial x^k} \right] \tag{9.387}$$

$$= \frac{1}{|g|^{1/2}} \frac{\partial}{\partial x^i} \left[|g|^{1/2} \left(g^{i1} \frac{\partial \Psi}{\partial x^1} + g^{i2} \frac{\partial \Psi}{\partial x^2} + g^{i3} \frac{\partial \Psi}{\partial x^3} \right) \right] \tag{9.388}$$

$$= \frac{1}{r^2 \sin\theta} \left[\frac{\partial}{\partial r} \left(r^2 \sin\theta \frac{\partial \Psi}{\partial r} \right) + \frac{\partial}{\partial \theta} \left(\frac{r^2 \sin\theta}{r^2} \frac{\partial \Psi}{\partial \theta} \right) + \frac{\partial}{\partial \phi} \left(\frac{r^2 \sin\theta}{r^2 \sin^2\theta} \frac{\partial \Psi}{\partial \phi} \right) \right]. \tag{9.389}$$

After simplifying, the **Laplacian** is obtained as

$$\boxed{\partial_i \partial^i \Psi = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial \Psi}{\partial r} \right) + \frac{1}{r^2 \sin\theta} \frac{\partial}{\partial \theta} \left(\sin\theta \frac{\partial \Psi}{\partial \theta} \right) + \frac{1}{r^2 \sin^2\theta} \frac{\partial^2 \Psi}{\partial \phi^2}.} \tag{9.390}$$

Here we have obtained a well-known formula in a rather straight forward manner, demonstrating the advantages of the tensor formalism. Note that even though the components of the metric tensor depend on position [Eq. (9.385)], the curvature tensor is zero:

$$R_{ijkl} = 0, \tag{9.391}$$

thus the space of the line element [Eq. (9.383)] is flat. However, for the metric

$$ds^2 = \left[\frac{1}{1 - r^2/R_0^2}\right] dr^2 + r^2 d\theta^2 + r^2 \sin^2\theta d\phi^2, \tag{9.392}$$

it can be shown that not all the components of R_{ijkl} vanish. In fact, this line element gives the distance between two infinitesimally close points on the surface of a hypersphere $(S - 3)$ with constant radius R_0.

9.7.6 Geodesics

Geodesics are defined as the shortest paths between two points in a given geometry. In flat space, they are naturally the straight lines. We can generalize the concept of straight lines as curves whose tangents remain constant along the curve. However, the constancy is now with respect to the covariant derivative. If we parametrize an arbitrary curve in terms of arclength, s, as $x^i(s)$, its tangent vector will be given as

$$t^i = \frac{dx^i}{ds}. \tag{9.393}$$

For geodesics, the covariant derivative of t^i must be zero; thus we obtain the equation of geodesics as

$$t^i_{;j}\frac{dx^j}{ds} = \left[\frac{dt^i}{dx^j} + \left\{\begin{matrix} i \\ jk \end{matrix}\right\} t^k\right]\frac{dx^j}{ds} = 0, \tag{9.394}$$

$$\boxed{\frac{d^2x^i}{ds^2} + \left\{\begin{matrix} i \\ jk \end{matrix}\right\}\frac{dx^j}{ds}\frac{dx^k}{ds} = 0.} \tag{9.395}$$

9.7.7 Invariance Versus Covariance

We have seen that scalars preserve their value under general coordinate transformations. Properties like the magnitude of a vector and the trace of a second-rank tensor also do not change under general coordinate transformations. Such properties are called **invariants**. They are very important in the study of the coordinate-independent properties of a system.

A very important property of tensors is that tensor equations preserve their form under coordinate transformations. For example, the tensor equation

$$A_{ij} = B_{ijkl}C_{kl} + kD_{ij} + E^k_{i;\, jk} + \cdots \tag{9.396}$$

transforms into

$$A'_{ij} = B'_{ijkl}C'_{kl} + kD'_{ij} + E'^{k}_{i;\,jk} + \cdots . \tag{9.397}$$

Under coordinate transformations, individual components of tensors change; however, the form of the tensor equation remains the same. This is called **covariance**. One of the early uses of tensors was in searching and expressing the properties of crystals that are independent on the choice of coordinates. However, the covariance of tensor equations reaches its full potential only with the introduction of the spacetime concept and the special and the general theories of relativity.

9.8 Spacetime and Four-Tensors

9.8.1 Minkowski Spacetime

In Newton's theory, the energy of a freely moving particle is given by the well-known expression for the kinetic energy as $E = \frac{1}{2}mv^2$. Since there is no limit to the energy that one could pump into a system, this formula implies that in principle, one could accelerate particles to any desired velocity. In classical physics, this makes it possible to construct infinitely fast signals to communicate with the other parts of the universe. Another property of Newton's theory is that time is universal, or absolute, that is, identical clocks carried by moving observers, uniform or accelerated, run at the same rate. Thus, once two observers synchronize their clocks, they will remain synchronized forever. In Newton's theory, this allows us to study systems with moving parts in terms of a single, universal, time parameter. With the discovery of the special theory of relativity, it became clear that clocks carried by moving observers run at different rates; thus rendering the usage of a single time parameter for all observers impossible.

After Einstein's introduction of the special theory of relativity, another remarkable contribution toward the understanding of time came with the introduction of the spacetime concept by Minkowski. Spacetime not only strengthened the mathematical foundations of special relativity but also paved the way to Einstein's theory of gravitation.

Minkowski spacetime is obtained by simply adding a time axis orthogonal to the Cartesian axis, thus treating time as another coordinate (Figure 9.17). A point in spacetime corresponds to an event. It is important to note that space and time are fundamentally different and cannot be treated symmetrically. For example, it is possible to be present at the same place at two different times; however, if we reverse the roles of space and time, and if space and time were symmetric, then it would also mean that we could be present at two different places at the same time. So far there is no evidence for this,

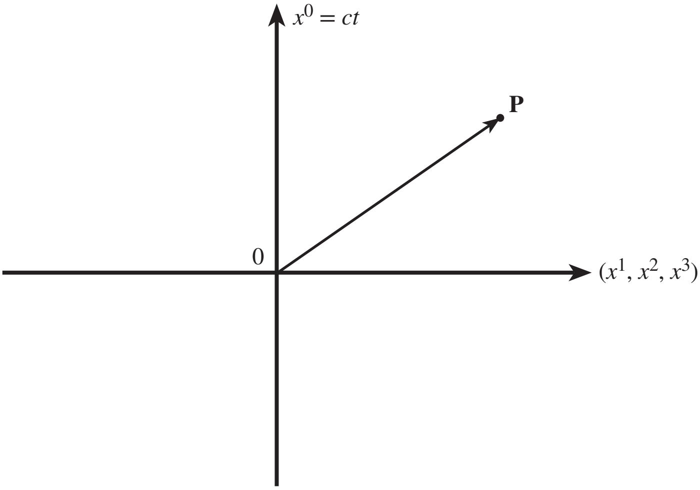

Figure 9.17 A point in Minkowski spacetime.

neither in the microrealm nor in the macrorealm. In relativity, even though space and time are treated on equal footing as independent coordinates, they are not treated symmetrically. This is evident in the Minkowski line element:

$$\boxed{ds^2 = c^2dt^2 - dx^2 - dy^2 - dz^2,} \tag{9.398}$$

where the signs of the spatial and the time coordinates are different. It is for this reason that Minkowski spacetime is called **pseudo-Euclidean**. In this line element, c is the speed of light representing the maximum velocity in nature. An interesting property of the Minkowski spacetime is that two events connected by light rays, like the emission of a photon from one galaxy and its subsequent absorption in another, have zero distance between them even though they are widely separated in spacetime.

9.8.2 Lorentz Transformations and Special Relativity

In Minkowski spacetime, there are infinitely many different ways to choose the orientation of the coordinate axis. However, a particular group of coordinate systems, which are related to each other by **linear transformations**:

$$\begin{aligned}
\bar{x}^0 &= a^0_0x^0 + a^0_1x^1 + a^0_2x^2 + a^0_3x^3,\\
\bar{x}^1 &= a^1_0x^0 + a^1_1x^1 + a^1_2x^2 + a^1_3x^3,\\
\bar{x}^2 &= a^2_0x^0 + a^2_1x^1 + a^2_2x^2 + a^2_3x^3,\\
\bar{x}^3 &= a^3_0x^0 + a^3_1x^1 + a^3_2x^2 + a^3_3x^3,
\end{aligned} \tag{9.399}$$

and which also preserve the **quadratic form**

$$(x^0)^2 - (x^1)^2 - (x^2)^2 - (x^3)^2, \tag{9.400}$$

have been extremely useful in special relativity. In these equations, we have written $x^0 = ct$ to emphasize the fact that time is treated as another coordinate.

In 1905, Einstein [2] published his celebrated paper on the **special theory of relativity**, which is based on two postulates:

First postulate of relativity: It is impossible to detect or measure uniform translatory motion of a system in free space.

Second postulate of relativity: The speed of light in free space is the maximum velocity in the universe, and it is the same for all uniformly moving observers.

In special relativity, two inertial observers K and $\overline{K}$, where $\overline{K}$ is moving uniformly with the velocity v along the common direction of the x^1- and $\overline{x}^1$-axes are related by the **Lorentz transformations** (Figure 9.18):

$$\boxed{\begin{aligned} \overline{x}^0 &= \frac{1}{\sqrt{1 - v^2/c^2}} \left[x^0 - \left(\frac{v}{c}\right) x^1\right], \\ \overline{x}^1 &= \frac{1}{\sqrt{1 - v^2/c^2}} \left[-\left(\frac{v}{c}\right) x^0 + x^1\right], \\ \overline{x}^2 &= x^2, \\ \overline{x}^3 &= x^3. \end{aligned}} \tag{9.401}$$

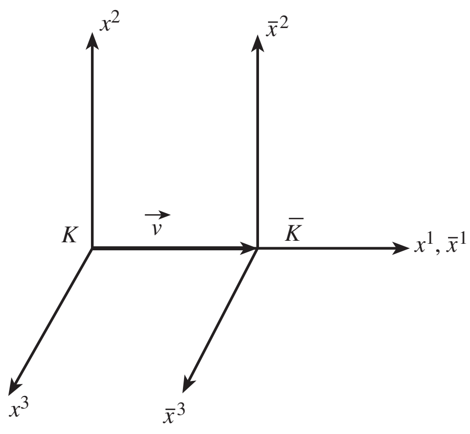

Figure 9.18 Lorentz transformations.

The **inverse transformation** is obtained by replacing v with $-v$ as

$$\boxed{\begin{aligned} x^0 &= \frac{1}{\sqrt{1-v^2/c^2}}\left[\bar{x}^0 + \left(\frac{v}{c}\right)\bar{x}^1\right], \\ x^1 &= \frac{1}{\sqrt{1-v^2/c^2}}\left[\left(\frac{v}{c}\right)\bar{x}^0 + \bar{x}^1\right], \\ x^2 &= \bar{x}^2, \\ x^3 &= \bar{x}^3. \end{aligned}} \tag{9.402}$$

When the axis in K and $\overline{K}$ remain parallel but the velocity $\vec{v}$ of frame $\overline{K}$ in frame K is arbitrary in direction, then the Lorentz transformation is generalized as

$$\boxed{\begin{aligned} \bar{x}^0 &= \gamma\left[x^0 - \left(\vec{\beta}\cdot\vec{x}\right)\right], \\ \vec{\bar{x}} &= \vec{x} + \frac{(\gamma-1)}{\beta^2}\left(\vec{\beta}\cdot\vec{x}\right)\vec{\beta} - \gamma\vec{\beta}x^0. \end{aligned}} \tag{9.403}$$

We have written $\gamma = 1/\sqrt{1-v^2/c^2}$ and $\vec{\beta} = \vec{v}/c$.

9.8.3 Time Dilation and Length Contraction

Two immediate and important consequences of the Lorentz transformation equations [Eq. (9.401)] are the **time dilation**:

$$\boxed{\Delta\bar{t} = \Delta t\left(1 - \frac{v^2}{c^2}\right)^{1/2}} \tag{9.404}$$

and the **length contraction** formulas:

$$\boxed{\Delta\bar{x}^1 = \Delta x^1\left(1 - \frac{v^2}{c^2}\right)^{1/2}.} \tag{9.405}$$

These formulas relate the time and the space intervals measured by two inertial observers $\overline{K}$ and K. The second formula is also known as the **Lorentz contraction**. The time dilation formula indicates that clocks carried by moving observers run slower compared to the clocks of the observer at rest. Similarly, the Lorentz contraction indicates that meter sticks carried by moving observers appear shorter to the observer at rest.

9.8.4 Addition of Velocities

Another important consequence of the Lorentz transformation is the formula for the addition of velocities, which relates the velocities measured in the K and

$\overline{K}$ frames by the formula

$$\boxed{u^1 = \frac{\overline{u}^1 + v}{1 + \overline{u}^1 v/c^2},} \tag{9.406}$$

where $u^1 = \frac{dx^1}{dt}$ and $\overline{u}^1 = \frac{d\overline{x}^1}{d\overline{t}}$ are the velocities measured in the K and the $\overline{K}$ frames, respectively. In the limit as $c \to \infty$, this formula reduces to the well-known Galilean result $u^1 = \overline{u}^1 + v$. Equation (9.406) indicates that even if we go to a frame moving with the speed of light, it is not possible to send signals faster than c.

If the axes in K and $\overline{K}$ remain parallel, but the velocity $\overrightarrow{v}$ of frame $\overline{K}$ in frame K is arbitrary in direction, then the parallel and the perpendicular components of velocity transform as

$$\boxed{u_{\parallel} = \frac{\overline{u}_{\parallel} + v}{1 + \overrightarrow{v} \cdot \overrightarrow{\overline{u}}/c^2},} \tag{9.407}$$

$$\boxed{\overrightarrow{u}_{\perp} = \frac{\overrightarrow{\overline{u}}_{\perp}}{\gamma(1 + \overrightarrow{v} \cdot \overrightarrow{\overline{u}}/c^2)}.} \tag{9.408}$$

In this notation, $u_{\parallel}$ and $\overrightarrow{u}_{\perp}$ refer to the parallel and perpendicular components with respect to $\overrightarrow{v}$ and $\gamma = (1 - v^2/c^2)^{-1/2}$.

9.8.5 Four-Tensors in Minkowski Spacetime

From the second postulate of relativity, **invariance** of the speed of light means

$$(d\overline{x}^0)^2 - \sum_{i=1}^{3} (d\overline{x}^i)^2 = (dx^0)^2 - \sum_{i=1}^{3} (dx^i)^2 = 0. \tag{9.409}$$

This can also be written as

$$\overline{g}_{\alpha\beta} d\overline{x}^{\alpha} d\overline{x}^{\beta} = g_{\alpha\beta} dx^{\alpha} dx^{\beta} = 0, \tag{9.410}$$

where the **metric** of the Minkowski spacetime is

$$\boxed{\overline{g}_{\alpha\beta} = g_{\alpha\beta} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}.} \tag{9.411}$$

We use the notation where the Greek indices take the values 0, 1, 2, 3 and the Latin indices run through 1, 2, 3. Note that even though the Minkowski spacetime is flat, because of the reversal of sign for the spatial components it is not Euclidean; thus the covariant and the contravariant indices differ in spacetime. Contravariant metric components can be obtained using [3]

$$g^{\alpha\beta} = \frac{|g_{\beta\alpha}|_{\text{cofactor}}}{\det g_{\alpha\beta}} \tag{9.412}$$

as

$$g^{\alpha\beta} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}. \tag{9.413}$$

Similar to the position vector in Cartesian coordinates, we can define a **position vector r** in Minkowski spacetime:

$$\mathbf{r} = x^\alpha = (x^0, x^1, x^2, x^3) = (x^0, \overrightarrow{r}), \tag{9.414}$$

where **r** defines the time and the position of an event. In terms of **linear transformations** [Eq. (9.399)], x^α transforms as

$$\boxed{\overline{x}^\alpha = a^\alpha_\beta x^\beta.} \tag{9.415}$$

For the **Lorentz transformations** [Eq. (9.401)], a^α_β is given as

$$\boxed{a^\alpha_\beta = \begin{bmatrix} \gamma & -\beta\gamma & 0 & 0 \\ -\beta\gamma & \gamma & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix},} \tag{9.416}$$

where for the general case [Eq. (9.403)] we have

$$a^\alpha_\beta = \begin{bmatrix} \gamma & -\beta_1\gamma & -\beta_2\gamma & -\beta_3\gamma \\ -\beta_1\gamma & 1 + \frac{(\gamma-1)\beta_1^2}{\beta^2} & \frac{(\gamma-1)\beta_1\beta_2}{\beta^2} & \frac{(\gamma-1)\beta_1\beta_3}{\beta^2} \\ -\beta_2\gamma & \frac{(\gamma-1)\beta_2\beta_1}{\beta^2} & 1 + \frac{(\gamma-1)\beta_2^2}{\beta^2} & \frac{(\gamma-1)\beta_2\beta_3}{\beta^2} \\ -\beta_3\gamma & \frac{(\gamma-1)\beta_3\beta_1}{\beta^2} & \frac{(\gamma-1)\beta_3\beta_2}{\beta^2} & 1 + \frac{(\gamma-1)\beta_3^2}{\beta^2} \end{bmatrix}. \tag{9.417}$$

For the general linear transformation [Eq. (9.399)], the matrix elements a^{α}_{β} can be obtained by

$$a^{\alpha}_{\beta} = \frac{d\overline{x}^{\alpha}}{dx^{\beta}}. \tag{9.418}$$

In Minkowski spacetime, the distance between two infinitesimally close points, that is, events, can be written in the following equivalent forms:

$$ds^2 = \begin{cases} dx^{\alpha} dx_{\alpha}, \\ (dx^0)^2 - (dx^1)^2 - (dx^2)^2 - (dx^3)^2, \\ g_{\alpha\beta} dx^{\alpha} dx^{\beta}. \end{cases} \tag{9.419}$$

In another inertial frame, ds^2 becomes

$$d\overline{s}^2 = \overline{g}_{\alpha\beta} d\overline{x}^{\alpha} d\overline{x}^{\beta}, \tag{9.420}$$

which after using Eqs. (9.411) and (9.415) can be written as

$$d\overline{s}^2 = \left[g_{\alpha\beta} a^{\alpha}_{\gamma} a^{\beta}_{\delta} \right] dx^{\gamma} dx^{\delta}. \tag{9.421}$$

If we restrict ourselves to transformations that preserve magnitude of vectors, we obtain the analog of the **orthogonality relation** [Eq. (9.38)]:

$$g_{\alpha\beta} a^{\alpha}_{\gamma} a^{\beta}_{\delta} = g_{\gamma\delta}. \tag{9.422}$$

The position vector in Minkowski spacetime is called a **four-vector** and its components transform as

$$\overline{x}^{\alpha} = a^{\alpha}_{\beta} x^{\beta}, \tag{9.423}$$

where its magnitude is a **four-scalar**.

An arbitrary four-vector, $A^{\alpha} = (A^0, A^1, A^2, A^3)$, is defined as a vector that transforms like the position vector x^{α} as

$$\overline{A}^{\alpha} = a^{\alpha}_{\beta} A^{\beta}. \tag{9.424}$$

The scalar product of two four-vectors, A^{α} and B^{α}, is a four-scalar:

$$A^{\alpha} B_{\alpha} = A_{\alpha} B^{\alpha} = \begin{cases} A^0 B_0 + A^1 B_1 + A^2 B_2 + A^3 B_3, \\ A_0 B^0 + A_1 B^1 + A_2 B^2 + A_3 B^3, \\ A_0 B_0 - A_1 B_1 - A_2 B_2 - A_3 B_3, \\ A^0 B^0 - A^1 B^1 - A^2 B^2 - A^3 B^3, \end{cases} \tag{9.425}$$

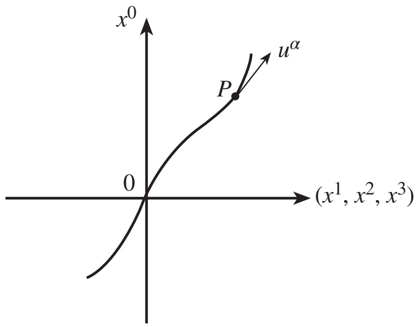

Figure 9.19 Worldline and four-velocity u^α.

In general, all tensor operations defined for the general tensors are valid in Minkowski spacetime with the Minkowski metric [Eq. (9.411)]. Higher-rank **four-tensors** can also be defined as

$$\overline{T}^{\alpha_1\alpha_2\cdots}_{\beta_1\beta_2\cdots} = \frac{\partial\overline{x}^{\alpha_1}}{\partial x^{\gamma_1}}\frac{\partial\overline{x}^{\alpha_2}}{\partial x^{\gamma_2}}\cdots\frac{\partial x^{\delta_1}}{\partial\overline{x}^{\beta_1}}\frac{\partial x^{\delta_2}}{\partial\overline{x}^{\beta_2}}\cdots T^{\gamma_1\gamma_2\cdots}_{\delta_1\delta_2\cdots} \tag{9.426}$$

9.8.6 Four-Velocity

Paths of observers in spacetime are called **worldlines** (Figure 9.19). Since spacetime increments form a four-vector, dx^α, they transform as

$$\begin{aligned} d\overline{x}^0 &= \frac{1}{\sqrt{1-v^2/c^2}}\left[dx^0 - \left(\frac{v}{c}\right)dx^1\right], \\ d\overline{x}^1 &= \frac{1}{\sqrt{1-v^2/c^2}}\left[-\left(\frac{v}{c}\right)dx^0 + dx^1\right], \\ d\overline{x}^2 &= dx^2, \\ d\overline{x}^3 &= dx^3. \end{aligned} \tag{9.427}$$

Dividing dx^α with a scalar, $d\tau = \frac{ds}{c}$, called the **proper time**, we obtain the **four-velocity** vector as

$$u^\alpha = \frac{dx^\alpha}{d\tau}. \tag{9.428}$$

Similarly, we can define **four-acceleration** as

$$a^\alpha = \frac{du^\alpha}{d\tau} = \frac{d^2x^\alpha}{d\tau^2}. \tag{9.429}$$

From the line element [Eq. (9.398)], it is seen that the **proper time**:

$$d\tau = \frac{ds}{c} = \left(1 - \frac{v^2}{c^2}\right)^{\frac{1}{2}} dt \tag{9.430}$$

is the time that the clocks carried by moving observers measure.

9.8.7 Four-Momentum and Conservation Laws

Using four-velocity, we can define a **four-momentum** as

$$p^\alpha = m_0 u^\alpha = m_0 \frac{dx^\alpha}{d\tau}, \tag{9.431}$$

where m_0 is the invariant **rest mass** of the particle. We can now express the energy and momentum conservation laws covariantly as the invariance of the magnitude of the four-momentum as

$$p^\alpha p_\alpha = m_0 u^\alpha u_\alpha = \text{const.} \tag{9.432}$$

To evaluate the constant, we use the line element and the definition of the proper time:

$$ds^2 = c^2 dt^2 - (dx^1)^2 - (dx^2)^2 - (dx^3)^2, \tag{9.433}$$

$$c^2 = \left(\frac{dx^0}{d\tau}\right)^2 - \left(\frac{dx^1}{d\tau}\right)^2 - \left(\frac{dx^2}{d\tau}\right)^2 - \left(\frac{dx^3}{d\tau}\right)^2 \tag{9.434}$$

$$= u^\alpha u_\alpha, \tag{9.435}$$

to obtain

$$p^\alpha p_\alpha = m_0^2 c^2. \tag{9.436}$$

Writing the left-hand side of Eq. (9.436) explicitly gives

$$p^0 p_0 + p^1 p_1 + p^2 p_2 + p^3 p_3 = m_0^2 c^2, \tag{9.437}$$

$$(p^0)^2 - (p^1)^2 - (p^2)^2 - (p^3)^2 = m_0^2 c^2. \tag{9.438}$$

Spatial components of the four-momentum are

$$p^i = m_0 \frac{dx^i}{d\tau}, \quad i = 1, 2, 3, \tag{9.439}$$

$$p^i = m_0 \frac{v^i}{\sqrt{1 - v^2/c^2}}. \tag{9.440}$$

Using this in Eq. (9.438), we obtain the **time component**, p^0, as

$$(p^0)^2 = m_0^2c^2 + \frac{m_0^2 v^2}{1 - v^2/c^2} \tag{9.441}$$

$$= m_0^2c^2 \left[1 + \frac{v^2/c^2}{(1 - v^2/c^2)}\right], \tag{9.442}$$

$$\boxed{p^0 = m_0 c\left[1 + \frac{v^2/c^2}{(1 - v^2/c^2)}\right]^{1/2}.} \tag{9.443}$$

To interpret p^0, we take its classical limit:

$$p^0 = m_0 c \left[1 + \frac{1}{2}\frac{v^2}{c^2} + \cdots \right] \tag{9.444}$$

$$\simeq \frac{1}{c}[m_0c^2 + \frac{1}{2}m_0v^2]. \tag{9.445}$$

The second term inside the square brackets is the classical expression for the kinetic energy of a particle; however, the first term is new to Newton's mechanics. It indicates that free particles, even when they are at rest, have energy due to their rest mass. This is the Einstein's famous formula

$$\boxed{E = m_0c^2,} \tag{9.446}$$

which indicates that mass and energy could be converted into each other. We can now interpret the time component of the four-momentum as E/c, where E is the total energy of the particle; thus the components of p^α become

$$\boxed{p^\alpha = (E/c, m_0u^i).} \tag{9.447}$$

We now write the **conservation of four-momentum** equation as

$$p^\alpha p_\alpha = \frac{E^2}{c^2} - \frac{m_0^2v^2}{\left(1 - \frac{v^2}{c^2}\right)}, \tag{9.448}$$

$$\boxed{p^\alpha p_\alpha = m_0^2c^2.} \tag{9.449}$$

Defining

$$m = \frac{m_0}{\left(1 - \frac{v^2}{c^2}\right)^{1/2}} \tag{9.450}$$

and calling

$$p^i = mv^i, \tag{9.451}$$

we obtain a relation between the energy and the momentum of a relativistic particle as

$$\boxed{E^2 = m_0^2 c^4 + p^2 c^2.} \tag{9.452}$$

9.8.8 Mass of a Moving Particle

Another important consequence of the special theory of relativity is Eq (9.450):

$$\boxed{m = \frac{m_0}{\left(1 - \frac{v^2}{c^2}\right)^{1/2}}.} \tag{9.453}$$

This is the mass of a particle moving with velocity v. It says that as the speed of a particle increases, its mass, that is, inertia, also increases, thus making it harder to accelerate. As the speed of a particle approaches the speed of light, its inertia approaches infinity, thus making it impossible to accelerate beyond c.

9.8.9 Wave Four-Vector

The phase of a wave, $\phi = \omega t - k^i x^i$, where there is a sum over i, is an invariant. This is so because it is merely a number equal to the number of wave crests getting past a given point. Therefore, we can write

$$\omega t - k^i x^i = \overline{\omega}\overline{t} - \overline{k}^i \overline{x}^i, \tag{9.454}$$

which immediately suggests a **wave four-vector**:

$$\boxed{k^\alpha = (k^0, k^i),} \tag{9.455}$$

$$k^\alpha = \left(\frac{\omega}{c}, \frac{2\pi}{\lambda^i}\right), \tag{9.456}$$

and λ^i is the wavelength along x^i. Because k^α is a four-vector, it transforms as

$$\boxed{\begin{aligned} \overline{k}^0 &= \gamma(k^0 - \overrightarrow{\beta} \cdot \overrightarrow{k}), \\ \overline{k}_\parallel &= \gamma(k_\parallel - \beta k^0). \end{aligned}} \tag{9.457}$$

We have written $\gamma = 1/\sqrt{1 - v^2/c^2}$ and $\overrightarrow{\beta} = \overrightarrow{v}/c$.

For light waves $|\overrightarrow{k}| = k^0$, $|\overrightarrow{\overline{k}}| = \overline{k}^0$; thus we obtain the familiar equations for the **Doppler shift**:

$$\omega = \gamma\overline{\omega}(1 - \beta\cos\theta), \tag{9.458}$$

$$\tan\overline{\theta} = \sin\theta/\gamma(\cos\theta - \beta), \tag{9.459}$$

where θ and $\overline{\theta}$ are the angles of $\overrightarrow{k}$ and $\overrightarrow{\overline{k}}$ with respect to $\overrightarrow{v}$, respectively. Note that because of the presence of γ, there is Doppler shift even when $\theta = \pi/2$, that is, when light is emitted perpendicular to the direction of motion.

9.8.10 Derivative Operators in Spacetime

Let us now consider the derivative operator, $\partial/\partial\overline{x}^{\alpha}$, calculated in the $\overline{K}$ frame. In terms of another inertial frame, K, it will be given as

$$\frac{\partial}{\partial\overline{x}^{\alpha}} = \frac{\partial x^{\beta}}{\partial\overline{x}^{\alpha}}\frac{\partial}{\partial x^{\beta}}, \tag{9.460}$$

thus $\partial/\partial x^{\beta}$ transforms like a covariant four-vector. In general, we write the **four-gradient** operator as

$$\partial^{\alpha} = \frac{\partial}{\partial x_{\alpha}} = \left(\frac{\partial}{\partial x^0}, -\overrightarrow{\nabla}\right), \tag{9.461}$$

$$\boxed{\partial_{\alpha} = \left(\frac{\partial}{\partial x^0}, \overrightarrow{\nabla}\right).} \tag{9.462}$$

The **four-divergence** of a four-vector is a four-scalar:

$$\boxed{\partial^{\alpha}A_{\alpha} = \partial_{\alpha}A^{\alpha} = \frac{\partial^0 A^0}{\partial x^0} + \overrightarrow{\nabla}\cdot\overrightarrow{A}.} \tag{9.463}$$

The **wave operator** or the **d'Alembert operator** in spacetime is written as

$$\boxed{\square = \partial^{\alpha}\partial_{\alpha} = \frac{\partial^2}{\partial(x^0)^2} - \overrightarrow{\nabla}^2.} \tag{9.464}$$

9.8.11 Relative Orientation of Axes in $\overline{K}$ and K Frames

Analogous to the orthogonal coordinates, any four-vector in Minkowski spacetime can be written in terms of basis vectors, $\widehat{\mathbf{e}}_{\alpha}$, as

$$\mathbf{A} = (A^0, A^1, A^2, A^3) \tag{9.465}$$
$$= \widehat{\mathbf{e}}_{\alpha}A^{\alpha}. \tag{9.466}$$

In terms of another Minkowski frame, the same four-vector can be written as

$$\mathbf{A} = \widehat{\overline{\mathbf{e}}}_{\alpha}\overline{A}^{\alpha}, \tag{9.467}$$

where $\widehat{\overline{\mathbf{e}}}_{\alpha}$ are the new basis vectors of the frame $\overline{K}$, which is moving with respect to K with velocity v along the common direction of the x^1- and $\overline{x}^1$-axes. Both $\widehat{\overline{\mathbf{e}}}_{\alpha}$ and $\widehat{\mathbf{e}}_{\alpha}$ are unit basis vectors along their axes in their respective frames. Because

A represents some physical property in Minkowski spacetime, Eqs. (9.466) and (9.467) are just different representations of **A**; hence, we can write

$$\hat{\mathbf{e}}_\alpha A^\alpha = \widehat{\bar{\mathbf{e}}}_{\alpha'} \overline{A}^{\alpha'}. \tag{9.468}$$

Using the transformation property of four-vectors, we write

$$\overline{A}^{\alpha'} = a^{\alpha'}_\beta A^\beta, \tag{9.469}$$

thus Eq. (9.468) becomes

$$\hat{\mathbf{e}}_\alpha A^\alpha = \widehat{\bar{\mathbf{e}}}_{\alpha'} a^{\alpha'}_\beta A^\beta. \tag{9.470}$$

We rearrange this as

$$A^\alpha \hat{\mathbf{e}}_\alpha = A^\beta \left(\widehat{\bar{\mathbf{e}}}_{\alpha'} a^{\alpha'}_\beta \right). \tag{9.471}$$

Since α and β are dummy indices, we can replace β with α to write

$$A^\alpha \hat{\mathbf{e}}_\alpha = A^\alpha \left(\widehat{\bar{\mathbf{e}}}_{\alpha'} a^{\alpha'}_\alpha \right), \tag{9.472}$$

which gives us the transformation law of the basis vectors as

$$\hat{\mathbf{e}}_\alpha = \widehat{\bar{\mathbf{e}}}_{\alpha'} a^{\alpha'}_\alpha. \tag{9.473}$$

Note that this is not a component transformation. It gives $\hat{\mathbf{e}}_\alpha$ as a linear combination of $\widehat{\bar{\mathbf{e}}}_{\alpha'}$. Using

$$a^{\alpha'}_\alpha = \begin{bmatrix} \gamma & -\beta\gamma & 0 & 0 \\ -\beta\gamma & \gamma & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \tag{9.474}$$

we obtain

$$\hat{\mathbf{e}}_0 = \gamma \widehat{\bar{\mathbf{e}}}_0 - \beta\gamma \widehat{\bar{\mathbf{e}}}_1, \tag{9.475}$$

$$\hat{\mathbf{e}}_1 = -\beta\gamma \widehat{\bar{\mathbf{e}}}_0 + \gamma \widehat{\bar{\mathbf{e}}}_1, \tag{9.476}$$

and its inverse as

$$\widehat{\bar{\mathbf{e}}}_0 = \gamma \hat{\mathbf{e}}_0 + \beta\gamma \hat{\mathbf{e}}_1, \tag{9.477}$$

$$\widehat{\bar{\mathbf{e}}}_1 = \beta\gamma \hat{\mathbf{e}}_0 + \gamma \hat{\mathbf{e}}_1. \tag{9.478}$$

The second set gives the orientation of the $\overline{K}$ axis in terms of the K axis. Since $\beta < 1$, relative orientation of the $\overline{K}$ axis with respect to the K axis can be shown as in Figure 9.20.

Similarly, using the first set, we can obtain the relative orientation of the K axis with respect to the $\overline{K}$ axis as shown in Figure 9.21.

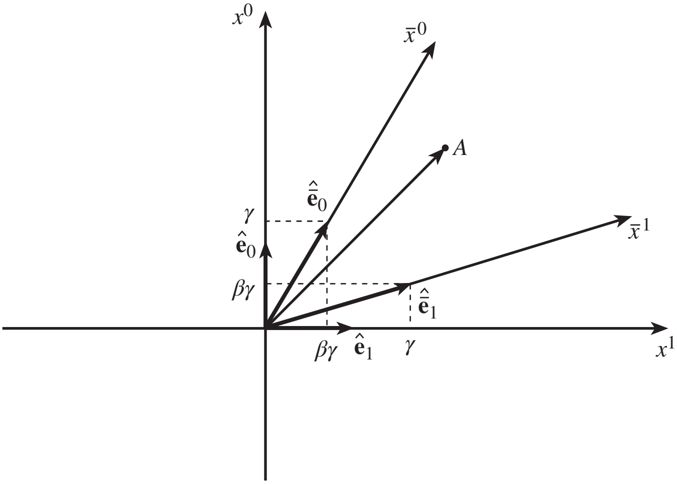

Figure 9.20 Orientation of the $\overline{K}$ axis with respect to the K frame.

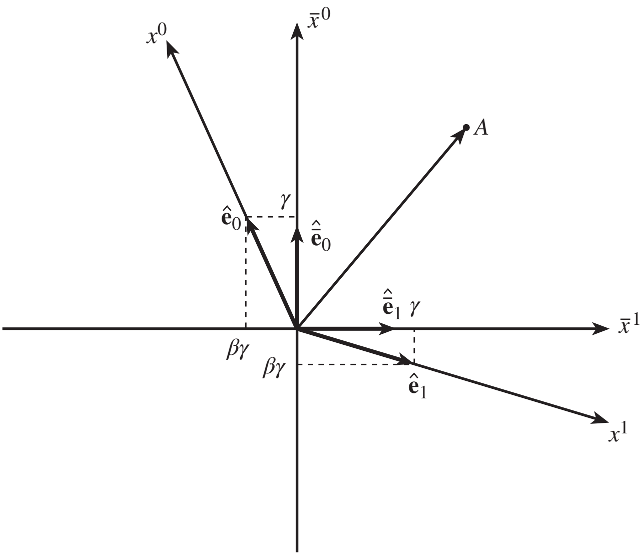

Figure 9.21 Orientation of the K axis with respect to the $\overline{K}$ frame.

9.9 Maxwell's Equations in Minkowski Spacetime

Before the spacetime formulation of special relativity, it was known that Maxwell's equations are covariant, that is, form-invariant, under Lorentz transformations. However, their covariance can be most conveniently expressed in terms of four-tensors.

First let us start with the **conservation of charge**, which can be expressed as

$$\boxed{\frac{\partial \rho}{\partial t} + \vec{\nabla} \cdot \vec{J} = 0,} \tag{9.479}$$

where ρ is the charge density and $\vec{J}$ is the current density in space. Defining a **four-current density** J^α as

$$J^\alpha = (\rho c, \vec{J}), \tag{9.480}$$

we can write Eq. (9.479) in covariant form as

$$\boxed{\partial_\alpha J^\alpha = 0,} \tag{9.481}$$

where ∂_α stands for covariant derivative [Eq. (9.461)]. **Maxwell's field equations**

$$\boxed{\begin{aligned} \vec{\nabla} \cdot \vec{E} &= 4\pi\rho, \\ \vec{\nabla} \times \vec{B} - \frac{1}{c}\frac{\partial \vec{E}}{\partial t} &= \frac{4\pi}{c}\vec{J}, \\ \vec{\nabla} \cdot \vec{B} &= 0, \\ \vec{\nabla} \times \vec{E} + \frac{1}{c}\frac{\partial \vec{B}}{\partial t} &= 0, \end{aligned}} \tag{9.482}$$

determine the electric and magnetic fields for a given charge, and current distribution. We now introduce the **field-strength tensor**, $F^{\alpha\beta}$, as

$$\boxed{F^{\alpha\beta} = \begin{bmatrix} 0 & -E_1 & -E_2 & -E_3 \\ E_1 & 0 & -B_3 & B_2 \\ E_2 & B_3 & 0 & -B_1 \\ E_3 & -B_2 & B_1 & 0 \end{bmatrix},} \tag{9.483}$$

where the covariant components of the field-strength tensor, $F_{\alpha\beta}$, are given as

$$F_{\alpha\beta} = g_{\alpha\gamma} g_{\delta\beta} F^{\gamma\delta} = \begin{bmatrix} 0 & E_1 & E_2 & E_3 \\ -E_1 & 0 & -B_3 & B_2 \\ -E_2 & B_3 & 0 & -B_1 \\ -E_3 & -B_2 & B_1 & 0 \end{bmatrix}. \tag{9.484}$$

Using $F^{\alpha\beta}$, the first two Maxwell's equations can be expressed in covariant form as

$$\boxed{\partial_\alpha F^{\alpha\beta} = \frac{4\pi}{c} J^\beta.} \tag{9.485}$$

For the remaining two Maxwell's equations, we introduce the **dual field-strength tensor**, $\widehat{F}^{\alpha\beta}$, which is related to the field strength tensor, $F_{\alpha\beta}$, through

$$\boxed{\widehat{F}^{\alpha\beta} = \frac{1}{2}\epsilon^{\alpha\beta\gamma\delta}F_{\gamma\delta} = \begin{bmatrix} 0 & -B_1 & -B_2 & -B_3 \\ B_1 & 0 & E_3 & -E_2 \\ B_2 & -E_3 & 0 & E_1 \\ B_3 & E_2 & -E_1 & 0 \end{bmatrix},} \tag{9.486}$$

where

$$\epsilon^{\alpha\beta\gamma\delta} = \begin{bmatrix} +1 \\ 0 \\ -1 \end{bmatrix} \begin{cases} \text{for even permutations,} \\ \text{when any of the two indices are equal,} \\ \text{for odd permutations.} \end{cases} \tag{9.487}$$

Now the remaining two Maxwell's equations can be written as

$$\boxed{\partial_\alpha \widehat{F}^{\alpha\beta} = 0.} \tag{9.488}$$

The motion of charged particles in an electromagnetic field is determined by the **Lorentz force equation**:

$$\boxed{\frac{d\vec{p}}{dt} = q\left(\vec{E} + \frac{\vec{v}}{c} \times \vec{B}\right),} \tag{9.489}$$

where $\vec{p}$ is the spatial momentum and $\vec{v}$ is the velocity of the charged particle. We can write this in covariant form by introducing the **four-momentum**:

$$p^\alpha = (p^0, \vec{p}) = m_0 u^\alpha, \tag{9.490}$$

where m_0 is the rest mass, u^α is the four-velocity, and $p^0 = E/c$. Using the derivative in terms of invariant proper time, we can write the Lorentz force equation [Eq. (9.489)] as

$$\frac{dp^\alpha}{d\tau} = m_0 \frac{du^\alpha}{d\tau}, \tag{9.491}$$

$$\boxed{\frac{dp^\alpha}{d\tau} = \frac{q}{c} F^{\alpha\beta} u_\beta.} \tag{9.492}$$

9.9.1 Transformation of Electromagnetic Fields

Because $F^{\alpha\beta}$ is a second-rank four-tensor, it transforms as

$$\overline{F}^{\alpha\beta} = \frac{d\overline{x}^{\alpha}}{dx^{\gamma}} \frac{d\overline{x}^{\beta}}{dx^{\delta}} F^{\gamma\delta}. \tag{9.493}$$

Given the values of $F^{\gamma\delta}$ in an inertial frame K, we can find it in another inertial frame $\overline{K}$ as

$$\overline{F}^{\alpha\beta} = a^{\alpha}_{\gamma} a^{\beta}_{\delta} F^{\gamma\delta}. \tag{9.494}$$

If $\overline{K}$ corresponds to an inertial frame moving with respect to K with velocity v along the common $\overline{x}_1$- and x_1-axes, the new components of $\overrightarrow{E}$ and $\overrightarrow{B}$ are

$$\boxed{\begin{aligned} \overline{E}_1 &= E_1, \\ \overline{E}_2 &= \gamma(E_2 - \beta B_3), \\ \overline{E}_3 &= \gamma(E_3 + \beta B_2), \end{aligned}} \tag{9.495}$$

$$\boxed{\begin{aligned} \overline{B}_1 &= B_1, \\ \overline{B}_2 &= \gamma(B_2 + \beta E_3), \\ \overline{B}_3 &= \gamma(B_3 - \beta E_2). \end{aligned}} \tag{9.496}$$

If $\overline{K}$ is moving with respect to K with $\overrightarrow{v}$, the transformation equations are given as

$$\boxed{\begin{aligned} \overrightarrow{\overline{E}} &= \gamma(\overrightarrow{E} + \overrightarrow{\beta} \times \overrightarrow{B}) - \frac{\gamma^2}{1+\gamma} \overrightarrow{\beta}(\overrightarrow{\beta} \cdot \overrightarrow{E}), \\ \overrightarrow{\overline{B}} &= \gamma(\overrightarrow{B} - \overrightarrow{\beta} \times \overrightarrow{E}) - \frac{\gamma^2}{1+\gamma} \overrightarrow{\beta}(\overrightarrow{\beta} \cdot \overrightarrow{B}), \end{aligned}} \tag{9.497}$$

where $\gamma = 1/(1-\beta^2)^{1/2}$ and $\overrightarrow{\beta} = \overrightarrow{v}/c$. Inverse transformations are easily obtained by interchanging $\overrightarrow{\beta}$ with $-\overrightarrow{\beta}$.

9.9.2 Maxwell's Equations in Terms of Potentials

The electric and magnetic fields can also be expressed in terms of the **potentials** $\overrightarrow{A}$ and ϕ as

$$\overrightarrow{E} = -\frac{1}{c}\frac{\partial \overrightarrow{A}}{\partial t} - \overrightarrow{\nabla}\phi, \tag{9.498}$$

$$\overrightarrow{B} = \overrightarrow{\nabla} \times \overrightarrow{A}. \tag{9.499}$$

In the **Lorentz gauge**,

$$\boxed{\frac{1}{c}\frac{\partial \phi}{\partial t} + \overrightarrow{\nabla} \cdot \overrightarrow{A} = 0,} \tag{9.500}$$

$\overrightarrow{A}$ and ϕ satisfy

$$\frac{1}{c^2}\frac{\partial^2 \overrightarrow{A}}{\partial t^2} - \overrightarrow{\nabla}^2 \overrightarrow{A} = \frac{4\pi}{c}\overrightarrow{J} \tag{9.501}$$

and

$$\frac{1}{c^2}\frac{\partial^2 \phi}{\partial t^2} - \overrightarrow{\nabla}^2 \phi = 4\pi\rho, \tag{9.502}$$

respectively. Defining a **four-potential**:

$$\boxed{A^\alpha = (\phi, \overrightarrow{A}),} \tag{9.503}$$

we can write Eqs. (9.501) and (9.502) in covariant form as

$$\boxed{\Box A^\alpha = \frac{4\pi}{c} J^\alpha,} \tag{9.504}$$

where the **d'Alembert operator** $\Box$ is defined as

$$\boxed{\Box = \frac{\partial^2}{d(x^0)^2} - \overrightarrow{\nabla}^2.} \tag{9.505}$$

Now the covariant form of the **Lorentz gauge** [Eq. (9.500)] becomes

$$\boxed{\partial_\alpha A^\alpha = 0.} \tag{9.506}$$

Field-strength tensor in terms of the **four-potential** can be written as

$$\boxed{F^{\alpha\beta} = \partial^\alpha A^\beta - \partial^\beta A^\alpha.} \tag{9.507}$$

9.9.3 Covariance of Newton's Dynamic Theory

The concept of relativity was not new to Newton. In fact, it was known that the dynamic equation of Newton:

$$\frac{d\overrightarrow{p}}{dt} = \overrightarrow{F}, \tag{9.508}$$

is covariant for all uniformly moving, that is, inertial, observers. However, the inertial observers in Newton's theory are related to each other by the **Galilean transformation**:

$$\bar{t} = t, \tag{9.509}$$

$$\bar{x}^1 = [x^1 - vt], \tag{9.510}$$

$$\bar{x}^2 = x^2, \tag{9.511}$$

$$\bar{x}^3 = x^3. \tag{9.512}$$

Note that the Lorentz transformation reduces to the Galilean transformation in the limit $c \to \infty$, or $v \ll c$. Before the special theory of relativity, it was already known that Maxwell's equations are covariant not under Galilean but under Lorentz transformations. Considering the success of Newton's theory, this was a conundrum, which took Einstein's genius to resolve by saying that Lorentz transformations are the correct transformation law between inertial observers that all laws of nature should obey. In this regard, we also need to write Newton's dynamic equation as a four-tensor equation in spacetime.

Using the definition of four-momentum:

$$p^\alpha = m_0 u^\alpha = (E/c,\ p^i) \tag{9.513}$$

and differentiating with respect to invariant proper time, we can write the Newton's dynamic equation in covariant form as

$$\frac{dp^\alpha}{d\tau} = F^\alpha, \tag{9.514}$$

where F^α is now the four-force. Note that the conservation of energy and momentum is now expressed covariantly as the conservation of four-momentum, that is,

$$p^\alpha p_\alpha = \frac{E^2}{c^2} - p^2 = m_0^2 c^2. \tag{9.515}$$

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Problems

1 For rotations about the z-axis, the transformation matrix is given as

$$\mathbf{R}_z(\theta) = \begin{bmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

Show that for two successive rotations by the amounts θ_1 and θ_2, the following is true:

$$\mathbf{R}_z(\theta_1 + \theta_2) = \mathbf{R}_z(\theta_2)\mathbf{R}_z(\theta_1).$$

2 Show that the rotation matrix $\mathbf{R}_z(\theta)$ is a second-rank tensor.

3 Using the properties of the permutation symbol and the Kronecker delta, prove the following identities in tensor notation:

(i) $\left[\vec{A} \times \vec{B}\right] \cdot \left[\vec{C} \times \vec{D}\right] = (\vec{A} \cdot \vec{C})(\vec{B} \cdot \vec{D}) - (\vec{A} \cdot \vec{D})(\vec{B} \cdot \vec{C})$,

(ii) $\left[\vec{A} \times \left[\vec{B} \times \vec{C}\right]\right] + \left[\vec{B} \times \left[\vec{C} \times \vec{A}\right]\right] + \left[\vec{C} \times \left[\vec{A} \times \vec{B}\right]\right] = 0$,

(iii) $\vec{A} \times \left[\vec{B} \times \vec{C}\right] = \vec{B}(\vec{A} \cdot \vec{C}) - \vec{C}(\vec{A} \cdot \vec{B})$.

4 Show that

$$\frac{\Delta V}{V} = e_{ii} = tr(e_{ij}).$$

5 We have written the moment (torque) of the force acting on a portion of a body as

$$M_{ik} = \oint_S (\sigma_{il}x_k - \sigma_{kl}x_i)ds_l + \int_V (\sigma_{ki} - \sigma_{ik})dV.$$

When the stress tensor is symmetric, $\sigma_{ki} = \sigma_{ik}$, obviously the volume integral on the right-hand side is zero. However, even when the stress tensor is not symmetric, under certain conditions it can be made symmetric. Show that if a stress tensor can be written as the divergence of a third-rank tensor antisymmetric in the first pair of indices:

$$\sigma_{ik} - \sigma_{ki} = 2\frac{\partial \Psi_{ikl}}{\partial x_l}, \quad \Psi_{ikl} = -\Psi_{kil},$$

then a third-rank tensor, $\chi_{ikl} = \Psi_{kli} + \Psi_{ilk} - \Psi_{ikl}$, antisymmetric in the last pair of indices, $\chi_{ikl} = -\chi_{ilk}$, can be found to transform σ_{ik} into symmetric form via the transformation

$$\sigma' = \sigma + \frac{\partial \chi_{ikl}}{\partial x_l}$$

as

$$\sigma'_{ik} = \frac{1}{2}(\sigma_{ik} + \sigma_{ki}) + \left(\frac{\partial \Psi_{ilk}}{\partial x_l} + \frac{\partial \Psi_{kli}}{\partial x_l} \right), \quad \sigma'_{ik} = \sigma'_{ki}.$$

In addition, show that the forces corresponding to the two stress tensors, σ' and σ, are identical.

6 Write the components of the strain tensor in

(i) Cylindrical coordinates,
(ii) Spherical coordinates.

7 The trace of a second-rank tensor is defined as $tr(A) = A^i_i$. Show that trace is invariant under general coordinate transformations.

8 Under general coordinate transformations, show that the volume element, $d^n x = dx^1 dx^2 \dots dx^n$, transforms as

$$d^n\overline{x} = d^n x \left| \frac{\partial \overline{x}}{\partial x} \right| = d^n x \left| \frac{\partial x}{\partial \overline{x}} \right|^{-1},$$

where $|\partial x / \partial \overline{x}|$ is the Jacobian of the transformation, which is defined as $|\partial x / \partial \overline{x}| = \det(\partial x^i / \partial \overline{x}^j)$.

9 Show the following relations between the permutation symbol and the Kronecker delta:

(i) $\displaystyle\sum_{i=1}^{3} \epsilon_{ijk}\epsilon_{ilm} = \delta_{jl}\delta_{km} - \delta_{jm}\delta_{kl},$

(ii) $\displaystyle\sum_{i=1}^{3}\sum_{j=1}^{3} \epsilon_{ijk}\epsilon_{ijm} = 2\delta_{km}.$

10 Evaluate

$$\sum_{ijk}\sum_{lmn} \epsilon_{ijk}\epsilon_{lmn} T_{il} T_{jm} T_{kn},$$

where T is an arbitrary matrix.

11 Using the symmetry of the Christoffel symbols, show that the curl of a vector, $\vec{v}$, can be written as

$$\left(\vec{\nabla} \times \vec{v}\right)_{ij} = v_{i;\,j} - v_{j;\,i} = \frac{\partial v_i}{\partial x^j} - \frac{\partial v_j}{\partial x^i}.$$

12 Prove that the covariant derivative of the metric tensor is zero.

13 Verify that

$$u^i_{;j} = \frac{\partial u^i}{\partial x^j} + \left\{ \begin{matrix} i \\ jk \end{matrix} \right\} u^k$$

transforms like a second-rank tensor.

14 Using the following symmetry properties:

$$E_{ijkl} = E_{jikl}, \quad E_{ijkl} = E_{ijlk}, \quad E_{ijkl} = E_{klij},$$

show that the elasticity tensor, E_{ijkl}, has 21 independent components.

15 Prove the following useful relation of the Christoffel symbol of the second kind:

$$\left\{ \begin{matrix} i \\ ik \end{matrix} \right\} = \frac{\partial(\ln\sqrt{|g|})}{\partial x^k}.$$

16 Show the following Christoffel symbols for a diagonal metric, where $g_{ij} = 0$ unless $i = j$:

$$\left\{ \begin{matrix} i \\ jk \end{matrix} \right\} = 0,$$

$$\left\{ \begin{matrix} i \\ jj \end{matrix} \right\} = -\frac{1}{2g_{ii}} \frac{\partial g_{jj}}{\partial x^i},$$

$$\left\{ \begin{matrix} i \\ ji \end{matrix} \right\} = \left\{ \begin{matrix} i \\ ij \end{matrix} \right\} = \frac{\partial}{\partial x^j}(\ln\sqrt{g_{ii}}),$$

$$\left\{ \begin{matrix} i \\ ii \end{matrix} \right\} = \frac{\partial}{\partial x^i}(\ln\sqrt{g_{ii}}).$$

In these equations, summation convention is not used and different letters imply different indices.

17 Show that the following tensor equation:

$$A_{ij} = c + B^{kl}_{ij} C_{kl} + E^k_{i;\,jk},$$

transforms as

$$A'_{ij} = c + B'^{kl}_{ij} C'_{kl} + E'^{k}_{i;\ jk}.$$

18 Find the expressions for the div and the grad operators for the following metrics:
(i) $ds^2 = dr^2 + \rho^2 d\theta^2 + dz^2,$
(ii) $ds^2 = \left[\frac{1}{1-kr^2/R^2}\right] dr^2 + r^2 d\theta^2 + r^2 \sin^2\theta d\phi^2,\ k = 0, 1, -1.$

19 Write the Laplacian operator for the following metrics and discuss what geometries they represent:
(i) $ds^2 = R^2(d\chi^2 + \sin^2\chi d\theta^2 + \sin^2\chi \sin^2\theta d\phi^2),\quad \chi \in [0, \pi],\quad \theta \in [0, \pi],$ $\phi \in [0, 2\pi],$
(ii) $ds^2 = R^2(d\chi^2 + \sinh^2\chi d\theta^2 + \sinh^2\chi \sin^2\theta d\phi^2),\quad \chi \in [0, \infty],\quad \theta \in [0, \pi],\ \phi \in [0, 2\pi].$

20 Write the line element for the elliptic cylindrical coordinates (u, v, z):

$$x = a \cosh u \cos v,$$
$$y = a \sinh u \sin v,$$
$$z = z.$$

21 Write the covariant and the contravariant components of the metric tensor for the parabolic cylindrical coordinates (u, v, z):

$$x = (1/2)(u^2 - v^2),$$
$$y = uv,$$
$$z = z.$$

22 Write the Laplacian in the parabolic coordinates (u, v, ϕ):

$$x = uv \cos\phi,$$
$$y = uv \sin\phi,$$
$$z = (1/2)(u^2 - v^2).$$

23 Calculate all the nonzero components of the Christoffel symbols for the metric in the line element

$$ds^2 = dr^2 + r^2 d\theta^2 + r^2 \sin^2\theta d\phi^2,\quad r \in [0, \infty],\ \theta \in [0, \pi],\ \phi \in [0, 2\pi].$$

24 Write the contravariant gradient of a scalar function in spherical polar coordinates.

25 Write the divergence operator in spherical polar coordinates.

26 Write the Laplace operator in cylindrical coordinates.

27 In four dimensions, spherical polar coordinates (r, χ, θ, ϕ) are defined as

$$\begin{aligned} x &= r\sin\chi\sin\theta\cos\phi, \\ y &= r\sin\chi\sin\theta\sin\phi, \\ z &= r\sin\chi\cos\theta, \\ w &= r\cos\chi. \end{aligned}$$

(i) Write the line element $ds^2 = dx^2 + dy^2 + dz^2 + dw^2$ in terms of (r, χ, θ, ϕ).
(ii) What are the ranges of (r, χ, θ, ϕ)?
(iii) Write the metric for the three-dimensional surface (S-3) of a hypersphere.

28 Which one of the following matrices are Cartesian tensors:
(i)

$$\begin{bmatrix} y^2 & -xy \\ -xy & x^2 \end{bmatrix},$$

(ii)

$$\begin{bmatrix} xy & y^2 \\ x^2 & -xy \end{bmatrix}.$$

29 Verify Eq. (9.363).

30 Show by direct substitution that the Bianchi identities [Eq. (9.367)] are true.

31 Verify Eqs. (9.377)–(9.381).

32 For the surface of a sphere, the metric can be written as $ds^2 = a^2(d\theta^2 + \sin^2\theta d\phi^2)$, where a is the radius of the sphere. Using the definition of the Riemann curvature tensor [Eq. (9.363)], evaluate R_{1212} and R, and verify that $K = 1/a^2$.

33 In the standard models of cosmology, the line element for a closed universe is given as

$$ds^2 = dt^2 - R_0(t)^2[d\chi^2 + \sin^2\chi d\theta^2 + \sin^2\chi\sin^2\theta d\phi^2], \quad c = 1,$$

where t is the universal time and χ, θ, and ϕ are the angular coordinates with the ranges $\chi \in [0, \pi]$, $\theta \in [0, \pi]$, $\phi \in [0, 2\pi]$.

For a static universe with constant radius, R_0, the wave equation for the massless conformal scalar field is given as

$$\Box\Phi(t, \chi, \theta, \phi) + \frac{1}{R_0^2}\Phi(t, \chi, \theta, \phi) = 0,$$

where $\Box$ is the d'Alembert wave operator, $\Box = g_{\mu\nu}\partial^\mu\partial_\nu$, and ∂_ν stands for the covariant derivative. The $\Box$ operator can also be written as [Eq. (9.330)]

$$\Box = g^{-1/2}\frac{\partial}{\partial x^\mu}\left[g^{1/2}g^{\mu\nu}\frac{\partial}{\partial x^\nu}\right],$$

where g is the absolute value of the determinant of the metric tensor, $g = R_0^6\sin^4\chi\sin^2\theta$.

(i) Write the wave equation for the massless conformal scalar field as

$$\left[\frac{1}{2g}\frac{\partial g}{\partial x^\mu}g^{\mu\nu}\partial_\nu + \frac{\partial g^{\mu\nu}}{\partial x^\mu}\partial_\nu + g^{\mu\nu}\partial_\mu\partial_\nu + \frac{1}{R_0^2}\right]\Phi = 0.$$

(ii) Using Einstein's summation convention and the identification

$$x^0 = t, \quad x^1 = \chi, \quad x^2 = \theta, \quad x^3 = \phi,$$

show that the wave equation becomes

$$\frac{\partial^2\Phi}{\partial t^2} - \frac{1}{R_0^2}\frac{\partial^2\Phi}{\partial\chi^2} - \frac{1}{R_0^2\sin^2\chi}\frac{\partial^2\Phi}{\partial\theta^2} - \frac{1}{R_0^2\sin^2\theta\sin^2\chi}\frac{\partial^2\Phi}{\partial\phi^2}$$
$$- \frac{2\cos\chi}{R_0^2\sin\chi}\frac{\partial\Phi}{\partial\chi} - \frac{\cos\theta}{R_0^2\sin^2\chi\sin\theta}\frac{\partial\Phi}{\partial\theta} + \frac{1}{R_0^2}\Phi = 0.$$

(iii) Using a separable solution of the form

$$\Phi(t, \chi, \theta, \phi) = T(t)X(\chi)Y(\theta, \phi),$$

show that the wave equation for the massless conformal scalar field reduces to

$$\left[\frac{1}{T(t)}\frac{d^2T(t)}{dt^2}\right] - \frac{1}{R_0^2}\left[\frac{1}{X(\chi)}\frac{d^2X(\chi)}{d\chi^2} + \frac{2\cos\chi}{\sin\chi}\frac{1}{X(\chi)}\frac{dX(\chi)}{d\chi} - 1\right]$$
$$- \frac{1}{R_0^2\sin^2\chi}\left[\frac{1}{Y(\theta,\phi)}\left(\frac{\partial^2Y(\theta,\phi)}{\partial\theta^2} + \frac{\cos\theta}{\sin\theta}\frac{\partial Y(\theta,\phi)}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2Y(\theta,\phi)}{\partial\phi^2}\right)\right]$$
$$= 0.$$

(iv) Using the separation of variables method, write the solutions for $T(t)$, $X(\chi)$, and $Y(\theta, \phi)$. Do not solve the differential equations, just compare them with the differential equations that the Gegenbauer polynomials and the spherical harmonics satisfy.

34 Using the four-current, $J^\alpha = (\rho c, \overrightarrow{J})$, and the field-strength tensor

$$F^{\alpha\beta} = \begin{bmatrix} 0 & -E_1 & -E_2 & -E_3 \\ E_1 & 0 & -B_3 & B_2 \\ E_2 & B_3 & 0 & -B_1 \\ E_3 & -B_2 & B_1 & 0 \end{bmatrix},$$

show that the Maxwell's field equations:

$$\overrightarrow{\nabla} \cdot \overrightarrow{E} = 4\pi\rho,$$

$$\overrightarrow{\nabla} \times \overrightarrow{B} - \frac{1}{c}\frac{\partial \overrightarrow{E}}{\partial t} = \frac{4\pi}{c}\overrightarrow{J},$$

$$\overrightarrow{\nabla} \cdot \overrightarrow{B} = 0,$$

$$\overrightarrow{\nabla} \times \overrightarrow{E} + \frac{1}{c}\frac{\partial \overrightarrow{B}}{\partial t} = 0,$$

can be written in covariant form as

$$\partial_\alpha F^{\alpha\beta} = \frac{4\pi}{c} J^\alpha,$$

$$\partial_\alpha \widehat{F}^{\alpha\beta} = 0.$$

The dual field-strength tensor $\widehat{F}^{\alpha\beta}$ is defined as

$$\widehat{F}^{\alpha\beta} = \frac{1}{2}\epsilon^{\alpha\beta\gamma\delta}F_{\gamma\delta} = \begin{bmatrix} 0 & -B_1 & -B_2 & -B_3 \\ B_1 & 0 & E_3 & -E_2 \\ B_2 & -E_3 & 0 & E_1 \\ B_3 & E_2 & -E_1 & 0 \end{bmatrix},$$

where $\epsilon^{\alpha\beta\gamma\delta}$ is the permutation symbol.

35 If $\overline{K}$ corresponds to an inertial frame moving with respect to K with velocity v along the x_1-axis, show that the new components of $\overrightarrow{E}$ and $\overrightarrow{B}$ become

$$\overline{E}_1 = E_1,$$

$$\overline{E}_2 = \gamma(E_2 - \beta B_3),$$

$$\overline{E}_3 = \gamma(E_3 + \beta B_2),$$

$$\overline{B}_1 = B_1,$$

$$\overline{B}_2 = \gamma(B_2 + \beta E_3),$$

$$\overline{B}_3 = \gamma(B_3 - \beta E_2).$$

36 Show that the field-strength tensor can also be written as $F^{\alpha\beta} = \partial^\alpha A^\beta - \partial^\beta A^\alpha$, where the four-potential is defined as $A^\alpha = (\phi, \vec{A})$ and

$$\vec{E} = -\frac{1}{c}\frac{\partial \vec{A}}{\partial t} - \vec{\nabla}\phi,$$
$$\vec{B} = \vec{\nabla} \times \vec{A}.$$

10

Continuous Groups and Representations

In ordinary parlance, the word symmetry is usually associated with beautiful. In fact, recent studies have shown that people with more symmetric bodies are more beautiful to humans. This is particularly interesting since the left–right symmetry of the human body is almost undetectable to the naked eye. In architecture and art, symmetry is used to build beautiful structures and patterns by distributing relatively simple building blocks according to a rule. Most of the symmetries around us are due to rotations and reflections. Symmetry in science usually means invariance of a given system under some operation. As in crystals and molecules, symmetries can be discrete, where applications of certain amounts of rotation, translation, or reflection produce the same structure. After the discovery of the Lagrangian formulation of mechanics, it became clear that the conservation laws are also due to the symmetries of the physical system. For example, conservation of angular momentum follows from the symmetry of a given system with respect to rotations, whereas the conservation of linear momentum follows from symmetry with respect to translations. In these symmetries, a system is carried from one identical state to another continuously; hence they are called continuous or Lie symmetries. With the discovery of quantum mechanics, the relation between conservation laws and symmetries has even become more important. Conservation of isospin and flavor in nuclear and particle physics are important tools in building theories. Similarly, gauge symmetry has become an important guide in constructing new models.

Group theory is the branch of mathematics that allows us to study symmetries in a systematic way. In this chapter, we discuss continuous groups and Lie algebras and their relation to coordinate transformations. We also discuss the representation theory and its applications. In particular, we concentrate on the representations of the rotation group, $R(3)$, and the special unitary group, $SU(2)$. An advanced treatment of spherical harmonics is given in terms of the rotation group and its representations. We also discuss the inhomogeneous Lorentz group and introduce its Lie algebra. We finally introduce symmetries of differential equations and the extension or prolongation of generators. Even though this chapter could be read independently, occasionally we refer to

Mathematical Methods in Science and Engineering, Second Edition. Selçuk Ş. Bayın.

results from Chapter 9. In particular, we recommend reading the sections on orthogonal and Lorentz transformations before reading this chapter.

10.1 Definition of a Group

The basic properties of rotations in three dimensions are just the properties that make a group. A **group** is an ensemble of elements:

$$G \in \{g_0, g_1, g_2, \dots\}, \tag{10.1}$$

with the following properties:

(i) For any two elements, $g_a, g_b \in G$, a **composition rule** is defined such that

$$g_a g_b \in G. \tag{10.2}$$

(ii) For any three elements of the group, $g_a, g_b, g_c \in G$, the **associative rule** is obeyed:

$$(g_a g_b) g_c = g_a (g_b g_c). \tag{10.3}$$

(iii) G contains the **unit element,** g_0, such that for any $g \in G$,

$$g g_0 = g_0 g = g. \tag{10.4}$$

(iv) For every $g \in G$, there exists an **inverse element**, $g^{-1} \in G$, such that

$$g g^{-1} = g^{-1} g = g_0. \tag{10.5}$$

10.1.1 Nomenclature

In n dimensions, the set, $\{\mathbf{A}\}$, of all linear transformations with $\det \mathbf{A} \neq 0$, forms a group called the **general linear group** in n dimensions, $GL(n)$.

We use the letter $\mathbf{A}$ for the transformation and its operator or its matrix representation. The matrix elements of $\mathbf{A}$ could be real or complex; thus, we also write $GL(n, R)$ or $GL(n, C)$. The **rotation group** in two dimensions is shown as $R(2)$. Elements of $R(2)$ are characterized by a single continuous parameter, θ, which is the angle of rotation. A group whose elements are characterized by a number of continuous parameters is called a **continuous group** or a **Lie group**. In a continuous group, the group elements can be generated continuously from the identity element. The rotation group in three dimensions is shown as $R(3)$. Elements of $R(3)$ are characterized in terms of three independent parameters, which are usually taken as the three **Euler angles**. $R(n)$ is a subgroup of $GL(n)$ and $R(n)$ is also a subgroup of the group of n-dimensional **orthogonal transformations**, $O(n)$. Elements of $O(n)$ satisfy $|\det \mathbf{A}|^2 = 1$. The set of all linear transformations with $\det \mathbf{A} = 1$ forms a group called the **special linear group**,

$SL(n,R)$ or $SL(n,C)$. Elements of $O(n)$ satisfying $\det \mathbf{A} = 1$ form the **special orthogonal group** shown as $SO(n)$, which is also a subgroup of $SL(n,R)$. The group of linear transformations acting on vectors in n-dimensional complex space and satisfying $|\det \mathbf{A}|^2 = 1$, is called the **unitary group** $U(n)$. If the elements of the unitary group also satisfy $\det \mathbf{A} = 1$, we have the **special unitary group** $SU(n)$. $SU(n)$ is a subgroup of $U(n)$. Groups with infinite number of elements like $R(n)$ are called **infinite groups**. A group with finite number of elements is called a **finite group**, where the number of elements in a finite group is called the **order** of the group. Elements of a group in general do not commute, that is, $g_a g_b$ for any two elements need not be equal to $g_b g_a$. If in a group for every pair $g_a g_b = g_b g_a$ holds, then the group is said to be **commutative** or **Abelian**.

10.2 Infinitesimal Ring or Lie Algebra

For a **continuous group** or a **Lie group,** G, if $\mathbf{A}(t) \in G$, we have seen that its generator, $\mathbf{X}$, [Eq. (9.72)] is given as

$$\boxed{\mathbf{X} = \mathbf{A}'(0).} \tag{10.6}$$

The ensemble $\{\mathbf{A}'(0)\}$ of transformations is called the **infinitesimal ring,** or the **Lie algebra** of G, and it is denoted by ${}^rG$.

Differentiating $\mathbf{A}(at) \in G$ with respect to t:

$$\mathbf{A}'(at) = a\mathbf{A}'(at), \tag{10.7}$$

where a is a constant and substituting $t = 0$ we get

$$a\mathbf{A}'(0) = a\mathbf{X}, \tag{10.8}$$

$$\mathbf{A}'(0) = \mathbf{X} \in {}^rG. \tag{10.9}$$

Also, if $\mathbf{A}(t)$ and $\mathbf{B}(t)$ are any two elements of G, then

$$\mathbf{C}(t) = \mathbf{A}(t)\mathbf{B}(t) \in G. \tag{10.10}$$

Differentiating this and substituting $t = 0$ and using the fact that

$$\mathbf{A}(0) = \mathbf{B}(0) = \mathbf{I}, \tag{10.11}$$

we obtain

$$\mathbf{C}'(0) = \mathbf{A}'(0) + \mathbf{B}'(0) = \mathbf{X} + \mathbf{Y}. \tag{10.12}$$

Hence,

$$\mathbf{X} + \mathbf{Y} \in {}^rG \quad \text{if } \mathbf{X}, \mathbf{Y} \in {}^rG. \tag{10.13}$$

Lie has proven some very interesting theorems about the relations between continuous groups and their generators. One of these is the **commutator**

$$[\mathbf{X}_i, \mathbf{X}_j] = \mathbf{X}_i\mathbf{X}_j - \mathbf{X}_j\mathbf{X}_i \tag{10.14}$$

$$= \sum_{k=1}^{n} c_{ij}^k \mathbf{X}_k, \tag{10.15}$$

which says that the commutator of two generators is always a linear combination of generators. The constants, c_{ij}^k, are called the **structure constants** of the group G, and n is the **dimension** of G.

10.2.1 Properties of ^rG

So far, we have shown the following properties of ^rG:

If $\mathbf{X}, \mathbf{Y} \in {}^rG$, then

(i) $a\mathbf{X} \in {}^rG$, where a is a real number, (10.16)

(ii) $\mathbf{X} + \mathbf{Y} = \mathbf{Y} + \mathbf{X} \in {}^rG$, (10.17)

(iii)

$$[\mathbf{X}_i, \mathbf{X}_j] = \mathbf{X}_i\mathbf{X}_j - \mathbf{X}_j\mathbf{X}_i \tag{10.18}$$

$$= \sum_{k=1}^{n} c_{ij}^k \mathbf{X}_k \in {}^rG. \tag{10.19}$$

This means that ^rG is a **vector space** with the multiplication defined in (iii). The **dimension** of this vector space is equal to the number, n, of the parameters of the group G; thus, one can define a basis $(\mathbf{X}_1, \mathbf{X}_2, \ldots, \mathbf{X}_n)$ such that every $\mathbf{X} \in {}^rG$ can be expressed as a linear combination of the basis vectors:

$$\mathbf{X} = x_1\mathbf{X}_1 + x_2\mathbf{X}_2 + \cdots + x_n\mathbf{X}_n, \quad x_n \in \mathbb{R}. \tag{10.20}$$

From these it is clear that a continuous group completely determines the structure of its Lie algebra. Lie has also proved the converse, that is, the local structure in some neighborhood of the identity of a continuous group is completely determined by the structure constants c_{ij}^k.

10.3 Lie Algebra of the Rotation Group $R(3)$

We have seen that the **generators** of the rotation group are given as [Eq. (9.80)]

$$\mathbf{X}_1 = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{bmatrix}, \quad \mathbf{X}_2 = \begin{bmatrix} 0 & 0 & -1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}, \quad \mathbf{X}_3 = \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}. \tag{10.21}$$

These generators satisfy the **commutation relation**

$$\boxed{[\mathbf{X}_i, \mathbf{X}_j] = -\epsilon_{ijk}\mathbf{X}_k,} \tag{10.22}$$

where ϵ_{ijk} is the permutation (Levi–Civita) symbol. Using these generators, we can write an arbitrary infinitesimal rotation as

$$\mathbf{r} \cong (\mathbf{I} + \mathbf{X}_1\varepsilon_1 + \mathbf{X}_2\varepsilon_2 + \mathbf{X}_3\varepsilon_3)\mathbf{r}(0), \tag{10.23}$$

$$\delta\mathbf{r} = (\mathbf{X}_1\varepsilon_1 + \mathbf{X}_2\varepsilon_2 + \mathbf{X}_3\varepsilon_3)\mathbf{r}(0). \tag{10.24}$$

Defining two vectors, that is, $\mathbf{\Theta}$ with the components

$$\mathbf{\Theta} = \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \end{bmatrix} \tag{10.25}$$

and

$$\mathbf{X} = \mathbf{X}_1\widehat{\mathbf{e}}_1 + \mathbf{X}_2\widehat{\mathbf{e}}_2 + \mathbf{X}_3\widehat{\mathbf{e}}_3, \tag{10.26}$$

we can write

$$\mathbf{r} \cong (\mathbf{I} + \mathbf{X}\cdot\mathbf{\Theta})\mathbf{r}(\mathbf{0}), \tag{10.27}$$

thus, $\delta\mathbf{r} \cong \mathbf{X}\cdot\mathbf{\Theta}$. The operator for finite rotations, where $\mathbf{\Theta}$ has now the components $(\theta_1, \theta_2, \theta_3)$, can be constructed by N successive infinitesimal rotations, each by the amount $\mathbf{\Theta}/N$, and in the $N \to \infty$ limit as

$$\mathbf{r} = \lim_{N\to\infty}\left(\mathbf{I} + \frac{1}{N}\mathbf{X}\cdot\mathbf{\Theta}\right)^N \mathbf{r}(0) \tag{10.28}$$

$$= \lim_{N\to\infty}\sum_{m=0}^{N}\frac{N!}{m!(N-m)!}\left(\frac{\mathbf{X}\cdot\mathbf{\Theta}}{N}\right)^m \mathbf{r}(0) \tag{10.29}$$

$$= e^{\ \mathbf{X}\cdot\mathbf{\Theta}}\mathbf{r}(0). \tag{10.30}$$

Euler's theorem [5] allows us to look at Eq. (10.23) as an **infinitesimal rotation** about a single axis along the unit normal:

$$\widehat{\mathbf{n}} = \frac{1}{\sqrt{\varepsilon_1^2 + \varepsilon_2^2 + \varepsilon_3^2}}\begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \end{bmatrix}, \tag{10.31}$$

by the amount

$$d\theta = \sqrt{\varepsilon_1^2 + \varepsilon_2^2 + \varepsilon_3^2}\ , \tag{10.32}$$

as

$$\boxed{\mathbf{r}(\theta) \cong (\mathbf{I} + \mathbf{X}\cdot\widehat{\mathbf{n}}d\theta)\mathbf{r}(0).} \tag{10.33}$$

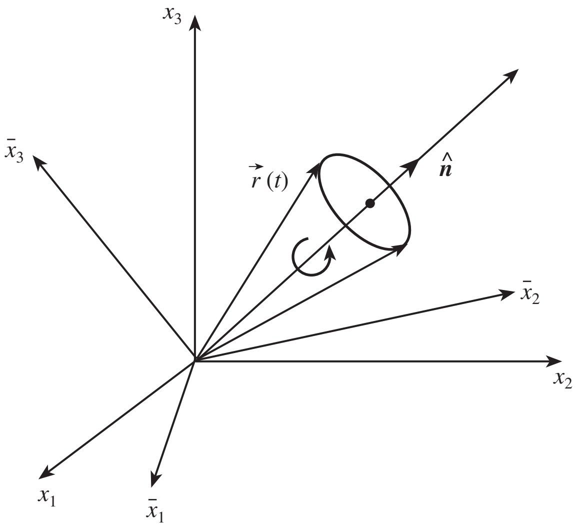


Figure 10.1 Rotation by θ about an axis along $\hat{\mathbf{n}}$.

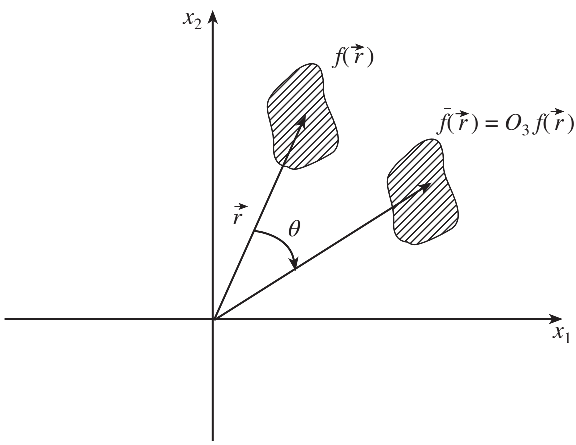


Figure 10.2 Effect of O_3 on $f(\mathbf{r})$.

For **finite rotations** (Figure 10.1) we write

$$\boxed{\mathbf{r}(\theta) = e^{\mathbf{X}\cdot\hat{\mathbf{n}}\theta}\mathbf{r}(0).} \tag{10.34}$$

10.3.1 Another Approach to ${}^{r}R(3)$

Let us approach ${}^{r}R(3)$ from the **operator**, that is, the **active** point of view. We now look for an operator, **O**, which acts on a function, $f(\mathbf{r})$, and rotates it clockwise, while keeping the coordinate axis fixed (Figure 10.2). Here $f(\mathbf{r})$ could be representing a physical system or a physical property. Instead of the Euler angles we use $(\theta_1, \theta_2, \theta_3)$, which represent rotations about the x_1- , x_2- , x_3-axes, respectively. For a counterclockwise rotation of the coordinate system about the x_3-axis we write

$$\bar{\mathbf{r}} = \mathbf{R}_3\mathbf{r}. \tag{10.35}$$

This induces the following change in $f(\mathbf{r})$:

$$\bar{f}(\mathbf{r}') = f(\mathbf{R}_3\mathbf{r}). \tag{10.36}$$

If $\mathbf{O}_3$ is an operator acting on $f(\mathbf{r})$, and since both views should agree, we write

$$\boxed{\mathbf{O}_3 f(\mathbf{r}) = \bar{f}(\mathbf{r}) = f(\mathbf{R}_3^{-1}\mathbf{r}).} \tag{10.37}$$

We now look for the generator of infinitesimal rotations of $\bar{f}(\mathbf{r})$ about the x_3-axis, which we show by $\overline{\mathbf{X}}_3$. Using Eq. (9.42), we write the rotation matrix $\mathbf{R}_3^{-1}$ as

$$\mathbf{R}_3^{-1}(\theta) = \mathbf{R}_3(-\theta).$$

For infinitesimal rotations we write $\theta_3 = \varepsilon_3$ and

$$\boxed{\mathbf{O}_3 = (\mathbf{I} - \overline{\mathbf{X}}_3\varepsilon_3).} \tag{10.38}$$

The minus sign in $\mathbf{O}_3$ indicates that the physical system is rotated clockwise (Figure 10.2), thus,

$$(\mathbf{I} - \overline{\mathbf{X}}_3\varepsilon_3)f(\mathbf{r}) = f(x_1\cos\varepsilon_3 - x_2\sin\varepsilon_3,\ x_1\sin\varepsilon_3 + x_2\cos\varepsilon_3,\ x_3), \tag{10.39}$$

$$\overline{\mathbf{X}}_3 f(\mathbf{r}) = -\left[\frac{f(x_1\cos\varepsilon_3 - x_2\sin\varepsilon_3,\ x_1\sin\varepsilon_3 + x_2\cos\varepsilon_3,\ x_3) - f(\mathbf{r})}{\varepsilon_3}\right], \tag{10.40}$$

$$\overline{\mathbf{X}}_3 f(\mathbf{r}) = -\left[\frac{f(x_1 - x_2\varepsilon_3,\ x_2 + x_1\varepsilon_3,\ x_3) - f(\mathbf{r})}{\varepsilon_3}\right]. \tag{10.41}$$

Using Taylor series expansion about the point (x_1, x_2, x_3) and taking the limit $\varepsilon_3 \to 0$ we obtain

$$\overline{\mathbf{X}}_3 f(\mathbf{r}) = -\left(x_1\frac{\partial}{\partial x_2} - x_2\frac{\partial}{\partial x_1}\right)f(\mathbf{r}), \tag{10.42}$$

thus,

$$\boxed{\overline{\mathbf{X}}_3 = -\left(x_1\frac{\partial}{\partial x_2} - x_2\frac{\partial}{\partial x_1}\right).} \tag{10.43}$$

Similarly, or by cyclic permutations of x_1, x_2, and x_3, we obtain the other operators as

$$\boxed{\overline{\mathbf{X}}_2 = -\left(x_3\frac{\partial}{\partial x_1} - x_1\frac{\partial}{\partial x_3}\right)} \tag{10.44}$$

and

$$\boxed{\overline{\mathbf{X}}_1 = -\left(x_2\frac{\partial}{\partial x_3} - x_3\frac{\partial}{\partial x_2}\right).} \tag{10.45}$$

Note that aside from a minus sign, $\overline{\mathbf{X}}_i$ satisfy the same commutation relations as $\mathbf{X}_i$, that is,

$$\boxed{\left[\overline{\mathbf{X}}_i, \overline{\mathbf{X}}_j\right] = \epsilon_{ijk}\overline{\mathbf{X}}_k.} \tag{10.46}$$

An arbitrary **infinitesimal rotation** of $f(\mathbf{r})$ can now be written as

$$\bar{f}(\mathbf{r}) \cong (\mathbf{I} - \overline{\mathbf{X}}_1\delta\theta_1 - \overline{\mathbf{X}}_2\delta\theta_2 - \overline{\mathbf{X}}_3\delta\theta_3)f(\mathbf{r}), \tag{10.47}$$

$$\boxed{\bar{f}(\mathbf{r}) \cong (\mathbf{I} - \overline{\mathbf{X}} \cdot \hat{\mathbf{n}}\delta\theta)f(\mathbf{r}),} \tag{10.48}$$

where $\hat{\mathbf{n}}$ and $\delta\theta$ are defined as in Eqs. (10.31) and (10.32). Now the **finite rotation operator** becomes

$$\boxed{\mathbf{O}f(\mathbf{r}) = e^{-\overline{\mathbf{X}} \cdot \hat{\mathbf{n}}\theta}f(\mathbf{r}).} \tag{10.49}$$

For applications in **quantum mechanics**, it is advantageous to adopt the view that the operator $\mathbf{O}$ still rotates the state function $f(\mathbf{r})$ counterclockwise, so that the direction of $\hat{\mathbf{n}}$ is positive when θ is measured with respect to the right-hand rule. In this regard, for the operator that rotates the physical system counterclockwise we write

$$\mathbf{O}f(\mathbf{r}) = e^{\overline{\mathbf{X}} \cdot \hat{\mathbf{n}}\theta}f(\mathbf{r}). \tag{10.50}$$

We will come back to this point later when we discuss angular momentum and quantum mechanics.

10.4 Group Invariants

It is obvious that for $R(3)$ the magnitude of a vector:

$$\widetilde{\mathbf{r}}\mathbf{r} = [x_1, x_2, x_3]\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = x_1^2 + x_2^2 + x_3^2, \tag{10.51}$$

is not changed through a rotation. A vector function $F(\mathbf{r})$ that remains unchanged by all $g \in G$, that is,

$$F(\mathbf{r}) = F(\bar{\mathbf{r}}), \tag{10.52}$$

is called a **group invariant**. We now determine a group whose invariant is $x_1^2 + x_2^2$. This group will naturally be a subgroup of $GL(2, R)$. An element of this group can be represented by the transformation

$$\begin{bmatrix} \bar{x}_1 \\ \bar{x}_2 \end{bmatrix} = \begin{bmatrix} a & b \\ c & d \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}. \tag{10.53}$$

From the group invariant

$$x_1^2 + x_2^2 = \bar{x}_1^2 + \bar{x}_2^2, \tag{10.54}$$

it follows that the transformation matrix elements must satisfy the relations

$$\begin{aligned} a^2 + c^2 &= 1, \\ b^2 + d^2 &= 1, \\ ab + cd &= 0. \end{aligned} \tag{10.55}$$

This means that only one of (a, b, c, d) could be independent. Choosing a new parameter as

$$a = \cos\theta, \tag{10.56}$$

we see that the transformation matrix has the following possible two forms:

$$\begin{bmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{bmatrix} \text{ and } \begin{bmatrix} \cos\theta & -\sin\theta \\ -\sin\theta & -\cos\theta \end{bmatrix}. \tag{10.57}$$

The first matrix is familiar; it corresponds to rotations, that is, $R(2)$. However, the determinant of the second matrix is

$$\det \begin{bmatrix} \cos\theta & -\sin\theta \\ -\sin\theta & -\cos\theta \end{bmatrix} = -1, \tag{10.58}$$

hence, the matrix can be written as

$$\begin{bmatrix} \cos\theta & -\sin\theta \\ -\sin\theta & -\cos\theta \end{bmatrix} = \begin{bmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}. \tag{10.59}$$

This is the reflection:

$$\begin{aligned} \bar{x}_1 &= x_1, \\ \bar{x}_2 &= -x_2, \end{aligned} \tag{10.60}$$

followed by a rotation. The group that leaves $x_1^2 + x_2^2$ invariant is called the **orthogonal group,** $O(2)$, where $R(2)$ is its subgroup with the determinant of all of its elements equal to one. $R(2)$ is also a subgroup of $SO(2)$, which includes rotations and translations.

10.4.1 Lorentz Transformations

As another example for a group invariant let us take

$$x^2 - y^2. \tag{10.61}$$

We can write this as

$$x^2 - y^2 = \begin{bmatrix} x & y \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix}. \tag{10.62}$$

For a linear transformation between $(\bar{x}, \bar{y})$ and (x, y), we write

$$\begin{bmatrix} \bar{x} \\ \bar{y} \end{bmatrix} = \begin{bmatrix} a & b \\ c & d \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix}. \tag{10.63}$$

Invariance of $(x^2 - y^2)$ can now be expressed as

$$\bar{x}^2 - \bar{y}^2 = \begin{bmatrix} \bar{x} & \bar{y} \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} \bar{x} \\ \bar{y} \end{bmatrix} \tag{10.64}$$

$$= \begin{bmatrix} x & y \end{bmatrix} \begin{bmatrix} a & c \\ b & d \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} a & b \\ c & d \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} \tag{10.65}$$

$$= \begin{bmatrix} x & y \end{bmatrix} \begin{bmatrix} a^2 - c^2 & ab - cd \\ ab - cd & b^2 - d^2 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} \tag{10.66}$$

$$= \begin{bmatrix} x & y \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} \tag{10.67}$$

$$= x^2 - y^2. \tag{10.68}$$

From the above equation, we see that for $(x^2 - y^2)$ to remain invariant under the transformation [Eq. (10.63)], components of the transformation matrix must satisfy

$$\begin{aligned} a^2 - c^2 &= 1, \\ b^2 - d^2 &= -1, \\ ab - cd &= 0. \end{aligned} \tag{10.69}$$

This means that only one of (a, b, c, d) can be independent. Defining a new parameter, χ, as

$$a = \cosh \chi, \tag{10.70}$$

we see that the transformation matrix in Eq. (10.63) can be written as

$$\begin{bmatrix} \cosh \chi & \sinh \chi \\ \sinh \chi & \cosh \chi \end{bmatrix}. \tag{10.71}$$

Introducing

$$\cosh \chi = \gamma, \tag{10.72}$$

$$\sinh \chi = -\gamma\beta, \tag{10.73}$$

$$\tanh \chi = -\beta, \tag{10.74}$$

where

$$\gamma = \frac{1}{\sqrt{1-\beta^2}}, \quad \beta = v/c, \tag{10.75}$$

and along with the identification

$$x = ct, \quad y = x, \tag{10.76}$$

we obtain

$$\begin{bmatrix} \bar{ct} \\ \bar{x} \end{bmatrix} = \begin{bmatrix} \gamma & -\beta\gamma \\ -\beta\gamma & \gamma \end{bmatrix} \begin{bmatrix} ct \\ x \end{bmatrix}. \tag{10.77}$$

This is nothing but the Lorentz transformation [Eq. (9.401)]:

$$\begin{aligned} \bar{ct} &= \frac{1}{\sqrt{1-(v/c)^2}}(ct - vx/c), \\ \bar{x} &= \frac{1}{\sqrt{1-(v/c)^2}}(x - vt), \end{aligned} \tag{10.78}$$

which leaves distances in spacetime:

$$(c^2t^2 - x^2), \tag{10.79}$$

invariant.

10.5 Unitary Group in Two Dimensions *U*(2)

Quantum mechanics is formulated in complex space. Hence, the components of the transformation matrix are in general complex numbers. The **scalar product** or the **inner product** of two vectors in n-dimensional complex space is defined as

$$\boxed{(\mathbf{x}, \mathbf{y}) = x_1^* y_1 + x_2^* y_2 + \cdots + x_n^* y_n,} \tag{10.80}$$

where x^* means the complex conjugate of x. **Unitary transformations** are linear transformations that leave the quadratic form

$$(\mathbf{x}, \mathbf{x}) = |\mathbf{x}|^2 = x_1^* x_1 + x_2^* x_2 + \cdots + x_n^* x_n \tag{10.81}$$

invariant. All such transformations form the **unitary group** $U(n)$. An element of $U(2)$ can be written as

$$\mathbf{u} = \begin{bmatrix} A & B \\ C & D \end{bmatrix}, \tag{10.82}$$

where A, B, C, and D are in general complex numbers. Invariance of $(\mathbf{x}, \mathbf{x})$ gives the **unitarity condition**:

$$\boxed{\mathbf{u}^\dagger \mathbf{u} = \mathbf{u}\mathbf{u}^\dagger = \mathbf{I},} \tag{10.83}$$

where

$$\boxed{\mathbf{u}^\dagger = \tilde{\mathbf{u}}^*} \tag{10.84}$$

is called the **Hermitian conjugate** of $\mathbf{u}$. Using the unitarity condition, we can write

$$\mathbf{u}^\dagger \mathbf{u} = \begin{bmatrix} A^* & C^* \\ B^* & D^* \end{bmatrix} \cdot \begin{bmatrix} A & B \\ C & D \end{bmatrix} \tag{10.85}$$

$$= \begin{bmatrix} |A|^2 + |C|^2 & A^*B + C^*D \\ AB^* + D^*C & |B|^2 + |D|^2 \end{bmatrix} \tag{10.86}$$

$$= \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \tag{10.87}$$

which gives

$$\begin{aligned} &|A|^2 + |C|^2 = 1, \\ &|B|^2 + |D|^2 = 1, \\ &A^*B + C^*D = 0. \end{aligned} \tag{10.88}$$

From elementary matrix theory [1], the inverse of $\mathbf{u}$ can be found as

$$\mathbf{u}^{-1} = \begin{bmatrix} D & -B \\ -C & A \end{bmatrix}. \tag{10.89}$$

Since for $U(2)$ the inverse of $\mathbf{u}$ is also equal to $\mathbf{u}^\dagger$ [Eq. (10.83)], we write

$$\mathbf{u}^{-1} = \mathbf{u}^\dagger, \tag{10.90}$$

$$\begin{bmatrix} D & -B \\ -C & A \end{bmatrix} = \begin{bmatrix} A^* & C^* \\ B^* & D^* \end{bmatrix}. \tag{10.91}$$

This gives $D = A^*$ and $C = -B^*$; thus, $\mathbf{u}$ becomes

$$\mathbf{u} = \begin{bmatrix} A & B \\ -B^* & A^* \end{bmatrix}. \tag{10.92}$$

Taking the determinant of the unitarity condition [Eq. (10.83)] and using the fact that

$$\det \mathbf{u}^{\dagger} = \det \mathbf{u}, \tag{10.93}$$

we obtain

$$|\det \mathbf{u}|^2 = 1. \tag{10.94}$$

10.5.1 Special Unitary Group *SU*(2)

In quantum mechanics, we are particularly interested in $SU(2)$, a subgroup of $U(2)$, where the group elements satisfy the condition

$$\det \mathbf{u} = 1. \tag{10.95}$$

For $SU(2)$, A and B in the transformation matrix

$$\mathbf{u} = \begin{bmatrix} A & B \\ -B^* & A^* \end{bmatrix}, \tag{10.96}$$

satisfy

$$\det \mathbf{u} = |A|^2 + |B|^2 = 1. \tag{10.97}$$

Expressing A and B as

$$\begin{aligned} A &= a + id, \\ B &= c + ib, \end{aligned} \tag{10.98}$$

we see that the unitary matrix has the form

$$\mathbf{u} = \begin{bmatrix} a + id & c + ib \\ -c + ib & a - id \end{bmatrix}. \tag{10.99}$$

This can be written as

$$\mathbf{u} = a\mathbf{I} + i(b\sigma_1 + c\sigma_2 + d\sigma_3), \tag{10.100}$$

where $\boldsymbol{\sigma}_i$ are the **Pauli spin matrices**:

$$\boxed{\sigma_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \ \sigma_2 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \ \sigma_3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix},} \tag{10.101}$$

which satisfy

$$\boxed{\begin{aligned} &\sigma_i^2 = 1, \\ &\sigma_i\sigma_j = -\sigma_j\sigma_i = i\sigma_k, \end{aligned}} \tag{10.102}$$

where (i, j, k) are cyclic permutations of $(1, 2, 3)$. The condition [Eq. (10.95)] on the determinant $\mathbf{u}$ gives

$$a^2 + b^2 + c^2 + d^2 = 1. \tag{10.103}$$

This allows us to choose (a, b, c, d) as

$$a = \cos\omega, \ b^2 + c^2 + d^2 = \sin^2\omega, \tag{10.104}$$

thus, Eq. (10.100) becomes

$$\mathbf{u}(\omega) = \mathbf{I}\cos\omega + i\mathbf{S}\sin\omega, \tag{10.105}$$

where we have defined

$$\mathbf{S} = \alpha\sigma_1 + \beta\sigma_2 + \gamma\sigma_3 \tag{10.106}$$

and

$$\begin{aligned} \alpha &= \frac{b}{(b^2 + c^2 + d^2)^{1/2}}, \\ \beta &= \frac{c}{(b^2 + c^2 + d^2)^{1/2}}, \\ \gamma &= \frac{d}{(b^2 + c^2 + d^2)^{1/2}}. \end{aligned} \tag{10.107}$$

Note that $\mathbf{u}$ in Eq. (10.82) has in general eight parameters. However, among these eight parameters we have five relations, four of which come from the unitarity condition [Eq. (10.83)]. We also have the condition fixing the value of the determinant [Eq. (10.95)] for $SU(2)$; thus, $SU(2)$ can only have three independent parameters. These parameters can be represented by a point on the three-dimensional surface (S-3) of a unit hypersphere defined by Eq. (10.103). In Eq. (10.105) we represent the elements of $SU(2)$ in terms of ω and (α, β, γ), where (α, β, γ) satisfies

$$\alpha^2 + \beta^2 + \gamma^2 = 1. \tag{10.108}$$

By changing (α, β, γ) on S-3 we can vary ω in

$$\mathbf{u}(\omega) = \mathbf{I}\cos\omega + \widetilde{\mathbf{X}}\sin\omega, \tag{10.109}$$

where we have defined $\widetilde{\mathbf{X}} = i\mathbf{S}$, hence $\widetilde{\mathbf{X}}^2 = -\mathbf{S}^2$.

10.5.2 Lie Algebra of *SU*(2)

In the previous section, we have seen that the elements of $SU(2)$ are given as

$$\boxed{\mathbf{u}(\omega) = \mathbf{I}\cos\omega + \widetilde{\mathbf{X}}\sin\omega.} \tag{10.110}$$

The 2×2 transformation matrix, $\mathbf{u}(\omega)$, transforms complex vectors:

$$\mathbf{v} = \begin{bmatrix} v_1 \\ v_2 \end{bmatrix}, \tag{10.111}$$

as

$$\boxed{\bar{\mathbf{v}} = \mathbf{u}(\omega)\mathbf{v}.} \tag{10.112}$$

The **infinitesimal transformations** of $SU(2)$, analogous to $R(3)$ [Eq. (10.33)], can be written as

$$\boxed{\begin{aligned}\mathbf{v}(\omega) &\cong (\mathbf{I} + \widetilde{\mathbf{X}}\delta\omega)\mathbf{v}(0),\\ \delta\mathbf{v} &= \widetilde{\mathbf{X}}\mathbf{v}(0)\delta\omega,\end{aligned}} \tag{10.113}$$

where the generator $\widetilde{\mathbf{X}}$ is obtained in terms of the generators $\widetilde{\mathbf{X}}_1, \widetilde{\mathbf{X}}_2, \widetilde{\mathbf{X}}_3$ [Eq. (10.109)] as

$$\widetilde{\mathbf{X}} = \mathbf{u}'(0) = i\mathbf{S}, \tag{10.114}$$

$$\widetilde{\mathbf{X}} = \alpha \begin{bmatrix} 0 & i \\ i & 0 \end{bmatrix} + \beta \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} + \gamma \begin{bmatrix} i & 0 \\ 0 & -i \end{bmatrix}. \tag{10.115}$$

Writing $\widetilde{\mathbf{X}}$ as

$$\widetilde{\mathbf{X}} = \alpha\widetilde{\mathbf{X}}_1 + \beta\widetilde{\mathbf{X}}_2 + \gamma\widetilde{\mathbf{X}}_3, \tag{10.116}$$

we identify the generators

$$\widetilde{\mathbf{X}}_1 = \begin{bmatrix} 0 & i \\ i & 0 \end{bmatrix}, \ \widetilde{\mathbf{X}}_2 = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}, \ \widetilde{\mathbf{X}}_3 = \begin{bmatrix} i & 0 \\ 0 & -i \end{bmatrix}, \tag{10.117}$$

where $\widetilde{\mathbf{X}}_i$ satisfy the following **commutation relation**:

$$\boxed{[\widetilde{\mathbf{X}}_i, \widetilde{\mathbf{X}}_j] = -2\epsilon_{ijk}\widetilde{\mathbf{X}}_k.} \tag{10.118}$$

We have seen that the generators of $R(3)$ satisfy [Eq. (10.22)]:

$$\boxed{[\mathbf{X}_i, \mathbf{X}_j] = -\epsilon_{ijk}\mathbf{X}_k,} \tag{10.119}$$

and the exponential form of the transformation matrix for finite rotations was [Eq. (10.34)]

$$\mathbf{r}(t) = e^{\mathbf{X}\cdot\hat{\mathbf{n}}\theta}\mathbf{r}(0). \tag{10.120}$$

If we make the correspondence

$$2\mathbf{X}_i \leftrightarrow \widetilde{\mathbf{X}}_i, \tag{10.121}$$

the two algebras are identical and the groups $SU(2)$ and $R(3)$ are called **isomorphic**. Defining a unit normal vector

$$\hat{\mathbf{n}} = (\alpha, \beta, \gamma), \tag{10.122}$$

we can now use Eq. (10.119) to write the exponential form of the transformation matrix for **finite rotations** in $SU(2)$ as

$$\mathbf{v}(t) = e^{\frac{1}{2}\widetilde{\mathbf{X}}\cdot\hat{\mathbf{n}}\theta}\mathbf{v}(0). \tag{10.123}$$

Since $\widetilde{\mathbf{X}} = i\mathbf{S}$, this gives us the **exponential form** of the transformation matrix for $SU(2)$:

$$\boxed{\mathbf{v}(t) = e^{\frac{1}{2}i\mathbf{S}\cdot\hat{\mathbf{n}}\theta}\mathbf{v}(0).} \tag{10.124}$$

Since in quantum mechanics the **active view**, where the vector is rotated counterclockwise, is preferred, the operator is taken as

$$e^{-\frac{1}{2}i\mathbf{S}\cdot\hat{\mathbf{n}}\theta}, \tag{10.125}$$

where $\mathbf{S}$ corresponds to the **spin** angular momentum operator:

$$\mathbf{S} = \alpha\sigma_1 + \beta\sigma_2 + \gamma\sigma_3. \tag{10.126}$$

In Section 10.9, we will see that the presence of the factor 1/2 in operator [Eq. (10.125)] is very important and it actually indicates that the correspondence between $SU(2)$ and $R(3)$ is **two-to-one**.

10.5.3 Another Approach to $'SU(2)$

Using the generators [Eq. (10.117)] and the transformation matrix [Eq. (10.110)] we can write

$$\widetilde{\mathbf{X}} = \alpha\widetilde{\mathbf{X}}_1 + \beta\widetilde{\mathbf{X}}_2 + \gamma\widetilde{\mathbf{X}} \tag{10.127}$$

and

$$\mathbf{u}(\alpha, \beta, \gamma) = (\mathbf{I}\cos\omega + \widetilde{\mathbf{X}}\sin\omega) \tag{10.128}$$

$$= \begin{bmatrix} \cos\omega + i\gamma\sin\omega & (\beta + i\alpha)\sin\omega \\ (-\beta + i\alpha)\sin\omega & \cos\omega - i\gamma\sin\omega \end{bmatrix}. \tag{10.129}$$

The transformation

$$\bar{\mathbf{v}} = \mathbf{u}(\omega)\mathbf{v} \tag{10.130}$$

induces the following change in a function $f(v_1, v_2)$:

$$\bar{f}(\bar{\mathbf{v}}) = f[\mathbf{u}(\alpha, \beta, \gamma)\mathbf{v}]. \tag{10.131}$$

Taking the **active view,** we define an operator $\mathbf{O}$, which acts on $f(\mathbf{v})$. Since both views should agree, we write

$$\boxed{\mathbf{O}f(\mathbf{r}) = \bar{f}(\mathbf{r}),} \tag{10.132}$$

where

$$\overline{f}(\mathbf{r}) = f[\mathbf{u}^{-1}(\alpha, \beta, \gamma)\mathbf{r}] = f[\mathbf{u}(-\alpha, -\beta, -\gamma)\mathbf{r}]. \tag{10.133}$$

For a given small ω, we can write $\mathbf{u}(-\alpha, -\beta, -\gamma)$ in terms of α, β, γ as

$$\mathbf{u}(-\alpha, -\beta, -\gamma) = \begin{bmatrix} 1 - i\gamma\omega & (-\beta - i\alpha)\omega \\ (\beta - i\alpha)\omega & 1 + i\gamma\omega \end{bmatrix}, \tag{10.134}$$

thus, we obtain

$$\overline{v}_1 = (1 - i\gamma\omega)v_1 + (-\beta - i\alpha)\omega v_2, \tag{10.135}$$

$$\overline{v}_2 = (\beta - i\alpha)\omega v_1 + (1 + i\gamma\omega)v_2. \tag{10.136}$$

Writing $\delta v_i = \overline{v}_i - v_i$, this becomes

$$\delta v_1 = -i\gamma\omega v_1 + (-\beta - i\alpha)\omega v_2, \tag{10.137}$$

$$\delta v_2 = (\beta - i\alpha)\omega v_1 + i\gamma\omega v_2. \tag{10.138}$$

We now write the effect of the operator $\mathbf{O}_1$, which induces infinitesimal changes in a function $f(v_1, v_2)$, as

$$(\mathbf{I} - \mathbf{O}_1\omega)f(v_1, v_2) = f(v_1, v_2) + \left[\frac{\partial f(v_1, v_2)}{\partial v_1}\frac{\partial(\delta v_1)}{\partial \alpha} + \frac{\partial f(v_1, v_2)}{\partial v_2}\frac{\partial(\delta v_2)}{\partial \alpha}\right] \tag{10.139}$$

$$= f(v_1, v_2) + \left[-i\omega v_2\frac{\partial f(v_1, v_2)}{\partial v_1} - i\omega v_1\frac{\partial f(v_1, v_2)}{\partial v_2}\right] \tag{10.140}$$

$$= f(v_1, v_2) - i\omega\left[v_2\frac{\partial}{\partial v_1} + v_1\frac{\partial}{\partial v_2}\right]f(v_1, v_2). \tag{10.141}$$

This gives the generator $\mathbf{O}_1$ as

$$\boxed{\mathbf{O}_1 = i\left[v_2\frac{\partial}{\partial v_1} + v_1\frac{\partial}{\partial v_2}\right].} \tag{10.142}$$

Similarly, we write

$$(\mathbf{I} - \mathbf{O}_2\omega)f(v_1, v_2) = f(v_1, v_2) + \left[\frac{\partial f(v_1, v_2)}{\partial v_1}\frac{\partial(\delta v_1)}{\partial \beta} + \frac{\partial f(v_1, v_2)}{\partial v_2}\frac{\partial(\delta v_2)}{\partial \beta}\right] \tag{10.143}$$

$$= f(v_1, v_2) + \left[-\omega v_2\frac{\partial f(v_1, v_2)}{\partial v_1} + \omega v_1\frac{\partial f(v_1, v_2)}{\partial v_2}\right] \tag{10.144}$$

$$= f(v_1, v_2) + \omega\left[-v_2\frac{\partial}{\partial v_1} + v_1\frac{\partial}{\partial v_2}\right]f(v_1, v_2) \tag{10.145}$$

and

$$(\mathbf{I} - \mathbf{O}_3\omega)f(v_1, v_2) = f(v_1, v_2) + \left[\frac{\partial f(v_1, v_2)}{\partial v_1}\frac{\partial(\delta v_1)}{\partial \gamma} + \frac{\partial f(v_1, v_2)}{\partial v_2}\frac{\partial(\delta v_2)}{\partial \gamma}\right] \tag{10.146}$$

$$= f(v_1, v_2) + \left[-i\omega v_1\frac{\partial f(v_1, v_2)}{\partial v_1} + i\omega v_2\frac{\partial f(v_1, v_2)}{\partial v_2}\right] \tag{10.147}$$

$$= f(v_1, v_2) + \omega i\left[v_2\frac{\partial}{\partial v_2} - v_1\frac{\partial}{\partial v_1}\right]f(v_1, v_2). \tag{10.148}$$

These give us the remaining generators as

$$\boxed{\mathbf{O}_2 = \left[v_2\frac{\partial}{\partial v_1} - v_1\frac{\partial}{\partial v_2}\right],} \tag{10.149}$$

$$\boxed{\mathbf{O}_3 = i\left[v_1\frac{\partial}{\partial v_1} - v_2\frac{\partial}{\partial v_2}\right],} \tag{10.150}$$

where $\mathbf{O}_i$ satisfy the commutation relation

$$\boxed{[\mathbf{O}_i, \mathbf{O}_j] = 2\epsilon_{ijk}\mathbf{O}_k.} \tag{10.151}$$

The sign difference with Eq. (10.118) is again due to the fact that in the passive view axes are rotated counterclockwise, while in the active view vectors are rotated clockwise.

10.6 Lorentz Group and Its Lie Algebra

The ensemble of objects, $[a^\alpha_\gamma]$, which preserve the length of **four-vectors** in Minkowski spacetime and which satisfy the relation

$$g_{\alpha\beta}a^\alpha_\gamma a^\beta_\delta = g_{\gamma\delta} \tag{10.152}$$

form the **Lorentz group**. If we exclude reflections and consider only the transformations that can be continuously generated from the identity transformation, we have the **homogeneous Lorentz group**. The group that includes reflections as well as the translations is called the **inhomogeneous Lorentz group** or the **Poincare group**. From now on we consider the homogeneous Lorentz group and omit the word homogeneous.

Given the coordinates of the position four-vector, x^α, in the K frame, elements of the Lorentz group, $[a^\alpha_\beta]$, give us the components, $\overline{x}^\alpha$, in the $\overline{K}$ frame as

$$\overline{x}^\alpha = a^\alpha_\beta x^\beta. \tag{10.153}$$

In matrix notation, we can write this as

$$\boxed{\overline{\mathbf{X}} = \mathbf{A}\mathbf{x},} \tag{10.154}$$

where

$$\overline{\mathbf{X}} = \begin{bmatrix} \overline{x}^0 \\ \overline{x}^1 \\ \overline{x}^2 \\ \overline{x}^3 \end{bmatrix}, \quad \mathbf{A} = \begin{bmatrix} a^0_0 & a^0_1 & a^0_2 & a^0_3 \\ a^1_0 & a^1_1 & a^1_2 & a^1_2 \\ a^2_0 & a^2_1 & a^2_2 & a^2_3 \\ a^3_0 & a^3_1 & a^3_2 & a^3_3 \end{bmatrix}, \quad \mathbf{x} = \begin{bmatrix} x^0 \\ x^1 \\ x^2 \\ x^3 \end{bmatrix}. \tag{10.155}$$

For transformations preserving the magnitude of four-vectors we write

$$\widetilde{\overline{\mathbf{x}}}\mathbf{g}\overline{\mathbf{x}} = \widetilde{\mathbf{x}}\mathbf{g}\mathbf{x}, \tag{10.156}$$

and after substituting Eq. (10.154), we obtain the analogue of the **orthogonality condition**:

$$\boxed{\widetilde{\mathbf{A}}\mathbf{g}\mathbf{A} = \mathbf{g}.} \tag{10.157}$$

Elements of the Lorentz group are 4×4 matrices, which means that they have 16 components. From the orthogonality condition [Eq. (10.157)], which is a symmetric matrix, we have 10 relations among these 16 components; thus, only six of them are independent. In other words, the Lorentz group is a six-parameter group. These six parameters can be conveniently thought of as the three Euler angles specifying the orientation of the spatial axis and the three components of $\overrightarrow{\beta}$ specifying the relative velocity of the two inertial frames.

Guided by our experience with $R(3)$, to find the generators of the Lorentz group we start with the ansatz that $\mathbf{A}$ can be written in exponential form as

$$\mathbf{A} = e^{\mathbf{L}}, \tag{10.158}$$

where $\mathbf{L}$ is a 4×4 matrix. From the theory of matrices we can write [4]

$$\det \mathbf{A} = \det e^{\mathbf{L}} = e^{Tr\mathbf{L}}. \tag{10.159}$$

Using this equation and considering only the proper Lorentz transformations, where $\det \mathbf{A} = 1$, we conclude that $\mathbf{L}$ is traceless. Thus, the generator of the proper Lorentz transformations is a real 4×4 traceless matrix.

We now multiply Eq. (10.157) from the left by $\mathbf{g}^{-1}$ and from the right by $\mathbf{A}^{-1}$ to write

$$\mathbf{g}^{-1}\widetilde{\mathbf{A}}\mathbf{g}[\mathbf{A}\mathbf{A}^{-1}] = \mathbf{g}^{-1}\mathbf{g}\mathbf{A}^{-1}, \tag{10.160}$$

which gives

$$\mathbf{g}^{-1}\widetilde{\mathbf{A}}\mathbf{g} = \mathbf{A}^{-1}. \tag{10.161}$$

Since for the Minkowski metric $\mathbf{g}^{-1} = \mathbf{g}$, this becomes

$$\mathbf{g}\widetilde{\mathbf{A}}\mathbf{g} = \mathbf{A}^{-1}. \tag{10.162}$$

Using Eq. (10.162) and the relations

$$\mathbf{g}^2 = \mathbf{I},\ \widetilde{\mathbf{A}} = e^{\widetilde{\mathbf{L}}},\ \mathbf{A}^{-1} = e^{-\mathbf{L}}, \tag{10.163}$$

we can also write

$$\mathbf{g}\widetilde{\mathbf{A}}\mathbf{g} = e^{\mathbf{g}\widetilde{\mathbf{L}}\mathbf{g}} = e^{-\mathbf{L}}; \tag{10.164}$$

Thus,

$$\mathbf{g}\widetilde{\mathbf{L}}\mathbf{g} = -\mathbf{L}. \tag{10.165}$$

Since $\widetilde{\mathbf{g}} = \mathbf{g}$, we obtain

$$\widetilde{\mathbf{gL}} = -\mathbf{gL}. \tag{10.166}$$

This equation shows that $\mathbf{gL}$ is an antisymmetric matrix. Considering that $\mathbf{g}$ is the Minkowski metric and $\mathbf{L}$ is traceless, we can write the general form of $\mathbf{L}$ as

$$\mathbf{L} = \begin{bmatrix} 0 & -L_{01} & -L_{02} & -L_{03} \\ -L_{01} & 0 & L_{12} & L_{13} \\ -L_{02} & -L_{12} & 0 & L_{23} \\ -L_{03} & -L_{13} & -L_{23} & 0 \end{bmatrix}. \tag{10.167}$$

Introducing six independent parameters, $(\beta_1, \beta_2, \beta_3)$ and $(\theta_1, \theta_2, \theta_3)$, this can also be written as

$$\boxed{\mathbf{L} = \beta_1\mathbf{V}_1 + \beta_2\mathbf{V}_2 + \beta_3\mathbf{V}_3 + \theta_1\mathbf{X}_1 + \theta_2\mathbf{X}_2 + \theta_3\mathbf{X}_3,} \tag{10.168}$$

where

$$\mathbf{V}_1 = \begin{bmatrix} 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix},\ \mathbf{V}_2 = \begin{bmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix},\ \mathbf{V}_3 = \begin{bmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{bmatrix}, \tag{10.169}$$

$$\mathbf{X}_1 = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{bmatrix},\ \mathbf{X}_2 = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix},\ \mathbf{X}_3 = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}. \tag{10.170}$$

Note that ($\mathbf{X}_1, \mathbf{X}_2$, and $\mathbf{X}_3$) are the generators of the infinitesimal rotations about the x^1-, x^2-, and x^3-axes [Eq. (9.80)], respectively, and ($\mathbf{V}_1, \mathbf{V}_2$, and $\mathbf{V}_3$) are the generators of the infinitesimal Lorentz transformations or **boosts** from one inertial observer to another moving with respect to each other with velocities (β_1, β_2, and β_3) along the x^1-, x^2-, and x^3-axes, respectively. These six generators satisfy the **commutation relations**

$$[\mathbf{X}_i, \mathbf{X}_j] = -\epsilon_{ijk}\mathbf{X}_k, \tag{10.171}$$

$$[\mathbf{X}_i, \mathbf{V}_j] = -\epsilon_{ijk}\mathbf{V}_k, \tag{10.172}$$

$$[\mathbf{V}_i, \mathbf{V}_j] = \epsilon_{ijk}\mathbf{X}_k. \tag{10.173}$$

The first of these three commutators is just the commutation relation for the rotation group $R(3)$; thus, the rotation group is also a subgroup of the Lorentz group. The second commutator shows that $\mathbf{V}_i$ transforms under rotation like a vector. The third commutator indicates that boosts in general do not commute, but more important than this, two successive boosts is equal to a boost plus a rotation (Figure 10.3), that is,

$$\mathbf{V}_i\mathbf{V}_j = \mathbf{V}_j\mathbf{V}_i + \epsilon_{ijk}\mathbf{X}_k. \tag{10.174}$$

Thus, boosts alone do not form a group. An important kinematic consequence of this is known as the **Thomas precession**.

We now define two unit three-vectors:

$$\hat{\mathbf{n}} = \frac{1}{\sqrt{\theta_1^2 + \theta_2^2 + \theta_3^2}} \begin{bmatrix} \theta_1 \\ \theta_2 \\ \theta_3 \end{bmatrix}, \tag{10.175}$$

$$\hat{\beta} = \frac{1}{\sqrt{\beta_1^2 + \beta_2^2 + \beta_3^2}} \begin{bmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \end{bmatrix}, \tag{10.176}$$

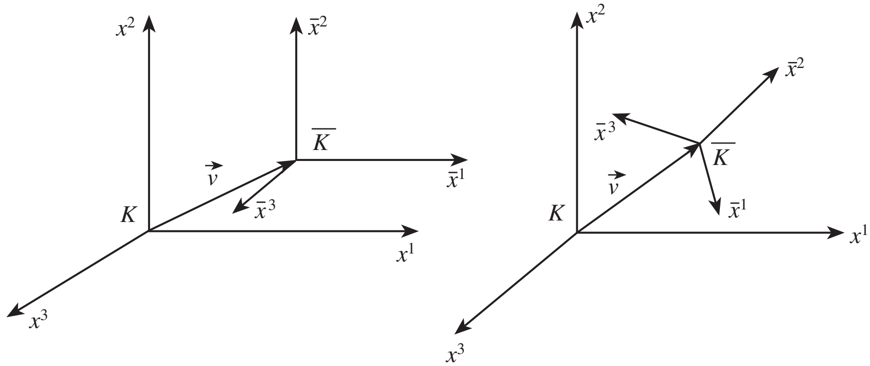


Figure 10.3 Boost and boost plus rotation.

and introduce the parameters

$$\theta = \sqrt{\theta_1^2 + \theta_2^2 + \theta_3^2} \text{ and } \beta = \sqrt{\beta_1^2 + \beta_2^2 + \beta_3^2}, \tag{10.177}$$

so that we can summarize these results as

$$\boxed{\mathbf{L} = \mathbf{X} \cdot \hat{\mathbf{n}}\theta + \mathbf{V} \cdot \hat{\beta}\beta,} \tag{10.178}$$

$$\boxed{\mathbf{A} = e^{\mathbf{X} \cdot \hat{\mathbf{n}}\theta + \mathbf{V} \cdot \hat{\beta}\beta}.} \tag{10.179}$$

For **pure rotations**, this reduces to the rotation matrix in Eq. (10.34):

$$\mathbf{A}_{\text{rot.}} = e^{\mathbf{X} \cdot \hat{\mathbf{n}}\theta}, \tag{10.180}$$

and for **pure boosts** it is equal to Eq. (9.417):

$$\mathbf{A}_{\text{boost}}(\beta) = e^{\mathbf{V} \cdot \hat{\beta}\beta} \tag{10.181}$$

$$= \begin{bmatrix} \gamma & -\beta_1\gamma & -\beta_2\gamma & -\beta_3\gamma \\ -\beta_1\gamma & 1 + \dfrac{(\gamma-1)\beta_1^2}{\beta^2} & \dfrac{(\gamma-1)\beta_1\beta_2}{\beta^2} & \dfrac{(\gamma-1)\beta_1\beta_3}{\beta^2} \\ -\beta_2\gamma & \dfrac{(\gamma-1)\beta_2\beta_1}{\beta^2} & 1 + \dfrac{(\gamma-1)\beta_2^2}{\beta^2} & \dfrac{(\gamma-1)\beta_2\beta_3}{\beta^2} \\ -\beta_3\gamma & \dfrac{(\gamma-1)\beta_3\beta_1}{\beta^2} & \dfrac{(\gamma-1)\beta_3\beta_2}{\beta^2} & 1 + \dfrac{(\gamma-1)\beta_3^2}{\beta^2} \end{bmatrix},$$

where $\beta_1 = v_1/c$, $\beta_2 = v_2/c$, $\beta_3 = v_3/c$. For a boost along the x_1 direction $\beta_1 = \beta$, $\beta_2 = \beta_3 = 0$, Eq. (10.181) reduces to

$$\mathbf{A}_{\text{boost}}(\beta_1) = \begin{bmatrix} \gamma & -\beta\gamma & 0 & 0 \\ -\beta\gamma & \gamma & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}. \tag{10.182}$$

Using the parametrization

$$-\beta_1 = \tanh \chi, \tag{10.183}$$

$$\gamma = \cosh \chi, \tag{10.184}$$

$$-\gamma\beta_1 = \sinh \chi, \tag{10.185}$$

Equation (10.181) becomes

$$\mathbf{A}_{\text{boost}}(\beta_1) = \begin{bmatrix} \cosh \chi & \sinh \chi & 0 & 0 \\ \sinh \chi & \cosh \chi & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \tag{10.186}$$

which is reminiscent of the rotation matrices [Eqs. (9.41) and (9.42)] with the hyperbolic functions instead of the trigonometric. Note that in accordance with our previous treatment in Section 10.2, the generator $\mathbf{V}_1$ can also be obtained from $\mathbf{V}_1 = \mathbf{A}'_{\text{boost}}(\beta_1 = 0)$. The other generators can also be obtained similarly.

10.7 Group Representations

A group with the general element g is an abstract concept. It gains practical meaning only when G is assigned physical operations, $D(g)$, to its elements that act in some space of objects called the **representation space**. These objects could be functions, vectors, and so on. As in the rotation group $R(3)$, group representations can be accomplished by assigning matrices to each element of G, which correspond to rotation matrices acting on vectors. Given a particular representation, $D(g)$, another representation can be constructed by a **similarity transformation**:

$$D'(g) = S^{-1}D(g)S. \tag{10.187}$$

Representations that are connected by a similarity transformation are called **equivalent representations**. Given two representations, $D^{(1)}(g)$ and $D^{(2)}(g)$, we can construct another representation:

$$D(g) = D^{(1)}(g) \oplus D^{(1)}(g) = \begin{bmatrix} D^{(1)}(g) & 0 \\ 0 & D^{(2)}(g) \end{bmatrix}, \tag{10.188}$$

where $D(g)$ is called the **product** of $D^{(1)}(g)$ and $D^{(2)}(g)$. If $D^{(1)}(g)$ has **dimension** n_1, that is, composed of $n_1 \times n_1$ matrices, and $D^{(2)}(g)$ has dimension n_2, the product representation has the dimension $n_1 + n_2$. $D(g)$ is also called a **reducible representation**. If $D(g)$ cannot be split into the sums of smaller representations by similarity transformations, it is called an **irreducible representation**. Irreducible representations are very important and they form the building blocks of the theory. A matrix that commutes with every element of an irreducible representation is a multiple of the unit matrix. We now present without proof an important lemma due to Schur for the criterion of irreducibility of a group representation.

10.7.1 Schur's Lemma

Let $D^{(1)}(g)$ and $D^{(2)}(g)$ be two irreducible representations with dimensions n_1 and n_2, and suppose that a matrix A exists such that

$$AD^{(1)}(g) = D^{(2)}(g)A \tag{10.189}$$

for all g in G. Then either $A = 0$, or $n_1 = n_2$ and $\det A \neq 0$, and the two representations, $D^{(1)}(g)$ and $D^{(2)}(g)$, are equivalent.

By a similarity transformation, if $D(g)$ can be written as

$$D(g) = \begin{bmatrix} D^{(1)}(g) & 0 & 0 & 0 \\ 0 & D^{(2)}(g) & 0 & 0 \\ 0 & 0 & D^{(2)}(g) & 0 \\ 0 & 0 & 0 & D^{(3)}(g) \end{bmatrix}, \tag{10.190}$$

we write

$$D(g) = D^{(1)}(g) \oplus 2D^{(2)}(g) \oplus D^{(3)}(g). \tag{10.191}$$

If $D^{(1)}(g)$, $D^{(2)}(g)$, and $D^{(3)}(g)$ cannot be reduced further, they are irreducible and $D(g)$ is called a **completely reducible representation**.

Every group has a trivial one-dimensional representation, where each group element is represented by the number one. In an irreducible representation, say $D^{(2)}(g)$ as in the above case, then every element of the representation space is transformed into another element of that space by the action of the group elements $D^{(2)}(g)$. For example, for the rotation group, $R(3)$, a three-dimensional representation is given by the rotation matrices and the representation space is the Cartesian vectors. In other words, rotations of a Cartesian vector always results in another Cartesian vector.

10.7.2 Group Character

The characterization of a representation by explicitly giving the matrices that represent the group elements is not possible, since by a similarity transformation one could always obtain a different set of matrices. Therefore, we need to identify properties that remain invariant under similarity transformations. One such property is the **trace** of a matrix. We now define the **group character,** $\chi^{(i)}(g)$, as the trace of the matrices $D^{(i)}(g)$:

$$\boxed{\chi^{(i)}(g) = \sum_{j=1}^{n_i} D_{jj}^{(i)}(g).} \tag{10.192}$$

10.7.3 Unitary Representation

Representation of a group by unitary (transformation) matrices is called **unitary representation**. Unitary transformations leave the quadratic form,

$$|\mathbf{x}|^2 = \sum_{i=1}^{n} |x_i|^2, \tag{10.193}$$

invariant, which is equivalent to the inner product in complex space:

$$(\mathbf{x}, \mathbf{y}) = \sum_{i=1}^{n} x_i^* y_i. \tag{10.194}$$

10.8 Representations of *R*(3)

We now construct the representations of the rotation group. Using Cartesian tensors we can easily construct the irreducible representations as

$$\begin{bmatrix} D^{(1)}(g) & 0 & 0 & 0 \\ 0 & D^{(3)}(g) & 0 & 0 \\ 0 & 0 & D^{(5)}(g) & 0 \\ 0 & 0 & 0 & \ddots \end{bmatrix}, \tag{10.195}$$

where $D^{(1)}(g)$ is the trivial representation, the number one, that acts on scalars. $D^{(3)}(g)$ are given as the 3×3 rotation matrices that act on vectors. The superscript 3 indicates the degrees of freedom, in this case the three independent components of a vector. $D^{(5)}(g)$ is the representation corresponding to the transformation matrices for the symmetric second-rank Cartesian tensors. In this case, the dimension of the representation comes from the fact that a second-rank symmetric tensor has six independent components; removing the trace leaves five. In general, a symmetric tensor of rank n has $(2n + 1)$ independent components; thus, the associated representation is $(2n + 1)$-dimensional.

10.8.1 Spherical Harmonics and Representations of *R*(3)

An elegant and also useful way of obtaining representations of $R(3)$ is to construct them through the transformation properties of the spherical harmonics. The trivial representation $D^{(1)}(g)$ simply consists of the transformation of Y_{00} onto itself. $D^{(3)}(g)$ describes the transformations of $Y_{(l=1)m}(\theta, \phi)$. The three spherical harmonics:

$$(Y_{1-1}, Y_{10}, Y_{11}), \tag{10.196}$$

under rotations transform into linear combinations of each other. In general, the transformation properties of the $(2l + 1)$ components of $Y_{lm}(\theta, \phi)$ generate the irreducible representations $D^{(2l+1)}(g)$ of $R(3)$.

10.8.2 Angular Momentum in Quantum Mechanics

In quantum mechanics, angular momentum, **L**, is a **differential operator** acting on a wave function $\Psi(x, y, z)$. It is obtained from the classical expression, $\vec{L} = \vec{r} \times \vec{p}$, with the replacement of the classical variables with their operator counterparts, $\vec{x} \to \vec{x}$ and $\vec{p} \to \frac{\hbar}{i}\vec{\nabla}$, as

$$\boxed{\mathbf{L} = -i\hbar \vec{r} \times \vec{\nabla}.} \tag{10.197}$$

In Cartesian coordinates, we write the components of **L** as (we set $\hbar = 1$)

$$L_x = i\overline{\mathbf{X}}_x = -i\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right), \tag{10.198}$$

$$L_y = i\overline{\mathbf{X}}_y = -i\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right), \tag{10.199}$$

$$L_z = i\overline{\mathbf{X}}_z = -i\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right). \tag{10.200}$$

In Eq. (10.46), we have seen that $\overline{\mathbf{X}}_i$ satisfy the commutation relation

$$[\overline{\mathbf{X}}_i, \overline{\mathbf{X}}_j] = \epsilon_{ijk}\overline{\mathbf{X}}_k, \tag{10.201}$$

Thus, L_i satisfy

$$[L_i, L_j] = i\epsilon_{ijk}L_k, \tag{10.202}$$

where the indices i, j, and k take the values 1, 2, and 3 which correspond to x, y, and z, respectively.

10.8.3 Rotation of the Physical System

We have seen that the effect of the operator, $e^{-\overline{\mathbf{X}}\cdot\hat{\mathbf{n}}\theta_n}$ [Eq. (10.49)], is to rotate a function clockwise about an axis pointing in the $\hat{\mathbf{n}}$ direction by θ_n. In quantum mechanics, we adhere to the right-handed screw convention, that is, when we curl the fingers of our right hand about the axis of rotation and in the direction of rotation, our thumb points along $\hat{\mathbf{n}}$. Hence, we work with the operator $e^{\overline{\mathbf{X}}\cdot\hat{\mathbf{n}}\theta_n}$, which rotates a function counterclockwise by θ_n (Figure 10.4). Using Eqs. (10.198)–(10.200) the quantum mechanical counterpart of the rotation operator now becomes

$$\boxed{\mathbf{R} = e^{-i\mathbf{L}\cdot\hat{\mathbf{n}}\theta_n}.} \tag{10.203}$$

For a rotation about the z-axis this gives

$$\mathbf{R}\Psi(r, \theta, \phi) = [e^{-iL_z\phi}]\Psi(r, \theta, \phi). \tag{10.204}$$

For a general rotation about an axis in the $\hat{\mathbf{n}}$ direction by θ_n we write

$$\mathbf{R}\Psi(x, y, z) = e^{-i\mathbf{L}\cdot\hat{\mathbf{n}}\theta_n}\Psi(x, y, z). \tag{10.205}$$

10.8.4 Rotation Operator in Terms of the Euler Angles

Using the **Euler angles** we can write the rotation operator $\mathbf{R} = e^{-i\mathbf{L}\cdot\hat{\mathbf{n}}\theta_n}$, as

$$\boxed{\mathbf{R} = e^{-i\gamma L_{z_2}}e^{-i\beta L_{y_1}}e^{-i\alpha L_z}.} \tag{10.206}$$

In this expression, we have used another convention commonly used in modern-day quantum mechanical discussions of angular momentum. It is

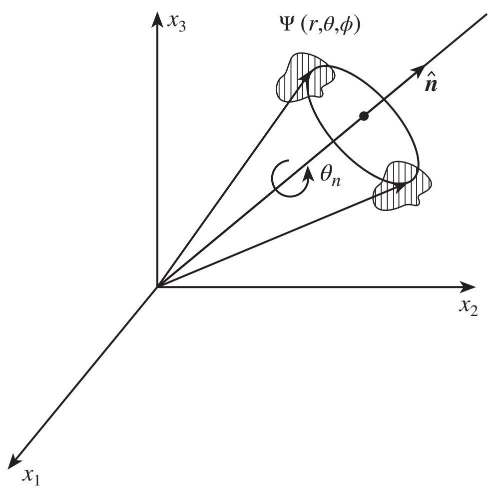


Figure 10.4 Counterclockwise rotation of the physical system by θ_n about $\hat{\mathbf{n}}$.

composed of the sequence of rotations, which starts with a counterclockwise rotation by α about the z-axis of the initial state of the system:

$$e^{-i\alpha L_z}: (x, y, z) \to (x_1, y_1, z_1), \tag{10.207}$$

followed by a counterclockwise rotation by β about y_1 of the intermediate axis.

$$e^{-i\beta L_{y_1}}: (x_1, y_1, z_1) \to (x_2, y_2, z_2) \tag{10.208}$$

and finally the desired orientation is reached by a counterclockwise rotation about the z_2-axis by γ:

$$e^{-i\gamma L_{z_2}}: (x_2, y_2, z_2) \to (x', y', z'). \tag{10.209}$$

10.8.5 Rotation Operator in the Original Coordinates

One of the disadvantages of the rotation operator expressed as

$$\mathbf{R} = e^{-i\mathbf{L}.\hat{\mathbf{n}}\theta_n} = e^{-i\gamma L_{z_2}} e^{-i\beta L_{y_1}} e^{-i\alpha L_z} \tag{10.210}$$

is that, except for the initial rotation about the z-axis, the remaining two rotations are performed about different sets of axis. Because we are interested in evaluating

$$\mathbf{R}\Psi(x, y, z) = \Psi(x', y', z'), \tag{10.211}$$

where (x, y, z) and (x', y', z') are two points in the same coordinate system, we need to express $\mathbf{R}$ as rotations entirely in terms of the original coordinate axis.

For this we first need to find how the operator $\mathbf{R}$ transforms under coordinate transformations. We now transform to a new coordinate system (x_n, y_n, z_n), where the z_n-axis is aligned with the $\hat{\mathbf{n}}$ direction (Figure 10.5). We show the matrix of this coordinate transformation with the letter R. We are interested in

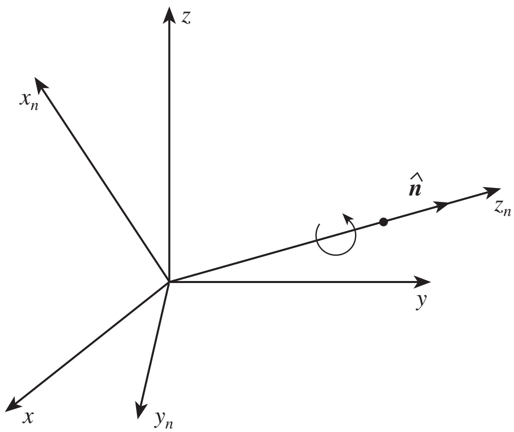


Figure 10.5 Transformation to the (x_n, y_n, z_n)-axis.

expressing the operator **R** in terms of the (x_n, y_n, z_n) coordinates. Action of R on the coordinates induces the following change in $\Psi(x, y, z)$:

$$R\Psi(x, y, z) = \Psi(x_n, y_n, z_n). \tag{10.212}$$

Similarly, for another point we write

$$R\Psi(x', y', z') = \Psi(x'_n, y'_n, z'_n). \tag{10.213}$$

Inverse transformations are naturally given as

$$R^{-1}\Psi(x_n, y_n, z_n) = \Psi(x, y, z) \tag{10.214}$$

and

$$R^{-1}\Psi(x'_n, y'_n, z'_n) = \Psi(x', y', z'). \tag{10.215}$$

Operating on Eq. (10.214) with **R** we get

$$\mathbf{R}R^{-1}\Psi(x_n, y_n, z_n) = \mathbf{R}\Psi(x, y, z). \tag{10.216}$$

Using Eq. (10.211), this becomes

$$\mathbf{R}R^{-1}\Psi(x_n, y_n, z_n) = \Psi(x', y', z'). \tag{10.217}$$

We now operate on this with R to write

$$R\mathbf{R}R^{-1}\Psi(x_n, y_n, z_n) = R\Psi(x', y', z') \tag{10.218}$$
$$= \Psi(x'_n, y'_n, z'_n), \tag{10.219}$$

where

$$\mathbf{R} = e^{-i\gamma L_{z_2}} e^{-i\beta L_{y_1}} e^{-i\alpha L_z}. \tag{10.220}$$

We now observe that

$$e^{-i\gamma L_{z_2}} = e^{-i\beta L_{y_1}} e^{-i\gamma L_{z_1}} e^{i\beta L_{y_1}} \tag{10.221}$$

to write

$$\mathbf{R} = e^{-i\beta L_{y_1}} e^{-i\gamma L_{z_1}} [e^{i\beta L_{y_1}} e^{-i\beta L_{y_1}}] e^{-i\alpha L_z}. \tag{10.222}$$

This may take a while to convince oneself. We recommend the reader first to plot all the axes in Eqs. (10.207)–(10.209) and then to operate on a radial vector drawn from the origin with (10.221). Finally, trace the orbit of the tip separately for each rotation while preserving the order of rotations. The operator inside the square brackets is the identity operator; thus,

$$\mathbf{R} = e^{-i\beta L_{y_1}} e^{-i\gamma L_{z_1}} e^{-i\alpha L_z}. \tag{10.223}$$

We now note the transformation

$$e^{-i\beta L_{y_1}} = e^{-i\alpha L_z} e^{-i\beta L_y} e^{i\alpha L_z} \tag{10.224}$$

to write

$$\mathbf{R} = e^{-i\alpha L_z} e^{-i\beta L_y} e^{i\alpha L_z} e^{-i\gamma L_{z_1}} e^{-i\alpha L_z}. \tag{10.225}$$

Since $z_1 = z$, this becomes

$$\mathbf{R} = e^{-i\alpha L_z} e^{-i\beta L_y} [e^{i\alpha L_z} e^{-i\alpha L_z}] e^{-i\gamma L_z}. \tag{10.226}$$

Again, the operator inside the square brackets is the identity operator, thus, giving **R** entirely in terms of the original coordinate system (x, y, z) as

$$\boxed{\mathbf{R} = e^{-i\alpha L_z} e^{-i\beta L_y} e^{-i\gamma L_z}.} \tag{10.227}$$

We can now find the effect of $\mathbf{R}(\alpha, \beta, \gamma)$ on $\Psi(x, y, z)$ as

$$\mathbf{R}(\alpha, \beta, \gamma)\Psi(x, y, z) = \Psi(x', y', z'), \tag{10.228}$$

$$e^{-i\alpha L_z} e^{-i\beta L_y} e^{-i\gamma L_z} \Psi(x, y, z) = \Psi(x', y', z'). \tag{10.229}$$

In spherical polar coordinates this becomes

$$\mathbf{R}(\alpha, \beta, \gamma)\Psi(r, \theta, \phi) = \Psi(r, \theta,' \phi'). \tag{10.230}$$

Expressing the components of the angular momentum operator in spherical polar coordinates (Figure 10.6):

$$x + iy = r \sin\theta e^{\pm i\phi}, \tag{10.231}$$

$$z = r\cos\theta, \tag{10.232}$$

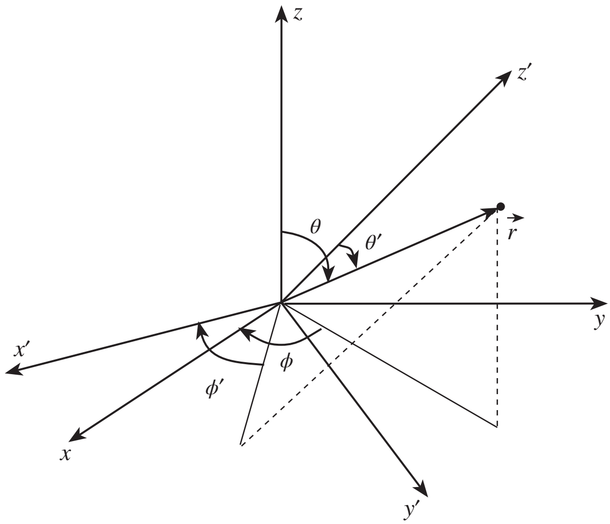


Figure 10.6 (x, y, z) and the (x', y', z') coordinates.

we obtain (we set $\hbar = 1$)

$$L_x = \left(i \cot\theta \cos\phi \frac{\partial}{\partial\phi} + i \sin\phi \frac{\partial}{\partial\theta} \right), \tag{10.233}$$

$$L_y = \left(i \cot\theta \sin\phi \frac{\partial}{\partial\phi} - i \cos\phi \frac{\partial}{\partial\theta} \right), \tag{10.234}$$

$$L_z = -i \frac{\partial}{\partial\phi}. \tag{10.235}$$

Using these we construct the operators

$$L_\pm = L_x \pm iL_y, \tag{10.236}$$

$$L^2 = L_x^2 + L_y^2 + L_z^2 \tag{10.237}$$

as

$$L_\pm = e^{\pm i\phi} \left(\pm \frac{\partial}{\partial\theta} + i \cot\theta \frac{\partial}{\partial\phi} \right), \tag{10.238}$$

$$L^2 = -\left[\frac{1}{\sin\theta} \left(\frac{\partial}{\partial\theta} \sin\theta \frac{\partial}{\partial\theta} \right) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} \right]. \tag{10.239}$$

Using Eqs. (10.233)–(10.235), we can now write Eq. (10.229) as

$$\boxed{[e^{-\alpha\partial/\partial\phi} e^{-\beta(\cos\phi\partial/\partial\theta - \sin\phi\cot\theta\partial/\partial\phi)} e^{-\gamma\partial/\partial\phi}]\Psi(r, \theta, \phi) = \Psi(r, \theta,' \phi'),} \tag{10.240}$$

which is now ready for applications to spherical harmonics $Y_{lm}(\theta, \phi)$.

10.8.6 Eigenvalue Equations for $L_z, L_\pm$, and L^2

In Chapter 8, we have established the following eigenvalue equations [Eqs. (8.191 and 8.192) and (8.209–8.211)]:

$$L_z Y_{lm}(\theta,\phi) = mY_{lm}(\theta,\phi), \tag{10.241}$$

$$L_- Y_{lm}(\theta,\phi) = \sqrt{(l+m)(l-m+1)}Y_{l,m-1}(\theta,\phi), \tag{10.242}$$

$$L_+ Y_{lm}(\theta,\phi) = \sqrt{(l-m)(l+m+1)}Y_{l,m+1}(\theta,\phi), \tag{10.243}$$

$$L^2 Y_{lm}(\theta,\phi) = l(l+1)Y_{lm}(\theta,\phi). \tag{10.244}$$

Using these and the definition $L_\pm = L_x \pm iL_y$ we can also write

$$\begin{aligned} L_x Y_{lm}(\theta,\phi) = {} & \frac{1}{2}\sqrt{(l-m)(l+m+1)}Y_{l,m+1}(\theta,\phi) \\ & + \frac{1}{2}\sqrt{(l+m)(l-m+1)}Y_{l,m-1}(\theta,\phi), \end{aligned} \tag{10.245}$$

$$\begin{aligned} L_y Y_{lm}(\theta,\phi) = {} & -\frac{i}{2}\sqrt{(l-m)(l+m+1)}Y_{l,m+1}(\theta,\phi) \\ & + \frac{i}{2}\sqrt{(l+m)(l-m+1)}Y_{l,m-1}(\theta,\phi). \end{aligned} \tag{10.246}$$

10.8.7 Fourier Expansion in Spherical Harmonics

We can expand a sufficiently smooth function, $F(\theta,\phi)$, in terms of spherical harmonics, which forms a complete and an orthonormal set as

$$F(\theta,\phi) = \sum_{l'=0}^{\infty}\sum_{m'=-l'}^{m'=l'} C_{l'm'}Y_{l'm'}(\theta,\phi), \tag{10.247}$$

where the expansion coefficients are given as

$$C_{l'm'} = \iint d\Omega Y^*_{l'm'}(\theta,\phi)F(\theta,\phi). \tag{10.248}$$

Spherical harmonics satisfy the orthogonality relation

$$\iint d\Omega Y^*_{l'm'}(\theta,\phi)Y_{lm}(\theta,\phi) = \delta_{ll'}\delta_{mm'} \tag{10.249}$$

and the completeness relation

$$\sum_{l=0}^{\infty}\sum_{m=-l}^{m=l} Y^*_{lm}(\theta',\phi')Y_{lm}(\theta,\phi) = \delta(\cos\theta - \cos\theta')\delta(\phi-\phi'), \tag{10.250}$$

where $d\Omega = \sin\theta\, d\theta\, d\phi$. In the study of angular momentum in quantum physics, we frequently need expansions of expressions like

$$\boxed{F_{lm}(\theta,\phi) = f(\theta,\phi)Y_{lm}(\theta,\phi)} \tag{10.251}$$

and

$$\boxed{G_{lm}(\theta,\phi) = O\left(\frac{\partial}{\partial\theta}, \frac{\partial}{\partial\phi}, \theta, \phi\right) Y_{lm}(\theta,\phi),} \tag{10.252}$$

where $O\left(\frac{\partial}{\partial\theta}, \frac{\partial}{\partial\phi}, \theta, \phi\right)$ is some differential operator.

For $F_{lm}(\theta,\phi)$ we can write

$$F_{lm}(\theta,\phi) = f(\theta,\phi)Y_{lm}(\theta,\phi) = \sum_{l'=0}^{\infty}\sum_{m'=-l'}^{m'=l'} C_{l'm'}Y_{l'm'}(\theta,\phi), \tag{10.253}$$

where the expansion coefficients are given as

$$C_{l'm'} = \iint d\Omega \;\; Y^*_{l'm'}(\theta,\phi)f(\theta,\phi)Y_{lm}(\theta,\phi), \tag{10.254}$$

which we rewrite as

$$\boxed{C_{l'm',lm} = \iint d\Omega \;\; Y^*_{l'm'}(\theta,\phi)f(\theta,\phi)Y_{lm}(\theta,\phi).} \tag{10.255}$$

For $G_{lm}(\theta,\phi)$ we can write

$$G_{lm}(\theta,\phi) = \sum_{l'=0}^{\infty}\sum_{m'=-l'}^{m'=l'} C_{l'm'}Y_{l'm'}(\theta,\phi), \tag{10.256}$$

where

$$C_{l'm'} = \iint d\Omega \;\; Y^*_{l'm'}(\theta,\phi)\left[O\left(\frac{\partial}{\partial\theta}, \frac{\partial}{\partial\phi}, \theta, \phi\right) Y_{lm}(\theta,\phi)\right] \tag{10.257}$$

$$= C_{l'm',lm}. \tag{10.258}$$

Based on these we can also write the expansion

$$f_1(\theta,\phi)[f_2(\theta,\phi)Y_{lm}(\theta,\phi)] = f_1(\theta,\phi)\left[\sum_{l'=0}^{\infty}\sum_{m'=-l'}^{m'=l'} C^{(2)}_{l'm',lm}Y_{l'm'}(\theta,\phi)\right] \tag{10.259}$$

$$= \sum_{l''=0}^{\infty}\sum_{m''=-l''}^{m''=l''}\sum_{l'=0}^{\infty}\sum_{m'=-l'}^{m'=l'} Y^*_{l''m''}(\theta,\phi)C^{(1)}_{l''m'',l'm'}C^{(2)}_{l'm',lm} \tag{10.260}$$

$$= \sum_{l''=0}^{\infty}\sum_{m''=-l''}^{m''=l''} C^{(1,2)}_{l''m'',lm}Y_{l''m''}(\theta,\phi), \tag{10.261}$$

where

$$\boxed{C^{(1,2)}_{l''m'',lm} = \sum_{l'=0}^{\infty}\sum_{m'=-l'}^{m'=l'} C^{(1)}_{l''m'',l'm'}C^{(2)}_{l'm',lm}.} \tag{10.262}$$

10.8.8 Matrix Elements of L_x, L_y, and L_z

Using the result [Eq. (10.258)], we can now evaluate $L_y Y_{(l=1)m}$ as

$$L_y Y_{(l=1)m} = \sum_{m'=-1}^{m'=1} C_{l'm',(l=1)m} Y_{l'm'}(\theta, \phi). \tag{10.263}$$

This gives the following matrix elements for the angular momentum operator $\mathbf{L}_y(l = 1)$:

$$(Y_{l'=1m'}, L_y Y_{l=1m}) = C_{l'=1m',l=1m} \tag{10.264}$$

$$= \iint d\Omega \ Y^*_{l'=1m'}(\theta, \phi) L_y Y_{l=1m}(\theta, \phi), \tag{10.265}$$

where we have dropped the brackets in the l indices. We now use Eq. (10.246):

$$L_y Y_{lm}(\theta, \phi) = -\frac{i}{2}\sqrt{(l-m)(l+m+1)}\, Y_{l,m+1}(\theta, \phi) + \frac{i}{2}\sqrt{(l+m)(l-m+1)}\, Y_{l,m-1}(\theta, \phi), \tag{10.266}$$

and the orthogonality relation [Eq. (10.249)] to write

$$[\mathbf{L}_y(l = 1)]_{mm'} = C_{l'=1m',l=1m} \tag{10.267}$$

$$= \begin{bmatrix} 0 & -\frac{i}{\sqrt{2}} & 0 \\ \frac{i}{\sqrt{2}} & 0 & -\frac{i}{\sqrt{2}} \\ 0 & \frac{i}{\sqrt{2}} & 0 \end{bmatrix}. \tag{10.268}$$

Operating on Eq. (10.263) with L_y and using Eq. (10.267), we can write

$$L_y^2 Y_{l=1m} = \sum_{m'=-1}^{m'=1} L_y Y_{l'=1m'}(\theta, \phi)[\mathbf{L}_y(l = 1)]_{m'm}, \tag{10.269}$$

to obtain the matrix elements of L_y^2 as

$$[\mathbf{L}_y^2(l = 1)]_{mm'} = \begin{bmatrix} 0 & -\frac{i}{\sqrt{2}} & 0 \\ \frac{i}{\sqrt{2}} & 0 & -\frac{i}{\sqrt{2}} \\ 0 & \frac{i}{\sqrt{2}} & 0 \end{bmatrix} \begin{bmatrix} 0 & -\frac{i}{\sqrt{2}} & 0 \\ \frac{i}{\sqrt{2}} & 0 & -\frac{i}{\sqrt{2}} \\ 0 & \frac{i}{\sqrt{2}} & 0 \end{bmatrix} \tag{10.270}$$

$$= \begin{bmatrix} 1/2 & 0 & -1/2 \\ 0 & 1 & 0 \\ -1/2 & 0 & 1/2 \end{bmatrix}. \tag{10.271}$$

Similarly, we find the other powers as

$$[\mathbf{L}_y(l = 1)]_{mm'} = [\mathbf{L}_y^3(l = 1)]_{mm'} = [\mathbf{L}_y^5(l = 1)]_{mm'} \tag{10.272}$$

$$\vdots$$

and

$$\begin{aligned}[\mathbf{L}_y^2(l=1)]_{mm'} &= [\mathbf{L}_y^4(l=1)]_{mm'} \\ &= [\mathbf{L}_y^6(l=1)]_{mm'} \\ &\vdots \end{aligned} \tag{10.273}$$

Using Eqs. (10.241)–(10.244) and the orthogonality relation [Eq. (10.249)], we can write the following matrix elements:

$$\mathbf{L}_x = (Y_{l'm'}, L_x Y_{lm}) \tag{10.274}$$

$$\begin{aligned} &= \frac{1}{2}\sqrt{(l-m)(l+m+1)}\delta_{ll'}\delta_{m'(m+1)} \\ &\quad + \frac{1}{2}\sqrt{(l+m)(l-m+1)}\delta_{ll'}\delta_{m'(m-1)}, \end{aligned} \tag{10.275}$$

$$\mathbf{L}_y = (Y_{l'm'}, L_y Y_{lm}) \tag{10.276}$$

$$\begin{aligned} &= -\frac{i}{2}\sqrt{(l-m)(l+m+1)}\delta_{ll'}\delta_{m'(m+1)} \\ &\quad + \frac{i}{2}\sqrt{(l+m)(l-m+1)}\delta_{ll'}\delta_{m'(m-1)}, \end{aligned} \tag{10.277}$$

$$\mathbf{L}_z = (Y_{l'm'}, L_z Y_{lm}) = m\delta_{ll'}\delta_{mm'}, \tag{10.278}$$

$$\mathbf{L}^2 = (Y_{l'm'}, L^2 Y_{lm}) = l(l+1)\delta_{ll'}\delta_{mm'}. \tag{10.279}$$

10.8.9 Rotation Matrices of the Spherical Harmonics

Since the effect of the **rotation operator**, $\mathbf{R}(\alpha,\beta,\gamma)$, on the spherical harmonics is to rotate them from (θ,ϕ) to new values, $(\theta,'\phi')$, we write

$$\mathbf{R}(\alpha,\beta,\gamma)Y_{lm}(\theta,\phi) = e^{-i\alpha L_z}e^{-i\beta L_y}e^{-i\gamma L_z}Y_{lm}(\theta,\phi) = Y_{lm}(\theta,'\phi'). \tag{10.280}$$

In spherical polar coordinates this becomes

$$e^{-\alpha\frac{\partial}{\partial\phi}}e^{-\beta\left(\cos\phi\frac{\partial}{\partial\theta}-\sin\phi\cot\theta\frac{\partial}{\partial\phi}\right)}e^{-\gamma\frac{\partial}{\partial\phi}}Y_{lm}(\theta,\phi) = Y_{lm}(\theta,'\phi'). \tag{10.281}$$

We now express $Y_{lm}(\theta,'\phi')$ in terms of the original $Y_{lm}(\theta,\phi)$ as

$$Y_{lm}(\theta,'\phi') = \sum_{l'm'} Y_{l'm'}(\theta,\phi)C_{l'm',lm}, \tag{10.282}$$

$$C_{l'm',lm} = \iint d\Omega\ Y^*_{l'm'}(\theta,\phi)\mathbf{R}(\alpha,\beta,\gamma)Y_{lm}(\theta,\phi). \tag{10.283}$$

Since the spherical harmonics are defined as

$$Y_{lm}(\theta,\phi) = \frac{\sin^m\theta}{\sqrt{2\pi}}\frac{d^m}{d(\cos\theta)^m}[P_{lm}(\cos\theta)]e^{im\phi}, \tag{10.284}$$

R does not change their l value [Eqs. (10.274)–(10.278)]. Hence, only the coefficients with $l = l'$ are nonzero in Eq. (10.283), thus, giving

$$C_{lm',lm} = \iint d\Omega Y^*_{lm'}(\theta,\phi)\mathbf{R}(\alpha,\beta,\gamma)Y_{lm}(\theta,\phi) = D^l_{m'm}(\alpha,\beta,\gamma), \tag{10.285}$$

thus,

$$\boxed{Y_{lm}(\theta,'\phi') = \sum_{m'=-l}^{m'=l} Y_{lm'}(\theta,\phi) D^{l}_{m'm}(\alpha,\beta,\gamma).} \tag{10.286}$$

$D^{l}_{m'm}(\alpha,\beta,\gamma)$ is called the **rotation matrix** of the **spherical harmonics**.

Using the definition [Eq. (10.227)] of $\mathbf{R}(\alpha,\beta,\gamma)$ we can construct the rotation matrix as

$$D^{l}_{m'm}(\alpha,\beta,\gamma) = \iint d\Omega Y^{*}_{lm'}(\theta,\phi) e^{-i\alpha L_z} e^{-i\beta L_y} [e^{-i\gamma L_z} Y_{lm}(\theta,\phi)] \tag{10.287}$$

$$= \iint d\Omega Y^{*}_{lm'}(\theta,\phi) e^{-i\alpha L_z} e^{-i\beta L_y} \left[e^{-\gamma \frac{\partial}{\partial\phi}} e^{im\phi} (\text{function of } \theta) \right] \tag{10.288}$$

$$= \iint d\Omega Y^{*}_{lm'}(\theta,\phi) e^{-i\alpha L_z} e^{-i\beta L_y} \left[\sum_{n=0}^{\infty} \frac{(-\gamma)^n}{n!} (im)^n Y_{lm}(\theta,\phi) \right] \tag{10.289}$$

$$= \iint d\Omega Y^{*}_{lm'}(\theta,\phi) e^{-i\alpha L_z} e^{-i\beta L_y} [e^{-i\gamma m} Y_{lm}(\theta,\phi)] \tag{10.290}$$

$$= \iint d\Omega e[^{-i\alpha L_z} Y_{lm'}(\theta,\phi)]^{*} e^{-i\beta L_y} [e^{-i\gamma m} Y_{lm}(\theta,\phi)] \tag{10.291}$$

$$= \iint d\Omega [e^{i\alpha L_z} Y^{*}_{lm'}(\theta,\phi)] e^{-i\beta L_y} [e^{-i\gamma m} Y_{lm}(\theta,\phi)], \tag{10.292}$$

$$\boxed{D^{l}_{m'm}(\alpha,\beta,\gamma) = e^{-i\alpha m'} \left[\iint d\Omega Y^{*}_{lm'}(\theta,\phi) \;\; e^{-i\beta L_y} Y_{lm}(\theta,\phi) \right] e^{-i\gamma m}.} \tag{10.293}$$

We have used the fact that L_z is a Hermitian operator, that is,

$$\int \Psi_1^{*} L_z \Psi_2 d\Omega = \int (L_z \Psi_1)^{*} \Psi_2 d\Omega. \tag{10.294}$$

Defining the **reduced rotation matrix** $d^{l}_{m'm}(\beta)$:

$$\boxed{d^{l}_{m'm}(\beta) = \iint d\Omega Y^{*}_{lm'}(\theta,\phi) \;\; e^{-i\beta L_y} Y_{lm}(\theta,\phi),} \tag{10.295}$$

we finally obtain

$$\boxed{D^{l}_{m'm}(\alpha,\beta,\gamma) = e^{-i\alpha m'} d^{l}_{m'm}(\beta) e^{-i\gamma m}.} \tag{10.296}$$

10.8.10 Evaluation of the $d^l_{m'm}(\beta)$ Matrices

For the low values of l it is relatively easy to evaluate $d^l_{m'm}(\beta)$. For example, for $l = 0$, $d^0_{m'm}(\beta) = 1$, which is the trivial 1×1 matrix.

For $l = 1$, we can write Eq. (10.295) as

$$d^1_{m'm}(\beta) = \iint d\Omega Y^*_{1m'}(\theta,\phi) \begin{pmatrix} 1+ \\ -i\beta L_y + i\beta^3 L_y^3/3! + \cdots \\ -\beta^2 L_y^2/2! + \beta^4 L_y^4/4! + \cdots \end{pmatrix} Y_{1m}(\theta,\phi). \tag{10.297}$$

Using the matrix elements of $(L_y)^n$ obtained in Section 10.8.8, we write this as

$$d^1_{m'm}(\beta) = \delta_{mm'} - i(L_y)_{mm'} \sin\beta + (L_y^2)_{mm'}(\cos\beta - 1) \tag{10.298}$$

$$= \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} - i \sin\beta \begin{bmatrix} 0 & -\frac{i}{\sqrt{2}} & 0 \\ \frac{i}{\sqrt{2}} & 0 & -\frac{i}{\sqrt{2}} \\ 0 & \frac{i}{\sqrt{2}} & 0 \end{bmatrix}$$

$$+ (\cos\beta - 1) \begin{bmatrix} 1/2 & 0 & -1/2 \\ 0 & 1 & 0 \\ -1/2 & 0 & 1/2 \end{bmatrix}. \tag{10.299}$$

Finally adding these we find

$$d^1_{m'm}(\beta) = \begin{matrix} & m=1 & m=0 & m=-1 \\ m'=1 & \frac{1}{2}(1+\cos\beta) & -\frac{\sin\beta}{\sqrt{2}} & \frac{1}{2}(1-\cos\beta) \\ m'=0 & \frac{\sin\beta}{\sqrt{2}} & \cos\beta & -\frac{\sin\beta}{\sqrt{2}} \\ m'=-1 & \frac{1}{2}(1-\cos\beta) & \frac{\sin\beta}{\sqrt{2}} & \frac{1}{2}(1+\cos\beta) \end{matrix}. \tag{10.300}$$

10.8.11 Inverse of the $d^l_{m'm}(\beta)$ Matrices

To find the inverse matrices we invert

$$Y_{lm}(\theta',\phi') = \mathbf{R}(\alpha,\beta,\gamma) Y_{lm}(\theta,\phi) \tag{10.301}$$

to write

$$Y_{lm}(\theta,\phi) = \mathbf{R}^{-1}(\alpha,\beta,\gamma) Y_{lm}(\theta',\phi') = \mathbf{R}(-\gamma,-\beta,-\alpha) Y_{lm}(\theta',\phi'). \tag{10.302}$$

Note that we have reversed the sequence of rotations because

$$\mathbf{R}^{-1}(\alpha,\beta,\gamma) = [\mathbf{R}(\alpha)\mathbf{R}(\beta)\mathbf{R}(\gamma)]^{-1} = \mathbf{R}(-\gamma)\mathbf{R}(-\beta)\mathbf{R}(-\alpha). \tag{10.303}$$

We can now write $Y_{lm}(\theta,\phi)$ in terms of $Y_{lm}(\theta',\phi')$ as

$$Y_{lm}(\theta,\phi) = \sum_{m''} Y_{lm''}(\theta',\phi') \left\{ \iint d\Omega Y^*_{lm''}[e^{i\gamma L_z} e^{i\beta L_y} e^{i\alpha L_z}] Y_{lm} \right\} \tag{10.304}$$

$$= \sum_{m''} Y_{lm''}(\theta',\phi') \iint d\Omega [Y^*_{lm''} e^{i\gamma L_z}] e^{i\beta L_y} [e^{i\alpha L_z} Y_{lm}]. \tag{10.305}$$

Using the fact that L_z is Hermitian, this can be written as

$$Y_{lm}(\theta,\phi) = \sum_{m''} Y_{lm''}(\theta',\phi') \iint d\Omega [e^{i\gamma L_z} Y_{lm''}]^* e^{i\beta L_y} Y_{lm} e^{i\alpha m}. \tag{10.306}$$

This leads to

$$Y_{lm}(\theta,\phi) = \sum_{m''} Y_{lm''}(\theta',\phi') e^{i\gamma m''} \left[\iint d\Omega Y^*_{lm''} e^{i\beta L_y} Y_{lm} \right] e^{i\alpha m} \tag{10.307}$$

$$= \sum_{m''} Y_{lm''}(\theta',\phi') e^{i\gamma m''} \left[\iint d\Omega Y_{lm} e^{-i\beta L_y} Y^*_{lm''} \right] e^{i\alpha m} \tag{10.308}$$

$$= \sum_{m''} Y_{lm''}(\theta',\phi') e^{i\gamma m''} [d^l_{mm''}(\beta)]^* e^{i\alpha m} \tag{10.309}$$

$$= \sum_{m''} Y_{lm''}(\theta',\phi') [e^{i\alpha m} [d^l_{mm''}(\beta)]^* e^{i\gamma m''}], \tag{10.310}$$

thus,

$$\boxed{Y_{lm}(\theta,\phi) = \sum\nolimits_{m''} Y_{lm''}(\theta',\phi') \quad [D^l_{mm''}(\alpha,\beta,\gamma)]^*,} \tag{10.311}$$

where we have used the fact that L_y is Hermitian and $L^*_y = -L_y$. This result can also be written as

$$\boxed{Y_{lm}(\theta,\phi) = \sum_{m''} Y_{lm''}(\theta',\phi') \quad D^l_{m''m}(-\gamma,-\beta,-\alpha),} \tag{10.312}$$

which implies

$$\boxed{D^l_{m''m}(\mathbf{R}^{-1}) = [D^l_{m''m}(\mathbf{R})]^{-1} = [D^l_{mm''}(\mathbf{R})]^*.} \tag{10.313}$$

10.8.12 Differential Equation for $d^l_{m'm}(\beta)$

From the definition of the Euler angles (Section 10.8.4) it is clear that the rotations (α,β,γ) are all performed about different sets of axes. Only the first rotation is about the z-axis of our original coordinates, that is,

$$-i\frac{\partial}{\partial\alpha} = L_z, \;\; \hbar = 1. \tag{10.314}$$

Similarly, we can write the components of the angular momentum vector about the other intermediate axes, that is, y_1 and the z_2-axis, in terms of the components of the angular momentum about the x-, y-, and z-axes as:

$$L_{y_1} = -i\frac{\partial}{\partial\beta} = -\sin\alpha L_x + \cos\alpha L_y \tag{10.315}$$

and

$$L_{z_2} = -i\frac{\partial}{\partial\gamma} = \sin\beta\cos\alpha L_x + \sin\beta\sin\alpha L_y + \cos\beta L_z. \tag{10.316}$$

Inverting these we obtain

$$L_x = -i\left[-\sin\alpha\frac{\partial}{\partial\beta} + \frac{\cos\alpha}{\sin\beta}\frac{\partial}{\partial\gamma} - \cos\alpha\cot\beta\frac{\partial}{\partial\alpha}\right], \tag{10.317}$$

$$L_y = -i\left[\cos\alpha\frac{\partial}{\partial\beta} + \frac{\sin\alpha}{\sin\beta}\frac{\partial}{\partial\gamma} - \sin\alpha\cot\beta\frac{\partial}{\partial\alpha}\right], \tag{10.318}$$

$$L_z = -i\frac{\partial}{\partial\alpha}. \tag{10.319}$$

We now construct L^2 as

$$L^2 = L_x^2 + L_y^2 + L_z^2 \tag{10.320}$$

$$= -\left[\frac{\partial^2}{\partial\beta^2} + \cot\beta\frac{\partial}{\partial\beta} + \frac{1}{\sin^2\beta}\left(\frac{\partial^2}{\partial\alpha^2} + \frac{\partial^2}{\partial\gamma^2} - 2\cos\beta\frac{\partial^2}{\partial\alpha\partial\gamma}\right)\right]. \tag{10.321}$$

We could use the L^2 operator either in terms of (α, β, γ) as

$$L^2\left(\frac{\partial}{\partial\alpha}, \frac{\partial}{\partial\beta}, \frac{\partial}{\partial\gamma}, \alpha, \beta, \gamma\right) \tag{10.322}$$

and act on $D^l_{m'm}(\alpha, \beta, \gamma)$, or in terms of (θ, ϕ) as

$$L^2\left(\frac{\partial}{\partial\theta}, \frac{\partial}{\partial\phi}, \theta, \phi\right) \tag{10.323}$$

and act on $Y_{lm}(\theta, \phi)$. We first write (we suppress derivatives in L^2)

$$L^2(\theta, \phi)Y_{lm}(\theta', \phi') = L^2(\alpha, \beta, \gamma)Y_{lm}(\theta', \phi') \tag{10.324}$$

and use Eq. (10.286) and

$$L^2(\theta, \phi)Y_{lm}(\theta, \phi) = l(l+1)Y_{lm}(\theta, \phi), \tag{10.325}$$

to write

$$\sum_{m'=-l}^{m'=l} Y_{lm'}(\theta, \phi)[l(l+1)D^l_{m'm}(\alpha, \beta, \gamma)] = \sum_{m'=-l}^{m'=l} Y_{lm'}(\theta, \phi)[L^2(\alpha, \beta, \gamma)D^l_{m'm}(\alpha, \beta, \gamma)]. \tag{10.326}$$

Since $Y_{lm'}(\theta,\phi)$ are linearly independent, this gives the differential equation that $D^l_{m'm}(\alpha,\beta,\gamma)$ satisfies as:

$$\boxed{\left[L^2\left(\frac{\partial}{\partial\alpha},\frac{\partial}{\partial\beta},\frac{\partial}{\partial\gamma},\alpha,\beta,\gamma\right)\right]D^l_{m'm}(\alpha,\beta,\gamma)=l(l+1)D^l_{m'm}(\alpha,\beta,\gamma).} \tag{10.327}$$

Using Eq. (10.321) for $L^2\left(\frac{\partial}{\partial\alpha},\frac{\partial}{\partial\beta},\frac{\partial}{\partial\gamma},\alpha,\beta,\gamma\right)$ and the derivatives

$$\frac{\partial^2}{\partial\alpha^2}D^l_{m'm}=-m'^2D^l_{m'm}, \tag{10.328}$$

$$\frac{\partial^2}{\partial\gamma^2}D^l_{m'm}=-m^2D^l_{m'm}, \tag{10.329}$$

$$\frac{\partial^2}{\partial\alpha\partial\gamma}D^l_{m'm}=-m'mD^l_{m'm}, \tag{10.330}$$

which follow from Eq. (10.296), we obtain the differential equation for $d^l_{m'm}(\beta)$ as

$$\boxed{\left\{\frac{d^2}{d\beta^2}+\cot\beta\frac{d}{d\beta}+\left[l(l+1)-\left(\frac{m^2+m'^2-2mm'\cos\beta}{\sin^2\beta}\right)\right]\right\}d^l_{m'm}(\beta)=0.} \tag{10.331}$$

Note that for

$$m'=0 \text{ or } m=0, \tag{10.332}$$

this reduces to the associated Legendre equation, which has the following solutions:

$$D^l_{0m}\propto Y^*_{lm}(\beta,\gamma), \tag{10.333}$$

$$D^l_{m'0}\propto Y^*_{lm'}(\beta,\alpha). \tag{10.334}$$

Also note that some books call $D^l_{mm'}(\mathbf{R})$ what we call $[D^l_{mm'}(\mathbf{R})]^{-1}$. Using the transformation

$$d^l_{m'm}(\beta)=\frac{y(\lambda_l,m',m,\beta)}{\sqrt{\sin\beta}}, \tag{10.335}$$

we can put Eq. (10.331) in the **second canonical form** of Chapter 8 as

$$\frac{d^2y(\lambda_l,m',m,\beta)}{d\beta^2} \tag{10.336}$$

$$+\left[\left(l(l+1)+\frac{1}{4}\right)-\left(\frac{m^2+m'^2-2mm'\cos\beta-\frac{1}{4}}{\sin^2\beta}\right)\right]y(\lambda_l,m',m,\beta)=0.$$

10.8.13 Addition Theorem for Spherical Harmonics

Spherical harmonics transform as [Eq. (10.286)]

$$Y_{lm}(\theta,'\phi') = \sum_{m'=-l}^{m'=l} Y_{lm'}(\theta,\phi) D^l_{m'm}(\alpha,\beta,\gamma), \tag{10.337}$$

with the inverse transformation given as

$$Y_{lm}(\theta,\phi) = \sum_{m'=-l}^{m'=l} D^{*l}_{mm'}(\alpha,\beta,\gamma) Y_{lm'}(\theta',\phi'), \tag{10.338}$$

where

$$D^l_{m'm}(\alpha,\beta,\gamma) = e^{-i\alpha m'} d^l_{m'm}(\beta) e^{-i\gamma m}. \tag{10.339}$$

We now prove an important theorem about spherical harmonics, which says that the sum

$$\sum_{m=-l}^{m=l} Y^*_{lm}(\theta_1,\phi_1) Y_{lm}(\theta_2,\phi_2) = I_l \tag{10.340}$$

is an invariant. This is the generalization of $\mathbf{r}_1 \cdot \mathbf{r}_2$ and the angles are defined as in Figure 10.7.

Before we prove this theorem, let us consider the special case $l = 1$, where

$$Y_{l=1,m=\pm1} = \mp\sqrt{\frac{3}{8\pi}} \sin\theta e^{\pm i\phi}, \tag{10.341}$$

$$Y_{l=1,m=0} = \sqrt{\frac{3}{4\pi}} \cos\theta. \tag{10.342}$$

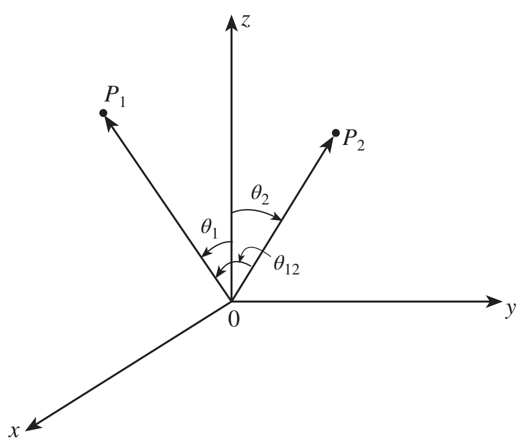


Figure 10.7 Definition of the angles in the addition theorem of the spherical harmonics.

Using Cartesian coordinates, we can write also these as

$$Y_{l=1,m=\pm1} = \mp\sqrt{\frac{3}{8\pi}}\frac{(x \pm iy)}{r}, \tag{10.343}$$

$$Y_{l=1,m=0} = \sqrt{\frac{3}{4\pi}}\frac{z}{r}. \tag{10.344}$$

We now evaluate I_1 as

$$I_1 = \frac{3}{4\pi}[\cos\theta_1\cos\theta_2 + \sin\theta_1\sin\theta_2\cos(\phi_1-\phi_2)] \tag{10.345}$$

$$= \frac{3}{4\pi}\cos\theta_{12} \tag{10.346}$$

$$= \frac{3}{4\pi}\frac{x_1x_2 + y_1y_2 + z_1z_2}{r_1r_2} = \frac{3}{4\pi}\frac{\mathbf{r}_1\cdot\mathbf{r}_2}{r_1r_2}. \tag{10.347}$$

To prove the invariance for a general l, we write

$$\sum_{m=-l}^{m=l} Y^*_{lm}(\theta'_1,\phi'_1)Y_{lm}(\theta'_2,\phi'_2)$$

$$= \sum_m \left[\sum_{m'm''} Y^*_{lm'}(\theta_1,\phi_1)Y_{lm''}(\theta_2,\phi_2)\right] D^{*l}_{m'm}(\alpha,\beta,\gamma)D^l_{m''m}(\alpha,\beta,\gamma) \tag{10.348}$$

$$= \left[\sum_{m'm''} Y^*_{lm'}(\theta_1,\phi_1)Y_{lm''}(\theta_2,\phi_2)\right]\sum_m D^{*l}_{m'm}(\alpha,\beta,\gamma)D^l_{m''m}(\alpha,\beta,\gamma). \tag{10.349}$$

Using Eqs. (10.311) and (10.312), we can write

$$D^l_{m''m}(\mathbf{R}^{-1}) = [D^l_{m''m}(\mathbf{R})]^{-1} = [D^l_{mm''}(\mathbf{R})]^*,$$

where $\mathbf{R}$ stands for $\mathbf{R}(\alpha,\beta,\gamma)$; hence

$$\sum_m D^{*l}_{m'm}(\alpha,\beta,\gamma)D^l_{m''m}(\alpha,\beta,\gamma) = \sum_m D^l_{m''m}(\mathbf{R})D^l_{mm'}(\mathbf{R}^{-1}) \tag{10.350}$$

$$= \sum_m D^l_{m''m}(\mathbf{R})[D^l_{mm'}(\mathbf{R})]^{-1} \tag{10.351}$$

$$= D^l_{m''m'}(\mathbf{R}\mathbf{R}^{-1}) \tag{10.352}$$

$$= \delta_{m''m'}. \tag{10.353}$$

We now use this in Eq. (10.349) to write

$$\sum_{m=-l}^{m=l} Y_{lm}^*(\theta_1', \phi_1') Y_{lm}(\theta_2', \phi_2') = \sum_{m'm''} Y_{lm'}^*(\theta_1, \phi_1) Y_{lm''}(\theta_2, \phi_2) \delta_{m''m'} \quad (10.354)$$

$$= \sum_{m} Y_{lm}^*(\theta_1, \phi_1) Y_{lm}(\theta_2, \phi_2) \quad (10.355)$$

$$= I_l, \quad (10.356)$$

thus, proving the theorem.

10.8.14 Determination of I_l in the Addition Theorem

Because I_l is an invariant, we can choose our axis and the location of the points, P_1 and P_2, conveniently (Figure 10.8). Thus, we can write

$$I_l = \sum_{m=-l}^{m=l} Y_{lm}^*(0, -) Y_{lm}(\theta_{12}, 0) \quad (10.357)$$

$$= Y_{l0}^*(0) Y_{l0}(\theta_{12}) \quad (10.358)$$

$$= \left(\sqrt{\frac{2l+1}{4\pi}} \right)^2 P_l(0) P_l(\cos\theta_{12}). \quad (10.359)$$

Using the value $P_l(0) = 1$, we complete the derivation of the addition theorem of the spherical harmonics as

$$\boxed{\sum_{m=-l}^{m=l} Y_{lm}^*(\theta_1, \phi_1) Y_{lm}(\theta_2, \phi_2) = \frac{2l+1}{4\pi} P_l(\cos\theta_{12}).} \quad (10.360)$$

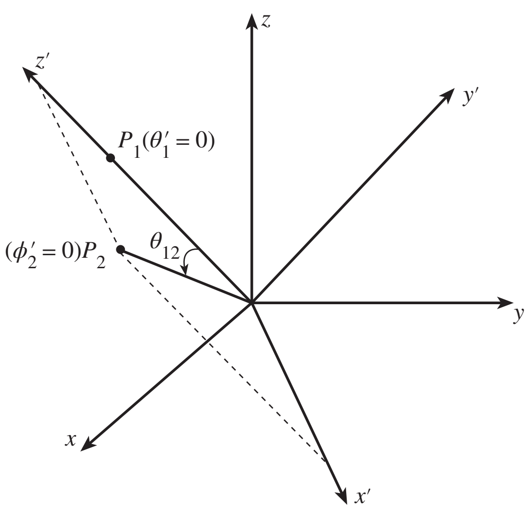
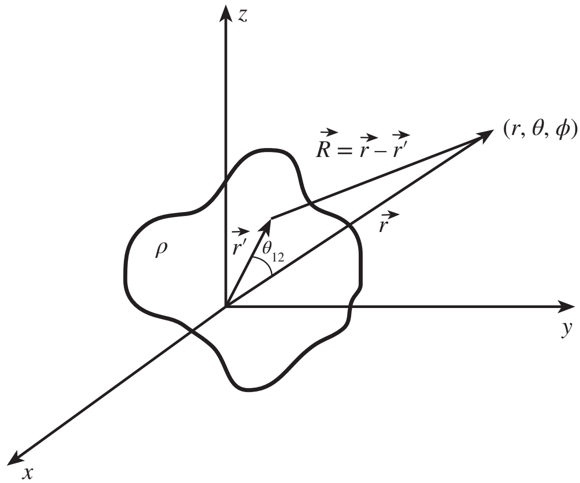


Figure 10.8 Evaluation of I_l.

Figure 10.9 Multipole expansion.



Example 10.1 ***Multipole expansion***
We now consider the electrostatic potential of an arbitrary charge distribution at (r, θ, ϕ) as shown in Figure 10.9. Given the charge density, $\rho(r', \theta', \phi')$, we can write the electrostatic potential, $\Phi((r, \theta, \phi)$, as

$$\Phi((r, \theta, \phi) = \iiint_{V''} \frac{\rho(r', \theta', \phi') r'^2 \sin\theta' dr' d\theta' d\phi'}{\sqrt{r'^2 + r^2 - 2rr' \cos\theta_{12}}}. \tag{10.361}$$

The integral is to be taken over the source variables (r', θ', ϕ'), while (r, θ, ϕ) denotes the field point. For a field point outside the source, we define a new variable, $t = r'/r$, to write

$$\Phi(r, \theta, \phi) = \iiint_{V'} \frac{\rho(r', \theta', \phi') r'^2 \sin\theta' dr' d\theta' d\phi'}{r\sqrt{1 + t^2 - 2t\cos\theta_{12}}}. \tag{10.362}$$

Using the generating function definition for the Legendre polynomials:

$$T(x, t) = \frac{1}{\sqrt{1 + t^2 - 2tx}} = \sum_{l=0}^{\infty} P_l(x) t^l, \quad |t| < 1, \tag{10.363}$$

Eq. (10.362) becomes

$$\Phi(r, \theta, \phi) = \sum_{l=0}^{\infty} \frac{1}{r^{l+1}} \iiint_{V'} \rho(r', \theta', \phi') r'^l P_l(\cos\theta_{12}) dv'. \tag{10.364}$$

Using the addition theorem [Eq. (10.360)], this can now be written as

$$\Phi(r, \theta, \phi) = \sum_{l,m} \frac{4\pi}{(2l + 1)} \frac{Y_{lm}(\theta, \phi)}{r^{l+1}} \left[\iiint_{V'} \rho(r', \theta', \phi') r'^l Y^*_{lm}(\theta', \phi') dv' \right], \tag{10.365}$$

where

$$\sum_{l,m} = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} . \tag{10.366}$$

The expression

$$q_{lm} = \iiint_{V'} \rho(r', \theta', \phi') r'^l Y_{lm}^*(\theta', \phi') dv' \tag{10.367}$$

is called the (lm)th multipole moment.

10.8.15 Connection of $D^l_{mm'}(\beta)$ with Spherical Harmonics

We are now going to prove two useful relations between the rotation matrix and the spherical harmonics:

$$\boxed{D^l_{m0}(\alpha, \beta, -) = \sqrt{\frac{4\pi}{(2l+1)}} Y_{lm}^*(\beta, \alpha)} \tag{10.368}$$

and

$$\boxed{D^l_{0m}(-, \beta, \gamma) = (-1)^m \sqrt{\frac{4\pi}{(2l+1)}} Y_{lm}^*(\beta, \gamma).} \tag{10.369}$$

We first establish the relation between $d^l_{m'm}(\beta)$ and the **Jacobi polynomials**. We have obtained the differential equation [Eq. (10.331)] that $d^l_{m'm}(\beta)$ satisfies as

$$\left\{ \frac{d^2}{d\beta^2} + \cot\beta \frac{d}{d\beta} + \left[l(l+1) - \frac{m^2 + m'^2 - 2mm' \cos\beta}{\sin^2\beta} \right] \right\} d^l_{m'm}(\beta) = 0. \tag{10.370}$$

Given the solution of the above equation:

$$d^l_{m'm}(\beta) = (-1)^{m'+m} \left[\frac{(l+m')!(l-m')!}{(l+m)!(l-m)!} \right]^{1/2} \sum_k \binom{l+m}{l-m'-k} \binom{l-m}{k} \times (-1)^{l-m'-k} \left(\cos\frac{\beta}{2} \right)^{2k+m'+m} \left(\sin\frac{\beta}{2} \right)^{2l-2k-m'-m}, \tag{10.371}$$

we can use the Jacobi polynomials:

$$P_n^{(a,b)}(x) = 2^{-n} \sum_{k=0}^{n} \binom{n+a}{k} \binom{n+b}{n-k} (x-1)^{n-k} (x+1)^k, \tag{10.372}$$

which satisfy the differential equation

$$(1-x^2)\frac{dy^2}{dx^2}+[b-a-(a+b+2)x]\frac{dy}{dx}+n(n+a+b+1)y(x)=0, \tag{10.373}$$

to express $d^l_{m'm}(\beta)$ as

$$d^l_{m'm}(\beta)=(-1)^{m'+m}\left[\frac{(l+m')!(l-m')!}{(l+m)!(l-m)!}\right]^{1/2}\left(\cos\frac{\beta}{2}\right)^{m'+m}\left(\sin\frac{\beta}{2}\right)^{m'-m} \times P^{(m'-m,m'+m)}_{l-m'}(\cos\beta). \tag{10.374}$$

Notes:

(i) The normalization constant of $d^l_{m'm}(\beta)$ can be evaluated via the integral

$$\int_{-1}^{1}(1-x)^a(1+x)^bP^{(a,b)}_n(x)P^{(a,b)}_m(x)dx = \frac{2^{a+b+1}}{2n+a+b+1}\frac{\Gamma(n+a+1)\Gamma(n+b+1)}{\Gamma(n+1)\Gamma(n+a+b+1)}\delta_{nm}. \tag{10.375}$$

Also note that the Jacobi polynomials are normalized so that

$$P^{(a,b)}_n(1)=\binom{n+a}{n}. \tag{10.376}$$

(ii) You can use Eq. (10.374) to check the matrix elements found in Problem 8 and in Eq. (10.300). You can use Mathematica® to obtain the needed Jacobi polynomials via the command "JacobiP[a,b,n,x]."

(iii) To see that $d^l_{m'm}(\beta)$ given in Eq. (10.374) is indeed a solution to Eq. (10.370), substitute

$$d^l_{m'm}(\beta)=C\left(\cos\frac{\beta}{2}\right)^{m'+m}\left(\sin\frac{\beta}{2}\right)^{m'-m}f(\cos\beta) \tag{10.377}$$

into Eq. (10.370), where C is an appropriate normalization constant, and then show that $f(\cos\beta)$ satisfies the Jacobi equation [Eq. (10.373)] with an appropriate choice of the parameters.

For the first relation [Eq.(10.368)], we need the value of $d^l_{m0}(\beta)$, which from Eq. (10.374) can be written as

$$d^l_{m0}(\beta)=(-1)^m\left[\frac{(l+m)!(l-m)!}{(l!)^2}\right]^{1/2}\frac{1}{2^m}(\sin^m\beta)P^{(m,m)}_{l-m}(x). \tag{10.378}$$

We now use the relation

$$P^{(m,m)}_{l-m}(x)=(-2)^m\frac{l!}{(l-m)!}(1-x^2)^{-m/2}P^{-m}_l(x), \tag{10.379}$$

to write

$$d^l_{m0}(\beta) = \left[\frac{(l+m)!}{(l-m)!}\right]^{1/2} P_l^{-m}(\cos\beta) \tag{10.380}$$

$$= (-1)^m \left[\frac{(l-m)!}{(l+m)!}\right]^{1/2} P_l^m(\cos\beta). \tag{10.381}$$

Using the definition [Eq. (10.296)]:

$$D^l_{m'm}(\alpha,\beta,\gamma) = e^{-i\alpha m'} d^l_{m'm}(\beta) e^{-i\gamma m}, \tag{10.382}$$

we write

$$D^l_{m0}(\alpha,\beta,\gamma) = e^{-i\alpha m} d^l_{m0}(\beta). \tag{10.383}$$

Since the spherical harmonics are defined as [Eq. (1.199)]

$$Y_l^m(\theta,\phi) = (-1)^m \sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}} e^{im\phi} P_l^m(\cos\theta), \tag{10.384}$$

Eqs. (10.383) and (10.381) yield the desired result in Eq. (10.368):

$$\boxed{D^l_{m0}(\alpha,\beta) = \sqrt{\frac{4\pi}{2l+1}} Y^*_{lm}(\beta,\alpha).} \tag{10.385}$$

For the second relation [Eq. (10.369)], we first show and then use the symmetry property:

$$d^l_{m'm}(-\beta) = d^l_{mm'}(\beta). \tag{10.386}$$

In Problem 9, the reader will get the chance to prove these relations via the addition theorem of spherical harmonics.

10.9 Irreducible Representations of *SU*(2)

From the physical point of view a very important part of the group theory is representing each element of the group with a linear transformation acting in a vector space. We now introduce the irreducible matrix representations of $SU(2)$. There is again the trivial one-dimensional representation $D^{(1)}$, where each group element is represented by the number one. Next, we have the two-dimensional representation $D^{(2)}$ provided by the matrices [Eq. (10.96)]

$$\mathbf{u} = \begin{bmatrix} A & B \\ -B^* & A^* \end{bmatrix}, \tag{10.387}$$

where $\det \mathbf{u} = |A|^2 + |B|^2 = 1$. These act on two-dimensional vectors in the complex plane, which we show as

$$\mathbf{w} = \begin{bmatrix} w_1 \\ w_2 \end{bmatrix}, \tag{10.388}$$

or

$$\mathbf{w} = w_\alpha, \quad \alpha = 1, 2. \tag{10.389}$$

For the higher-order representations we need to define tensors, such that each element of the group corresponds to transformations of the various components of a tensor into each other. Such a representation is called generated by tensors. In this regard, $D^{(1)}$ is generated by scalars, $D^{(2)}$ is generated by vectors, and $D^{(3)}$ is generated by symmetric second-rank tensors $w_{\alpha\beta}$. In general, $D^{(n)}$ is generated by completely symmetric tensors with $(n-1)$ indices, $w_{\alpha_1\alpha_2\ldots\alpha_{n-1}}$, as

$$\begin{bmatrix} D^{(1)} & 0 & 0 & . & 0 \\ 0 & D^{(2)} & 0 & .. & 0 \\ 0 & 0 & D^{(3)} & \ldots & 0 \\ . & .. & \ldots & \ddots & 0 \\ 0 & 0 & 0 & 0 & D^{(n)} \end{bmatrix}. \tag{10.390}$$

If $w_{\alpha_1\alpha_2\cdots\alpha_{n-1}}$ is not symmetric with respect to any of the two indices, then we can contract those two indices and obtain a symmetric tensor of rank two less than the original one; thus, $w_{\alpha_1\alpha_2} \ldots \alpha_{n-1}$ is not irreducible because it contains the smaller representation generated by the contracted tensor.

10.10 Relation of *SU*(2) and *R*(3)

We have seen that the general element, $\mathbf{u}$, of $SU(2)$ is given as Eq. (10.387). We now define a matrix operator in this space as

$$P = \begin{bmatrix} z & x - iy \\ x + iy & -z \end{bmatrix}, \tag{10.391}$$

where (x, y, z) are real quantities. However, we will interpret them as the coordinates of a point. Under the action of $\mathbf{u}$, P transforms as

$$P' = \mathbf{u}P\mathbf{u}^{-1}, \tag{10.392}$$

which is nothing but a similarity transformation. For unitary operators $\mathbf{u}$ satisfies

$$\mathbf{u}^{-1} = \mathbf{u}^\dagger = \widetilde{\mathbf{u}}^*. \tag{10.393}$$

Also note that P is **Hermitian**, $P^\dagger = P$, and traceless. Because of the Hermitian property, trace and the determinant of a matrix are invariant under similarity transformations, hence we can write

$$P' = \begin{bmatrix} z' & x' - iy' \\ x' + iy' & -z' \end{bmatrix}, \tag{10.394}$$

where (x', y', z') are again real and satisfy

$$-\det P' = (x'^2 + y'^2 + z'^2) \tag{10.395}$$

$$= (x^2 + y^2 + z^2) \tag{10.396}$$

$$= -\det P. \tag{10.397}$$

This is just the orthogonality condition, which requires that the magnitude of a vector, $r = (x, y, z)$, remain unchanged. In summary, for every element of $SU(2)$ we can associate an orthogonal transformation in three dimensions.

We have seen that the orientation of a system in three dimensions can be completely specified by the three Euler angles (ϕ, θ, ψ). A given orientation can be obtained by three successive rotations. We now find the corresponding operators in $SU(2)$. For convenience we first define

$$x_+ = x + iy, \tag{10.398}$$

$$x_- = x - iy. \tag{10.399}$$

This allows us to write the first transformation, which corresponds to rotation about the z-axis as

$$\begin{aligned} x'_+ &= e^{-i\phi} x_+, \\ x'_- &= e^{i\phi} x_-, \\ z' &= z. \end{aligned} \tag{10.400}$$

In $SU(2)$ this corresponds to the transformation

$$P' = \begin{bmatrix} z' & x'_- \\ x'_+ & -z' \end{bmatrix} \tag{10.401}$$

$$= \begin{bmatrix} A & B \\ -B^* & A^* \end{bmatrix} \begin{bmatrix} z & x_- \\ x_+ & -z \end{bmatrix} \begin{bmatrix} A^* & -B \\ B^* & A \end{bmatrix}. \tag{10.402}$$

On performing the multiplications we get

$$x'_+ = -2B^*A^*z - B^{*2}x_- + A^{*2}x_+, \tag{10.403}$$

$$x'_- = -2ABz + A^2x_- - B^2x_+, \tag{10.404}$$

$$z' = (|A|^2 - |B|^2)z + AB^*x_- + BA^*x_+. \tag{10.405}$$

Comparing this with Eq. (10.400) gives

$$B = B^* = 0, \tag{10.406}$$

$$A^2 = e^{i\phi}. \tag{10.407}$$

Thus,

$$\boxed{\mathbf{u}_\phi = \begin{bmatrix} e^{i\phi/2} & 0 \\ 0 & e^{-i\phi/2} \end{bmatrix}.} \tag{10.408}$$

Similarly, we obtain the other matrices as

$$\boxed{\mathbf{u}_\theta = \begin{bmatrix} \cos\theta/2 & i\sin\theta/2 \\ i\sin\theta/2 & \cos\theta/2 \end{bmatrix}} \tag{10.409}$$

and

$$\boxed{\mathbf{u}_\psi = \begin{bmatrix} e^{i\psi/2} & 0 \\ 0 & e^{-i\psi/2} \end{bmatrix}.} \tag{10.410}$$

For the complete sequence we can write

$$\mathbf{u} = \mathbf{u}_\psi \mathbf{u}_\theta \mathbf{u}_\phi \tag{10.411}$$

$$= \begin{bmatrix} e^{i\psi/2} & 0 \\ 0 & e^{-i\psi/2} \end{bmatrix} \begin{bmatrix} \cos\theta/2 & i\sin\theta/2 \\ i\sin\theta/2 & \cos\theta/2 \end{bmatrix} \begin{bmatrix} e^{i\phi/2} & 0 \\ 0 & e^{-i\phi/2} \end{bmatrix}, \tag{10.412}$$

which is

$$\boxed{\mathbf{u} = \begin{bmatrix} e^{i(\psi+\phi)/2}\cos\theta/2 & ie^{i(\psi-\phi)/2}\sin\theta/2 \\ ie^{-i(\psi-\phi)/2}\sin\theta/2 & e^{-i(\psi+\phi)/2}\cos\theta/2 \end{bmatrix}.} \tag{10.413}$$

In terms of the three Euler angles the four independent parameters of $\mathbf{u}$ [Eq. (10.99)] are now given as

$$A = a + id = e^{i(\psi+\phi)/2}\cos\theta/2, \tag{10.414}$$

$$B = c + ib = ie^{i(\psi-\phi)/2}\sin\theta/2. \tag{10.415}$$

The presence of half-angles in these matrices is interesting. If we examine $\mathbf{u}_\phi$, for $\phi = 0$ it becomes

$$\mathbf{u}_\phi(0) = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \tag{10.416}$$

which corresponds to the identity matrix in $R(3)$. However, for $\phi = 2\pi$, which also gives the identity matrix in $R(3)$, $\mathbf{u}_\phi$ corresponds to

$$\mathbf{u}_\phi(2\pi) = \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix} \tag{10.417}$$

in $SU(2)$. Hence, the correspondence (isomorphism) between $SU(2)$ and $R(3)$ is two-to-one. The matrices $(\mathbf{u}, -\mathbf{u})$ in $SU(2)$ correspond to a single matrix in $R(3)$. The complex two-dimensional vector space is called the **spinor space**.

It turns out that in quantum mechanics the wave function, at least parts of it, must be composed of spinors. The double-valued property and the half-angles are associated with the fact that spin is half-integer.

10.11 Group Spaces

10.11.1 Real Vector Space

We have seen that the elements of $R(3)$ act in a real vector space and transform vectors into other vectors. A real vector space, V, where $\vec{v}_1, \vec{v}_2, \vec{v}_3$ are any three elements of V, is defined as a collection of objects, that is, vectors, with the following properties:

1. Addition of vectors results in another vector:
$$\vec{v}_1 + \vec{v}_2 \in V. \tag{10.418}$$
2. Addition is commutative:
$$\vec{v}_1 + \vec{v}_2 = \vec{v}_2 + \vec{v}_1. \tag{10.419}$$
3. Addition is associative:
$$(\vec{v}_1 + \vec{v}_2) + \vec{v}_3 = \vec{v}_1 + (\vec{v}_2 + \vec{v}_3). \tag{10.420}$$
4. There exists a null vector, $\vec{0}$, such that for any $\vec{v} \in V$
$$\vec{v} + \vec{0} = \vec{v}. \tag{10.421}$$
5. For each $\vec{v} \in V$ there exists an inverse $(-\vec{v})$ such that
$$\vec{v} + (-\vec{v}) = 0. \tag{10.422}$$
6. Multiplication of a vector, $\vec{v}$, with the number 1 leaves it unchanged:
$$1\vec{v} = \vec{v}. \tag{10.423}$$
7. A vector multiplied with a scalar, c, is another vector:
$$c\vec{v} \in V. \tag{10.424}$$

A set of vectors, $\vec{u}_i \in V, i = 1, 2, \ldots, n$, is said to be **linearly independent** if the equality

$$c_1\vec{u}_1 + c_2\vec{u}_2 + \cdots + c_n\vec{u}_n = 0, \quad c_i \in \mathbb{R}, \tag{10.425}$$

can only be satisfied for the trivial case

$$c_1 = c_2 = \cdots = c_n = 0. \tag{10.426}$$

In an N-dimensional vector space, we can find N linearly independent unit basis vectors,

$$\hat{\mathbf{e}}_i \in V, \quad i = 1, 2, \ldots, n, \tag{10.427}$$

such that any vector $\vec{v} \in V$ can be expressed as a linear combination of these vectors as

$$\vec{v} = c_1\hat{\mathbf{e}}_1 + c_2\hat{\mathbf{e}}_2 + \cdots + c_n\hat{\mathbf{e}}_n. \tag{10.428}$$

10.11.2 Inner Product Space

In addition to the above properties, introduction of **scalar** or **inner product** enriches the vector space concept significantly and makes physical applications easier. In Cartesian coordinates the inner product, also called the **dot product**, is defined as

$$\boxed{(\vec{v}_1, \vec{v}_2) = \vec{v}_1 \cdot \vec{v}_2 = v_{1x}v_{2x} + v_{1y}v_{2y} + v_{1z}v_{2z}.} \tag{10.429}$$

Generalization to arbitrary dimensions is obvious. The inner product makes it possible to define the **norm** or **magnitude,** $|\vec{v}|$, of a vector as

$$\boxed{|\vec{v}| = (\vec{v} \cdot \vec{v})^{1/2},} \tag{10.430}$$

where θ_{12} is the angle between two vectors:

$$\boxed{\cos\theta_{12} = \frac{\vec{v}_1 \cdot \vec{v}_2}{|\vec{v}_1||\vec{v}_2|}.} \tag{10.431}$$

Basic properties of the inner product are:

1. $$\vec{v}_1 \cdot \vec{v}_2 = \vec{v}_2 \cdot \vec{v}_1, \tag{10.432}$$
2. $$\vec{v}_1 \cdot (a\vec{v}_2 + b\vec{v}_3) = a(\vec{v}_1 \cdot \vec{v}_2) + b(\vec{v}_1 \cdot \vec{v}_3), \tag{10.433}$$

   where a and b are real numbers. A vector space with the definition of an inner product is also called an **inner product space**.

10.11.3 Four-Vector Space

In Section 9.8, we have extended the vector concept to Minkowski spacetime as four-vectors, where the elements of the Lorentz group act on four-vectors and transform them into other four-vectors. For four-vector spaces properties (1)–(7) still hold; however, the inner product of two four-vectors A^α and B^α is now defined as

$$A_\alpha B^\alpha = g_{\alpha\beta}A^\alpha B^\beta = A^0B^0 - A^1B^1 - A^2B^2 - A^3B^3, \tag{10.434}$$

where $g_{\alpha\beta}$ is the Minkowski metric.

10.11.4 Complex Vector Space

Allowing complex numbers, we can also define complex vector spaces in the complex plane. For complex vector spaces properties (1)–(7) still hold; however, the **inner product** in n dimensions is now defined as

$$\boxed{\vec{v}_1 \cdot \vec{v}_2 = \sum_{i=1}^{n} v_{1i}^* v_{2i},} \tag{10.435}$$

where the complex conjugate must be taken to ensure a real value for the **norm** (magnitude) of a vector, that is,

$$\boxed{|\vec{v}| = (\vec{v} \cdot \vec{v})^{1/2} = \left(\sum_{i=1}^{n} v_i^* v_i \right)^{1/2}.} \tag{10.436}$$

Note that the inner product in the complex plane is no longer symmetric, that is,

$$\vec{v}_1 \cdot \vec{v}_2 \neq \vec{v}_2 \cdot \vec{v}_1, \tag{10.437}$$

however,

$$(\vec{v}_1 \cdot \vec{v}_2) = (\vec{v}_2 \cdot \vec{v}_1)^* \tag{10.438}$$

is true.

10.11.5 Function Space and Hilbert Space

We now define a vector space L_2, whose elements are complex valued functions of a real variable x, which are square integrable in the interval $[a, b]$. L_2 is also called the **Hilbert space**. By square integrable it is meant that the integral, $\int_a^b |f(x)|^2 dx$, exists and is finite. Proof of the fact that the space of square integrable functions satisfies the properties of a vector space is rather technical, and we refer to books like Courant and Hilbert [3] and Morse and Feshbach [11]. The inner product in L_2 is defined as

$$(f_1, f_2) = \int_a^b f_1^*(x) f_2(x) dx. \tag{10.439}$$

In the presence of a **weight function**, $w(x)$, the **inner product** becomes

$$\boxed{(f_1, f_2) = \int_a^b f_1^*(x) f_2(x) w(x) dx.} \tag{10.440}$$

Analogous to choosing a set of basis vectors in ordinary vector space, a major problem in L_2 is to find a suitable complete and an orthonormal set of functions, $\{u_m(x)\}$, such that a given $f(x) \in L_2$ can be expanded as

$$f(x) = \sum_{m=0}^{\infty} c_m u_m(x). \tag{10.441}$$

Orthogonality of $\{u_m(x)\}$ is expressed as

$$(u_m, u_n) = \int_a^b u_m^*(x) u_n(x) dx = \delta_{mn}, \tag{10.442}$$

where we have taken $w(x) = 1$ for simplicity. Using the orthogonality relation [Eq. (10.442)] we can free the expansion coefficients, c_m, under the summation sign [Eq. (10.441)] as

$$c_m = (u_m, f) = \int_a^b u_m^*(x) f(x) dx. \tag{10.443}$$

In physical applications $\{u_m(x)\}$ is usually taken as the eigenfunction set of a Hermitian operator. Substituting Eq. (10.443) back into Eq. (10.441) a formal expression for the **completeness** of the set $\{u_m(x)\}$ is obtained as

$$\sum_{m=0}^{\infty} u_m^*(x') u_m(x) = \delta(x - x'). \tag{10.444}$$

10.11.6 Completeness

Proof of the completeness of the eigenfunction set is rather technical for our purposes and can be found in Courant and Hilbert [3, vol. 1, p. 427]. What is important for us is that any sufficiently well behaved and at least piecewise continuous function, $F(x)$, can be expressed as an **infinite series** in terms of the set $\{u_m(x)\}$ as

$$F(x) = \sum_{m=0}^{\infty} a_m u_m(x). \tag{10.445}$$

Convergence of this series to $F(x)$ could be approached via the variation technique, and it could be shown that for a Sturm–Liouville system the limit [9, p. 338].

$$\lim_{N\to\infty} \int_a^b \left[F(x) - \sum_{m=0}^{N} a_m u_m(x)\right]^2 \omega(x) dx \to 0 \tag{10.446}$$

is true. In this case we say that in the interval $[a, b]$ the series $\sum_{m=0}^{\infty} a_m u_m(x)$ converges to $F(x)$ in the mean. **Convergence in the mean** does not imply **point-to-point** or **uniform convergence**:

$$\boxed{\lim_{N\to\infty} \sum_{m=0}^{N} a_m u_m(x) \to F(x).} \tag{10.447}$$

However, for most practical situations convergence in the mean will accompany point-to-point convergence and will be sufficient. We conclude this section by quoting a theorem from Courant and Hilbert [3, p. 427].

Expansion theorem: Any piecewise continuous function defined in the fundamental domain $[a, b]$ with a square integrable first derivative could be expanded in an eigenfunction series $F(x) = \sum_{m=0}^{\infty} a_m u_m(x)$, which converges absolutely and uniformly in all subdomains free of points of discontinuity. At the points of discontinuity it represents the arithmetic mean of the right- and the left-hand limits.

In this theorem, the function does not have to satisfy the boundary conditions. This theorem also implies convergence in the mean; however, the converse is not true.

10.12 Hilbert Space and Quantum Mechanics

In quantum mechanics a physical system is completely described by giving its state or the wave function, $\Psi(x)$, in Hilbert space. To every physical observable there corresponds a Hermitian differential operator acting on the functions in Hilbert space. Because of their Hermitian nature, these operators have real eigenvalues, which are the allowed physical values of the corresponding observable. These operators are usually obtained from their classical definitions by replacing position, momentum, and energy with their operator counterparts. In position space the replacements

$$\overrightarrow{r} \to \overrightarrow{r}, \tag{10.448}$$

$$\overrightarrow{p} \to -i\hbar\overrightarrow{\nabla}, \tag{10.449}$$

$$E \to i\hbar\frac{\partial}{\partial t} \tag{10.450}$$

have been rather successful. Using these, the angular momentum operator is obtained as

$$\overrightarrow{L} = \overrightarrow{r} \times \overrightarrow{p} = -i\hbar\overrightarrow{r} \times \overrightarrow{\nabla}. \tag{10.451}$$

In Cartesian coordinates components of $\overrightarrow{L}$ are given as

$$L_1 = -i\hbar \left(x_2 \frac{\partial}{\partial x_3} - x_3 \frac{\partial}{\partial x_2} \right), \tag{10.452}$$

$$L_2 = -i\hbar \left(x_3 \frac{\partial}{\partial x_1} - x_1 \frac{\partial}{\partial x_3} \right), \tag{10.453}$$

$$L_3 = -i\hbar \left(x_1 \frac{\partial}{\partial x_2} - x_2 \frac{\partial}{\partial x_1} \right), \tag{10.454}$$

where L_i satisfies the commutation relation

$$[L_i, L_j] = i\hbar\epsilon_{ijk}L_k. \tag{10.455}$$

10.13 Continuous Groups and Symmetries

In everyday language, the word **symmetry** is usually associated with familiar operations like rotations and reflections. In scientific parlance, we have a broader definition in terms of general operations performed in the parameter space of a given system, where symmetry means that a given system is invariant under a certain operation. A system could be represented by a Lagrangian, a state function, or a differential equation. In our previous Sections, we have discussed examples of continuous groups and their generators. The theory of continuous groups was invented by Lie when he was studying symmetries of differential equations. He also introduced a method for integrating differential equations once the symmetries are known. In what follows we discuss **extension** or the **prolongation** of generators of continuous groups so that they could be applied to differential equations.

10.13.1 Point Groups and Their Generators

In two dimensions general **point transformations** can be defined as

$$\begin{aligned} \overline{x} &= \overline{x}(x, y), \\ \overline{y} &= \overline{y}(x, y), \end{aligned} \tag{10.456}$$

where x and y are two variables that are not necessarily the Cartesian coordinates. All we require is that this transformation form a continuous group so that finite transformations can be generated continuously from the identity element. We assume that these transformations depend on at least on one parameter, ε; hence we write

$$\boxed{\begin{aligned} \overline{x} &= \overline{x}(x, y; \varepsilon), \\ \overline{y} &= \overline{y}(x, y; \varepsilon). \end{aligned}} \tag{10.457}$$

A well-known example is the orthogonal transformation:

$$\begin{aligned} \overline{x} &= x\cos\varepsilon + y\sin\varepsilon, \\ \overline{y} &= -x\sin\varepsilon + y\cos\varepsilon, \end{aligned} \tag{10.458}$$

which corresponds to counterclockwise rotations about the z-axis by the amount ε. If we expand Eq. (10.457) about $\varepsilon = 0$ we get

$$\begin{aligned} \overline{x}(x, y; \varepsilon) &= x + \varepsilon\alpha(x, y) + \cdots , \\ \overline{y}(x, y; \varepsilon) &= y + \varepsilon\beta(x, y) + \cdots , \end{aligned} \tag{10.459}$$

where

$$\alpha(x, y) = \left.\frac{\partial \overline{x}}{\partial \varepsilon}\right|_{\varepsilon=0}, \tag{10.460}$$

$$\beta(x, y) = \left.\frac{\partial \overline{y}}{\partial \varepsilon}\right|_{\varepsilon=0}. \tag{10.461}$$

If we define the operator

$$\boxed{\mathbf{X} = \alpha(x, y)\frac{\partial}{\partial x} + \beta(x, y)\frac{\partial}{\partial y},} \tag{10.462}$$

we can write Eq. (10.459) as

$$\begin{aligned} \overline{x}(x, y; \varepsilon) &= x + \varepsilon\mathbf{X}x + \cdots , \\ \overline{y}(x, y; \varepsilon) &= y + \varepsilon\mathbf{X}y + \cdots . \end{aligned} \tag{10.463}$$

The operator $\mathbf{X}$ is called the **generator** of the infinitesimal point transformation. For infinitesimal rotations about the z-axis, this agrees with our previous result [Eq. (10.43)] as

$$\mathbf{X}_z = y\frac{\partial}{\partial x} - x\frac{\partial}{\partial y}. \tag{10.464}$$

Similarly, the generator for the point transformation

$$\overline{x} = x + \varepsilon, \ \ \overline{y} = y, \tag{10.465}$$

which corresponds to translation along the x-axis, is

$$\mathbf{X} = \frac{\partial}{\partial x}. \tag{10.466}$$

10.13.2 Transformation of Generators and Normal Forms

We have given the generators in terms of the (x, y) variables [Eq. (10.462)]. However, we would also like to know how they look in another set of variables, say (u, v):

$$\begin{aligned} u &= u(x, y), \\ v &= v(x, y). \end{aligned} \tag{10.467}$$

For this we first generalize [Eq. (10.462)] to n variables as

$$\boxed{\mathbf{X} = a^i(x^j)\frac{\partial}{\partial x^i}, \quad i = 1, 2, \ldots, n.} \tag{10.468}$$

Note that we used the Einstein summation convention for the index i. Defining new variables by $\overline{x}^i = \overline{x}^i(x^j)$, we obtain

$$\frac{\partial}{\partial x^i} = \frac{\partial \overline{x}^j}{\partial x^i}\frac{\partial}{\partial \overline{x}^j}. \tag{10.469}$$

When substituted in Eq. (10.468), this gives the generator in terms of the new variables as

$$\mathbf{X} = \left[a^i \frac{\partial \overline{x}^j}{\partial x^i}\right]\frac{\partial}{\partial \overline{x}^j} = \overline{a}^j \frac{\partial}{\partial \overline{x}^j}, \tag{10.470}$$

where

$$\overline{a}^j = \frac{\partial \overline{x}^j}{\partial x^i} a^i. \tag{10.471}$$

Note that if we operate on x^j with $\mathbf{X}$ we get

$$\mathbf{X}x^j = a^i \frac{\partial x^j}{\partial x^i} = a^j. \tag{10.472}$$

Similarly,

$$\mathbf{X}\overline{x}^j = \overline{a}^i \frac{\partial \overline{x}^j}{\partial \overline{x}^i} = \overline{a}^j. \tag{10.473}$$

In other words, the coefficients in the definition of the generator can be found by simply operating on the coordinates with the generator; hence, we can write

$$\boxed{\mathbf{X} = (\mathbf{X}x^i)\frac{\partial}{\partial x^i}} \tag{10.474}$$

or

$$\boxed{\mathbf{X} = (\mathbf{X}\overline{x}^i)\frac{\partial}{\partial \overline{x}^i}.} \tag{10.475}$$

We now consider the generator for rotations about the z-axis [Eq. (10.464)] in plane polar coordinates:

$$\rho = (x^2 + y^2)^{1/2}, \tag{10.476}$$

$$\phi = \arctan(y/x). \tag{10.477}$$

Applying Eq. (10.474), we obtain the generator as

$$\mathbf{X} = (\mathbf{X}\rho)\frac{\partial}{\partial r} + (\mathbf{X}\phi)\frac{\partial}{\partial \phi} \tag{10.478}$$

$$= \left[\left(y\frac{\partial}{\partial x} - x\frac{\partial}{\partial y}\right)(x^2+y^2)^{\frac{1}{2}}\right]\frac{\partial}{\partial r} + \left[\left(y\frac{\partial}{\partial x} - x\frac{\partial}{\partial y}\right)\arctan\left(\frac{y}{x}\right)\right]\frac{\partial}{\partial \phi} \tag{10.479}$$

$$= [0]\frac{\partial}{\partial r} + [-1]\frac{\partial}{\partial \phi} \tag{10.480}$$

$$= -\frac{\partial}{\partial \phi}. \tag{10.481}$$

Naturally, the plane polar coordinates in two dimensions or in general the spherical polar coordinates are the natural coordinates to use in rotation problems. This brings out the obvious question: Is it always possible to find a new definition of variables so that the generator of the one-parameter group of transformations looks like

$$\mathbf{X} = \frac{\partial}{\partial s}\ ? \tag{10.482}$$

We will not go into the proof, but the answer to this question is yes, where the above form of the generator is called the **normal form**.

10.13.3 The Case of Multiple Parameters

Transformations can also depend on multiple parameters. For a group of transformations with m parameters we write

$$\boxed{\overline{x}^i = \overline{x}^i(x^j;\varepsilon_\mu), \quad i,j = 1,2,\dots,n \text{ and } \mu = 1,2,\dots,m.} \tag{10.483}$$

We now associate a generator for each parameter as

$$\boxed{\mathbf{X}_\mu = a^i_\mu(x^j)\frac{\partial}{\partial x^i}, \quad i = 1,2,\dots,n,} \tag{10.484}$$

where

$$\boxed{a^i_\mu(x^j) = \left.\frac{\partial x^i}{\partial \varepsilon_\mu}\right|_{\varepsilon_\mu=0}.} \tag{10.485}$$

The generator of a general transformation can now be given as a linear combination of the individual generators as

$$\mathbf{X} = c^\mu \mathbf{X}_\mu, \quad \mu = 1,2,\dots,m. \tag{10.486}$$

We have seen examples of this in $R(3)$ and $SU(2)$. In fact, $\mathbf{X}_\mu$ forms the Lie algebra of the m-dimensional group of transformations.

10.13.4 Action of Generators on Functions

We have already seen that the action of the generators of the rotation group $R(3)$ on a function $f(\mathbf{r})$ are given as

$$f'(\mathbf{r}) = (\mathbf{I} - \overline{\mathbf{X}}_1\delta\theta_1 - \overline{\mathbf{X}}_2\delta\theta_2 - \overline{\mathbf{X}}_3\delta\theta_3)f(\mathbf{r}) \tag{10.487}$$

$$= (\mathbf{I} - \overline{\mathbf{X}} \cdot \widehat{\mathbf{n}}\delta\theta)f(\mathbf{r}), \tag{10.488}$$

where the generators are given as

$$\overline{\mathbf{X}}_1 = -\left(x_2\frac{\partial}{\partial x_3} - x_3\frac{\partial}{\partial x_2}\right), \tag{10.489}$$

$$\overline{\mathbf{X}}_2 = -\left(x_3\frac{\partial}{\partial x_1} - x_1\frac{\partial}{\partial x_3}\right), \tag{10.490}$$

$$\overline{\mathbf{X}}_3 = -\left(x_1\frac{\partial}{\partial x_2} - x_2\frac{\partial}{\partial x_1}\right). \tag{10.491}$$

The minus sign in Eq. (10.488) means that the physical system is rotated clockwise by θ about an axis pointing in the $\widehat{\mathbf{n}}$ direction. Now the change in $f(\mathbf{r})$ is given as

$$\delta f(\mathbf{r}) = -(\overline{\mathbf{X}} \cdot \widehat{\mathbf{n}})f(\mathbf{r})\delta\theta. \tag{10.492}$$

If a system represented by $f(\mathbf{r})$ is symmetric under the rotation generated by $(\overline{\mathbf{X}} \cdot \widehat{\mathbf{n}})$, that is, it does not change, then we have

$$(\overline{\mathbf{X}} \cdot \widehat{\mathbf{n}})f(\mathbf{r}) = 0. \tag{10.493}$$

For rotations about the z-axis, in spherical polar coordinates this means

$$\frac{\partial}{\partial\phi}f(\mathbf{r}) = 0, \tag{10.494}$$

that is, $f(\mathbf{r})$ does not depend on ϕ explicitly.

For a general transformation, we can define two vectors

$$\mathbf{r} = \begin{bmatrix} x^1 \\ x^2 \\ \vdots \\ x^n \end{bmatrix}, \quad \mathbf{e} = \begin{bmatrix} \varepsilon^1 \\ \varepsilon^2 \\ \vdots \\ \varepsilon^m \end{bmatrix}, \tag{10.495}$$

where ε^μ are small, so that

$$f'(\mathbf{r}) = (\mathbf{I} - \mathbf{X}_1\varepsilon^1 - \mathbf{X}_2\varepsilon^2 - \cdots - \mathbf{X}_m\varepsilon^m)f(\mathbf{r}) \tag{10.496}$$

$$= (\mathbf{I} - \mathbf{X}_\mu \cdot \widehat{\mathbf{e}}^\mu e)f(\mathbf{r}), \tag{10.497}$$

where $\widehat{\mathbf{e}}^\mu$ is a unit vector in the direction of $\mathbf{e}$:

$$\widehat{\mathbf{e}}^\mu = \mathbf{e}/e, \quad e = |\mathbf{e}| = [(\varepsilon^1)^2 + (\varepsilon^2)^2 + \cdots + (\varepsilon^m)^2]^{1/2}, \tag{10.498}$$

and the generators are defined as in Eq. (10.484).

10.13.5 Extension or Prolongation of Generators

To find the effect of infinitesimal point transformations on a differential equation

$$D(x, y', y'', \dots, y^{(n)}) = 0, \tag{10.499}$$

we first need to find how the derivatives, $y^{(n)}$, transform. For the point transformation

$$\begin{aligned} \overline{x} &= \overline{x}(x, y; \varepsilon), \\ \overline{y} &= \overline{y}(x, y; \varepsilon), \end{aligned} \tag{10.500}$$

we can write

$$\overline{y}' = \frac{d\overline{y}}{d\overline{x}} \tag{10.501}$$

$$= \frac{d\overline{y}(x, y; \varepsilon)}{d\overline{x}(x, y; \varepsilon)} \tag{10.502}$$

$$= \frac{(\partial\overline{y}/\partial x) + (\partial\overline{y}/\partial y)y'}{(\partial\overline{x}/\partial x) + (\partial\overline{x}/\partial y)y'} \tag{10.503}$$

$$= \overline{y}'(x, y, y'; \varepsilon). \tag{10.504}$$

Other derivatives can also be written as

$$\begin{aligned} \overline{y}'' &= \frac{d\overline{y}'}{d\overline{x}} = \overline{y}''(x, y, y', y''; \varepsilon), \\ &\vdots \\ \overline{y}^{(n)} &= \frac{d\overline{y}^{(n-1)}}{d\overline{x}} = \overline{y}^{(n)}(x, y, y', \dots, y^{(n)}; \varepsilon). \end{aligned} \tag{10.505}$$

What is actually needed are the generators of the following infinitesimal transformations:

$$\begin{aligned} \overline{x} &= x + \varepsilon\alpha(x, y) + \cdots, \\ \overline{y} &= y + \varepsilon\beta(x, y) + \cdots, \\ \overline{y}' &= y' + \varepsilon\beta^{[1]}(x, y, y') + \cdots, \\ &\vdots \\ \overline{y}^{(n)} &= y^{(n)} + \varepsilon\beta^{[n]}(x, y, y', \dots, y^{(n)}) + \cdots, \end{aligned} \tag{10.506}$$

where

$$\alpha(x, y) = \left.\frac{\partial\overline{x}}{\partial\varepsilon}\right|_{\varepsilon=0}, \quad \beta(x, y) = \left.\frac{\partial\overline{y}}{\partial\varepsilon}\right|_{\varepsilon=0} \tag{10.507}$$

and

$$\beta^{[1]} = \left.\frac{\partial\overline{y}'}{\partial\varepsilon}\right|_{\varepsilon=0}, \dots, \quad \beta^{[n]} = \left.\frac{\partial\overline{y}^{(n)}}{\partial\varepsilon}\right|_{\varepsilon=0}. \tag{10.508}$$

Also note that $\beta^{[n]}$ is not the nth derivative of β. For reasons to become clear shortly, we use $\mathbf{X}$ for all the generators in Eq. (10.506) and write

$$\begin{aligned}
\bar{x} &= x + \varepsilon \mathbf{X} x + \cdots , \\
\bar{y} &= y + \varepsilon \mathbf{X} y + \cdots , \\
\bar{y}' &= y' + \varepsilon \mathbf{X} y' + \cdots , \\
&\vdots \\
\bar{y}^{(n)} &= y^{(n)} + \varepsilon \mathbf{X} y^{(n)} + \cdots .
\end{aligned} \tag{10.509}$$

We now define the **extension** or the **prolongation** of the generator

$$\mathbf{X} = \alpha(x,y)\frac{\partial}{\partial x} + \beta(x,y)\frac{\partial}{\partial y} \tag{10.510}$$

as

$$\boxed{\mathbf{X} = \alpha\frac{\partial}{\partial x} + \beta\frac{\partial}{\partial y} + \beta^{[1]}\frac{\partial}{\partial y'} + \cdots + \beta^{[n]}\frac{\partial}{\partial y^{(n)}}.} \tag{10.511}$$

To find the coefficients, $\beta^{[n]}$, we start with Eq. (10.506) and use it in Eq. (10.503):

$$\bar{y}' = \frac{d\bar{y}}{d\bar{x}} \tag{10.512}$$

$$= \frac{y' + \varepsilon(d\beta/dx) + \cdots}{1 + \varepsilon(d\alpha/dx) + \cdots} \tag{10.513}$$

$$= y' + \varepsilon\left(\frac{d\beta}{dx} - y'\frac{d\alpha}{dx}\right) + \cdots . \tag{10.514}$$

Comparing with [Eq. (10.506)]:

$$\bar{y}' = y' + \varepsilon\beta^{[1]} + \cdots , \tag{10.515}$$

we obtain $\beta^{[1]}$ as

$$\beta^{[1]} = \left(\frac{d\beta}{dx} - y'\frac{d\alpha}{dx}\right). \tag{10.516}$$

Similarly, we write

$$\bar{y}^{(n)} = \frac{d}{d\bar{x}}\bar{y}^{(n-1)} = y^{(n)} + \varepsilon\beta^{[n]} + \cdots \tag{10.517}$$

$$= \frac{d}{dx}\left[y^{(n-1)} + \varepsilon\beta^{[n-1]}\right]\frac{dx}{d\bar{x}} + \cdots \tag{10.518}$$

$$= y^{(n)} + \varepsilon\left(\frac{d\beta^{[n-1]}}{dx} - y^{(n)}\frac{d\alpha}{dx}\right) + \cdots \tag{10.519}$$

and obtain

$$\beta^{[n]} = \frac{d\beta^{[n-1]}}{dx} - y^{(n)}\frac{d\alpha}{dx}. \tag{10.520}$$

This can also be written as

$$\boxed{\beta^{[n]} = \frac{d^n(\beta - y'\alpha)}{dx^n} + y^{(n+1)}\alpha.} \tag{10.521}$$

The first two terms give

$$\beta^{[1]} = \frac{d\beta(x,y)}{dx} - y'\frac{d\alpha(x,y)}{dx} \tag{10.522}$$

$$= \frac{\partial\beta}{\partial x} + y'\left(\frac{\partial\beta}{\partial y} - \frac{\partial\alpha}{\partial x}\right) - y'^2\frac{\partial\alpha}{\partial y} \tag{10.523}$$

and

$$\beta^{[2]} = \frac{d^2(\beta - y'\alpha)}{dx^2} + y^{(3)}\alpha \tag{10.524}$$

$$= \frac{\partial^2\beta}{\partial x^2} + \left(2\frac{\partial^2\beta}{\partial x\partial y} - \frac{\partial^2\alpha}{\partial x^2}\right)y' + \left(\frac{\partial^2\beta}{\partial y^2} - 2\frac{\partial^2\alpha}{\partial x\partial y}\right)y'^2 \tag{10.525}$$

$$- \frac{\partial^2\alpha}{\partial y^2}y'^3 + \left(\frac{\partial\beta}{\partial y} - 2\frac{\partial\alpha}{\partial x} - 3\frac{\partial\alpha}{\partial y}y'\right)y''.$$

For the infinitesimal rotations about the z-axis, the extended generator can now be written as

$$\mathbf{X} = y\frac{\partial}{\partial x} - x\frac{\partial}{\partial y} - (1 + y'^2)\frac{\partial}{\partial y'} - 3y'y''\frac{\partial}{\partial y''} - (3y''^2 + 4y'y''')\frac{\partial}{\partial y'''} + \cdots. \tag{10.526}$$

For the extension of the generator for translations along the x-axis, we obtain

$$\mathbf{X} = \frac{\partial}{\partial x}. \tag{10.527}$$

10.13.6 Symmetries of Differential Equations

We are now ready to discuss the symmetry of differential equations under point transformations, which depend on at least one parameter. To avoid some singular cases we confine our discussion to differential equations [12]:

$$D(x, y', y'', \ldots, y^{(n)}) = 0, \tag{10.528}$$

which can be solved for the highest derivative as

$$D = y^{(n)} - \widetilde{D}(x, y', y'', \ldots, y^{(n-1)}) = 0. \tag{10.529}$$

For example, the differential equation

$$D = 2y'' + y'^2 + y = 0 \tag{10.530}$$

satisfies this property, whereas

$$D = (y'' - y' + x)^2 = 0 \tag{10.531}$$

does not.

For the point transformation

$$\bar{x} = \bar{x}(x, y; \varepsilon),$$
$$\bar{y} = \bar{y}(x, y; \varepsilon), \tag{10.532}$$

we say the differential equation is symmetric, if the solutions, $y(x)$, of Eq. (10.529) are mapped into other solutions, $\bar{y} = \bar{y}(\bar{x})$, of

$$D = \bar{y}^{(n)} - \widetilde{D}(\bar{x}, \bar{y}', \bar{y}'', \ldots, \bar{y}^{(n-1)}) = 0. \tag{10.533}$$

Expanding D with respect to ε about $\varepsilon = 0$ we write

$$D(\bar{x}, \bar{y}', \bar{y}'', \ldots, \bar{y}^{(n)}; \varepsilon) = D(\bar{x}, \bar{y}', \bar{y}'', \ldots, \bar{y}^{(n)}; \varepsilon)|_{\varepsilon=0} + \frac{\partial D(\bar{x}, \bar{y}', \bar{y}'', \ldots, \bar{y}^{(n)}; \varepsilon)}{\partial \varepsilon}|_{\varepsilon=0}\, \varepsilon + \cdots . \tag{10.534}$$

For infinitesimal transformations we keep only the linear terms in ε:

$$D(\bar{x}, \bar{y}', \bar{y}'', \ldots, \bar{y}^{(n)}; \varepsilon) - D(\bar{x}, \bar{y}', \bar{y}'', \ldots, \bar{y}^{(n)}; \varepsilon)|_{\varepsilon=0} = \frac{\partial D}{\partial \bar{x}}\frac{\partial \bar{x}}{\partial \varepsilon} + \frac{\partial D}{\partial \bar{y}}\frac{\partial \bar{y}}{\partial \varepsilon} + \cdots + \frac{\partial D}{\partial \bar{y}^{(n)}}\frac{\partial \bar{y}^{(n)}}{\partial \varepsilon}|_{\varepsilon=0}\varepsilon. \tag{10.535}$$

In the presence of symmetry, Eq. (10.533) must be true for all ε; thus, the left-hand side of Eq. (10.535) is zero, and we obtain a formal expression for symmetry as

$$\left[\alpha\frac{\partial D}{\partial x} + \beta\frac{\partial D}{\partial y} + \cdots + \beta^{[n]}\frac{\partial D}{\partial y^{(n)}}\right] = 0, \tag{10.536}$$

$$\left[\alpha\frac{\partial}{\partial x} + \beta\frac{\partial}{\partial y} + \cdots + \beta^{[n]}\frac{\partial}{\partial y^{(n)}}\right] D = 0, \tag{10.537}$$

$$\mathbf{X}D = 0. \tag{10.538}$$

Note that the symmetry of a differential equation is independent of the choice of the variables used. Using an arbitrary point transformation only changes the form of the generator. We now summarize these results in terms of a theorem [12].

Theorem 10.1 An ordinary differential equation, which could be written as

$$D = \bar{y}^{(n)} - \widetilde{D}(\bar{x}, \bar{y}', \bar{y}'', \ldots, \bar{y}^{(n-1)}) = 0, \tag{10.539}$$

admits a group of symmetries with the generator $\mathbf{X}$, if and only if

$$\mathbf{X}D \equiv 0 \tag{10.540}$$

holds. Note that we have written $\mathbf{X}D \equiv 0$ instead of $\mathbf{X}D = 0$ to emphasize the fact that Eq. (10.540) must hold for every solution $y(x)$ of $D = 0$.

For example, the differential equation

$$D = y'' + a_0 y' + b_0 y = 0 \tag{10.541}$$

admits the symmetry transformation

$$\begin{aligned} \overline{x} &= 0, \\ \overline{y} &= (1+\varepsilon)y, \end{aligned} \tag{10.542}$$

since D does not change when we multiply y (also y' and y'') with a constant factor. Using Eq. (10.511) the generator of this transformation can be written as

$$\mathbf{X} = y\frac{\partial}{\partial y} + y'\frac{\partial}{\partial y'} + y''\frac{\partial}{\partial y''}, \tag{10.543}$$

which gives

$$\mathbf{X}D = \left[y\frac{\partial}{\partial y} + y'\frac{\partial}{\partial y'} + y''\frac{\partial}{\partial y''}\right](y'' + a_0 y' + b_0 y) \tag{10.544}$$

$$= (y'' + a_0 y' + b_0 y). \tag{10.545}$$

Considered with $D = 0$, this gives $\mathbf{X}D = 0$.

We have mentioned that one can always find a new variable, say $\widetilde{x}$, where a generator appears in its normal form as

$$\mathbf{X} = \frac{\partial}{\partial \widetilde{x}}. \tag{10.546}$$

If $\mathbf{X}$ generates a symmetry of a given differential equation, which can be solved for its highest derivative as

$$D = \overline{y}^{(n)} - \widetilde{D}(\overline{x}, \overline{y}', \overline{y}'', \ldots, \overline{y}^{(n-1)}) = 0, \tag{10.547}$$

then we can write

$$\mathbf{X}D = \frac{\partial D}{\partial \widetilde{x}} = 0, \tag{10.548}$$

which means that in normal coordinates D does not depend explicitly on the independent variable $\widetilde{x}$.

Note that restricting our discussion to differential equations that could be solved for the highest derivative guards us from singular cases where all the first derivatives of D are zero. For example, for the differential equation

$$D = (y'' - y' + x)^2 = 0, \tag{10.549}$$

all the first-order derivatives are zero for $D = 0$:

$$\frac{\partial D}{\partial y''} = 2(y'' - y' + x) = 0, \tag{10.550}$$

$$\frac{\partial D}{\partial y'} = -2(y'' - y' + x) = 0, \tag{10.551}$$

$$\frac{\partial D}{\partial y} = 0, \tag{10.552}$$

$$\frac{\partial D}{\partial x} = 2(y'' - y' + x) = 0. \tag{10.553}$$

Thus, $\mathbf{X}D = 0$ holds for any linear operator, and in normal coordinates even though $\frac{\partial D}{\partial \widetilde{x}} = 0$, we can no longer say that D does not depend on $\widetilde{x}$ explicitly.

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Problems

1 Consider the following linear group in two dimensions:

$$x' = ax + by,$$
$$y' = cx + dy.$$

Show that the four infinitesimal generators are given as

$$X_1 = x\frac{\partial}{\partial x},\ X_2 = y\frac{\partial}{\partial x},\ X_3 = x\frac{\partial}{\partial y},\ X_4 = y\frac{\partial}{\partial y}$$

and find their commutators.

2 Show that

$$\det \mathbf{A} = \det e^{\mathbf{L}} = e^{Tr\mathbf{L}},$$

where $\mathbf{L}$ is an $n \times n$ matrix. Use the fact that the determinant and the trace of a matrix are invariant under similarity transformations. Then make a similarity transformation that puts $\mathbf{L}$ into diagonal form.

3 Verify the transformation matrix

$$\mathbf{A}_{\text{boost}}(\beta) = e^{\mathbf{V}\cdot\hat{\beta}\beta}$$
$$= \begin{bmatrix} \gamma & -\beta_1\gamma & -\beta_2\gamma & -\beta_3\gamma \\ -\beta_1\gamma & 1+\dfrac{(\gamma-1)\beta_1^2}{\beta^2} & \dfrac{(\gamma-1)\beta_1\beta_2}{\beta^2} & \dfrac{(\gamma-1)\beta_1\beta_3}{\beta^2} \\ -\beta_2\gamma & \dfrac{(\gamma-1)\beta_2\beta_1}{\beta^2} & 1+\dfrac{(\gamma-1)\beta_2^2}{\beta^2} & \dfrac{(\gamma-1)\beta_2\beta_3}{\beta^2} \\ -\beta_3\gamma & \dfrac{(\gamma-1)\beta_3\beta_1}{\beta^2} & \dfrac{(\gamma-1)\beta_3\beta_2}{\beta^2} & 1+\dfrac{(\gamma-1)\beta_3^2}{\beta^2} \end{bmatrix},$$

where $\beta_1 = \dfrac{v_1}{c}$, $\beta_2 = \dfrac{v_2}{c}$, $\beta_3 = \dfrac{v_3}{c}$.

4 Show that the generators $\mathbf{V}_i$ [Eq. (10.169)]:

$$\mathbf{V}_1 = \begin{bmatrix} 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix},\ \mathbf{V}_2 = \begin{bmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix},\ \mathbf{V}_3 = \begin{bmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{bmatrix},$$

can also be obtained from $\mathbf{V}_i = \mathbf{A}'_{\text{boost}}(\beta_i = 0)$.

5 Given the charge distribution, $\rho(\overrightarrow{r}) = r^2 e^{-r}\sin^2\theta$, make a multipole expansion of the potential and evaluate all the nonvanishing multipole moments. What is the potential for large distances?

6 Go through the details of the derivation of the differential equation that $d^l_{m'm}(\beta)$ satisfies:

$$\left\{\frac{d^2}{d\beta^2}+\cot\beta\frac{d}{d\beta}+\left[l(l+1)-\left(\frac{m^2+m'^2-2mm'\cos\beta}{\sin^2\beta}\right)\right]\right\}d^l_{m'm}(\beta)=0.$$

7 Using the substitution $d^l_{m'm}(\beta)=\frac{y(\lambda_l,m',m,\beta)}{\sqrt{\sin\beta}}$ in Problem 6, show that the second canonical form of the differential equation for $d^l_{m'm}(\beta)$ (Chapter 8) is given as

$$\frac{d^2y(\lambda_l,m',m,\beta)}{d\beta^2}+\left[l(l+1)+\frac{1}{4}-\left(\frac{m^2+m'^2-2mm'\cos\beta-\frac{1}{4}}{\sin^2\beta}\right)\right]y(\lambda_l,m',m,\beta)=0.$$

8 Using the result of Problem 7, solve the differential equation for $d^l_{mm'}(\beta)$ by the factorization method.

(i) Considering m as a parameter, find the normalized step-up and step-down operators, $£_+(m+1)$ and $£_-(m)$, which change the index m while keeping the index m' fixed.

(ii) Considering m' as a parameter, find the normalized step-up and step-down operators $£'_+(m'+1)$ and $£'_-(m')$, which change the index m' while keeping the index m fixed. Show that $|m|\le l$ and $|m'|\le l$.

(iii) Find the normalized functions with $m=m'=l$.

(iv) For $l=2$, construct the full matrix $d^2_{m'm}(\beta)$.

(v) By transforming the differential equation for $d^l_{mm'}(\beta)$ into an appropriate form, find the step-up and step-down operators that shift the index l for fixed m and m', giving the **normalized** functions $d^l_{mm'}(\beta)$.

(vi) Using the result in part (v) derive a recursion relation for $(\cos\beta)d^l_{mm'}(\beta)$. That is, express this as a combination of $d^{l'}_{mm'}(\beta)$ with $l'=l\pm1,\ldots$.

Note: This is a difficult problem and requires knowledge of the material discussed in Chapter 8.

9 Show that

(i)
$$D^l_{m0}(\alpha,\beta,-)=\sqrt{\frac{4\pi}{(2l+1)}}Y^*_{lm}(\beta,\alpha),$$

(ii)
$$D^l_{0m}(-,\beta,\gamma)=(-1)^m\sqrt{\frac{4\pi}{(2l+1)}}Y^*_{lm}(\beta,\gamma).$$

Hint: Use the invariant

$$\sum_{m=-l}^{m=l}Y^*_{lm}(\theta_1,\phi_1)Y_{lm}(\theta_2,\phi_2)$$

with

$$(\theta_1, \phi_1) = (\beta, \alpha) \text{ and } (\theta_2, \phi_2) = (\theta, \phi), \quad \theta_{12} = \theta',$$

and

$$[D^l_{mm'}(\alpha, \beta, \gamma)]^{-1} = [D^l_{m'm}(\alpha, \beta, \gamma)]^* = D^l_{mm'}(-\gamma, -\beta, -\alpha).$$

10 For $l = 2$ construct the matrices $\mathbf{L}^k_y = (L^k_y)_{mm'}$ for $k = 0, 1, 2, 3, 4, \ldots$ and show that the matrices with $k \geq 5$ can be expressed as linear combinations of these. Use this result to check the result in part (iv) of Problem 8.

11 We have studied spherical harmonics $Y_{lm}(\theta, \phi)$, which are single-valued functions of (θ, ϕ) for $l = 0, 1, 2, \ldots$. However, the factorization method also gave us a second family of solutions corresponding to the eigenvalues $\lambda = J(J+1)$ with $M = J, (J-1), \ldots, 0, \ldots, -(J-1), -J$, where $J = 0, 1/2, 3/2, \ldots$.
For $J = 1/2$, find the 2×2 matrix of the y component of the angular momentum operator, that is, the generalization of our $[\mathbf{L}_y]_{mm'}$. Show that the matrices for $\mathbf{L}^2_y, \mathbf{L}^3_y, \mathbf{L}^4_y, \ldots$ are simply related to the 2×2 unit matrix and the matrix $[\mathbf{L}_y]_{MM'}$. Calculate the d-function for $J = 1/2$, $d^{J=1/2}_{MM'}(\beta)$, with M and M' taking values $+1/2$ or $-1/2$.

12 Using the definition of the Hermitian operators, $\int \Psi^*_1 \pounds \Psi_2 dx = \int (\pounds \Psi_1)^* \Psi_2 dx$, show that

$$\iint d\Omega Y^*_{lm''} e^{i\gamma L_z} e^{i\beta L_y} e^{-i\alpha L_z} Y_{lm} = e^{i\gamma m''} \left[\iint d\Omega Y_{lm} e^{-i\beta L_y} Y^*_{lm''} \right] e^{i\alpha m}.$$

13 Convince yourself that the relations

$$e^{-i\beta L_{y_1}} = e^{-i\alpha L_z} e^{-i\beta L_y} e^{i\alpha L_z},$$
$$e^{-i\gamma L_{z_2}} = e^{-i\beta L_{y_1}} e^{-i\gamma L_{z_1}} e^{i\beta L_{y_1}},$$

used in the derivation of the rotation matrix in terms of the original set of axes are true.

14 Show that $D^l_{mm''}(R)$ satisfy $\sum_{m''} [D^l_{m'm''}(R)][D^l_{m''m}(R^{-1})] = \delta_{m'm}$.

15 Show that the extended generator of

$$\mathbf{X} = x\frac{\partial}{\partial x} + y\frac{\partial}{\partial y}$$

is given as

$$\mathbf{X} = x\frac{\partial}{\partial x} + y\frac{\partial}{\partial y} - y''\frac{\partial}{\partial y''} - 2y'''\frac{\partial}{\partial y'''} + \cdots.$$

16 Find the extension of

$$\mathbf{X} = xy\frac{\partial}{\partial x} + y^2\frac{\partial}{\partial y}$$

up to third order.

17 Express the generator $\mathbf{X} = x(\partial/\partial x) + y(\partial/\partial y)$ in terms of $u = y/x$, $v = xy$.

18 Using induction, show that

$$\beta^{[n]} = \frac{d\beta^{[n-1]}}{dx} - y^{(n)}\frac{d\alpha}{dx}$$

can be written as

$$\beta^{[n]} = \frac{d^n(\beta - y'\alpha)}{dx^n} + y^{(n+1)}\alpha.$$

19 Does the following transformation form a group?

$$\overline{x} = x, \; \overline{y} = ay + a^2y^2, \quad a \text{ is a constant.}$$

11

Complex Variables and Functions

Even though the complex numbers do not exist in nature directly, they are very useful in physics and engineering applications:

1. In the theory of complex functions, there are pairs of functions called the conjugate harmonic functions. They are useful in finding solutions of the Laplace equation in two dimensions.
2. The method of analytic continuation is a very important tool in finding solutions of differential equations and evaluating definite integrals.
3. Infinite series, infinite products, asymptotic solutions, and stability calculations are other areas, where the complex techniques are very helpful.
4. Even though the complex techniques are very useful in certain problems of physics and engineering, which are essentially defined in the real domain, complex numbers appear as an essential part of the physical theory in quantum mechanics.

11.1 Complex Algebra

A **complex number**, $a + ib$, where $i = \sqrt{-1}$, can be defined by giving a pair of **real numbers** (a, b) representing the real and the imaginary parts, respectively. A convenient way to represent complex numbers is to introduce the complex ***z*-plane** (Figure 11.1), where a point is shown as

$$z = (x, y) = x + iy. \tag{11.1}$$

Using plane polar coordinates, where $x = r\cos\theta$ and $y = r\sin\theta$, we can write a complex number as (Figure 11.1)

$$z = r(\cos\theta + i\sin\theta), \tag{11.2}$$

Mathematical Methods in Science and Engineering, Second Edition. Selçuk Ş. Bayın.

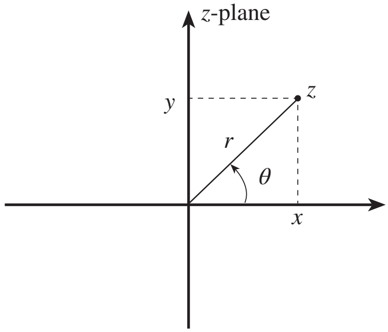


Figure 11.1 A point in the complex z-plane.

which is also equal to

$$z = re^{i\theta}. \tag{11.3}$$

Here, θ is called the **argument** and r, or $|z|$ is the **modulus** given as $r = \sqrt{x^2 + y^2}$. Algebraic manipulations with complex numbers can be done according to the following rules:

(i) **Addition:**

$$z_1 + z_2 = (x_1 + iy_1) + (x_2 + iy_2) \tag{11.4}$$

$$= (x_1 + x_2) + i(y_1 + y_2). \tag{11.5}$$

(ii) **Multiplication** with a constant c:

$$cz = c(x + iy) \tag{11.6}$$

$$= cx + icy. \tag{11.7}$$

(iii) **Product** of complex numbers:

$$z_1 \cdot z_2 = (x_1 + iy_1)(x_2 + iy_2) \tag{11.8}$$

$$= (x_1x_2 - y_1y_2) + i(x_1y_2 + y_1x_2). \tag{11.9}$$

(iv) **Division:**

$$\frac{z_1}{z_2} = \frac{(x_1 + iy_1)}{(x_2 + iy_2)} \tag{11.10}$$

$$= \frac{(x_1 + iy_1)}{(x_2 + iy_2)} \frac{(x_2 - iy_2)}{(x_2 - iy_2)} \tag{11.11}$$

$$= \frac{[(x_1x_2 + y_1y_2) + i(y_1x_2 - x_1y_2)]}{(x_2^2 + y_2^2)}. \tag{11.12}$$

The **conjugate** of a complex number is defined as

$$z^* = x - iy. \tag{11.13}$$

The modulus of a complex number can now be written as

$$r = |z| = \sqrt{zz^*} = \sqrt{x^2 + y^2}. \tag{11.14}$$

The **De Moivre's formula:**

$$\boxed{e^{in\theta} = (\cos\theta + i\sin\theta)^n = \cos n\theta + i\sin n\theta} \tag{11.15}$$

and the following relations:

$$|z_1| - |z_2| \le |z_1 + z_2| \le |z_1| + |z_2|, \tag{11.16}$$

$$|z_1 z_2| = |z_1||z_2|, \tag{11.17}$$

$$\arg\left(z_1 z_2\right) = \arg z_1 + \arg z_2 \tag{11.18}$$

are very useful in calculations with complex numbers.

11.2 Complex Functions

We can define a **complex function**, w, as (Figure 11.2)

$$w = f(z) = u(x, y) + iv(x, y). \tag{11.19}$$

As an example for complex functions, we can give polynomials like

$$f(z) = z^2 = (x + iy)^2 = (x^2 - y^2) + i(2xy), \tag{11.20}$$

$$f(z) = 3z^4 + 2z^3 + 2iz. \tag{11.21}$$

Trigonometric functions and some other well-known functions can also be defined in the complex plane as

$$\sin z, \quad \cos z, \quad \ln z, \quad \sinh z, \quad \sqrt{z}. \tag{11.22}$$

However, as we will see, one must be very careful with multivaluedness.

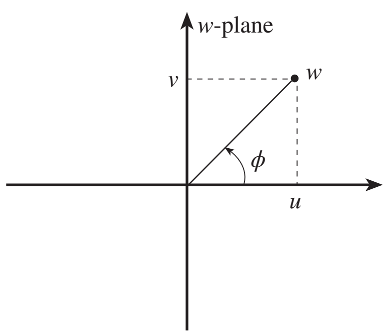


Figure 11.2 A point in the w-plane.

11.3 Complex Derivatives and Cauchy–Riemann Conditions

As in real analysis, we can define the **derivative** of a complex function, $f(z)$, at some point z as

$$\frac{df(z)}{dz} = \lim_{\triangle z\to 0} \frac{f(z+\triangle z)-f(z)}{\triangle z} \tag{11.23}$$

$$= \lim_{\triangle z\to 0} \left[\frac{\triangle u}{\triangle z} + i\frac{\triangle v}{\triangle z}\right]. \tag{11.24}$$

For this derivative to be meaningful, it must be independent of the direction in which the limit $\triangle z \to 0$ is taken. If we approach z parallel to the real axis, $\triangle z = \triangle x$, we find the derivative as

$$\frac{df}{dz} = \frac{\partial u}{\partial x} + i\frac{\partial v}{\partial x}. \tag{11.25}$$

On the other hand, if we approach z parallel to the imaginary axis, $\Delta z = i\Delta y$, the derivative becomes

$$\frac{df}{dz} = -i\frac{\partial u}{\partial y} + \frac{\partial v}{\partial y}. \tag{11.26}$$

For the derivative to exist at z, these two expressions must agree; thus giving the **Cauchy–Riemann conditions** as

$$\boxed{\frac{\partial u(x,y)}{\partial x} = \frac{\partial v(x,y)}{\partial y},} \tag{11.27}$$

$$\boxed{\frac{\partial v(x,y)}{\partial x} = -\frac{\partial u(x,y)}{\partial y},} \tag{11.28}$$

which are **necessary and sufficient.**

11.3.1 Analytic Functions

If the derivative of a function, $f(z)$, exists not only at z_0 but also at every other point in some neighborhood of z_0, then we say that $f(z)$ is **analytic** at z_0.

Example 11.1 ***Analytic functions***
The function $f(z) = z^2 + 5z^3$, like all other polynomials, is analytic in the entire z-plane. On the other hand, even though the function $f(z) = |z|$ satisfies the Cauchy–Riemann conditions at $z = 0$, it is not analytic at any other point in the z-plane.

If a function is analytic in the entire z-plane, it is called an **entire function**. All polynomials are entire functions. If a function is analytic at every point in the neighborhood of z_0 except at z_0, we call z_0 an **isolated singular point**.

Example 11.2 ***Analytic functions***
If we take the derivative of $f(z) = 1/z$, we find $f'(z) = -1/z^2$, which means that $z = 0$ is an isolated singular point of this function. At all other points, this function is analytic.

Theorem 11.1 If $f(z)$ is analytic in some domain of the z-plane, then the partial derivatives of all orders of $u(x, y)$ and $v(x, y)$ exist. The $u(x, y)$ and $v(x, y)$ functions of such a function satisfy the Laplace equations:

$$\vec{\nabla}^2_{xy} u(x,y) = \frac{\partial^2 u(x,y)}{\partial x^2} + \frac{\partial^2 u(x,y)}{\partial y^2} = 0, \tag{11.29}$$

$$\vec{\nabla}^2_{xy} v(x,y) = \frac{\partial^2 v(x,y)}{\partial x^2} + \frac{\partial^2 v(x,y)}{\partial y^2} = 0. \tag{11.30}$$

Proof: We use the first Cauchy–Riemann condition [Eq. (11.27)] and differentiate with respect to x to get

$$\frac{\partial u}{\partial x} = \frac{\partial v}{\partial y}, \tag{11.31}$$

$$\frac{\partial^2 u}{\partial x^2} = \frac{\partial^2 v}{\partial x \partial y}. \tag{11.32}$$

Similarly, we write the second condition [Eq. (11.28)] and differentiate with respect to y to get

$$\frac{\partial v}{\partial x} = -\frac{\partial u}{\partial y}, \tag{11.33}$$

$$\frac{\partial^2 u}{\partial y^2} = -\frac{\partial^2 v}{\partial y \partial x}. \tag{11.34}$$

Adding Eqs. (11.32) and (11.34) gives

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = \frac{\partial^2 v}{\partial x \partial y} - \frac{\partial^2 v}{\partial x \partial y} = 0. \tag{11.35}$$

One can show Eq. (11.30) in exactly the same way. The $u(x, y)$ and $v(x, y)$ functions are called **harmonic functions**, whereas the pair of functions (u, v) are called **conjugate harmonic functions**.

11.3.2 Harmonic Functions

Harmonic functions have very useful properties in applications. Given an analytic function, $w(z) = u(x, y) + iv(x, y)$:

1. The two families of curves defined as $u = c_i$ and $v = d_i$, where c_i and d_i are real numbers, are orthogonal to each other:

$$\vec{\nabla} u \cdot \vec{\nabla} v = \frac{\partial u}{\partial x}\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y}\frac{\partial v}{\partial y} \tag{11.36}$$

$$= \frac{\partial u}{\partial x}\left(-\frac{\partial u}{\partial y}\right) + \left(\frac{\partial u}{\partial y}\right)\left(\frac{\partial u}{\partial x}\right) = 0, \tag{11.37}$$

where we have used the Cauchy–Riemann conditions [Eqs. (11.27) and (11.28)].

2. If we differentiate an analytic function, $w(z)$, we get

$$\frac{dw}{dz} = \left(\frac{\partial u}{\partial x} + i\frac{\partial v}{\partial x}\right)\frac{dx}{dz} + \left(\frac{\partial u}{\partial y} + i\frac{\partial v}{\partial y}\right)\left(\frac{dy}{dz}\right)(-i^2) \tag{11.38}$$

$$= \left(\frac{\partial u}{\partial x} - i\frac{\partial u}{\partial y}\right)\left(\frac{dx + idy}{dz}\right) \tag{11.39}$$

$$= \frac{\partial u}{\partial x} - i\frac{\partial u}{\partial y}, \tag{11.40}$$

the modulus of which is

$$\left|\frac{dw}{dz}\right| = \sqrt{\left(\frac{\partial u}{\partial x}\right)^2 + \left(\frac{\partial u}{\partial y}\right)^2}. \tag{11.41}$$

Harmonic functions are very useful in electrostatics. If we identify $u(x, y)$ as the potential, the electric field, $\vec{E}$, becomes

$$\vec{E} = -\vec{\nabla} u, \tag{11.42}$$

and the magnitude of the electric field is given by the modulus of dw/dz :

$$|\vec{E}| = \left|\frac{dw}{dz}\right|. \tag{11.43}$$

3. If $\Psi(u, v)$ satisfies the Laplace equation in the w-plane:

$$\frac{\partial^2 \Psi(u, v)}{\partial u^2} + \frac{\partial^2 \Psi(u, v)}{\partial v^2} = 0, \tag{11.44}$$

where u and v are conjugate harmonic functions, then $\Psi(x, y)$ will satisfy the Laplace equation in the z-plane:

$$\frac{\partial^2 \Psi(x, y)}{\partial x^2} + \frac{\partial^2 \Psi(x, y)}{\partial y^2} = 0. \tag{11.45}$$

Example 11.3 ***Analytic functions***
Let us discuss the analyticity and the differentiability of the function

$$f(z) = \frac{x^2y^2(x+iy)}{x^2+y^2}. \tag{11.46}$$

We first write the u and v functions as

$$u(x,y) = \frac{x^3y^2}{x^2+y^2}, \tag{11.47}$$

$$v(x,y) = \frac{x^2y^3}{x^2+y^2} \tag{11.48}$$

and then evaluate the following partial derivatives:

$$\frac{\partial u}{\partial x} = \frac{x^2y^2(x^2+3y^2)}{(x^2+y^2)^2}, \quad \frac{\partial u}{\partial y} = \frac{2x^5y}{(x^2+y^2)^2}, \tag{11.49}$$

$$\frac{\partial v}{\partial x} = \frac{2xy^5}{(x^2+y^2)^2}, \quad \frac{\partial v}{\partial y} = \frac{x^2y^2(3x^2+y^2)}{(x^2+y^2)^2}. \tag{11.50}$$

Substituting these into the Cauchy–Riemann conditions:

$$\begin{aligned} \frac{\partial u}{\partial x} &= \frac{\partial v}{\partial y}, \\ \frac{\partial v}{\partial x} &= -\frac{\partial u}{\partial y}, \end{aligned} \tag{11.51}$$

we obtain

$$\frac{x^2y^2(x^2+3y^2)}{(x^2+y^2)^2} = \frac{x^2y^2(3x^2+y^2)}{(x^2+y^2)^2}, \tag{11.52}$$

$$\frac{2xy^5}{(x^2+y^2)^2} = -\frac{2x^5y}{(x^2+y^2)^2}. \tag{11.53}$$

These two conditions can be satisfied simultaneously only at the origin. In conclusion, the derivative exists at the origin but the function is analytic nowhere. This is also apparent from the expression of $f(z)$ as

$$f(z) = -\frac{z}{16(zz^*)}(z+z^*)^2(z-z^*)^2, \tag{11.54}$$

which depends on z^* explicitly.

Important: Cauchy–Riemann conditions are necessary for the derivative to exist at a given point z_0. It is only when the partial derivatives of u and v are continuous at z_0 that they become both necessary and sufficient. In this case, one should check that the partial derivatives of u and v are indeed continuous at $z = 0$, hence the derivative of $f(z)$ [Eq. (11.46)] exists at $z = 0$ [2].

11.4 Mappings

A real function, $y = f(x)$, which defines a curve in the xy-plane, can be interpreted as an **operator** that maps a point on the x-axis to a point on the y-axis (Figure 11.3), which is not very interesting. However, in the complex plane, a function,

$$w = f(z) = u(x, y) + iv(x, y), \tag{11.55}$$

maps a point (x, y) in the z-plane to another point (u, v) in the w-plane, which implies that curves and domains in the z-plane are mapped to other curves and domains in the w-plane. This has rather interesting consequences in applications.

Example 11.4 ***Translation***
Let us consider the function

$$w = z + z_0. \tag{11.56}$$

Since this means

$$u = x + x_0, \tag{11.57}$$

$$v = y + y_0, \tag{11.58}$$

a point (x, y) in the z-plane is mapped into the translated point $(x + x_{0,}\ y + y_0)$ in the w-plane.

Example 11.5 ***Rotation***
Consider the function

$$w = zz_0. \tag{11.59}$$

Using $w = \rho e^{i\phi}$, $z = re^{i\theta}$, and $z_0 = r_0 e^{i\theta_0}$, we write w in plane polar coordinates as

$$\rho e^{i\phi} = rr_0 e^{i(\theta+\theta_0)}. \tag{11.60}$$

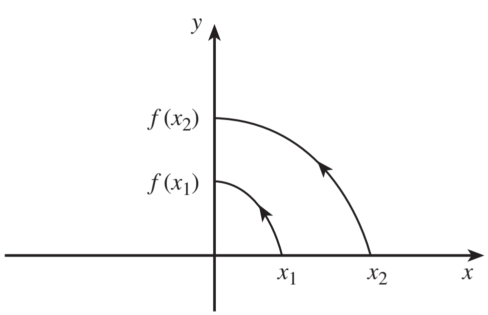


Figure 11.3 It is not interesting to look at real functions as mappings.

In the w-plane, this means,

$$\rho = rr_0, \tag{11.61}$$

$$\phi = \theta + \theta_0. \tag{11.62}$$

Two things have changed:

(i) Modulus r has increased or decreased by a factor r_0.
(ii) Argument θ has changed by θ_0.
If we take $z_0 = i$, this mapping (function) corresponds to a pure rotation by $\pi/2$.

Example 11.6 ***Inversion***
The function

$$w(z) = \frac{1}{z} \tag{11.63}$$

can be written as

$$\rho e^{i\phi} = \frac{1}{re^{i\theta}} = \frac{1}{r}e^{-i\theta}. \tag{11.64}$$

This gives

$$\rho = \frac{1}{r}, \tag{11.65}$$

$$\phi = -\theta, \tag{11.66}$$

which means that a point inside the unit circle in the z-plane is mapped to a point outside the unit circle, plus a reflection about the u-axis in the w-plane (Figure 11.4).

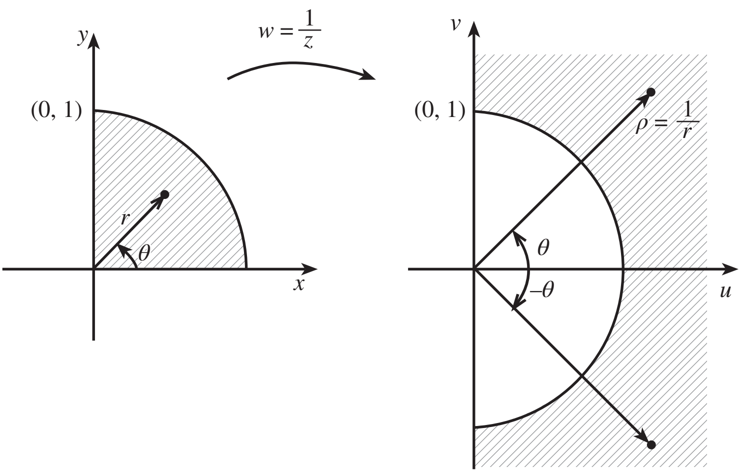


Figure 11.4 Inversion maps circles to circles.

Example 11.7 ***Inversion function***
Let us now see how inversion:

$$w(z) = \frac{1}{z}, \tag{11.67}$$

maps curves in the z-plane to the w-plane. We first write

$$w = u + iv \tag{11.68}$$

$$= \frac{1}{x + iy} \tag{11.69}$$

$$= \frac{1}{x + iy} . \frac{x - iy}{x - iy} \tag{11.70}$$

$$= \frac{x}{\left(x^2 + y^2\right)} - i\frac{y}{\left(x^2 + y^2\right)}. \tag{11.71}$$

This gives us the transformation $(x, y) \rightarrow (u, v)$:

$$u = \frac{x}{x^2 + y^2}, \quad v = \frac{-y}{x^2 + y^2} \tag{11.72}$$

and its inverse as

$$x = \frac{u}{u^2 + v^2}, \quad y = \frac{-v}{u^2 + v^2}. \tag{11.73}$$

We are now ready to see how a circle in the z-plane,

$$x^2 + y^2 = r^2, \tag{11.74}$$

is mapped to the w-plane by inversion. Using Eqs. (11.73) and (11.74), we see that this circle is mapped to

$$\frac{u^2}{(u^2 + v^2)^2} + \frac{v^2}{(u^2 + v^2)^2} = r^2, \tag{11.75}$$

$$u^2 + v^2 = \frac{1}{r^2} = \rho^2, \tag{11.76}$$

which is another circle with the radius $1/r$ or ρ.
Next, let us consider a straight line in the z-plane:

$$y = c_1. \tag{11.77}$$

Using Eq. (11.73), this becomes

$$-\frac{v}{u^2 + v^2} = c_1 \tag{11.78}$$

or

$$u^2 + v^2 + \frac{v}{c_1} + \frac{1}{(2c_1)^2} = \frac{1}{(2c_1)^2}, \tag{11.79}$$

$$u^2 + \left(v + \frac{1}{2c_1}\right)^2 = \frac{1}{(2c_1)^2}. \tag{11.80}$$

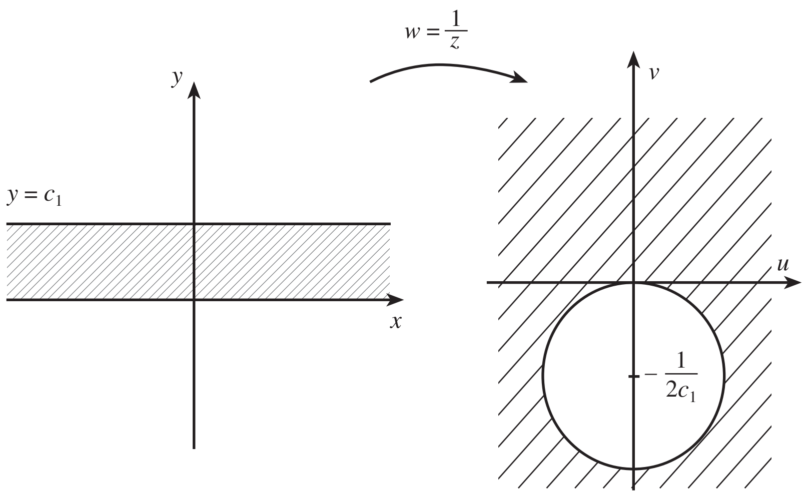


Figure 11.5 Inversion maps straight lines to circles.

This is nothing but a circle with the radius $1/2c_1$ and with its center located at $(0, -1/2c_1)$; thus inversion maps straight lines in the z-plane to circles in the w-plane (Figure 11.5).

All the mappings we have discussed so for are **one-to-one** mappings, that is, a single point in the z-plane is mapped to a single point in the w-plane.

Example 11.8 ***Two-to-one mapping***
We now consider the function

$$w = z^2 \tag{11.81}$$

and write it in plane polar coordinates as

$$w = \rho e^{i\theta}. \tag{11.82}$$

Using $z = re^{i\theta}$, ρ and ϕ become

$$\rho = r^2, \tag{11.83}$$

$$\phi = 2\theta. \tag{11.84}$$

The factor of two in front of the θ is crucial. This means that the first quarter in the z-plane, $0 \leq \theta \leq \frac{\pi}{2}$, is mapped to the upper half of the w-plane, $0 \leq \phi < \pi$. On the other hand, the upper half of the z-plane, $0 \leq \theta < \pi$, is mapped to the entire w-plane, $0 \leq \phi < 2\pi$. In other words, the lower half of the z-plane is mapped to the already covered (used) entire w-plane. Hence, in order to cover the z-plane once, we have to cover the w-plane twice. This is called a **two-to-one** mapping. Two different points in the z-plane,

$$z_0 \tag{11.85}$$

and

$$z_0 e^{-i\pi} = -z_0 \tag{11.86}$$

are mapped to the same point in the w-plane as

$$w = z_0^2. \tag{11.87}$$

We now consider the exponential function

$$w = e^z. \tag{11.88}$$

Writing

$$\rho e^{i\phi} = e^{x+iy}, \tag{11.89}$$

where

$$\rho = e^x \tag{11.90}$$

and

$$\phi = y, \tag{11.91}$$

we see that in the z-plane, the $0 \leq y < 2\pi$ band is mapped to the entire w-plane; thus in the z-plane, all the other parallel bands given as

$$x + i(y + 2n\pi), \quad n \quad \text{integer}, \tag{11.92}$$

are mapped to the already covered w-plane. In this case, we say that we have a **many-to-one** mapping.

Let us now consider the function

$$w = \sqrt{z}, \tag{11.93}$$

In plane polar coordinates, we write

$$\rho e^{i\phi} = \sqrt{r} e^{i\theta/2}, \tag{11.94}$$

thus

$$\rho = \sqrt{r} \text{ and } 2\phi = \theta. \tag{11.95}$$

In this case, the point

$$r = r_0, \quad \theta = 0, \tag{11.96}$$

is mapped to

$$w = \sqrt{r_0}, \tag{11.97}$$

while the point

$$r = r_0, \quad \theta = 2\pi, \tag{11.98}$$

is mapped to

$$w = \sqrt{r_0}e^{i\pi} = -\sqrt{r_0} \tag{11.99}$$

in the w-plane. However, the coordinates (11.96) and (11.98) represent the same point in the z-plane. In other words, a single point in the z-plane is mapped to two distinct points, except at the origin, in the w-plane. This is called a **one-to-two** mapping.

To define a square root as a single-valued function so that for a given value of z a single value of w results, all we have to do is to cut out the $\theta = 2\pi$ line from the z-plane. This line is called the **cut line** or the **branch cut,** and the point $z = 0$, where this line ends, is called the **branch point** (Figure 11.6). What is important here is to find a region in the z-plane where our function is single valued and then extend this region over the entire z-plane without our function becoming multivalued. As seen from Figures 11.7a and b, the problem is at the origin:

$$z = 0. \tag{11.100}$$

For any region that does not include the origin, our function will be single valued. However, for any region that includes the origin, where θ changes between $[0, 2\pi]$, we will run into the multivaluedness problem. In order to extend the region in which our function is single valued, we start with a region R, where our function is single valued, and then extend it without including the origin so that we cover a maximum of the z-plane (Figure 11.7b–f). The only way to do this is to exclude the points on a curve, usually taken as a straight line, that starts from the origin and then extends all the way to infinity.

As seen from Figure 11.8, for the square root, $f(z) = \sqrt{z}$, for any path that does not cross the cut line our function is single valued and the value it takes is called the branch I value:

$$\text{I. branch} \qquad w_1(z) = \sqrt{r}e^{\theta/2}, \quad 0 \le \theta < 2\pi.$$

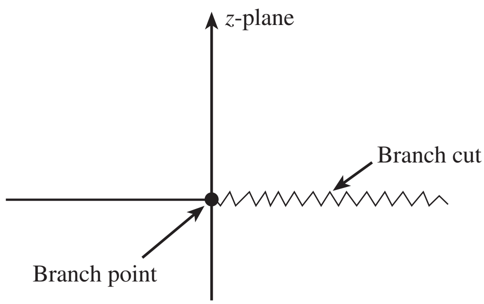


Figure 11.6 Cut line ends at a branch point.

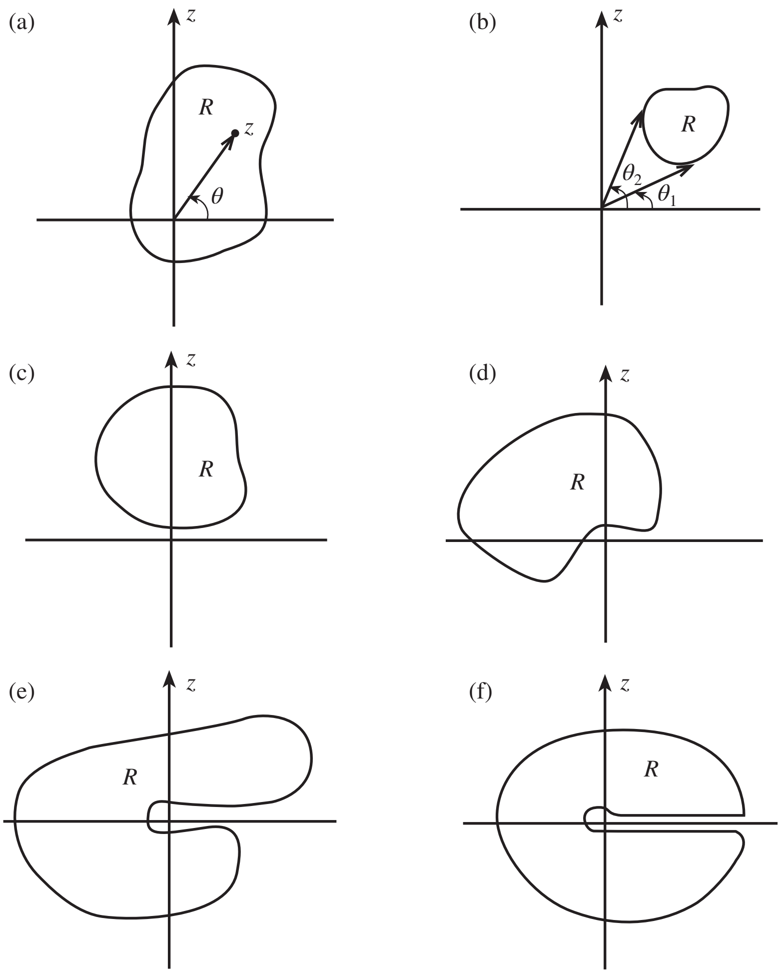


Figure 11.7 (a) For every point z in every region R that contains the origin, θ has the full range $[0, 2\pi]$, hence $\sqrt{z}$ is multivalued. (b) For every region R that does not include the origin, $\sqrt{z}$ is single valued. (b)–(f) For a single valued definition of the function $w = \sqrt{z}$, we extend the region R in (b) without including the origin.

For the range $2\pi \leq \theta < 4\pi$, since the cut line is crossed once, our function will take the branch II value given as

$$\text{II. branch} \qquad w_2(z) = -\sqrt{r}e^{\theta/2}, \quad 2\pi \leq \theta < 4\pi.$$

Square root function has two branch values. In cases where θ increases continuously, as in rotation problems, we switch from one branch value to another

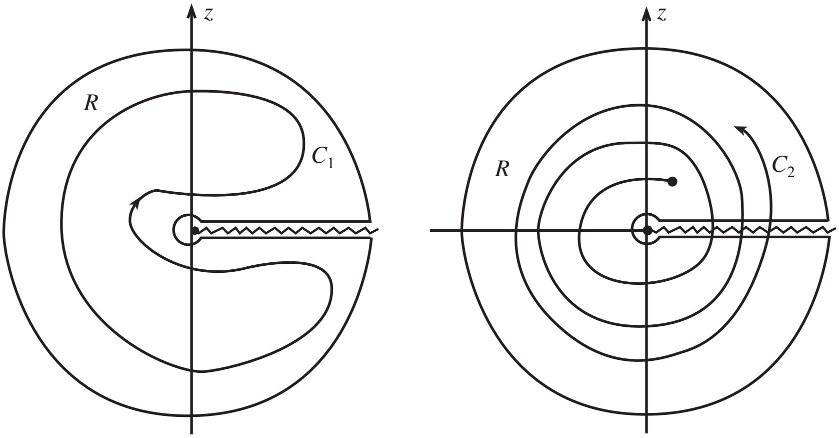


Figure 11.8 Each time we cross the cut line, $w = z^{1/2}$ changes from one branch value to another.

each time we cross over the cut line. This situation can be conveniently shown by the **Riemann sheets** (Figure 11.9).

Riemann sheets for this function are two parallel sheets sewn together along the cut line. As long as we remain in one of the sheets, our function is single valued and takes only one of the branch values. Whenever we cross the cut line, we find ourselves on the other sheet and the function switches to the other branch value.

Example 11.9 $\quad w(z) = \ln z$ ***function***
In the complex plane, the ln function is defined as

$$w(z) = \ln z = \ln r + i\theta. \tag{11.101}$$

It has infinitely many branches; thus infinitely many Riemann sheets as

$$\begin{array}{ll} \text{branch } 0 & w_0(z) = \ln r + i\theta, \\ \text{branch } 1 & w_1(z) = \ln r + i(\theta + 1(2\pi)), \\ \text{branch } 2 & w_2(z) = \ln r + i(\theta + 2(2\pi)), \\ \vdots & \vdots \\ \text{branch } n & w_n(z) = \ln r + i(\theta + n(2\pi)), \end{array} \tag{11.102}$$

where $0 \leq \theta < 2\pi, \quad n = 0, 1, 2, \ldots$.

Example 11.10 $\quad w(z) = \sqrt{z^2 - 1}$ ***function***
To investigate the branches of the function

$$w(z) = \sqrt{z^2 - 1}, \tag{11.103}$$

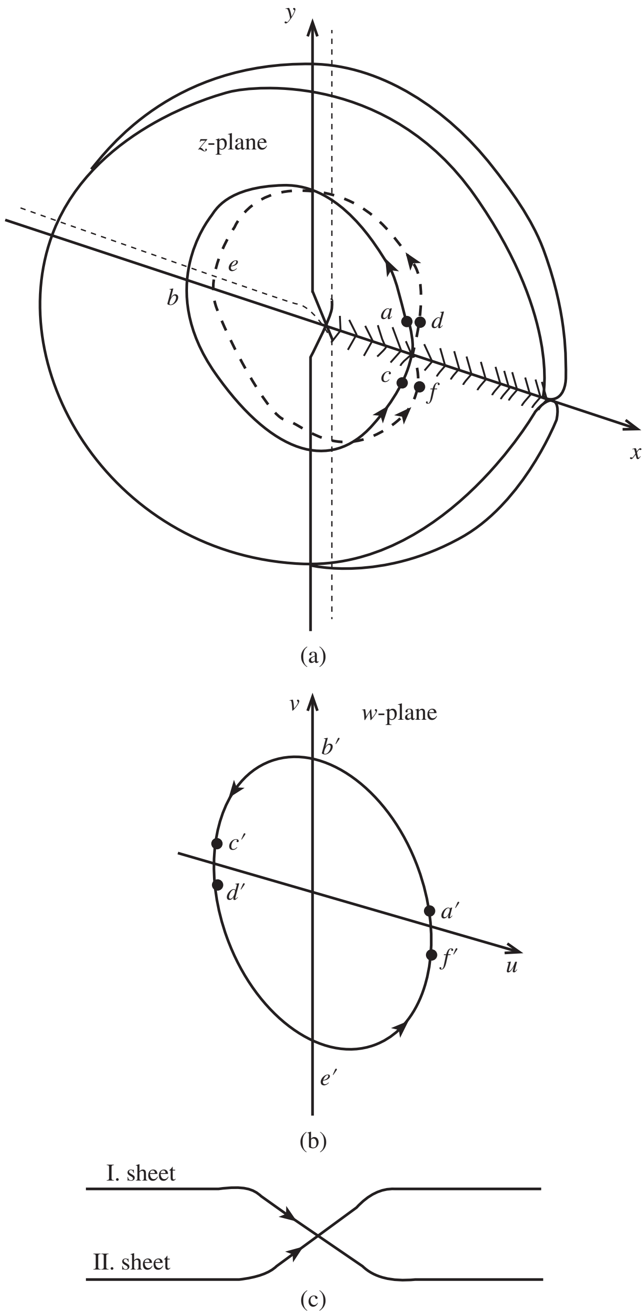


Figure 11.9 Riemann sheets for the $w = z^{1/2}$ function.

we define

$$(z-1)=r_1e^{i\theta_1}\,,\quad (z+1)=r_2e^{i\theta_2} \tag{11.104}$$

and write

$$w(z)=\rho e^{i\phi} \tag{11.105}$$

$$=\sqrt{(z-1)(z+1)} \tag{11.106}$$

$$=\sqrt{r_1r_2}e^{i(\theta_1+\theta_2)/2}. \tag{11.107}$$

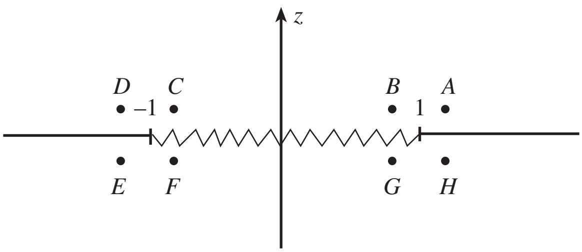
This function has two branch points located at $x=+1$ and $x=-1$. We place the cut lines along the real axis and to the right of the branch points. This choice gives the ranges of θ_1 and θ_2 as

$$0\le\theta_1<2\pi, \tag{11.108}$$

$$0\le\theta_2<2\pi. \tag{11.109}$$

We now investigate the limits of the points A, B, C, D, F, G, H in the z-plane as they approach the real axis and the corresponding points in the w-plane (Figure 11.10):

Figure 11.10 Cut lines for $\sqrt{z^2-1}$.



(11.110)

Point	θ_1	θ_2	ϕ	$\sqrt{z^2-1}$
A	0	0	0	single valued
H	2π	2π	2π	single valued
B	π	0	$\pi/2$	double valued
G	π	2π	$3\pi/2$	double valued
C	π	0	$\pi/2$	double valued
F	π	2π	$3\pi/2$	double valued
D	π	π	π	single valued
E	π	π	π	single valued

Points A and H, which approach the same point in the z-plane, also go to the same point in the w-plane. In other words, where the two cut lines overlap our

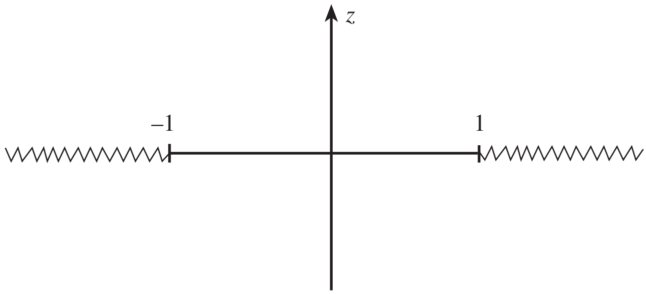


Figure 11.11 A different choice for the cut lines of $\sqrt{z^2 - 1}$.

function is single valued. For pairs (B, G) and (C, F), even though the corresponding points approach the same point in the z-plane, they are mapped to different points in the w-plane. For points D and E, the function is again single valued. For this case, the cut lines are now shown as in Figure 11.10. The first and second branch values for this function are given as

$$w_1(z) = \sqrt{r_1 r_2} e^{i(\theta_1+\theta_2)/2}, \tag{11.111}$$

$$w_2(z) = \sqrt{r_1 r_2} e^{i(\theta_1+\theta_2+2\pi)/2}. \tag{11.112}$$

Riemann sheets for this function will be two parallel sheets sewn together in the middle between points −1 and +1.

For this function, another choice for the cut lines is given as in Figure 11.11, where

$$0 \le \theta_1 < 2\pi, \tag{11.113}$$

$$-\pi \le \theta_2 < \pi. \tag{11.114}$$

Example 11.11 ***Mappings***

We now find the Riemann surfaces on which the function

$$w = \sqrt[3]{(z-1)(z-2)(z-3)} \tag{11.115}$$

is single valued. We have discussed the square root function, $w = \sqrt{z}$, in detail, which has a branch point at $z = 0$ and two branch values:

$$w = \sqrt{r} e^{i(\theta+2\pi k)/2}, \tag{11.116}$$

where $0 \le \theta < 2\pi$ and $k = 0, 1$. In general, the function

$$w = z^{1/n} \tag{11.117}$$

has a single branch point at $z = 0$, but n branch values given by

$$w = \sqrt[n]{r} e^{i(\theta+2\pi k)/n}, \quad 0 \le \theta < 2\pi, \quad k = 0, 1, \dots, n-1. \tag{11.118}$$

In the case of the square root function, there are two Riemann sheets connected along the branch cut (Figure 11.9). For both of the above cases [Eqs. (11.116) and (11.118)], branch cuts are chosen to be along the positive real axis. For $w = z^{1/n}$, there are n Riemann sheets connected along the cut line. For the function,

$$w = \sqrt[n]{z - z_0}\ , \tag{11.119}$$

the situation is not very different. There are n Riemann sheets connected along a suitably chosen branch cut, which ends at the branch point z_0. For the function,

$$w = \sqrt[3]{z - z_0}\ , \tag{11.120}$$

for a full revolution about z_0 in the z-plane, where θ goes from 0 to 2π, the corresponding point in the w-plane completes only 1/3 of a revolution, where ϕ changes from 0 to $2\pi/3$. In other words, for a single revolution in the w-plane, one has to complete three revolutions in the z-plane. In this case, the three branch values are given as

$$w = \sqrt[3]{r}e^{i(\theta+2\pi k)/3}, \quad 0 \le \theta < 2\pi,\ k = 0, 1, 2, \tag{11.121}$$

where $r = |z - z_0|$. To avoid multiple revolutions in the z-plane, we need three Riemann sheets. For the function at hand:

$$w = \sqrt[3]{(z-1)(z-2)(z-3)}, \tag{11.122}$$

we have three branch points located at the points

$$z_1 = 1, \quad z_2 = 1, \quad z_3 = 1. \tag{11.123}$$

We choose the branch cuts to be along the real axis and to the right of the corresponding branch point as shown in Figure 11.12. We can now write

$$z - 1 = r_1 e^{i\theta_1}, \tag{11.124}$$

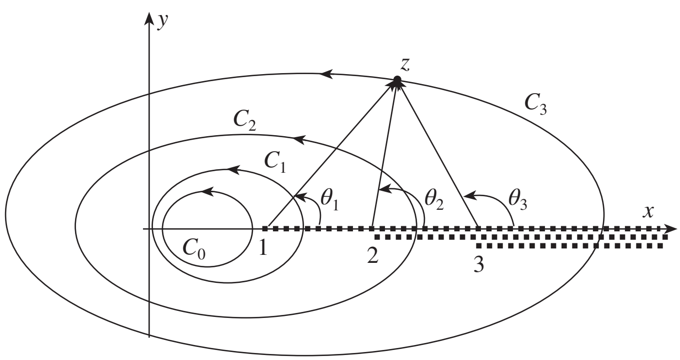


Figure 11.12 Branch cuts for Example 11.11.

$$z - 2 = r_2 e^{i\theta_2}, \tag{11.125}$$

$$z - 3 = r_3 e^{i\theta_3}, \tag{11.126}$$

where $0 \leq \theta_1, \theta_2, \theta_3 < 2\pi$. The corresponding branch values for the cube root function are now given as

$$\sqrt[3]{z-1} = \sqrt[3]{r_1}\ e^{i(\theta_1+2\pi k)/3}, \quad 0 \leq \theta_1 < 2\pi, \quad k = 0, 1, 2, \tag{11.127}$$

$$\sqrt[3]{z-2} = \sqrt[3]{r_2}\ e^{i(\theta_2+2\pi l)/3}, \quad 0 \leq \theta_2 < 2\pi, \quad l = 0, 1, 2, \tag{11.128}$$

$$\sqrt[3]{z-3} = \sqrt[3]{r_3}\ e^{i(\theta_3+2\pi m)/3}, \quad 0 \leq \theta_3 < 2\pi, \quad m = 0, 1, 2. \tag{11.129}$$

Hence for

$$w = \sqrt[3]{(z-1)(z-2)(z-3)} = \rho e^{i\phi}, \tag{11.130}$$

where

$$\rho = \sqrt[3]{r_1 r_2 r_3}, \quad \phi = (\theta_1 + \theta_2 + \theta_3)/3, \tag{11.131}$$

the branch values are given as

$$w = \sqrt[3]{r_1 r_2 r_3}\ e^{i(\theta+2\pi(k+l+m))/3}, \tag{11.132}$$

where k, l, m take the values

$$k = 0, 1, 2, \tag{11.133}$$

$$l = 0, 1, 2, \tag{11.134}$$

$$m = 0, 1, 2. \tag{11.135}$$

For points on a closed path, C_0, that does not include any of the branch points, the function [Eq. (11.122)] is single valued and takes its first branch value, that is, $k = l = m = 0$. For the path C_1, only one of the branch points, $z = 1$, is within the path, hence there are three branch values corresponding to the (k, l, m) values

$$(k, l, m) = \begin{cases} (0, 0, 0), \\ (1, 0, 0), \\ (2, 0, 0). \end{cases} \tag{11.136}$$

For the path C_2, both $z = 1$ and $z = 2$ are within the path, hence when we complete a full circuit, we cross over both of the branch cuts. In this case, the three branch values are given by

$$(k, l, m) = \begin{cases} (0, 0, 0), \\ (1, 1, 0), \\ (2, 2, 0). \end{cases} \tag{11.137}$$

For the third path C_3, all three of the branch points are within the path, hence to complete a full circuit, one has to cross over all three of the branch cuts. In this

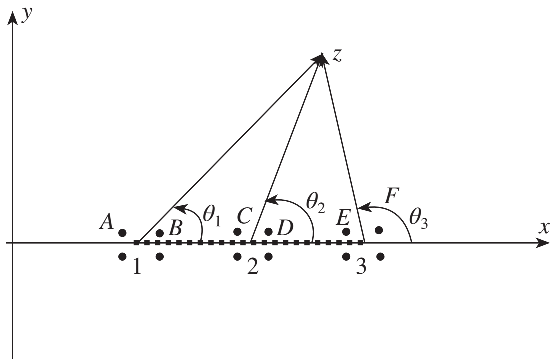


Figure 11.13 Points below the real axis, which are symmetric to A, B, C, D, E, F, are A', B', C', D', E', F', respectively.

case, the function is single valued and (k, l, m) take the values

$$(k, l, m) = \begin{cases} (0, 0, 0), \\ (1, 1, 1), \\ (2, 2, 2). \end{cases} \tag{11.138}$$

In other words, for the points to the right of $z = 3$, the three branch cuts combine to cancel each other's effect, thus producing a single valued function (Figure 11.13). To see the situation along the real axis, where the branch cuts overlap, we construct the following table, where the points are defined as in Figure 11.13:

Point\angle	θ_1	θ_2	θ_3	ϕ
A	π	π	π	π
B	0	π	π	$2\pi/3$
C	0	π	π	$2\pi/3$
D	0	0	π	$\pi/3$
E	0	0	π	$\pi/3$
F	0	0	0	0
A'	π	π	π	π
B'	2π	π	π	$4\pi/3$
C'	2π	π	π	$4\pi/3$
D'	2π	2π	π	$5\pi/3$
E'	2π	2π	π	$5\pi/3$
F'	2π	2π	2π	$6\pi/3$

, (11.139)

which gives

A, A'	Same pt. in the ω-plane.	
B, B'	Not single valued.	
C, C'	Not single valued.	
D, D'	Not single valued.	(11.140)
E, E'	Not single valued.	
F, F'	Same pt. in the ω-plane.	

From this table, we see that the 3 Riemann sheets are sewn together along the dotted lines between the points $z = 1$ and $z = 3$ as shown in Figure 11.13.

11.4.1 Conformal Mappings

To see an interesting property of analytic functions, we differentiate

$$w = f(z) \tag{11.141}$$

at z_0, where the modulus and the arguments of the derivative are given as $\left|\frac{df}{dz}\right|_{z_0}$ and α, respectively. We now use polar coordinates to write the modulus:

$$\lim_{\Delta z\to 0}\left|\frac{\Delta w}{\Delta z}\right| = \left|\frac{dw}{dz}\right|_{z_0} \tag{11.142}$$

$$= \left|\frac{df}{dz}\right|_{z_0}, \tag{11.143}$$

and the argument (Figure 11.14) as

$$\arg \left.\frac{df}{dz}\right|_{z_0} = \alpha = \arg \lim_{\Delta z\to 0}\left(\frac{\Delta w}{\Delta z}\right), \tag{11.144}$$

$$\alpha = \lim_{\Delta z\to 0} \arg[\Delta w] - \lim_{\Delta z\to 0} \arg[\Delta z]. \tag{11.145}$$

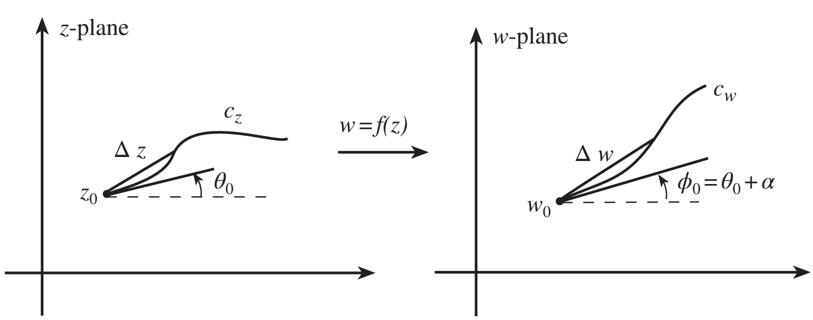


Figure 11.14 Angles in conformal mapping.

Since the function $f(z)$ maps a curve, c_z, in the z-plane to another curve, c_w, in the w-plane, from the arguments [Eq. (11.145)], we see that if the slope of c_z at z_0 is θ_0, then the slope of c_w at w_0 is$\alpha + \theta_0$. For a pair of curves intersecting at z_0, the angle between their tangents in the w- and z-planes will be equal:

$$\phi_2 - \phi_1 = (\theta_2 + \alpha) - (\theta_1 + \alpha) \tag{11.146}$$

$$= \theta_2 - \theta_1. \tag{11.147}$$

Since analytic functions **preserve angles** between the curves they map (Figure 11.14), they are called **conformal mappings** or **transformations**.

11.4.2 Electrostatics and Conformal Mappings

Conformal mappings are very useful in electrostatic and laminar (irrotational) flow problems, where the Laplace equation must be solved. Even though the method is restricted to cases with one translational symmetry, it allows analytic solution of some complex boundary value problems.

Example 11.12 ***Conformal mappings and electrostatics***
Let us consider two conductors held at potentials V_1 and V_2 with hyperbolic cross sections

$$x^2 - y^2 = c_1 \text{ and } x^2 - y^2 = c_2. \tag{11.148}$$

We want to find the equipotentials and the electric field lines. In the complex z-plane, the problem can be shown as in Figure 11.15. We use the conformal mapping

$$w = z^2 = x^2 - y^2 + i(2xy), \tag{11.149}$$

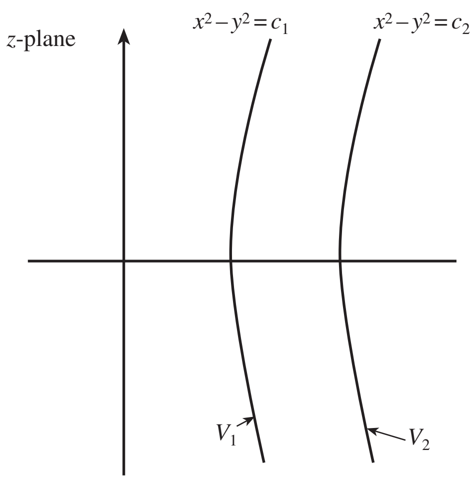


Figure 11.15 Two plates with hyperbolic cross sections.

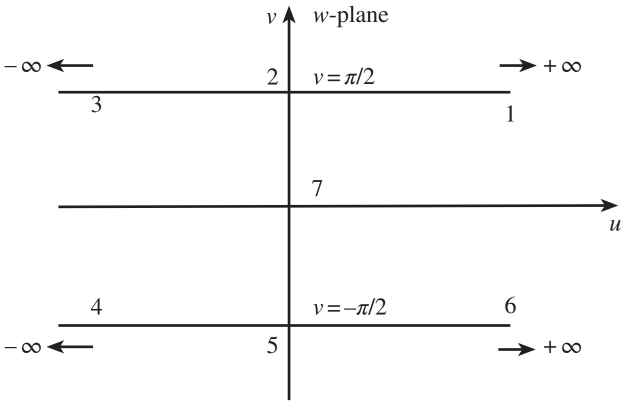


Figure 11.16 Equipotentials and electric field lines in the w-plane.

to map these hyperbolae to straight lines,

$$u = c_1 \text{ and } u = c_2, \tag{11.150}$$

in the w-plane (Figure 11.16). The problem is now reduced to finding the equipotentials and the electric field lines between two infinitely long parallel plates held at potentials V_1 and V_2, where the electric field lines are given by the family of lines:

$$v = C_j \tag{11.151}$$

and the equipotentials are given by the lines perpendicular to these as

$$u = c_i. \tag{11.152}$$

Because the problem is in the z-plane, we make the inverse transformation to obtain the electric field lines:

$$(v =)\ 2xy = C_j \tag{11.153}$$

and the equipotentials as

$$(u =)\ x^2 - y^2 = c_i. \tag{11.154}$$

To find the equipotential surfaces in three dimensions, these curves must be extended along the direction of the normal to the plane of the paper.

Example 11.13 ***Electrostatics and conformal mappings***
We now find the equipotentials and the electric field lines inside two conductors with semicircular cross sections separated by an insulator and held at potentials $+V_0$ and $-V_0$, respectively (Figure 11.17). The equation of a circle in the z-plane is given as

$$x^2 + y^2 = 1. \tag{11.155}$$

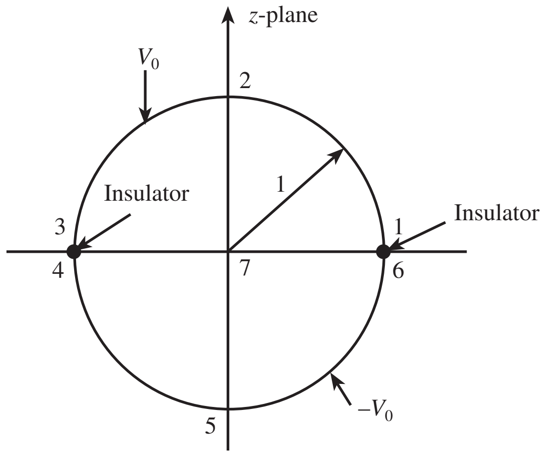


Figure 11.17 Two conductors with semicircular cross sections.

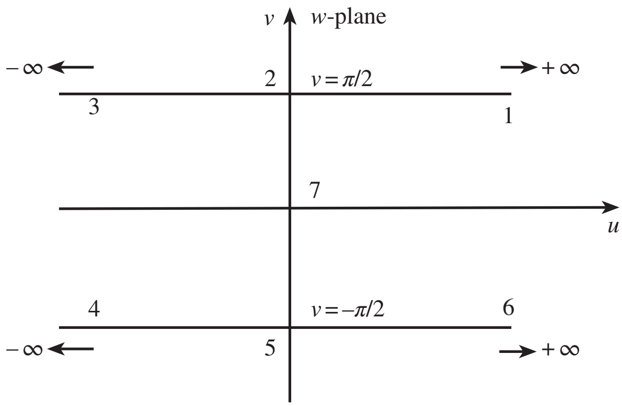


Figure 11.18 Two semicircular conductors in the *w*-plane.

We use the conformal mapping

$$w(z) = \ln\left(\frac{1+z}{1-z}\right), \tag{11.156}$$

to map these semicircles into straight lines in the w-plane (Figure 11.18). Using Eq. (11.156), we write

$$u + iv = \ln\frac{1+x+iy}{1-x-iy} \tag{11.157}$$

$$= \ln\left[\frac{1-x^2-y^2+2iy}{1-2x+x^2+y^2}\right] \tag{11.158}$$

and express the argument of the ln function as $Re^{i\alpha}$:

$$u + iv = \ln R + i\alpha. \tag{11.159}$$

Now the v function is found as

$$v = \alpha \tag{11.160}$$

$$= \tan^{-1}\frac{2y}{1-(x^2+y^2)}. \tag{11.161}$$

From the limits,

$$\lim_{\substack{x^2+y^2\to 1\\ y>0}}\left[\tan^{-1}\frac{2y}{1-(x^2+y^2)}\right] = \frac{\pi}{2} \tag{11.162}$$

and

$$\lim_{\substack{x^2+y^2\to 1\\ y<0}}\left[\tan^{-1}\frac{2y}{1-(x^2+y^2)}\right] = -\frac{\pi}{2}, \tag{11.163}$$

we see that the two semicircles in the z-plane are mapped to two straight lines given as

$$v = \frac{\pi}{2} \text{ and } v = -\frac{\pi}{2}. \tag{11.164}$$

Equipotential surfaces in the w-plane can now be written easily as

$$V(v) = \frac{2V_0}{\pi}v. \tag{11.165}$$

Using Eq. (11.161), we transform this into the z-plane to find the equipotentials:

$$V = \frac{2V_0}{\pi}\tan^{-1}\left[\frac{2y}{1-(x^2+y^2)}\right] \tag{11.166}$$

$$= \frac{2V_0}{\pi}\tan^{-1}\left[\frac{2r\sin\theta}{1-r^2}\right]. \tag{11.167}$$

Because this problem has translational symmetry perpendicular to the plane of the paper, equipotential surfaces in three dimensions can be found by extending these curves in that direction. The solution to this problem has been found rather easily and in closed form. Compare this with the separation of variables method, where the solution is given in terms of the Legendre polynomials as an infinite series. However, applications of conformal mapping are limited to problems with one translational symmetry, where the problem can be reduced to two dimensions. Even though there are tables [3] of conformal mappings, it is not always easy as in this case to find an analytic expression for the needed mapping.

11.4.3 Fluid Mechanics and Conformal Mappings

For laminar (irrotational) and frictionless flow, conservation of mass is given as the continuity equation

$$\frac{\partial\rho}{\partial t} + \vec{\nabla}\cdot(\rho\vec{v}) = 0, \tag{11.168}$$

where $\rho(\vec{r}, t)$ and $\vec{v}(\vec{r}, t)$ represent the density and the velocity of a fluid element. For stationary flow $\partial\rho/\partial t = 0$, thus Eq. (11.168) becomes

$$\vec{\nabla} \cdot (\rho\vec{v}) = 0. \tag{11.169}$$

Also, a lot of realistic situations can be approximated by the incompressible fluid equation of state $\rho =$ constant. This further reduces Eq. (11.169) to

$$\vec{\nabla} \cdot \vec{v} = 0. \tag{11.170}$$

This equation alone is not sufficient to determine the velocity field $\vec{v}(\vec{r}, t)$. If the flow is irrotational, it will also satisfy

$$\vec{\nabla} \times \vec{v} = 0, \tag{11.171}$$

thus the two equations:

$$\vec{\nabla} \cdot \vec{v} = 0, \tag{11.172}$$

$$\vec{\nabla} \times \vec{v} = 0, \tag{11.173}$$

completely specify the kinematics of laminar, frictionless flow of incompressible fluids. These equations are also the expressions of the linear and angular momentum conservation laws for the fluid elements. Fluid elements in laminar flow follow streamlines, where the velocity, $\vec{v}(\vec{r}, t)$, at a given point is tangent to the streamline at that point.

Equations (11.172) and (11.173) are the same as Maxwell's equations in electrostatics. Following the definition of electrostatic potential, we use Eq. (11.173) to define a **velocity potential** as

$$\vec{v}(\vec{r}, t) = \vec{\nabla}\Phi(\vec{r}, t). \tag{11.174}$$

Substituting this into Eq. (11.172), we obtain the Laplace equation:

$$\vec{\nabla}^2 \Phi(\vec{r}, t) = 0. \tag{11.175}$$

We should note that even though $\Phi(\vec{r}, t)$ is known as the velocity potential, it is very different from the electrostatic potential.

Example 11.14 ***Flow around an obstacle of height h***
Let us consider laminar flow around an infinitely long and thin obstacle of height h. Since the problem has translational symmetry, we can treat it in two dimensions as in Figure 11.19, where we search for a solution of the Laplace equation in the region R.

Even though the velocity potential satisfies the Laplace equation like the electrostatic potential, we have to be careful with the boundary conditions. In electrostatics, electric field lines are perpendicular to the equipotentials; hence the test particles can only move perpendicular to the conducting surfaces. In the

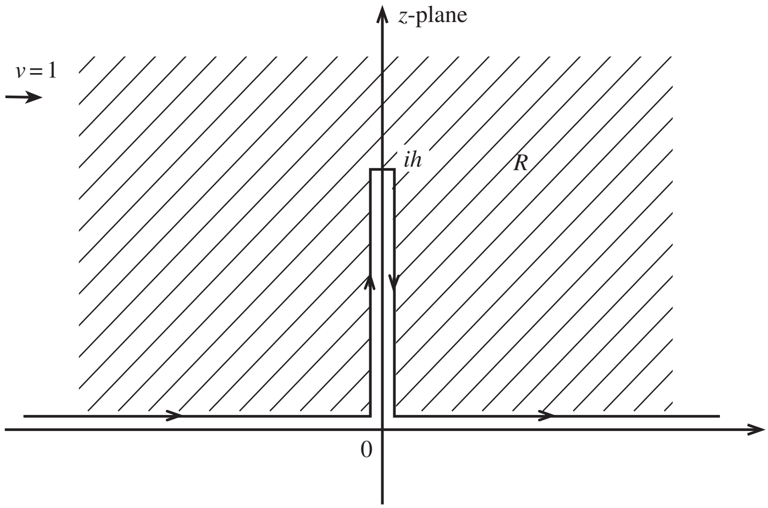


Figure 11.19 Flow around a wall of height *h*.

laminar flow case, where the fluid elements follow the contours of the bounding surfaces, motion perpendicular to the surfaces is not allowed. For points far away from the obstacle, we take the flow lines as parallel to the x-axis. As we approach the obstacle, the flow lines follow the contours of the surface. For points away from the obstacle, we set $v_\infty = 1$. We now look for a transformation that maps the region R in the z-plane to the upper half of the w-plane. Naturally, the lower boundary of the region R in Figure 11.19 will be mapped to the real axis of the w-plane. We now construct this transformation in three steps: We first use

$$w_1 = z^2 \tag{11.176}$$

to map the region R to the entire w_1-plane. Here, the obstacle is between 0 and $-h^2$. As our second step, we translate the obstacle to the interval between 0 and h^2 by

$$w_2 = z^2 + h^2. \tag{11.177}$$

Finally, we map the w_2-plane to the upper half of the w-plane by

$$w = \sqrt{w_2}. \tag{11.178}$$

The complete transformation from the z-plane to the w-plane can be written as (Figure 11.20)

$$w = \sqrt{z^2 + h^2}. \tag{11.179}$$

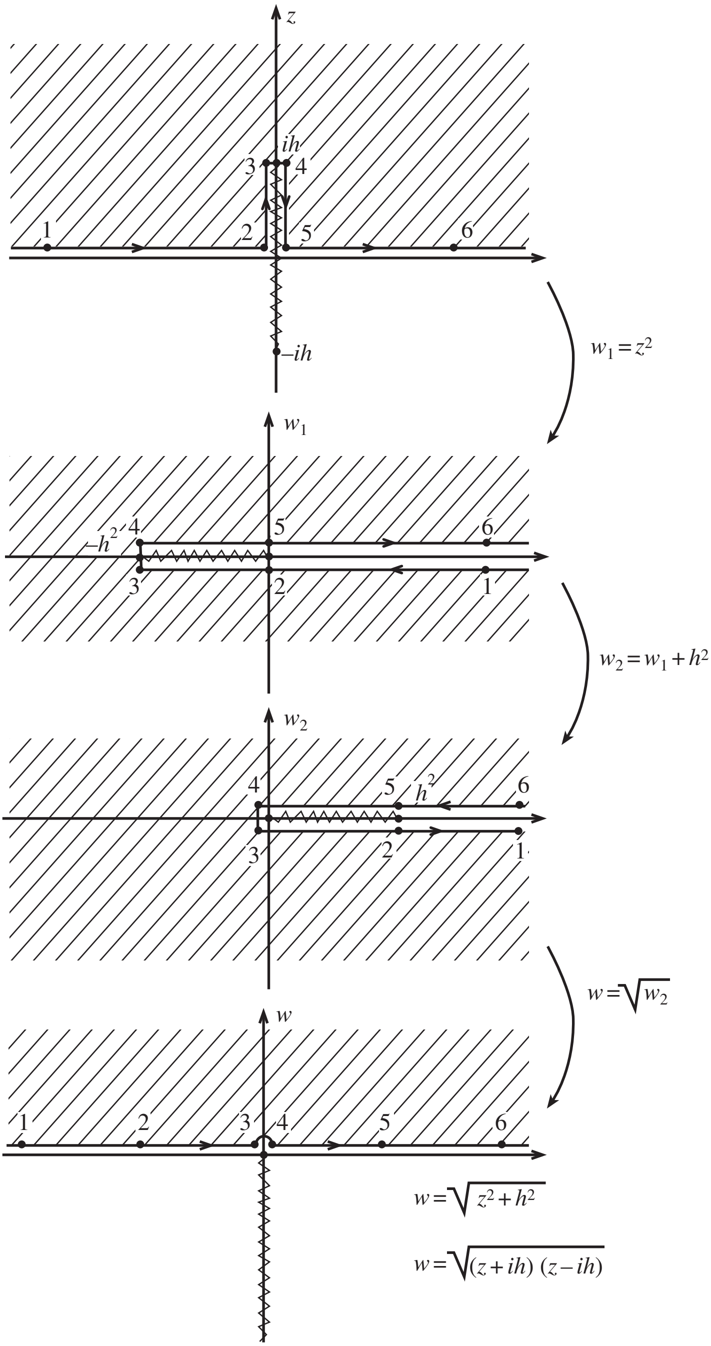


Figure 11.20 Transition from the z-plane to the w-plane.

The Laplace equation can now be easily solved in the upper half of the w-plane, yielding the streamlines as

$$v = c_j. \tag{11.180}$$

Curves perpendicular to the streamlines gives the velocity equipotentials as

$$u = b_j. \tag{11.181}$$

Transforming back to the z-plane, we find the streamlines as the curves

$$c_j = \mathrm{Im}\left[\sqrt{z^2 + h^2}\right], \tag{11.182}$$

and the velocity of the fluid elements that are tangents to the streamlines (Figure 11.21) as

$$|\vec{v}| = \left|\frac{dw}{dz}\right|. \tag{11.183}$$

Example 11.15 ***Mappings***
We now show that the transformation

$$w = \frac{z+1}{1-z}, \tag{11.184}$$

maps the following region:

$$x \le 0, \quad -\infty < y < \infty, \tag{11.185}$$

to the unit disc in the w-plane. We first use the general expression

$$w = \frac{az+b}{cz+d} \tag{11.186}$$

and its inverse

$$z = \frac{dw-b}{-cw+a}, \tag{11.187}$$

to write

$$z = \frac{w-1}{w+1}. \tag{11.188}$$

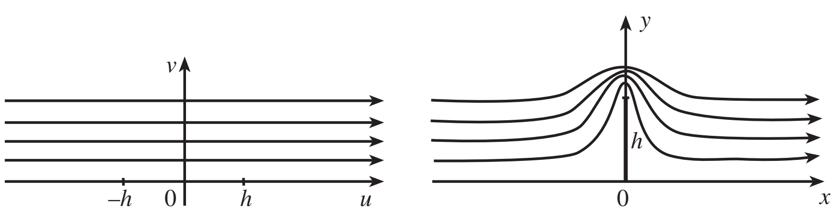


Figure 11.21 Streamlines in the w and z-planes.

Using $w = u + iv$, we write

$$x + iy = \frac{(u-1)+iv}{(u+1)+iv} \cdot \frac{(u+1)-iv}{(u+1)-iv} \tag{11.189}$$

$$= \frac{(u^2+v^2-1)+i(2v)}{(u+1)^2+v^2} \tag{11.190}$$

and obtain the following relations:

$$x = \frac{(u^2+v^2-1)}{(u+1)^2+v^2}, \quad y = \frac{2v}{(u+1)^2+v^2}. \tag{11.191}$$

For $x \leq 0$, these imply

$$u^2 + v^2 \leq 1, \tag{11.192}$$

which is the unit disc with its center located at the origin.

Example 11.16 ***Mappings***

We now determine the image of the horizontal strip:

$$-\pi/2 < \text{Im } z < \pi/2, \tag{11.193}$$

under the transformation

$$w = \frac{e^z - 1}{e^z + 1}. \tag{11.194}$$

We first write the inverse of the above mapping:

$$e^z = \frac{w+1}{1-w}, \tag{11.195}$$

and then rewrite it as

$$e^x e^{iy} = \frac{(u+1)+iv}{(1-u)-iv}, \tag{11.196}$$

$$e^x(\cos y + i \sin y) = \frac{(1-u^2-v^2)+2iv}{(1-u)^2+v^2}. \tag{11.197}$$

For $y = \pm\pi/2$, this gives

$$\pm i e^x = \frac{(1-u^2-v^2)+2iv}{(1-u)^2+v^2}, \tag{11.198}$$

which implies the unit circle:

$$1 = u^2 + v^2. \tag{11.199}$$

We can find the images of the points A, B, C, D, E, F as A', B', C', D', E', F', respectively (Figure 11.22). Also see Example 11.13.

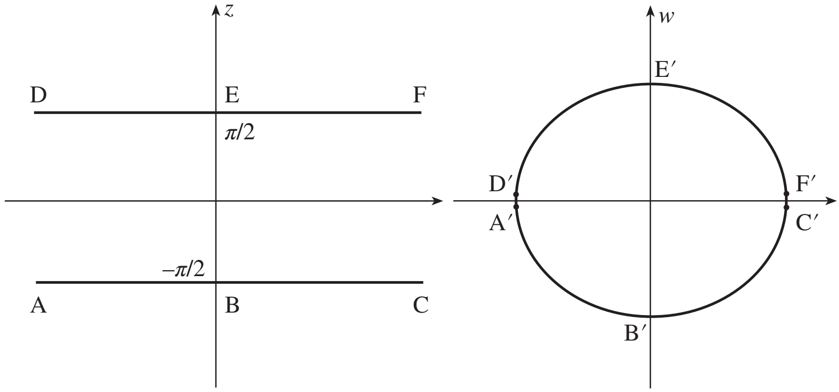


Figure 11.22 Mapping for Example 11.16.

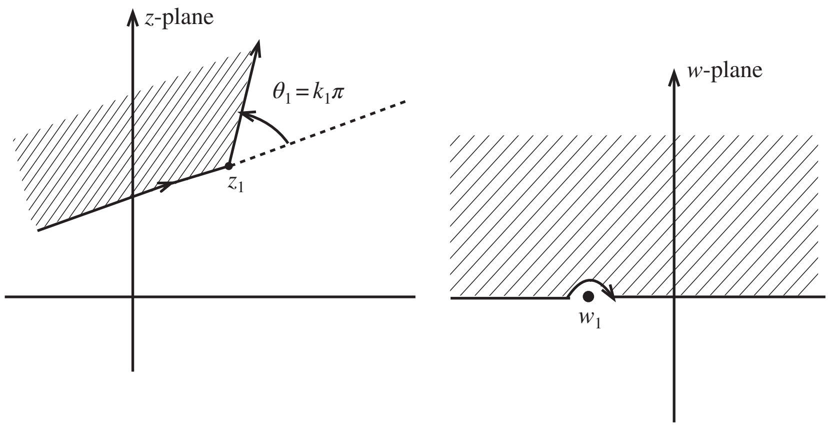


Figure 11.23 Schwarz–Christoffel transformation maps the inside of a polygon to the upper half of the w-plane.

11.4.4 Schwarz–Christoffel Transformations

We have seen that analytic transformations are also conformal mappings, which preserve angles. We now introduce the **Schwarz–Christoffel** transformations, where the transformation is not analytic at isolated number of points. Schwarz–Christoffel transformations map the inside of a polygon in the z-plane, to the upper half of the w-plane (Figure 11.23). To construct the Schwarz–Christoffel transformation, let us consider the function

$$\frac{dz}{dw} = A(w - w_1)^{-k_1}, \tag{11.200}$$

where A is complex, k_1 is real, and w_1 is a point on the u-axis. Comparing the arguments of both sides in Eq. (11.200), we get

$$\arg\left(\frac{dz}{dw}\right) = \lim_{\Delta w\to 0}[\arg\Delta z - \arg\Delta w], \tag{11.201}$$

$$\lim_{\Delta w\to 0}[\arg\Delta z - \arg\Delta w] = \begin{cases} \arg A - k_1\pi, & w < w_1, \\ \arg A, & w > w_1. \end{cases} \tag{11.202}$$

As we move along the positive u-axis

$$\lim_{\Delta w\to 0}\arg\Delta w = \arg[dw] = 0, \tag{11.203}$$

hence we can write

$$\lim_{\Delta w\to 0}[\arg\Delta z] = \arg[dz] = \begin{cases} \arg A - k_1\pi, & w < w_1, \\ \arg A, & w > w_1. \end{cases} \tag{11.204}$$

For a constant A, this means that the transformation [Eq. (11.200)] maps the parts of the u-axis; $w < w_1$ and $w > w_1$, to two line segments meeting at z_0 in the z-plane. Thus

$$A(w - w_1)^{-k_1} \tag{11.205}$$

corresponds to one of the vertices of a polygon with the exterior angle $k_1\pi$ and located at z_1. For a polygon with n-vertices, we can write the **Schwarz–Christoffel transformation** as

$$\boxed{\frac{dz}{dw} = A(w - w_1)^{-k_1}(w - w_2)^{-k_2}\cdots(w - w_n)^{-k_n}.} \tag{11.206}$$

Because the exterior angles of a polygon add up to 2π, powers, k_i, should satisfy the condition

$$\boxed{\sum_{i=1} k_i = 2.} \tag{11.207}$$

Integrating Eq. (11.206), we get

$$z = A\int^w (w - w_1)^{-k_1}(w - w_2)^{-k_2}\cdots(w - w_n)^{-k_n}dw + B, \tag{11.208}$$

where B is a complex integration constant. In general, A determines the orientation and B fixes the location of the polygon in the z-plane. In a Schwarz–Christoffel transformation, there are all together $2n + 4$ parameters, that is, n w_is, n k_is, and 4 parameters from the complex constants A and B. A polygon can be specified by giving the coordinates of its n vertices in the z-plane. Along with the constraint [Eq. (11.207)], this determines the $2n + 1$ of the parameters in the transformation. This means that we have the freedom to choose the locations of the three w_i on the real axis of the w-plane.

Example 11.17 ***Schwarz–Christoffel transformation***
We now construct the Schwarz–Christoffel transformation that maps the region shown in Figure 11.24 into the upper half of the w-plane. Such transformations are frequently needed in applications. To construct the Schwarz–Christoffel transformation, we define a polygon whose inside, in the limit as $z_3 \to -\infty$, goes to the desired region (Figure 11.25). Using the freedom in defining the Schwarz–Christoffel transformation, we map the points z_1, z_2, and z_3 to the following points in the w-plane:

$$w_1 = -1, \quad w_2 = +1, \quad w_3 \to -\infty. \tag{11.209}$$

We now write the Schwarz–Christoffel transformation as

$$\frac{dz}{dw} = c(w+1)^{-k_1}(w-1)^{-k_2}(w-w_3)^{-k_3}. \tag{11.210}$$

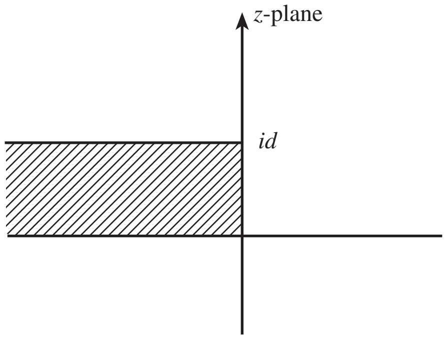


Figure 11.24 Region we map in Example 11.17.

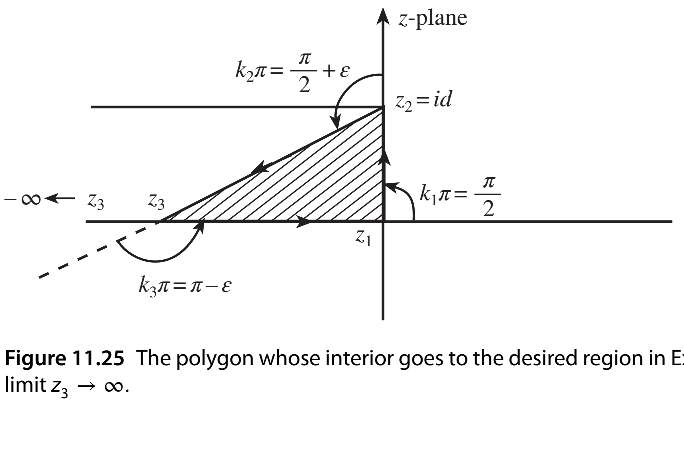


Figure 11.25 The polygon whose interior goes to the desired region in Example 11.17 in the limit $z_3 \to \infty$.

Powers k_1, k_2, and k_3 are determined from the figure as $\frac{1}{2}$, $\frac{1}{2}$, and 1, respectively. Note, how the signs of k_i are chosen as plus because of the counterclockwise directions shown in Figure 11.25. Because the constant c is still arbitrary, we define a new finite complex number A:

$$\lim_{w_3 \to -\infty} \frac{c}{(-w_3)^{k_3}} \to A, \tag{11.211}$$

so that the Schwarz–Christoffel transformation becomes

$$\frac{dz}{dw} = A(w+1)^{-\frac{1}{2}}(w-1)^{-\frac{1}{2}} \tag{11.212}$$

$$= \frac{A}{\sqrt{w^2-1}}. \tag{11.213}$$

This can be integrated as

$$z = A \cosh^{-1} w + B, \tag{11.214}$$

where the constants A and B are found from the locations of the vertices:

$$z = 0 \to w = -1, \tag{11.215}$$

$$z = id \to w = +1, \tag{11.216}$$

as

$$A = \frac{d}{\pi} \text{ and } B = id. \tag{11.217}$$

Example 11.18 ***Semi-infinite parallel plate capacitor***
We now calculate the fringe effects of a semi-infinite parallel plate capacitor. Making use of the symmetry of the problem, we can concentrate on the region shown in Figure 11.26. To find a Schwarz–Christoffel transformation that maps this region to the upper half of the w-plane, we choose the points on the real w-axis as

$$\begin{aligned} z_1 \to\ & w_1 \to -\infty, \\ z_4 \to\ & w_4 \to +\infty, \\ z_2 \to\ & w_2 = -1, \\ z_3 \to\ & w_3 = 0. \end{aligned} \tag{11.218}$$

Since $k_2 = -1$ and $k_3 = 1$, we can write

$$\frac{dz}{dw} = c(w+1)^{-k_2}(w-0)^{-k_3} \tag{11.219}$$

$$= c\frac{(w+1)}{w} = c\left(1 + \frac{1}{w}\right). \tag{11.220}$$

Integrating this gives

$$z = c(w + \ln w) + D. \tag{11.221}$$

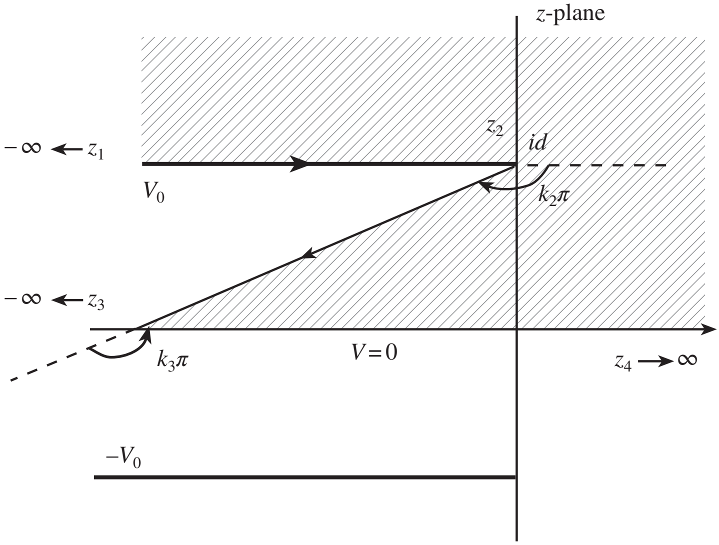


Figure 11.26 Semi-infinite parallel plate capacitor.

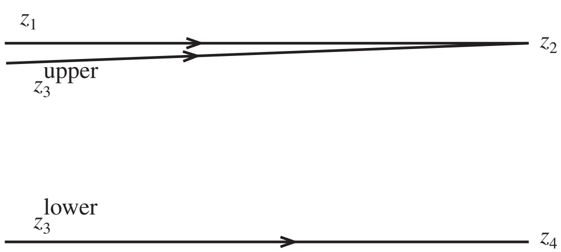


Figure 11.27 Limit of the point z_3.

If we substitute $w = |w|e^{i\phi}$, Eq. (11.221) becomes

$$z = c[|w|e^{i\phi} + \ln|w| + i\phi] + D. \tag{11.222}$$

Considering the limit in Figure 11.27, we can write

$$z_3^{\text{upper}} - z_3^{\text{lower}} = id. \tag{11.223}$$

Using Eq. (11.222), this becomes

$$z_3^{\text{upper}} - z_3^{\text{lower}} = c\left[0 + i\left(\phi_3^{\text{upper}} - \phi_3^{\text{lower}}\right)\right] \tag{11.224}$$

$$= ci(\pi - 0), \tag{11.225}$$

thus determining the constant c as $c = d/\pi$. On the other hand, considering that the vertex $z_2 = id$ is mapped to the point -1 in the w-plane, we write

$$id = \frac{d}{\pi}(-1 + i\pi) + D \tag{11.226}$$

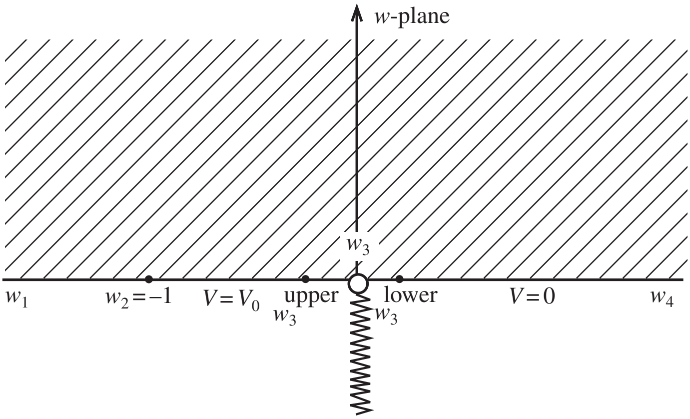


Figure 11.28 w-Plane for the semi-infinite parallel plate capacitor.

and determine D as $D = d/\pi$. This determines the Schwarz–Christoffel transformation

$$z = \frac{d}{\pi}[w + \ln w + 1], \tag{11.227}$$

which maps the region shown in Figure 11.26 to the upper half w-plane shown in Figure 11.28. We now consider the transformation

$$\bar{z} = \frac{d}{\pi} \ln w \quad \text{or} \quad w = e^{\bar{z}\pi/d}, \tag{11.228}$$

which maps the region in Figure 11.28 to the region shown in Figure 11.29 in the $\bar{z}$-plane. In the $\bar{z}$-plane, equipotentials are easily written as

$$\bar{y} = \text{const.} = \frac{V}{V_0}d \quad \text{or} \quad V(\bar{y}) = \frac{V_0}{d}\bar{y}. \tag{11.229}$$

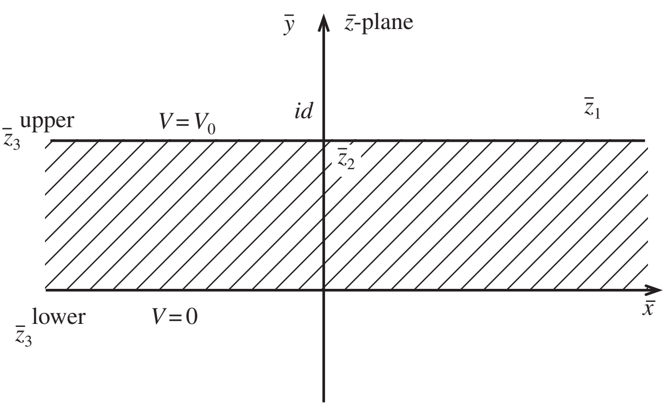


Figure 11.29 $\bar{z}$-Plane for the semi-infinite parallel plate capacitor.

Using the inverse transformation in Eq. (11.227), we write

$$z = x + iy \tag{11.230}$$
$$= \frac{d}{\pi}\left\{e^{\bar{x}\pi/d}\left[\cos\left(\frac{V}{V_0}\pi\right) + i\sin\left(\frac{V}{V_0}\pi\right)\right] + 1\right\} + \bar{x} + i\frac{V}{V_0}d,$$

which gives us the parametric expression of the equipotentials in the z-plane (Figure 11.30):

$$x = \frac{d}{\pi}\left[e^{\bar{x}\pi/d}\cos\left(\frac{V}{V_0}\pi\right) + 1\right] + \bar{x}, \tag{11.231}$$

$$y = \frac{d}{\pi}e^{\bar{x}\pi/d}\sin\left(\frac{V}{V_0}\pi\right) + \frac{V}{V_0}d. \tag{11.232}$$

Similarly, the electric field lines in the $\bar{z}$-plane are written as

$$\bar{x} = \text{const.} \tag{11.233}$$

Transforming back to the z-plane, with the definitions

$$\frac{\bar{x}\pi}{d} = \kappa \quad \text{and} \quad \theta = \frac{\bar{y}\pi}{d}, \tag{11.234}$$

we get

$$x = \frac{d}{\pi}[e^{\kappa}\cos\theta + 1] + \kappa\frac{d}{\pi}, \tag{11.235}$$

$$y = \frac{d}{\pi}[e^{\kappa}\sin\theta + \theta]. \tag{11.236}$$

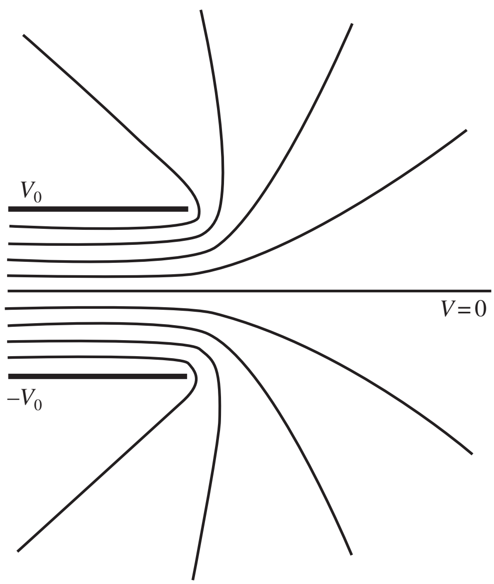


Figure 11.30 Equipotentials for the semi-infinite parallel plate capacitor.

Example 11.19 ***Schwarz–Christoffel transformation***
Let us now find the Schwarz–Christoffel transformation that maps the semi-infinite strip: $-\pi/2 < x < \pi/2$, to the upper half w-plane, $v > 0$. We will also use this result to solve the Laplace equation within the given strip satisfying the following boundary conditions:

$$V(x,0) = 1, \tag{11.237}$$

$$V(-\pi/2, y) = V(\pi/2, y) = 0. \tag{11.238}$$

We start by mapping the points $(\pm\pi/2, 0)$ in the z-plane to $(\pm 1, 0)$ in the w-plane, respectively (Figure 11.31). We also map the point z_3 to ∞. Schwarz–Christoffel transformation can now be written as

$$\frac{dz}{dw} = A(w+1)^{-k_1}(w-1)^{-k_2}(w-\infty)^{-k_3}, \tag{11.239}$$

where

$$k_1 = k_2 = 1/2, \quad k_3 = 1. \tag{11.240}$$

We again absorb ∞ into the arbitrary constant A and define a new constant C_0 to write

$$\frac{dz}{dw} = C_0(w^2-1)^{-1/2}, \tag{11.241}$$

which upon integration yields

$$z = C_0 \cosh^{-1} w + C_1. \tag{11.242}$$

Since

$$\begin{aligned} z_1 &= (-\pi/2, 0) &\rightarrow \quad w_1 &= (-1, 0), \\ z_2 &= (\pi/2, 0) &\rightarrow \quad w_2 &= (1, 0) \end{aligned} \tag{11.243}$$

we determine C_0 and C_1 as

$$C_0 = i, \tag{11.244}$$

$$C_1 = \pi/2, \tag{11.245}$$

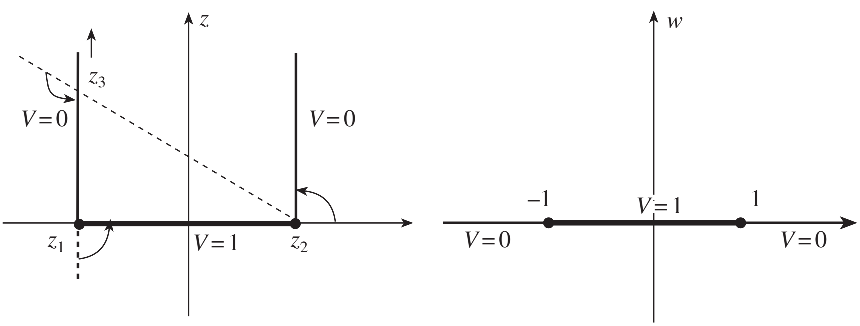


Figure 11.31 Schwarz–Christoffel transformation for Example 11.19.

and write

$$z = i \cosh^{-1} w + \pi/2. \tag{11.246}$$

From the electromagnetic theory or the potential theory, the solution of the Laplace equation in the w-plane is given as

$$V(u, v) = \frac{v}{\pi} \int_{-\infty}^{+\infty} \frac{V(\xi, 0) d\xi}{(u - \xi)^2 + v^2}, \tag{11.247}$$

which can be integrated to yield

$$V(u, v) = \frac{1}{\pi} \tan^{-1} \left[\frac{2v}{u^2 + v^2 - 1} \right]. \tag{11.248}$$

One should check that the above $V(u, v)$ does indeed satisfies the Laplace equation in the w-plane with the following boundary conditions:

$$V(u, 0) = 1 \quad \text{for} \quad -1 < u < 1, \tag{11.249}$$

$$V(u, v) = 0 \quad \text{elsewhere}. \tag{11.250}$$

For the solution in the z-plane, we need the transformation equations from (u, v) to (x, y). Using Eq. (11.246), we write

$$w = \cosh \left(\frac{z - \pi/2}{i} \right) \tag{11.251}$$

$$= \sin x \cosh y + i \sinh y \cos x, \tag{11.252}$$

thus obtaining the needed relations as

$$u = \sin x \cosh y, \tag{11.253}$$

$$v = \sinh y \cos x. \tag{11.254}$$

The solution in the z-plane can now be written as

$$V(x, y) = \frac{1}{\pi} \tan^{-1} \left[\frac{2 \sinh y \cos x}{\sin^2 x \cosh^2 y + \sinh^2 y \cos^2 x - 1} \right]. \tag{11.255}$$

Note: The transformation we obtained [Eq. (11.246)]:

$$z = i[\cosh^{-1} w - i\pi/2] \tag{11.256}$$

can in general be written as

$$z = -i[A \cosh^{-1} w + B], \tag{11.257}$$

where the constants, A and B, depend on the orientation and the location of the strip in the z-plane. If you compare this with the horizontal strip used in Example 11.17, the factor $-i$ is essentially rotating the domain by $-\pi/2$.

Example 11.20 ***Schwarz–Christoffel transformation***
We now construct the Schwarz–Christoffel mapping that transforms the bent line, A, B, C, D, in the w-plane with the points

$$(-2, 1), \quad (-1, 0), \quad (1, 0), \quad (2, -1), \tag{11.258}$$

respectively, into a straight line along the real axis in the z-plane.

We first map point B to $(-1, 0)$ and C to $(1, 0)$ as shown in Figure 11.32. Differential form of the transform is written as

$$\frac{dw}{dz} = A(z - z_1)^{-k_1}(z - z_2)^{-k_2}, \tag{11.259}$$

where k_1 and k_2 are determined as

$$k_1\pi = \pi/4 \to k_1 = 1/4, \tag{11.260}$$
$$k_2\pi = -\pi/4 \to k_2 = -1/4. \tag{11.261}$$

Equation (11.259) now becomes

$$\frac{dw}{dz} = A(z + 1)^{1/4}(z - 1)^{-1/4} \tag{11.262}$$
$$= A\left(\frac{z - 1}{z + 1}\right)^{1/4}, \tag{11.263}$$

which upon integration yields

$$w = A \int \left(\frac{z - 1}{z + 1}\right)^{1/4} dz + B \tag{11.264}$$
$$= A\left[\frac{-2u}{u^4 - 1} + \frac{1}{2}\ln\left|\frac{u - 1}{u + 1}\right| - \tan^{-1}u\right] + B, \tag{11.265}$$

where

$$u = \left(\frac{z - 1}{z + 1}\right)^{1/4}. \tag{11.266}$$

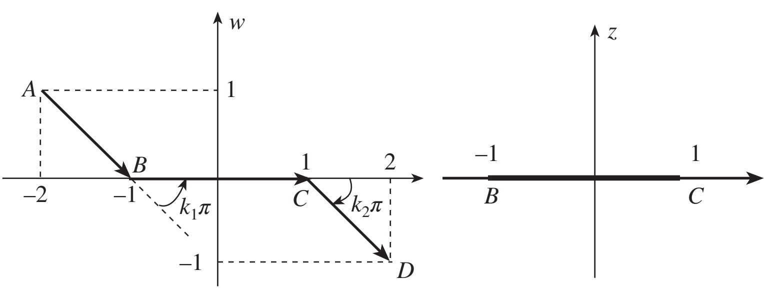


Figure 11.32 Schwarz–Christoffel transfomation for Example 11.20.

Using the fact that

$$z = 1 \rightarrow w = 1, \tag{11.267}$$

$$z = -1 \rightarrow w = -1, \tag{11.268}$$

we obtain two equations:

$$1 = B + A\pi/2, \tag{11.269}$$

$$-1 = B + A\pi/2, \tag{11.270}$$

hence determine the integration constants A and B as

$$A = \frac{4}{\pi(i-1)}, \quad B = \frac{1+i}{1-i}. \tag{11.271}$$

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Problems

1 For conjugate harmonic pairs, show that if $\Psi(u, v)$ satisfies the Laplace equation:

$$\frac{\partial^2 \Psi(u,v)}{\partial u^2} + \frac{\partial^2 \Psi(u,v)}{\partial v^2} = 0,$$

in the w-plane, then $\Psi(x, y)$ satisfies

$$\frac{\partial^2 \Psi(x,y)}{\partial x^2} + \frac{\partial^2 \Psi(x,y)}{\partial y^2} = 0$$

in the z-plane.

2 Show that

$$u(x,y) = \sin x \cosh y + x^2 - y^2 + 4xy$$

is a harmonic function and find its conjugate.

3 Show that

$$u(x,y) = \sin 2x/(\cosh 2y + \cos 2x)$$

can be the real part of an analytic function $f(z)$. Find its imaginary part and express $f(z)$ explicitly as a function of z.

4 Check the differentiability and the analyticity of the function

$$f(z) = \begin{cases} \frac{x^3 - y^3}{x^2 + y^2} + i\frac{x^3 + y^3}{x^2 + y^2}, & |z| \neq 0, \\ 0, & z = 0. \end{cases}$$

5 Using cylindrical coordinates and the method of separation of variables, find the equipotentials and the electric field lines inside two conductors with semi-circular cross sections separated by an insulator and held at potentials $+V_0$ and $-V_0$, respectively (Figure 11.17). Compare your result with Example 11.13 and show that the two methods agree.

6 With the aid of a computer program plot the equipotentials and the electric field lines found in Example 11.18 for the semi-infinite parallel plate capacitor.

7 In a two-dimensional potential problem, the surface ABCD is at potential V_0 and the surface EFG is at potential zero. Find the transformation (in differential form) that maps the region R into the upper half of the w-plane (Figure 11.33). Do not integrate but determine all the constants.

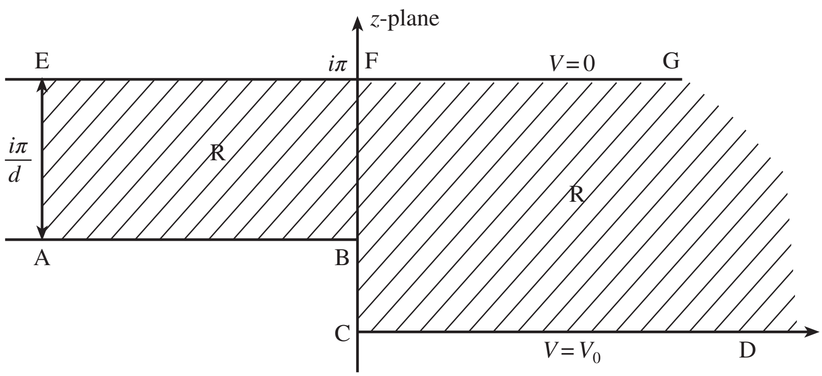


Figure 11.33 Two-dimensional equipotential problem.

8 Given the following two-dimensional potential problem in Figure 11.34, The surface ABC is held at potential V_0 and the surface DEF is at potential zero. Find the transformation that maps the region R into upper half of the w-plane. Do not integrate but determine all the constants in the differential form of the transformation.

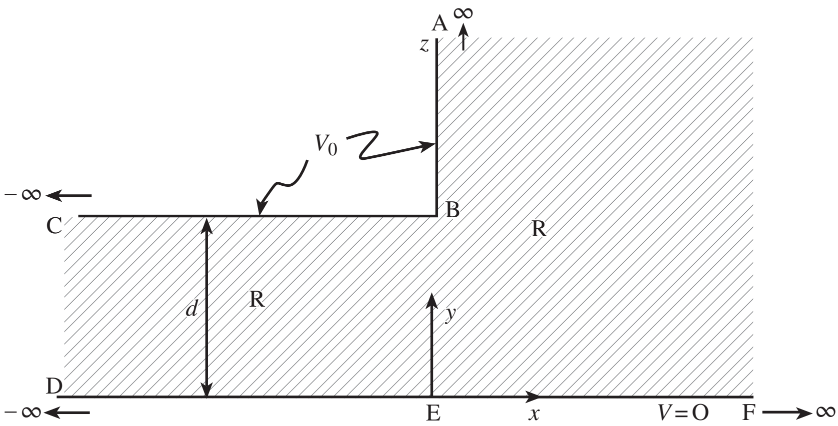


Figure 11.34 Schwarz–Christoffel transformation.

9 Find the Riemann surface on which

$$\sqrt{(z-1)(z-2)(z-3)}$$

is single valued and analytic except at $z = 1, 2, 3$.

10 Find the singularities of

$$f(z) = \tanh z.$$

11 Show that the transformation

$$\frac{w}{2} = \tan^{-1}\left(\frac{iz}{a}\right),$$

or

$$w = -i \ln \left[\frac{1+\frac{z}{a}}{1-\frac{z}{a}}\right],$$

maps the $v =$ const. lines to circles in the z-plane.

12 Show that the transformation

$$w = i\frac{1-z}{1+z},$$

maps the upper half of the unit disc,

$$y \geq 0,\ x^2 + y^2 \leq 1,$$

to the first quadrant, $u \geq 0$, $v \geq 0$, of the w-plane.

13 Use the transformation given in Problem 11 to find the equipotentials and the electric field lines for the electrostatics problem of two infinite parallel cylindrical conductors, each of radius R and separated by a distance of d, and held at potentials $+V_0$ and $-V_0$, respectively.

14 Consider the electrostatics problem for the rectangular region surrounded by metallic plates as shown in Figure 11.35. The top plate is held at potential V_0, while the bottom and the right sides are grounded ($V = 0$). The two plates are separated by an insulator. Find the equipotentials and the electric field lines and plot.

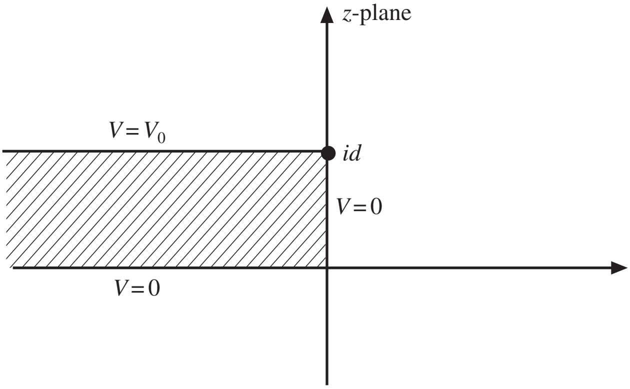
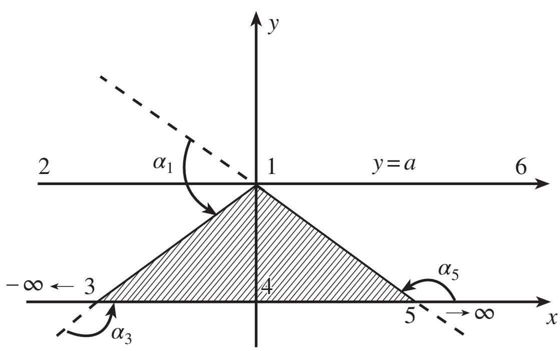


Figure 11.35 Rectangular region surrounded by metallic plates.

15 Map the real w-axis to the triangular region shown in Figure 11.36 in the limit

$$x_5 \to \infty$$
and
$$x_3 \to -\infty.$$

Figure 11.36 Triangular region.



16 Find the equipotentials and the electric field lines for a conducting circular cylinder held at potential V_0 and parallel to a grounded infinite conducting plane (Figure 11.37). Hint: Use the transformation $z = a \tanh iw/2$.

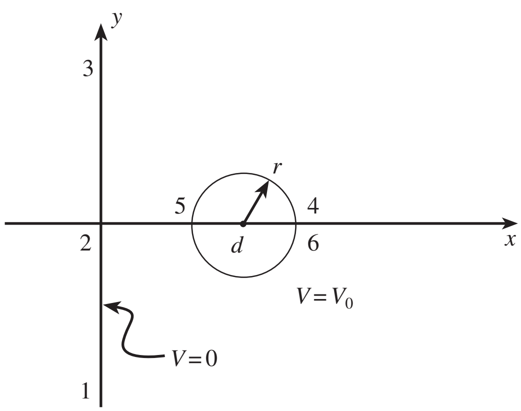


Figure 11.37 Conducting circular cylinder parallel to infinite metallic plate.

12

Complex Integrals and Series

In this chapter, we first introduce the complex integral theorems. Despite their simplicity, these theorems are incredibly powerful and establish the basis of complex techniques in applied mathematics. Using analytic continuation, we show how these theorems can be used to evaluate some of the frequently encountered definite integrals in science and engineering. In conjunction with our discussion of definite integrals, we also introduce the gamma and the beta functions, which frequently appear in applications. Next, we introduce complex power series, that is, the Taylor and the Laurent series and discuss classification of singular points. Finally, we discuss the integral representations of special functions.

12.1 Complex Integral Theorems

12.1.1 Cauchy–Goursat Theorem

Let C be a closed contour in a simply connected domain (Figure 12.1). If a given function, $f(z)$, is analytic within and on this contour, then the following integral is true:

$$\boxed{\oint_C f(z)dz = 0.} \tag{12.1}$$

Proof: If we write the function $f(z)$ as $f(z) = u + iv$, the above integral [Eq. (12.1)] becomes

$$\oint_C (u + iv)(dx + idy) = \oint (udx - vdy) + i \oint (vdx + udy). \tag{12.2}$$

Using the Stokes theorem:

$$\oint_C \vec{A} \cdot d\vec{l} = \iint_S (\vec{\nabla} \times \vec{A}) \cdot \hat{\mathbf{n}}\, ds, \tag{12.3}$$

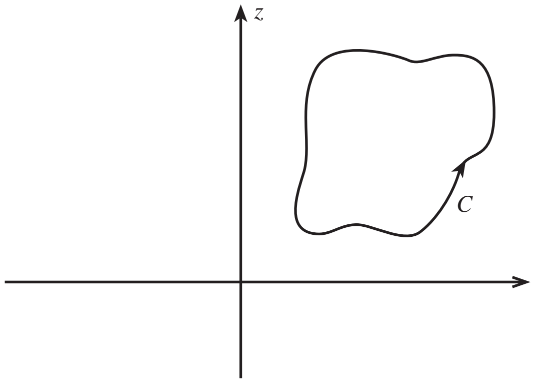


Figure 12.1 Contour for the Cauchy–Goursat theorem.

we can also write this as

$$\oint_C (u + iv)(dx + idy) = \iint_S \left(-\frac{dv}{dx} - \frac{du}{dy}\right) ds + \iint_S \left(\frac{du}{dx} - \frac{dv}{dy}\right) ds, \tag{12.4}$$

where S is an oriented surface bounded by the closed path C. Because the Cauchy–Riemann conditions, $\partial u/\partial x = \partial v/\partial y$ and $\partial v/\partial x = -\partial u/\partial y$, are satisfied within and on the closed path C, the right-hand side of Eq. (12.4) is zero, thus proving the theorem.

12.1.2 Cauchy Integral Theorem

If $f(z)$ is analytic within and on a closed path, C, in a simply connected domain (Figure 12.2) and if z_0 is a point inside the path C, then we can write the integral

$$\boxed{\frac{1}{2\pi i}\oint_C \frac{f(z)dz}{(z - z_0)} = f(z_0).} \tag{12.5}$$

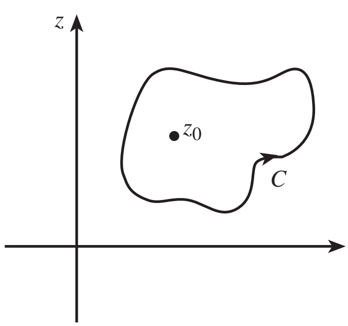


Figure 12.2 Contour for the Cauchy integral theorem.

Proof: To prove this theorem, we modify the contour in Figure 12.2 and use the one in Figure 12.3, where we can use the Cauchy–Goursat theorem to write

$$\oint_{C+L_1+L_2+C_0} \frac{f(z)dz}{(z-z_0)} = 0. \tag{12.6}$$

This integral must be evaluated in the limit as the radius of the path C_0 goes to zero. Since the function $f(z)$ is analytic within and on C, the integrals over L_1 and L_2 cancel each other. In addition, noting that the integral over C_0 is taken clockwise, we write

$$\frac{1}{2\pi i}\oint_C \frac{f(z)dz}{(z-z_0)} = \frac{1}{2\pi i}\oint_{C_0} \frac{f(z)dz}{(z-z_0)}, \tag{12.7}$$

where both integrals are now taken counterclockwise. The integral on the left-hand side is what we want. For the integral on the right-hand side, we can write

$$\frac{1}{2\pi i}\oint_{C_0} \frac{f(z)dz}{(z-z_0)} = \frac{1}{2\pi i} f(z_0)\oint_{C_0} \frac{dz}{(z-z_0)} + \frac{1}{2\pi i}\oint_{C_0} \frac{f(z)-f(z_0)}{(z-z_0)}dz. \tag{12.8}$$

Using the substitution $z - z_0 = R_0 e^{i\theta}$ on C_0, the first integral on the right-hand side can be evaluated easily, giving

$$\frac{1}{2\pi i} f(z_0)\oint_{C_0} \frac{dz}{(z-z_0)} = \frac{1}{2\pi i} f(z_0) i \int_0^{2\pi} \frac{R_0 e^{i\theta} d\theta}{R_0 e^{i\theta}} = f(z_0). \tag{12.9}$$

The second integral on the right-hand side of Eq. (12.8), which we call I_2, can be bounded from above as

$$|I_2| \le \int_{C_0} \left|\frac{f(z)-f(z_0)}{z-z_0}\right| |dz| \le M \cdot L, \tag{12.10}$$

where M is the maximum value that $(f(z) - f(z_0))/(z - z_0)$ can take on C_0:

$$M = \max\left|\frac{f(z)-f(z_0)}{z-z_0}\right| = \max\frac{|f(z)-f(z_0)|}{|z-z_0|} \tag{12.11}$$

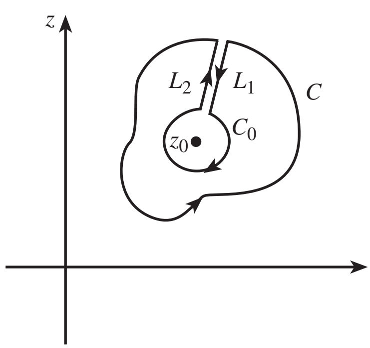


Figure 12.3 The modified contour for the Cauchy integral theorem.

and L is the circumference, $L = 2\pi R_0$, of C_0. Now let ϵ be a given small number such that on C_0

$$|f(z) - f(z_0)| < \epsilon \tag{12.12}$$

is satisfied. Because $f(z)$ is analytic within and on C, no matter how small an ϵ is given, we can always find a sufficiently small radius δ:

$$|z - z_0| \leq R_0 = \delta, \tag{12.13}$$

such that the condition (12.12) is satisfied; thus we can write

$$|I_2| \leq M \cdot L = 2\pi\epsilon. \tag{12.14}$$

From the limit $\epsilon \to 0$ as $\delta \to 0$, it follows that $|I_2| \to 0$; thus the desired result is obtained:

$$\frac{1}{2\pi i}\oint_C \frac{f(z)dz}{(z - z_0)} = f(z_0). \tag{12.15}$$

Note that the following limit:

$$\lim_{z\to z_0} \frac{f(z) - f(z_0)}{z - z_0}, \tag{12.16}$$

is actually the definition of the derivative of $f(z)$ evaluated at z_0. Because $f(z)$ is analytic within and on the contour, $C, f'(z)$ exists and hence M in Eq. (12.10) is finite. Thus, $|I_2| \to 0$ as $R_0 \to 0$.

12.1.3 Cauchy Theorem

Because the position of the point z_0 is arbitrary in the Cauchy integral theorem, we can treat it as a parameter and differentiate Eq. (12.5) with respect to z_0 as

$$f'(z_0) = \left.\frac{df}{dz}\right|_{z=z_0} = \frac{1}{2\pi i}\oint_C \frac{f(z)dz}{(z - z_0)^2}. \tag{12.17}$$

After n-fold differentiation, we obtain a very useful formula:

$$\boxed{f^{(n)}(z_0) = \left.\frac{d^n f}{dz^n}\right|_{z=z_0} = \frac{n!}{2\pi i}\oint_C \frac{f(z)dz}{(z - z_0)^{n+1}}.} \tag{12.18}$$

Example 12.1 ***Contour integrals***
Let $f(z)$ be an analytic function within and on a simple closed curve, C, and let z_0 be a point not on C. If

$$I_1 = \oint_C \frac{f'(z)dz}{(z - z_0)} \tag{12.19}$$

and

$$I_2 = \oint_C \frac{f(z)dz}{(z-z_0)^2}, \tag{12.20}$$

then show that $I_1 = I_2$ and evaluate I_1 in terms of z_0.

Solution

When z_0 is within C, using the Cauchy integral theorem [Eq. (12.5)] and the Cauchy theorem [Eq. (12.18)], we can write

$$f'(z_0) = \frac{1}{2\pi i}\oint_C \frac{f'(z)dz}{(z-z_0)} \tag{12.21}$$

and

$$\frac{2\pi i}{n!} f^{(n)}(z_0) = \oint_C \frac{f(z)dz}{(z-z_0)^{n+1}}, \tag{12.22}$$

hence

$$I_1 = I_2 = 2\pi i f'(z_0). \tag{12.23}$$

When z_0 is outside of C, and $f'(z)/(z-z_0)$ and $f(z)/(z-z_0)^2$ are analytic within and on C, then $I_1 = I_2 = 0$.

Example 12.2 ***Contour integrals***

Evaluate the integral

$$I = \oint_C z^m z^{*n} dz, \quad m, n \text{ are integers,} \tag{12.24}$$

over the unit circle.

Solution

Over the unit circle, we write $z = e^{i\theta}$, $dz = izd\theta$, hence

$$I = i\int_0^{2\pi} e^{i(m+1-n)\theta} d\theta \tag{12.25}$$

$$= \frac{i}{i(m+1-n)} e^{i(m+1-n)\theta}\Big|_0^{2\pi} \tag{12.26}$$

$$= \begin{cases} 2\pi i, & m+1 = n, \\ 0, & m+1 \neq n. \end{cases} \tag{12.27}$$

12.2 Taylor Series

Let us expand a function $f(z)$ about z_0, where it is analytic. In addition, let z_1 be the nearest singular point of $f(z)$ to z_0. If $f(z)$ is analytic on and inside a closed contour, C, we can use the Cauchy integral theorem [Eq. (12.5)] to write

$$f(z) = \frac{1}{2\pi i} \oint_C \frac{f(z')dz'}{(z' - z)}, \tag{12.28}$$

where z' is a point on the contour and z is a point inside the contour C (Figure 12.4). We can now write Eq. (12.28) as

$$f(z) = \frac{1}{2\pi i} \oint_C \frac{f(z')dz'}{[(z' - z_0) - (z - z_0)]} \tag{12.29}$$

$$= \frac{1}{2\pi i} \oint_C \frac{f(z')dz'}{(z' - z_0)\left[1 - \frac{(z - z_0)}{(z' - z_0)}\right]}. \tag{12.30}$$

Choosing the contour, C, as the circle centered at z_0 and passing through z', we see that the inequality $|z - z_0| < |z' - z_0|$ is satisfied. We can now use the

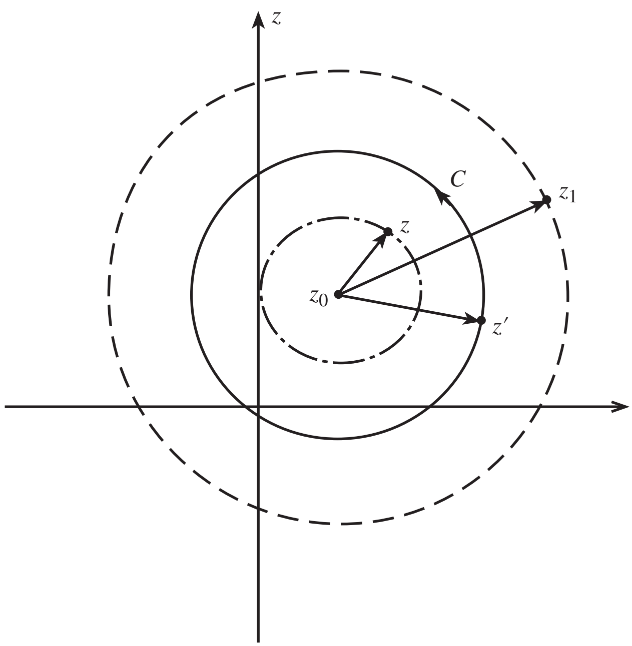


Figure 12.4 Contour C for the Taylor series.

binomial formula:

$$\frac{1}{1-t} = 1 + t + t^2 + \cdots = \sum_{n=0}^{\infty} t^n, \quad |t| < 1, \tag{12.31}$$

to write

$$f(z) = \frac{1}{2\pi i} \oint_C \sum_{n=0}^{\infty} \frac{(z - z_0)^n}{(z' - z_0)^{n+1}} f(z')dz'. \tag{12.32}$$

Interchanging the integral and the summation signs, we find

$$f(z) = \frac{1}{2\pi i} \sum_{n=0}^{\infty} (z - z_0)^n \oint_C \frac{f(z')dz'}{(z' - z_0)^{n+1}}, \tag{12.33}$$

which gives the **Taylor series** expansion of $f(z)$ as

$$\boxed{f(z) = \sum_{n=0}^{\infty} A_n (z - z_0)^n.} \tag{12.34}$$

Using the Cauchy theorem [Eq. (12.18)], we can write the expansion coefficients as

$$\boxed{A_n = \frac{1}{n!} f^{(n)}(z_0) = \frac{1}{2\pi i} \oint_C \frac{f(z')dz'}{(z' - z_0)^{n+1}}.} \tag{12.35}$$

This expansion is unique and valid in the region $|z - z_0| < |z_1 - z_0|$, where $f(z)$ is analytic.

12.3 Laurent Series

Sometimes $f(z)$ is analytic inside an annular region as shown in Figure 12.5. For a closed contour in the annular region, C, composed of the parts C_1, C_2, L_1, and L_2, where our function is analytic within and on C, using the Cauchy integral theorem [Eq. (12.5)], we can write

$$f(z) = \frac{1}{2\pi i} \oint_{C=C_1+C_2+L_1+L_2} \frac{f(z')dz'}{(z' - z)}. \tag{12.36}$$

Here z' is a point on C and z is a point inside C. In the limit as the straight line segments of the contour approach each other, integrals over L_1 and L_2 cancel; hence, we can also write

$$f(z) = \frac{1}{2\pi i} \oint_{C_1} \frac{f(z')dz'}{(z' - z)} - \frac{1}{2\pi i} \oint_{C_2} \frac{f(z')dz'}{(z' - z)}, \tag{12.37}$$

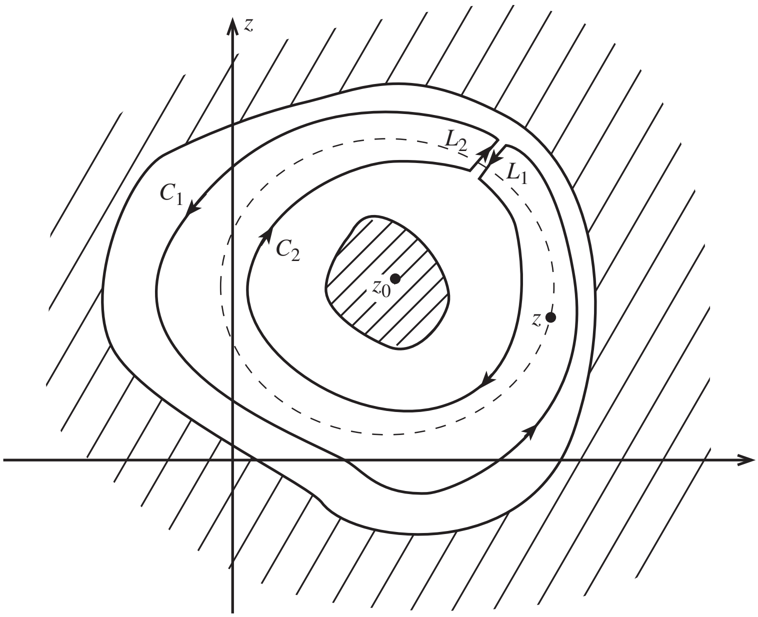


Figure 12.5 Laurent series are defined in an annular region.

where both integrals are taken counterclockwise. Since the inequality $|z' - z_0| > |z - z_0|$ is satisfied on C_1 and $|z' - z_0| < |z - z_0|$ is satisfied on C_2, we can write the above equation as

$$f(z) = \frac{1}{2\pi i}\oint_{C_1} \frac{f(z')dz'}{[(z' - z_0) - (z - z_0)]} - \frac{1}{2\pi i}\oint_{C_2} \frac{f(z')dz'}{-[(z - z_0) - (z' - z_0)]} \tag{12.38}$$

$$= \frac{1}{2\pi i}\oint_{C_1} \frac{f(z')dz'}{(z' - z_0)\left[1 - \frac{z - z_0}{z' - z_0}\right]} + \frac{1}{2\pi i}\oint_{C_2} \frac{f(z')dz'}{(z - z_0)\left[1 - \frac{z' - z_0}{z - z_0}\right]}. \tag{12.39}$$

We now use the binomial formula and interchange the integral and the summation signs to obtain the **Laurent expansion** valid at each point inside the annular region as

$$f(z) = \sum_{n=0}^{\infty} (z - z_0)^n \left[\frac{1}{2\pi i}\oint_{C_1} \frac{f(z')dz'}{(z' - z_0)^{n+1}}\right] + \sum_{n=0}^{\infty} \frac{1}{(z - z_0)^{n+1}} \left[\frac{1}{2\pi i}\oint_{C_2} \frac{f(z')dz'}{(z' - z_0)^{-n}}\right]. \tag{12.40}$$

Since $f(z)$ is analytic inside the annular region R, for any point z inside R, we can deform the two contours continuously into each other and use the contour

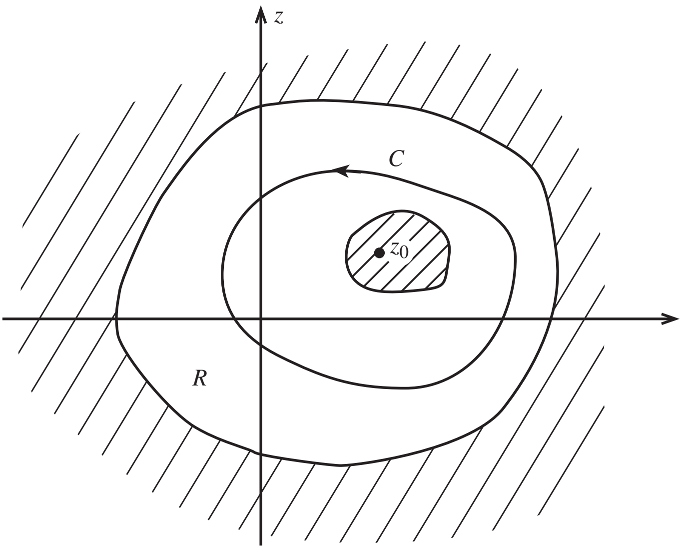


Figure 12.6 Another contour for the Laurent series.

in Figure 12.6 to write the **Laurent series** as

$$\boxed{f(z) = \sum_{n=-\infty}^{\infty} a_n (z - z_0)^n,} \tag{12.41}$$

$$\boxed{a_n = \frac{1}{2\pi i} \oint_C \frac{f(z')dz'}{(z' - z_0)^{n+1}}.} \tag{12.42}$$

Example 12.3 ***Taylor series***
We find the series expansion of $f(z) = 1/\sqrt{z^2 - 1}$ in the interval $|z| < 1$ about the origin. Since this function is analytic inside the unit circle (Figure 12.7), we need the Taylor series

$$f(z) = \sum_{n=0}^{\infty} \frac{a_n}{n!} z^n. \tag{12.43}$$

Using

$$a_n = \left[\frac{d^n f}{dz^n}\right]_{z=0}, \tag{12.44}$$

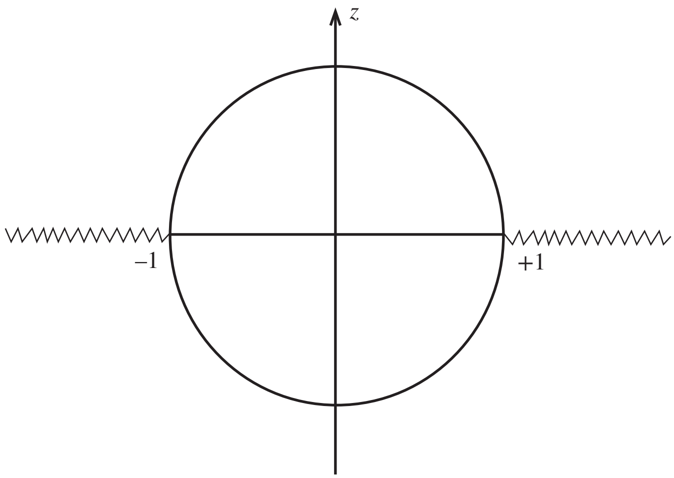


Figure 12.7 For the $1/\sqrt{z^2-1}$ function, we write the Taylor series in the region $|z| < 1$.

we write the Taylor series as

$$f(z) = \frac{1}{i}\left[1 + \frac{1}{2}z^2 + \frac{3}{8}z^4 + \frac{5}{16}z^6 + \cdots\right]. \tag{12.45}$$

Example 12.4 ***Laurent series***

We now expand the same function, $f(z) = 1/\sqrt{z^2-1}$, in the region $|z| > 1$. We place the cutline outside our region of interest between the points -1 and 1 (Figure 12.8). The outer boundary of the annular region in which $f(z)$ is analytic could be taken as a circle with infinite radius, while the inner boundary is a circle with radius infinitesimally larger than 1. We now write the Laurent series about $z = 0$ as

$$f(z) = \sum_{n=-\infty}^{\infty} a_n z^n, \tag{12.46}$$

where the expansion coefficients are given as

$$a_n = \frac{1}{2\pi i}\oint_C \frac{1}{z'^{n+1}} \frac{dz'}{\sqrt{z'^2-1}}. \tag{12.47}$$

In this integral, z' is a point on the contour C, which could be taken as any closed path inside the annular region where $f(z)$ is analytic. To evaluate the coefficients with $n \geq 0$, we first deform our contour so that it hugs the outer boundary of our annular region, which is a circle with infinite radius. For points on this contour,

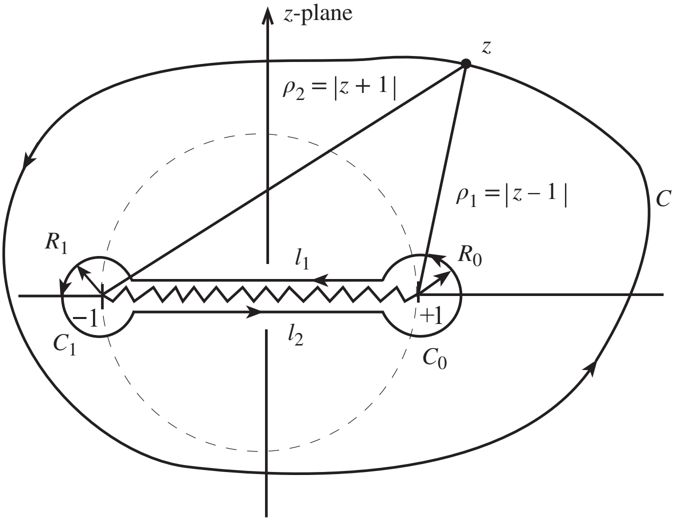


Figure 12.8 For the $1/\sqrt{z^2-1}$ function, we write the Laurent series in the region $|z|>1$.

we write $z' = Re^{i\theta}$ and evaluate the coefficients $a_n (n \geq 0)$ in the limit $R \to \infty$ as

$$a_{n(n\geq 0)} = \lim_{R\to\infty} \frac{1}{2\pi i} \oint_C \frac{dz'}{z'^{n+1}\sqrt{z'^2-1}} \tag{12.48}$$

$$= \lim_{R\to\infty} \frac{1}{2\pi i} \int \frac{iRe^{i\theta} d\theta}{R^{n+2} e^{i(n+2)\theta}} \tag{12.49}$$

$$= 0. \tag{12.50}$$

To pick the coefficients with the negative values of n, we take our contour as a circle with radius infinitesimally larger than 1. Because $f(z)$ is analytic everywhere except the cutline, these coefficients can be evaluated by shrinking the contour to a bone shape so that it hugs the cutline as shown in Figure 12.8; thus

$$a_{n(n<0)} = \frac{1}{2\pi i} \oint_{\underset{C_1}{\circlearrowleft} + \underset{l_1}{\leftarrow} + \underset{l_2}{\rightarrow} + \underset{C_0}{\circlearrowleft}} \frac{1}{z'^{n+1}} \frac{dz'}{\sqrt{z'^2-1}}. \tag{12.51}$$

We evaluate the integrals over C_0 and C_1 in the limit as their radiuses go to zero. First, let us consider the integral over C_0, where $z' - 1 = R_0 e^{i\theta_0}$. The contribution of this to a_n is zero:

$$\lim_{R_0\to 0} \frac{1}{2\pi i} \int_{\underset{C_0}{\circlearrowleft}\,-\pi}^{\pi} \frac{(+1)^{|n|-1}}{\sqrt{2}} \frac{R_0 i e^{i\theta_0} d\theta_0}{\sqrt{R_0} e^{\frac{1}{2}\theta_0}} \to 0. \tag{12.52}$$

Similarly, the contribution of C_1 is also zero, thus leaving us with

$$a_{n(n<0)} = \frac{1}{2\pi i} \oint_{\overleftarrow{l_1}+\overrightarrow{l_2}} \frac{1}{z'^{n+1}} \frac{1}{\sqrt{z'^2 - 1}} \, dz'. \tag{12.53}$$

Integrals over l_1 and l_2 can be evaluated by defining the parameters

$$\begin{aligned} z' - 1 &= \rho_1 e^{i\theta_1}, \quad 0 \le \theta_1 < 2\pi, \\ z' + 1 &= \rho_2 e^{i\theta_2}, \quad 0 \le \theta_2 < 2\pi, \end{aligned} \tag{12.54}$$

and writing

$$a_{n(n<0)} = \frac{1}{2\pi i} \left[\int_{L_1} \frac{z'^{|n|-1} dz'}{\sqrt{|z' - 1||z' + 1| e^{i\theta_1} e^{i\theta_2}}} + \int_{L_2} \frac{z'^{|n|-1} dz'}{\sqrt{|z' - 1||z' + 1| e^{i\theta_1} e^{i\theta_2}}} \right], \tag{12.55}$$

$$a_{n(n<0)} = \frac{1}{2\pi i} \left[\int_1^{-1} \frac{x^{|n|-1} dx}{e^{i\frac{\pi}{2}} \sqrt{(1 - x)(1 + x)}} + \int_{-1}^{1} \frac{x^{|n|-1} dx}{e^{i\frac{3\pi}{2}} \sqrt{(1 - x)(1 + x)}} \right], \tag{12.56}$$

$$a_{n(n<0)} = -\frac{(-1)^{|n|}}{2\pi} \int_{-1}^{1} \frac{x^{|n|-1} dx}{\sqrt{1 - x^2}} + \frac{1}{2\pi} \int_{-1}^{1} \frac{x^{|n|-1} dx}{\sqrt{1 - x^2}}. \tag{12.57}$$

We finally obtain the coefficients as

$$a_{-|n|} = \frac{1}{2\pi} \left[1 - (-1)^{|n|}\right] \int_{-1}^{1} \frac{x^{|n|-1} dx}{\sqrt{1 - x^2}}, \tag{12.58}$$

$$a_{-|n|} = \left\{ \begin{array}{ll} 0, & |n| = \text{even}, \\ \dfrac{(|n| - 1)!}{2^{|n|-1} [(|n| - 1)/2!]^2}, & |n| = \text{odd}. \end{array} \right\} \tag{12.59}$$

This gives the Laurent expansion for the region $|z| > 1$ and about the origin as

$$\frac{1}{\sqrt{z^2 - 1}} = \frac{1}{z} + \frac{1}{2z^3} + \frac{3}{8}\frac{1}{z^5} + \frac{5}{16}\frac{1}{z^7} + \cdots. \tag{12.60}$$

Example 12.5 ***Laurent series – a short cut***

In the previous example, we found the Laurent expansion of the function $f(z) = 1/\sqrt{z^2 - 1}$ about the origin and in the region $|z| > 1$. We used the contour integral definition of the coefficients. However, using the uniqueness of power series and appropriate binomial expansions, we can also evaluate the same series. First, we write $f(z)$ as

$$f(z) = \frac{1}{\sqrt{z^2 - 1}} \tag{12.61}$$

$$= \frac{1}{(z+1)^{\frac{1}{2}}} \frac{1}{(z-1)^{\frac{1}{2}}} \tag{12.62}$$

$$= \frac{1}{z^{\frac{1}{2}}} \frac{1}{\left(1+\frac{1}{z}\right)^{\frac{1}{2}}} \frac{1}{z^{\frac{1}{2}}} \frac{1}{\left(1-\frac{1}{z}\right)^{\frac{1}{2}}} \tag{12.63}$$

$$= \frac{1}{z}\left(1+\frac{1}{z}\right)^{-\frac{1}{2}}\left(1-\frac{1}{z}\right)^{-\frac{1}{2}}. \tag{12.64}$$

Since for the region $|z| > 1$ the inequality $1/z < 1$ is satisfied, we can use the binomial formula for the factors $\left(1+\frac{1}{z}\right)^{-\frac{1}{2}}$ and $\left(1-\frac{1}{z}\right)^{-\frac{1}{2}}$ to write the Laurent expansion as

$$f(z) = \frac{1}{z}\left[1 + \frac{1}{2z} + \frac{3}{8z^2} + \frac{5}{16z^3} + \cdots\right]\left[1 - \frac{1}{2z} + \frac{3}{8z^2} - \frac{5}{16z^3} + \cdots\right] \tag{12.65}$$

$$= \frac{1}{z} + \frac{1}{2z^3} + \frac{3}{8z^3} + \cdots , \tag{12.66}$$

which is the same as our previous result [Eq. (12.60)].

12.4 Classification of Singular Points

Using the Laurent series, we can classify singular points of a function.

Definition 12.1 ***Isolated singular point*** If a function is not analytic at z_0 but analytic at every other point in some neighborhood of z_0, then z_0 is called an isolated singular point.

Definition 12.2 ***Singular point of order*** m In the Laurent series of a function:

$$f(z) = \sum_{n=-\infty}^{\infty} a_n (z - z_0)^n, \tag{12.67}$$

if for $n < -m$, where $m > 0$, $a_n = 0$ but $a_m \neq 0$, then z_0 is called a singular point of order m.

Definition 12.3 ***Essential singular point*** If m is infinity, then z_0 is called an essential singular point.

Definition 12.4 ***Simple Pole*** In Definition 12.2, if $m = 1$, then z_0 is called a simple pole.

Definition 12.5 ***Entire function*** When a function is analytic in the entire z-plane, it is called an entire function.

12.5 Residue Theorem

If a function $f(z)$ is analytic within and on the closed contour C except for a finite number of isolated singular points (Figure 12.9), then we can write the integral

$$\boxed{\oint_C f(z)dz = 2\pi i \sum_{n=0}^{N} R_n,} \tag{12.68}$$

where R_n is the **residue** of $f(z)$ at the nth isolated singular point. The residue at z_n is defined as the coefficient of the $1/(z - z_n)$ term in the Laurent expansion of $f(z)$.

Proof: We change the contour C as shown in Figure 12.10 and use the Cauchy–Goursat theorem [Eq. (12.1)] to write

$$\oint_C f(z)dz = \left[\sum_{n=0}^{N}\left[\oint_{c_n[\circlearrowright]} + \oint_{l_n[\rightarrow]} + \oint_{l_n[\leftarrow]}\right] + \oint_{C'[\circlearrowleft]}\right] f(z)dz = 0. \tag{12.69}$$

Straight line segments of the integral cancel each other. Integrals over the small circles are evaluated clockwise and in the limit as their radius goes to zero. Since

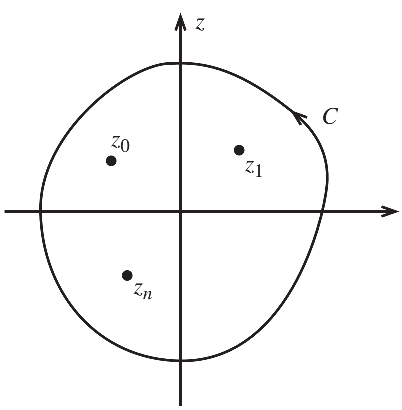


Figure 12.9 In the residue theorem, a function has finite number of isolated singular points.

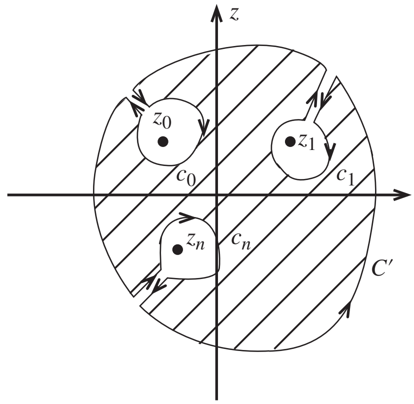


Figure 12.10 Contour for the residue theorem.

the integral over the closed path C' is equal to the integral over the closed path C, we write

$$\oint_C f(z)dz = \sum_{n=0}^{N} \oint_{c_n[\circlearrowleft]} f(z)dz, \tag{12.70}$$

where the integrals over c_n are now evaluated counterclockwise. Using the Laurent series expansion of $f(z)$ about z_0, the integral of the terms with the positive powers of $(z - z_0)$ gives

$$\oint_{c_0} (z - z_0)^n dz = 0, \quad n \geq 0. \tag{12.71}$$

On the other hand, for the negative powers of $(z - z_0)$, we have

$$\oint_{c_n} \frac{dz}{(z - z_0)^n} = \lim_{R_0 \to 0} \int_0^{2\pi} \frac{iR_0 e^{i\theta_0} d\theta_0}{R_0^n e^{in\theta_0}}, \quad n \geq 1 \tag{12.72}$$

$$= \lim_{R_0 \to 0} \frac{i}{R_0^{n-1}} \int_0^{2\pi} e^{-i(n-1)\theta_0} d\theta_0 \tag{12.73}$$

$$= \begin{cases} 0, & n = 2, 3, \ldots, \\ 2\pi i, & n = 1. \end{cases} \tag{12.74}$$

We repeat this for all the other poles to get

$$\oint_C f(z)dz = \sum_{n=0}^{N} \oint_{c_n} f(z)dz \tag{12.75}$$

$$= 2\pi i \sum_{n=0}^{N} R_n. \tag{12.76}$$

Example 12.6 ***Residue theorem***
If a function has an isolated pole of order m:

$$f(z) = \sum_{n=0}^{\infty} a_n (z - z_0)^n + \frac{b_1}{(z - z_0)} + \cdots + \frac{b_m}{(z - z_0)^m}, \tag{12.77}$$

we first show that its residue at z_0 can be given as

$$\text{Res}[f(z_0)] = \frac{1}{(m-1)!} \lim_{z \to z_0} \frac{d^{m-1}}{dz^{m-1}} [(z - z_0)^m f(z)] \tag{12.78}$$

and then find the residues of

$$f(z) = \frac{z}{(z+1)^2 (z-1)}. \tag{12.79}$$

Next, we evaluate the integral:

$$I = \oint_C \frac{z\,dz}{(z+1)^2 (z-1)}, \tag{12.80}$$

over the contours, C_1 and C_2, shown in Figure 12.11.

Solution
If $f(z)$ has a pole of order m, then $g(z) = (z - z_0)^m f(z)$ is analytic at z_0:

$$g(z) = \sum_{n=0}^{\infty} a_n (z - z_0)^{n+m} + b_m + b_{m-1}(z - z_0) + \cdots + b_1 (z - z_0)^{m-1}, \tag{12.81}$$

hence

$$\lim_{z \to z_0} \frac{dg(z)}{dz} = b_{m-1}, \tag{12.82}$$

$$\lim_{z \to z_0} \frac{d^2 g(z)}{dz^2} = 2! b_{m-2}, \tag{12.83}$$

$$\vdots$$

$$\lim_{z \to z_0} \frac{d^{m-1} g(z)}{dz^{m-1}} = (m-1)! b_1. \tag{12.84}$$

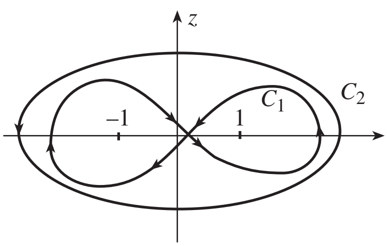


Figure 12.11 Contours for Example 12.6.

Since $\mathrm{Res}[f(z_0)] = b_1$, we can write

$$\mathrm{Res}[f(z_0)] = \frac{1}{(m-1)!} \lim_{z\to z_0} \frac{d^{m-1}g(z)}{dz^{m-1}}, \tag{12.85}$$

thus proving the desired result. The given function:

$$f(z) = \frac{z}{(z+1)^2(z-1)}, \tag{12.86}$$

has a second-order isolated pole at $z = -1$ and a first-order isolated pole $z = 1$; hence, we can find its residues as

$$\mathrm{Res}[f(1)] = \frac{1}{0!} \lim_{z\to 1} \frac{d^{1-1}}{dz^{1-1}} \left[(z-1)\frac{z}{(z+1)^2(z-1)} \right] = \frac{1}{4} \tag{12.87}$$

and

$$\mathrm{Res}[f(-1)] = \frac{1}{(2-1)!} \frac{d^{2-1}}{dz^{2-1}} \lim_{z\to -1} \left[(z+1)^2 \frac{z}{(z+1)^2(z-1)} \right] = -\frac{1}{4}. \tag{12.88}$$

We can now evaluate the integral for path C_1 as

$$I = \oint_{C_1} \frac{z\,dz}{(z+1)^2(z-1)} = 2\pi i \left[\frac{1}{4} - \left(-\frac{1}{4} \right) \right] = \pi i \tag{12.89}$$

and for C_2 as

$$I = \oint_{C_2} \frac{z\,dz}{(z+1)^2(z-1)} = 2\pi i \left[\frac{1}{4} + \left(-\frac{1}{4} \right) \right] = 0. \tag{12.90}$$

12.6 Analytic Continuation

When we discussed harmonic functions and mappings, we saw that analytic functions have very interesting properties. It is for this reason that it is very important to determine the region where a function is analytic and, if possible, to extend this region to other parts of the z-plane. This process is called **analytic continuation**. Sometimes functions like polynomials and trigonometric functions, which are defined on the real axis as

$$f(x) = a_0 + a_1 x + a_2 x^2 + \cdots + a_n x^n, \tag{12.91}$$

$$f(x) = \sin x, \tag{12.92}$$

can be analytically continued to the entire z-plane by simply replacing the real variable x with z as

$$f(z) = a_0 + a_1 z + a_2 z^2 + \cdots + a_n z^n, \tag{12.93}$$

$$f(z) = \sin z. \tag{12.94}$$

However, analytic continuation is not always this easy. Let us now consider different series expansions of the function

$$f(z) = \frac{1}{1-z} + \frac{2}{2-z}. \tag{12.95}$$

This function has two isolated singular points at $z = 1$ and $z = 2$. We first make a Taylor series expansion about $z = 0$. We write

$$f(z) = \frac{1}{(1-z)} + \frac{1}{\left(1 - \frac{z}{2}\right)} \tag{12.96}$$

and use the binomial formula:

$$(1-x)^{-1} = \sum_{n=0}^{\infty} x^n \tag{12.97}$$

to obtain

$$f(z) = \sum_{n=0}^{\infty} \left(1 + \frac{1}{2^n}\right) z^n, \quad |z| < 1. \tag{12.98}$$

This expansion is naturally valid up to the nearest singular point at $z = 1$. Similarly, we can make another expansion, this time valid in the interval $1 < |z| < 2$ as

$$f(z) = -\left(\frac{1}{z}\right) \frac{1}{\left(1 - \frac{1}{z}\right)} + \frac{1}{\left(1 - \frac{z}{2}\right)} \tag{12.99}$$

$$= -\frac{1}{z} \sum_{n=0}^{\infty} \left(\frac{1}{z}\right)^n + \sum_{n=0}^{\infty} \left(\frac{z}{2}\right)^n \tag{12.100}$$

$$= 1 + \sum_{n=1}^{\infty} \left[\left(\frac{z}{2}\right)^n - \frac{1}{z^n}\right]. \tag{12.101}$$

Finally for $|z| > 2$, we obtain

$$f(z) = -\frac{1}{z}\left(\frac{1}{1 - \frac{1}{z}}\right) - \left(\frac{2}{z}\right) \frac{1}{\left(1 - \frac{2}{z}\right)} \tag{12.102}$$

$$= -\sum_{n=1}^{\infty} \left[\frac{1}{z^n} + \frac{2^n}{z^n}\right]. \tag{12.103}$$

These three expansions of the same function [Eq. (12.96)] are valid for the intervals $|z| < 1$, $1 < |z| < 2$, and $|z| > 2$, respectively. Naturally, it is not practical to use these series definitions, where each one is valid in a different part of the z-plane, when a closed expression like

$$f(z) = \frac{1}{1-z} + \frac{2}{2-z} \tag{12.104}$$

exists for the entire z-plane. However, it is not always possible to find a closed expression like this. Let us assume that we have a function with a finite number of isolated singular points at $z_1, z_2, \dots, z_n$. Taylor series expansion of this function about a regular point z_0 will be valid only up to the nearest singular point z_1 (Figure 12.12). In such cases, we can accomplish analytic continuation by successive Taylor series expansions, where each expansion is valid up to the nearest singular point (Figure 12.13). We should make a note that during this process, we are not making the function analytic at the points where it is singular.

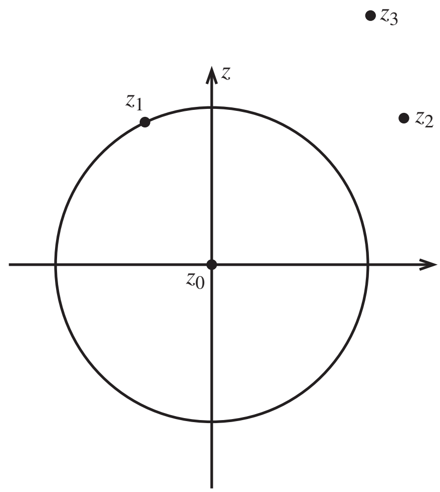


Figure 12.12 A function with isolated singular points at z_1, z_2, and z_3.

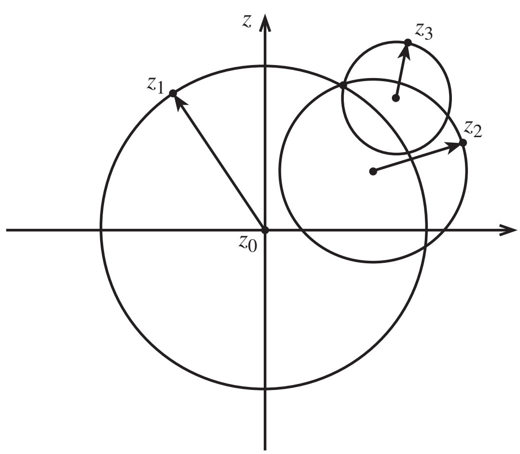


Figure 12.13 Analytic continuation by successive Taylor series expansions.

12.7 Complex Techniques in Taking Some Definite Integrals

Many of the definite integrals encountered in physics and engineering can be evaluated by using the complex integral theorems and analytic continuation:

Type I. Integrals of the form

$$\boxed{I = \int_0^{2\pi} R(\cos\theta, \sin\theta)d\theta,} \tag{12.105}$$

where R is a rational function:

$$R = \frac{a_1\cos\theta + a_2\sin\theta + a_3\cos^2\theta + \cdots}{b_1\cos\theta + b_2\sin\theta + b_3\cos^2\theta + b_4\sin^2\theta + \cdots}, \tag{12.106}$$

can be converted into a complex contour integral over the **unit circle** by the substitutions

$$\cos\theta = \frac{1}{2}\left(z + \frac{1}{z}\right),\ \sin\theta = \frac{1}{2i}\left(z - \frac{1}{z}\right) \tag{12.107}$$

and

$$z = e^{i\theta},\ d\theta = -i\left(\frac{dz}{z}\right) \tag{12.108}$$

as

$$\boxed{I = -i\oint_C R\left[\frac{1}{2}\left(z + \frac{1}{z}\right), \frac{1}{2i}\left(z - \frac{1}{z}\right)\right]\frac{dz}{z}.} \tag{12.109}$$

Example 12.7 ***Complex contour integration techniques***
Let us evaluate the integral

$$I = \int_0^{2\pi} \frac{d\theta}{a + \cos\theta}, \quad a > 1. \tag{12.110}$$

Using Eqs. (12.107) and (12.108), we can write this integral as

$$I = -i\oint_{|z|=1} \frac{dz}{\left(a + \frac{z}{2} + \frac{2}{2z}\right)z} \tag{12.111}$$

$$= -2i\oint_{|z|=1} \frac{dz}{z^2 + 2az + 1}. \tag{12.112}$$

The denominator can be factorized as $(z - \alpha)(z - \beta)$, where

$$\alpha = -a + (a^2 - 1)^{\frac{1}{2}}, \tag{12.113}$$

$$\beta = -a - (a^2 - 1)^{\frac{1}{2}}. \tag{12.114}$$

For $a > 1$, we have $|\alpha| < 1$ and $|\beta| > 1$; thus only the root $z = \alpha$ is present inside the unit circle. We can now use the Cauchy integral theorem [Eq. (12.5)] to find

$$I = -2i(2\pi i)\frac{1}{\alpha - \beta} = \frac{2\pi}{(a^2 - 1)^{\frac{1}{2}}}. \tag{12.115}$$

Example 12.8 ***Complex contour integral techniques***
We now consider the integral

$$I = \frac{1}{2\pi}\int_0^{2\pi} \sin^{2l}\theta d\theta. \tag{12.116}$$

We can use Eqs. (12.107) and (12.108) to write I as a contour integral over the unit circle as

$$I = \frac{(-1)^l}{2\pi}\frac{(-i)}{2^{2l}}\oint \frac{dz}{z}\left(z - \frac{1}{z}\right)^{2l}. \tag{12.117}$$

We can now evaluate this integral by using the residue theorem [Eq. (12.68)] as

$$I = \frac{(-1)^l}{2\pi}\frac{(-i)}{2^{2l}}2\pi i\left[\text{residue of } \frac{1}{z}\left(z - \frac{1}{z}\right)^{2l} \text{at} \quad z = 0\right]. \tag{12.118}$$

Using the binomial formula, we can write

$$\frac{1}{z}\left(z - \frac{1}{z}\right)^{2l} = \frac{1}{z}\sum_{k=0}^{2l} \frac{(2l)!}{(2l - k)!k!}(z^{2l-k})\left(-\frac{1}{z}\right)^k, \tag{12.119}$$

where the residue we need is the coefficient of the $1/z$ term. This can be found as

$$(-1)^l\frac{(2l)!}{(l!)^2}, \tag{12.120}$$

and the result of the definite integral I becomes

$$I = \frac{(2l)!}{2^{2l}(l!)^2}. \tag{12.121}$$

Type II. Integrals given as

$$\boxed{I = \int_{-\infty}^{\infty} dxR(x),} \tag{12.122}$$

where $R(x)$ is a rational function:

$$R(x) = \frac{a_0 + a_1x + a_2x^2 + \cdots + a_nx^n}{b_0 + b_1x + b_2x^2 + \cdots + b_mx^m}, \tag{12.123}$$

(a) with no singular points on the real axis,
(b) $|R(z)|$ goes to zero at least as $1/|z^2|$ in the limit as $|z| \to \infty$.

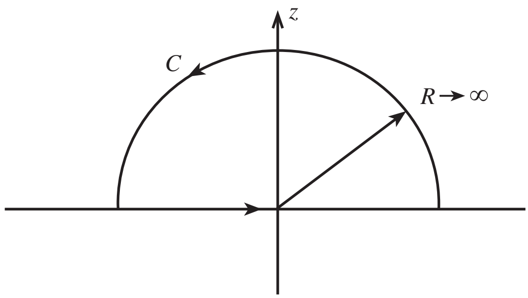


Figure 12.14 Contour for the type II integrals.

Under these conditions, I has the same value with the complex contour integral

$$\boxed{I = \oint_C R(z)dz,} \tag{12.124}$$

where C is a semicircle in the upper half of the z-plane considered in the limit as the radius goes to infinity (Figure 12.14). Proof is fairly straightforward if we write I as

$$I = \oint_C R(z)dz = \int_{-\infty}^{\infty} R(x)dx + \oint_{\frown} R(z)dz \tag{12.125}$$

and note that the integral over the semicircle vanishes in the limit as the radius goes to infinity. We can now evaluate I using the residue theorem.

Example 12.9 ***Complex contour integral techniques***
Let us evaluate the integral

$$I = \int_{-\infty}^{\infty} \frac{dx}{(1+x^2)^n}, \quad n = 1, 2, \ldots . \tag{12.126}$$

Since the conditions of the above technique are satisfied, we write

$$I = \oint_C \frac{dz}{(z+i)^n (z-i)^n}. \tag{12.127}$$

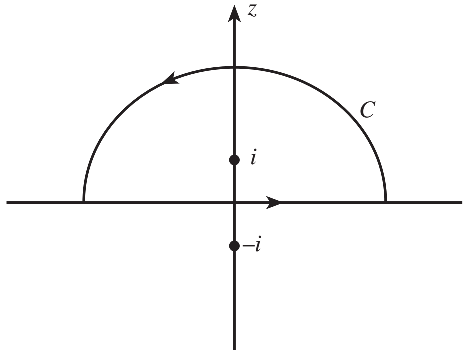
Only the singular point $z = i$ is inside the contour C (Figure 12.15); thus we can write I as

$$I = 2\pi i \left[\text{residue of } \left(\frac{1}{(z+i)^n (z-i)^n} \right) \text{ at } z = i \right]. \tag{12.128}$$

To find the residue, we write

$$f(z) = \frac{1}{(z+i)^n} = \sum_{k=0}^{\infty} A_k (z-i)^k \tag{12.129}$$

Figure 12.15 Contour for Example 12.9.



and extract the coefficient A_{n-1} as

$$A_{n-1} = \frac{1}{(n-1)!} \frac{d^{n-1}f}{dz^{n-1}}\bigg|_{z=i} \tag{12.130}$$
$$= \frac{1}{(n-1)!}(-1)^{n-1} \frac{n(n+1)(n+2)\cdots(2n-2)}{(z+i)^{2n-1}}\bigg|_{z=i}.$$

This gives the value of the integral I as

$$I = \frac{2\pi i}{(n-1)!} \quad \frac{(-1)^{n-1}}{2^{2n-1}} \frac{(2n-2)!i}{(n-1)!(-1)^n}. \tag{12.131}$$

Type III. Integrals of the type

$$\boxed{I = \int_{-\infty}^{\infty} dx R(x) e^{i\kappa x},} \tag{12.132}$$

where κ is a real parameter and $R(x)$ is a rational function with

(a) no singular points on the real axis,
(b) in the limit as $|z| \to \infty$, $|R(z)| \to 0$ independent of θ.

Under these conditions, we can write the integral I as the contour integral:

$$\boxed{I = \oint_C R(z) e^{i\kappa z} dz,} \tag{12.133}$$

where the contour C is shown in Figure 12.16. To show that this is true, we have to show the limit

$$I_A = \lim_{R\to\infty} \oint_{\curvearrowleft} R(z) e^{i\kappa z} dz \to 0. \tag{12.134}$$

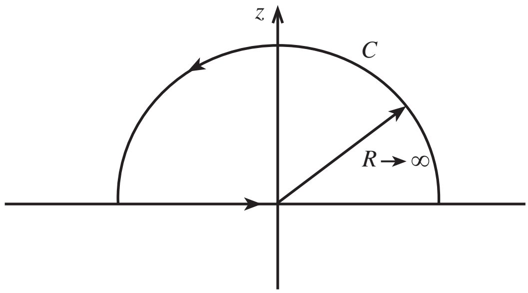


Figure 12.16 Contour C in the limit $R \to \infty$ for type III integrals.

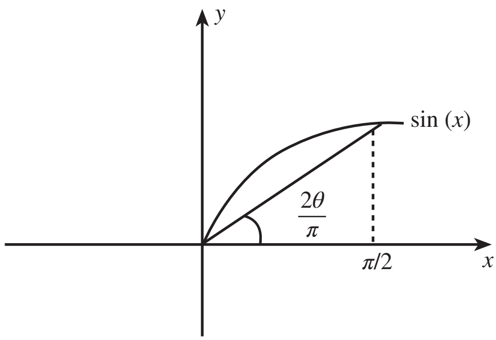


Figure 12.17 Upper bound calculation for type III integrals.

We start by taking the moduli of the quantities in the integrand to put an upper limit to this integral as

$$|I_A| \le \int_0^{\pi} |R(z)| \left| e^{i\kappa(\rho\cos\theta + i\rho\sin\theta)} \right| |\rho i e^{i\theta}| d\theta. \tag{12.135}$$

We now call the maximum value that $R(z)$ takes in the interval $[0, 2\pi]$ as $M(\rho) = \max |R(z)|$ and improve this bound as

$$|I_A| \le \rho M(\rho) \int_0^{\pi} e^{-\kappa\rho\sin\theta} d\theta, \tag{12.136}$$

$$|\, I_A| \le 2\rho M(\rho) \int_0^{\frac{\pi}{2}} e^{-\kappa\rho\sin\theta} d\theta. \tag{12.137}$$

Since the straight line segment shown in Figure 12.17, in the interval $[0, \pi/2]$, is always less than the $\sin\theta$ function, we can also write Eq. (12.137) as

$$|I_A| \le 2\rho M(\rho) \int_0^{\frac{\pi}{2}} e^{-2\kappa\rho\frac{\theta}{\pi}} d\theta. \tag{12.138}$$

This integral can easily be taken to yield

$$|I_A| \leq 2\rho M(\rho)\frac{\pi}{2\kappa\rho}(1 - e^{-\kappa\rho}), \tag{12.139}$$

$$|I_A| \leq M(\rho)\frac{\pi}{\kappa}(1 - e^{-\kappa\rho}). \tag{12.140}$$

From here, we see that in the limit as $\rho \to \infty$, the value of the integral I_A goes to zero, that is,

$$\lim_{\rho\to\infty} |I_A| \to 0. \tag{12.141}$$

This result is also called **Jordan's lemma**.

Example 12.10 ***Complex contour integral techniques***
In calculating dispersion relations, we frequently encounter integrals like

$$f(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dkg(k)e^{ikx}. \tag{12.142}$$

Let us consider a case where $g(k)$ is given as

$$g(k) = \frac{ik}{(k^2 + \mu^2)}. \tag{12.143}$$

(i) For $x > 0$, we can write

$$f(x) = \frac{i}{\sqrt{2\pi}}\oint_C \frac{dkke^{ikx}}{(k + i\mu)(k - i\mu)}. \tag{12.144}$$

In this integral, k is now a point in the complex k-plane. Because we have a pole, $k = i\mu$, inside our contour, we use the Cauchy integral theorem [Eq. (12.5)] to find

$$f(x) = 2\pi i\frac{i}{\sqrt{2\pi}}\frac{i\mu}{2i\mu}e^{-\mu x} \tag{12.145}$$

$$= -\sqrt{\frac{\pi}{2}}e^{-\mu x}. \tag{12.146}$$

(ii) For $x < 0$, we complete our contour C from below to find

$$f(x) = \frac{i}{2\pi}\oint \frac{ke^{-ik|x|}dk}{(k - i\mu)(k + i\mu)} \tag{12.147}$$

$$= -2\pi i\frac{i}{\sqrt{2\pi}}\left(\frac{-i\mu}{-2i\mu}\right)e^{-\mu|x|} \tag{12.148}$$

$$= \sqrt{\frac{\pi}{2}}e^{-\mu|x|}. \tag{12.149}$$

Type IV. Integrals of the type

$$I = \int_0^\infty dx x^{\lambda-1} R(x), \tag{12.150}$$

where

(a) $\lambda \neq$ integer,
(b) $R(x)$ is a rational function with no poles on the positive real axis and the origin,
(c) in the limit as $|z| \to 0$, $|z^\lambda R(z)| \to 0$,
(d) in the limit as $|z| \to \infty$, $|z^\lambda R(z)| \to 0$.

Under these conditions, we can evaluate the integral, I, as the following contour integral:

$$I = \oint_C z^{\lambda-1} R(z) dz = \frac{\pi(-1)^{\lambda-1}}{\sin \pi\lambda} \sum_{\text{inside } C} \text{residues of } [z^{\lambda-1} R(z)], \tag{12.151}$$

where C is the closed contour shown in Figure 12.18.

Proof: Let us write the integral I as a complex contour integral:

$$\oint_C z^{\lambda-1} R(z) dz. \tag{12.152}$$

In the limit as the radius of the small circle goes to zero, the integral over the contour C_i goes to zero because of **c**. Similarly, in the limit as the radius of the

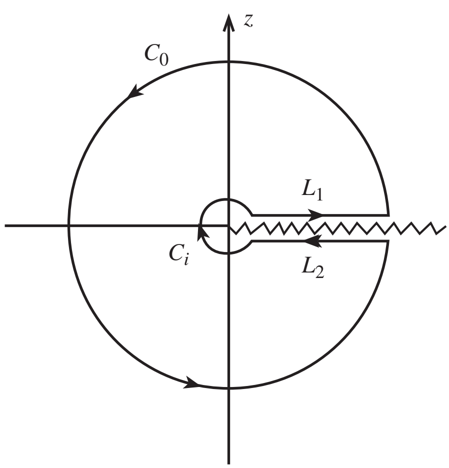


Figure 12.18 Contour for the type IV integrals.

large circle goes to infinity, the integral over C_0 goes to zero because of **d**. This leaves us with

$$\oint_C z^{\lambda-1}R(z)dz = \oint_{\to L_1} z^{\lambda-1}R(z)dz + \oint_{\leftarrow L_2} z^{\lambda-1}R(z)dz. \tag{12.153}$$

We can now evaluate the integrals on the left-hand side by using the residue theorem. But first, we write the right-hand side as

$$\oint_{\to L_1 + \leftarrow L_2} z^{\lambda-1}R(z)dz = \int_0^\infty x^{\lambda-1}R(x)dx + \int_\infty^0 x^{(\lambda-1)}e^{2i\pi(\lambda-1)}R(x)dx \tag{12.154}$$

$$= (1 - e^{2\pi i(\lambda-1)}) \int_0^\infty dx x^{\lambda-1}R(x), \tag{12.155}$$

which when substituted into Eq. (12.153) gives

$$2\pi i \sum_{\text{inside } C} \text{residues of } [z^{\lambda-1}R(z)] = -\frac{2i \sin \pi\lambda}{e^{-i\pi\lambda}} \int_0^\infty dx x^{\lambda-1}R(x). \tag{12.156}$$

After rearranging, we obtain the desired integral:

$$\boxed{\int_0^\infty x^{\lambda-1}R(x)dx = \frac{\pi(-1)^{\lambda-1}}{\sin \pi\lambda} \sum_{\text{inside } C} \text{residues of } [z^{\lambda-1}R(z)].} \tag{12.157}$$

12.8 Gamma and Beta Functions

12.8.1 Gamma Function

An important application of the type IV integrals is encountered in the definition of the gamma and the beta functions, which are frequently encountered in science and engineering applications. The **gamma function** is defined for all x as

$$\boxed{\Gamma(x) = \lim_{N\to\infty} \left\{ \frac{N!N^x}{x[x+1][x+2]\cdots[x+N]} \right\}.} \tag{12.158}$$

The integral definition of the gamma function, even though restricted to $x > 0$, is also very useful:

$$\boxed{\Gamma(x) = \int_0^\infty y^{x-1} \exp(-y)dy.} \tag{12.159}$$

Using integration by parts, we can write this as

$$\Gamma(x) = -\int_0^\infty d(e^{-y})y^{x-1} = (x-1)\int_0^\infty dye^{-y}y^{x-2}, \tag{12.160}$$

which gives the formula

$$\boxed{\Gamma(x) = (x-1)\Gamma(x-1).} \tag{12.161}$$

This is one of the most important properties of the gamma function. For the positive integer values of x, this formula gives

$$n = 1, \tag{12.162}$$

$$\Gamma(1) = 1, \tag{12.163}$$

$$\Gamma(n+1) = n!. \tag{12.164}$$

Besides, if we write

$$\Gamma(x-1) = \frac{\Gamma(x)}{(x-1)}, \tag{12.165}$$

we can also define the gamma function for the negative integer arguments. Even though this expression gives infinity for the values of $\Gamma(0)$, $\Gamma(-1)$, and for all the other negative integer arguments, their ratios are finite:

$$\frac{\Gamma(-n)}{\Gamma(-N)} = [-N][-N+1]\cdots[-N-2][-N-1], \tag{12.166}$$

$$\boxed{\frac{\Gamma(-n)}{\Gamma(-N)} = [-1]^{N-n}\frac{N!}{n!}.} \tag{12.167}$$

For some n values, the gamma function takes the following values:

$\Gamma\left(-\frac{3}{2}\right) = \frac{4}{3}\sqrt{\pi}$	$\Gamma(1) = 1$
$\Gamma(-1) = \pm\infty$	$\Gamma\left(\frac{3}{2}\right) = \frac{1}{2}\sqrt{\pi}$
$\Gamma\left(-\frac{1}{2}\right) = -2\sqrt{\pi}$	$\Gamma(2) = 1$
$\Gamma(0) = \pm\infty$	$\Gamma\left(\frac{5}{2}\right) = \frac{3}{4}\sqrt{\pi}$
$\Gamma\left(\frac{1}{2}\right) = \sqrt{\pi}$	$\Gamma(3) = 2.$

The inverse of the gamma function, $1/\Gamma(x)$, is single valued and always finite with the limit

$$\lim_{x\to\infty} \frac{1}{\Gamma(x)} = \frac{x^{\frac{1}{2}-x}}{\sqrt{2\pi}} \exp(x). \tag{12.168}$$

12.8.2 Beta Function

Let us write the product of two gamma functions as

$$\Gamma(n+1)\Gamma(m+1) = \int_0^\infty e^{-u}u^n du \int_0^\infty e^{-v}v^m dv. \tag{12.169}$$

Using the transformation $u = x^2$ and $v = y^2$, we can write

$$\Gamma(n+1)\Gamma(m+1) = \left(2\int_0^\infty e^{-x^2}x^{2n+1}dx\right)\left(2\int_0^\infty e^{-y^2}y^{2m+1}dy\right) \tag{12.170}$$

$$= 4\int_0^\infty \int_0^\infty e^{-(x^2+y^2)}x^{2n+1}y^{2n+1}dx\,dy. \tag{12.171}$$

In plane polar coordinates, this becomes

$$\Gamma(n+1)\Gamma(m+1) = 4\int_0^\infty dr \int_0^{\pi/2} d\theta e^{-r^2}\ r^{2n+2m+2+1}\cos^{2n+1}\theta\sin^{2m+1}\theta \tag{12.172}$$

$$= \left[2\int_0^\infty dr e^{-r^2} r^{2n+2m+2+1}\right]\left[2\int_0^{\pi/2} d\theta \sin^{2m+1}\theta\cos^{2n+1}\theta\right]. \tag{12.173}$$

The first term on the right-hand side is $\Gamma(m+n+2)$ while the second term is called the **beta function** $B(m+1, n+1)$. Thus, the beta function is related to the gamma function through the relation

$$B(m+1, n+1) = \frac{\Gamma(n+1)\Gamma(m+1)}{\Gamma(m+n+2)}. \tag{12.174}$$

Another definition of the beta function is obtained by the substitutions $\sin^2\theta = t$ and $t = x/(1-x)$ as

$$B(m+1, n+1) = \int_0^\infty \frac{x^m dx}{(1+x)^{m+n+2}}. \tag{12.175}$$

Using the substitution $x = y/(1-y)$, we can also write

$$\boxed{B(p,q) = \int_0^1 y^{p-1}[1-y]^{q-1}dy, \quad p > 0, \quad q > 0.} \tag{12.176}$$

To calculate the value of $B\left(\frac{1}{2},\frac{1}{2}\right)$, we have to evaluate the integral [Eq. (12.175)]

$$B\left(\frac{1}{2},\frac{1}{2}\right) = \int_0^\infty dx \frac{x^{\frac{1}{2}-1}}{(1+x)}, \tag{12.177}$$

which is type IV [Eq. (12.150)]; hence, using Eq. (12.151), we find its value as

$$B\left(\frac{1}{2},\frac{1}{2}\right) = -\pi \frac{(-1)^{-1/2}(-1)^{-1/2}}{\sin \pi/2} = \pi. \tag{12.178}$$

Finally, using Eq. (12.174), we write

$$B\left(\frac{1}{2},\frac{1}{2}\right) = \frac{\left[\Gamma\left(\frac{1}{2}\right)\right]^2}{\Gamma(1)}, \tag{12.179}$$

to obtain

$$\Gamma\left(\frac{1}{2}\right) = \sqrt{\pi}. \tag{12.180}$$

Similarly,

$$\Gamma\left(\frac{1}{2}+n\right) = \frac{(2n)!\sqrt{\pi}}{4^n n!}, \tag{12.181}$$

$$\Gamma\left(\frac{1}{2}-n\right) = \frac{(-4)^n n!\sqrt{\pi}}{(2n)!}. \tag{12.182}$$

Another useful function related to the gamma function is the **digamma function**, $\Psi(x)$, which is defined as

$$\boxed{\Psi(x) = \frac{1}{\Gamma(x)}\frac{d\Gamma(x)}{dx}.} \tag{12.183}$$

The digamma function satisfies the recursion relation

$$\Psi(x+1) = \Psi(x) + x^{-1}, \tag{12.184}$$

from which we obtain

$$\Psi(n+1) = \Psi(1) + \sum_{j=1}^{n} \frac{1}{j}. \tag{12.185}$$

The value of $\Psi(1)$ is given in terms of the **Euler constant** γ as

$$-\Psi(1) = \gamma = 0.5772157. \tag{12.186}$$

12.8.3 Useful Relations of the Gamma Functions

Among the useful relations of the gamma function, we can write

$$\Gamma(-x) = \frac{-\pi \csc(\pi x)}{\Gamma(x+1)}, \tag{12.187}$$

$$\Gamma(2x) = \frac{4^x \Gamma(x)\Gamma(x+\frac{1}{2})}{2\sqrt{\pi}}, \tag{12.188}$$

$$\Gamma(nx) = \sqrt{\frac{2\pi}{n}} \left[\frac{n^x}{\sqrt{2\pi}}\right]^n \prod_{k=0}^{n-1} \Gamma\left(x + \frac{k}{n}\right). \tag{12.189}$$

In calculating ratios like

$$\frac{\Gamma(j-q)}{\Gamma(-q)} \text{ and } \frac{\Gamma(j-q)}{\Gamma(j+1)}, \tag{12.190}$$

the ratio

$$\boxed{\frac{\Gamma(j-q)}{\Gamma(-q)\Gamma(j+1)} = \frac{[-1]^j}{j!} \sum_{m=0}^{j} S_j^{(m)} q^m} \tag{12.191}$$

is very useful. Here $S_j^{(m)}$ are the **Stirling numbers** of the first type:

$$S_{j+1}^{(m)} = S_j^{(m-1)} - jS_j^{(m)}, \quad S_0^{(0)} = 1 \tag{12.192}$$

and for the others

$$S_0^{(m)} = S_j^{(0)} = 0. \tag{12.193}$$

In terms of the **binomial coefficients**, this ratio can also be written as

$$\frac{\Gamma(j-q)}{\Gamma(-q)\Gamma(j+1)} = \binom{j-q-1}{j} \tag{12.194}$$

$$= [-1]^j \binom{q}{j}. \tag{12.195}$$

12.8.4 Incomplete Gamma and Beta Functions

Both the beta and the gamma functions have their incomplete forms. The definition of the **incomplete beta function** with respect to x is given as

$$\boxed{B_x(p,q) = \int_0^x y^{p-1}[1-y]^{q-1}dy.} \tag{12.196}$$

On the other hand, the **incomplete gamma** function is defined by

$$\gamma^*(c,x) = \frac{c^{-x}}{\Gamma(x)} \int_0^c y^{(x-1)} \exp(-y)dy, \tag{12.197}$$

or as

$$\gamma^*(c,x) = \exp(-x) \sum_{j=0}^{\infty} \frac{x^j}{\Gamma(j+c+1)}. \tag{12.198}$$

In this equation, $\gamma^*(c,x)$ is a single-valued analytic function of c and x. Among the useful relations of $\gamma^*(c,x)$, we can give

$$\gamma^*(c-1,x) = x\gamma^*(c,x) + \frac{\exp(-x)}{\Gamma(c)}, \tag{12.199}$$

$$\gamma^*\left(\frac{1}{2},x\right) = \frac{\mathrm{erf}(\sqrt{x})}{\sqrt{x}}. \tag{12.200}$$

12.8.5 Analytic Continuation of the Gamma Function

We have seen that the gamma function with real argument is defined as [Eq. (12.159)]

$$\Gamma(x) = \int_0^\infty dt\ e^{-t}t^{x-1}, \quad x > 0. \tag{12.201}$$

This formula can be analytically continued to the right-hand side of the z-plane easily as

$$\Gamma(z) = \int_0^\infty dt\, e^{-t}t^{z-1}, \quad \mathrm{Re}\, z > 0. \tag{12.202}$$

The above integral is convergent only for $\mathrm{Re}\, z > 0$. A definition valid in the entire z-plane exists and has been given by Hankel as

$$\Gamma(z) = \frac{1}{2i\sin \pi z} \int_C dt\, e^t t^{z-1}, \tag{12.203}$$

where the integral is now taken in the complex t-plane over the contour shown in Figure (12.19). In this definition, the branch cut of t^{z-1} is located along the negative real axis as

$$t^{z-1} = e^{(z-1)\ln t} = e^{(z-1)(\ln|t|+i\theta)}, \quad -\pi \le \theta < \pi. \tag{12.204}$$

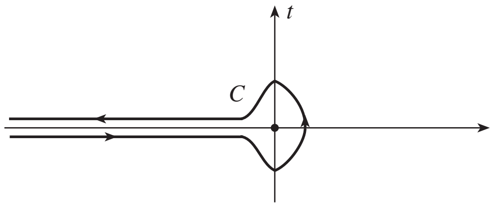


Figure 12.19 Contour for the Hankel definition of $\Gamma(z)$.

As we deform the contour without touching the branch point and without crossing over the branch cut, the integral in Eq. (12.203) reduces to two integrals over straight paths; one just over the branch cut and the other just below:

$$\int_C dt\ e^t t^{z-1} = \int_C dt\ e^t e^{(z-1)(\ln|t|+i\theta)} \tag{12.205}$$

$$= \int_0^{-\infty} dt\ e^t e^{(z-1)(\ln|t|+i\pi)} + \int_{-\infty}^0 dt\ e^t e^{(z-1)(\ln|t|-i\pi)} \tag{12.206}$$

$$= -\int_0^{\infty} dt\ e^{-t} e^{(z-1)\ln|t|}[e^{i(z-1)\pi} - e^{-i(z-1)\pi}] \tag{12.207}$$

$$= 2i \sin \pi z \int_0^{\infty} dt\ e^{-t} e^{(z-1)\ln|t|}. \tag{12.208}$$

Substituting this into Eq. (12.203) gives Eq. (12.202), thus proving their equivalence.

Equation (12.203) tells us that $\Gamma(z)$ has simple poles located at $z = -n$, $n = 0, 1, 2, \ldots$. Near the poles, we can write

$$\sin \pi z = (-1)^n \sin \pi(z+n) \tag{12.209}$$

$$\simeq (-1)^n \pi(z+n). \tag{12.210}$$

In addition, at $z = -n$, we can collapse the contour in Eq. (12.203):

$$\int_C dt\ e^t t^{z-1}, \tag{12.211}$$

to a closed contour about the origin. Thus, considering that near the origin t^{-n-1} is single valued, we obtain the integral

$$\int_C dt\ e^t t^{-n-1} = \frac{1}{n!} 2\pi i. \tag{12.212}$$

In other words,

$$\Gamma(z) \simeq \frac{(-1)^n}{n!} \frac{1}{z+n}, \tag{12.213}$$

which gives the residues of $\Gamma(z)$ at $z = -n$ as $(-1)^n/n!$.

Finally, we use Eq. (12.174):

$$B(u, v) = \frac{\Gamma(u)\Gamma(v)}{\Gamma(u+v)} \tag{12.214}$$

and the definition of the beta function [Eq. (12.175)]:

$$B(u,v) = \int_0^\infty dt \frac{t^{u-1}}{(1+t)^{u+v}}, \tag{12.215}$$

with the identifications

$$u = z, \quad v = 1 - z, \tag{12.216}$$

to write

$$\Gamma(z)\Gamma(1-z) = \Gamma(1)B(z, 1-z) = \int_0^\infty dt \frac{t^{z-1}}{1+t}. \tag{12.217}$$

Evaluating the above integral, which is type IV [Eq. (12.157)], gives the following useful property of the gamma function [Eq. (12.187)]:

$$\boxed{\Gamma(z)\Gamma(1-z) = \frac{\pi}{\sin \pi z}.} \tag{12.218}$$

Writing the above result as

$$\frac{1}{\Gamma(z)} = \frac{\sin \pi z}{\pi}\Gamma(1-z) \tag{12.219}$$

and substituting Eq. (12.203) for $\Gamma(1-z)$, one obtains

$$\boxed{\frac{1}{\Gamma(z)} = \frac{1}{2\pi i}\int_C dt\, e^t t^{-z}.} \tag{12.220}$$

12.9 Cauchy Principal Value Integral

Sometimes we encounter integrals with poles on the real axis, such as the integral

$$\boxed{I = \int_{-\infty}^{\infty} \frac{f(x)}{(x-a)} dx,} \tag{12.221}$$

which is undefined (divergent) at $x = a$. However, because the problem is only at $x = a$, we can modify this integral by first integrating up to an infinitesimally close point to a, $(a - \delta)$, and then continue integration on the other side from an arbitrarily close point, $(a + \delta)$, to infinity, that is, define the integral I as

$$I = \lim_{\delta \to 0} \left[\int_{-\infty}^{a-\delta} \frac{f(x)dx}{(x-a)} + \int_{a+\delta}^{\infty} \frac{f(x)dx}{(x-a)} \right] \tag{12.222}$$

$$= P \int_{-\infty}^{\infty} \frac{f(x)}{(x-a)} dx. \tag{12.223}$$

This is called taking the **Cauchy principal value** of the integral, and it is shown as

$$\int_{-\infty}^{\infty} \frac{f(x)}{(x-a)} dx \to P \int_{-\infty}^{\infty} \frac{f(x)}{(x-a)} dx. \tag{12.224}$$

If $f(z)$ is analytic in the upper half z-plane, that is, as $|z| \to \infty$, $f(z) \to 0$ for $y > 0$, we can evaluate the Cauchy principal value of the integral [Eq. (12.221)] by using the contour in Figure 12.20. In this case, we write

$$\oint_C \frac{f(z)dz}{(z-a)} = \left[\oint_{\substack{c_R[\curvearrowleft] \\ R\to\infty}} dz + \lim_{\begin{bmatrix} R\to\infty \\ \delta\to 0 \end{bmatrix}} \oint_{-R}^{a-\delta} dz + \oint_{\substack{c_\delta[\curvearrowright] \\ \delta\to 0}} dz + \lim_{\begin{bmatrix} R\to\infty \\ \delta\to 0 \end{bmatrix}} \oint_{a+\delta}^{R} dz \right] \frac{f(z)}{(z-a)} \tag{12.225}$$

and evaluate this integral by using the residue theorem as

$$\oint_C \frac{f(z)}{(z-a)} dz = 2\pi i \sum_{\text{inside } C} \text{residues of } \left[\frac{f(z)}{z-a} \right]. \tag{12.226}$$

If $f(z)/(z-a)$ does not have any isolated singular points inside the closed contour C (Figure 12.20), the left-hand side of Eq. (12.225) is zero, thus giving the Cauchy principal value of the integral [Eq. (12.224)] as

$$P \int_{-\infty}^{\infty} \frac{f(x)}{x-a} dx = -\lim_{\delta\to 0} \oint_{c_\delta[\curvearrowright]} \frac{f(z)}{(z-a)} dz - \lim_{R\to\infty} \oint_{c_R[\curvearrowleft]} \frac{f(z)}{(z-a)} dz. \tag{12.227}$$

From the condition $f(z) \to 0$ as $|z| \to \infty$ for $y > 0$, the second integral over c_R on the right-hand side is zero. To evaluate the integral over the small arc

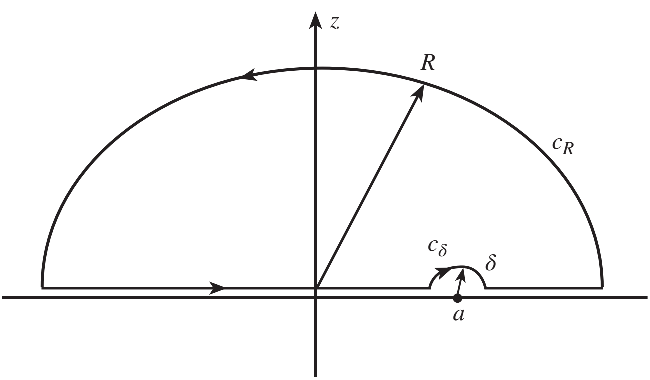


Figure 12.20 Contour C for the Cauchy principal value integral.

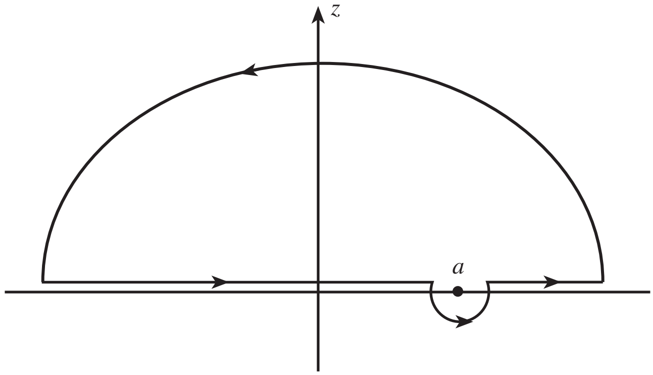


Figure 12.21 Another contour for the Cauchy principal value calculation.

c_δ, we write $z - a = \rho e^{i\theta}$ and $dz = id\theta\rho e^{i\theta}$, and find the Cauchy principal value as

$$P\int_{-\infty}^{\infty} \frac{f(x)dx}{(x-a)} = -i\int_{\pi}^{0} d\theta f(a), \tag{12.228}$$

$$\boxed{P\int_{-\infty}^{\infty} \frac{f(x)dx}{(x-a)} = i\pi f(a).} \tag{12.229}$$

Another contour that we can use to find the Cauchy principal value is given in Figure 12.21. In this case, the pole at $x = a$ is inside our contour. Using the residue theorem, we obtain

$$P\int_{-\infty}^{\infty} \frac{f(x)dx}{(x-a)} = -i\int_{\pi}^{2\pi} d\theta f(a) + 2\pi i f(a) \tag{12.230}$$

$$= -i\pi f(a) + 2\pi i f(a) = i\pi f(a). \tag{12.231}$$

As expected, the Cauchy principal value is the same for both choices of detour about $z = a$.

If $f(z)$ is analytic in the lower half of the z-plane, that is, $f(z) \to 0$ as $|z| \to \infty$ for $y < 0$, then the Cauchy principal value is given as

$$\boxed{P\int_{-\infty}^{\infty} \frac{f(x)dx}{(x-a)} = -i\pi f(a).} \tag{12.232}$$

In this case, we again have two choices for the detour around the singular point on the real axis. Again the Cauchy principal value is $-i\pi f(a)$ for both choices.

Example 12.11 ***Cauchy principal value integral***
Let us now evaluate the integral

$$I = \int_{-\infty}^{\infty} \frac{x \sin x dx}{[x^2 - k^2 r^2]}. \tag{12.233}$$

We write I as $I = I_1 + I_2$, where

$$I_1 = \frac{1}{2i} \int_{-\infty}^{\infty} \frac{x e^{ix} dx}{(x - kr)(x + kr)}, \tag{12.234}$$

$$I_2 = -\frac{1}{2i} \int_{-\infty}^{\infty} \frac{x e^{-ix} dx}{(x - kr)(x + kr)}. \tag{12.235}$$

For I_1, we choose our path in the z-plane as in Figure 12.22 to obtain

$$\begin{aligned} I_1 &= \frac{1}{2i} \left\{ i\pi \left[\frac{z e^{iz}}{z + kr} \right]_{z=kr} + i\pi \left[\left[\frac{z e^{ix}}{z - kr} \right]_{z=-kr} \right] \right\} \\ &= \frac{\pi}{2} \cos kr. \end{aligned} \tag{12.236}$$

For the integral I_2, we use the path in Figure 12.23 to obtain

$$\begin{aligned} I_2 &= -\frac{1}{2i} \left\{ -i\pi \left[\frac{z e^{-iz}}{z + kr} \right]_{z=kr} - i\pi \left[\left[\frac{z e^{-iz}}{z - kr} \right]_{z=-kr} \right] \right\} \\ &= \frac{\pi}{2} \cos kr. \end{aligned} \tag{12.237}$$

Hence, the divergent integral

$$I = \int_{-\infty}^{\infty} \frac{x \sin x dx}{[x^2 - k^2 r^2]}, \tag{12.238}$$

can now be replaced with its Cauchy principal value as

$$I = P \int_{-\infty}^{\infty} \frac{x \sin x dx}{[x^2 - k^2 r^2]} = \pi \cos kr. \tag{12.239}$$

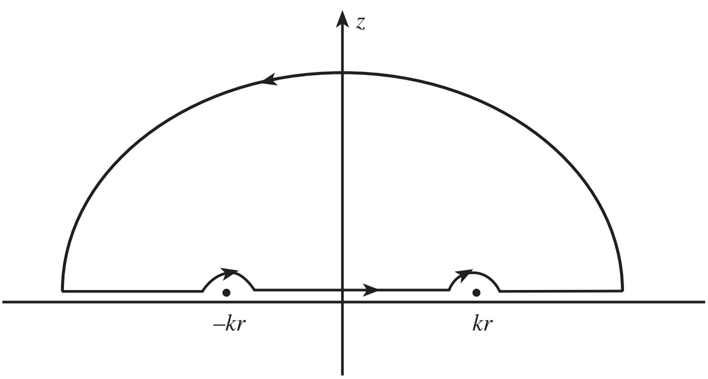


Figure 12.22 Contour for I_1.

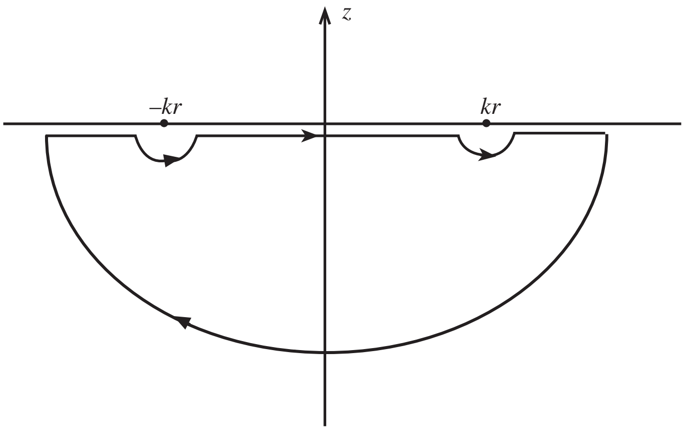


Figure 12.23 Contour for I_2.

12.10 Integral Representations of Special Functions

12.10.1 Legendre Polynomials

Let us write the Rodriguez formula for the Legendre polynomials:

$$P_l(x) = \frac{1}{2^l l!}\frac{d^l}{dx^l}(x^2-1)^l. \tag{12.240}$$

Using the Cauchy formula [Eq. (12.18)]:

$$\left.\frac{d^l f(z)}{dz^l}\right|_{z_0} = \frac{l!}{2\pi i}\oint \frac{f(z)dz}{(z-z_0)^{l+1}}, \tag{12.241}$$

with $z_0 = x$ and $f(z) = (z^2-1)^l$, we obtain

$$\left.\frac{d^l}{dz^l}(z^2-1)^l\right|_{z=x} = \frac{l!}{2\pi i}\oint \frac{(z'^2-1)^l dz'}{(z'-x)^{l+1}}. \tag{12.242}$$

This gives the complex contour integral representation of the Legendre polynomials:

$$\boxed{P_l(x) = \frac{1}{2\pi i}\frac{1}{2^l}\oint_C \frac{(z'^2-1)^l dz'}{(z'-x)^{l+1}},} \tag{12.243}$$

which is also called the **Schläfli integral formula**, where the contour is given in Figure 12.24. Using the Schläfli formula [Eq. (12.243)] and the residue theorem, we can obtain the Legendre polynomials as

$$P_l(x) = \frac{1}{2^l}\left[\text{residue of}\left[\frac{(z^2-1)^l}{(z-x)^{l+1}}\right]\text{ at } x\right]. \tag{12.244}$$

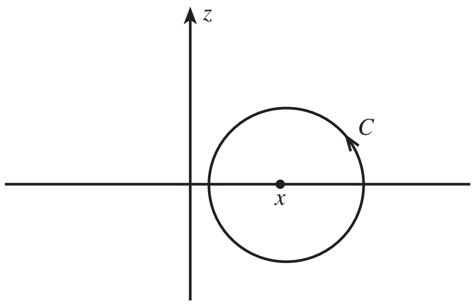


Figure 12.24 Contour for the Schläfli formula of Legendre polynomials.

We use the binomial formula to write $(z^2 - 1)^l$ in powers of $(z - x)$ as

$$(z^2 - 1)^l = \sum_{k=0}^{l} \frac{l!(-1)^k}{k!(l-k)!} z^{2(l-k)} \tag{12.245}$$

$$= \sum_{k=0}^{l} \frac{l!(-1)^k}{k!(l-k)!} [z - x + x]^{2l-2k} \tag{12.246}$$

$$= \sum_{k=0}^{l} \frac{l!(-1)^k}{k!(l-k)!} \sum_{j=0}^{2l-2k} \frac{(2l-2k)!}{(2l-2k-j)!j!} (z-x)^j x^{2l-2k-j}. \tag{12.247}$$

For the residue, we need the coefficient of $(z - x)^l$; hence, we need the $j = l$ term in the above series, which is

$$\text{coefficient of } (z-x)^l = \sum_{k=0}^{[l/2]} \frac{l!(-1)^k}{k!(l-k)!} \frac{(2l-2k)!}{(l-2k)!l!} x^{l-2k}. \tag{12.248}$$

Using this in Eq. (12.244), we finally obtain $P_l(x)$ as

$$\boxed{P_l(x) = \sum_{k=0}^{[l/2]} \frac{(-1)^k}{k!(l-k)!} \frac{(2l-2k)!}{(l-2k)!} \frac{x^{l-2k}}{2^l}.} \tag{12.249}$$

12.10.2 Laguerre Polynomials

The generating function, $T(x, t)$, of the Laguerre polynomials is defined as

$$T(x,t) = \frac{\exp(-xt/(1-t))}{1-t} = \sum_{n=0}^{\infty} L_n(x) t^n. \tag{12.250}$$

The Taylor series expansion of the generating function:

$$T(x,t) = \frac{\exp(-xt/(1-t))}{1-t}, \tag{12.251}$$

about the origin in the complex t-plane gives

$$T(x,t) = \sum_{n=0}^{\infty} \frac{1}{n!} T^{(n)}(x,0)t^n, \tag{12.252}$$

where

$$\begin{aligned} T^{(n)}(x,0) &= \frac{n!}{2\pi i} \oint_C \frac{T(x,t)dt}{t^{n+1}} \\ &= \frac{n!}{2\pi i} \oint_C \frac{\exp(-xt/(1-t))dt}{(1-t)t^{n+1}}. \end{aligned} \tag{12.253}$$

Since $T(x,t)$ is analytic within and on the contour, where C is a circle with unit radius that includes the origin but excludes $t = 1$, we use the above derivatives to write

$$T(x,t) = \sum_{n=0}^{\infty} \frac{1}{n!} \left[\frac{n!}{2\pi i} \oint_C \frac{\exp(-xt/(1-t))dt}{(1-t)t^{n+1}} \right] t^n, \tag{12.254}$$

which when compared with the right-hand side of Eq. (12.250), $\sum_{n=0}^{\infty} L_n(x)t^n$, yields

$$\boxed{L_n(x) = \frac{1}{2\pi i} \oint_C \frac{\exp(-xt/(1-t))}{(1-t)t^{n+1}} dt.} \tag{12.255}$$

Note that this is valid for a region enclosed by a circle centered at the origin with unit radius. To obtain $L_n(z)$ valid for the whole complex plane one might expand $T(x,t)$ about $t = 1$ in Laurent series.

Another contour integral representation of the Laguerre polynomials can be obtained by using the Rodriguez formula:

$$L_n(x) = \frac{e^x}{n!} \frac{d^n}{dx^n}(x^n e^{-x}). \tag{12.256}$$

Using

$$\frac{d(x^n e^{-x})}{dx^n} = \frac{n!}{2\pi i} \oint_C \frac{f(z)dz}{(z-z_0)^{n+1}} \tag{12.257}$$

and taking z_0 as a point on the real axis with $f(z) = z^n e^{-z}$, we can write

$$\frac{2\pi i}{n!} f^{(n)}(x) = \oint_C \frac{z^n e^{-z} dz}{(z-x)^{n+1}}, \tag{12.258}$$

where C is a circle centered at some point $z = x$, thus obtaining

$$\boxed{L_n(x) = \frac{1}{2\pi i} \oint_C \frac{z^n e^{x-z} dz}{(z-x)^{n+1}}.} \tag{12.259}$$

12.10.3 Bessel Functions

Using the generating function definition of $J_n(x)$ [2]:

$$\exp\left[\frac{x}{2}\left(t-\frac{1}{t}\right)\right] = \sum_{-\infty}^{\infty} t^n J_n(x), \tag{12.260}$$

we can write the integral definition

$$J_n(x) = \frac{1}{2\pi i}\oint_C \frac{\exp\left[\frac{x}{2}\left(t-\frac{1}{t}\right)\right]}{t^{n+1}}dt, \tag{12.261}$$

where t is now a point on the complex t-plane and C is a closed contour enclosing the origin. We can extend this definition to the complex z-plane as the **Schläfli definition**:

$$\boxed{J_n(z) = \frac{1}{2\pi i}\oint_C \frac{\exp\left[\frac{z}{2}\left(t-\frac{1}{t}\right)\right]}{t^{n+1}}dt, \quad |\arg z| < \frac{\pi}{2},} \tag{12.262}$$

where $J_n(z)$ satisfies the differential equation [Eq. (5.17)]

$$\boxed{\left[z^2\frac{d^2}{dz^2} + z\frac{d}{dz} + (z^2 - n^2)\right] J_n(z) = 0.} \tag{12.263}$$

One can check this by substituting Eq. (12.262) into Eq. (12.263). To extend this definition to the noninteger values of n, we write the integral

$$g_n(z) = \frac{1}{2\pi i}\int_{C'} \frac{\exp\left[\frac{z}{2}\left(t-\frac{1}{t}\right)\right]}{t^{n+1}}dt, \ |\arg z| < \frac{\pi}{2}, \tag{12.264}$$

where C' is a path in the complex t-plane. We operate on $g_n(z)$ with the Bessel's differential operator to write

$$\left[z^2\frac{d^2}{dz^2} + z\frac{d}{dz} + (z^2 - n^2)\right] g_n(z) \tag{12.265}$$

$$= \frac{1}{2\pi i}\int_{C'} \frac{dt}{t^{n+1}} \exp\left[\frac{z}{2}\left(t-\frac{1}{t}\right)\right]\left\{\frac{z^2}{4}\left(t-\frac{1}{t}\right)^2 + \frac{z}{2}\left(t-\frac{1}{t}\right) + z^2 - n^2\right\} \tag{12.266}$$

$$= \frac{1}{2\pi i}\int_{C'} dt\frac{d}{dt}\left\{\frac{\exp\left[\frac{z}{2}\left(t-\frac{1}{t}\right)\right]}{t^n}\left[\frac{z}{2}\left(t+\frac{1}{t}\right)+n\right]\right\} \tag{12.267}$$

$$= \frac{1}{2\pi i}[G_n(z,t_2) - G_n(z,t_1)], \tag{12.268}$$

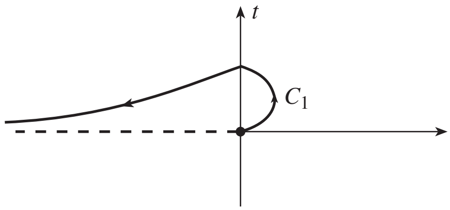


Figure 12.25 Contour for $\frac{1}{2}H_n^{(1)}(z)$.

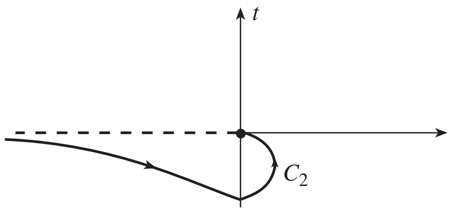


Figure 12.26 Contour for $\frac{1}{2}H_n^{(2)}(z)$.

where

$$G_n(z,t) = \frac{\exp\left[\frac{z}{2}\left(t-\frac{1}{t}\right)\right]}{t^n}\left[\frac{z}{2}\left(t+\frac{1}{t}\right)+n\right] \tag{12.269}$$

and t_1 and t_2 are the end points of the path C'. Obviously, for a path that makes the difference in Eq. (12.228) zero, we have a solution of the Bessel's equation. For the integer values of n, choosing C' as a closed path that encloses the origin does the job, which reduces to the Schläfli definition [Eq. (12.262)]. For the noninteger values of n, we have a branch cut, which we choose to be along the negative real axis. Along the real axis, $G_n(z,t)$ has the limits $G_n(z,t) \to 0$ as $t \to 0^+$ and $t \to -\infty$. Hence, the two paths, C_1 and C_2, shown in Figures (12.25) and (12.26) give two linearly independent solutions corresponding to $H_n^{(1)}(z)$ and $H_n^{(2)}(z)$, respectively. Their sum gives

$$\boxed{\frac{1}{2}\left[H_n^{(1)}(z) + H_n^{(2)}(z)\right] = J_n(z).} \tag{12.270}$$

We can now write $J_n(z)$ for general n as

$$\boxed{J_n(z) = \frac{1}{2\pi i}\int_C \frac{\exp\left[\frac{z}{2}\left(t-\frac{1}{t}\right)\right]}{t^{n+1}}dt, \quad |\arg z| < \frac{\pi}{2},} \tag{12.271}$$

where the contour is given in Figure (12.27). For the integer values of n, there is no need for a branch cut; hence, the contour can be deformed into C as shown in Figure (12.28). Furthermore, since the integrand is now single valued, we can also collapse the contour to one enclosing the origin (Figure 12.29).

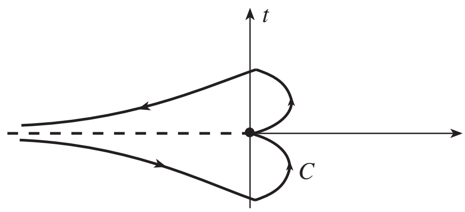


Figure 12.27 $J_n(z) = \frac{1}{2}[H_n^{(1)}(z) + H_n^{(2)}(z)]$.

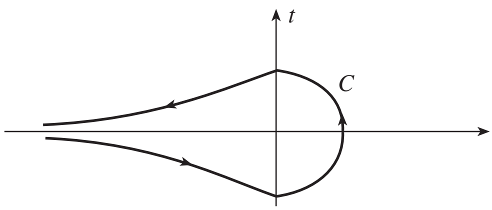


Figure 12.28 For the integer values n, there is no need for the branch cut; hence, the contour for the integral definition of $J_n(z)$ can be deformed into C.

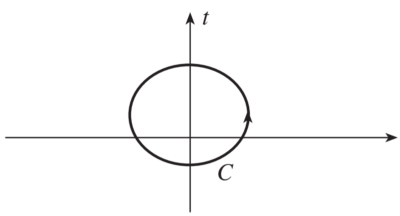


Figure 12.29 The contour for $J_n(z)$, where n takes integer values, can be taken as any closed path enclosing the origin.

In Eq. (12.271), we now make the transformation $t = 2s/z$ to write

$$J_n(z) = \frac{1}{2\pi i}\left(\frac{z}{2}\right)^n \int_C ds \frac{\exp\left[s - \frac{z^2}{4s}\right]}{s^{n+1}}. \tag{12.272}$$

Expanding $e^{-z^2/4s}$:

$$e^{-z^2/4s} = \sum_{r=0}^{\infty} \frac{(-1)^r}{r!} \frac{z^{2r}}{2^{2r}s^r}, \tag{12.273}$$

we write

$$J_n(z) = \left(\frac{z}{2}\right)^n \sum_{r=0}^{\infty} \frac{(-1)^r}{r!} \quad \left(\frac{z}{2}\right)^{2r} \frac{1}{2\pi i} \int_C ds\ e^s s^{-n-r-1}. \tag{12.274}$$

The integral is nothing but one of the integral representations of the **gamma function** [Eq. (12.220)]:

$$\frac{1}{\Gamma(z)} = \frac{1}{2\pi i} \int_C dt\ e^t t^{-z}, \tag{12.275}$$

which leads to the series expression of $J_n(z)$:

$$J_n(z) = \left(\frac{z}{2}\right)^n \sum_{r=0}^{\infty} \frac{(-1)^r}{r!\Gamma(n+r+1)} \left(\frac{z}{2}\right)^{2r}. \tag{12.276}$$

An other useful formula can be obtained by using the contour integral representation in Eq. (12.262) and the substitution $t = e^{i\theta}$, which allows us to write

$$J_n(z) = \frac{1}{2\pi i} \int_0^{2\pi} \frac{e^{iz\sin\theta}}{e^{(n+1)i\theta}} ie^{i\theta} d\theta \tag{12.277}$$

$$= \frac{1}{2\pi} \int_0^{2\pi} e^{i(z\sin\theta - n\theta)} d\theta. \tag{12.278}$$

This yields the **Bessel's integral** [Eq. (5.60)] as

$$J_n(z) = \frac{1}{\pi} \int_0^{\pi} \cos(n\theta - z\sin\theta) d\theta. \tag{12.279}$$

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Problems

1 Use the contour integral representation of the Laguerre polynomials:

$$L_n(x) = \frac{1}{2\pi i} \oint \frac{z^n e^{x-z} dz}{(z-x)^{n+1}},$$

where C is a circle centered at x, to obtain the coefficients, C_k, in the expansion

$$L_n(x) = \sum_{k=0}^{n} C_k x^{n-k}.$$

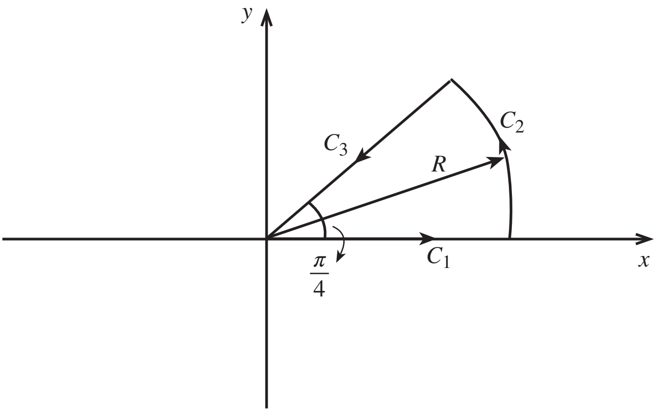

Figure 12.30 Contour for problem 5.

2 Establish the following contour integral representation for the Hermite polynomials:

$$H_n(x) = \frac{(-1)^n n!}{2\pi i} e^{x^2} \oint_C \frac{e^{-z^2} dz}{(z-x)^{n+1}},$$

where C encloses the point x. Use this result to derive the series expansion

$$H_n(x) = \sum_{j=0}^{[n/2]} (-1)^j \frac{2^{n-2j} x^{n-2j} n!}{(n-2j)! j!}.$$

3 Using Taylor series prove the Cauchy–Goursat theorem, $\oint_C f(z)dz = 0$, where $f(z)$ is an analytic function within and on the closed contour C in a simply connected domain.

4 Find the Laurent expansions of the function

$$f(z) = \frac{1}{1-z} + \frac{2}{(2-z)}$$

about the origin for the regions $|z| < 1$, $|z| > 2$, and $1 < |z| < 2$. Use two different methods and show that the results agree with each other.

5 Using the path in Figure 12.30, evaluate the integral

$$\int_0^\infty e^{-ix^2} dx.$$

6 Evaluate the following integrals:

(i) $$\int_0^{2\pi} \frac{(\cos 3\theta)d\theta}{5 - 4\cos\theta},$$

(ii) $$\int_{-\infty}^{\infty} \frac{\sin x\; dx}{x^2 + 4x + 5},$$

(iii) $$\int_0^{\infty} \frac{\ln(x^2 + 1)dx}{x^2 + 1},$$

(iv) $$\int_0^{\infty} \frac{dx}{1 + x^5},$$

(v) $$\int_0^{\infty} \frac{\sin x\; dx}{x},$$

(vi) $$\int_0^{\infty} \frac{dx}{a^3 + x^3},$$

(vii) $$\int_{-\infty}^{\infty} \frac{x^2 dx}{(x + 1)(x^2 + 2x + 2)},$$

(viii) $$\int_{-\infty}^{\infty} \frac{x^{2a-1}}{b^2 + x^2} dx,$$

(ix) $$\int_0^{2\pi} \frac{\sin^2\theta\; d\theta}{a + b\cos\theta},$$

(x) $$\int_{-\infty}^{\infty} \frac{\sin x\; dx}{x(a^2 + x^2)}.$$

7 Evaluate the following Cauchy principal value integral:

$$P\int_0^{\infty} \frac{dx}{[(x - x_0)^2 + a^2](x - x_1)}, \quad x_1 > x_0.$$

8 Using the generating function for the polynomials $P_{nm}(x)$:

$$\frac{e^{-xt/(1-t)}}{(1 - t)^{m+1}} = \sum_{n=0}^{\infty} P_{nm}(x)t^n, \quad |t| < 1,\; m = \text{positive},$$

establish a contour integral representation in the complex t-plane. Use this representation to find $A(n, m, k)$ in

$$P_{nm}(x) = \sum_{k=0}^{n} A(n, m, k)x^k.$$

9 Use contour integral techniques to evaluate

$$\int_{-\infty}^{\infty} \frac{\sin^2 x \, dx}{x^2(1 + x^2)}.$$

10 The Jacobi polynomials, $P_n^{(a,b)}(\cos\theta)$, where n = positive integer and a, b are arbitrary real numbers, are defined by the Rodriguez formula:

$$P_n^{(a,b)}(x) = \frac{(-1)^n}{2^n n!(1-x)^a(1+x)^b} \frac{d^n}{dx^n}[(1-x)^{n+a}(1+x)^{n+b}], \quad |x| < 1.$$

(i) Find a contour integral representation for this polynomial valid for $|x| < 1$.

(ii) Use this to show that the polynomial can be expanded as

$$P_n^{(a,b)}(\cos\theta) = \sum_{k=0}^{n} A(n, a, b, k)\left(\sin\frac{\theta}{2}\right)^{2n-2k}\left(\cos\frac{\theta}{2}\right)^{2k}.$$

(iii) Determine the coefficients $A(n, a, b, k)$ for the special case, where a and b are both integers.

11 For a function $F(z)$ analytic everywhere in the upper half plane and on the real axis with the property

$$F(z) \to b \text{ as } |z| \to \infty, \; b \text{ is a real constant,}$$

show the following Cauchy principal value integrals:

$$F_R(z) = b + \frac{1}{\pi} P \int_{-\infty}^{\infty} \frac{F_I(x')dx'}{x' - x}$$

and

$$F_I(z) = -\frac{1}{\pi} P \int_{-\infty}^{\infty} \frac{F_R(x')dx'}{x' - x}.$$

12 Given the following contour integral definition of the spherical Hankel function of the first kind:

$$h_l^{(1)}(x) = \frac{(-1)^l 2^l l!}{\pi x^{l+1}} \oint_C \frac{e^{-ixz}dz}{(z^2 - 1)^{l+1}},$$

where the contour C encloses the point $x = -1$, show that $h_l^{(1)}(x)$ can be written as

$$h_l^{(1)}(x) = \sum_{k=0}^{\infty} A(k,l) \frac{e^{i[x-\beta(l,k)]}}{x^{k+1}},$$

In addition,

(i) show that this series breaks of at the $k = l$th term,
(ii) by using the contour integral definition given above, find explicitly the constants $A(k,l)$ and $\beta(l,k)$.

13 Another definition for the gamma function is given as

$$\Gamma(x) = x^{x-\frac{1}{2}} e^{-x} \sqrt{2\pi} e^{\theta(x)/12x}, \quad x > 0,$$

where $\theta(x)$ is a function satisfying $0 < \theta(x) < 1$. Using the above definition, show the limit

$$\lim_{x\to\infty} \frac{\Gamma(x+1)}{x^{x+\frac{1}{2}} e^{-x} \sqrt{2\pi}} = 1.$$

When x is an integer, this gives the **Stirling's approximation** to $x!$ as $x \to \infty$:

$$x! \sim x^{x+\frac{1}{2}} e^{-x} \sqrt{2\pi}.$$

14 Show that

$$\Gamma(x+1) = x\Gamma(x), \quad x > 0$$

and

$$\Gamma(n+1) = n!, \quad n = \text{integer} > 0.$$

15 Show that

$$\begin{aligned}(1+x)^{1/2} &= \sum_{n=0}^{\infty} \binom{1/2}{n} x^n = 1 + \frac{x}{2} - \frac{x^2}{8} + \frac{x^3}{16} - \cdots \\ &= 1 + \frac{x}{2} + \sum_{n=2}^{\infty} (-1)^{n-1} \frac{(2n-3)!!}{(2n)!!} x^n,\end{aligned}$$

where the **double factorial** means

$$\begin{aligned}(2n+1)!! &= 1 \cdot 3 \cdot 5 \cdots (2n+1), \\ (2n)!! &= 2 \cdot 4 \cdot 6 \cdots (2n).\end{aligned}$$

16 Use the factorization method (Chapter 8) to show that the spherical Hankel functions of the first kind,

$$h_l^{(1)} = j_l + in_l,$$

can be expressed as

$$\begin{aligned} h_l^{(1)}(x) &= (-1)^l x^l \left[\frac{1}{x}\frac{d}{dx}\right]^l h_0^{(1)}(x) \\ &= (-1)^l x^l \left[\frac{1}{x}\frac{d}{dx}\right]^l \left(\frac{-ie^{ix}}{x}\right). \end{aligned}$$

Hint: First define

$$u_l(x) = y_l(x)/x^{l+1}$$

in

$$y_l'' + \left[1 - \frac{l(l+1)}{x^2}\right] y_l = 0.$$

Using this result, define $h_l^{(1)}(x)$ as a contour integral in the complex j'-plane, $j' = t' + is'$, where

$$\frac{d}{dt} = \frac{1}{x}\frac{d}{dx}.$$

Indicate your contour, C, by clearly showing the singularities that must be avoided.

17 Using the integral definition of $h_l^{(1)}(x)$ found in the previous problem and the transformation

$$z'' = -\frac{[2j']^{1/2}}{x},$$

show that an even more useful integral definition can be obtained as

$$h_l^{(1)}(x) = \frac{(-1)^l 2^l l!}{\pi x^{l+1}} \oint_{C_{z''}} \frac{e^{-ixz} dz''}{[(z''-1)(z''+1)]^{l+1}}.$$

Compare the two contours, C and $C_{z''}$.

18 If $f(z)$ is analytic in the lower half of the z-plane:

$$f(z) \to 0 \text{ as } |z| \to \infty \text{ for } y < 0,$$

then show that the following Cauchy principal value integral is true:

$$P \int_{-\infty}^{\infty} \frac{f(x)dx}{(x-a)} = -i\pi f(a).$$

Identify your two choices for the detour around the singular point on the real axis and show that the Cauchy principal value is $-i\pi f(a)$ for both choices.

13

Fractional Calculus

The integral form of the **diffusion equation** is written as

$$\boxed{\frac{\partial}{\partial t}\iiint_V c\left(\overrightarrow{r},t\right) dv = -\oint_S \overrightarrow{J}\left(\overrightarrow{r},t\right)\cdot d\overrightarrow{s},} \tag{13.1}$$

where $c\left(\overrightarrow{r},t\right)$ is the concentration of particles and $\overrightarrow{J}\left(\overrightarrow{r},t\right)$ is the current density. The left-hand side of this equation gives the rate of change of the number of particles in volume V, and the right-hand side gives the number of particles flowing past the boundary, S, of volume V, per unit time. In the absence of sources or sinks, these terms are naturally equal. Using the Gauss theorem we can write the above equation as

$$\frac{\partial}{\partial t}\iiint_V c\left(\overrightarrow{r},t\right) dv + \iiint_V \overrightarrow{\nabla}\cdot\overrightarrow{J}\left(\overrightarrow{r},t\right) dv = 0, \tag{13.2}$$

$$\iiint_V \left[\frac{\partial}{\partial t}c\left(\overrightarrow{r},t\right) + \overrightarrow{\nabla}\cdot\overrightarrow{J}\left(\overrightarrow{r},t\right)\right] dv = 0. \tag{13.3}$$

For an arbitrary volume element, we can set the expression inside the square brackets to zero, thus obtaining the partial differential equation to be solved for concentration:

$$\boxed{\frac{\partial}{\partial t}c\left(\overrightarrow{r},t\right) + \overrightarrow{\nabla}\cdot\overrightarrow{J}\left(\overrightarrow{r},t\right) = 0.} \tag{13.4}$$

With a given relation between $c\left(\overrightarrow{r},t\right)$ and $\overrightarrow{J}\left(\overrightarrow{r},t\right)$, we can now solve this equation for $c\left(\overrightarrow{r},t\right)$. Since particles have a tendency to flow from regions of high to low concentration, as a first approximation, we can assume a linear relation between the current density and the gradient of concentration as $\overrightarrow{J} = -k\overrightarrow{\nabla}c\left(\overrightarrow{r},t\right)$. The proportionality constant, k, is called the diffusion

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constant. We can now write the **diffusion equation** as

$$\boxed{\frac{\partial}{\partial t}c\left(\overrightarrow{r},t\right)-k\overrightarrow{\nabla}^{2}c\left(\overrightarrow{r},t\right)=0,} \tag{13.5}$$

which is also called the **Fick's equation**.

Einstein noticed that in a diffusion process concentration is also proportional to the probability, $P\left(\overrightarrow{r},t\right)$, of finding a diffusing particle at position $\overrightarrow{r}$ and time t. Thus, the probability distribution satisfies the same differential equation as the concentration. For a particle starting its motion from the origin, probability distribution can be found as

$$P\left(\overrightarrow{r},t\right)=\frac{1}{(4\pi kt)^{3/2}}\exp\left(-\frac{r^2}{4kt}\right). \tag{13.6}$$

This means that even though the average displacement of a particle is zero:

$$\langle\overrightarrow{r}\rangle=0, \tag{13.7}$$

the mean square displacement, $\langle\overrightarrow{r}^{2}\rangle=\langle\overrightarrow{r}^{2}\rangle-\langle\overrightarrow{r}\rangle^2$, is nonzero and depends on time as

$$\langle\overrightarrow{r}^{2}\rangle=\int r^2P\left(\overrightarrow{r},t\right)d^3r=6kt. \tag{13.8}$$

In other words, the particle slowly drifts away from its initial position. What is significant in this equation is the relation

$$\boxed{\langle r^2(t)\rangle\propto t.} \tag{13.9}$$

For the particle to cover twice the distance, time must be increased by a factor of four. This scaling property results from the diffusion equation where the time derivative is of first order and the space derivative is of second order. However, it has been experimentally determined that for some processes this relation goes as

$$\boxed{\langle r^2(t)\rangle\propto t^{\alpha},\quad \alpha\neq 1.} \tag{13.10}$$

In terms of the diffusion equation this would imply

$$\boxed{\frac{\partial^{\alpha}}{\partial t^{\alpha}}P\left(\overrightarrow{r},t\right)-k_{\alpha}\overrightarrow{\nabla}^{2}P\left(\overrightarrow{r},t\right)=0,\qquad k_{\alpha}\neq 1.} \tag{13.11}$$

However, what does this mean? Is a fractional derivative possible? If a fractional derivative is possible, can we also have a fractional integral? Actually, the geometric interpretation of derivative as the slope and integral as the area are so natural that most of us have not even thought of the possibility of fractional derivatives and integrals, let alone their meaning. On the other hand, the history of fractional calculus dates back as far as Leibniz (1695), and results have been accumulated over the past years in various branches of mathematics. The situation on the applied side of this intriguing branch of mathematics is now changing rapidly, and there are a growing number of research areas in science and engineering that make use of fractional calculus. Chemical analysis of fluids, heat transfer, diffusion, Schrödinger equation, and material science are some areas where fractional calculus is used. Interesting applications to economy, finance, and earthquake science should also be expected. It is well known that in the study of nonlinear situations and in the study of processes away from equilibrium fractal curves and surfaces are encountered, where ordinary mathematical techniques are not sufficient. In this regard, the relation between fractional calculus and fractals is also being actively investigated. Fractional calculus also offers us some useful mathematical techniques in evaluating definite integrals and finding sums of infinite series. In this chapter, we introduce some of the basic properties of fractional calculus along with some mathematical techniques and their applications.

13.1 Unified Expression of Derivatives and Integrals

13.1.1 Notation and Definitions

In our notation we follow Oldham and Spanier [15], where a detailed treatment of the subject along with a survey of the history and various applications can be found. Unless otherwise specified, we use n and N for positive integers, q and Q for any number. The nth derivative of a function, $f(x)$, is shown as $\frac{d^n f}{dx^n}$. Since an integral is the inverse of a derivative, we write

$$\frac{d^{-1}f}{d[x]^{-1}} = \int_0^x f(x_0)dx_0. \tag{13.12}$$

Successive integrations will be shown as

$$\frac{d^{-2}f}{d[x]^{-2}} = \int_0^x dx_1 \int_0^{x_1} f(x_0)dx_0, \tag{13.13}$$

$$\vdots$$

$$\frac{d^{-n}f}{d[x]^{-n}} = \int_0^x dx_{n-1} \int_0^{x_{n-1}} dx_{n-2} \cdots \int_0^{x_2} dx_1 \int_0^{x_1} f(x_0)dx_0. \tag{13.14}$$

When the lower limit differs from zero, we will write

$$\frac{d^{-1}f}{[d(x-a)]^{-1}} = \int_a^x f(x_0)dx_0, \tag{13.15}$$

$$\vdots$$

$$\frac{d^{-n}f}{[d(x-a)]^{-n}} = \int_a^x dx_{n-1} \int_a^{x_{n-1}} dx_{n-2} \cdots \int_a^{x_2} dx_1 \int_a^{x_1} f(x_0)dx_0. \quad (13.16)$$

We should remember that even though the equation

$$\frac{d^n}{[d(x-a)]^n} = \frac{d^n}{[dx]^n} \quad (13.17)$$

is true for derivatives, it is not true for integrals, that is,

$$\frac{d^{-n}}{[d(x-a)]^{-n}} \neq \frac{d^{-n}}{[dx]^{-n}}. \quad (13.18)$$

The nth derivative is frequently written as $f^{(n)}(x)$. Hence for n successive integrals we will also use

$$f^{(-n)} = \int_{a_n}^x dx_{n-1} \int_{a_{n-1}}^{x_{n-1}} dx_{n-2} \cdots \int_{a_2}^{x_2} dx_1 \int_{a_1}^{x_1} f(x_0)dx_0. \quad (13.19)$$

When there is no room for confusion, in general, we also write

$$\frac{d^q f(x)}{[d(x-0)]^q} = \begin{cases} d^q f(x)/[dx]^q, \\ d^q f(x)/dx^q, \\ f^{(q)}(x), \end{cases} \quad (13.20)$$

where q can take any positive or negative value. The value of a differintegral at $x = b$ is shown as

$$\left.\frac{d^q f(x)}{[d(x-a)]^q}\right|_{x=b} = \frac{d^q f}{[d(x-a)]^q}(b). \quad (13.21)$$

Other commonly used expressions for differintegrals are:

$$\frac{d^q f(x)}{[d(x-a)]^q} = \begin{cases} {}_a\mathbf{D}_x^q f(x), \\ \mathbf{D}_a^q f(x). \end{cases} \quad (13.22)$$

13.1.2 The *n*th Derivative of a Function

Before we introduce the differintegral, we derive a unified expression for the derivative and integral for integer orders. We first write the definition of a derivative as

$$\frac{d^1 f}{dx^1} = \frac{df(x)}{dx} = \lim_{\delta x \to 0} \{[\delta x]^{-1}[f(x) - f(x - \delta x)]\}. \quad (13.23)$$

Similarly, the second- and third-order derivatives can be written as

$$\frac{d^2f}{dx^2} = \lim_{\delta x \to 0} \{[\delta x]^{-2}[f(x) - 2f(x - \delta x) + f(x - 2\delta x)]\}, \tag{13.24}$$

$$\frac{d^3f}{dx^3} = \lim_{\delta x \to 0} \{[\delta x]^{-3}[f(x) - 3f(x - \delta x) + 3f(x - 2\delta x) - f(x - 3\delta x)]\}. \tag{13.25}$$

Since the coefficients in these equations are the binomial coefficients, for the nth derivative we can write

$$\frac{d^nf}{dx^n} = \lim_{\delta x \to 0} \left\{ [\delta x]^{-n} \sum_{j=0}^{n} [-1]^j \binom{n}{j} f(x - j\delta x) \right\}. \tag{13.26}$$

In these equations, we have assumed that all the derivatives exist. In addition, we have assumed that $[\delta x]$ goes to zero continuously, that is, by taking all values on its way to zero. For a unified representation with the integral, we are going to need a restricted limit. For this we divide the interval $[x - a]$ into N equal segments as $\delta_N x = [x - a]/N$, $N = 1, 2, 3, \ldots$. In this expression a is a number smaller than x. Thus, Eq. (13.26) becomes

$$\frac{d^nf}{[dx]^n} = \lim_{\delta_N x \to 0} \left\{ [\delta_N x]^{-n} \sum_{j=0}^{n} [-1]^j \binom{n}{j} f(x - j\delta_N x) \right\}. \tag{13.27}$$

Since the binomial coefficients $\binom{n}{j}$ are zero for the $j > n$ values, we can also write

$$\frac{d^nf}{[dx]^n} = \lim_{\delta_N x \to 0} \left\{ [\delta_N x]^{-n} \sum_{j=0}^{N-1} [-1]^j \binom{n}{j} f(x - j\delta_N x) \right\}. \tag{13.28}$$

Now, assuming that this limit is also valid in the continuum limit, we write the ***n*th derivative** as

$$\boxed{\frac{d^nf}{[dx]^n} = \lim_{N \to \infty} \left\{ \left[\frac{x-a}{N}\right]^{-n} \sum_{j=0}^{N-1} [-1]^j \binom{n}{j} f\left(x - j\left[\frac{x-a}{N}\right]\right) \right\}.} \tag{13.29}$$

13.1.3 Successive Integrals

We now concentrate on the expression for n successive integrations of $f(x)$. Because an integral of integer order is defined as area, we express it as a

Riemann sum:

$$\frac{d^{-1}f}{[d(x-a)]^{-1}} = \int_a^x f(x_0)dx_0 \tag{13.30}$$

$$= \lim_{\delta_N x\to 0}\{\delta_N x[f(x)+f(x-\delta_N x)+f(x-2\delta_N x)+ \tag{13.31}$$

$$\cdots + f(a+\delta_N x)]\}$$

$$= \lim_{\delta_N x\to 0}\left\{\delta_N x\sum_{j=0}^{N-1} f(x-j\delta_N x)\right\}. \tag{13.32}$$

As before, we have taken $\delta_N x = [x-a]/N$. We also write the Riemann sum for the double integral as

$$\frac{d^{-2}f}{[d(x-a)]^{-2}} = \int_a^x dx_1\int_a^{x_1} f(x_0)dx_0 \tag{13.33}$$

$$= \lim_{\delta_N x\to 0}\{[\delta_N x]^2[f(x)+2f(x-\delta_N x)+3f(x-2\delta_N x)+ \tag{13.34}$$

$$\cdots + Nf(a+\delta_N x)]\}$$

$$= \lim_{\delta_N x\to 0}\left\{[\delta_N x]^2\sum_{j=0}^{N-1}[j+1]f(x-j\delta_N x)\right\} \tag{13.35}$$

and for the triple integral as

$$\frac{d^{-3}f}{[d(x-a)]^{-3}} = \int_a^x dx_2\int_a^{x_2} dx_1\int_a^{x_1} f(x_0)dx_0 \tag{13.36}$$

$$= \lim_{\delta_N x\to 0}\{[\delta_N x]^3\sum_{j=0}^{N-1}\frac{[j+1][j+2]}{2}f(x-j\delta_N x)\}. \tag{13.37}$$

Similarly for n-**fold integration** we write

$$\frac{d^{-n}f}{[d(x-a)]^{-n}} = \lim_{\delta_N x\to 0}\left\{[\delta_N x]^n\sum_{j=0}^{N-1}\binom{j+n-1}{j}f(x-j\delta_N x)\right\}, \tag{13.38}$$

$$\boxed{\frac{d^{-n}f}{[d(x-a)]^{-n}} = \lim_{N\to\infty}\left\{\left[\frac{x-a}{N}\right]^n\sum_{j=0}^{N-1}\binom{j+n-1}{j}f\left(x-j\left[\frac{x-a}{N}\right]\right)\right\}.} \tag{13.39}$$

Compared to Eq. (13.29), the binomial coefficients in this equation are going as

$$\binom{j+n-1}{j}$$

and all the terms are positive.

13.1.4 Unification of Derivative and Integral Operators

Using Eqs. (13.29) and (13.39) and also making use of the relation

$$[-1]^j \binom{n}{j} = \binom{j+n-1}{j} = \frac{\Gamma(j-n)}{\Gamma(-n)\Gamma(j+1)}, \tag{13.40}$$

we can write a **unified expression** for both the derivative and integral of order n as

$$\boxed{\frac{d^n f}{[d(x-a)]^n} = \lim_{N\to\infty} \left\{ \frac{\left[\frac{x-a}{N}\right]^{-n}}{\Gamma(-n)} \sum_{j=0}^{N-1} \frac{\Gamma(j-n)}{\Gamma(j+1)} f\left(x - j\frac{[x-a]}{N}\right) \right\}.} \tag{13.41}$$

In this equation, n takes integer values of both signs.

13.2 Differintegrals

13.2.1 Grünwald's Definition of Differintegrals

Considering that the gamma function in the above formula is valid for all n, we obtain the most general and basic definition of differintegral given by Grünwald, also called the **Grünwald–Letnikov definition**, as

$$\boxed{\frac{d^q f}{[d(x-a)]^q} = \lim_{N\to\infty} \left\{ \frac{\left[\frac{x-a}{N}\right]^{-q}}{\Gamma(-q)} \sum_{j=0}^{N-1} \frac{\Gamma(j-q)}{\Gamma(j+1)} f\left(x - j\left[\frac{x-a}{N}\right]\right) \right\}.} \tag{13.42}$$

In this expression q can take all values. A major advantage of this definition is that the differintegral is found by using only the values of the function without the need for its derivatives or integrals. On the other hand, evaluation of the infinite series could pose practical problems in applications. In this formula even though the gamma function, $\Gamma(-q)$, is infinite for the positive integer values of q, their ratio, $\Gamma(j-q)/\Gamma(-q)$, is finite.

We now show that for a positive integer n and for all q values the following relation is true:

$$\boxed{\frac{d^n}{dx^n} \frac{d^q f}{[d(x-a)]^q} = \frac{d^{n+q} f}{[d(x-a)]^{n+q}}, \quad n \geq 0.} \tag{13.43}$$

Using $\delta_N x = [x-a]/N$, we can write

$$\frac{d^q f}{[d(x-a)]^q} = \lim_{N\to\infty} \left\{ \frac{[\delta_N x]^{-q}}{\Gamma(-q)} \sum_{j=0}^{N-1} \frac{\Gamma(j-q)}{\Gamma(j+1)} f(x - j\delta_N x) \right\}. \tag{13.44}$$

If we further divide the interval $a \le x' \le x - \delta_N x$ into $N-1$ equal pieces we can write

$$\begin{aligned} &\frac{d^q f}{[d(x-a)]^q}(x-\delta_N x) \\ &= \lim_{N\to\infty} \left\{ \frac{[\delta_N x]^{-q}}{\Gamma(-q)} \sum_{j=0}^{N-2} \frac{\Gamma(j-q)}{\Gamma(j+1)} f(x-\delta_N x - j\delta_N x) \right\} \quad (13.45)\\ &= \lim_{N\to\infty} \left\{ \frac{[\delta_N x]^{-q}}{\Gamma(-q)} \sum_{j=1}^{N-1} \frac{\Gamma(j-q-1)}{\Gamma(j)} f(x - j\delta_N x) \right\}. \quad (13.46)\end{aligned}$$

Taking the derivative of Eq. (13.44) and using Eq. (13.46) gives

$$\begin{aligned} &\frac{d}{dx}\frac{d^q f}{[d(x-a)]^q} \\ &= \lim_{N\to\infty} \left\{ [\delta_N x]^{-1} \left[\frac{d^q f}{[d(x-a)]^q}(x) - \frac{d^q f}{[d(x-a)]^q}(x-\delta_N x) \right] \right\} \quad (13.47)\end{aligned}$$

$$= \lim_{N\to\infty} \left\{ \frac{[\delta_N x]^{-q-1}}{\Gamma(-q)} \left[\Gamma(-q) f(x) + \sum_{j=1}^{N-1} \left\{ \frac{\Gamma(j-q)}{\Gamma(j+1)} - \frac{\Gamma(j-q-1)}{\Gamma(j)} \right\} f(x - j\delta_N x) \right] \right\}. \tag{13.48}$$

We now use the following relation among gamma functions:

$$\frac{\Gamma(j-q)}{\Gamma(j+1)} - \frac{\Gamma(j-q-1)}{\Gamma(j)} = \frac{\Gamma(-q)}{\Gamma(-q-1)} \frac{\Gamma(j-q-1)}{\Gamma(j+1)}, \tag{13.49}$$

to write Eq. (13.48) as

$$\frac{d}{dx}\frac{d^q f}{[d(x-a)]^q} = \lim_{N\to\infty} \left\{ \frac{[\delta_N x]^{-q-1}}{\Gamma(-q-1)} \left[\sum_{j=0}^{N-1} \frac{\Gamma(j-q-1)}{\Gamma(j+1)} f(x - j\delta_N x) \right] \right\} \tag{13.50}$$

$$= \frac{d^{q+1} f}{[d(x-a)]^{q+1}}. \tag{13.51}$$

The general formula can be shown by assuming this to be true for $(n-1)$ and then showing it for n.

13.2.2 Riemann–Liouville Definition of Differintegrals

Another commonly used definition of the differintegral is given by **Riemann and Liouville**. Assume that the following integral is given:

$$I_n(x) = \int_a^x (x-\xi)^{n-1} f(\xi) d\xi, \tag{13.52}$$

where n is an integer greater than zero and a is a constant. Using the formula

$$\frac{d}{dx}\int_{A(x)}^{B(x)} F(x,\xi)d\xi = \int_{A(x)}^{B(x)} \frac{\partial F(x,\xi)}{\partial x} d\xi + F(x,B(x))\frac{dB(x)}{dx} - F(x,A(x))\frac{dA(x)}{dx}, \tag{13.53}$$

we find the derivative of I_n as

$$\frac{dI_n}{dx} = (n-1)\int_a^x (x-\xi)^{n-2} f(\xi)d\xi + [(x-\xi)^{n-1} f(\xi)]_{\xi=x}. \tag{13.54}$$

For $n > 1$ this gives us

$$\frac{dI_n}{dx} = (n-1)I_{n-1} \tag{13.55}$$

and for $n = 1$

$$\frac{dI_1}{dx} = f(x). \tag{13.56}$$

Differentiating Eq. (13.54) k times we find

$$\frac{d^k I_n}{dx^k} = (n-1)(n-2)\cdots(n-k)I_{n-k}, \tag{13.57}$$

which gives us

$$\frac{d^{n-1} I_n}{dx^{n-1}} = (n-1)! I_1(x), \tag{13.58}$$

or

$$\frac{d^n I_n}{dx^n} = (n-1)! f(x). \tag{13.59}$$

Using the fact that $I_n(a) = 0$ for $n \geq 1$, from Eqs. (13.58) and (13.59) we see that $I_n(x)$ and all of its $(n-1)$ derivatives evaluated at $x = a$ are zero. This gives us

$$I_1(x) = \int_a^x f(x_1)dx_1, \tag{13.60}$$

$$I_2(x) = \int_a^x I_1(x_2)dx_2 = \int_a^x \int_a^{x_2} f(x_1)dx_1dx_2, \tag{13.61}$$

$$\vdots \tag{13.62}$$

$$I_n(x) = (n-1)! \int_a^x \int_a^{x_n} \cdots \int_a^{x_3} \int_a^{x_2} f(x_1)dx_1 dx_2 \cdots dx_{n-1}dx_n. \quad (13.63)$$

From these equations, we obtain a very useful formula also known as the **Cauchy formula**:

$$\int_a^x \int_a^{x_n} \cdots \int_a^{x_3} \int_a^{x_2} f(x_1)dx_1 \cdots dx_{n-1}dx_n = \frac{1}{(n-1)!} \int_a^x (x-\xi)^{n-1} f(\xi)d\xi. \quad (13.64)$$

To obtain the Riemann–Liouville definition of the differintegral, we write the above equation for all $q < 0$ as

$$\left[\frac{d^q f}{[d(x-a)]^q}\right]_{R-L} = \frac{1}{\Gamma(-q)} \int_a^x \left[x - x'\right]^{-q-1} f(x')dx', \quad q < 0. \quad (13.65)$$

However, this formula is valid only for the $q < 0$ values. In this definition, $[..]_{R-L}$ denotes the fact that differintegral is being evaluated by the Riemann–Liouville definition. Later, when we show that this definition agrees with the Grünwald definition for all q, we drop the subscript.

We first show that for $q < 0$ and for a finite function $f(x)$ in the interval $a \leq x' \leq x$, the two definitions agree. We now calculate the difference between the two definitions as

$$\Delta = \frac{d^q f}{[d(x-a)]^q} - \left[\frac{d^q f}{[d(x-a)]^q}\right]_{R-L}. \quad (13.66)$$

Using the definitions in Eqs. (13.42) and (13.65), and changing the range of the integral, we write Δ as

$$\Delta = \lim_{N\to\infty} \left\{ \frac{[\delta_N x]^{-q}}{\Gamma(-q)} \sum_{j=0}^{N-1} \frac{\Gamma(j-q)}{\Gamma(j+1)} f(x - j\delta_N x) \right\} - \frac{1}{\Gamma(-q)} \int_0^{x-a} \frac{f(x-x')}{x'^{1+q}} dx'. \quad (13.67)$$

We write the integral in the second term as a Riemann sum to get

$$\Delta = \lim_{N\to\infty} \left\{ \frac{[\delta_N x]^{-q}}{\Gamma(-q)} \sum_{j=0}^{N-1} \frac{\Gamma(j-q)}{\Gamma(j+1)} f(x - j\delta_N x) \right\} - \lim_{N\to\infty} \left\{ \sum_{j=0}^{N-1} \frac{f(x - j\delta_N x)\delta_N x}{\Gamma(-q)[j\delta_N x]^{1+q}} \right\}. \quad (13.68)$$

Taking $\delta_N x = (x-a)/N$, this becomes

$$\Delta = \lim_{N\to\infty}\left\{\frac{[\delta_N x]^{-q}}{\Gamma(-q)}\sum_{j=0}^{N-1} f(x-j\delta_N x)\left[\frac{\Gamma(j-q)}{\Gamma(j+1)} - j^{-1-q}\right]\right\} \tag{13.69}$$

$$= \frac{[x-a]^{-q}}{\Gamma(-q)}\lim_{N\to\infty}\sum_{j=0}^{N-1} f\left(\frac{Nx-jx+ja}{N}\right)N^q\left[\frac{\Gamma(j-q)}{\Gamma(j+1)} - j^{-1-q}\right]. \tag{13.70}$$

We now write the sum on the right-hand side as two terms, the first from 0 to $(j-1)$ and the other from j to $(n-1)$. Also, assuming that j is sufficiently large so that we can use the approximation

$$\Gamma(j-q)/\Gamma(j+1) \simeq j^{-1-q}[1+q(q+1)/2j+0(j^{-2})], \tag{13.71}$$

we obtain

$$\Delta = \frac{[x-a]^{-q}}{\Gamma(-q)}\lim_{N\to\infty}\left\{\sum_{j=0}^{J-1} f\left(\frac{Nx-jx+ja}{N}\right)N^q\left[\frac{\Gamma(j-q)}{\Gamma(j+1)} - j^{-1-q}\right]\right\} \tag{13.72}$$

$$+\frac{[x-a]^{-q}}{\Gamma(-q)}\lim_{N\to\infty}\left\{\frac{1}{N}\sum_{j=J}^{N-1} f\left(\frac{Nx-jx+ja}{N}\right)\left[\frac{j}{N}\right]^{-2-q}\left[\frac{q(q+1)}{2N}+\frac{0(j^{-1})}{N}\right]\right\}.$$

In the first sum, for $q < -1$, the quantity inside the parentheses is finite and in the limit as $N \to \infty$, because of the N^q factor going to zero. Similarly, for $q \leq -2$, the second term also goes to zero as $N \to \infty$. Thus, we have shown that in the interval $a \leq x' \leq x$, for a finite function $f(x)$ and for $q \leq -2$, the two definitions agree:

$$\frac{d^q f}{[d(x-a)]^q} = \left[\frac{d^q f}{[d(x-a)]^q}\right]_{R-L}, \quad q \leq -2. \tag{13.73}$$

To see that the Riemann–Liouville definition agrees with the Grünwald definition [Eq. (13.42)] for all q, as in the Grünwald definition, we require the Riemann–Liouville definition to satisfy Eq. (13.43):

$$\left[\frac{d^q f}{[d(x-a)]^q}\right]_{R-L} = \frac{d^n}{dx^n}\left[\frac{d^{q-n} f}{[d(x-a)]^{q-n}}\right]_{R-L}. \tag{13.74}$$

In the above formula, for a given q, if we choose n as $q-n \leq -2$ and use Eq. (13.73) to write

$$\left[\frac{d^q f}{[d(x-a)]^q}\right]_{R-L} = \frac{d^n}{dx^n}\left[\frac{d^{q-n} f}{[d(x-a)]^{q-n}}\right], \tag{13.75}$$

we see that the Grünwald definition and the Riemann–Liouville definition agree with each other for all q values:

$$\left[\frac{d^q f}{[d(x-a)]^q}\right]_{R-L} = \left[\frac{d^q f}{[d(x-a)]^q}\right]. \tag{13.76}$$

We can now drop the subscript $R-L$.

Riemann–Liouville definition:

For $q < 0$, the differintegral is evaluated by using the formula

$$\left[\frac{d^q f}{[d(x-a)]^q}\right] = \frac{1}{\Gamma(-q)} \int_a^x [x-x']^{-q-1} f(x')dx', \quad q < 0. \tag{13.77}$$

For $q \geq 0$, we use

$$\left[\frac{d^q f}{[d(x-a)]^q}\right] = \frac{d^n}{dx^n}\left[\frac{1}{\Gamma(n-q)} \int_a^x [x-x']^{-(q-n)-1} f(x')dx'\right], \quad q \geq 0, \tag{13.78}$$

where the integer n must be chosen such that $(q - n) < 0$.

The Riemann–Liouville definition has found widespread application. In this definition the integral in Eq. (13.77) is convergent only for the $q < 0$ values. However, for the $q \geq 0$ values the problem is circumvented by imposing the condition $n > q$ in Eq. (13.78). The fact that we have to evaluate an n-fold derivative of an integral somewhat reduces the practicality of the Riemann–Liouville definition for the $q \geq 0$ values.

13.3 Other Definitions of Differintegrals

The Grünwald and Riemann–Liouville definitions are the most basic definitions of differintegral, and they have been used widely. In addition to these, we can also define differintegral via the Cauchy integral formula and also by using integral transforms. Even though these definitions are not as useful as the Grünwald and Riemann–Liouville definitions, they are worth discussing to show that other definitions are possible and when they are implemented properly, they agree with the basic definitions. Sometimes fractional derivatives and fractional integrals are treated separately. However, their unification as the "differintegral" brings the two notions closer than one usually assumes and avoids confusion between different definitions.

13.3.1 Cauchy Integral Formula

We have seen that for a function $f(z)$ analytic on and inside a closed contour C, the nth derivative is given as

$$\frac{d^n f(z)}{dz^n} = \frac{n!}{2\pi i} \oint_C \frac{f(z')dz'}{(z'-z)^{n+1}}, \quad n \geq 0 \text{ and integer}, \tag{13.79}$$

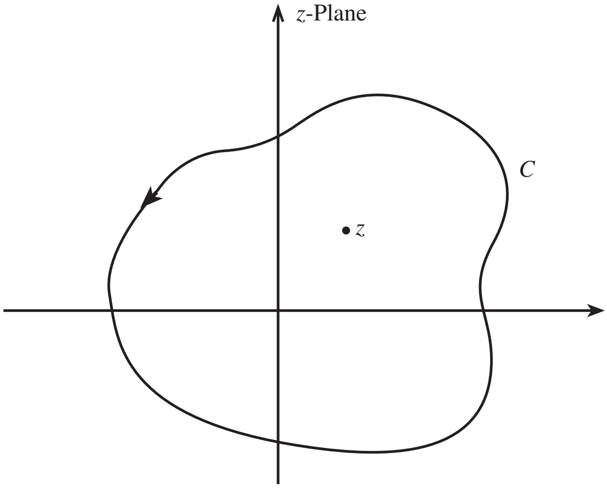

Figure 13.1 Contour C for the Cauchy integral formula.

where z' denotes a point on the contour C and z is a point inside C (Figure 13.1). We rewrite this formula for an arbitrary q and take z as a point on the real axis:

$$\frac{d^q f(x)}{dx^q} = \frac{\Gamma(q+1)}{2\pi i} \oint_C \frac{f(z')dz'}{(z'-x)^{q+1}}. \tag{13.80}$$

For the path shown in Figure 13.1, this formula is valid only for the positive integer values of q. For the negative integer values of q it is not defined because $\Gamma(q+1)$ diverges. However, it can still be used to define differintegrals for the negative but different than integer values of q. Now, x is a branch point; hence we have to be careful with the direction of the cut line. Thus, our path is no longer as shown in Figure 13.1. We choose our cut line along the real axis and to the left of our branch point. We now modify the contour as shown in Figure 13.2 and write our definition of differintegral for the negative, noninteger values of q as

$$\frac{d^q f(x)}{dx^q} = \frac{\Gamma(q+1)}{2\pi i} \oint_C \frac{f(z')dz'}{(z'-x)^{q+1}}, \quad q < 0 \text{ and } \neq \text{integer}. \tag{13.81}$$

The integral is evaluated over the contour C in the limit as the radius goes to infinity.

Evaluating the integral in Eq. (13.81), as it stands, is not easy. Thus, we modify our contour to C' as shown in Figure 13.3. Since the function

$$\frac{f(z')}{(z'-x)^{q+1}} \tag{13.82}$$

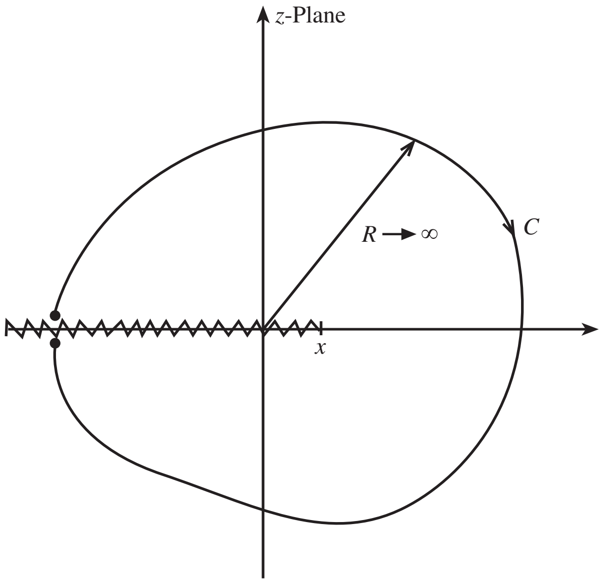

Figure 13.2 Contour C in the differintegral formula.

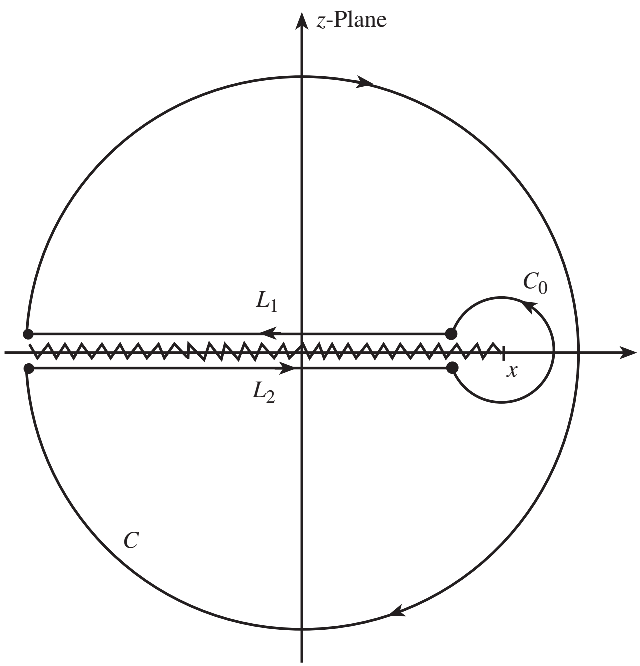

Figure 13.3 Contour $C' = C + C_0 + L_1 + L_2$ in the differintegral formula.

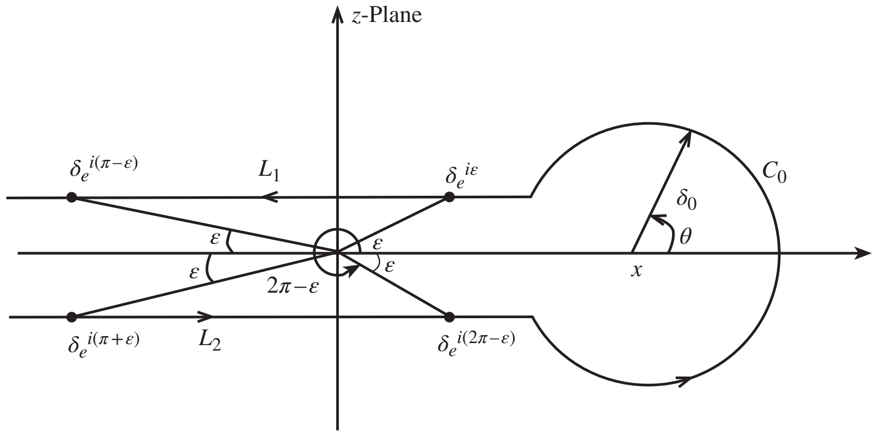

Figure 13.4 Contours for the $\oint_{\leftarrow L_1}$, $\oint_{\rightarrow L_2}$, and $\oint_{C_0}$ integrals.

is analytic within and on the closed contour C', we can write

$$\oint_{C'} \frac{f(z')dz'}{(z'-x)^{q+1}} = 0, \tag{13.83}$$

where the contour C' has the parts $\circlearrowright C' = \circlearrowright C + \circlearrowleft C_0 + \leftarrow L_1 + \rightarrow L_2$. We see that the integral we need to evaluate in Eq. (13.81) is equal to the negative of the integral (Figure 13.4)

$$\oint_{\circlearrowleft C_0 + \leftarrow L_1 + \rightarrow L_2} \frac{f(z')dz'}{(z'-x)^{q+1}}. \tag{13.84}$$

Part of the integral over C_0 is taken in the limit as the radius of the contour goes to zero. For a point on the contour, we write $z' - x = \delta_0 e^{i\theta}$. Thus, for $q < 0$ and noninteger, we can write

$$\lim_{\delta_0 \to 0} \oint_{C_0} f(z') \frac{\delta_0 i e^{i\theta} d\theta}{\delta_0^{q+1} e^{i(q+1)\theta}} = \lim_{\delta_0 \to 0} f(x) i \delta_0^{-q_i} \int_{-\pi}^{\pi} e^{-iq\theta} d\theta, \tag{13.85}$$

which goes to zero in the limit $\delta_0 \to 0$. For the C_0 integral to be zero in the limit $\delta_0 \to 0$, we have taken q as negative. Using this result, we can write the integral in Eq. (13.81) as

$$\oint_C \frac{f(z')dz'}{(z'-x)^{q+1}} = -\left[\oint_{\leftarrow L_1} \frac{f(z')dz'}{(z'-x)^{q+1}} + \oint_{\rightarrow L_2} \frac{f(z')dz'}{(z'-x)^{q+1}}\right] \tag{13.86}$$

$$= \left[\oint_{\rightarrow L_1} \frac{f(z')dz'}{(z'-x)^{q+1}} - \oint_{\rightarrow L_2} \frac{f(z')dz'}{(z'-x)^{q+1}}\right]. \tag{13.87}$$

Now we have to evaluate the integral $\left[\oint_{\to L_1} - \oint_{\to L_2}\right]$. We first evaluate the part for $[-\infty, 0]$, which gives zero as $\varepsilon \to 0$:

$$\int_{-\infty}^{0} \frac{f(\delta e^{i(\pi-\varepsilon)})d\delta e^{i(\pi-\varepsilon)}}{(\delta e^{i(\pi-\varepsilon)} - x)^{q+1}} - \int_{-\infty}^{0} \frac{f(\delta e^{i(\pi+\varepsilon)})d\delta e^{i(\pi+\varepsilon)}}{(\delta e^{i(\pi+\varepsilon)} - x)^{q+1}}$$

$$= \left[e^{i(\pi-\varepsilon)} - e^{i(\pi+\varepsilon)}\right] \int_{-\infty}^{0} \frac{f(\delta e^{i(\pi-\varepsilon)})d\delta}{(-\delta - x)^{q+1}} \tag{13.88}$$

$$= \lim_{\varepsilon\to 0} \left[e^{i(\pi-\varepsilon)} - e^{i(\pi+\varepsilon)}\right] \int_{-\infty}^{0} \frac{f(\delta e^{i(\pi-\varepsilon)})d\delta}{(-\delta - x)^{q+1}} = 0. \tag{13.89}$$

Writing the remaining part of the integral we get

$$\oint_C \frac{f(z')dz'}{(z' - x)^{q+1}} = \lim_{\delta_0,\varepsilon\to 0} \left[\int_0^x \frac{f(\delta e^{i\varepsilon})e^{i\varepsilon}d\delta}{(\delta - x)^{q+1}e^{i(q+1)\varepsilon}} - \int_0^x \frac{f(\delta e^{i(2\pi-\varepsilon)})e^{i(2\pi-\varepsilon)}d\delta}{(\delta - x)^{q+1}e^{i(q+1)(2\pi-\varepsilon)}}\right]. \tag{13.90}$$

After taking the limit, $\delta_0 \to 0$ and $\varepsilon \to 0$, we substitute this into the definition [Eq. (13.81)] to obtain

$$\frac{d^q f(x)}{dx^q} = \frac{\Gamma(q+1)}{2\pi i} \left[1 - e^{-i(q+1)2\pi}\right] \int_0^x \frac{f(\delta)d\delta}{(\delta - x)^{q+1}}, \quad q < 0 \text{ and noninteger,} \tag{13.91}$$

which after simplification becomes

$$\frac{d^q f(x)}{dx^q} = \frac{\Gamma(q+1)}{2\pi i} \left[2i\sin(\pi q)\right](-1)^q \int_0^x \frac{f(\delta)d\delta}{(\delta - x)^{q+1}} \tag{13.92}$$

$$= -\frac{\Gamma(q+1)}{\pi} \left[\sin(\pi q)\right] \int_0^x \frac{f(\delta)d\delta}{(x - \delta)^{q+1}}. \tag{13.93}$$

To see that this agrees with the Riemann–Liouville definition, we use the following relation of the gamma function:

$$\Gamma(-q) = \frac{-\pi \csc(\pi q)}{\Gamma(q+1)}, \tag{13.94}$$

and write

$$\boxed{\frac{d^q f(x)}{dx^q} = \frac{1}{\Gamma(-q)} \int_0^x \frac{f(\delta)d\delta}{(x - \delta)^{q+1}}, \quad q < 0 \text{ and noninteger.}} \tag{13.95}$$

This is nothing but the Riemann–Liouville definition. Using Eq. (13.78), we can extend this definition to positive values of q.

13.3.2 Riemann Formula

We now evaluate the differintegral of $f(x) = x^p$, which is very useful in writing the differintegrals of functions with Taylor series. Using Eq. (13.92), we write

$$\frac{d^q x^p}{dx^q} = \frac{\Gamma(q+1)}{\pi}\sin(\pi q)(-1)^q \int_0^x \frac{\delta^p \, d\delta}{(\delta - x)^{q+1}}, \tag{13.96}$$

$$\frac{d^q x^p}{dx^q} = \frac{\Gamma(q+1)}{\pi}\sin(\pi q)(-1)^q \int_0^x \frac{\delta^p \, d\delta}{x^{q+1}\left(\frac{\delta}{x} - 1\right)^{q+1}}. \tag{13.97}$$

We define $\delta/x = s$ so that Eq. (13.97) becomes

$$\frac{d^q x^p}{dx^q} = -\frac{\Gamma(q+1)}{\pi}\sin(\pi q)x^{p-q} \int_0^1 \frac{s^p \, ds}{(1-s)^{q+1}}. \tag{13.98}$$

Remembering the definition of the beta function:

$$B(p,q) = \int_0^1 y^{p-1}[1-y]^{q-1}dy, \quad p > 0, \ q > 0, \tag{13.99}$$

we can write Eq. (13.98) as

$$\frac{d^q x^p}{dx^q} = -\frac{\Gamma(q+1)}{\pi}\sin(\pi q)x^{p-q}B(p+1,-q). \tag{13.100}$$

Also using Eq. (13.94) and the relation between the beta and the gamma functions:

$$B(p+1,-q) = \frac{\Gamma(p+1)\Gamma(-q)}{\Gamma(p+1-q)}, \tag{13.101}$$

we obtain the result as

$$\frac{d^q x^p}{dx^q} = \frac{\Gamma(p+1)x^{p-q}}{\Gamma(p+1-q)}, \quad p > -1, \ q < 0. \tag{13.102}$$

Limits on the parameters p and q follow from the conditions of convergence for the beta integral.

For $q \geq 0$, as in the Riemann–Liouville definition, we write

$$\frac{d^q x^p}{dx^q} = \frac{d^n}{dx^n}\left[\frac{d^{q-n} x^p}{dx^{q-n}}\right] \tag{13.103}$$

and choose the integer n as $q - n < 0$. We now evaluate the differintegral inside the square brackets using Eq. (13.78) as

$$\frac{d^q x^p}{dx^q} = \frac{d^n}{dx^n}\left[\frac{\Gamma(p+1)x^{p-q+n}}{\Gamma(p-q+n+1)}\right] \tag{13.104}$$

$$= \frac{\Gamma(p+1)x^{p-q}}{\Gamma(p-q+1)}, \quad q \geq 0. \tag{13.105}$$

Combining this with the result in Eq. (13.102) we obtain a formula valid for all q as

$$\boxed{\frac{d^q x^p}{dx^q} = \frac{\Gamma(p+1)x^{p-q}}{\Gamma(p-q+1)}, \quad p > -1.} \tag{13.106}$$

This formula is also known as the **Riemann formula**. It is a generalization of the formula

$$\frac{d^n x^m}{dx^n} = \frac{m!}{(m-n)!}x^{m-n}, \tag{13.107}$$

for $p > -1$, where m and n are positive integers. For $p \leq -1$, the beta function is divergent, hence a generalization valid for all p values is yet to be found.

13.3.3 Differintegrals via Laplace Transforms

For $q < 0$, we can define differintegrals by using Laplace transforms as

$$\frac{d^q f}{dx^q} = \pounds^{-1}[s^q \tilde{f}(s)], \quad q < 0, \tag{13.108}$$

where $\tilde{f}(s)$ is the Laplace transform of $f(x)$. To show that this agrees with the Riemann–Liouville definition, we make use of the convolution theorem:

$$\pounds \int_0^x f(u)g(x-u)du = \tilde{f}(s)\tilde{g}(s) \tag{13.109}$$

and take $g(x)$ as $g(x) = 1/x^{q+1}$, where its Laplace transform is

$$\tilde{g}(s) = \int_0^\infty e^{-sx} \frac{dx}{x^{q+1}} = \Gamma(-q)s^q. \tag{13.110}$$

Using the Laplace transform of $f(x)$:

$$\tilde{f}(s) = \int_0^\infty e^{-sx} f(x)dx, \tag{13.111}$$

in Eq. (13.108), we write

$$\left[\frac{d^q f}{dx^q}\right]_L = \pounds^{-1}[s^q \tilde{f}(s)], \quad q < 0, \tag{13.112}$$

$$\left[\frac{d^q f}{dx^q}\right]_L = \frac{1}{\Gamma(-q)} \int_0^x \frac{f(\tau)d\tau}{(x-\tau)^{q+1}}, \tag{13.113}$$

$$\left[\frac{d^q f}{dx^q}\right]_L = \left[\frac{d^q f}{dx^q}\right]_{R-L}, \quad q < 0. \tag{13.114}$$

The subscripts L and $R-L$ denote the method used in evaluating the differintegral. Thus, the two methods agree for $q < 0$.

For $q > 0$, the differintegral definition by the Laplace transforms is given as (Section 13.6.1)

$$\left[\frac{d^q f}{dx^q}\right]_L = \pounds^{-1}\left[s^q\tilde{f}(s) - \sum_{k=0}^{n-1} s^k \frac{d^{q-1-k}f}{dx^{q-1-k}}(0)\right], \quad q > 0, \tag{13.115}$$

or as

$$\left[\frac{d^q f}{dx^q}\right]_L = \pounds^{-1}\left[s^q\tilde{f}(s) - \frac{d^{q-1}f}{dx^{q-1}}(0) - \cdots - s^{n-1}\frac{d^{q-n}f}{dx^{q-n}}(0)\right]. \tag{13.116}$$

In this definition, $q > 0$ and the integer n must be chosen such that the inequality $n-1 < q \leq n$ is satisfied. The differintegrals on the right-hand side are all evaluated via the L method. To show that the methods agree we write

$$A(x) = \frac{1}{\Gamma(n-q)}\int_0^x \frac{f(\tau)d\tau}{(x-\tau)^{q-n+1}}, \quad q < n, \tag{13.117}$$

and use the convolution theorem to find its Laplace transform as

$$\tilde{A}(s) = \pounds\left[\frac{1}{\Gamma(n-q)}\int_0^x \frac{f(\tau)d\tau}{(x-\tau)^{q-n+1}}\right] = s^{q-n}\tilde{f}(s), \quad q-n < 0. \tag{13.118}$$

This gives us the relation $s^q\tilde{f}(s) = s^n\tilde{A}(s)$. Using the Riemann–Liouville definition [Eqs. (13.77)–(13.78)], we can write

$$A(0) = \left[\frac{d^{(q-n)}f}{dx^{(q-n)}}(0)\right]_{R-L}. \tag{13.119}$$

Since $q-n < 0$ and because of Eq. (13.114), we can write

$$A(0) = \left[\frac{d^{(q-n)}f}{dx^{(q-n)}}(0)\right]_{L}. \tag{13.120}$$

From the definition of $A(x)$, we can also write

$$A(x) = \frac{1}{\Gamma(n-q)}\int_0^x \frac{f(\tau)d\tau}{(x-\tau)^{q-n+1}}, \quad q-n < 0, \tag{13.121}$$

$$= \left[\frac{d^{(q-n)}f(x)}{dx^{(q-n)}}\right]_{R-L} = \left[\frac{d^{(q-n)}f(x)}{dx^{(q-n)}}\right]_{L}. \tag{13.122}$$

As in the Grünwald and Riemann–Liouville definitions we assume that the $[..]_L$ definition also satisfies the relation [Eq. (13.43)]

$$\frac{d^n}{dx^n}\frac{d^q f(x)}{dx^q} = \frac{d^{n+q}f(x)}{dx^{n+q}}, \tag{13.123}$$

where n a is positive integer and q takes all values. We can now write

$$\frac{d^{n-1}A(x)}{dx^{n-1}} = \frac{d^{n-1}}{dx^{n-1}}\left[\frac{d^{q-n}f(x)}{dx^{q-n}}\right]_L = \left[\frac{d^{q-1}f(x)}{dx^{q-1}}\right]_L, \tag{13.124}$$

which gives

$$\left[\frac{d^{q-1}f(0)}{dx^{q-1}}\right]_L = \left[\frac{d^{n-1}A(0)}{dx^{n-1}}\right]. \tag{13.125}$$

Similarly, we find the other terms in Eq. (13.116) to write

$$\left[\frac{d^q f}{dx^q}\right]_L = \pounds^{-1}\left[s^n\tilde{A}(s) - \frac{d^{n-1}A}{dx^{n-1}}(0) - \cdots - s^{n-1}A(0)\right] \tag{13.126}$$

$$= \pounds^{-1}\left[s^n\tilde{A}(s) - s^{n-1}A(0) - \cdots - \frac{d^{n-1}A}{dx^{n-1}}(0)\right] \tag{13.127}$$

$$= \pounds^{-1}\left[\pounds\left[\frac{d^n A}{dx^n}\right]_{R-L}\right] = \left[\frac{d^n A}{dx^n}\right]_{R-L}. \tag{13.128}$$

Using Eq. (13.117), we can now write

$$\left[\frac{d^q f}{dx^q}\right]_L = \frac{d^n}{dx^n}\left[\frac{1}{\Gamma(n-q)}\int_0^x \frac{f(\tau)d\tau}{(x-\tau)^{q-n+1}}\right] \tag{13.129}$$

$$= \frac{1}{\Gamma(n-q)}\frac{d^n}{dx^n}\int_0^x \frac{f(\tau)d\tau}{(x-\tau)^{q-n+1}}, \quad n > q, \tag{13.130}$$

$$= \left[\frac{d^q f}{dx^q}\right]_{R-L}, \quad q > 0, \tag{13.131}$$

which shows that also for $q > 0$, both definitions agree.

In Eq. (13.116), if the function $f(x)$ satisfies the **boundary conditions**

$$\boxed{\frac{d^{q-1}f}{dx^{q-1}}(0) = \cdots = \frac{d^{q-n}f}{dx^{q-n}}(0) = 0, \quad q > 0,} \tag{13.132}$$

we can write a differintegral definition valid for all q values via the Laplace transform as

$$\boxed{\left[\frac{d^q f}{dx^q}\right]_L = \pounds^{-1}[s^q\tilde{f}(s)].} \tag{13.133}$$

However, because the boundary conditions [Eq. (13.132)] involve fractional derivatives, this will create problems in interpretation and application.

13.4 Properties of Differintegrals

In this section, we introduce the basic properties of differintegrals. These properties are also useful in generating new differintegrals from the known ones.

13.4.1 Linearity

We express the **linearity** of differintegrals as

$$\frac{d^q[f_1+f_2]}{[d(x-a)]^q} = \frac{d^q f_1}{[d(x-a)]^q} + \frac{d^q f_2}{[d(x-a)]^q}. \tag{13.134}$$

13.4.2 Homogeneity

Homogeneity of differintegrals is expressed as

$$\frac{d^q(C_0 f)}{[d(x-a)]^q} = C_0 \frac{d^q f}{[d(x-a)]^q}, \quad C_0 \text{ is any constant.} \tag{13.135}$$

Both of these properties could easily be seen from the Grünwald definition [Eq. (13.42)].

13.4.3 Scale Transformations

We express the **scale transformation** of a function with respect to the lower limit, a, as $f(x) \to f(\gamma x - \gamma a + a)$, where γ is a constant scale factor. If the lower limit is zero, this means that $f(x) \to f(\gamma x)$. If the lower limit differs from zero, the scale change is given as

$$\frac{d^q f(\gamma X)}{[d(x-a)]^q} = \gamma^q \frac{d^q f(\gamma X)}{[d(\gamma X - a)]^q}, \quad X = x + [a - a\gamma]/\gamma. \tag{13.136}$$

This formula is most useful when a is zero:

$$\frac{d^q f(\gamma x)}{[dx]^q} = \gamma^q \frac{d^q f(\gamma x)}{[d(\gamma x)]^q}. \tag{13.137}$$

13.4.4 Differintegral of a Series

Using the linearity of the differintegral operator, we can find the differintegral of a uniformly convergent series for all q values as

$$\frac{d^q}{[d(x-a)]^q} \sum_{j=0}^{\infty} f_j(x) = \sum_{j=0}^{\infty} \frac{d^q f_j}{[d(x-a)]^q}. \tag{13.138}$$

Differintegrated series are also uniformly convergent in the same interval. For functions with power series expansions, using the Riemann formula we can write

$$\frac{d^q}{[d(x-a)]^q} \sum_{j=0}^{\infty} a_i [x-a]^{p+(j/n)} = \sum_{j=0}^{\infty} a_j \frac{\Gamma\left(\frac{pn+j+n}{n}\right)}{\Gamma\left(\frac{pn-qn+j+n}{n}\right)} [x-a]^{p-q+(j/n)}, \tag{13.139}$$

where q can take any value, but $p + (j/n) > -1$, $a_0 \neq 0$, and n is a positive integer.

13.4.5 Composition of Differintegrals

When working with differintegrals one always has to remember that operations like

$$d^q d^Q = d^Q d^q, \tag{13.140}$$

$$d^q d^Q = d^{q+Q}, \tag{13.141}$$

$$d^q f = g \to f = d^{-q} g \tag{13.142}$$

are valid only under certain conditions. In these operations problems are not just restricted to the noninteger values of q and Q.

When n and N are positive integer numbers, from the properties of derivatives and integrals we can write

$$\frac{d^n}{[d(x-a)]^n}\left\{\frac{d^N f}{[d(x-a)]^N}\right\} = \frac{d^{n+N} f}{[d(x-a)]^{n+N}} = \frac{d^N}{[d(x-a)]^N}\left\{\frac{d^n f}{[d(x-a)]^n}\right\} \tag{13.143}$$

and

$$\frac{d^{-n}}{[d(x-a)]^{-n}}\left\{\frac{d^{-N} f}{[d(x-a)]^{-N}}\right\} = \frac{d^{-n-N} f}{[d(x-a)]^{-n-N}}$$
$$= \frac{d^{-N}}{[d(x-a)]^{-N}}\left\{\frac{d^{-n} f}{[d(x-a)]^{-n}}\right\}. \tag{13.144}$$

However, if we look at the operation

$$\frac{d^{\pm n}}{[d(x-a)]^{\pm n}}\left\{\frac{d^{\mp N} f}{[d(x-a)]^{\mp N}}\right\}, \tag{13.145}$$

the result is not always

$$\frac{d^{\pm n \mp N} f}{[d(x-a)]^{\pm n \mp N}}. \tag{13.146}$$

Assume that the function $f(x)$ has continuous Nth-order derivative in the interval $[a, b]$ and let us take the integral of this Nth-order derivative as

$$\int_a^x f^{(N)}(x_1)dx_1 = f^{(N-1)}(x)|_a^x = f^{(N-1)}(x) - f^{(N-1)}(a). \tag{13.147}$$

We integrate this once more:

$$\int_a^x \left(\int_a^{x_2} f^{(N)}(x_1)dx_1\right) dx_2$$
$$= \int_a^x \left[f^{(N-1)}(x) - f^{(N-1)}(a)\right] dx \tag{13.148}$$
$$= f^{(N-2)}(x) - f^{(N-2)}(a) - (x-a)f^{(N-1)}(a) \tag{13.149}$$

and repeat the process n times to get

$$\int_a^x \cdots \int_a^x f^{(N)}(x)(dx)^n = f^{(N-n)}(x) - f^{(N-n)}(a) - (x-a)f^{(N-n+1)}(a) - \frac{(x-a)^2}{2!}f^{(N-n+2)}(a) \cdots - \frac{(x-a)^{n-1}}{(n-1)!}f^{(N-1)}(a). \tag{13.150}$$

Since

$$\frac{d^{-n}}{[d(x-a)]^{-n}}\left\{\frac{d^N f}{[d(x-a)]^N}\right\} = \int_a^x \cdots \int_a^x f^{(N)}(x)(dx)^n, \tag{13.151}$$

we write

$$\frac{d^{-n}}{[d(x-a)]^{-n}}\left\{\frac{d^N f}{[d(x-a)]^N}\right\} = f^{(N-n)}(x) - \sum_{k=0}^{n-1}\frac{[x-a]^k}{k!}f^{(N+k-n)}(a). \tag{13.152}$$

Writing Eq. (13.152) for $N = 0$ gives us

$$\frac{d^{-n}f}{[d(x-a)]^{-n}} = f^{(-n)}(x) - \sum_{k=0}^{n-1}\frac{[x-a]^k}{k!}f^{(k-n)}(a). \tag{13.153}$$

We differentiate this to get

$$\frac{d}{dx}\left\{\frac{d^{-n}f}{[d(x-a)]^{-n}}\right\} = f^{(1-n)}(x) - \sum_{k=1}^{n-1}\frac{[x-a]^{k-1}}{(k-1)!}f^{(k-n)}(a). \tag{13.154}$$

After N-fold differentiation we obtain

$$\frac{d^N}{dx^N}\left\{\frac{d^{-n}f}{[d(x-a)]^{-n}}\right\} = f^{(N-n)}(x) - \sum_{k=N}^{n-1}\frac{[x-a]^{k-N}}{(k-N)!}f^{(k-n)}(a). \tag{13.155}$$

For $N \geq n$, remembering that differentiation does not depend on the lower limit and also observing that in this case the summation in Eq. (13.155) is empty, we write

$$\frac{d^N}{[d(x-a)]^N}\left\{\frac{d^{-n}f}{[d(x-a)]^{-n}}\right\} = \frac{d^{N-n}f}{[d(x-a)]^{N-n}} = f^{(N-n)}(x). \tag{13.156}$$

On the other hand, for $N < n$, we use Eq. (13.153) to write

$$\frac{d^{N-n}f}{[d(x-a)]^{N-n}} = f^{(N-n)}(x) - \sum_{k=0}^{n-N-1}\frac{[x-a]^k}{k!}f^{(k+N-n)}(a). \tag{13.157}$$

This equation also contains Eq. (13.156). In Eq. (13.155) we now make the transformation

$$k \to k + N \tag{13.158}$$

to write

$$\frac{d^N}{[d(x-a)]^N}\left\{\frac{d^{-n}f}{[d(x-a)]^{-n}}\right\} = f^{(N-n)}(x) - \sum_{k=0}^{n-N-1}\frac{[x-a]^k}{k!}f^{(k+N-n)}(a). \tag{13.159}$$

Because the right-hand sides of Eqs. (13.159) and (13.157) are identical, we obtain the composition rule for n successive integrations followed by N differentiations as

$$\boxed{\frac{d^N}{[d(x-a)]^N}\left\{\frac{d^{-n}f}{[d(x-a)]^{-n}}\right\} = \frac{d^{N-n}f}{[d(x-a)]^{N-n}}.} \tag{13.160}$$

To find the composition rule for the cases where the differentiations are performed before the integrations, we turn to Eq. (13.152) and write the sum in two pieces as

$$\frac{d^{-n}}{[d(x-a)]^{-n}}\left\{\frac{d^N f}{[d(x-a)]^N}\right\} = f^{(N-n)}(x) - \sum_{k=0}^{n-N-1}\frac{[x-a]^k}{k!}f^{(N+k-n)}(a)$$
$$- \sum_{k=n-N}^{n-1}\frac{[x-a]^k}{k!}f^{(N+k-n)}(a). \tag{13.161}$$

Comparing this with Eq. (13.157), we now obtain the composition rule for the cases where N-fold differentiation is performed before n successive integrations as

$$\boxed{\frac{d^{-n}}{[d(x-a)]^{-n}}\left\{\frac{d^N f}{[d(x-a)]^N}\right\} = \frac{d^{N-n}f}{[d(x-a)]^{N-n}} - \sum_{k=n-N}^{n-1}\frac{[x-a]^k}{k!}f^{(N+k-n)}(a).} \tag{13.162}$$

Example 13.1 ***Composition of differintegrals***
For the function $f(x) = e^{-3x}$, we first calculate the derivative

$$\frac{d}{[dx]}\left\{\frac{d^{-3}f(x)}{[dx]^{-3}}\right\}. \tag{13.163}$$

Using Eqs. (13.160) and (13.153), we find

$$\frac{d}{[dx]}\left\{\frac{d^{-3}f(x)}{[dx]^{-3}}\right\} = \frac{d^{-2}f(x)}{[dx]^{-2}} = \frac{e^{-3x}}{9} + \frac{x}{3} - \frac{1}{9}. \tag{13.164}$$

On the other hand, for the case where the order of the operators are reversed:

$$\frac{d^{-3}}{[dx]^{-3}}\left\{\frac{df(x)}{[dx]}\right\}, \tag{13.165}$$

we use Eq. (13.162). Since $N = 1$ and $n = 3$, k takes only the value 2, thus giving

$$\frac{d^{-3}}{[dx]^{-3}}\left\{\frac{df(x)}{[dx]}\right\} = \frac{e^{-3x}}{9} + \frac{x}{3} - \frac{1}{9} - \frac{x^2}{2}, \tag{13.166}$$

which is different from Eq. (13.164)

13.4.5.1 Composition Rule for General q and Q

When q and Q take any value, composition of differintegrals as

$$\frac{d^q}{[d(x-a)]^q}\left[\frac{d^Q f}{[d(x-a)]^Q}\right] = \frac{d^{q+Q} f}{[d(x-a)]^{q+Q}} \tag{13.167}$$

is possible only under certain conditions. It is needless to say that we assume all the required differintegrals exist. Assuming that a series expansion for $f(x)$ can be given as

$$f(x) = \sum_{j=0}^{\infty} a_j [x-a]^{p+j}, \quad p \text{ is a noninteger such that } p + j > -1, \tag{13.168}$$

it can be shown that the composition rule [Eq. (13.167)] is valid only for functions satisfying the condition

$$\boxed{f(x) - \frac{d^{-Q}}{[d(x-a)]^{-Q}}\left[\frac{d^Q f}{[d(x-a)]^Q}\right] = 0.} \tag{13.169}$$

In general, for functions that can be expanded as in Eq. (13.168), differintegrals are composed as [15]

$$\frac{d^q}{[d(x-a)]^q}\left[\frac{d^Q f}{[d(x-a)]^Q}\right] = \frac{d^{q+Q} f}{[d(x-a)]^{q+Q}} - \frac{d^{q+Q}}{[d(x-a)]^{q+Q}}\left\{f - \frac{d^{-Q}}{[d(x-a)]^{-Q}}\left[\frac{d^Q f}{[d(x-a)]^Q}\right]\right\}. \tag{13.170}$$

For such functions, violation of the condition in Eq. (13.169) can be shown to result from the fact that $\frac{d^Q f}{[d(x-a)]^Q}$ vanishes even though $f(x)$ is different from zero. From here we see that, even though the operators $\frac{d^Q}{[d(x-a)]^Q}$ and $\frac{d^{-Q}}{[d(x-a)]^{-Q}}$ are in general inverses of each other, this is not always true.

In practice it is difficult to apply the composition rule as given in Eq. (13.170). Because the violation of Eq. (13.169) is equivalent to the vanishing of the derivative $\frac{d^Q f(x)}{[dx]^Q}$, let us first write the differintegral of $f(x)$ as

$$\frac{d^Q f(x)}{[dx]^Q} = \sum_{j=0}^{\infty} a_j \frac{d^Q x^{p+j}}{[dx]^Q} = \sum_{j=0}^{\infty} a_j \frac{\Gamma(p+j+1)x^{p+j-Q}}{\Gamma(p+j-Q+1)}, \tag{13.171}$$

where for simplicity we have set $a = 0$. Because the condition $p + j > -1$, or $p > -1$, the gamma function in the numerator is always different from zero and finite. For the $Q < p + 1$ values, the gamma function in the denominator is always finite; thus the condition in Eq. (13.169) is satisfied. For the remaining cases, the condition in Eq. (13.169) is violated. We now check the equivalent condition $\frac{d^Q f(x)}{[dx]^Q} = 0$, to identify the terms responsible for the violation of condition in Eq. (13.169). For the derivative $\frac{d^Q f(x)}{[dx]^Q}$ to vanish, from Eq. (13.171) it is seen that the gamma function in the denominator must diverge for all $a_j \neq 0$, that is,

$$p + j - Q + 1 = 0, -1, -2, \ldots . \tag{13.172}$$

For a given p (> -1) and positive Q, j will eventually make $(p - Q + j + 1)$ positive; therefore, we can write

$$p + j = Q - 1, Q - 2, \ldots , Q - m, \tag{13.173}$$

where m is an integer satisfying

$$0 < Q < m < Q + 1. \tag{13.174}$$

For the j values that make $(p - Q + j + 1)$ positive, the gamma function in the denominator is finite, and the corresponding terms in the series satisfy the condition in Eq. (13.169). Thus, the problem is located to the terms with the j values satisfying Eq. (13.173). Now, in general for an arbitrary diffferintegrable function we can write the expression

$$f(x) - \frac{d^{-Q}}{[dx]^{-Q}} \left[\frac{d^Q f}{[dx]^Q} \right] = c_0 x^{Q-1} + c_1 x^{Q-2} + \cdots + c_m x^{Q-m}, \tag{13.175}$$

where $c_1, c_2, \ldots , c_m$ are arbitrary constants. Note that the right-hand side of Eq. (13.175) is exactly composed of the terms that vanish when $\frac{d^Q f(x)}{[dx]^Q} \neq 0$, that is, when Eq. (13.169) is satisfied. This formula, which is very useful in finding solutions of extraordinary differential equations can now be used in Eq. (13.170) to compose differintegrals.

Another useful formula is obtained when Q takes integer values N in Eq. (13.170). We apply the composition rule [Eq. (13.170)] with Eq. (13.152) written for $n = N$, and use the generalization of the Riemann formula:

$$\frac{d^q (x-a)^p}{[d(x-a)]^q} = \frac{\Gamma(p+1)(x-a)^{p-q}}{\Gamma(p-q+1)}, \quad p > -1, \tag{13.176}$$

to obtain

$$\frac{d^q}{[d(x-a)]^q}\left[\frac{d^N f}{[d(x-a)]^N}\right]$$
$$= \frac{d^{q+N}f}{[d(x-a)]^{q+N}} - \frac{d^{q+N}}{[d(x-a)]^{q+N}}\left\{f - \frac{d^{-N}}{[d(x-a)]^{-N}}\left[\frac{d^N f}{[d(x-a)]^N}\right]\right\} \tag{13.177}$$

$$= \frac{d^{q+N}f}{[d(x-a)]^{q+N}} - \sum_{k=0}^{N-1}\frac{[x-a]^{k-q-N}f^{(k)}(a)}{\Gamma(k-q-N+1)}. \tag{13.178}$$

Example 13.2 ***Composition of differintegrals***

We now consider the function $f(x) = x^{-1/2}$ for the values $a = 0$, $Q = 1/2$, $q = -1/2$. Since the condition in Eq. (13.169) is not satisfied, that is,

$$x^{-1/2} - \frac{d^{-\frac{1}{2}}}{[dx]^{-\frac{1}{2}}}\left[\frac{d^{\frac{1}{2}}x^{-1/2}}{[dx]^{\frac{1}{2}}}\right] = x^{-1/2} - \frac{d^{-\frac{1}{2}}}{[dx]^{-\frac{1}{2}}}\left[\frac{\Gamma\left(\frac{1}{2}\right)}{\Gamma(0)}x^{-1}\right] = x^{-1/2} - 0 \neq 0, \tag{13.179}$$

we have to use Eq. (13.170):

$$\frac{d^{-\frac{1}{2}}}{[dx]^{-\frac{1}{2}}}\frac{d^{\frac{1}{2}}x^{-1/2}}{[dx]^{\frac{1}{2}}} = \frac{d^{-\frac{1}{2}+\frac{1}{2}}x^{-1/2}}{[dx]^{-\frac{1}{2}+\frac{1}{2}}} - \frac{d^{-\frac{1}{2}+\frac{1}{2}}}{[dx]^{-\frac{1}{2}+\frac{1}{2}}}\left\{x^{-1/2} - \frac{d^{-\frac{1}{2}}}{[dx]^{-\frac{1}{2}}}\left[\frac{d^{\frac{1}{2}}x^{-1/2}}{[dx]^{\frac{1}{2}}}\right]\right\}. \tag{13.180}$$

Since

$$\frac{d^{\frac{1}{2}}x^{-1/2}}{[dx]^{\frac{1}{2}}} = 0,$$

we have

$$\frac{d^{-\frac{1}{2}}}{[dx]^{-\frac{1}{2}}}\left\{\frac{d^{\frac{1}{2}}x^{-1/2}}{[dx]^{\frac{1}{2}}}\right\} = 0,$$

which leads to

$$\frac{d^{-\frac{1}{2}}}{[dx]^{-\frac{1}{2}}}\frac{d^{\frac{1}{2}}x^{-1/2}}{[dx]^{\frac{1}{2}}} = \frac{d^{-\frac{1}{2}+\frac{1}{2}}x^{-1/2}}{[dx]^{-\frac{1}{2}+\frac{1}{2}}} - \frac{d^{-\frac{1}{2}+\frac{1}{2}}}{[dx]^{-\frac{1}{2}+\frac{1}{2}}}(x^{-1/2} - 0) \tag{13.181}$$

$$= x^{-1/2} - x^{-1/2} = 0. \tag{13.182}$$

Contrary to what we expect

$$\frac{d^{-\frac{1}{2}}}{[dx]^{-\frac{1}{2}}}$$

is not the inverse of

$$\frac{d^{\frac{1}{2}}}{[dx]^{\frac{1}{2}}}$$

for $x^{-1/2}$.

Example 13.3 ***Inverse of differintegrals***
Consider the function $f(x) = x$ for the values $Q = 2$ and $a = 0$. Since

$$\frac{d^2x}{[dx]^2} = 0$$

is true, contrary to our expectations we find

$$\frac{d^{-2}}{[dx]^{-2}}\frac{d^2x}{[dx]^2} = 0.$$

The problem is again that the function $f(x) = x$ does not satisfy the condition in Eq. (13.169).

13.4.6 Leibniz Rule

The differintegral of qth order of the multiplication of two functions, $f(x)$ and $g(x)$, is given by the formula

$$\frac{d^q[f(x)g(x)]}{[d(x-a)]^q} = \sum_{j=0}^{\infty}\binom{q}{j}\frac{d^{q-j}f(x)}{[d(x-a)]^{q-j}}\frac{d^jg(x)}{[d(x-a)]^j}, \tag{13.183}$$

where the binomial coefficients are to be calculated by replacing the factorials with the corresponding gamma functions.

13.4.7 Right- and Left-Handed Differintegrals

The Riemann–Liouville definition of differintegral was given as

$$\boxed{\frac{d^qf(t)}{[d(t-a)]^q} = \frac{1}{\Gamma(k-q)}\left(\frac{d}{dt}\right)^k\int_a^t(t-\tau)^{k-q-1}f(\tau)d\tau,} \tag{13.184}$$

where k is an integer satisfying

$$\begin{aligned} &k = 0 && \text{for } q < 0, \\ &k-1 < q < k && \text{for } q \geq 0. \end{aligned} \tag{13.185}$$

This is also called the **right-handed** Riemann–Liouville definition. If $f(t)$ is a function representing a dynamic process, in general t is a time-like variable. The principle of causality justifies the usage of the right-handed derivative because the present value of a differintegral is determined from the past values of $f(t)$

starting from an initial time $t = a$. Similar to the advanced potentials, it is also possible to define a **left-handed** Riemann–Liouville differintegral as

$$\frac{d^q f(t)}{[d(b-t)]^q} = \frac{1}{\Gamma(k-q)}\left(-\frac{d}{dt}\right)^k \int_t^b (\tau - t)^{k-q-1} f(\tau)d\tau, \tag{13.186}$$

where k is again an integer satisfying Eq. (13.185). Even though for dynamic processes it is difficult to interpret the left-handed definition, in general the boundary or the initial conditions determine which definition is to be used. It is also possible to give a left-handed version of the Grünwald definition. In this chapter, unless otherwise stated, we confine ourselves to the right-handed definition.

We also use the notation

$${}_0\mathbf{I}_t^q[f(t)] = \frac{1}{\Gamma(q)}\int_0^t \frac{f(\tau)d\tau}{(t-\tau)^{1-q}}, \quad q > 0, \tag{13.187}$$

to generalize the fractional Riemann–Liouville integral as the **right-** and **left-handed** Riemann–Liouville integrals, respectively, as

$${}_{a^+}\mathbf{I}_t^q[f(t)] = \frac{1}{\Gamma(q)}\int_a^t (t-\tau)^{q-1} f(\tau)d\tau, \tag{13.188}$$

$${}_{b^-}\mathbf{I}_t^q[f(t)] = \frac{1}{\Gamma(q)}\int_t^b (\tau - t)^{q-1} f(\tau)d\tau, \tag{13.189}$$

where $a < t < b$ and $q > 0$. In applications we frequently encounter cases with $a = -\infty$ or $b = \infty$. Fractional integrals with either the lower or the upper limit is taken as infinity are also called the **Weyl fractional integral**. Some authors may reverse the definitions of the right- and the left-handed derivatives. Sometimes ${}_{a^+}\mathbf{I}_t^q$ and ${}_{b^-}\mathbf{I}_t^q$ are also called **progressive** and **regressive**, respectively.

The **right**- and the **left-handed** Riemann–Liouville derivatives [Eq. (13.78)] of order $q > 0$ are defined and shown [Eq. (13.22)] as

$${}_{a^+}\mathbf{D}_t^q f(t) = \frac{d^n}{dt^n}\left({}_{a^+}\mathbf{I}_t^{n-q}[f(t)]\right), \tag{13.190}$$

$${}_{b^-}\mathbf{D}_t^q f(t) = (-1)^n \frac{d^n}{dt^n}\left({}_{b^-}\mathbf{I}_t^{n-q}[f(t)]\right), \tag{13.191}$$

where $a < t < b$ and $n > q$.

The following **composition rules** hold for the d^n/dt^n and the ${}_{a^+}\mathbf{I}_t^n f(t)$ operators [Eqs. (13.160) and (13.161)]:

$$\frac{d^n}{dt^n}\left[{}_{a^+}\mathbf{I}_t^n f(t)\right] = f(t), \tag{13.192}$$

$$\left[{}_{a^+}\mathbf{I}_t^n\right]\frac{d^n f(t)}{dt^n} = f(t) - \sum_{k=0}^{n-1}\frac{f^{(k)}(a^+)}{k!}(t-a)^k. \tag{13.193}$$

The corresponding equations for the left-handed integrals are given as

$$\frac{d^n}{dt^n}\left[{}_{b^-}\mathbf{I}_t^n f(t)\right] = (-1)^n f(t), \tag{13.194}$$

$$\left[{}_{b^-}\mathbf{I}_t^n\right]\frac{d^n f(t)}{dt^n} = (-1)^n\left[f(t) - \sum_{k=0}^{n-1}\frac{f^{(k)}(b^-)}{k!}(b-t)^k\right]. \tag{13.195}$$

13.4.8 Dependence on the Lower Limit

We now discuss the dependence of the differintegral

$$\frac{d^q f(x)}{[d(x-a)]^q}$$

on the lower limit. For $q < 0$, using Eq. (13.184) we write the difference:

$$\delta = \frac{d^q f(x)}{[d(x-a)]^q} - \frac{d^q f(x)}{[d(x-b)]^q}, \tag{13.196}$$

as

$$\delta = \frac{1}{\Gamma(-q)}\int_a^x (x-\tau)^{-q-1} f(\tau)d\tau - \frac{1}{\Gamma(-q)}\int_b^x (x-\tau)^{-q-1} f(\tau)d\tau \tag{13.197}$$

$$= \frac{1}{\Gamma(-q)}\int_a^b (x-\tau)^{-q-1} f(\tau)d\tau \tag{13.198}$$

$$= \frac{1}{\Gamma(-q)}\int_a^b (x-b+b-\tau)^{-q-1} f(\tau)d\tau \tag{13.199}$$

$$= \frac{1}{\Gamma(-q)}\int_a^b \left[\sum_{l=0}^{\infty}\binom{-l-q}{l}(x-b)^{-q-1-l}(b-\tau)^l\right] f(\tau)d\tau. \tag{13.200}$$

For the binomial coefficients we write

$$\binom{-l-q}{l} = \frac{\Gamma(-q)}{\Gamma(-q-l)\Gamma(l+1)} \tag{13.201}$$

to obtain

$$\delta = \int_a^b \left[\sum_{l=0}^{\infty} \frac{(x-b)^{-q-1-l}(b-\tau)^l}{\Gamma(-q-l)\Gamma(l+1)} \right] f(\tau)d\tau \tag{13.202}$$

$$= \sum_{l=0}^{\infty} \left[\frac{(x-b)^{-q-1-l}}{\Gamma(-q-l)} \right] \left[\int_a^b \frac{(b-\tau)^l f(\tau)d\tau}{\Gamma(l+1)} \right] \tag{13.203}$$

$$= \sum_{l=0}^{\infty} \frac{d^{q+l+1}[1]}{[d(x-b)]^{q+l+1}} \frac{d^{-l-1}f(b)}{[d(b-a)]^{-l-1}}, \tag{13.204}$$

$$= \sum_{l=1}^{\infty} \frac{d^{q+l}[1]}{[d(x-b)]^{q+l}} \frac{d^{-l}f(b)}{[d(b-a)]^{-l}}. \tag{13.205}$$

Even though we have obtained this expression for $q < 0$, it is also valid for all q [15]. For $q = 0, 1, 2, \ldots$, that is, for ordinary derivatives, we have $\delta = 0$ as expected. For $q = -1$, the above equation simplifies to

$$\delta = \frac{d^{-1}f(b)}{[d(b-a)]^{-1}} = \int_a^b f(\tau)d\tau. \tag{13.206}$$

For all other values of q, δ not only depends on a and b but also on x. This is due to the fact that the differintegral, except when it reduces to an ordinary derivative, is a global operator and requires a knowledge of $f(x)$ over the entire space. This is apparent from the Riemann–Liouville definition [Eq. (13.184)], which is given as an integral, $\int_a^x dx$, and the Grünwald definition [Eq. (13.42)] which is given as an infinite series that makes use of the values of the function over the entire range $[a, x]$.

13.5 Differintegrals of Some Functions

In this section, we discuss differintegrals of some selected functions. For an extensive list and a discussion of the differintegrals of functions of mathematical physics we refer the reader to Oldham and Spanier [15].

13.5.1 Differintegral of a Constant

We first take the number 1 and find its differintegral using the Grünwald definition [Eq. (13.42)] as

$$\frac{d^q[1]}{[d(x-a)]^q} = \lim_{N\to\infty} \left\{ \left[\frac{N}{x-a} \right]^q \sum_{j=0}^{N-1} \frac{\Gamma(j-q)}{\Gamma(j+1)\Gamma(-q)} \right\}. \tag{13.207}$$

Using the properties of gamma functions:

$$\sum_{j=0}^{N-1} \Gamma(j-q)/\Gamma(-q)\Gamma(j+1) = \Gamma(N-q)/\Gamma(1-q)\Gamma(N), \tag{13.208}$$

and the $\lim_{N\to\infty}[N^q\Gamma(N-q)/\Gamma(N)] = 1$, we find

$$\frac{d^q[1]}{[d(x-a)]^q} = \frac{[x-a]^{-q}}{\Gamma(1-q)}. \tag{13.209}$$

When q takes integer values, this reduces to the expected result. For an arbitrary constant C_0, including zero, the differintegral is

$$\frac{d^q[C_0]}{[d(x-a)]^q} = C_0\frac{d^q[1]}{[d(x-a)]^q}, \tag{13.210}$$

$$\boxed{\frac{d^q[C_0]}{[d(x-a)]^q} = C_0\frac{[x-a]^{-q}}{\Gamma(1-q)}.} \tag{13.211}$$

13.5.2 Differintegral of $[x-a]$

For the differintegral of $[x-a]$, we again use Eq. (13.42) and write

$$\frac{d^q[x-a]}{[d(x-a)]^q} = \lim_{N\to\infty}\left\{\left[\frac{N}{x-a}\right]^q \sum_{j=0}^{N-1}\frac{\Gamma(j-q)}{\Gamma(-q)\Gamma(j+1)}\left[\frac{Nx-jx+ja}{N}-a\right]\right\} \tag{13.212}$$

$$= [x-a]^{1-q}\lim_{N\to\infty}\left[\left\{N^q\sum_{j=0}^{N-1}\frac{\Gamma(j-q)}{\Gamma(-q)\Gamma(j+1)}\right\} - \left\{[N]^{q-1}\sum_{j=0}^{N-1}\frac{j\Gamma(j-q)}{\Gamma(-q)\Gamma(j+1)}\right\}\right]. \tag{13.213}$$

In addition to the properties used in Section 13.5.1, we also use the following relation between the gamma functions:

$$\sum_{j=0}^{N-1} \Gamma(j-q)/\Gamma(-q)\Gamma(j) = (-q)\Gamma(N-q)/\Gamma(2-q)\Gamma(N-1), \tag{13.214}$$

to obtain

$$\frac{d^q[x-a]}{[d(x-a)]^q} = [x-a]^{1-q}\left[\frac{1}{\Gamma(1-q)} + \frac{q}{\Gamma(2-q)}\right], \tag{13.215}$$

$$\boxed{\frac{d^q[x-a]}{[d(x-a)]^q} = \frac{[x-a]^{1-q}}{\Gamma(2-q)}.} \tag{13.216}$$

We now use the Riemann–Liouville formula to find the same differintegral. We first write

$$\frac{d^q[x-a]}{[d(x-a)]^q} = \frac{1}{\Gamma(-q)} \int_a^x \frac{[x'-a]dx'}{[x-x']^{q+1}}. \tag{13.217}$$

For $q < 0$, we make the transformation $y = x - x'$ and write

$$\frac{d^q[x-a]}{[d(x-a)]^q} = \frac{1}{\Gamma(-q)} \int_a^{x-a} \frac{[x-a-y]dy}{y^{q+1}} \tag{13.218}$$

$$= \frac{1}{\Gamma(-q)} \left[\int_a^{x-a} \frac{[x-a]dy}{y^{q+1}} + \int_a^{x-a} \frac{dy}{y^q} \right] \tag{13.219}$$

$$= \frac{1}{\Gamma(-q)} \left[\frac{[x-a]^{1-q}}{-q} + \frac{[x-a]^{1-q}}{1-q} \right] \tag{13.220}$$

$$= \frac{[x-a]^{1-q}}{[-q][1-q]\Gamma(-q)}, \tag{13.221}$$

which leads us to

$$\frac{d^q[x-a]}{[d(x-a)]^q} = \frac{[x-a]^{1-q}}{\Gamma(2-q)}, \quad q < 0. \tag{13.222}$$

For the positive values of q, we use Eq. (13.43) to write:

$$\frac{d^q[x-a]}{[d(x-a)]^q} = \frac{d^n}{dx^n} \left[\frac{d^{q-n}[x-a]}{[d(x-a)]^{q-n}} \right] \tag{13.223}$$

and choose n such that $q - n < 0$ is satisfied. Using the Riemann formula [Eq. (13.106)] we write

$$\frac{d^{q-n}[x-a]}{[d(x-a)]^{q-n}} = \frac{\Gamma(2)[x-a]^{1-q+n}}{\Gamma(2-q+n)}, \tag{13.224}$$

which leads to the following result:

$$\frac{d^q[x-a]}{[d(x-a)]^q} = \frac{d^n}{[d(x-a)]^n} \left[\frac{[x-a]^{1-q+n}}{\Gamma(2-q+n)} \right] = \frac{\Gamma(2-q+n)}{\Gamma(2-q)} \frac{[x-a]^{1-q}}{\Gamma(2-q+n)}, \tag{13.225}$$

$$\boxed{\frac{d^q[x-a]}{[d(x-a)]^q} = \frac{[x-a]^{1-q}}{\Gamma(2-q)}.} \tag{13.226}$$

This is now valid for all q.

13.5.3 Differintegral of $[x-a]^p$ $(p > -1)$

There is no restriction on p other than $p > -1$. We start with the Riemann–Liouville definition and write

$$\frac{d^q[x-a]^p}{[d(x-a)]^q} = \frac{1}{\Gamma(-q)} \int_a^x \frac{[x'-a]^p dx'}{[x-x']^{q+1}}, \quad q < 0. \tag{13.227}$$

Using the transformation $x' - a = v$, the above equation becomes

$$\frac{d^q[x-a]^p}{[d(x-a)]^q} = \frac{1}{\Gamma(-q)} \int_0^{x-a} \frac{v^p dv}{[x-a-v]^{q+1}}. \tag{13.228}$$

We now make another transformation, $v = (x-a)u$, to write

$$\frac{d^q[x-a]^p}{[d(x-a)]^q} = \frac{(x-a)^{p-q}}{\Gamma(-q)} \int_0^1 u^p(1-u)^{-q-1} du, \quad q < 0. \tag{13.229}$$

Using the definition of the beta function [Eq. (12.176)] and its relation with the gamma functions [Eq. (12.174)], we finally obtain

$$\frac{d^q[x-a]^p}{[d(x-a)]^q} = \frac{[x-a]^{p-q}}{\Gamma(-q)} B(p+1, -q), \tag{13.230}$$

$$\boxed{\frac{d^q[x-a]^p}{[d(x-a)]^q} = \frac{\Gamma(p+1)[x-a]^{p-q}}{\Gamma(p-q+1)},} \tag{13.231}$$

where $q < 0$ and $p > -1$. Actually, we could remove the restriction on q and use Eq. (13.231) for all q. See the derivation of the Riemann formula with the substitution $x \to x - a$.

13.5.4 Differintegral of $[1 - x]^p$

To find a formula valid for all p and q values we write $1 - x = 1 - a - (x - a)$ and use the binomial formula to write

$$(1-x)^p = \sum_{j=0}^{\infty} \frac{\Gamma(p+1)}{\Gamma(j+1)\Gamma(p-j+1)} (-1)^j (1-a)^{p-j} (x-a)^j. \tag{13.232}$$

We now use Eq. (13.139) and the Riemann formula [Eq. (13.106)], along with the properties of gamma and the beta functions to find

$$\boxed{\frac{d^q[1-x]^p}{[d(x-a)]^q} = \frac{(1-x)^{p-q}}{\Gamma(-q)} B_x(-q, q-p), \quad |x| < 1,} \tag{13.233}$$

where B_x is the incomplete beta function [Eq. (12.196)].

13.5.5 Differintegral of $\exp(\pm x)$

We first write the Taylor series of the exponential function as

$$\exp(\pm x) = \sum_{j=0}^{\infty} \frac{[\pm x]^j}{\Gamma(j+1)}$$

and use the Riemann formula [Eq. (13.106)] to obtain

$$\boxed{\frac{d^q \exp(\pm x)}{dx^q} = \frac{\exp(\pm x)}{x^q}\gamma^*(-q, \pm x),} \tag{13.234}$$

where γ^* is the incomplete gamma function [Eq. (12.197)].

13.5.6 Differintegral of ln (*x*)

To find the differintegral of $\ln x$, we first write the Riemann–Liouville derivative:

$$\frac{d^q \ln x}{dx^q} = \frac{1}{\Gamma(-q)}\int_0^x \frac{\ln x' dx'}{[x - x']^{q+1}}, \quad q < 0, \tag{13.235}$$

and then make the substitution $y = (x - x')/x$, to write

$$\frac{d^q \ln x}{dx^q} = \frac{x^{-q} \ln x}{\Gamma(-q)}\int_0^1 \frac{dy}{y^{q+1}} + \frac{x^{-q}}{\Gamma(-q)}\int_0^1 \frac{\ln(1-y)dy}{y^{q+1}}. \tag{13.236}$$

The first integral is easily evaluated as $1/(-q)$. Using integration by parts, the second integral can be written as

$$\int_0^1 \frac{\ln(1-y)dy}{y^{q+1}} = \frac{1}{q}\int_0^1 \ln(1-y)d(1-y^{-q}) \tag{13.237}$$

$$= \frac{(1-y^{-q})\ln(1-y)}{q}\Bigg|_0^1 + \frac{1}{q}\int_0^1 \frac{(1-y^{-q})dy}{1-y} \tag{13.238}$$

$$= \frac{1}{q}\int_0^1 \frac{1-y^{-q}}{1-y}dy. \tag{13.239}$$

Using the integral definition of the **digamma function** $\Psi(x)$:

$$\Psi(x+1) = -\gamma + \int_0^1 \frac{1-t^x}{1-t}dt, \tag{13.240}$$

where γ is the **Euler constant**:

$$\gamma = 0.5772157,$$

we find

$$\int_0^1 \frac{\ln(1-y)dy}{y^{q+1}} = \frac{1}{q}[\gamma + \Psi(1-q)]. \tag{13.241}$$

Using these in Eq. (13.236), we obtain

$$\frac{d^q \ln x}{dx^q} = \frac{x^{-q}\ln x}{(-q)\Gamma(-q)} + \frac{x^{-q}}{(-q)\Gamma(-q)}[-\gamma - \Psi(1-q)] \tag{13.242}$$

$$= \frac{x^{-q}}{\Gamma(1-q)}[\ln x - \gamma - \Psi(1-q)]. \tag{13.243}$$

Even though this result is obtained for $q < 0$, using analyticity, we can use it for all values of q [15]:

$$\boxed{\frac{d^q \ln(x)}{dx^q} = \frac{x^{-q}}{\Gamma(1-q)} \left[\ln(x) - \gamma - \psi(1-q)\right].} \tag{13.244}$$

The **digamma function**, $\psi(x)$, is defined in terms of the gamma function as

$$\psi(x) = \frac{1}{\Gamma(x)} \frac{d\Gamma(x)}{dx}. \tag{13.245}$$

Example 13.4 ***Digamma function***

We prove the following useful relation between the **digamma function** and the **gamma function**:

$$\frac{\Psi(1-n)}{\Gamma(1-n)} = (-1)^n \Gamma(n), \quad n = 1, 2, \ldots . \tag{13.246}$$

Proof: We start with the identity $\Gamma(-x)\Gamma(x+1) = -\pi \csc(\pi x)$, or with $\Gamma(x)\Gamma(1-x) = \pi \csc(\pi x)$, and differentiate to write:

$$\frac{d\Gamma(x)}{dx}\Gamma(1-x) + \Gamma(x)\frac{d\Gamma(1-x)}{dx} = -\pi^2 \frac{\cos(\pi x)}{\sin^2(\pi x)}, \tag{13.247}$$

$$\frac{d\Gamma(x)}{dx}\Gamma(1-x) + \Gamma(x)\frac{d\Gamma(1-x)}{d(1-x)}\frac{d(1-x)}{dx} = -\pi^2 \cos(\pi x)\csc^2(\pi x), \tag{13.248}$$

$$\frac{d\Gamma(x)}{dx}\Gamma(1-x) - \Gamma(x)\frac{d\Gamma(1-x)}{d(1-x)} = -\pi^2 \cos(\pi x)\csc^2(\pi x). \tag{13.249}$$

Rearranging, we obtain

$$\frac{1}{\Gamma(x)}\frac{d\Gamma(x)}{dx} - \frac{1}{\Gamma(1-x)}\frac{d\Gamma(1-x)}{d(1-x)} = -\frac{\pi^2 \cos(\pi x)}{\Gamma(1-x)\Gamma(x)}\csc^2(\pi x) \tag{13.250}$$

$$= -\frac{\pi^2 \cos(\pi x)}{\Gamma(1-x)\Gamma(x)} \frac{\Gamma^2(1-x)\Gamma^2(x)}{\pi^2} \tag{13.251}$$

$$= -\cos(\pi x)\Gamma(1-x)\Gamma(x), \tag{13.252}$$

which is nothing but $\Psi(x) - \Psi(1-x) = -\cos(\pi x)\Gamma(1-x)\Gamma(x)$. For $x = n$, where $n = 1, 2, 3, \ldots$, this becomes

$$\frac{\Psi(n)}{\Gamma(1-n)} - \frac{\Psi(1-n)}{\Gamma(1-n)} = -(-1)^n \Gamma(n), \quad n = 1, 2, 3, \ldots . \tag{13.253}$$

Since $\Psi(n)$ is finite for $n = 1, 2, 3, \ldots$, and the gamma function with a negative integer argument is infinite, the first term vanishes, thus proving the desired identity:

$$\boxed{\frac{\Psi(1-n)}{\Gamma(1-n)} = (-1)^n \Gamma(n), \quad n = 1, 2, 3, \ldots .} \tag{13.254}$$

13.5.7 Some Semiderivatives and Semi-Integrals

We conclude this section with a table of the frequently used semiderivatives and semi-integrals of some functions:

f	$d^{\frac{1}{2}} f / [dx]^{\frac{1}{2}}$	$d^{-\frac{1}{2}} f / [dx]^{-\frac{1}{2}}$
C	$C/\sqrt{\pi x}$	$2C\sqrt{x/\pi}$
$1/\sqrt{x}$	0	$\sqrt{\pi}$
$\sqrt{x}$	$\sqrt{\pi}/2$	$x\sqrt{\pi}/2$
x	$2\sqrt{x/\pi}$	$\frac{4}{3}x^{3/2}\sqrt{\pi}$
$x^\mu (\mu > -1)$	$[\Gamma(\mu+1)/\Gamma(\mu+1/2)]x^{\mu-1/2}$	$\Gamma(\mu+1)/\Gamma(\mu+3/2)]x^{\mu+1/2}$
$\exp(x)$	$1/\sqrt{\pi x} + \exp(x)\mathrm{erf}(\sqrt{x})$	$\exp(x)\mathrm{erf}(\sqrt{x})$
$\ln x$	$\ln(4x)/\sqrt{\pi x}$	$2\sqrt{\pi/x}[\ln(4x) - 2]$
$\exp(x)\mathrm{erf}(\sqrt{x})$	$\exp(x)$	$\exp(x) - 1$

13.6 Mathematical Techniques with Differintegrals

13.6.1 Laplace Transform of Differintegrals

The Laplace transform of a differintegral is defined as

$$£\left\{\frac{d^q f}{dx^q}\right\} = \int_0^\infty \exp(-sx) \frac{d^q f}{dx^q} dx, \quad s > 0. \tag{13.255}$$

When q takes integer values, Laplace transform of derivatives and integrals are given, respectively, as

$$£\left\{\frac{d^q f}{dx^q}\right\} = s^q £\{f\} - \sum_{k=0}^{q-1} s^{q-1-k} \frac{d^q f}{dx^q}(0), \quad q = 1, 2, 3 \ldots, \tag{13.256}$$

$$£\left\{\frac{d^q f}{dx^q}\right\} = s^q £\{f\}, \quad q = 0, -1, -2, \ldots. \tag{13.257}$$

We can unify these equations as

$$£\left\{\frac{d^n f}{dx^n}\right\} = s^n £\{f\} - \sum_{k=0}^{n-1} s^k \frac{d^{n-1-k} f}{dx^{q-1-k}}(0), \quad n = 0, \pm 1, \pm 2, \pm 3, \ldots. \tag{13.258}$$

In this equation, we can replace the upper limit in the sum by any number greater than $n-1$. We are now going to show that this expression is generalized for all q values as

$$£\left\{\frac{d^q f}{dx^q}\right\} = s^q £\{f\} - \sum_{k=0}^{n-1} s^k \frac{d^{q-1-k} f}{dx^{q-1-k}}(0), \tag{13.259}$$

where n is an integer satisfying the inequality $n-1 < q \leq n$.

We first consider the $q < 0$ case. We write the Riemann–Liouville definition:

$$\frac{d^q f}{dx^q} = \frac{1}{\Gamma(-q)} \int_0^x \frac{f(x')dx'}{[x-x']^{q+1}}, \quad q < 0, \tag{13.260}$$

and use the convolution theorem:

$$£\left\{\int_0^\infty f_1(x-x') f_2(x')\right\} = £\{f_1(x)\}£\{f_2(x)\}, \tag{13.261}$$

where we take $f_1(x) = x^{-q-1}$ and $f_2(x) = f(x)$ to write

$$£\left\{\frac{d^q f}{dx^q}\right\} = \frac{1}{\Gamma(-q)} £\{x^{-1-q}\}£\{f\} = s^q £\{f\}. \tag{13.262}$$

For the $q < 0$ values, the sum in Eq. (13.259) is empty. Thus, we see that the expression in Eq. (13.259) is valid for all $q < 0$ values. For the $q > 0$ case, we write the condition [Eq. (13.43)] that the Grünwald and Riemann–Liouville definitions satisfy as

$$\frac{d^n}{dx^n}\frac{d^{q-n} f}{dx^{q-n}} = \frac{d^q f}{dx^q}, \tag{13.263}$$

where n is positive integer, and choose n as

$$n - 1 < q < n. \tag{13.264}$$

We now take the Laplace transform of Eq. (13.263) to find

$$£\left\{\frac{d^q f}{dx^q}\right\} = £\left\{\frac{d^n}{dx^n}\left[\frac{d^{q-n} f}{dx^{q-n}}\right]\right\} \tag{13.265}$$

$$= s^n £\left\{\frac{d^{q-n} f}{dx^{q-n}}\right\} - \sum_{k=0}^{n-1} s^k \frac{d^{n-1-k}}{dx^{n-1-k}}\left[\frac{d^{q-n} f}{dx^{q-n}}\right](0), \quad q - n < 0. \tag{13.266}$$

Since $q - n < 0$, from Eqs. (13.260)–(13.262) the first term on the right-hand side becomes $s^q £\{f\}$. When $n - 1 - k$ takes integer values, the term,

$$\frac{d^{n-1-k}}{dx^{n-1-k}}\left[\frac{d^{q-n}f}{dx^{q-n}}\right](0),$$

under the summation sign with the $q - n < 0$ condition and the composition formula [Eq. (13.263)], can be written as

$$\frac{d^{q-1-k}f}{dx^{q-1-k}}(0).$$

This leads us to the Laplace transform of differintegrals as

$$\boxed{£\left\{\frac{d^q f}{dx^q}\right\} = s^q £\{f\} - \sum_{k=0}^{n-1} s^k \frac{d^{q-1-k}f}{dx^{q-1-k}}(0), \quad 0 < q \neq 1, 2, 3 \ldots.} \tag{13.267}$$

We could satisfy this equation for the integer values of q by taking the condition $n - 1 < q \leq n$ instead of Eq. (13.264).

Example 13.5 ***Heat transfer equation***

We consider the heat transfer equation for a semi-infinite slab:

$$\frac{\partial T(x,t)}{\partial t} = K\frac{\partial^2 T(x,t)}{\partial x^2}, \quad t \in [0,\infty],\ x \in [0,\infty], \tag{13.268}$$

where K is the heat transfer coefficient, which depends on conductivity, density, and the specific heat of the slab. We take $T(x,t)$ as the difference of the local temperature from the ambient temperature, where t is the time and x is the distance from the surface of interest. As the boundary conditions we take

$$T(x,0) = 0 \tag{13.269}$$

and

$$T(\infty,t) = 0. \tag{13.270}$$

Taking the Laplace transform of Eq. (13.268) with respect to t we get

$$£\left\{\frac{\partial T(x,t)}{\partial t}\right\} = K£\left\{\frac{\partial^2 T(x,t)}{\partial x^2}\right\}, \tag{13.271}$$

$$s\tilde{T}(x,s) - T(x,0) = K\frac{\partial^2 \tilde{T}(x,s)}{\partial x^2}, \tag{13.272}$$

$$s\tilde{T}(x,s) = K\frac{\partial^2 \tilde{T}(x,s)}{\partial x^2}. \tag{13.273}$$

Using the boundary condition [Eq. (13.270)], we can immediately write the solution, which is finite for all x as

$$\tilde{T}(x,s) = F(s)e^{-x\sqrt{s/K}}. \tag{13.274}$$

In this solution, $F(s)$ is the Laplace transform of the boundary condition $T(0,t)$:

$$F(s) = £\{T(0,t)\}, \tag{13.275}$$

which remains unspecified. In most of the engineering applications we are interested in the heat flux, which is given as

$$J(x,t) = -k\frac{\partial T(x,t)}{\partial x}, \tag{13.276}$$

where k is the conductivity. Or, in particular, we are interested in the surface flux:

$$J(0,t) = -k\left.\frac{\partial T(x,t)}{\partial x}\right|_{x=0}, \tag{13.277}$$

which could be monitored quite easily. To find the surface flux we differentiate Eq. (13.274) with respect to x:

$$\frac{\partial \tilde{T}(x,s)}{\partial x} = -\sqrt{s/K}F(s)e^{-x\sqrt{s}} \tag{13.278}$$

and eliminate $F(s)$ by using Eq. (13.274) to get

$$\frac{\partial \tilde{T}(x,s)}{\partial x} = -\sqrt{s/K}\tilde{T}(x,s). \tag{13.279}$$

We now use Eq. (13.267) with $q = 1/2$ and choose $n = 1$:

$$£\left\{\frac{d^{1/2}T(x,t)}{dt^{1/2}}\right\} = s^{1/2}£\{T(x,t)\} - \frac{d^{-1/2}T(x,0)}{dt^{-1/2}}. \tag{13.280}$$

Using the other boundary condition [Eq. (13.269)], the second term on the right-hand side is zero; thus, we write

$$£\left\{\frac{d^{1/2}T(x,t)}{dt^{1/2}}\right\} = s^{1/2}£\{T(x,t)\} = s^{1/2}\tilde{T}(x,s). \tag{13.281}$$

Substituting Eq. (13.279) into this equation and taking the inverse Laplace transform we get

$$\frac{d^{1/2}T(x,t)}{dt^{1/2}} = -\sqrt{K}\frac{\partial T(x,t)}{\partial x}. \tag{13.282}$$

Using this in the surface heat flux expression, we finally obtain

$$J(0,t) = -k\left.\frac{\partial T(x,t)}{\partial x}\right|_{x=0} = \frac{k}{\sqrt{K}}\frac{d^{1/2}T(0,t)}{dt^{1/2}}. \tag{13.283}$$

The importance of this result is that the surface heat flux is given in terms of the surface temperature distribution $T(0,t)$, which is experimentally easier to measure.

13.6.2 Extraordinary Differential Equations

An equation composed of the differintegrals of an unknown function is called an **extraordinary** differential equation. Naturally, solutions of such equations involve some constants and integrals. A simple example of such an equation can be given as $\frac{d^q f(x)}{dx^q} = F(x)$, where q is any number, $F(x)$ is a given function, and $f(x)$ is the unknown function. For simplicity, we have taken the lower limit, a, as zero. We would like to write the solution of this equation simply as $f(x) = \frac{d^{-q}F(x)}{dx^{-q}}$. However, we have seen that the operators $\frac{d^{-q}}{dx^{-q}}$ and $\frac{d^q}{dx^q}$ are not the inverses of each other unless the condition [Eq. (13.169)]:

$$f(x) - \frac{d^{-q}}{dx^{-q}} \frac{d^q f(x)}{dx^q} = 0,$$

is satisfied. It is for this reason that extraordinary differential equations are in general much more difficult to solve. One of the most frequently encountered differential equation in science is $dx(t)/dt = -\alpha x(t)^n$, where for $n = 1$ the solution is given as an exponential function: $x(t) = x_0 \exp(-\alpha t)$, while for $n \neq 1$, the solutions are given with a power dependence: $x(t)^{1-n} = \alpha(n-1)(t-t_0)$. On the other hand, the solutions of

$$\frac{d^n x(t)}{dt^n} = (\mp\alpha)^n x(t), \quad n = 1, 2, \ldots \tag{13.284}$$

are the **Mittag–Leffler** functions:

$$x(t) = x_0 E_n[(\mp\alpha t)^n], \tag{13.285}$$

which correspond to extrapolations between exponential and power dependence. A fractional generalization of Eq. (13.284) can be written as

$$\frac{d^{-q}N(t)}{[d(t)]^{-q}} = -\alpha^{-q}[N(t) - N_0], \quad q > 0, \tag{13.286}$$

which is frequently encountered in kinetic theory, where its solutions are given in terms of the Mittag–Leffler functions as $N(t) = N_0 E_q(-\alpha^q t^q)$.

13.6.3 Mittag–Leffler Functions

Mittag–Leffler functions are encountered in many different branches of science like biology, chemistry, kinetic theory, and Brownian motion. They are defined by the series (Figure 13.5)

$$\boxed{E_q(x) = \sum_{k=0}^{\infty} \frac{x^k}{\Gamma(qk+1)}, \quad q > 0.} \tag{13.287}$$

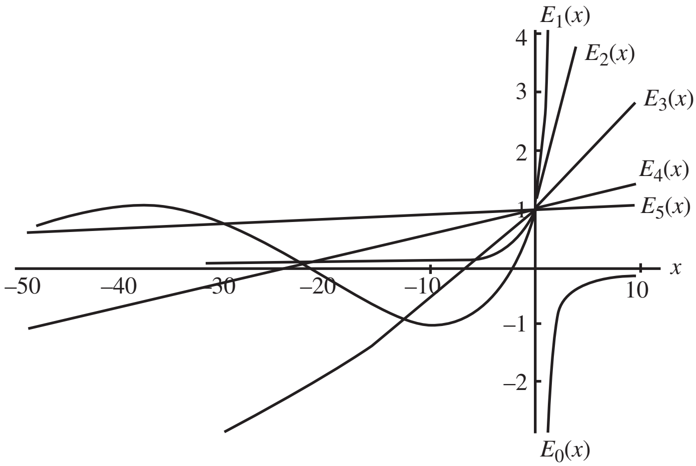

Figure 13.5 Mittag–Leffler functions.

For some integer values of q the Mittag–Leffler functions are given as

$$E_0(x) = \frac{1}{1-x}, \tag{13.288}$$

$$E_1(x) = \exp(x), \tag{13.289}$$

$$E_2(x) = \cosh\left(\sqrt{x}\right), \tag{13.290}$$

$$E_3(x) = \frac{1}{3}\left[\exp\left(\sqrt[3]{x}\right) + 2\exp\left(-\sqrt[3]{x}/2\right)\cos\left(\frac{\sqrt{3}}{2}\sqrt[3]{x}\right)\right], \tag{13.291}$$

$$E_4(x) = \frac{1}{2}\left[\cos\left(\sqrt[4]{x}\right) + \cosh\left(\sqrt[4]{x}\right)\right]. \tag{13.292}$$

A frequently encountered Mittag–Leffler function is given for $q = 1/2$, which can be written in terms of the error function as

$$E_{1/2}\left(\pm\sqrt{x}\right) = \exp(x)[1 + \mathrm{erf}\left(\pm\sqrt{x}\right)], \quad x > 0. \tag{13.293}$$

13.6.4 Semidifferential Equations

In applications we frequently encounter extraordinary differential equations like

$$\frac{d^3 f(x)}{dx^3} + \sin(x)\frac{d^{3/2} f(x)}{dx^{3/2}} = \exp(2x), \tag{13.294}$$

$$\frac{d^{-1/2} f(x)}{dx^{-1/2}} - 4\frac{d^{3/2} f(x)}{dx^{3/2}} + 5f(x) = x, \tag{13.295}$$

which involves semiderivatives of the unknown function $f(x)$. However, an equation like

$$\frac{d^4 f(x)}{dx^4} - \frac{d^3 f(x)}{dx^3} + 5f(x) = \frac{d^{3/2} F(x)}{dx^{3/2}}, \tag{13.296}$$

where $F(x)$ is a known function is not considered to be a semidifferential equation.

Example 13.6 ***Semidifferential equation solution***
Consider the following semidifferential equation:

$$\frac{d^{1/2}}{dx^{1/2}} f(x) + af(x) = 0, \quad a = \text{constant}. \tag{13.297}$$

Applying the operator $\frac{d^{1/2}}{dx^{1/2}}$ to this equation and using the composition rule [Eq. (13.170)] with Eq. (13.175), and with m taken as 1 we get

$$\frac{df(x)}{dx} - C_1 x^{-3/2} + a\frac{d^{1/2}}{dx^{1/2}} f(x) = 0. \tag{13.298}$$

Using Eq. (13.297), again we find

$$\frac{df(x)}{dx} - a^2 f(x) = C_1 x^{-3/2}. \tag{13.299}$$

This is now a first-order ordinary differential equation the solution of which is given as

$$f(x) = C\exp(a^2 x) + C_1 \exp(a^2 x) \int_0^x \exp(-a^2 x') x'^{-3/2} dx'. \tag{13.300}$$

What is new here is that the solution involves two integration constants and a divergent integral. However, this integral can be defined by using the incomplete gamma function $\gamma^*(c, x)$:

$$\gamma^*(c, x) = \frac{c^{-x}}{\Gamma(x)} \int_0^c x'^{x-1} \exp(-x') dx' = \exp(-x) \sum_{j=0}^{\infty} \frac{x^j}{\Gamma(j + c + 1)}, \tag{13.301}$$

where $\gamma^*(c, x)$ is a single-valued and an analytic function of c and x. Using the relations

$$\gamma^*(c - 1, x) = x\gamma^*(c, x) + \frac{\exp(-x)}{\Gamma(c)} \quad \text{and} \quad \gamma^*\left(\frac{1}{2}, x\right) = \frac{\operatorname{erf}\left(\sqrt{x}\right)}{\sqrt{x}}, \tag{13.302}$$

we can evaluate the divergent integral $I = \int_0^x \exp(-a^2 x') x'^{-3/2} dx'$ as

$$I = -2a\sqrt{\pi}\operatorname{erf}\left(\sqrt{a^2 x}\right) - 2a\frac{\exp(-a^2 x)}{\sqrt{a^2 x}}. \tag{13.303}$$

Substituting this into Eq. (13.300), we find the solution

$$f(x) = C\exp(a^2x) + C_1\exp(a^2x)\left[-2a\sqrt{\pi}\mathrm{erf}\left(\sqrt{a^2x}\right) - \frac{2a\exp(-a^2x)}{\sqrt{a^2x}}\right] \tag{13.304}$$

$$= C\exp(a^2x) - 2a\sqrt{\pi}C_1\exp(a^2x) \quad \mathrm{erf}\left(\sqrt{a^2x}\right) - \frac{2aC_1}{\sqrt{a^2x}}. \tag{13.305}$$

This solution still contains two arbitrary constants. To check that it satisfies the semidifferential Eq. (13.297), we first find its semiderivative as

$$\frac{d^{1/2}f}{dx^{1/2}} = a\left[\frac{C}{\sqrt{\pi a^2x}} + C\exp(a^2x) \quad \mathrm{erf}(\sqrt{a^2x}) - 2a\sqrt{\pi}C_1\exp(a^2x)\right],$$

where we have used the scale transformation formula [Eq. (13.137)] and the semiderivatives given in Section 13.5.7. Substituting the above equation into Eq. (13.297) gives

$$a\left[\frac{C}{\sqrt{\pi a^2x}} + C\exp(a^2x) \quad \mathrm{erf}\left(\sqrt{a^2x}\right) - 2a\sqrt{\pi}C_1\exp(a^2x)\right]$$
$$= -a\left[-\frac{2aC_1}{\sqrt{a^2x}} - 2a\sqrt{\pi}C_1\exp(a^2x) \quad \mathrm{erf}\left(\sqrt{a^2x}\right) + C\exp(a^2x)\right], \tag{13.306}$$

thus, we obtain a relation between C and C_1 as $C/\sqrt{\pi} = 2aC_1$. Now the final solution is obtained as

$$f(x) = C\exp(a^2x)\left[1 - \mathrm{erf}\left(a\sqrt{x}\right)\right] - \frac{C}{a^2\sqrt{\pi x}}. \tag{13.307}$$

13.6.5 Evaluating Definite Integrals by Differintegrals

We have seen how analytic continuation and complex integral theorems can be used to evaluate definite integrals. Fractional calculus can also be used for evaluating some definite integrals. Using the transformation

$$x' = x - x\lambda \tag{13.308}$$

and the Riemann–Liouville definition [Eqs. (13.77)–(13.78)], we can write the differintegral of the function x^q as

$$\frac{d^qx^q}{dx^q} = \frac{1}{\Gamma(-q)}\int_0^1 \frac{[1-\lambda]^q d\lambda}{\lambda^{q+1}} = \Gamma(q+1), \tag{13.309}$$

where $-1 < q < 0$ and we have used Eq. (13.231) to write

$$d^qx^q/dx^q = \Gamma(q+1). \tag{13.310}$$

Making one more transformation, $t = -\ln(\lambda)$, we obtain the following definite integral:

$$\int_0^\infty \frac{dt}{[\exp(t) - 1]^{-q}} = \Gamma(-q)\Gamma(q+1) = -\pi \csc(q\pi), -1 < q < 0. \tag{13.311}$$

We can also use the transformation [Eq. (13.308)] in the Riemann–Liouville definition for an arbitrary function to write

$$\int_0^1 f(x - x\lambda) d(\lambda^{-q}) = \Gamma(1-q) x^q \frac{d^q f(x)}{dx^q}, \quad q < 0. \tag{13.312}$$

If we also make the replacements $\lambda^{-q} \to t$ and $-1/q \to p$, where p is positive but does not have to be an integer, to obtain the formula

$$\boxed{\int_0^1 f(x - xt^p) dt = \Gamma\left(\frac{p+1}{p}\right) x^{-1/p} \frac{d^{-1/p} f(x)}{dx^{-1/p}}, \quad p > 0,} \tag{13.313}$$

this is very useful in the evaluation of some definite integrals.

As a special case we may choose $x = 1$ to write

$$\boxed{\int_0^1 f(1 - t^p) dt = \Gamma\left(\frac{p+1}{p}\right) \left. \frac{d^{-1/p} f(x)}{dx^{-1/p}} \right|_{x=1}.} \tag{13.314}$$

Example 13.7 ***Evaluation of some definite integrals by differintegrals***

Using differintegrals we can evaluate the definite integral $\int_0^1 \exp(2 - 2t^{2/3}) dt$. Using Eq. (13.313) with $x = 2$ and $p = 2/3$ along with Eq. (13.234) we find

$$\int_0^1 \exp(2 - 2t^{2/3}) dt = \Gamma\left(\frac{5}{2}\right) 2^{-3/2} \left. \frac{d^{-3/2}(\exp x)}{dx^{-3/2}} \right|_{x=2} \tag{13.315}$$

$$= \Gamma\left(\frac{5}{2}\right) 2^{-3/2} \left[\frac{\exp(x)}{x^{-3/2}} \gamma^* \left(\frac{3}{2}, x\right) \right]_{x=2} \tag{13.316}$$

$$= (3\sqrt{\pi} e^2/4) \gamma^* \left(\frac{3}{2}, 2\right). \tag{13.317}$$

In 1972, Osler [17] gave the integral version of the **Leibniz rule** [Eq. (13.183)], which can be useful in evaluating some definite integrals as

$$\boxed{\frac{d^q[f(x)g(x)]}{dx^q} = \int_{-\infty}^{\infty} \binom{q}{\lambda + \gamma} \frac{d^{q-\gamma-\lambda} f(x)}{dx^{q-\gamma-\lambda}} \frac{d^{\gamma+\lambda} g(x)}{dx^{\gamma+\lambda}} d\lambda,} \tag{13.318}$$

where γ is any constant.

Example 13.8 ***Evaluation of definite integrals by differintegrals***
In the Osler formula [Eq. (13.318)], we may choose $f(x) = x^{\alpha}$, $g(x) = x^{\beta}$, $\gamma = 0$ to write

$$\frac{d^q[x^{\alpha+\beta}]}{dx^q} = \int_{-\infty}^{\infty} \frac{\Gamma(q+1)\Gamma(\alpha+1)\Gamma(\beta+1)x^{\alpha-q+\lambda+\beta-\lambda}d\lambda}{\Gamma(q-\lambda+1)\Gamma(\lambda+1)\Gamma(\alpha-q+\lambda+1)\Gamma(\beta-\lambda+1)}. \tag{13.319}$$

Using the derivative [Eq. (13.231)]:

$$\frac{d^q[x^{\alpha+\beta}]}{dx^q} = \frac{\Gamma(\alpha+\beta+1)x^{\alpha+\beta-q}}{\Gamma(\alpha+\beta-q+1)}, \tag{13.320}$$

and after simplification, we obtain the definite integral

$$\frac{\Gamma(\alpha+\beta+1)}{\Gamma(\alpha+\beta-q+1)} = \int_{-\infty}^{\infty} \frac{\Gamma(q+1)\Gamma(\alpha+1)\Gamma(\beta+1)d\lambda}{\Gamma(q-\lambda+1)\Gamma(\lambda+1)\Gamma(\alpha-q+\lambda+1)\Gamma(\beta-\lambda+1)}. \tag{13.321}$$

Furthermore, if we set $\beta = 0$ and $\alpha = q$, we can use the relation

$$\Gamma(\lambda+1)\Gamma(1-\lambda) = \lambda\pi/\sin\lambda\pi, \tag{13.322}$$

to obtain the following useful result:

$$\boxed{\int_{-\infty}^{\infty} \frac{\sin(\lambda\pi)d\lambda}{\lambda\Gamma(\lambda+1)\Gamma(q-\lambda+1)} = \frac{\pi}{\Gamma(q+1)}.} \tag{13.323}$$

13.6.6 Evaluation of Sums of Series by Differintegrals

In 1970, Osler [16] gave the summation version of the **Leibniz rule**, which is very useful in finding sums of infinite series:

$$\frac{d^q[u(x)v(x)]}{dx^q} = \sum_{n=-\infty}^{\infty} \binom{q}{n+\gamma} \frac{d^{q-n-\gamma}u}{dx^{q-n-\gamma}} \frac{d^{\gamma+n}v}{dx^{\gamma+n}} \tag{13.324}$$

$$= \sum_{n=-\infty}^{\infty} \frac{\Gamma(q+1)}{\Gamma(q-\gamma-n+1)\Gamma(\gamma+n+1)} \frac{d^{q-\gamma-n}u(x)}{dx^{q-\gamma-n}} \frac{d^{\gamma+n}v(x)}{dx^{\gamma+n}}, \tag{13.325}$$

where γ is any constant.

Example 13.9 ***Evaluation of sums of series by differintegrals***
In the above formula, we choose $u(x) = x^{\alpha}$, $v(x) = x^{\beta}$, $\gamma = 0$ and use Eq. (13.231) to obtain the sum

$$\sum_{n=-\infty}^{\infty} \frac{\Gamma(q+1)\Gamma(\alpha+1)\Gamma(\beta+1)}{\Gamma(q-n+1)\Gamma(n+1)\Gamma(\alpha-q+n+1)\Gamma(\beta-n+1)} = \frac{\Gamma(\alpha+\beta+1)}{\Gamma(\alpha+\beta-q+1)}. \tag{13.326}$$

Furthermore, we set $\alpha = -1/2$, $\beta = 1/2$, $q = -1/2$ to get the useful result

$$\sum_{n=0}^{\infty} \frac{[(2n)!]^2}{2^{4n}(n!)^4(1-2n)} = \frac{2}{\pi}. \tag{13.327}$$

13.6.7 Special Functions Expressed as Differintegrals

Using Eq. (13.325), we can also express hypergeometric functions and some special functions as differintegrals [16]:

$$\text{Hypergeometric Functions}: F(\alpha,\beta,\gamma,x) = \frac{\Gamma(\gamma)x^{1-\gamma}}{\Gamma(\beta)} \frac{d^{\beta-\gamma}}{dx^{\beta-\gamma}}\left(\frac{x^{\beta-1}}{(1-x)^{\alpha}}\right),$$

$$\text{Confluent Hypergeometric Functions}: M(\alpha,\gamma,x) = \frac{\Gamma(\gamma)x^{1-\gamma}}{\Gamma(\alpha)} \frac{d^{\alpha-\gamma}}{dx^{\alpha-\gamma}}\left(e^{x}x^{\alpha-1}\right),$$

$$\text{Bessel Functions}: J_{\nu}(x) = \frac{x^{-\nu}}{2^{\nu}\sqrt{\pi}} \frac{d^{-\nu-1/2}}{d(x^2)^{-\nu-1/2}}\left(\frac{\cos x}{x}\right),$$

$$\text{Legendre Polynomials}: P_{\nu}(x) = \frac{1}{\Gamma(\nu+1)2^{\nu}} \frac{d^{\nu}}{d(1-x)^{\nu}}\left(1-x^2\right)^{\nu},$$

$$\text{Incomplete Gamma Function}: \gamma^{*}(\alpha,x) = \Gamma(\alpha)e^{-x}\frac{d^{-\alpha}e^{x}}{dx^{-\alpha}}.$$

13.7 Caputo Derivative

In 1960s, Caputo introduced another definition of fractional derivative, which he used to study dissipation effects in linear viscoelasticity problems. Caputo derivative is based on a modification of the Laplace transform of differintegrals and found widespread use in applications.

Laplace transform of a differintegral is given as [Eq. (13.267)]

$$£\left\{\frac{d^q f(t)}{dt^q}\right\} = s^q \tilde{f}(s) - \sum_{k=0}^{n-1} s^k \frac{d^{q-1-k}f}{dx^{q-1-k}}(0) \tag{13.328}$$

$$= s^q \tilde{f}(s) - f^{(q-1)}(0) - sf^{(q-2)}(0) - \cdots - s^{n-1}f^{(q-n)}(0), \tag{13.329}$$

where n is an integer satisfying $n-1 < q \leq n$. For $0 < q < 1$, we take $n = 1$, thus obtaining

$$£\left\{\frac{d^q f(t)}{dt^q}\right\} = s^q \tilde{f}(s) - f^{(q-1)}(0). \tag{13.330}$$

Due to the difficulty in imposing boundary conditions with fractional derivatives, **Caputo** defined the Laplace transform for $0 < q < 1$ as

$$£\left\{\frac{d^q f(t)}{dt^q}\right\} = s^q \tilde{f}(s) - s^{q-1}f(0) = s^{q-1}\left(s\tilde{f}(s) - f(0)\right), \tag{13.331}$$

the inverse of which gives

$$\frac{d^q f(t)}{dt^q} = £^{-1}\{s^{q-1}\ (s\tilde{f}(s) - f(0))\}. \tag{13.332}$$

Using the convolution theorem, $\int_0^t f(u)g(t-u)du = £^{-1}\{F(s)G(s)\}$, with the definitions $F(s) = s\tilde{f}(s) - f(0)$ and $G(s) = s^{q-1}$, yields the fractional derivative known as the **Caputo derivative**:

$$\boxed{\left[\frac{d^q f(t)}{dt^q}\right]_C = \frac{1}{\Gamma(1-q)} \int_0^t \left(\frac{df(\tau)}{d\tau}\right) \frac{d\tau}{(t-\tau)^q}, \quad 0 < q < 1,} \tag{13.333}$$

which was used by him to model dissipation effects in linear viscosity.

13.7.1 Caputo and the Riemann–Liouville Derivative

We now write the Riemann–Liouville derivative [Eq. (13.78)] for $0 < q < 1$ as

$$\left[\frac{d^{q+1} f(t)}{dt^{q+1}}\right]_{R-L} = \frac{d^n}{dt^n}\left[\frac{1}{\Gamma(n-q-1)} \int_0^t \frac{f(\tau)d\tau}{(t-\tau)^{q+1-n+1}}\right], \tag{13.334}$$

where n is a positive integer satisfying $n - q - 1 > 0$. Choosing $n = 2$ yields

$$\left[\frac{d^{q+1} f(t)}{dt^{q+1}}\right]_{R-L} = \frac{d^2}{dt^2}\left[\frac{1}{\Gamma(1-q)} \int_0^t \frac{f(\tau)d\tau}{(t-\tau)^q}\right]. \tag{13.335}$$

Similarly, we write

$$\left[\frac{d^{1+q} f(t)}{dt^{1+q}}\right]_{R-L} = \frac{d^n}{dt^n}\left[\frac{1}{\Gamma(n-1-q)} \int_0^t \frac{f(\tau)d\tau}{(t-\tau)^{1+q-n+1}}\right] \tag{13.336}$$

and choose $n = 2$:

$$\left[\frac{d^{1+q} f(t)}{dt^{1+q}}\right]_{R-L} = \frac{d^2}{dt^2}\left[\frac{1}{\Gamma(1-q)} \int_0^t \frac{f(\tau)d\tau}{(t-\tau)^q}\right], \tag{13.337}$$

thus verifying the relation

$$\left[\frac{d^{q+1} f(t)}{dt^{q+1}}\right]_{R-L} = \left[\frac{d^{1+q} f(t)}{dt^{1+q}}\right]_{R-L}. \tag{13.338}$$

Returning to the Caputo derivative [Eq. (13.333)], we write

$$\frac{d}{dt}\left[\frac{d^q f(t)}{dt^q}\right]_C = \frac{1}{\Gamma(1-q)} \frac{d}{dt} \int_0^t \frac{df(\tau)}{d\tau} \frac{d\tau}{(t-\tau)^q}. \tag{13.339}$$

As in the Riemann–Liouville and Grünwald definitions [Eqs. (13.43) and (13.74)], we impose the condition

$$\frac{d}{dt}\left[\frac{d^q f(t)}{dt^q}\right] = \frac{d^{1+q} f(t)}{dt^{1+q}}, \tag{13.340}$$

to get

$$\left[\frac{d^{1+q}f(t)}{dt^{1+q}}\right]_C = \frac{1}{\Gamma(1-q)}\frac{d}{dt}\int_0^t \frac{df(\tau)}{d\tau}\frac{d\tau}{(t-\tau)^q}. \tag{13.341}$$

Definition of the Riemann–Liouville derivative and Eq. (13.338) allows us to write

$$\left[\frac{d^{1+q}f(t)}{dt^{1+q}}\right]_C = \left[\frac{d^q}{dt^q}\left(\frac{df(t)}{dt}\right)\right]_{R-L}. \tag{13.342}$$

Using the composition rule [Eq. (13.170)] of differintegrals, $d^q d^Q f = d^{q+Q} f - d^{q+Q}[f - d^{-Q} d^Q f]$, we write the right-hand side of Eq. (13.342) as

$$\left[\frac{d^q}{dt^q}\left(\frac{df(t)}{dt}\right)\right]_{R-L} = \left[\frac{d^{q+1}f(t)}{dt^{q+1}}\right]_{R-L} - \left[\frac{d^{q+1}}{dt^{q+1}}\right]_{R-L}\left[f(t) - \frac{d^{-1}}{dt^{-1}}\frac{d}{dt}f(t)\right]. \tag{13.343}$$

Also using Eq. (13.162):

$$\frac{d^{-n}f^{(N)}(t)}{[d(t-a)]^{-n}} = f^{(N-n)}(t) - \sum_{k=n-N}^{n-1}\frac{[t-a]^k}{k!}f^{(N+k-n)}(a), \tag{13.344}$$

with $n = 1$, $N = 1$, and $a = 0$, we have $d^{-1}d^1 f(t) = f(t) - f^{(1+0-1)}(0) = f(t) - f(0)$. Thus,

$$\left[\frac{d^q}{dt^q}\left(\frac{df(t)}{dt}\right)\right]_{R-L} = \left[\frac{d^{q+1}f(t)}{dt^{q+1}}\right]_{R-L} - \left[\frac{d^{q+1}}{dt^{q+1}}\right]_{R-L}[f(t) - f(t) + f(0)] \tag{13.345}$$

$$= \left[\frac{d^{q+1}f(t)}{dt^{q+1}}\right]_{R-L} - \left[\frac{d^{q+1}}{dt^{q+1}}\right]_{R-L} f(0). \tag{13.346}$$

Using this in Eq. (13.342) we write

$$\left[\frac{d^{1+q}f(t)}{dt^{1+q}}\right]_C = \left[\frac{d^{q+1}f(t)}{dt^{q+1}}\right]_{R-L} - \left[\frac{d^{q+1}}{dt^{q+1}}\right]_{R-L} f(0). \tag{13.347}$$

Also using Eq. (13.338):

$$\left[\frac{d^{q+1}f(t)}{dt^{q+1}}\right]_{R-L} = \left[\frac{d^{1+q}f(t)}{dt^{1+q}}\right]_{R-L}, \tag{13.348}$$

and the Riemann–Liouville derivative of a constant [Eq. (13.211)]:

$$\left[\frac{d^{q+1}}{dt^{q+1}}f(0)\right]_{R-L} = \frac{t^{-q-1}f(0)}{\Gamma(-q)}, \tag{13.349}$$

we finally obtain the relation between the Riemann–Liouville derivative and the Caputo derivative as

$$\boxed{\left[\frac{d^q f(t)}{dt^q}\right]_C = \left[\frac{d^q f(t)}{dt^q}\right]_{R-L} - \frac{t^{-q}f(0)}{\Gamma(1-q)}, \quad 0 < q < 1.} \tag{13.350}$$

From the above equation, it is seen that the Caputo and the Riemann–Liouville derivatives agree when $f(0) = 0$. Furthermore, unlike the $R-L$ derivative the Caputo derivative of a constant, C_0, is zero:

$$\left[\frac{d^q C_0}{dt^q}\right]_C = \left[\frac{d^q C_0}{dt^q}\right]_{R-L} - \frac{t^{-q}C_0}{\Gamma(1-q)} = \frac{t^{-q}C_0}{\Gamma(1-q)} - \frac{t^{-q}C_0}{\Gamma(1-q)} = 0. \tag{13.351}$$

To display the clear distinction between the two definitions of fractional derivatives, we use the Riemann–Liouville definition of fractional integrals [Eq. (13.77)] to introduce the fractional integral operator ${}_0\mathbf{I}_t^q$:

$${}_0\mathbf{I}_t^q[f(t)] = \frac{1}{\Gamma(q)}\int_0^t \frac{f(\tau)d\tau}{(t-\tau)^{1-q}}, \quad q > 0, \tag{13.352}$$

which allows us to define the **Riemann–Liouville** and the **Caputo** derivatives of arbitrary order, $q > 0$, respectively, as

$$\left[\frac{d^q f(t)}{dt^q}\right]_{R-L} = \frac{d^n}{dt^n}\left({}_0\mathbf{I}_t^{n-q}[f(t)]\right), \quad n > q,\ q > 0, \tag{13.353}$$

$$\left[\frac{d^q f(t)}{dt^q}\right]_C = {}_0\mathbf{I}_t^{n-q}\left[\frac{d^n}{dt^n}f(t)\right], \quad n > q,\ q > 0, \tag{13.354}$$

where n is the smallest integer greater than q, that is, $n-1 < q < n$. Notice how the order of the $\frac{d^n}{dt^n}$ and the ${}_0\mathbf{I}_t^{n-q}$ operators reverses. We can also write the above equations as

$${}_0^{R-L}\mathbf{D}_t^q f(t) = \frac{d^n}{dt^n}\left({}_0\mathbf{I}_t^{n-q}[f(t)]\right), \tag{13.355}$$

$${}_0^{C}\mathbf{D}_t^q f(t) = {}_0\mathbf{I}_t^{n-q}\left[\frac{d^n}{dt^n}f(t)\right]. \tag{13.356}$$

Taking the **Laplace transform** of these derivatives yields

$$\pounds\left\{{}_0^{R-L}\mathbf{D}_t^q f(t)\right\} = s^q\tilde{f}(s) - \sum_{k=0}^{n-1} s^k\left({}_0^{R-L}\mathbf{D}_t^{q-k-1}f(t)\right)\Big|_{t=0}, \quad n-1 < q \le n, \tag{13.357}$$

and

$$\pounds\left\{{}_0^{C}\mathbf{D}_t^q f(t)\right\} = s^q\tilde{f}(s) - \sum_{k=0}^{n-1} s^{q-k-1}\left.\frac{d^k f(t)}{dt^k}\right|_{t=0}, \quad n-1 < q \le n. \tag{13.358}$$

Since the Laplace transform of the Caputo derivative requires only the values of the function and its ordinary derivatives at $t = 0$, it has a clear advantage over the Riemann–Liouville derivative when it comes to imposing the initial conditions. Eq. (13.350) can be generalized for all $q > 0$ as

$$\boxed{{}_0^C\mathbf{D}_t^q f(t) = {}_0^{R-L}\mathbf{D}_t^q f(t) - \sum_{k=0}^{n-1} \frac{t^{k-q}}{\Gamma(k-q+1)} f^{(k)}(0^+), \quad n-1 < q < n,\ q > 0.} \tag{13.359}$$

In other words, the two derivatives are not equal unless $f(t)$ and its first $n-1$ derivatives vanish at $t = 0$ [7].

13.7.2 Mittag–Leffler Function and the Caputo Derivative

The **Mittag–Leffler** function, $E_q(x)$, is the generalization of the exponential function, $e^x = \sum_{n=0}^{\infty} t^n/n! = \sum_{n=0}^{\infty} t^n/\Gamma(n+1)$, as

$$E_q(x) = \sum_{n=0}^{\infty} \frac{t^{qn}}{\Gamma(qn+1)}, \quad q > 0. \tag{13.360}$$

We now consider the following fractional differential equation:

$$\boxed{{}_0^C\mathbf{D}_x^q y(x) = \omega y(x), \quad y(0) = y_0,\ 0 < q < 1,} \tag{13.361}$$

where ${}_0^C\mathbf{D}_x^q$ stands for the Caputo derivative, and write its Laplace transform, $s^q\tilde{y} - s^{q-1}y_0 = \omega\tilde{y}$, as

$$\tilde{y}(s) = \frac{s^{q-1}y_0}{s^q - \omega}. \tag{13.362}$$

Using the geometric series, $\sum_{n=0}^{\infty} x^n = 1/(1-x)$, we can write $\tilde{y}$ as

$$\tilde{y}(s) = y_0 \sum_{n=0}^{\infty} \frac{\omega^n}{s^{1+qn}}, \tag{13.363}$$

which can be inverted easily to yield the solution:

$$y(x) = y_0 \sum_{n=0}^{\infty} \frac{\omega^n x^{qn}}{\Gamma(qn+1)} = y_0 E_q(\omega x^q). \tag{13.364}$$

Another notation used in literature is

$$\boxed{y(x) = y_0 E_q(\omega; x),} \tag{13.365}$$

where $E_q(\omega; x)$ satisfies

$$\boxed{{}_0^C\mathbf{D}_x^q E_q(\omega; x) = \omega E_q(\omega; x), \quad E_q(\omega; 0) = 1.} \tag{13.366}$$

13.7.3 Right- and Left-Handed Caputo Derivatives

The **right-handed** Caputo derivative is defined as

$$\boxed{{}^{C}_{a^+}\mathbf{D}^q_r f(r) = {}_{a^+}\mathbf{I}^{n-q}_r f^{(n)}(r) = \frac{1}{\Gamma(n-q)}\int_a^r \frac{f^{(n)}(\tau)d\tau}{(r-\tau)^{1-n+q}}, \quad q>0,} \tag{13.367}$$

where n is the next integer higher than q. Note that for $0<q<1$, $a=0$ and $n=1$, we obtain Eq. (13.333).

The **left-handed** Caputo derivative is defined as

$$\boxed{{}^{C}_{b^-}\mathbf{D}^q_r f(r) = (-1)^n {}_{b^-}\mathbf{I}^{n-q}_r f^{(n)}(r) = \frac{(-1)^n}{\Gamma(n-q)}\int_r^b \frac{f^{(n)}(\tau)d\tau}{(\tau-r)^{1-n+q}}, \quad q>0,} \tag{13.368}$$

where n is again the next integer higher than q. We reserve the letter a for the lower limit of the integral operators and the letter b for the upper limit, hence we will ignore the superscripts in a^+ and b^-.

Note the following important relation between the **left-handed Riemann–Liouville** and the **Caputo** derivatives [5]:

$$\boxed{{}^{R-L}_{b}\mathbf{D}^q_t g(t) = {}^{C}_{b}\mathbf{D}^q_t g(t) + \sum_{k=0}^{n-1} \frac{(-1)^{q-k}(b-t)^{k-q}}{\Gamma(k-q+1)}[\mathbf{D}^k_t g(t)]_{t=b},} \tag{13.369}$$

where $q \in (n-1, n]$. When $g(t)$ satisfies the boundary conditions $\mathbf{D}^k_t g(b) = 0$, $k = 0, 1, \ldots, n-1$, Eq. (13.369) implies ${}^{R-L}_{b}\mathbf{D}^q_t g(t) = {}^{C}_{b}\mathbf{D}^q_t g(t)$.

Example 13.10 ***Left-handed Caputo derivative of 1/r***
The left-handed Caputo derivative of $1/r$ for $0<q<1$, $k=1$ and $b=\infty$ is calculated as follows:

$$ {}^{C}_{\infty}\mathbf{D}^q_r\left(\frac{1}{r}\right) = \frac{-1}{\Gamma(1-q)}\int_r^\infty \frac{(-1/\tau^2)d\tau}{(\tau-r)^q} \tag{13.370}$$

$$ = \frac{-1}{\Gamma(1-q)}\int_r^\infty (-1)\tau^{-(q+2)}\left(1-\frac{r}{\tau}\right)^{-q}d\tau. \tag{13.371}$$

Defining $t = r/\tau$ we write

$$ {}^{C}_{\infty}\mathbf{D}^q_r\left(\frac{1}{r}\right) = \frac{1}{\Gamma(1-q)}\int_1^0 \left(\frac{r}{t}\right)^{-(q+2)}(1-t)^{-q}\left(-\frac{rdt}{t^2}\right) \tag{13.372}$$

$$ = \frac{-r^{-(q+1)}}{\Gamma(1-q)}\int_1^0 \frac{(1-t)^{-q}}{t^{-q}}dt = \frac{r^{-(q+1)}}{\Gamma(1-q)}\int_0^1 t^q(1-t)^{-q}dt. \tag{13.373}$$

Using the definition of the beta function [Eqs. (12.174) and (12.176)] this gives

$$ {}_{\infty}^{C}\mathbf{D}_r^q \left(\frac{1}{r}\right) = r^{-(q+1)}\Gamma(1+q), \quad 0<q<1. \tag{13.374}$$

Note that as $q \to 1$, one does not get the expected result, that is, $D_r^1(1/r) = -1/r^2$. Actually, in general, one has [5]

$$ \lim_{q\to n} \left[{}_{b}^{C}\mathbf{D}_r^q f(r)\right] = (-1)^n f^{(n)}(r). \tag{13.375}$$

13.7.4 A Useful Relation of the Caputo Derivative

We now derive the following relation of the Caputo derivative:

$$ \boxed{ {}_{0}^{C}\mathbf{D}_t^{1-q} \left[{}_{0}^{C}\mathbf{D}_t^q f(t)\right] = \frac{df(t)}{dt} - \frac{\left[{}_{0}^{C}\mathbf{D}_t^q f(t)\right]_0}{\Gamma(q)t^{1-q}}, \quad 0<q<1,} \tag{13.376}$$

which is very useful in obtaining the effective potential for fractional quantum mechanics.

Proof: Using the relation between the Caputo derivative and the Riemann–Liouville derivative [Eq. (13.350)], we can write

$$ {}_{0}^{C}\mathbf{D}_t^{1-q} \left[{}_{0}^{C}\mathbf{D}_t^q f(t)\right] = {}_{0}^{R-L}\mathbf{D}_t^{1-q} \left[{}_{0}^{C}\mathbf{D}_t^q f(t)\right] - \frac{\left[{}_{0}^{C}\mathbf{D}_t^q f(t)\right]_0}{\Gamma(q)t^{1-q}}. \tag{13.377}$$

Using Eq. (13.350) again, the first term on the right-hand side of the above equation becomes

$$ {}_{0}^{R-L}\mathbf{D}_t^{1-q} \left[{}_{0}^{C}\mathbf{D}_t^q f(t)\right] = {}_{0}^{R-L}\mathbf{D}_t^{1-q} \left[{}_{0}^{R-L}\mathbf{D}_t^q f(t) - \frac{f(0)}{\Gamma(1-q)t^q}\right] \tag{13.378}$$

$$ = {}_{0}^{R-L}\mathbf{D}_t^{1-q} \left[{}_{0}^{R-L}\mathbf{D}_t^q f(t)\right] - {}_{0}^{R-L}\mathbf{D}_t^{1-q} \left[\frac{f(0)}{\Gamma(1-q)t^q}\right] \tag{13.379}$$

$$ = {}_{0}^{R-L}\mathbf{D}_t^{1-q} \left[{}_{0}^{R-L}\mathbf{D}_t^q f(t)\right] - {}_{0}^{R-L}\mathbf{D}_t^{1-q} \left[\frac{C}{t^q}\right], \tag{13.380}$$

where $C = f(0)/\Gamma(1-q)$. Using Eq. (13.170) for the composition of fractional derivatives:

$$ {}_{0}^{R-L}\mathbf{D}_t^q \left[{}_{0}^{R-L}\mathbf{D}_t^Q f(t)\right] $$
$$ = {}_{0}^{R-L}\mathbf{D}_t^{q+Q} f(t) - {}_{0}^{R-L}\mathbf{D}_t^{q+Q} f(t) \left\{ f - {}_{0}^{R-L}\mathbf{D}_t^{-Q} \left[{}_{0}^{R-L}\mathbf{D}_t^Q f(t)\right] \right\}, \tag{13.381}$$

with $q = 1 - q$ and $Q = q$, we write the first term on the right-hand side of Eq. (13.380) as

$$
\begin{aligned}
&{}^{R-L}_{0}\mathbf{D}^{1-q}_{t}\left[{}^{R-L}_{0}\mathbf{D}^{q}_{t}f(t)\right] \\
&={}^{R-L}_{0}\mathbf{D}^{1-q+q}_{t}f(t) - {}^{R-L}_{0}\mathbf{D}^{1-q+q}_{t}\left[f(t) - {}^{R-L}_{0}\mathbf{D}^{-q}_{t}\left({}^{R-L}_{0}\mathbf{D}^{q}_{t}f(t)\right)\right] \qquad (13.382)\\
&= \frac{df(t)}{dt} - \frac{d}{dt}\left[f(t) - {}^{R-L}_{0}\mathbf{D}^{-q}_{t}\left({}^{R-L}_{0}\mathbf{D}^{q}_{t}f(t)\right)\right]. \qquad (13.383)
\end{aligned}
$$

Assuming ${}^{R-L}_{0}\mathbf{D}^{q}_{t}f(t) \neq 0$, we have ${}^{R-L}_{0}\mathbf{D}^{-q}_{t}({}^{R-L}_{0}\mathbf{D}^{q}_{t}f(t)) = f(t)$, therefore ${}^{R-L}_{0}\mathbf{D}^{1-q}_{t}\left[{}^{R-L}_{0}\mathbf{D}^{q}_{t}f(t)\right] = \frac{df(t)}{dt}$. Substituting this into Eq. (13.380), we obtain

$$
{}^{R-L}_{0}\mathbf{D}^{1-q}_{t}\left[{}^{C}_{0}\mathbf{D}^{q}_{t}f(t)\right] = \frac{df(t)}{dt} - {}^{R-L}_{0}\mathbf{D}^{1-q}_{t}\left[\frac{C}{t^{q}}\right], \quad C = f(0)/\Gamma(1-q). \qquad (13.384)
$$

For the second term on the right-hand side, we now use the Leibniz rule [Eq. (13.183)]:

$$
{}^{R-L}_{0}\mathbf{D}^{q}_{t}[f(t)g(t)] = \sum_{j=0}^{\infty}\binom{q}{j}\left({}^{R-L}_{0}\mathbf{D}^{q-j}_{t}f(t)\right)\left({}^{R-L}_{0}\mathbf{D}^{j}_{t}g(t)\right) \qquad (13.385)
$$

and write

$$
{}^{R-L}_{0}\mathbf{D}^{1-q}_{t}(Ct^{-q}) = \sum_{j=0}^{\infty}\binom{1-q}{j}\ {}^{R-L}_{0}\mathbf{D}^{q-j}_{t}(t^{-q})\,{}^{R-L}_{0}\mathbf{D}^{j}_{t}C. \qquad (13.386)
$$

Since j is an integer and C is a constant, ${}^{R-L}_{0}\mathbf{D}^{j}_{t}C = d^{j}C/dt^{j} = 0$, hence only the $j = 0$ term survives. Since $\Gamma(0) = \infty$, we obtain

$$
{}^{R-L}_{0}\mathbf{D}^{1-q}_{t}\left(\frac{f(0)}{\Gamma(1-q)t^{q}}\right) = \binom{1-q}{0}\ {}^{R-L}_{0}\mathbf{D}^{q}_{t}(t^{-q})\,{}^{R-L}_{0}C \qquad (13.387)
$$

$$
= \left(\frac{f(0)}{\Gamma(1-q)}\right)\left(\frac{\Gamma(2-q)}{\Gamma(1)\Gamma(2-q)}\right)\frac{\Gamma(1-q)}{\Gamma(0)}t^{-1} = 0. \qquad (13.388)
$$

Substituting this into Eq. (13.384) gives

$$
{}^{R-L}_{0}\mathbf{D}^{1-q}_{t}\left[{}^{C}_{0}\mathbf{D}^{q}_{t}f(t)\right] = df(t)/dt, \qquad (13.389)
$$

which when substituted back into Eq. (13.377) yields the desired result:

$$
\boxed{{}^{C}_{0}\mathbf{D}^{1-q}_{t}\left[{}^{C}_{0}\mathbf{D}^{q}_{t}f(t)\right] = \frac{df(t)}{dt} - \frac{\left[{}^{C}_{0}\mathbf{D}^{q}_{t}f(t)\right]_{0}}{\Gamma(q)t^{1-q}}, \quad 0 < q < 1.} \qquad (13.390)
$$

13.8 Riesz Fractional Integral and Derivative

13.8.1 Riesz Fractional Integral

Another fractional derivative commonly encountered in applications is the **Riesz derivative**. Unlike the Caputo derivative, which is defined in terms of its Laplace transform, the Riesz derivative is defined in terms of its **Fourier transform**. It is used to define **fractional Laplacian** encountered in many different branches of science and engineering.

Since the Riesz derivative is defined through its Fourier transform, we start with a review of the basic properties of the Fourier transforms. The Fourier transform, $F(\omega)$, of an absolutely integrable function, $f(t)$, in the interval $(-\infty, \infty)$, along with its inverse, is defined as

$$F(\omega) = \mathcal{F}\{f(t)\} = \int_{-\infty}^{\infty} e^{-i\omega t} f(t)\, dt, \quad \omega \text{ is real}, \tag{13.391}$$

$$f(t) = \mathcal{F}^{-1}\{F(\omega)\} = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{i\omega t} F(\omega)\, d\omega. \tag{13.392}$$

If $F(\omega)$ and $G(\omega)$ are the Fourier transforms of $f(t)$ and $g(t)$, respectively, the **convolution** of $f(t)$ with $g(t), f * g$, is defined as $f * g = \int_{-\infty}^{\infty} f(t-\tau)g(\tau)d\tau = \int_{-\infty}^{\infty} f(\tau)g(t-\tau)d\tau$. The Fourier transform of a convolution, $\mathcal{F}\{f * g\}$, is equal to the product of the Fourier transforms $F(\omega)$ and $G(\omega)$ as $\mathcal{F}\{f * g\} = F(\omega)\cdot G(\omega)$. Granted that as $t \to \pm\infty$ all the required derivatives vanish, that is, $f(f), f'(t), \ldots, f^{(n-1)}(t) \to 0$ as $t \to \pm\infty$, the Fourier transform of a derivative, $\mathcal{F}\{f^{(n)}(t)\}$, is given as

$$\mathcal{F}\{f^{(n)}(t)\} = (i\omega)^n F(\omega). \tag{13.393}$$

To find the Fourier transform of the fractional **Riemann–Liouville integral** [Eq. (13.77) with $a = -\infty$.]:

$${}_{-\infty}\mathbf{I}_t^q g(t) = {}_{-\infty}\mathbf{D}_t^{-q} g(t) = \frac{1}{\Gamma(q)}\int_{-\infty}^{t} (t-\tau)^{q-1} g(\tau) d\tau, \quad q > 0, \tag{13.394}$$

we first write the Laplace transform of the function

$$h(t) = \frac{t^{q-1}}{\Gamma(q)}, \quad q > 0: \tag{13.395}$$

$$\pounds\{h(t)\} = \frac{1}{\Gamma(q)}\int_0^{\infty} t^{q-1} e^{-st} dt = s^{-q}, \tag{13.396}$$

and then substitute $s = i\omega$ to obtain the Fourier transform of

$$h_+(t) = \begin{cases} \frac{t^{q-1}}{\Gamma(q)}, & t > 0, \\ 0, & t \le 0, \end{cases} \tag{13.397}$$

as

$$\mathcal{F}\{h_+(t)\} = H_+(\omega) = (i\omega)^{-q}. \tag{13.398}$$

In this case the convergence of the integral in Eq. (13.396) restricts q to $0 < q < 1$. We now write the convolution of $g(t)$ with $h_+(t)$ as

$$h_+(t) * g(t) = \int_{-\infty}^{\infty} h_+(t-\tau)g(\tau)\,d\tau = \frac{1}{\Gamma(q)}\int_{-\infty}^{t} (t-\tau)^{q-1}g(\tau)\,d\tau, \tag{13.399}$$

which is nothing but ${}_{-\infty}\mathbf{D}_t^{-q}g(t)$:

$$h_+(t) * g(t) = {}_{-\infty}\mathbf{D}_t^{-q}g(t). \tag{13.400}$$

We finally use Eq. (13.398) to obtain

$$\boxed{\mathcal{F}\{{}_{-\infty}\mathbf{D}_t^{-q}g(t)\} = (i\omega)^{-q}G(\omega),} \tag{13.401}$$

where $G(\omega)$ is the Fourier transform of $g(t)$.

To find the Fourier transform of

$${}_{\infty}\mathbf{D}_t^{-q}g(t) = \frac{1}{\Gamma(q)}\int_t^{\infty} (\tau-t)^{q-1}g(\tau)\,d\tau, \quad 0 < q < 1, \tag{13.402}$$

we again make use of the Laplace transform

$$\pounds\{h(t)\} = \frac{1}{\Gamma(q)}\int_0^{\infty} t^{q-1}e^{-st}dt = s^{-q}, \quad q > 0, \tag{13.403}$$

and substitute $s = -i\omega$ to get

$$\pounds\{h(t)\} = \frac{1}{\Gamma(q)}\int_0^{\infty} t^{q-1}e^{i\omega t}dt = (-i\omega)^{-q}, \quad 0 < q < 1. \tag{13.404}$$

We then let $t \to -t$ in the above integral to write

$$\pounds\{h(t)\} = \frac{1}{\Gamma(q)}\int_{-\infty}^{0} (-t)^{q-1}e^{-i\omega t}dt = (-i\omega)^{-q}, \quad 0 < q < 1. \tag{13.405}$$

This is nothing but the Fourier transform of the function

$$h_-(t) = \begin{cases} 0, & t \geq 0, \\ \dfrac{(-t)^{q-1}}{\Gamma(q)}, & t < 0, \end{cases} \tag{13.406}$$

as

$$\mathcal{F}\{h_{\_}(t)\} = H_{\_}(\omega) = \int_{-\infty}^{\infty} h_{\_}(t)e^{-i\omega t}dt \tag{13.407}$$

$$= \left[\int_{-\infty}^{0} h_{\_}(t)e^{-i\omega t}dt + \int_{0}^{\infty} h_{\_}(t)e^{-i\omega t}dt\right] \tag{13.408}$$

$$= \frac{1}{\Gamma(q)}\int_{-\infty}^{0} (-t)^{q-1}e^{-i\omega t}dt \tag{13.409}$$

$$= (-i\omega)^{-q}. \tag{13.410}$$

We now employ the convolution theorem to write

$$h_{\_}(t) * g(t) = \int_{-\infty}^{\infty} h_{\_}(t-\tau)g(\tau)\,d\tau \tag{13.411}$$

$$= \int_{-\infty}^{t} h_{\_}(t-\tau)g(\tau)\,d\tau + \int_{t}^{\infty} h_{\_}(t-\tau)g(\tau)\,d\tau \tag{13.412}$$

$$= \frac{1}{\Gamma(q)}\int_{t}^{\infty} (\tau - t)^{q-1}g(\tau)\,d\tau \tag{13.413}$$

$$= {}_{\infty}\mathbf{D}_t^{-q}g(t), \tag{13.414}$$

which yields the Fourier transform $\mathcal{F}\{{}_{\infty}\mathbf{D}_t^{-q}g(t)\}$ as

$$\mathcal{F}\{{}_{\infty}\mathbf{D}_t^{-q}g(t)\} = H_{\_}(\omega)G(\omega), \tag{13.415}$$

$$\boxed{\mathcal{F}\{{}_{\infty}\mathbf{D}_t^{-q}g(t)\} = (-i\omega)^{-q}G(\omega).} \tag{13.416}$$

Summary

We have obtained the following Fourier transforms of fractional integrals:

$$\boxed{\mathcal{F}\{{}_{-\infty}\mathbf{D}_t^{-q}g(t)\} = (i\omega)^{-q}G(\omega),} \tag{13.417}$$

$$\boxed{\mathcal{F}\{{}_{\infty}\mathbf{D}_t^{-q}g(t)\} = (-i\omega)^{-q}G(\omega).} \tag{13.418}$$

We can now combine these equations to write

$$\mathcal{F}\left\{\left[{}_{-\infty}\mathbf{D}_t^{-q} + {}_{\infty}\mathbf{D}_t^{-q}\right]g(t)\right\} = \left[(i\omega)^{-q} + (-i\omega)^{-q}\right]G(\omega) \tag{13.419}$$

$$= |\omega|^{-q}\left[i^{-q} + (-i)^{-q}\right]G(\omega) \tag{13.420}$$

$$= \left(2\cos\frac{q\pi}{2}\right)|\omega|^{-q}G(\omega), \tag{13.421}$$

hence

$$\mathcal{F}\left\{\frac{\left[{}_{-\infty}\mathbf{D}_t^{-q} + {}_{\infty}\mathbf{D}_t^{-q}\right]}{2\cos\left(\frac{q\pi}{2}\right)} g(t)\right\} = |\omega|^{-q} G(\omega). \tag{13.422}$$

The combined expression:

$$\boxed{\mathbf{R}_t^{-q} g(t) = \frac{\left[{}_{-\infty}\mathbf{D}_t^{-q} + {}_{\infty}\mathbf{D}_t^{-q}\right] g(t)}{2\cos\left(\frac{q\pi}{2}\right)}, \quad q > 0,\ q \neq 1, 3, 5, \dots,} \tag{13.423}$$

or

$$\boxed{\mathbf{R}_t^{-q} g(t) = \frac{1}{2\Gamma(q)\cos\left(\frac{q\pi}{2}\right)} \int_{-\infty}^{\infty} (t-\tau)^{q-1} g(\tau) d\tau, \quad q > 0,\ q \neq 1, 3, 5, \dots} \tag{13.424}$$

is called the **Riesz fractional integral** or the **Riesz potential**. The Riesz fractional integral for $0 < q < 1$ is evaluated through its Fourier transform as

$$\boxed{\mathcal{F}\left\{\mathbf{R}_t^{-q} g(t)\right\} = |\omega|^{-q} G(\omega), \quad 0 < q < 1.} \tag{13.425}$$

13.8.2 Riesz Fractional Derivative

To find the Fourier transform of fractional derivatives, we write the **Riemann–Liouville** definition [Eq. (13.78)] with $a = -\infty$ as

$$\begin{aligned} {}_{-\infty}\mathbf{D}_t^q g(t) &= \frac{1}{\Gamma(n-q)} \int_{-\infty}^{t} (t-\tau)^{-q-1+n} g^{(n)}(\tau) d\tau, \quad q > 0, && (13.426)\\ &= {}_{-\infty}\mathbf{D}_t^{q-n} g^{(n)}(t), \quad n-1 < q < n. && (13.427) \end{aligned}$$

We assume reasonable behavior of $g(t)$ and its derivatives:

$$g(x), g'(x), \dots, g^{(n-1)}(x) \to 0 \ \text{ as } x \to \pm\infty. \tag{13.428}$$

In general, when there is no indication of the type in ${}_a\mathbf{D}_t^q g(t)$ we mean $R-L$. However, in this case due to the boundary conditions used as $x \to \pm\infty$, the Riemann–Liouville and the Caputo definitions of the fractional derivatives agree. Since $q - n < 0$, using Eq. (13.417) we can write the Fourier transform of ${}_{-\infty}\mathbf{D}_t^q g(t)$ as

$$\begin{aligned} \mathcal{F}\left\{{}_{-\infty}\mathbf{D}_t^q g(t)\right\} &= (i\omega)^{q-n} \mathcal{F}\left\{g^{(n)}(t)\right\}, \quad q > 0 && (13.429)\\ &= (i\omega)^{q-n} (i\omega)^n G(\omega), && (13.430) \end{aligned}$$

hence

$$\boxed{\mathcal{F}\{{}_{-\infty}\mathbf{D}_t^q g(t)\} = (i\omega)^q G(\omega),} \tag{13.431}$$

where we have used the result in Eq. (13.393). Similarly, one can show that

$$\boxed{\mathcal{F}\{{}_{\infty}\mathbf{D}_t^q g(t)\} = (-i\omega)^q G(\omega).} \tag{13.432}$$

We now combine the results in Eqs. (13.431) and (13.432) to write

$$\mathcal{F}\left\{\left[{}_{-\infty}\mathbf{D}_t^q + {}_{\infty}\mathbf{D}_t^q\right] g(t)\right\} = \left[(i\omega)^q + (-i\omega)^q\right] G(\omega). \tag{13.433}$$

For real ω, this becomes

$$\mathcal{F}\left\{\left[{}_{-\infty}\mathbf{D}_t^q + {}_{\infty}\mathbf{D}_t^q\right] g(t)\right\} = \left(2\cos\frac{q\pi}{2}\right) |\omega|^q G(\omega), \quad \omega \text{ real}. \tag{13.434}$$

Defining the derivative $\mathbf{D}_t^q g(t) = ({}_{-\infty}\mathbf{D}_t^q + {}_{\infty}\mathbf{D}_t^q) g(t)$, we see that $\mathbf{D}_t^q g(t)$ does not have the desired Fourier transform neither at $q = 1$ nor at $q = 2$, that is,

$$\mathcal{F}\{\mathbf{D}_t^1 g(t)\} \neq i\omega G(\omega), \tag{13.435}$$

$$\mathcal{F}\{\mathbf{D}_t^2 g(t)\} \neq (i\omega)^2 G(\omega) = -|\omega|^2 G(\omega). \tag{13.436}$$

For $0 < q \leq 2$, $q \neq 1$, the **Riesz fractional derivative** is usually defined with a minus sign as [8]

$$\mathbf{R}_t^q g(t) = -\frac{\left[{}_{-\infty}\mathbf{D}_t^q + {}_{\infty}\mathbf{D}_t^q\right] g(t)}{2\cos(q\pi/2)}, \quad 0 < q \leq 2,\ q \neq 1, \tag{13.437}$$

$$\mathcal{F}\{\mathbf{R}_t^q g(t)\} = -\frac{(i\omega)^q + (-i\omega)^q}{2\cos(q\pi/2)} G(\omega). \tag{13.438}$$

This form of the Riesz derivative allows analytic continuation and thus the correct implementation of the complex contour integral theorems encountered in some applications. For real ω, $\mathcal{F}\{\mathbf{R}_t^q g(t)\}$ [Eq. (13.438)] can be written as

$$\boxed{\mathcal{F}\{\mathbf{R}_t^q g(t)\} = -|\omega|^q G(\omega).} \tag{13.439}$$

This definition of the Riesz derivative has the desired Fourier transform for $q = 2$, but still does not reproduce the standard result for $q = 1$. Therefore, the above definition is generally written as valid for $0 < q \leq 2$, $q \neq 1$.

The minus sign in the definition of the Riesz derivative [Eq. (13.437)] is introduced by hand to recover the $q = 2$ case as [3]

$$\mathbf{R}_t^2 g(t) = -\frac{1}{2\pi}\int_{-\infty}^{\infty} |\omega|^2 G(\omega) e^{i\omega t} d\omega = \frac{1}{2\pi}\int_{-\infty}^{\infty} G(\omega)\left[\frac{d^2}{dt^2} e^{i\omega t}\right] d\omega \tag{13.440}$$

$$= \frac{d^2}{dt^2}\left[\frac{1}{2\pi}\int_{-\infty}^{\infty} G(\omega) e^{i\omega t} d\omega\right] = \frac{d^2}{dt^2} g(t). \tag{13.441}$$

In general, the Riesz derivative is related to the power $q/2$ of the positive definite operator $-\mathbf{D}_t^2 g(t) = -d^2 g(t)/dt^2$ as

$$-\mathbf{R}_t^q g(t) = \left(-\frac{d^2}{dt^2}\right)^{q/2} g(t). \tag{13.442}$$

13.8.3 Fractional Laplacian

Using the following definitions of the three-dimensional Fourier transforms:

$$\Phi(\vec{k},t) = \int_{-\infty}^{\infty} d^3\vec{r}\ \Psi\left(\vec{r},t\right) e^{-i\vec{k}\cdot\vec{r}}, \tag{13.443}$$

$$\Psi\left(\vec{r},t\right) = \frac{1}{(2\pi)^3}\int_{-\infty}^{\infty} d^3\vec{k}\ \Phi(\vec{k},t)e^{i\vec{k}\cdot\vec{r}}, \tag{13.444}$$

we can introduce the fractional Laplacian as.

$$\boxed{\Delta^{q/2}\Psi\left(\vec{r},t\right) = -\frac{1}{(2\pi)^3}\int_{-\infty}^{\infty} d^3\vec{k}\,\Phi(\vec{k},t)|k|^q e^{i\vec{k}\cdot\vec{r}}.} \tag{13.445}$$

13.9 Applications of Differintegrals in Science and Engineering

13.9.1 Fractional Relaxation

Exponential relaxation is governed by the differential equation

$$\boxed{\frac{df(t)}{dt} = -\frac{f(t)}{\tau}, \quad \tau > 0,} \tag{13.446}$$

where τ is a constant. For the initial condition $f(0) = f_0$, the solution is the exponential function, $f(t) = f_0 e^{-t/\tau}$. We now write Eq. (13.446) in integral form as

$$\int df = -\frac{1}{\tau}\int f(t)\,dt, \tag{13.447}$$

$$f(t) - f_0 = -\left(\frac{1}{\tau}\right)\ {}_0\mathbf{D}_t^{-1} f(t), \tag{13.448}$$

where ${}_0\mathbf{D}_t^{-1}$ is the standard **Riemann integral** operator ${}_0\mathbf{D}_t^{-1} = \int_0^t dt'$. Using the replacement ${}_0\mathbf{D}_t^{-1} f(t) \to {}_0\mathbf{D}_t^{-\alpha} f(t)$, $\alpha > 0$, where ${}_0\mathbf{D}_t^{-\alpha}$ is the fractional **Riemann–Liouville integral** [Eq. (13.394)], we can write the fractional relaxation equation as

$$f(t) - f_0 = -\left(\frac{1}{\tau^\alpha}\right)\ {}_0\mathbf{D}_t^{-\alpha} f(t). \tag{13.449}$$

Operating on this with ${}_0\mathbf{D}_t^\alpha$ gives

$$ {}_0\mathbf{D}_t^\alpha f(t) - {}_0\mathbf{D}_t^\alpha f_0 = -\tau^{-\alpha} f(t), \tag{13.450} $$

$$ {}_0\mathbf{D}_t^\alpha f(t) - f_0 \frac{t^{-\alpha}}{\Gamma(1-\alpha)} = -\tau^{-\alpha} f(t), \tag{13.451} $$

where we have used the fractional derivative of a constant [Eq. (13.211)]. Using the relation between the **Riemann–Liouville** and the **Caputo** derivatives [Eq. (13.350)], we can also write this as

$$ \boxed{{}_0^C\mathbf{D}_t^\alpha f(t) = -\tau^{-\alpha} f(t), \quad 0 < \alpha < 1.} \tag{13.452} $$

Using Eq. (13.361) the solution is immediately written as the **Mittag–Leffler** function:

$$ \boxed{f(t) = f_0 E_\alpha(-(t/\tau)^\alpha).} \tag{13.453} $$

The series expansion of this solution is

$$ f(t) = f_0 \sum_{k=0}^{\infty} \frac{(-1)^k}{\Gamma(1+\alpha k)} (t/\tau)^{\alpha k}, \tag{13.454} $$

which reduces to the exponential relaxation as $\alpha \to 1$.

13.9.2 Continuous Time Random Walk (CTRW)

We have seen that the diffusion equation is given as

$$ \frac{\partial c\left(\vec{r},t\right)}{\partial t} = -\vec{\nabla}\cdot\vec{J}\left(\vec{r},t\right), \tag{13.455} $$

where $\vec{J}\left(\vec{r},t\right)$ represents the current density and $c\left(\vec{r},t\right)$ is the concentration of particles. As a first approximation we can assume a linear relation between $\vec{J}$ and the gradient of concentration, $\vec{\nabla}c$, as $\vec{J} = -k\vec{\nabla}c$, where k is the diffusion constant. This gives the partial differential equation to be solved for $c\left(\vec{r},t\right)$ as

$$ \boxed{\frac{\partial c\left(\vec{r},t\right)}{\partial t} = k\vec{\nabla}^2 c\left(\vec{r},t\right).} \tag{13.456} $$

To prove the molecular structure of matter, Einstein studied the random motion of particles in suspension in a fluid. This motion is also known as the **Brownian motion** and results from the random collisions of the fluid molecules with the particles in suspension. Since diffusion is basically many particles undergoing Brownian motion at the same time, division of the concentration, $c(r,t)$, by the total number of particles, N, gives the probability of finding a particle at position $\vec{r}$ and time t as $P\left(\vec{r},t\right) = c\left(\vec{r},t\right)/N$.

Thus, the probability, $P\left(\vec{r},t\right)$, satisfies the same differential equation as the concentration:

$$\frac{\partial P\left(\vec{r},t\right)}{\partial t} = k\vec{\nabla}^2 P\left(\vec{r},t\right). \tag{13.457}$$

In d dimensions, for a particle initially at the origin, the solution of Eq. (13.457) is a Gaussian:

$$P\left(\vec{r},t\right) = \frac{1}{(4\pi kt)^{d/2}} \exp\left(-\frac{r^2}{4kt}\right). \tag{13.458}$$

In Brownian motion, even though the **mean** distance covered by the particle is zero, $\langle r(t)\rangle = \int \vec{r} P\left(\vec{r},t\right) d\vec{r} = 0$, the **mean square** distance is given as

$$\langle r^2(t)\rangle = \int r^2 P\left(\vec{r},t\right) d\vec{r} = 2k(d)t. \tag{13.459}$$

This equation sets the scale of the process as

$$\langle r^2(t)\rangle \propto t. \tag{13.460}$$

Hence the root mean square of the distance covered by a particle is

$$\sqrt{\langle r^2(t)\rangle} \propto t^{1/2}. \tag{13.461}$$

In Figure 13.6, the first figure shows the distance covered by a Brown particle. In Brownian motion or Einstein random walk, even though the particles are hit by the fluid particles symmetrically, they slowly drift away from the origin with the relation [Eq. (13.461)].

In Einstein's theory of random walk steps are taken with equal intervals. Recently, theories in which steps are taken according to a waiting distribution, $\Psi(t)$, have been developed. This distribution function essentially carries information about the **delays** and the **traps** present in the system. Thus, in a way, it incorporates memory effects into the random walk process. These theories are called **continuous time random walk** (CTRW) theories. In **CTRW**, if the integral $\tau = \int t\Psi(t)dt$, that gives the average waiting time of the system is finite, we can study the problem by taking the diffusion constant in Eq. (13.457) as $a^2/2\tau$. If the average waiting time is divergent, as in

$$\Psi(t) \propto \frac{1}{(1+t/\tau)^{1+\alpha}}, \quad 0 < \alpha < 1, \tag{13.462}$$

the situation changes dramatically. In CTRW theories $\langle r^2\rangle$ in general grows as $\langle r^2\rangle \propto t^\alpha$. Compared to Einstein's theory, in **anomalous diffusion** cases with $\alpha < 1$ are called **subdiffusive** and less distance is covered by the particle (Figure 13.6b), while the $\alpha > 1$ cases are called **superdiffusive** and more distance is covered. In CTRW theories, waiting times between steps varies. This is reminiscent of stock markets or earthquakes, where there could be long waiting times before the system makes the next move. For $\alpha = 1/2$

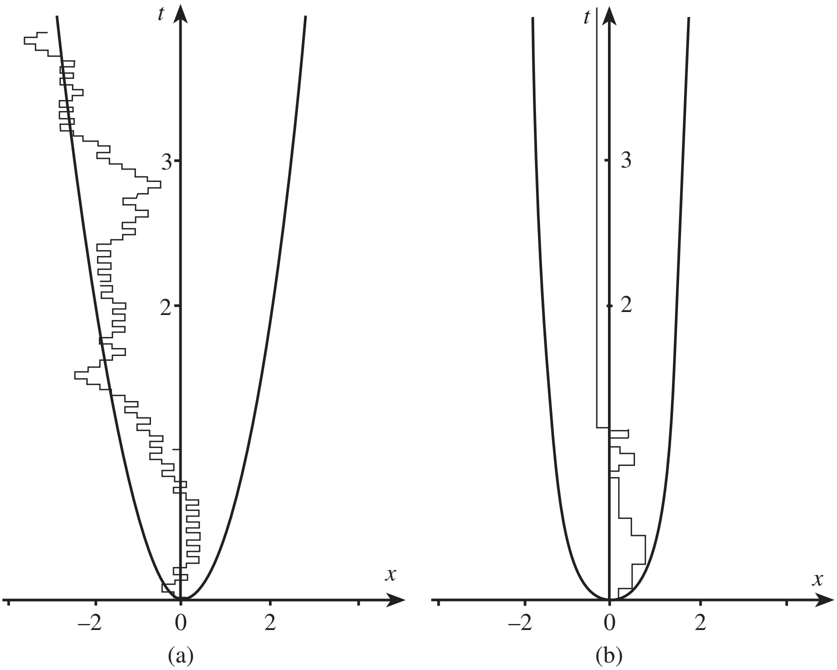

Figure 13.6 Random walk and CTRW.

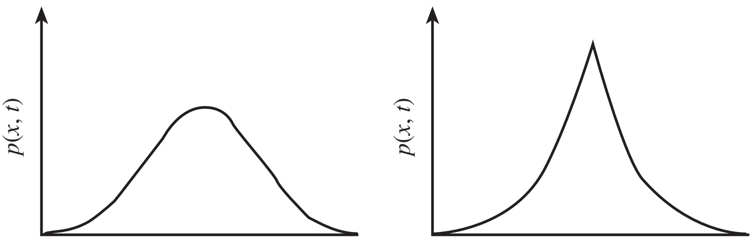

Figure 13.7 Probability distribution in random walk and CTRW.

the root mean square distance covered is $\sqrt{\langle r^2 \rangle} \propto t^{1/4}$ and the probability distribution $P\left(\overrightarrow{r}, t\right)$ behaves like the second curve in Figure 13.7, which has a cusp compared to a Gaussian [13, 22].

Fractional calculus has been successfully applied to the **anomalous diffusion** phenomenon with the **time fractional** form of the **diffusion equation** [Eq. (13.457)]:

$$\frac{\partial^\alpha P\left(\overrightarrow{r}, t\right)}{[\partial(t)]^\alpha} = k_\alpha \overrightarrow{\nabla}^2 P\left(\overrightarrow{r}, t\right), \tag{13.463}$$

where α is a real number.

13.9.3 Time Fractional Diffusion Equation

The time fractional diffusion equation with the **Riemann–Liouville** derivative is written as

$$\boxed{{}_0\mathbf{D}_t^{\alpha} u(x,t) = D_\alpha^2 \frac{\partial^2 u(x,t)}{\partial x^2}, \quad t>0, -\infty < x < \infty,\ 0<\alpha<1,} \tag{13.464}$$

where D_α is a constant with the appropriate units. Using the boundary conditions $\lim_{x\to\pm\infty} u(x,t) \to 0$ and ${}_0D_t^{\alpha-1}u(x,0) = \phi(x)$, we write the Fourier transform [Eqs. (13.391) and (13.392)] with respect to x and its inverse, respectively, as

$$\mathcal{F}\left\{{}_0\mathbf{D}_t^{\alpha} u(x,t)\right\} = D_\alpha^2 \mathcal{F}\left\{\frac{\partial^2 u(x,t)}{\partial x^2}\right\}, \tag{13.465}$$

$${}_0\mathbf{D}_t^{\alpha} \overline{u}(k,t) = -D_\alpha^2 k^2 \overline{u}(k,t), \tag{13.466}$$

where $\mathcal{F}\{u(x,t)\} = \overline{u}(k,t)$. We now take the Laplace transform [Eq. (13.255)] of Eq. (13.466) with respect to t to write the Fourier–Laplace transform of the solution as

$$\boxed{\tilde{\overline{u}}(k,s) = \frac{\overline{\phi}(k)}{s^\alpha + k^2 D_\alpha^2},} \tag{13.467}$$

where $\overline{\phi}(k) = \mathcal{F}\{{}_0\mathbf{D}_t^{\alpha-1}\overline{u}(k,0)\}$. Before we find the solution by inverting $\tilde{\overline{u}}(k,s)$, we evaluate the following useful Laplace transform [12]:

$$\mathcal{L}\left\{x^{\beta-1}E_{\alpha,\beta}(ax^\alpha)\right\} = \int_0^\infty e^{-sx} x^{\beta-1} E_{\alpha,\beta}(ax^\alpha)\,dx, \tag{13.468}$$

where $E_{\alpha,\beta}(x)$ is the **generalized Mittag–Leffler** function:

$$\boxed{E_{\alpha,\beta}(x) = \sum_{k=0}^{\infty} \frac{x^{\alpha k}}{\Gamma(ak+\beta)}.} \tag{13.469}$$

The Laplace transform in Eq. (13.468) can be evaluated as

$$\mathcal{L}\left\{x^{\beta-1}E_{\alpha,\beta}(ax^\alpha)\right\} = \int_0^\infty e^{-sx} x^{\beta-1} \left[\sum_{k=0}^{\infty} \frac{a^k x^{\alpha k}}{\Gamma(ak+\beta)}\right] dx \tag{13.470}$$

$$= \sum_{k=0}^{\infty} \frac{a^k}{\Gamma(ak+\beta)} \int_0^\infty e^{-sx} x^{\alpha k+\beta-1} dx, \tag{13.471}$$

$$\boxed{\mathcal{L}\left\{x^{\beta-1}E_{\alpha,\beta}(ax^\alpha)\right\} = \frac{s^{\alpha-\beta}}{s^\alpha - a}, \quad \operatorname{Re}\alpha,\ \operatorname{Re}\beta > 0,\ |as^{-\alpha}| < 1.} \tag{13.472}$$

For our case, $\alpha = \beta$ and $a = -k^2 D_\alpha^2$, hence we write the needed inverse Laplace transform as

$$\overline{u}(k,t) = \mathcal{L}^{-1}\left\{\tilde{\overline{u}}(k,s)\right\} = \overline{\phi}(k)\mathcal{L}^{-1}\left\{\frac{1}{s^\alpha + k^2 D_\alpha^2}\right\} \tag{13.473}$$

$$= \overline{\phi}(k)t^{\alpha-1}E_{\alpha,\alpha}(-k^2 D_\alpha^2 t^\alpha). \tag{13.474}$$

Finally, we find the inverse Fourier transform:

$$u(x,t) = \mathcal{F}^{-1}\left\{t^{\alpha-1}E_{\alpha,\alpha}(-k^2 D_\alpha^2 t^\alpha)\overline{\phi}(k)\right\} \tag{13.475}$$

$$= \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-ikx}t^{\alpha-1}E_{\alpha,\alpha}(-k^2 D_\alpha^2 t^\alpha)\overline{\phi}(k)dk, \tag{13.476}$$

and substitute $\overline{\phi}(k) = \int_{-\infty}^{\infty} e^{ikx'}\phi(x')dx'$ to write

$$u(x,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-ikx}t^{\alpha-1}E_{\alpha,\alpha}(-k^2 D_\alpha^2 t^\alpha)\left[\int_{-\infty}^{\infty} e^{ikx'}\phi(x')dx'\right]dk \tag{13.477}$$

$$= \frac{1}{2\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dkdx'\,t^{\alpha-1}E_{\alpha,\alpha}(-k^2 D_\alpha^2 t^\alpha)e^{-ik(x-x')}\phi(x'). \tag{13.478}$$

Since for even $f(k)$ we can use the identity

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-ikx}f(k)dk = \frac{1}{\pi}\int_0^{\infty}\cos(kx)f(k)dk, \tag{13.479}$$

we obtain the final solution as

$$\boxed{u(x,t) = \int_{-\infty}^{\infty} dx'\,\phi(x')G(x,x'),} \tag{13.480}$$

where $G(x,x')$ is given as

$$\boxed{G(x,x') = \frac{1}{\pi}\int_0^{\infty} dk t^{\alpha-1}E_{\alpha,\alpha}(-k^2 D_\alpha^2 t^\alpha)\cos k(x-x').} \tag{13.481}$$

13.9.4 Fractional Fokker–Planck Equations

In standard diffusion, particles move because of their random collisions with the molecules. However, there could also exist a deterministic force due to some external agent like gravity, external electromagnetic fields, etc. Effects of such forces can be included by taking the current density as

$$\vec{J}\left(\vec{r},t\right) = -k\vec{\nabla}P\left(\vec{r},t\right) + \mu\vec{F}(\vec{r})P\left(\vec{r},t\right), \tag{13.482}$$

where $\vec{F}(\vec{r}) = -\vec{\nabla}V(\vec{r})$ is the external force.

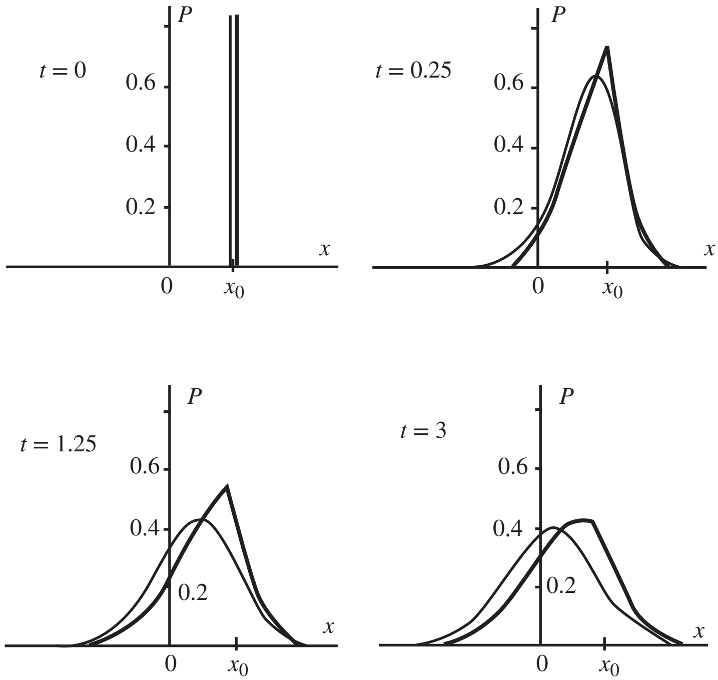

Figure 13.8 Evolution of the probability distribution with position *x* and time *t* in arbitrary units for the harmonic oscillator potential.

The diffusion equation now becomes

$$\frac{\partial P\left(\vec{r},t\right)}{\partial t} = \vec{\nabla}\cdot\left[k\vec{\nabla}P\left(\vec{r},t\right) - \mu\vec{F}(\vec{r})P\left(\vec{r},t\right)\right], \tag{13.483}$$

which is called the **Fokker–Planck equation**. If we consider particles moving under the influence of a harmonic oscillator potential, $V(x) = \frac{1}{2}bx^2$, the probability distribution for particles initially concentrated at some point x_0 is given as shown in Figure 13.8 by the thin curves. When we study the same phenomenon using the **time fractional** Fokker–Planck equation:

$$\frac{\partial^{\alpha}P\left(\vec{r},t\right)}{[\partial(t)]^{\alpha}} = \vec{\nabla}\cdot\left[k\vec{\nabla}P\left(\vec{r},t\right) - \mu\vec{F}(\vec{r})P\left(\vec{r},t\right)\right], \tag{13.484}$$

with $\alpha = 1/2$, the general behavior of the probability distribution looks like the thick curves in Figure 13.8. Both distributions become Gaussian for large times. However, for the fractional Fokker–Planck case, it not only takes longer but also initially it is very different from a Gaussian and shows CTRW characteristics [13, 22].

For the standard diffusion case the distribution is always a Gaussian. For the cases known as superdiffusive, $\alpha > 1$, use of the fractional derivatives in the Fokker–Planck equation and the diffusion equation are not restricted to time derivatives. Chaotic diffusion and Lévy processes, which relate far away points and regions are also active areas of research. In such cases, **Riesz derivative** [Eq. (13.437)] and **fractional Laplacian** [Eq. (13.445)] found wide spread use. Among other applications of fractional calculus, **image processing** is discussed in Sethares and Bayin [21] and applications to quantum mechanics and space fractional diffusion equation will be discussed in Chapter 19.

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Problems

1 Show that the following differintegral is valid for all q values:

$$\frac{d^q[x-a]^p}{[d(x-a)]^q} = \frac{\Gamma(p+1)[x-a]^{p-q}}{\Gamma(p-q+1)}, \quad p > -1.$$

2 Derive the following formula:

$$\frac{d^q[1-x]^p}{[d(x-a)]^q} = \frac{(1-x)^{p-q}}{\Gamma(-q)} B_x(-q, q-p), \ -1 < x < 1.$$

3 Show that the differintegral of an exponential function is given as

$$\frac{d^q \exp(\pm x)}{dx^q} = \frac{\exp(\pm x)}{x^q} \gamma^*(-q, \pm x).$$

4 Show that the upper limit $(n-1)$ in the summation

$$£\left\{\frac{d^n f}{dx^n}\right\} = s^n £\{f\} - \sum_{k=0}^{n-1} s^k \frac{d^{n-1-k} f}{dx^{n-1-k}}(0), \quad n = 0, \pm 1, \pm 2, \pm 3 \dots,$$

can be replaced by any number greater than $n-1$.

5 Show that the solution of the following extraordinary differential equation:

$$\frac{df}{dx} + \frac{d^{1/2}f}{dx^{1/2}} - 2f = 0,$$

is given as

$$f(x) = \frac{C}{3}(2\exp(4x)\ \text{erfc}\ (2\sqrt{x}) + \exp(x)\ \text{erfc}(-\sqrt{x})),$$

where $\text{erfc}(x) = 1 - \text{erf}(x)$.

6 Show the integral

$$\int_0^1 \sin\left(\sqrt{1-t^2}\right) dt = 0.69123$$

by using differintegrals.

7 Using both the Riemann–Liouville and the Caputo definitions of the fractional derivative find the solutions of the fractional evolution equation:

$$\left(\frac{d^q x(t)}{dt^q}\right)_{R\text{–}L \text{ or } C} = \alpha_0 x(t), \quad 0 < q \leq 1.$$

8 Compare the solutions of the anomalous diffusion equation:

$$\left(\frac{\partial^q C(x,t)}{\partial t^q}\right)_{R\text{–}L \text{ or } C} = -D_0 \frac{\partial^2 C(x,t)}{\partial x^2}, \quad 0 < q \leq 1,$$

found by the Riemann–Liouville and the Caputo definitions of the fractional derivative.

9 Show the following differintegral:

$$\frac{d^q \exp(c_0 - c_1 x)}{[d(x-a)]^q} = \frac{\exp(c_0 - c_1 x)}{[x-a]^q} \gamma^*(-q, -c_1(x-a)).$$

10 Using the relation $\Psi(1-n)/\Gamma(1-n) = (-1)^n \Gamma(n)$, show that the following differintegral of $1/x$:

$$\frac{d^q(1/x)}{[d(x-1)]^q} = \frac{x^{-(q+1)}}{\Gamma(-q)}[\ln x - \gamma - \Psi(-q)]$$
$$+ \sum_{l=1}^{\infty} (x-1)^{-(q+1+l)} \frac{[\gamma + \Psi(1+l)]}{\Gamma(-q-l)l!},$$

reduces to the usual results for the integer values of q. For the negative integer values of q show only for the first three values: $q = -1, -2, -3$.

11 Verify the Fourier transform used in the definition of the Riesz fractional integral: $\mathcal{F}\{h_+(t)\} = (i\omega)^{-q}, 0 < q < 1$, where

$$h_+(t) = \begin{cases} \frac{t^{q-1}}{\Gamma(q)}, & t > 0, \\ 0, & t \leq 0, \end{cases}$$

by using complex contour integration.

12 Using complex contour integration show that the Fourier transform of $h_-(t)$:

$$h_-(t) = \begin{cases} 0, & t \geq 0, \\ \frac{(-t)^{q-1}}{\Gamma(q)}, & t < 0, \end{cases}$$

which is used in the definition of the Riesz fractional integral, is given as $\mathcal{F}\{h_-(t)\} = (-i\omega)^{-q}, 0 < q < 1$.

13 Justify equation

$$\mathcal{F}\left\{{}_{\infty}\mathbf{D}_t^q g(t)\right\} = (-i\omega)^q G(\omega), \quad q > 0,$$

by using complex contour integration. Also show that the Riemann–Liouville, Grünwald, and the Caputo definitions of the fractional derivative agree.

14 Show that for real ω the following Fourier transform:

$$\mathcal{F}\left\{\left[{}_{-\infty}\mathbf{D}_t^q + {}_{\infty}\mathbf{D}_t^q\right] g(t)\right\} = \left[(i\omega)^q + (-i\omega)^q\right] G(\omega)$$

can be written as

$$\mathcal{F}\left\{\left[{}_{-\infty}\mathbf{D}_t^q + {}_{\infty}\mathbf{D}_t^q\right] g(t)\right\} = \left(2\cos\frac{q\pi}{2}\right) |\omega|^q G(\omega).$$

15 Show that the solution of the following fractional integral equation:

$$N(t) - N_0 t^{\mu-1} = \tau^{\nu}\ {}_0D_t^{-\nu} N(t), \quad \nu,\ \mu > 0,$$

with the initial condition $N(0) = N_0$, is given in terms of the generalized Mittag–Leffler function: $E_{\alpha,\beta}(x) = \sum_{n=0}^{\infty} x^n/\Gamma(\alpha n + \beta)$.

16 Show that the inverse Laplace transform

$$\mathcal{L}^{-1}\left\{\frac{s^{-1}}{1 - as^{-\alpha}}\right\},$$

where a is a constant, is the Mittag–Leffler function.

17 Evaluate the following inverse Laplace transform:

$$\mathcal{L}^{-1}\left\{\frac{s^{-2}}{1+\omega^2 s^{-\alpha}}\right\}.$$

18 **Fractional harmonic oscillator**: Introducing fractional calculus into a given branch of science is usually straight forward. One simply replaces the time or the space derivatives in the equation of motion by their fractional counterparts. For example, for the classical harmonic oscillator we can replace

$$\frac{d^2x(t)}{dt^2} + \omega_0^2 x(t) = 0, \quad \omega_0^2 = \frac{k}{m_0},$$

with

$$\left(\frac{d^\alpha x(t)}{dt^\alpha}\right)_{R-L \text{ or } C} + \omega_0^2 x(t) = 0, \quad 1 < \alpha \leq 2.$$

i) Find the solution of the above fractional differential equation for the $R-L$ and the Caputo derivatives and discuss the boundary conditions.
ii) Discuss the general nature of the solution. Try plotting [4].

19 Show that a second representation of the Riesz derivative can be given as

$$\mathbf{R}_t^q g(t) = \frac{\Gamma(1+q)\sin q\pi/2}{\pi}\int_0^\infty \frac{g(t+\xi)-2g(t)+g(t-\xi)}{\xi^{1+q}}d\xi,$$

for $0 < q < 1$ [3].

14

Infinite Series

In physics and engineering, sometimes physical properties can only be expressed in terms of infinite sums. We also frequently encounter differential or integral equations that can only be solved by the method of infinite series. In working with infinite series, the first thing that needs to be checked is their convergence. In this regard, we start by introducing the commonly used tests of convergence for series of numbers and then extend our discussion to series of functions and power series. We then introduce some analytic techniques for evaluating infinite sums. We also discuss asymptotic series and the method of steepest descent and saddle-point integrals. We also introduce the Padé approximants, which is a very effective tool in finding sums of series whose only a few terms are known. Infinite products, which are closely related to infinite series, are also discussed in this chapter. In conjunction with the Casimir effect, we show how finite and meaningful results can be obtained from some of the divergent series in physics by the method of regularization and renormalization.

14.1 Convergence of Infinite Series

We write an infinite series with the general term a_n as

$$\sum_{n=1}^{\infty} a_n = a_1 + a_2 + \cdots. \tag{14.1}$$

Summation of the first N terms is called the Nth **partial sum** of the series. If the Nth partial sum of a series has the limit

$$\lim_{N\to\infty} \sum_{n=1}^{N} a_n \to S, \tag{14.2}$$

Mathematical Methods in Science and Engineering, Second Edition. Selçuk Ş. Bayın.

we say the series is **convergent** and write the infinite series as

$$\sum_{n=1}^{\infty} a_n = S. \tag{14.3}$$

If S is infinity, we say the series is **divergent**. When a series is not convergent, it is divergent. The nth term of a convergent series always satisfies the limit

$$\lim_{n\to\infty} a_n \to 0. \tag{14.4}$$

However, the converse is not true.

Example 14.1 ***Harmonic series***
Even though the nth term of the harmonic series :

$$\sum_{n=1}^{\infty} a_n, \quad a_n = \frac{1}{n}, \tag{14.5}$$

goes to zero as $n \to \infty$, the series diverges.

14.2 Absolute Convergence

If the series constructed by taking the absolute values of the terms of a given series:

$$\sum_{n=1}^{\infty} |a_n|, \tag{14.6}$$

is convergent, then we say the series is **absolutely convergent**. An absolutely convergent series is also convergent, but the converse is not true. Series that are convergent but not absolutely convergent are called **conditionally convergent**. In working with series, absolute convergence is a very important property.

Example 14.2 ***Conditionally convergent series***
The series

$$1 - \frac{1}{2} + \frac{1}{3} - \cdots = \sum_{n=1}^{\infty} (-1)^{n+1}\frac{1}{n} \tag{14.7}$$

converges to $\ln 2$. However, since it is not absolutely convergent, it is only conditionally convergent.

14.3 Convergence Tests

There exist a number of tests for checking the convergence of a given series. In what follows we give some of the most commonly used tests for convergence.

The tests are ordered in increasing level of complexity. In practice, one starts with the simplest test and, if the test fails, moves on to the next one. In the following tests, we either consider series with positive terms or take the absolute value of the terms; hence we check for **absolute convergence**.

14.3.1 Comparison Test

The simplest test for convergence is the **comparison test**. We compare a given series term by term with another series, the convergence or divergence of which has been established. Let two series with the general terms a_n and b_n be given. For all $n \geq 1$, if $|a_n| \leq |b_n|$ is true and if the series $\sum_{n=1}^{\infty} |b_n|$ is convergent, then the series $\sum_{n=1}^{\infty} a_n$ is also convergent. Similarly, if $\sum_{n=1}^{\infty} a_n$ is divergent, then the series $\sum_{n=1}^{\infty} |b_n|$ is also divergent.

Example 14.3 ***Comparison test***
Consider the series with the general term $a_n = n^{-p}$, where $p = 0.999$. We compare this series with the harmonic series which has the general term $b_n = n^{-1}$. Since for $n \geq 1$, we can write $n^{-1} < n^{-0.999}$ and since the harmonic series is divergent, we also conclude that the series $\sum_{n=1}^{\infty} n^{-p}$ is divergent.

14.3.2 Ratio Test

For the series $\sum_{n=1}^{\infty} a_n$, let $a_n \neq 0$ for all $n \geq 1$. When we find the limit

$$\lim_{n\to\infty} \left| \frac{a_{n+1}}{a_n} \right| = r, \tag{14.8}$$

for $r < 1$, the series is convergent; for $r > 1$, the series is divergent; and for $r = 1$, the test is inconclusive.

14.3.3 Cauchy Root Test

For the series $\sum_{n=1}^{\infty} a_n$, when we find the limit

$$\lim_{n\to\infty} \sqrt[n]{|a_n|} = l, \tag{14.9}$$

for $l < 1$, the series is convergent; for $l > 1$, the series is divergent; and for $l = 1$, the test is inconclusive.

14.3.4 Integral Test

Let $a_n = f(n)$ be the general term of a given series with positive terms. If for $n > 1, f(n)$ is continuous and a monotonic decreasing function, that is, $f(n + 1) < f(n)$, then the series converges or diverges with the integral

$$\int_1^{\infty} f(x)dx. \tag{14.10}$$

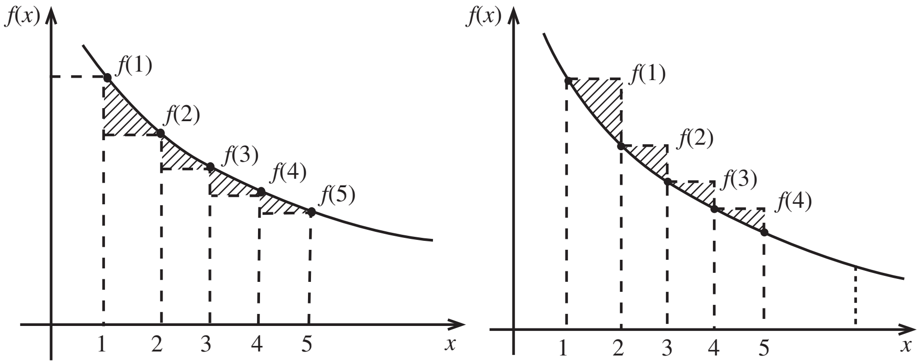

Figure 14.1 Integral test.

Proof: As shown in Figure 14.1, we can put a lower and an upper bound to the series $\sum_{n=1}^{\infty} a_n$ as

$$\int_1^{N+1} f(x)dx < \sum_{n=1}^{N} a_n, \tag{14.11}$$

$$\sum_{n=1}^{N} a_n < \int_1^{N} f(x)dx + a_1. \tag{14.12}$$

From here it is apparent that in the limit as $N \to \infty$, if the integral $\int_1^N f(x)dx$ is finite, then the series $\sum_{n=1}^{\infty} a_n$ is convergent. If the integral diverges, then the series also diverges.

Example 14.4 ***Integral test***

Let us consider the Riemann zeta function

$$\xi(s) = 1 + \frac{1}{2^s} + \frac{1}{3^s} + \cdots. \tag{14.13}$$

To use the ratio test, we make use of the binomial formula and write

$$\frac{a_{n+1}}{a_n} = \left(\frac{n}{n+1}\right)^s = \left(1 + \frac{1}{n}\right)^{-s} \tag{14.14}$$

$$\simeq 1 - \frac{s}{n} + \cdots. \tag{14.15}$$

In the limit as $n \to \infty$, this gives $\frac{a_{n+1}}{a_n} \to 1$; thus the ratio test fails. However, using the integral test, we find

$$\int_1^{\infty} \frac{dx}{x^s} = \left.\frac{x^{-s+1}}{-s+1}\right|_1^{\infty} = \begin{cases} 1/(s-1), & s > 1, \Rightarrow \text{ series is convergent,} \\ \infty, & s < 1 \Rightarrow \text{ series is divergent.} \end{cases} \tag{14.16}$$

14.3.5 Raabe Test

For a series with positive terms, $a_n > 0$, when we find the limit

$$\lim_{n\to\infty} n\left(\frac{a_n}{a_{n+1}} - 1\right) = m, \tag{14.17}$$

for $m > 1$, the series is convergent and for $m < 1$, the series is divergent. For $m = 1$, the Raabe test is inconclusive.

The Raabe test can also be expressed as follows: Let N be a positive integer independent of n. For all $n \geq N$, if

$$n\left(\frac{a_n}{a_{n+1}} - 1\right) \geq P > 1 \tag{14.18}$$

is true, then the series is convergent and if

$$n\left(\frac{a_n}{a_{n+1}} - 1\right) \leq 1 \tag{14.19}$$

is true, then the series is divergent.

Example 14.5 ***Raabe test***
For the series $\sum_{n=1}^{\infty} 1/n^2$, the ratio test is inconclusive. However, using the Raabe test, we see that it converges:

$$\lim_{n\to\infty} n\left(\frac{a_n}{a_{n+1}} - 1\right) = \lim_{n\to\infty} n\left(\frac{(n+1)^2}{n^2} - 1\right) \tag{14.20}$$

$$= \lim_{n\to\infty}\left(2 + \frac{1}{n}\right) = 2 > 1. \tag{14.21}$$

Example 14.6 ***Raabe test***
The second form of the Raabe test shows that the harmonic series $\sum_{n=1}^{\infty} 1/n$ is divergent. This follows from the fact that for all n values,

$$n\left(\frac{a_n}{a_{n+1}} - 1\right) = n\left(\frac{n+1}{n} - 1\right) = 1. \tag{14.22}$$

When the available tests fail, we can also use theorems like the Cauchy theorem.

14.3.6 Cauchy Theorem

A given series, $\sum_{n=1}^{\infty} a_n$, with positive decreasing terms, $a_n \geq a_{n+1} \geq \cdots \geq 0$, converges or diverges with the series

$$\sum_{n=1}^{\infty} c^n a_{c^n} = ca_c + c^2 a_{c^2} + c^3 a_{c^3} + \cdots, \quad c \text{ an integer}. \tag{14.23}$$

Example 14.7 ***Cauchy theorem***
Let us check the convergence of the series

$$\frac{1}{2\ln^{\alpha}2}+\frac{1}{3\ln^{\alpha}3}+\frac{1}{4\ln^{\alpha}4}+\cdots=\sum_{n=2}^{\infty}\frac{1}{n\ln^{\alpha}n}, \tag{14.24}$$

using the Cauchy theorem for $\alpha \geq 0$. Choosing the value of c as 2, we construct the series $\sum_{n=1}^{\infty} 2^n a_{2^n} = 2a_2 + 4a_4 + 8a_8 + \cdots$, where the general term is given as

$$2^k a_{2^k} = 2^k \frac{1}{2^k \ln^{\alpha} 2^k} = \left(\frac{1}{\ln^{\alpha} 2}\right)\frac{1}{k^{\alpha}}. \tag{14.25}$$

Since the series

$$\frac{1}{\ln^{\alpha}2}\sum_{n=1}^{\infty}\frac{1}{n^{\alpha}}$$

converges for $\alpha > 1$, our series is also convergent for $\alpha > 1$. On the other hand, for $\alpha \leq 1$, both series are divergent.

14.3.7 Gauss Test and Legendre Series

Legendre series are given as

$$\sum_{n=0}^{\infty} a_{2n}x^{2n} \text{ and } \sum_{n=0}^{\infty} a_{2n+1}x^{2n+1}, \; x \in [-1,1], \tag{14.26}$$

where both series have the same recursion relation:

$$a_{n+2} = a_n \frac{(n-l)(l+n+1)}{(n+1)(n+2)}, \quad n = 0, 1, \ldots . \tag{14.27}$$

For $|x| < 1$, the convergence of both series can be established using the ratio test. For the even series, the general term is given as $u_n = a_{2n}x^{2n}$; hence we write the ratio

$$\frac{u_{n+1}}{u_n} = \frac{a_{2(n+1)}x^{2(n+1)}}{a_{2n}x^{2n}} = \frac{(2n-l)(2n+l+1)x^2}{(2n+1)(2n+2)}, \tag{14.28}$$

$$\lim_{n\to\infty}\left|\frac{u_{n+1}}{u_n}\right| = x^2. \tag{14.29}$$

Using the ratio test, we conclude that the Legendre series with the even terms is convergent for the interval $x \in (-1, 1)$. The argument and the conclusion for the other series are exactly the same. However, at the end points, the ratio test fails. For these points, we can use the Gauss test:

Gauss test:

Let $\sum_{n=0}^{\infty} u_n$ be a series with positive terms. If for $n \geq N$, where N is a given constant, we can write

$$\frac{u_n}{u_{n+1}} \simeq 1 + \frac{\mu}{n} + 0\left(\frac{1}{n^i}\right), \quad i > 0, \tag{14.30}$$

where $0\,(1/n^i)$ means that for a given function $f(n)$, the $\lim_{n\to\infty}\{f(n)/(n^i)\}$ is finite, then the series $\sum_{n=0}^{\infty} u_n$ converges for $\mu > 1$ and diverges for $\mu \leq 1$. Note that there is no case here where the test fails.

Example 14.8 ***Legendre series***
We now investigate the convergence of the Legendre series at the end points, $x = \pm 1$, using the Gauss test. We find the required ratio as

$$\frac{u_n}{u_{n+1}} = \frac{(2n+1)(2n+2)}{(2n-l)(2n+l+1)} = \frac{4n^2+6n+2}{4n^2+2n-l(l+1)} \tag{14.31}$$

$$\simeq 1 + \frac{1}{n} + \frac{l(l+1)(1+n)}{[4n^2+2n-l(l+1)]n}. \tag{14.32}$$

From the limit,

$$\lim_{n\to\infty} \frac{l(l+1)(1+n)}{[4n^2+2n-l(l+1)]n} \bigg/ \left(\frac{1}{n^2}\right) = \frac{l(l+1)}{4}, \tag{14.33}$$

we see that this ratio is constant and goes as $O(1/n^2)$. Since $\mu = 1$ in $\frac{u_n}{u_{n+1}}$, we conclude that the Legendre series, both the even and the odd series, diverge at the end points.

Example 14.9 ***Chebyshev series***
The Chebyshev equation is given as

$$(1-x^2)\frac{d^2y}{dx^2} - x\frac{dy}{dx} + n^2 y = 0. \tag{14.34}$$

Let us find finite solutions of this equation in the interval $x \in [-1, 1]$ using the Frobenius method. We substitute the following series and its derivatives into the Chebyshev equation:

$$y = \sum_{k=0}^{\infty} a_k x^{k+\alpha}, \tag{14.35}$$

$$y' = \sum_{k=0}^{\infty} a_k (k+\alpha) x^{k+\alpha-1}, \tag{14.36}$$

$$y'' = \sum_{k=0}^{\infty} a_k (k+\alpha)(k+\alpha-1) x^{k+\alpha-2}, \tag{14.37}$$

to get

$$\sum_{k=0}^{\infty} a_k (k+\alpha)(k+\alpha-1) x^{k+\alpha-2} - \sum_{k=0}^{\infty} a_k (k+\alpha)(k+\alpha-1) x^{k+\alpha} - \sum_{k=0}^{\infty} a_k (k+\alpha) x^{k+\alpha} + n^2 \sum_{k=0}^{\infty} a_k x^{k+\alpha} = 0. \tag{14.38}$$

After rearranging, we first get

$$a_0\alpha(\alpha-1)x^{\alpha-2}+a_1\alpha(\alpha+1)x^{\alpha-1}+\sum_{k=2}^{\infty}a_k(k+\alpha)(k+\alpha-1)x^{k+\alpha-2}$$
$$+\sum_{k=0}^{\infty}a_kx^{k+\alpha}[n^2-(k+\alpha)^2]=0 \tag{14.39}$$

and then

$$a_0\alpha(\alpha-1)x^{\alpha-2}+a_1\alpha(\alpha+1)x^{\alpha-1}+\sum_{k=0}^{\infty}a_{k+2}(k+\alpha+2)(k+\alpha+1)x^{k+\alpha}$$
$$+\sum_{k=0}^{\infty}a_kx^{k+\alpha}[n^2-(k+\alpha)^2]=0. \tag{14.40}$$

This gives the indicial equation as

$$a_0\alpha(\alpha-1)=0,\quad a_0\neq 0. \tag{14.41}$$

The remaining coefficients are determined by

$$a_1\alpha(\alpha+1)=0 \tag{14.42}$$

and the recursion relation:

$$a_{k+2}=\frac{(k+\alpha)^2-n^2}{(k+\alpha+2)(k+\alpha+1)}a_k,\quad k=0,1,2,\ldots. \tag{14.43}$$

Since $a_0\neq 0$, roots of the indicial equation are 0 and 1. Choosing the smaller root gives the general solution with the recursion relation

$$a_{k+2}=\frac{k^2-n^2}{(k+2)(k+1)}a_k \tag{14.44}$$

and the series solution of the Chebyshev equation is obtained as

$$y(x)=a_0\left(1-\frac{n^2}{2}x^2-\frac{n^2(2^2-n^2)}{4\cdot 3\cdot 2}x^4-\cdots\right)$$
$$+a_1\left(x+\frac{(1-n^2)}{3\cdot 2}x^3+\frac{(3^2-n^2)(1-n^2)}{5\cdot 4\cdot 3\cdot 2}x^5+\cdots\right). \tag{14.45}$$

We now investigate the convergence of these series. Since the argument for both series is the same, we study the series with the general term $u_k=a_{2k}x^{2k}$ and write

$$\left|\frac{u_{k+1}}{u_k}\right|=\left|\frac{a_{2k+2}x^{2k+2}}{a_{2k}x^{2k}}\right|=\left|\frac{a_{2k+2}}{a_{2k}}\right|x^2. \tag{14.46}$$

This gives the limit

$$\lim_{k\to\infty}\left|\frac{a_{2k+2}}{a_{2k}}\right|x^2=x^2. \tag{14.47}$$

Using the ratio test, it is clear that this series converges for the interval $(-1, 1)$. However, at the end points, the ratio test fails, where we now use the Raabe test. We first evaluate the ratio

$$\lim_{k\to\infty} k\left[\frac{a_{2k}}{a_{2k+2}} - 1\right] = \lim_{k\to\infty} k\left[\frac{(2k+2)(2k+1)}{(2k)^2 - n^2} - 1\right] \tag{14.48}$$

$$= \lim_{k\to\infty} k\left[\frac{6k+2+n^2}{(2k)^2 - n^2}\right] = \frac{3}{2} > 1, \tag{14.49}$$

which indicates that the series is convergent at the end points as well. This means that for the polynomial solutions of the Chebyshev equation, restricting n to integer values is an additional assumption, which is not required by the finite solution condition at the end points. The same conclusion is also valid for the series with the odd powers.

14.3.8 Alternating Series

For a given series of the form $\sum_{n=1}^{\infty}(-1)^{n+1}a_n$, if a_n is positive for all n, then the series is called an **alternating series**. In an alternating series for sufficiently large values of n, if a_n is monotonic decreasing or constant and the limit as $n \to \infty$, $a_n \to 0$ is true, then the series is convergent. This is also known as the **Leibniz rule**.

Example 14.10 ***Leibniz rule***
In the alternating series,

$$\sum_{n=1}^{\infty}(-1)^{n+1}\frac{1}{n} = 1 - \frac{1}{2} + \frac{1}{3} - \frac{1}{4} + \cdots, \tag{14.50}$$

since $\frac{1}{n} > 0$ and $\frac{1}{n} \to 0$ as $n \to \infty$, the series is convergent.

14.4 Algebra of Series

Absolute convergence is very important in working with series. It is only for absolutely convergent series that ordinary algebraic manipulations like addition, subtraction, multiplication, etc., can be done without problems:

1. An absolutely convergent series can be rearranged without affecting the sum.
2. Two absolutely convergent series can be multiplied. The result is another absolutely convergent series, which converges to the product of the individual series sums.

All these operations that look very natural, when applied to conditionally convergent series may lead to erroneous results.

Example 14.11 ***Conditionally convergent series***
The following conditionally convergent series:

$$\sum_{n=1}^{\infty} (-1)^{n+1}\frac{1}{n} = 1 - \frac{1}{2} + \frac{1}{3} - \frac{1}{4} + \cdots \tag{14.51}$$

$$= 1 - \left(\frac{1}{2} - \frac{1}{3}\right) - \left(\frac{1}{4} - \frac{1}{5}\right) - \cdots \tag{14.52}$$

$$= 1 - 0.167 - 0.05 - \cdots, \tag{14.53}$$

obviously converges to some number less than one, actually to ln 2 or 0.693. We now rearrange this sum as

$$\left(1 + \frac{1}{3} + \frac{1}{5}\right) - \left(\frac{1}{2}\right) + \left(\frac{1}{7} + \frac{1}{9} + \frac{1}{11} + \frac{1}{13} + \frac{1}{15}\right) - \left(\frac{1}{4}\right)$$
$$+ \left(\frac{1}{17} + \cdots + \frac{1}{25}\right) - \left(\frac{1}{6}\right) + \left(\frac{1}{27} + \cdots + \frac{1}{35}\right) - \left(\frac{1}{8}\right) + \cdots, \tag{14.54}$$

and consider each term in parenthesis as the terms of a new series. Partial sums of this new series are

$$\begin{aligned} s_1 &= 1.5333, & s_2 &= 1.0333, \\ s_3 &= 1.5218, & s_4 &= 1.2718, \\ s_5 &= 1.5143, & s_6 &= 1.3476, \cdots. \\ s_7 &= 1.5103, & s_8 &= 1.3853, \\ s_9 &= 1.5078, & s_{10} &= 1.4078, \end{aligned} \tag{14.55}$$

It is now seen that this alternating series added in this order converges to 3/2. What we have done is very simple. First, we added positive terms until the partial sum was equal or just above 3/2 and then subtracted negative terms until the partial sum fell just below 3/2. In this process, we have neither added nor subtracted anything from the series; we have simply added its terms in a different order. By a suitable arrangement of its terms, a conditionally convergent series can be made to converge to any desired value or even to diverge. This result is also known as the **Riemann theorem**.

14.4.1 Rearrangement of Series

Let us write the partial sum of a double series as $\sum_{i=1}^{n}\sum_{j=1}^{m} a_{ij} = s_{nm}$. If the limit $s_{nm} \to s$ as $(n, m) \to \infty$ exists, then we can write $\sum_{i=1}^{\infty}\sum_{j=1}^{\infty} a_{ij} = s$ and say that the double series, $\sum_{i,j=1}^{\infty} a_{ij}$, is convergent and converges to s. When a double series, $\sum_{i=0}^{\infty}\sum_{j=0}^{\infty} a_{ij}$, converges absolutely, that is, when $\sum_{i=0}^{\infty}\sum_{j=0}^{\infty}|a_{ij}|$ is convergent, then we can rearrange its terms without affecting the sum. For example, consider the double series $\sum_{i=0}^{\infty}\sum_{j=0}^{\infty} a_{ij}$ and define new dummy variables q and p as $i = q \geq 0$ and $j = p - q \geq 0$. Now the sum becomes

$$\sum_{i=0}^{\infty}\sum_{j=0}^{\infty} a_{ij} = \sum_{p=0}^{\infty}\sum_{q=0}^{p} a_{q(p-q)}, \tag{14.56}$$

$$\begin{aligned} & a_{00} + a_{01} + a_{02} + \cdots \\ & + a_{10} + a_{11} + a_{12} + \cdots \\ & + a_{20} + a_{21} + a_{22} + \cdots \\ & \vdots \\ & = a_{00} \\ & + a_{01} + a_{10} \\ & + a_{02} + a_{11} + a_{20} \\ & + a_{03} + a_{12} + a_{21} + a_{30} \\ & \vdots \end{aligned} \tag{14.57}$$

Another rearrangement can be obtained by the definitions $i = s \geq 0$ and $j = r - 2s \geq 0$, s $\leq \frac{r}{2}$, as

$$\sum_{i=0}^{\infty}\sum_{j=0}^{\infty} a_{ij} = \sum_{r=0}^{\infty}\sum_{s=0}^{[r/2]} a_{s,r-2s} = (a_{00}) + (a_{01}) + (a_{02} + a_{10}) + (a_{03} + a_{11}) + \cdots. \tag{14.58}$$

14.5 Useful Inequalities About Series

For the following useful inequalities about series, we take $\frac{1}{p} + \frac{1}{q} = 1$:

Hölder's Inequality: If $a_n \geq 0$, $b_n \geq 0$, $p > 1$, then

$$\sum_{n=1}^{\infty} a_n b_n \leq \left(\sum_{n=1}^{\infty} a_n^p\right)^{1/p} \cdot \left(\sum_{n=1}^{\infty} b_n^q\right)^{1/q}. \tag{14.59}$$

Minkowski's Inequality: If $a_n \geq 0$, $b_n \geq 0$, and $p \geq 1$, then

$$\left[\sum_{n=1}^{\infty} (a_n + b_n)^p\right]^{1/p} \leq \left(\sum_{n=1}^{\infty} a_n^p\right)^{1/p} + \left(\sum_{n=1}^{\infty} b_n^p\right)^{1/p}. \tag{14.60}$$

Schwarz–Cauchy Inequality: If $a_n \geq 0$ and $b_n \geq 0$, then

$$\left(\sum_{n=1}^{\infty} a_n b_n\right)^2 \leq \left(\sum_{n=1}^{\infty} a_n^2\right) \cdot \left(\sum_{n=1}^{\infty} b_n^2\right). \tag{14.61}$$

Thus, if the series $\sum_{n=1}^{\infty} a_n^2$ and $\sum_{n=1}^{\infty} b_n^2$ converges, then the series $\sum_{n=1}^{\infty} a_n b_n$ also converges.

14.6 Series of Functions

We can also define series of functions with the general term $u_n = u_n(x)$. In this case, partial sums, S_n, are also functions of x :

$$S_n(x) = u_1(x) + u_2(x) + \cdots + u_n(x). \tag{14.62}$$

If the limit $S_n(x) \to S(x)$ as $n \to \infty$ is true, then we can write $\sum_{n=1}^{\infty} u_n(x) = S(x)$. In studying the properties of series of functions, we need a new concept called the **uniform convergence**.

14.6.1 Uniform Convergence

For a given positive small number ε, if there exists a number N independent of x for $x \in [a, b]$, and if for all $n \geq N$, we can say the inequality

$$|s(x) - s_n(x)| < \varepsilon \tag{14.63}$$

is true, then the series with the general term $u_n(x)$ is uniformly convergent in the interval $[a, b]$. This also means that for a uniformly convergent series, for a given error margin, ε, we can always find a number N independent of x such that the remainder of the series: $\left|\sum_{i=N+1}^{\infty} u_i(x)\right|$, is always less than ε for all x in the interval $[a, b]$. Uniform convergence can also be shown as in Figure 14.2.

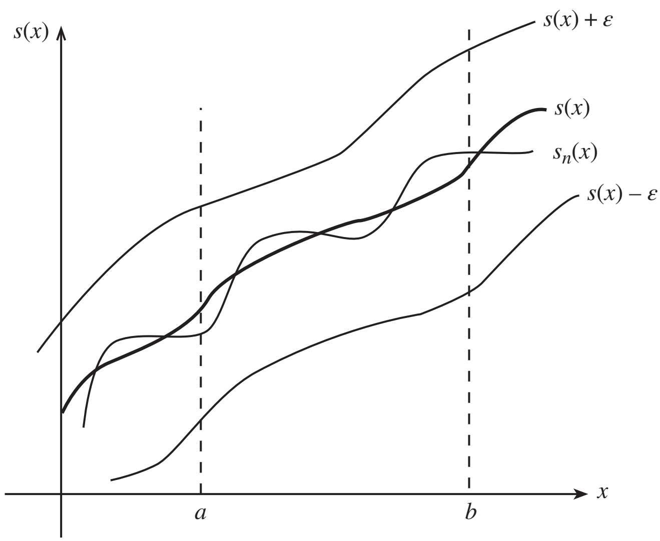

Figure 14.2 Uniform convergence is very important.

14.6.2 Weierstrass M-Test

For uniform convergence, the most commonly used test is the **Weierstrass M-test** or in short the **M-test**: Let us say that we found a series of numbers $\sum_{i=1}^{\infty} M_i$, such that for all x in $[a, b]$ the inequality $M_i \geq |u_i(x)|$ is true. Then the uniform convergence of the series of functions $\sum_{i=1}^{\infty} u_i(x)$, in the interval $[a, b]$, follows from the convergence of the series of numbers $\sum_{i=1}^{\infty} M_i$. Note that because the absolute values of $u_i(x)$ are taken, the M-test also checks absolute convergence. However, it should be noted that absolute convergence and uniform convergence are two independent concepts and neither of them implies the other.

Example 14.12 ***M-test***
The following series are uniformly convergent, but not absolutely convergent:

$$\sum_{n=1}^{\infty} \frac{(-1)^n}{n + x^4}, \quad -\infty < x < \infty, \tag{14.64}$$

$$\sum_{n=1}^{\infty} (-1)^{n-1} \frac{x^n}{n} = \ln(1 + x), \quad 0 \leq x \leq 1, \tag{14.65}$$

while the series, the so-called **Riemann zeta function**:

$$\zeta(x) = \frac{1}{1^x} + \frac{1}{2^x} + \cdots + \frac{1}{n^x} + \cdots \tag{14.66}$$

converges uniformly and absolutely in the interval $[a, \infty)$, where a is any number greater than 1. Because the M-test checks for uniform and absolute convergence together, for conditionally convergent series, we can use the **Abel test**.

14.6.3 Abel Test

Let a series with the general term $u_n(x) = a_n f_n(x)$ be given. If the series of numbers $\sum a_n = A$ is convergent and if the functions $f_n(x)$ are bounded, $0 \leq f_n(x) \leq M$, and monotonic decreasing, $f_{n+1}(x) \leq f_n(x)$, in the interval $[a, b]$, then the series $\sum u_n(x)$ is uniformly convergent in $[a, b]$.

Example 14.13 ***Uniform convergence***
The series

$$\sum_{n=0}^{\infty} (1 - x)x^n = \begin{cases} 1, & 0 \leq x < 1, \\ 0, & x = 1, \end{cases} \tag{14.67}$$

is absolutely convergent but not uniformly convergent in $[0, 1]$.

From the definition of uniform convergence, it is clear that any series $f(x) = \sum_{n=1}^{\infty} u_n(x)$, where all $u_n(x)$ are continuous functions, cannot be uniformly convergent in any interval containing a discontinuity of $f(x)$.

14.6.4 Properties of Uniformly Convergent Series

For a uniformly convergent series, the following are true:

1. If $u_n(x)$ for all n are continuous, then the series $f(x) = \sum_{n=1}^{\infty} u_n(x)$ is also continuous.
2. Provided $u_n(x)$ are continuous for all n in $[a, b]$, then the series can be integrated as
$$\int_a^b f(x)dx = \int_a^b dx \left[\sum_{n=1}^{\infty} u_n(x)\right] = \sum_{n=1}^{\infty} \int_a^b u_n(x)dx, \tag{14.68}$$
where the integral sign can be interchanged with the summation sign.
3. If for all n in the interval $[a, b]$, $u_n(x)$ and $\frac{d}{dx}u_n(x)$ are continuous, and the series $\sum_{n=1}^{\infty} \frac{d}{dx}u_n(x)$ is uniformly convergent, then we can differentiate the series term by term as
$$\frac{d}{dx}f(x) = \frac{d}{dx}\left[\sum_{n=1}^{\infty} u_n(x)\right] = \sum_{n=1}^{\infty} \frac{d}{dx}u_n(x). \tag{14.69}$$

14.7 Taylor Series

Let us assume that a function has a continuous nth derivative, $f^{(n)}(x)$, in the interval $[a, b]$. Integrating this derivative, we get
$$\int_a^x f^{(n)}(x_1)dx_1 = f^{(n-1)}(x_1)\Big|_a^x = f^{(n-1)}(x) - f^{(n-1)}(a). \tag{14.70}$$
Integrating again gives
$$\begin{aligned}\int_a^x \left(\int_a^{x_2} f^{(n)}(x_1)dx_1\right) dx_2 &= \int_a^x \left[f^{(n-1)}(x_2) - f^{(n-1)}(a)\right] dx_2 \\ &= f^{(n-2)}(x) - f^{(n-2)}(a) - (x-a)f^{(n-1)}(a)\end{aligned} \tag{14.71}$$
and after n-fold integrations, we get
$$\begin{aligned}\int_a^x \cdots \int_a^x f^{(n)}(x)(dx)^n &= f(x) - f(a) - (x-a)f'(a) \\ &\quad - \frac{(x-a)^2}{2!}f''(a) \\ &\quad \cdots - \frac{(x-a)^{n-1}}{(n-1)!}f^{(n-1)}(a).\end{aligned} \tag{14.72}$$

We now solve this equation for $f(x)$ to write

$$\begin{aligned} f(x) =& f(a) + (x-a)f'(a) + \frac{(x-a)^2}{2!}f''(a) + \cdots \\ &+ \frac{(x-a)^{n-1}}{(n-1)!}f^{(n-1)}(a) + \int_a^x \cdots \int_a^x f^{(n)}(x)(dx)^n. \end{aligned} \tag{14.73}$$

In this equation, $R_n = \int_a^x \cdots \int_a^x f^{(n)}(x)(dx)^n$ is called the **remainder**, which can also be written as

$$R_n = \frac{(x-a)^n}{n!}f^{(n)}(\xi), \quad a \le \xi \le x. \tag{14.74}$$

Note that Eq. (14.73) is exact. If $R_n \to 0$ as $n \to \infty$, we have a series expansion of the function $f(x)$ in terms of the positive powers of $(x - a)$ as

$$f(x) = \sum_{n=0}^{\infty} \frac{f^{(n)}(a)}{n!}(x-a)^n. \tag{14.75}$$

This is called the **Taylor series** expansion of $f(x)$ about the point $x = a$.

14.7.1 Maclaurin Theorem

In the Taylor series, if we take the point of expansion as the origin, we obtain the **Maclaurin series**:

$$f(x) = \sum_{n=0}^{\infty} \frac{f^{(n)}(0)}{n!}x^n. \tag{14.76}$$

14.7.2 Binomial Theorem

We now write the Taylor series for the function $f(x) = (1 + x)^m$ about $x = 0$ as

$$(1+x)^m = 1 + mx + \frac{m(m-1)}{2!}x^2 + \cdots + R_n, \tag{14.77}$$

$$R_n = \frac{x^n}{n!}(1+\xi)^{m-n}m(m-1)\cdots(m-n+1), \tag{14.78}$$

where m can be negative and noninteger and ξ is a point such that $0 \le \xi < x$. Since for $n > m$, the function $(1 + \xi)^{m-n}$ takes its maximum value for $\xi = 0$, we can write the following upper bound for the remainder term:

$$R_n \le \frac{x^n}{n!}m(m-1)\cdots(m-n+1). \tag{14.79}$$

From Eq. (14.79), it is seen that in the interval $0 \le x < 1$ the remainder goes to zero as $n \to \infty$; thus we obtain the binomial formula as

$$(1+x)^m = \sum_{n=0}^{\infty} \frac{m!}{n!(m-n)!}x^n = \sum_{n=0}^{\infty} \binom{m}{n} x^n. \tag{14.80}$$

It can easily be shown that this series is convergent in the interval $-1 < x < 1$. Note that for $m = n$ (integer), the sum automatically terminates after a finite number of terms, where the quantity

$$\binom{m}{n} = \frac{m!}{n!(m-n)!} \tag{14.81}$$

is called the **binomial coefficient**.

Example 14.14 ***Relativistic kinetic energy***
The binomial formula is probably one of the most widely used formulas in science and engineering. An important application of the binomial formula was given by Einstein in his celebrated paper where he announced his famous formula for the energy of a freely moving particle of mass m as $E = mc^2$. In this equation, c is the speed of light and m is the mass of the moving particle, which is related to the rest mass m_0 by

$$m = m_0 \Big/ \left(1 - \frac{v^2}{c^2}\right)^{1/2}, \tag{14.82}$$

where v is the velocity. Relativistic kinetic energy can be defined by subtracting the rest energy from the energy in motion as

$$\text{K.E.} = mc^2 - m_0c^2. \tag{14.83}$$

Since $v < c$, we can use the binomial formula to write the kinetic energy as

$$\text{K.E.} = m_0c^2 + \frac{1}{2}m_0v^2 + \frac{3}{8}m_0v^2\left(\frac{v^2}{c^2}\right) + \frac{5}{16}m_0v^2\left(\frac{v^2}{c^2}\right)^2 + \cdots - m_0c^2 \tag{14.84}$$

and after simplifying we obtain

$$\text{K.E.} = \frac{1}{2}m_0v^2 + \frac{3}{8}m_0v^2\left(\frac{v^2}{c^2}\right) + \frac{5}{16}m_0v^2\left(\frac{v^2}{c^2}\right)^2 + \cdots. \tag{14.85}$$

From here, we see that in the nonrelativistic limit, that is, $v/c \ll 1$ or when $c \to \infty$, the above formula reduces to the well-known classical expression for the kinetic energy as K.E. $\cong \frac{1}{2}m_0v^2$.

14.7.3 Taylor Series with Multiple Variables

For a function with two independent variables, $f(x,y)$, the Taylor series is given as

$$\begin{aligned} f(x,y) =& f(a,b) + (x-a)\frac{\partial f}{\partial x} + (x-b)\frac{\partial f}{\partial y} \\ &+ \frac{1}{2!}\left[(x-a)^2\frac{\partial^2 f}{\partial x^2} + 2(x-a)(y-b)\frac{\partial^2 f}{\partial x \partial y} + (y-b)^2\frac{\partial^2 f}{\partial y^2}\right] \end{aligned}$$

$$+\frac{1}{3!}\left[(x-a)^3\frac{\partial^3 f}{\partial x^3}+3(x-a)^2(y-b)\frac{\partial^3 f}{\partial x^2\partial y}\right.$$
$$\left.+3(x-a)(y-b)^2\frac{\partial^3 f}{\partial x\partial y^2}+(y-b)^3\frac{\partial^3 f}{\partial y^3}\right]+\cdots. \tag{14.86}$$

All the derivatives are evaluated at the point (a, b). In the presence of m independent variables, Taylor series becomes

$$f(x_1,x_2,\ldots,x_m)=\sum_{n=0}^{\infty}\frac{1}{n!}\left\{\left[\sum_{i=1}^{m}(x_j-x_{j0})\frac{\partial}{\partial x_i}\right]^n f(x_1,x_2,\ldots,x_m)\right\}_{x_{10},x_{20},\ldots,x_{m0}}. \tag{14.87}$$

14.8 Power Series

Series with their general term given as $u_n(x) = a_n x^n$ are called **power series**:

$$f(x)=a_0+a_1x+a_2x^2+\cdots=\sum_{n=0}^{\infty}a_nx^n, \tag{14.88}$$

where the coefficients, a_n, are independent of x. To use the ratio test, we write

$$\left|\frac{u_{n+1}}{u_n}\right|=\left|\frac{a_{n+1}x^{n+1}}{a_nx^n}\right|=\left|\frac{a_{n+1}}{a_n}\right||x| \tag{14.89}$$

and find $\lim_{n\to\infty}\left|\frac{a_{n+1}}{a_n}\right|=\frac{1}{R}$. Hence the condition for the convergence of a power series is obtained as $|x| < R \Rightarrow -R < x < R$, where R is called the **radius of convergence**. At the end points, the ratio test fails; hence these points must be analyzed separately.

Example 14.15 ***Power series***
For the power series,

$$1+x+\frac{x^2}{2}+\frac{x^3}{3}+\cdots+\frac{x^n}{n}+\cdots, \tag{14.90}$$

the radius of convergence R is 1; thus the series converges in the interval $-1 < x < 1$. On the other hand, at the end point, $x = 1$, it is divergent while at the other end point, $x = -1$, it is convergent.

Example 14.16 ***Power series***
The radius of convergence can also be zero. For the series,

$$1+x+2!x^2+3!x^3+\cdots+n!x^n+\cdots, \tag{14.91}$$

the ratio

$$\frac{a_{n+1}}{a_n} = \frac{(n+1)!}{n!} = n+1 \tag{14.92}$$

gives

$$\lim_{n\to\infty}(n+1) = \frac{1}{R} \to \infty, \tag{14.93}$$

hence the radius of convergence is zero. Note that this series converges only for $x = 0$.

Example 14.17 ***Power series***
For the power series

$$1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \cdots + \frac{x^n}{n!} + \cdots, \tag{14.94}$$

we find

$$\frac{a_{n+1}}{a_n} = \frac{n!}{(n+1)!} = \frac{1}{n+1} \tag{14.95}$$

and

$$\lim_{n\to\infty}\frac{1}{n+1} = \frac{1}{R} \to 0. \tag{14.96}$$

Hence the radius of convergence is infinity. This series converges for all x values.

14.8.1 Convergence of Power Series

If a power series is convergent in the interval $-R < x < R$, then it is uniformly and absolutely convergent in any subinterval S:

$$-S \leq x \leq S, \quad \text{where} \quad 0 < S < R. \tag{14.97}$$

This can be seen by taking $M_i = |a_i|S^i$ in the M-test.

14.8.2 Continuity

In a power series, since every term, $u_n(x) = a_n x^n$, is a continuous function and since in the interval $-S \leq x \leq S$, the series $f(x) = \sum a_n x^n$ is uniformly convergent, $f(x)$ is also a continuous function. Considering that in Fourier series, even though the $u_n(x)$ functions are Continuous, we expand discontinuous functions shaped like a saw tooth, this is an important property.

14.8.3 Differentiation and Integration of Power Series

In the interval of uniform convergence, a power series can be differentiated and integrated as often as desired. These operations do not change the radius of convergence.

14.8.4 Uniqueness Theorem

Let us assume that a function has two power series expansions about the origin with overlapping radii of convergence, that is,

$$f(x) = \sum_{n=0}^{\infty} a_n x^n \Rrightarrow -R_a < x < R_a \tag{14.98}$$

$$= \sum_{n=0}^{\infty} b_n x^n \Rrightarrow -R_b < x < R_b, \tag{14.99}$$

then $b_n = a_n$ is true for all n. Hence the power series is unique.

Proof: Let us write

$$\sum_{n=0}^{\infty} a_n x^n = \sum_{n=0}^{\infty} b_n x^n \Rrightarrow -R < x < R, \tag{14.100}$$

where R is equal to the smaller of the two radii R_a and R_b. If we set $x = 0$ in this equation, we find $a_0 = b_0$. Using the fact that a power series can be differentiated as often as desired, we differentiate the above equation once to write

$$\sum_{n=1}^{\infty} a_n n x^{n-1} = \sum_{n=1}^{\infty} b_n n x^{n-1}. \tag{14.101}$$

We again set $x = 0$, this time to find $a_1 = b_1$. Similarly, by repeating this process, we show that $a_n = b_n$ for all n.

14.8.5 Inversion of Power Series

Consider the power series expansion of the function $y(x) - y_0$ in powers of $(x - x_0)$ as

$$y - y_0 = a_1(x - x_0) + a_2(x - x_0)^2 + \cdots, \tag{14.102}$$

that is,

$$y - y_0 = \sum_{n=1}^{\infty} a_n (x - x_0)^n. \tag{14.103}$$

Sometimes it is desirable to express this series as

$$x - x_0 = \sum_{n=1}^{\infty} b_n (y - y_0)^n. \tag{14.104}$$

For this, we can substitute Eq. (14.104) into Eq. (14.103) and compare equal powers of $(y - y_0)$ to get the new coefficients, b_n, as

$$b_1 = \frac{1}{a_1}, \tag{14.105}$$

$$b_2 = -\frac{a_2}{a_1^3}, \tag{14.106}$$

$$b_3 = \frac{1}{a_1^5}\left(2a_2^2 - a_1 a_3\right), \tag{14.107}$$

$$b_4 = \frac{1}{a_1^7}\left(5a_1 a_2 a_3 - a_1^2 a_4 - 5a_2^3\right), \tag{14.108}$$

$$\vdots$$

A closed expression for these coefficients can be found using the residue theorem as

$$\boxed{b_n = \frac{1}{n!}\left[\frac{d^{n-1}}{dt^{n-1}}\left(\frac{t}{w(t)}\right)^n\right]_{t=0},} \tag{14.109}$$

where $w(t) = \sum_{n=1}^{\infty} a_n t^n$.

14.9 Summation of Infinite Series

After we conclude that a given series is convergent, the next and most important thing we need in applications is the value or the function that it converges. For uniformly convergent series, it is sometimes possible to identify an unknown series as the derivative or the integral of a known series. In this section, we introduce some analytic techniques to evaluate the sums of infinite series. We start with the Euler–Maclaurin sum formula, which has important applications in quantum field theory and Green's function calculations. Next, we discuss how some infinite series can be summed using the residue theorem. Finally, we show that differintegrals can also be used to sum infinite series.

14.9.1 Bernoulli Polynomials and their Properties

In deriving the Euler–Maclaurin sum formula, we make use of the properties of the **Bernoulli polynomials**, $B_s(x)$, where their **generating function** definition is given as

$$\frac{te^{xt}}{e^t - 1} = \sum_{s=0}^{\infty} B_s(x)\frac{t^s}{s!}, \quad |t| < 2\pi. \tag{14.110}$$

Some of the Bernoulli polynomials are given as follows:

Bernoulli Polynomials

$$\begin{aligned} B_0(x) &= 1, \\ B_1(x) &= x - \frac{1}{2}, \\ B_2(x) &= x^2 - x + \frac{1}{6}, \\ B_3(x) &= x\left(x - \frac{1}{2}\right)(x-1), \\ B_4(x) &= x^4 - 2x^3 + x^2 - \frac{1}{30}, \\ B_5(x) &= x\left(x - \frac{1}{2}\right)(x-1)\left(x^2 - x - \frac{1}{3}\right). \end{aligned} \tag{14.111}$$

Values of the Bernoulli polynomials at $x = 0$ are known as the **Bernoulli numbers**:

$$B_s = B_s(0), \tag{14.112}$$

where the first nine of them are given below:

Bernoulli numbers

$$\begin{array}{llll} B_0 = 1,\ B_1 = -\frac{1}{2}, & B_2 = \frac{1}{6}, & B_3 = 0, & B_4 = -\frac{1}{30}, \\ B_5 = 0,\ B_6 = \frac{1}{42}, & B_7 = 0, & B_8 = -\frac{1}{30}, & \dots . \end{array} \tag{14.113}$$

Some of the important properties of the Bernoulli polynomials can be listed as follows:

1.

$$B_s(x) = \sum_{j=0}^{s} \binom{s}{j} B_{s-j} x^j. \tag{14.114}$$

2.

$$B_s'(x) = sB_{s-1}(x),\ \int_0^1 B_s(x)dx = 0,\ s \geq 1. \tag{14.115}$$

3.

$$B_s(1-x) = (-1)^s B_s(x). \tag{14.116}$$

Note that when we write $B_s(1-x)$, we mean the Bernoulli polynomial with the argument $(1-x)$. The Bernoulli numbers are shown as B_s.

4.

$$\sum_{j=1}^{n} j^s = \frac{1}{(s+1)} \left\{B_{s+1}(n+1) - B_{s+1}\right\}, \ s \geq 1. \tag{14.117}$$

5.

$$\sum_{j=1}^{\infty} \frac{1}{j^{2s}} = (-1)^{s-1}(2\pi)^{2s} \frac{B_{2s}}{2(2s)!}, \ s \geq 1. \tag{14.118}$$

6.

$$\int_0^{\infty} \frac{x^{2s-1}}{e^{2\pi x} - 1} dx = (-1)^{s-1} \frac{B_{2s}}{4s}, \ s \geq 1. \tag{14.119}$$

7. In the interval [0, 1] and for $s \geq 1$, the only zeroes of $B_{2s+1}(x)$ are 0, $\frac{1}{2}$, and 1. In the same interval, 0 and 1 are the only zeroes of $(B_{2s}(x) - B_{2s})$. Bernoulli polynomials also satisfy the inequality

$$|B_{2s}(x)| \leq |B_{2s}|, \ 0 \leq x \leq 1. \tag{14.120}$$

8. The **Bernoulli periodic function**, which is continuous and has the period 1, is defined as

$$P_s(x) = B_s(x - [x]), \tag{14.121}$$

where $[x]$ means the greatest integer in the interval $(x - 1, x]$. The Bernoulli periodic function also satisfies the relations

$$P_s'(x) = sP_{s-1}(x), \quad s = 1, 2, 3, \ldots \tag{14.122}$$

and

$$P_s(1) = (-1)^s P_s(0), \quad s = 0, 1, 2, 3, \ldots. \tag{14.123}$$

14.9.2 Euler–Maclaurin Sum Formula

Using the fact that $B_0(x) = 1$, we write the integral $\int_0^1 f(x)dx$ as

$$\int_0^1 f(x)dx = \int_0^1 f(x)B_0(x)dx. \tag{14.124}$$

After using the relation $B_1'(x) = B_0(x) = 1$, Eq. (14.124) becomes

$$\int_0^1 f(x)dx = \int_0^1 f(x)B_0(x)dx = \int_0^1 f(x)B_1'(x)dx, \tag{14.125}$$

which can be integrated by parts to give

$$\int_0^1 f(x)dx = f(x)B_1(x)|_0^1 - \int_0^1 f'(x)B_1(x)dx \tag{14.126}$$

$$= \frac{1}{2}[f(1) + f(0)] - \int_0^1 f'(x)B_1(x)dx, \tag{14.127}$$

where we used $B_1(1) = \frac{1}{2}$, and $B_1(0) = -\frac{1}{2}$. In the above integral [Eq. (14.127)], we now use $B_1(x) = \frac{1}{2}B_2'(x)$ and integrate by parts again to obtain

$$\int_0^1 f(x)dx = \frac{1}{2}[f(1) + f(0)] - \frac{1}{2!}[f'(1)B_2(1) - f'(0)B_2(0)] + \frac{1}{2!}\int_0^1 f''(x)B_2(x)dx. \tag{14.128}$$

Using the values,

$$\begin{aligned} B_{2n}(1) = B_{2n}(0) = B_{2n} \qquad & n = 0, 1, 2, \ldots, \\ B_{2n+1}(1) = B_{2n+1}(0) = 0 \qquad & n = 1, 2, 3, \ldots, \end{aligned} \tag{14.129}$$

and continuing like this, we obtain

$$\int_0^1 f(x)dx = \frac{1}{2}[f(1) + f(0)] - \sum_{p=1}^{q} \frac{B_{2p}}{(2p)!}\left[f^{(2p-1)}(1) - f^{(2p-1)}(0)\right] + \frac{1}{(2q)!}\int_0^1 f^{(2q)}(x)B_{2q}(x)dx. \tag{14.130}$$

This equation is called the **Euler–Maclaurin sum formula**. We have assumed that all the necessary derivatives of $f(x)$ exist and q is an integer greater than one.

We now change the limits of the integral from $\int_0^1$ to $\int_1^2$:

$$\int_1^2 f(x)dx = \int_0^1 f(y+1)dy \tag{14.131}$$

and repeat the above steps for $f(y+1)$ to obtain

$$\begin{aligned} \int_0^1 f(y+1)dy = {} & \frac{1}{2}[f(2) + f(1)] \\ & - \sum_{p=1}^{q} \frac{B_{2p}}{(2p)!}\left[f^{(2p-1)}(2) - f^{(2p-1)}(1)\right] \\ & + \frac{1}{(2q)!}\int_0^1 f^{(2q)}(y+1)P_{2q}(y)dy, \end{aligned} \tag{14.132}$$

where we used the Bernoulli periodic function [Eq. (14.121)]. Making the transformation $y + 1 = x$, we write

$$\begin{aligned} \int_1^2 f(x)dx &= \int_0^1 f(y+1)dy, \\ &= \frac{1}{2}[f(2) + f(1)] \end{aligned} \tag{14.133}$$

$$-\sum_{p=1}^{q}\frac{B_{2p}}{(2p)!}\left[f^{(2p-1)}(2)-f^{(2p-1)}(1)\right]$$

$$+\frac{1}{(2q)!}\int_0^1 f^{(2q)}(x)P_{2q}(x-1)dx. \tag{14.134}$$

Repeating this for the interval [2, 3], we write

$$\int_2^3 f(x)dx = \frac{1}{2}[f(3)+f(2)]$$

$$-\sum_{p=1}^{q}\frac{B_{2p}}{(2p)!}\left[f^{(2p-1)}(3)-f^{(2p-1)}(2)\right]$$

$$+\frac{1}{(2q)!}\int_2^3 f^{(2q)}(x)P_{2q}(x-2)dx. \tag{14.135}$$

Integrals for the other intervals can be written similarly. Since the integral for the interval $[0, n]$ can be written as

$$\int_0^n f(x)dx = \int_0^1 f(x)dx + \int_1^2 f(x)dx + \cdots + \int_{n-1}^n f(x)dx, \tag{14.136}$$

we substitute the formulas found above in the right-hand side to obtain

$$\int_0^n f(x)dx = \frac{1}{2}f(0)+f(1)+f(2)+\cdots+\frac{1}{2}f(n)$$

$$-\sum_{p=1}^{q}\frac{B_{2p}}{(2p)!}\left[f^{(2p-1)}(n)-f^{(2p-1)}(0)\right]$$

$$+\frac{1}{(2q)!}\int_0^n f^{(2q)}(x)P_{2q}(x)dx. \tag{14.137}$$

We used the fact that the function $P_{2q}(x)$ is periodic with the period 1. Rearranging this, we write

$$\sum_{j=0}^{n} f(j) = \int_0^n f(x)dx + \frac{1}{2}[f(0)+f(n)]$$

$$+\sum_{p=1}^{q-1}\frac{B_{2p}}{(2p)!}\left[f^{(2p-1)}(n)-f^{(2p-1)}(0)\right] \tag{14.138}$$

$$+\frac{B_{2q}}{(2q)!}\left[f^{(2q-1)}(n)-f^{(2q-1)}(0)\right]-\frac{1}{(2q)!}\int_0^n f^{(2q)}(x)P_{2q}(x)dx.$$

The last two terms on the right-hand side can be written under the same integral sign, which gives us the final form of the **Euler–Maclaurin sum formula** as

$$\sum_{j=0}^{n} f(j) = \int_0^n f(x)dx + \frac{1}{2}[f(0) + f(n)] + \sum_{p=1}^{q-1} \frac{B_{2p}}{(2p)!} \left[f^{(2p-1)}(n) - f^{(2p-1)}(0)\right] + \int_0^n \frac{\left[B_{2q} - B_{2q}(x - [x])\right]}{(2q)!} f^{(2q)}(x)dx. \quad (14.139)$$

In this derivation, we assumed that $f(x)$ is continuous and has all the required derivatives. This is a very versatile formula that can be used in several ways. When q is chosen as a finite number, it allows us to evaluate a given series as an integral plus some correction terms. When q is chosen as infinity, it could allow us to replace a slowly converging series with a rapidly converging one. If we take the integral to the left-hand side, it can be used for numerical evaluation of integrals.

14.9.3 Using Residue Theorem to Sum Infinite Series

Some of the infinite series can be summed using the residue theorem. First, we take a rectangular contour C_N in the z-plane with the corners as shown in Figure 14.3. We now prove a property that will be useful to us shortly.

Lemma 14.1 On the contour C_N, the inequality $|\cot \pi z| < A$ is always satisfied, where A is a constant independent of N.

We prove this by considering the parts of C_N with $y > \frac{1}{2}$, $-\frac{1}{2} \leq y \leq \frac{1}{2}$, and $y < -\frac{1}{2}$, separately.

1. **Case for** $y > \frac{1}{2}$**:**
   We write a complex number as $z = x + iy$; thus

$$|\cot \pi z| = \left|\frac{e^{i\pi z} + e^{-i\pi z}}{e^{i\pi z} - e^{-i\pi z}}\right| = \left|\frac{e^{i\pi x-\pi y} + e^{-i\pi x+\pi y}}{e^{i\pi x-\pi y} - e^{-i\pi x+\pi y}}\right|. \quad (14.140)$$

   Using the triangle inequality:

$$|z_1| - |z_2| \leq |z_1 + z_2| \leq |z_1| + |z_2|, \quad (14.141)$$

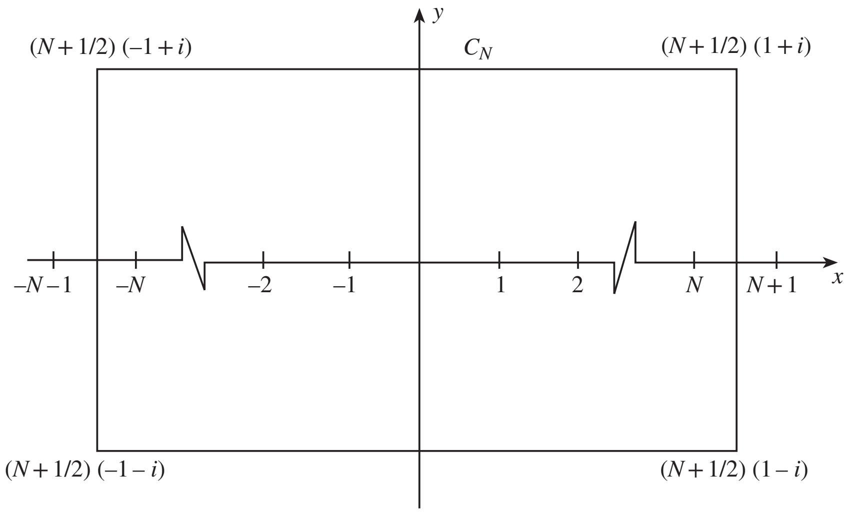

Figure 14.3 Contour for finding series sums using the residue theorem.

and considering that $y > \frac{1}{2}$, we find

$$|\cot \pi z| \leq \frac{|e^{i\pi x-\pi y}| + |e^{-i\pi x+\pi y}|}{|e^{-i\pi x+\pi y}| - |e^{i\pi x-\pi y}|} \tag{14.142}$$

$$\leq \frac{e^{-\pi y} + e^{\pi y}}{e^{\pi y} - e^{-\pi y}} = \frac{1 + e^{-2\pi y}}{1 - e^{-2\pi y}} \tag{14.143}$$

$$\leq \frac{1 + e^{-\pi}}{1 - e^{-\pi}} = A_1. \tag{14.144}$$

2. **Case for** $y < -\frac{1}{2}$: Following the procedure of the first case, we find

$$|\cot \pi z| \leq \frac{|e^{i\pi x-\pi y}| + |e^{-i\pi x+\pi y}|}{|e^{i\pi x-\pi y}| - |e^{-i\pi x+\pi y}|} = \frac{e^{-\pi y} + e^{\pi y}}{e^{-\pi y} - e^{\pi y}} \tag{14.145}$$

$$\leq \frac{1 + e^{2\pi y}}{1 - e^{2\pi y}} \leq \frac{1 + e^{-\pi}}{1 - e^{-\pi}} = A_1. \tag{14.146}$$

3. **Case for** $-\frac{1}{2} \leq y \leq \frac{1}{2}$: A point on the right-hand side of C_N can be written as $z = N + \frac{1}{2} + iy$; thus for $-\frac{1}{2} \leq y \leq \frac{1}{2}$, we obtain

$$|\cot \pi z| = \left|\cot \pi \left(N + \frac{1}{2} + iy\right)\right| = \left|\cot \left(\frac{\pi}{2} + i\pi y\right)\right| \tag{14.147}$$

$$= |\tanh \pi y| \leq \tanh \left(\frac{\pi}{2}\right) = A_2. \tag{14.148}$$

Similarly, a point on the left-hand side of C_N is written as $z = -N - \frac{1}{2} + iy$, which gives us

$$|\cot \pi z| = \left|\cot \pi \left(-N - \frac{1}{2} + iy\right)\right| = \left|\cot \left(\frac{\pi}{2} + i\pi y\right)\right| \tag{14.149}$$

$$= |\tanh \pi y| \leq \tanh \left(\frac{\pi}{2}\right) = A_2. \tag{14.150}$$

Choosing the greater of the A_1 and A_2 and calling it A proves that on C_N the inequality $|\cot \pi z| < A$ is satisfied. We also note that A is a constant independent of N. Actually, since $A_2 < A_1$, we could also write $|\cot \pi z| \leq A_1 = \cot \frac{\pi}{2}$.

We now state the following useful theorem:

Theorem 14.1 If a function $f(z)$ satisfies the inequality $|f(z)| \leq \frac{M}{|z|^k}$ on the contour C_N, where $k > 1$ and M is a constant independent of N, then the sum of the series $\sum_{j=-\infty}^{\infty} f(j)$ is given as

$$\boxed{\sum_{j=-\infty}^{\infty} f(j) = -\begin{bmatrix}\text{Sum of the Residues of } (\pi \cot \pi z f(z)) \\ \text{at the isolated singular points of } f(z)\end{bmatrix}.} \tag{14.151}$$

Proof:

1. Case: Let us assume that $f(z)$ has a finite number of isolated singular points. In this case, we choose the number N such that the closed contour C_N encloses all of the singular points of $f(z)$. On the other hand, $\cot \pi z$ has poles at the points $z = n$, $n = 0, \pm 1, \pm 2, \ldots$, where the residues of the function $\pi \cot \pi z f(z)$ at these points are given as

$$\lim_{z \to n}(z - n)\pi \cot \pi z f(z) = \lim_{z \to n} \pi \frac{(z - n)f(z) \cos \pi z}{\sin z\pi} = f(n). \tag{14.152}$$

For this result, we used the L'Hopital's rule and assumed that $f(z)$ has no poles at the points $z = n$. Using the residue theorem, we can now write

$$\oint_{C_N} \pi \cot \pi z f(z) dz = \sum_{n=-N}^{N} f(n) + S, \tag{14.153}$$

where S represents the sum of the finite number of residues of $\pi \cot \pi z f(z)$ at the poles of $f(z)$. We can put an upper bound to the integral on the left as

$$\oint_{C_N} \pi \cot \pi z f(z) dz \leq \left| \oint_{C_N} \pi \cot \pi z f(z) dz \right| \leq \oint_{C_N} \pi |\cot \pi z| |f(z)| |dz|. \tag{14.154}$$

Since on the contour $f(z)$ satisfies $|f(z)| \leq M/|z|^k$, this becomes

$$\left| \oint_{C_N} \pi \cot \pi z f(z) dz \right| \leq \frac{\pi A M}{N^k}(8N + 4), \tag{14.155}$$

where $(8N + 4)$ is the length of C_N. From here, we see that as $N \to \infty$, the value of the integral in Eq. (14.153) goes to zero:

$$\lim_{N \to \infty} \oint_{C_N} \pi \cot \pi z f(z) dz = 0, \tag{14.156}$$

hence we can write

$$\sum_{n=-\infty}^{\infty} f(n) = -S. \tag{14.157}$$

2. Case: If $f(z)$ has infinitely many singular points, the result can be obtained similarly by an appropriate limiting process.

Example 14.18 ***Series sum by the residue theorem***
In quantum field theory and in Green's function calculations, we occasionally encounter series like

$$\sum_{n=0}^{\infty} \frac{1}{n^2 + a^2}, \quad a > 0, \tag{14.158}$$

where $f(z) = 1/(z^2 + a^2)$ has two isolated singular points located at $z = \pm ia$ and satisfies the conditions of the above theorem. The residue of $\pi \cot \pi z/(z^2 + a^2)$ at $z = ia$ is found as

$$\lim_{z\to ia}(z - ia)\frac{\pi \cot \pi z}{(z + ia)(z - ia)} = \frac{\pi \cot \pi ia}{2ia} = -\frac{\pi}{2a} \coth \pi a. \tag{14.159}$$

Similarly, the residue at $z = -ia$ is $-\frac{\pi}{2a}$ coth πa; thus using the conclusion of the above theorem [Eq. (14.151)], we can write

$$\sum_{n=-\infty}^{\infty} \frac{1}{n^2 + a^2} = \frac{\pi}{a} \coth \pi a. \tag{14.160}$$

From this result, we obtain the needed sum, $\sum_{n=0}^{\infty} \frac{1}{n^2+a^2}$, as follows:

$$\sum_{n=-\infty}^{\infty} \frac{1}{n^2 + a^2} = \sum_{n=-\infty}^{-1} \frac{1}{n^2 + a^2} + \frac{1}{a^2} + \sum_{n=1}^{\infty} \frac{1}{n^2 + a^2}, \tag{14.161}$$

$$2\sum_{n=1}^{\infty} \frac{1}{n^2 + a^2} + \frac{1}{a^2} = \frac{\pi}{a} \coth \pi a, \tag{14.162}$$

$$\sum_{n=0}^{\infty} \frac{1}{n^2 + a^2} = \frac{\pi}{2a} \coth \pi a + \frac{1}{2a^2}. \tag{14.163}$$

14.9.4 Evaluating Sums of Series by Differintegrals

Using differintegrals (Chapter 13), in 1970, Osler [5] gave the following summation version of the Leibniz rule, which is very useful in finding sums of infinite series:

$$\frac{d^q[u(x)v(x)]}{dx^q} = \sum_{n=-\infty}^{\infty} \binom{q}{n+\gamma} \frac{d^{q-\gamma-n}u}{dx^{q-\gamma-n}} \frac{d^{\gamma+n}v}{dx^{\gamma+n}} \tag{14.164}$$

$$= \sum_{n=-\infty}^{\infty} \frac{\Gamma(q+1)}{\Gamma(q-\gamma-n+1)\Gamma(\gamma+n+1)} \frac{d^{q-\gamma-n}u}{dx^{q-\gamma-n}} \frac{d^{\gamma+n}v}{dx^{\gamma+n}}, \tag{14.165}$$

where γ is any constant.

Example 14.19 ***Evaluating sums of series by differintegrals***
In the above formula, if we choose $u = x^a$, $v = x^b$, and $\gamma = 0$, and use the differintegral

$$\frac{d^q x^p}{dx^q} = \frac{\Gamma(p+1)x^{p-q}}{\Gamma(p-q+1)}, \tag{14.166}$$

where $p > -1$, we find the sum

$$\frac{\Gamma(a+b+1)}{\Gamma(a+b-q+1)} = \sum_{n=0}^{\infty} \frac{\Gamma(q+1)\Gamma(a+1)\Gamma(b+1)}{\Gamma(q-n+1)\Gamma(n+1)\Gamma(a-q+n+1)\Gamma(b-n+1)}.$$

14.10 Asymptotic Series

Asymptotic series are frequently encountered in applications. They are generally used in numerical evaluation of certain functions approximately. Two typical functions, $I_1(x)$ and $I_2(x)$, where asymptotic series are used for their evaluation are given as

$$\boxed{I_1(x) = \int_x^{\infty} e^{-u} f(u) du,} \tag{14.167}$$

$$\boxed{I_2(x) = \int_0^{\infty} e^{-u} f\left(\frac{u}{x}\right) du.} \tag{14.168}$$

In astrophysics, we frequently work on gasses obeying the Maxwell–Boltzman distribution, where we encounter gamma functions defined as

$$\boxed{I(x,p) = \int_x^{\infty} e^{-u} u^{-p} du = \Gamma(1-p,x), \quad x, \; p > 0.} \tag{14.169}$$

We now calculate $I(x,p)$ for large values of x. We first start by integrating the above integral by parts twice to get

$$I(x,p) = \frac{e^{-x}}{x^p} - p \int_x^{\infty} e^{-u} u^{-p-1} du \tag{14.170}$$

and then

$$I(x,p) = \frac{e^{-x}}{x^p} - \frac{pe^{-x}}{x^{p+1}} + p(p+1) \int_x^{\infty} e^{-u} u^{-p-2} du. \tag{14.171}$$

We keep on integrating by parts to obtain the series

$$I(x,p) = e^{-x}\left[\frac{1}{x^p} - \frac{p}{x^{p+1}} + \frac{p(p+1)}{x^{p+2}} - \cdots + (-1)^{n-1}\frac{(p+n-2)!}{(p-1)!x^{p+n-1}}\right] + (-1)^n \frac{(p+n-1)!}{(p-1)!} \int_x^{\infty} e^{-u} u^{-p-n} du. \tag{14.172}$$

This is a rather interesting series, where the ratio test gives

$$\lim_{n\to\infty}\frac{|u_{n+1}|}{|u_n|}=\lim_{n\to\infty}\frac{(p+n)!}{(P+n-1)!}\frac{1}{x}=\lim_{n\to\infty}\frac{p+n}{x}\to\infty. \tag{14.173}$$

Thus the series diverges for all finite values of x. Before we discard this series as useless in calculating the values of the function $I(x,p)$, let us write the absolute value of the difference of $I(x,p)$ and the nth partial sum, S_n, as

$$|I(x,p)-S_n(x,p)|\le\left|(-1)^{n+1}\frac{(p+n)!}{(p-1)!}\int_x^\infty e^{-u}u^{-p-n-1}du\right|=|R_n(x,p)|. \tag{14.174}$$

Using the transformation $u=v+x$, we can write the above integral as

$$\int_x^\infty e^{-u}u^{-p-u-1}du=e^{-x}\int_0^\infty e^{-v}(v+x)^{-p-n-1}dv \tag{14.175}$$

$$=\frac{e^{-x}}{x^{p+n+1}}\int_0^\infty e^{-v}\left(1+\frac{v}{x}\right)^{-p-n-1}dv. \tag{14.176}$$

For the large values of x, using the limit

$$\lim_{x\to\infty}\int_0^\infty e^{-v}\left(1+\frac{v}{x}\right)^{-p-n-1}dv\to 1, \tag{14.177}$$

we find

$$\boxed{|R_n|=|I(x,p)-S_n(x,p)|\approx\frac{(p+n)!}{(p-1)!}\frac{e^{-x}}{x^{p+n+1}},} \tag{14.178}$$

which shows that for sufficiently large values of x, we can use S_n [Eq. (14.172)] for evaluating the values of the function $I(x,p)$ to sufficient accuracy. Naturally, the R_n value of the partial sum depends on the desired accuracy. For this reason, such series are sometimes called **asymptotic** or **semi-convergent** series.

Example 14.20 ***Asymptotic expansions***

We now consider the integral $I=\int_0^x e^{-t^2}dt$ and use the expansion

$$e^{-t^2}=1-\frac{t^2}{1!}+\frac{t^4}{2!}-\frac{t^6}{3!}+\cdots,\quad r=\infty, \tag{14.179}$$

to write

$$I=\int_0^x e^{-t^2}dt=x-\frac{x^3}{3\cdot 1!}+\frac{x^5}{5\cdot 2!}-\frac{x^7}{7\cdot 3!}+\cdots,\quad r=\infty, \tag{14.180}$$

where r is the radius of convergence. For small values of x, this series can be used to evaluate I to any desired level of accuracy. However, even though this series is convergent for all x, it is not practical to use for large x. For the large values of x, we can use the method of asymptotic expansions. Writing

$$I = \int_0^x e^{-t^2} dt = \int_0^\infty e^{-t^2} dt - \int_x^\infty e^{-t^2} dt \tag{14.181}$$

$$= \frac{\sqrt{\pi}}{2} - \left[\int_x^\infty \left(-\frac{1}{2t} \right) d(e^{-t^2}) \right] \tag{14.182}$$

and integrating by parts, we obtain

$$I = \frac{\sqrt{\pi}}{2} - \left[\frac{e^{-x^2}}{2x} - \frac{1}{2} \int_x^\infty \frac{e^{-t^2}}{t^2} dt \right]. \tag{14.183}$$

Repeated application of integration by parts, after n times, yields

$$\int_x^\infty e^{-t^2} dt \tag{14.184}$$

$$= \frac{e^{-x^2}}{2x} \left[1 - \frac{1}{2x^2} + \frac{1 \cdot 3}{(2x^2)^2} - \cdots + (-1)^{n-1} \frac{1 \cdot 3 \cdot 5 \cdots (2n-3)}{(2x^2)^{n-1}} \right] + R_n,$$

where

$$R_n = (-1)^n \frac{1 \cdot 3 \cdot 5 \cdots (2n-1)}{2^n} \int_x^\infty \frac{e^{-t^2}}{t^{2n}} dt. \tag{14.185}$$

As $n \to \infty$, this series diverges for all x. However, using the inequalities

$$\int_x^\infty \frac{e^{-t^2}}{t^{2n}} dt < \frac{1}{x^{2n}} \int_x^\infty e^{-t^2} dt, \tag{14.186}$$

$$\int_x^\infty e^{-t^2} dt < \frac{e^{-x^2}}{2x}, \tag{14.187}$$

we see that the remainder satisfies

$$|R_n| < \frac{1 \cdot 3 \cdot 5 \cdots (2n-1)}{2^{n+1} x^{2n+1}} e^{-x^2}. \tag{14.188}$$

Hence $|R_n|$ can be made sufficiently small by choosing n sufficiently large, thus the series in Eq. (14.184) can be used to evaluate I as

$$I = \frac{\sqrt{\pi}}{2} - \frac{e^{-x^2}}{2x} \left[1 - \frac{1}{2x^2} + \frac{1 \cdot 3}{(2x^2)^2} - \cdots + (-1)^{n-1} \frac{1 \cdot 3 \cdot 5 \cdots (2n-3)}{(2x^2)^{n-1}} \right] - R_n. \tag{14.189}$$

For $x = 5$, if we choose $n = 13$, we have $|R_n| < 10^{-20}$.

14.11 Method of Steepest Descent

Frequently, we encounter integrals that cannot be evaluated exactly. Even though nowadays modern computers can be used to evaluate almost any integral numerically, methods for obtaining approximate expressions of various types of integrals remain extremely useful. Having an approximate yet an analytic expression for a given integral, not only allows us to push further with the analytic approach, but also helps us to understand and interpret the results better. In this regard, in the previous section, we have introduced the asymptotic series. We now introduce two more useful methods for obtaining approximate values of integrals, that is, the method of **steepest descent** and the **saddle-point integrals**. They are both closely related to the **asymptotic series**.

Consider the integral

$$I = \int_{x_1}^{x_2} dx\, F(x), \tag{14.190}$$

where the range could be infinite. We now write I as

$$I = \int_{x_1}^{x_2} dx\, e^{f(x)}, \tag{14.191}$$

where $f(x)$ is defined as $f(x) = \ln[F(x)]$. If $f(x)$ has a steep maximum at x_0, where

$$f'(x_0) = \frac{1}{F(x_0)} F'(x_0) = 0 \tag{14.192}$$

and $F''(x_0) < 0$, we can approximate $f(x)$ in the neighborhood of x_0 by taking only the first two nonzero terms of the Taylor series:

$$f(x) = f(x_0) + f'(x_0)(x - x_0) + \frac{1}{2!} f''(x_0)(x - x_0)^2 + \cdots, \tag{14.193}$$

as

$$f(x) \simeq f(x_0) + \frac{1}{2!} f''(x_0)(x - x_0)^2. \tag{14.194}$$

If the range includes the point x_0, we can write I as

$$I = \int_{x_1}^{x_2} dx\, F(x) \tag{14.195}$$

$$= \int_{x_1}^{x_2} dx\, e^{f(x)} \tag{14.196}$$

$$\simeq \int_{x_1}^{x_2} dx\, \exp\left[f(x_0) + \frac{1}{2} f''(x_0)(x - x_0)^2 \right] \tag{14.197}$$

$$\simeq F(x_0) \int_{x_1}^{x_2} dx\, e^{-\frac{1}{2}|f''(x_0)|(x-x_0)^2}. \tag{14.198}$$

If the end points do not contribute to the integral significantly, we can replace I with

$$I \simeq F(x_0) \int_{-\infty}^{\infty} dx\, e^{-\frac{1}{2}|f''(x_0)|(x-x_0)^2}, \tag{14.199}$$

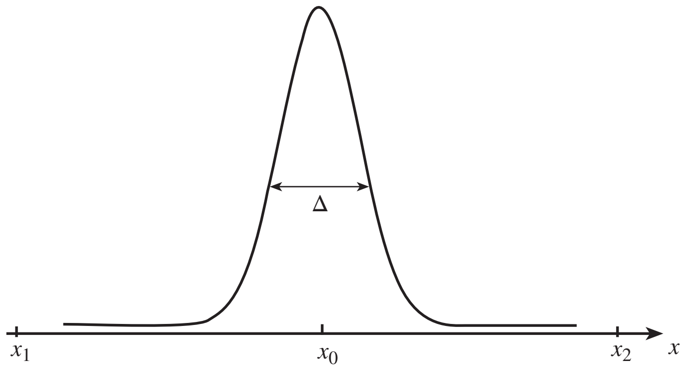

Figure 14.4 In one dimension, the method of steepest descent allows us to approximate the integrand in Eq. (14.190), $F(x)$, that has a high maximum at x_0 with a Gaussian, $F(x_0)e^{-\frac{1}{2}|f''(x_0)|(x-x_0)^2}$, where the width, Δ, is $\Delta \propto 1/\sqrt{|f''(x_0)|}$ and $f(x) = \ln[F(x)]$.

where the integrand:

$$e^{-\frac{1}{2}\left|f''(x_0)\right|(x-x_0)^2}, \tag{14.200}$$

is a Gaussian as shown in Figure 14.4.

We can now evaluate the integral in Eq. (14.199) to obtain the approximate expression

$$I \simeq \sqrt{\frac{2\pi}{|f''(x_0)|}}\, F(x_0). \tag{14.201}$$

Example 14.21 ***Method of steepest descent***

Evaluate the integral

$$\Gamma(x+1) = \int_0^\infty t^x e^{-t} dt \tag{14.202}$$

for large x.

Solution: We first rewrite the integrand as

$$F(x;t) = e^{f(x;t)} = t^x e^{-t} = e^{x \ln t - t}, \tag{14.203}$$

hence determine $f(x;t)$ as

$$f(x;t) = x \ln t - t. \tag{14.204}$$

Evaluating the first two derivatives with respect to t:

$$f'(x;t) = \frac{x}{t} - 1, \tag{14.205}$$

$$f''(x;t) = -\frac{x}{t^2}, \tag{14.206}$$

we see that the maximum of $f(x;t)$ is located at $t = x$. Finally, using Eq. (14.201), we obtain the approximate value of $\Gamma(x+1)$ as

$$\boxed{\Gamma(x+1) \simeq \sqrt{2\pi x}x^x e^{-x},} \tag{14.207}$$

which is good for large x. When x is an integer, n, this is nothing but the **Stirling's approximation** of the **factorial** $n!$.

Important:

(i) Note that the large x condition assures us that the coefficient of the third order term in the Taylor series expansion about $t = x$:

$$f(x;t) = f(x;x) + \frac{1}{2!}f''(x;x)(t-x)^2 + \frac{1}{3!}f''(x;x)(t-x)^3 + \cdots, \tag{14.208}$$

is negligible for t values near x. That is,

$$\left|\frac{1}{3!}f''(x;x)(t-x)^3 \Big/ \frac{1}{2!}f''(x;x)(t-x)^2\right| = \frac{2}{3}\left|\frac{t-x}{x}\right| \ll 1. \tag{14.209}$$

(ii) The approximate formula we have obtained in Eq. (14.207) is nothing but the first term in the asymptotic expansion of $\Gamma(x+1)$:

$$\boxed{n! = \sqrt{2\pi n}n^n e^{-n}\left(1 + \frac{1}{12n} + \frac{1}{288n^2} + \cdots\right).} \tag{14.210}$$

(iii) A Series expansion of the integrand in Eq. (14.202) would not be useful.

14.12 Saddle-Point Integrals

In general, the method of steepest descent is applicable to contour integrals of the form

$$I(\alpha) = \int_C F(z)\,dz \tag{14.211}$$

$$= \int_C e^{\alpha f(z)}\,dz, \tag{14.212}$$

where α is large and positive and C is a path in the complex plane where the end points do not contribute significantly to the integral. The method of steepest descent works if the function $f(z)$ has a maximum at some point z_0 on the contour. However, if the function is analytic, we can always deform the contour so that it passes through the point z_0 without altering the value of the integral.

From the theory of complex functions (Chapter 11), we know that the real and the imaginary parts, u and v, of an analytic function:

$$f(z) = u(x, y) + iv(x, y), \tag{14.213}$$

satisfy the Laplace equation:

$$\nabla^2 u(x, y) = 0, \tag{14.214}$$

and

$$\nabla^2 v(x, y) = 0. \tag{14.215}$$

From Eq. (14.214), it is seen that if $\frac{\partial^2 u}{\partial x^2} < 0$, then $\frac{\partial^2 u}{\partial y^2} > 0$. The same conclusion also holds for $v(x, y)$. Using Theorem 1.4 in [2, p. 18], we conclude that the point z_0, where

$$\left.\frac{\partial u}{\partial x}\right|_{z_0} = \left.\frac{\partial u}{\partial y}\right|_{z_0} = 0, \tag{14.216}$$

must be a saddle point of the surface $u(x, y)$. At z_0 the surface looks like a saddle or a mountain pass (Figure 14.5).

By the Cauchy–Riemann conditions, we also infer that

$$\left.\frac{\partial v}{\partial x}\right|_{z_0} = \left.\frac{\partial v}{\partial y}\right|_{z_0} = 0, \tag{14.217}$$

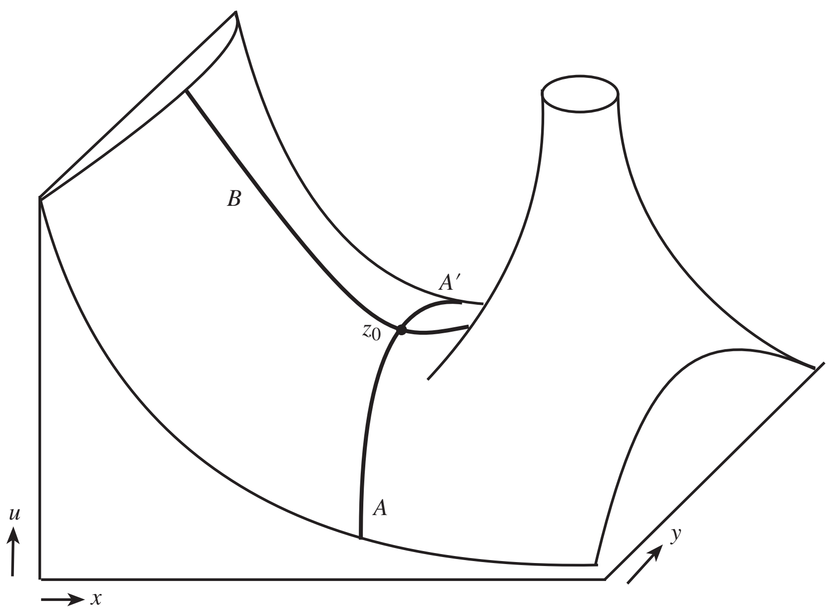

Figure 14.5 The path AA' is the path that follows the steepest descent. The path B is perpendicular to AA', hence it follows the ridges.

hence $\frac{df(z_0)}{dz} = 0$. In other words, a saddle point of $u(x, y)$ is also a saddle point of $v(x, y)$.

About the saddle point, we can write the Taylor series

$$f(z) = f(z_0) + \frac{1}{2!}f''(z_0)(z - z_0)^2 + \frac{1}{3!}f'''(z_0)(z - z_0)^2 + \cdots \tag{14.218}$$

and for points on the contour near the saddle point, we can use the approximation

$$f(z) \simeq f(z_0) + \frac{1}{2}f''(z_0)(z - z_0)^2. \tag{14.219}$$

Using polar representations of $f''(z_0)$ and $(z - z_0)$:

$$f''(z_0) = \rho_0 e^{i\phi_0}, \tag{14.220}$$

$$(z - z_0) = re^{i\theta}, \tag{14.221}$$

where z is a point on the contour, we can approximate the integral $I(\alpha)$ [Eq. (14.212)] by

$$I(\alpha) \simeq \int_{C'} dz\ e^{\alpha\left[f(z_0)+\frac{1}{2}f''(z_0)(z-z_0)^2\right]} \tag{14.222}$$

$$\simeq \int_{C'} dr\ e^{i\theta} e^{\alpha\left[f(z_0)+\frac{1}{2}\rho_0 e^{i\phi_0} r^2 e^{i2\theta}\right]} \tag{14.223}$$

$$\simeq e^{\alpha f(z_0)} \int_{C'} dr\ e^{i\theta} e^{\alpha\frac{1}{2}\rho_0 r^2 e^{i(\phi_0+2\theta)}} \tag{14.224}$$

$$\simeq e^{\alpha f(z_0)} \int_{C'} dr\ e^{i\theta} e^{\alpha\frac{1}{2}\rho_0 r^2[\cos(\phi_0+2\theta)+i\sin(\phi_0+2\theta)]}, \tag{14.225}$$

where C' is now a contour that passes through the saddle point z_0. We are now looking for directions, that is, the θ values, that allow us to approximate the value of this integral only using the values of $f(z)$ in the neighborhood of z_0. Note that for points near the saddle Point, the surface is nearly flat, hence θ varies very slowly, hence we have written

$$dz \simeq dr\ e^{i\theta}. \tag{14.226}$$

We can also take $e^{i\theta}$ outside the integral sign to write

$$I(\alpha) \simeq e^{\alpha f(z_0)}\ e^{i\theta} \int_{C'} dr\ e^{\alpha\frac{1}{2}\rho_0 r^2[\cos(\phi_0+2\theta)+i\sin(\phi_0+2\theta)]}. \tag{14.227}$$

The integrand has two factors:

$$e^{\alpha\frac{1}{2}\rho_0 r^2[\cos(\phi_0+2\theta)]} \tag{14.228}$$

and

$$e^{i\alpha\frac{1}{2}\rho_0 r^2[\sin(\phi_0+2\theta)]}. \tag{14.229}$$

The first factor is an exponential, which could be decaying or growing depending on the sign of the cosine, while the second factor oscillates wildly for large α. For this method to work effectively, we have to pick a direction that makes the exponential decay in the fastest possible way, thus justifying the name **steepest descent**, while suppressing the effect of the wildly fluctuating second factor. From the following table, we see that the paths that follow the steepest descent from the saddle point, z_0, are the ones that follow the directions that make

$$\cos(\phi_0 + 2\theta) = -1. \tag{14.230}$$

Since for these paths

$$\sin(\phi_0 + 2\theta) = 0, \tag{14.231}$$

they also eliminate the concerns caused by the wildly fluctuating second factor. If we take

$$(\phi_0 + 2\theta) = \pi, \tag{14.232}$$

the direction that we have to follow becomes

$$\theta = -\frac{\phi_0}{2} + \frac{\pi}{2}, \tag{14.233}$$

where ϕ_0 is determined from Eq. (14.220).

Choice of angles in the saddle-point method:

$(\phi_0 + 2\theta)$	$[\cos(\phi_0 + 2\theta) + i\sin(\phi_0 + 2\theta)]$	θ
0	$+1$	$-\frac{\phi_0}{2}$
π	-1	$-\frac{\phi_0}{2} + \frac{\pi}{2}$
2π	$+1$	$-\frac{\phi_0}{2} + \pi$
3π	-1	$-\frac{\phi_0}{2} + \frac{3\pi}{2}$
4π	$+1$	$-\frac{\phi_0}{2} + 2\pi$

Every time we change θ, that is, the direction that we start moving at z_0, by $\pi/2$, the quantity

$$[\cos(\phi_0 + 2\theta) + i\sin(\phi_0 + 2\theta)] \tag{14.234}$$

changes its value from $+1$ to -1. Depending on which direction we are passing through the saddle point, the directions that correspond to the steepest descent are given as

$$\theta = -\frac{\phi_0}{2} \pm \frac{\pi}{2}. \tag{14.235}$$

For these directions, the integrand in Eq. (14.227) is a Gaussian, hence for large positive α, only the points very close to z_0 contribute to the integral. The directions perpendicular to these follow the ridges and give rise to exponentially

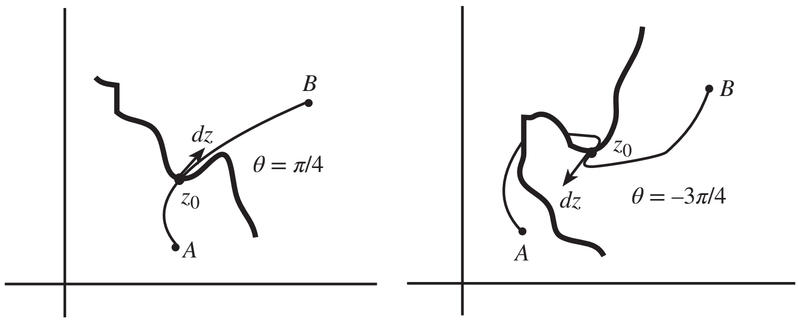

Figure 14.6 Two possible *mountain ranges*: For the one on the left, we use + and for the one on the right, we use − in Eq. (14.235).

increasing functions in Eq. (14.227). Any direction in between will compromise the advantages of this method. Keep in mind that usually this method gives the first term in the asymptotic expansion of $I(\alpha)$ for large α. To choose the correct sign in Eq. (14.235), we need to look at the topography more carefully and see which way to deform the contour. For example, for $\phi_0 = \pi/2$, in Figure 14.6, we show two possible topographies that require the + and the − signs, respectively. In these figures, dz is a tangent vector to the path at z_0 pointing in the direction we move.

In the light of these, we now write an approximate expression for $I(\alpha)$ as

$$I(\alpha) \simeq e^{\alpha f(z_0)} \int_{-\infty}^{\infty} e^{-\alpha \frac{1}{2}\rho_0 r^2} e^{i\theta}\, dr \tag{14.236}$$

$$\simeq \sqrt{\frac{2\pi}{\alpha\rho_0}}\, e^{\alpha f(z_0)} e^{i\theta}, \tag{14.237}$$

where θ takes one of the values

$$\theta = -\frac{\phi_0}{2} \pm \frac{\pi}{2} \tag{14.238}$$

and

$$\phi_0 = \tan^{-1}\left[\frac{\mathrm{Im}\, f''(z_0)}{\mathrm{Re}\, f''(z_0)}\right]. \tag{14.239}$$

Note that since for large α, only points near z_0 contribute to the integral, we have taken the limits in Eq. (14.236) as $\pm\infty$.

Example 14.22 ***Saddle-point integrals***

Let us evaluate $\Gamma(z+1)$ using the definition

$$\Gamma(z) = \int_0^{\infty} e^{-t} t^{z-1} dt, \ \mathrm{Re} z > 0, \tag{14.240}$$

via the saddle-point method. We start by writing

$$\Gamma(z+1) = \int_0^\infty e^{-t} t^z dt \tag{14.241}$$

$$= \int_0^\infty e^{-t+z\ln t} dt. \tag{14.242}$$

Using the polar representation of z as $z = \alpha e^{i\beta}$, we rewrite Eq. (14.242):

$$\Gamma(z+1) = \int_0^\infty \exp\left[\alpha\left(\ln t - \frac{t}{z}\right)e^{i\beta}\right] dt, \tag{14.243}$$

and compare with $\Gamma(z+1) = \int_0^\infty e^{\alpha f(t)} dt$ to obtain

$$f(t) = \left(\ln t - \frac{t}{z}\right)e^{i\beta}. \tag{14.244}$$

The first two derivatives of $f(t)$ are easily found as

$$f'(t) = \left(\frac{1}{t} - \frac{1}{z}\right)e^{i\beta}, \tag{14.245}$$

$$f''(t) = -\frac{1}{t^2}e^{i\beta}. \tag{14.246}$$

Setting the first derivative to zero, we obtain the saddle point, t_0, as $f'(t_0) = 0 \Rightarrow t_0 = z$. This gives $f(t_0) = (\ln z - 1)e^{i\beta}$ and

$$f''(t_0) = -\frac{e^{i\beta}}{z^2} = -\frac{1}{\alpha^2}e^{-i\beta}. \tag{14.247}$$

Using the polar representation, $f''(t_0) = \rho_0 e^{i\phi_0}$, we obtain $\rho_0 = 1/\alpha^2$, $\phi_0 = \pi - \beta$. We now have to decide between the two possibilities for θ:

$$\theta = -\frac{\pi-\beta}{2} + \frac{\pi}{2} = \frac{\beta}{2} \tag{14.248}$$

and

$$\theta = -\frac{\pi-\beta}{2} - \frac{\pi}{2} = -\pi + \frac{\beta}{2}. \tag{14.249}$$

In our previous example, where z was real, $\beta = 0$ and $\theta = 0$, it seems that $\theta = \beta/2$ is the right choice. This gives the steepest descent approximation of $\Gamma(z+1)$ as

$$\Gamma(z+1) \simeq \sqrt{2\pi\alpha}\; e^{z\ln z - z}\; e^{i\beta/2}, \tag{14.250}$$

$$\boxed{\Gamma(z+1) \simeq \sqrt{2\pi} z^{z+\frac{1}{2}} e^{-z}.} \tag{14.251}$$

Even though the integral definition [Eq. (14.241)] is valid for Re $z > 0$, the above result is good for $|z| \gg 1$, provided that we stay away from the negative real axis where we have a branch cut.

Example 14.23 ***Saddle-point integrals***
We now show that the approximate expression for $\Gamma(z+1)$ obtained via the saddle-point method:

$$\Gamma(z+1) \simeq \sqrt{2\pi}\, z^{z+\frac{1}{2}} e^{-z}, \tag{14.252}$$

is only the first term in the asymptotic expansion of $\Gamma(z+1)$.
We first write Eq. (14.240):

$$\Gamma(z) = \int_0^\infty e^{-t} t^{z-1} dt, \quad \operatorname{Re} z > 0, \tag{14.253}$$

as

$$\Gamma(z+1) = \int_0^\infty dt\, e^{f(t)}, \tag{14.254}$$

where

$$f(t) = -t + z \ln t. \tag{14.255}$$

The saddle point,

$$f'(t_0) = 0, \tag{14.256}$$

of $f(t)$ is located at $t_0 = z$. We now expand $f(t)$ about the saddle point to write

$$f(t) = f(z) + A_1(t-z) + A_2(t-z)^2 + A_3(t-z)^3 + \cdots, \tag{14.257}$$

where

$$A_k = \frac{1}{k!} \frac{d^k f(z)}{dt^k}.$$

Substituting $f(t)$ [Eq. (14.255)] into Eq. (14.257), we obtain

$$f(t) = [-z + z \ln z] - \frac{(t-z)^2}{2z} + \frac{(t-z)^3}{3z^2} - \frac{(t-z)^4}{4z^3} + \cdots, \tag{14.258}$$

which when substituted into Eq. (14.254) gives

$$\Gamma(z+1) = z^z e^{-z} \int_0^\infty dt \exp\left[-\frac{(t-z)^2}{2z} + \frac{(t-z)^3}{3z^2} - \frac{(t-z)^4}{4z^3} + \cdots\right]. \tag{14.259}$$

To simplify, we use the substitution $s = (t-z)/\sqrt{2z}$ to get

$$\Gamma(z+1) = \sqrt{2z}\, z^z e^{-z} \int_{-\sqrt{z/2}}^\infty ds \exp\left[-s^2 + \frac{s^3}{3}\sqrt{\frac{8}{z}} - \frac{s^4}{z} + \cdots\right]. \tag{14.260}$$

We now write this as

$$\Gamma(z+1) \simeq \sqrt{2z}\, z^z e^{-z} \int_{-\sqrt{z/2}}^\infty ds\, e^{-s^2} \exp\left(\frac{s^3}{3}\sqrt{\frac{8}{z}} - \frac{s^4}{z}\right) \tag{14.261}$$

and then expand the exponential to get

$$\Gamma(z+1) \simeq \sqrt{2z}\, z^z e^{-z} \int_{-\sqrt{z/2}}^{\infty} ds\, e^{-s^2} \left[1 + \left(\frac{s^3}{3}\sqrt{\frac{8}{z}} - \frac{s^4}{z} \right) + \frac{1}{2!}\left(\frac{s^3}{3}\sqrt{\frac{8}{z}} - \frac{s^4}{z} \right)^2 + \cdots \right], \tag{14.262}$$

which when the integrals are evaluated yields the series

$$\Gamma(z+1) \simeq \sqrt{2\pi}\, z^{z+1/2} e^{-z} \left[1 + \frac{1}{12z} + \frac{1}{288z^2} + \cdots \right]. \tag{14.263}$$

For integers, $z = n$, this gives the **asymptotic expansion** of the factorial:

$$\boxed{n! \simeq \sqrt{2\pi} n^{n+1/2} e^{-n} \left[1 + \frac{1}{12n} + \frac{1}{288n^2} + \cdots \right],} \tag{14.264}$$

the first term of which is the well-known **Stirling's formula** valid for large n:

$$\boxed{n! \simeq \sqrt{2\pi} n^{n+1/2} e^{-n}.} \tag{14.265}$$

Keep in mind that the several steps of this derivation lacks the desired rigor, but nevertheless produces the right answer [Eq. (14.210)].

14.13 Padé Approximants

We have seen how to use contour integrals and Euler–Maclaurin sum formula to sum series. Both techniques required that the general term of the series be known. In applications, we frequently encounter situations where only the first few terms of the series can be determined. Furthermore, these terms may not be sufficient to reveal the general term of the series. We are now going to introduce an intriguing technique that will allow us to evaluate series sums to very high levels of accuracy.

As an example, consider the series

$$f(x) = 1 + x - \frac{5}{2}x^2 + \frac{13}{2}x^3 - \frac{141}{8}x^4 + \cdots, \tag{14.266}$$

where only the first five terms are known. Let us first introduce the general method.

Consider a series whose first M terms are given:

$$f(x; M) = \sum_{i=0}^{M} a_i x^i. \tag{14.267}$$

We write $f(x;M)$ as the ratio of two polynomials:

$$f(x;M) = \frac{P(x;N)}{Q(x;L)}, \tag{14.268}$$

where

$$P(x;N) = \sum_{j=0}^{N} p_j x^j, \tag{14.269}$$

$$Q(x;L) = \sum_{k=0}^{L} q_k x^k, \tag{14.270}$$

and $M = N + L$. We have $(N + L + 2) = M + 2$ unknowns, where $(N + 1)$ p_j's and $(L + 1)$ q_k's, are to be determined from the known $M + 1$ values of a_i. We now write Eq. (14.268) as

$$f(x;M)\left(\sum_{k=0}^{L} q_k x^k\right) = \left(\sum_{j=0}^{N} p_j x^j\right), \tag{14.271}$$

$$\left(\sum_{i=0}^{M} a_i x^i\right)\left(\sum_{k=0}^{L} q_k x^k\right) = \left(\sum_{j=0}^{N} p_j x^j\right), \tag{14.272}$$

$$(a_0 + a_1 x + \cdots + a_M x^M)(q_0 + q_1 x + \cdots + q_L x^L) = (p_0 + p_1 x + \cdots + a_N x^N). \tag{14.273}$$

Since when $P(x;N)$ and $Q(x;L)$ are multiplied with the same constant, $f(x;M)$ does not change, hence we can set $q_0 = 1$, thus obtaining

$$(a_0 + a_1 x + \cdots + a_M x^M)(1 + q_1 x + \cdots + q_L x^L) = (p_0 + p_1 x + \cdots + p_N x^N). \tag{14.274}$$

We now have $N + L + 1 = M + 1$ unknowns, $p_0, p_1, \ldots, p_N;\ q_1, \ldots, q_L$, to be determined from the $N + 1$ values of a_i, $i = 0, 1, \ldots, M$. Expanding Eq. (14.274) and equating the coefficients of the equal powers of x gives the following $M + 1$ equations:

$$\begin{aligned}
a_0 &= p_0, \\
a_1 + a_0 q_1 &= p_1, \\
a_2 + a_1 q_1 + a_0 q_2 &= p_2, \\
&\vdots \\
a_N + a_{N-1} q_1 + \cdots + a_0 q_N &= p_N, \\
a_{N+1} + a_N q_1 + \cdots + a_{N-L+1} q_L &= 0, \\
&\vdots \\
a_{N+L} + a_{N+L-1} q_1 + \cdots + a_N q_L &= 0,
\end{aligned} \tag{14.275}$$

for the $M + 1$ unknowns, where we have taken

$$a_i = 0 \quad \text{when } i > M, \tag{14.276}$$

$$p_j = 0 \quad \text{when } j > N, \tag{14.277}$$

$$q_k = 0 \quad \text{when } k > L. \tag{14.278}$$

The first $N + 1$ equations can be written as

$$\begin{pmatrix} p_0 \\ p_1 \\ \vdots \\ p_N \end{pmatrix} = \begin{pmatrix} a_0 & 0 & \cdots & 0 \\ a_1 & a_0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ a_N & a_{N-1} & \cdots & a_0 \end{pmatrix} \begin{pmatrix} 1 \\ q_1 \\ \vdots \\ q_N \end{pmatrix}, \tag{14.279}$$

while the remaining equations become

$$\begin{pmatrix} a_N & a_{N-1} & \cdots & a_{N-L+1} \\ a_{N+1} & a_N & \cdots & a_{N-L+2} \\ \vdots & \vdots & \vdots & \vdots \\ a_M & a_{M-1} & \cdots & a_N \end{pmatrix} \begin{pmatrix} q_1 \\ q_2 \\ \vdots \\ q_L \end{pmatrix} = - \begin{pmatrix} a_{N+1} \\ a_{N+2} \\ \vdots \\ a_M \end{pmatrix}. \tag{14.280}$$

These are two sets of linear equations. Since a_i's are known, we can solve the second set for the q_k values, which when substituted into the first set will yield the p_j values. For a review of linear algebra and techniques on solving systems of linear equations, we recommend Bayin [2].

Let us now return to the series in Eq. (14.266), where $M = 4$ and choose $N = L = 2$. Using the values

$$a_0 = 1, \quad a_1 = 1, \quad a_2 = -\frac{5}{2}, \quad a_3 = \frac{13}{2}, \quad a_4 = -\frac{141}{8}, \tag{14.281}$$

the two linear systems to be solved becomes:

$$\begin{pmatrix} a_2 & a_1 \\ a_3 & a_2 \end{pmatrix} \begin{pmatrix} q_1 \\ q_2 \end{pmatrix} = - \begin{pmatrix} a_3 \\ a_4 \end{pmatrix}, \tag{14.282}$$

$$\begin{pmatrix} -\frac{5}{2} & 1 \\ \frac{13}{2} & -\frac{5}{2} \end{pmatrix} \begin{pmatrix} q_1 \\ q_2 \end{pmatrix} = - \begin{pmatrix} \frac{13}{2} \\ -\frac{141}{8} \end{pmatrix} \tag{14.283}$$

and

$$\begin{pmatrix} p_0 \\ p_1 \\ p_2 \end{pmatrix} = \begin{pmatrix} a_0 & 0 & \cdots \\ a_1 & a_0 & \cdots \\ a_2 & a_1 & a_0 \end{pmatrix} \begin{pmatrix} 1 \\ q_1 \\ q_2 \end{pmatrix}, \tag{14.284}$$

$$\begin{pmatrix} p_0 \\ p_1 \\ p_2 \end{pmatrix} = \begin{pmatrix} 1 & 0 & \cdots \\ 1 & 1 & \cdots \\ -\frac{5}{2} & 1 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ q_1 \\ q_2 \end{pmatrix}. \tag{14.285}$$

The first set yields the values of q_k as

$$\begin{pmatrix} q_1 \\ q_2 \end{pmatrix} = \begin{pmatrix} \frac{11}{2} \\ \frac{29}{4} \end{pmatrix}. \tag{14.286}$$

Using these values in the second set, we obtain

$$\begin{pmatrix} p_0 \\ p_1 \\ p_2 \end{pmatrix} = \begin{pmatrix} 1 \\ \frac{13}{2} \\ \frac{41}{4} \end{pmatrix}. \tag{14.287}$$

Thus, we obtain the **Padé approximant,** $f^{(2,2)}(x)$, as

$$f^{(2,2)}(x) = \frac{1 + \frac{13}{2}x + \frac{41}{4}x^2}{1 + \frac{11}{2}x + \frac{29}{4}x^2}. \tag{14.288}$$

To interpret this result, it is time to reveal the truth about the five terms we have in Eq. (14.266). They are just the first five terms of the Taylor series expansion of

$$F(x) = \sqrt{\frac{1+4x}{1+2x}}. \tag{14.289}$$

This function has a pole at $x = -\frac{1}{2}$ and a branch point at $x = -\frac{1}{4}$. In other words, the Taylor series:

$$f(x) = 1 + x - \frac{5}{2}x^2 + \frac{13}{2}x^3 - \frac{141}{8}x^4 + \cdots, \tag{14.290}$$

converges only for $|x| \leq \frac{1}{4}$. We now construct the following table to compare $F(x), f(x)$, and $f^{(2,2)}(x)$ for various values of x:

x	0	1/4	1/2	1	3.0	7.0
F(x)	1	1.1547	1.22474	1.29099	1.36277	1.39044
$f(x)$	1	1.12646	0.585938	−11.625	−1270.63	−40202.6
$f^{(2,2)}(x)$	1	1.1547	1.22472	1.29091	1.36254	1.39012
$f^{(1,3)}(x)$	1	1.15426	1.2196	1.24966	0.89702	0.316838
$f^{(1,1)}(x)$	1	1.15428	1.2199	1.2513	0.712632	−2.91771

The last two rows are the other two Padé approximants corresponding to the choices $(N, L) = (1, 3)$ and $(N, L) = (3, 1)$, respectively:

$$f^{(1,3)}(x) = \frac{1 + \frac{363}{100}x}{1 + \frac{263}{100}x - \frac{13}{100}x^2 + \frac{41}{200}x^3} \tag{14.291}$$

and

$$f^{(3,1)}(x) = \frac{1 + \frac{193}{52}x + \frac{11}{52}x^2 - \frac{29}{104}x^3}{1 + \frac{141}{52}x}. \tag{14.292}$$

From this table, it is seen that the Padé approximant, $f^{(2,2)}(x)$, approximates the function $F(x)$ much better than the Taylor series, $f(x)$, truncated after the fifth term. It is also interesting that $f^{(2,2)}(x)$ remains to be an excellent approximation even outside the domain, $|x| > 1/4$, where the Taylor series ceases to be valid. In this case, the symmetric Padé approximant; $f^{(2,2)}(x)$, gives a much better approximation than its antisymmetric counterparts.

Definition 14.1 For a given function, $f(x)$, the Padé approximant $R_{N/L}(x) \equiv [N, L]$, of order (N, L) is defined as the rational function

$$\boxed{R_{N/L}(x) = \frac{p_0 + p_1 x + p_2 x^2 + \cdots + p_N x^N}{1 + q_1 x + q_2 x^2 + \cdots + q_L x^L},} \tag{14.293}$$

where $R_{N/L}(x)$ agrees with $f(x)$ to the highest possible order, that is,

$$\boxed{f(x) - R_{N/L}(x) = c_{N+L+1} x^{N+L+1} + c_{N+L+2} x^{N+L+2} + \cdots.} \tag{14.294}$$

In other words, the first $(N + L)$ terms of the Taylor series expansion of $R_{N/L}(x)$ exactly cancel the first $(N + L + 1)$ terms of the Taylor series of $f(x)$. For a given (N, L), the Padé approximant is **unique**. Padé approximants will often be a superior approximation to a function, compared to the one obtained by truncating the Taylor series. As in the above example, it may even work where the Taylor series do not.

14.14 Divergent Series in Physics

So far, we have seen how to test a series for convergence and introduced some techniques for evaluating infinite sums. In quantum field theory, we occasionally encounter divergent series corresponding to physical properties like energy and mass. These divergences are naturally due to some pathologies in our theory, which are expected to disappear in the next generation of field theories. However, even within the existing theories, it is sometimes possible to obtain meaningful results that agree with the experiments to an incredibly high degree of accuracy. The process of obtaining finite and meaningful results from divergent series is accomplished in two steps. The first step is called the **regularization**, where the divergent pieces are written out explicitly. The second step is the **renormalization**, where the divergent pieces identified in the first part are subtracted by suitable physical arguments. Whether a given theory is renormalizable or not is very important. In 1999, Gerardus't Hooft and J. G. Martinus Veltman received the Nobel Prize for showing that Salam and Weinberg's theory of unified electromagnetic and weak interactions is renormalizable. On the other hand, quantum gravity is nonrenormalizable because it contains infinitely many divergent pieces.

14.14.1 Casimir Effect and Renormalization

To demonstrate the regularization and the renormalization procedure, we consider massless conformal scalar field in one-dimensional box with length L. Using the periodic boundary conditions, we find the eigenfrequencies as

$$\omega_n = \frac{2\pi cn}{L}, \qquad n = 0, 1, 2, \ldots, \tag{14.295}$$

where each frequency is twofold degenerate. In quantum field theory, vacuum energy is a divergent expression given by the infinite sum

$$\overline{E}_0 = \sum_n g_n \frac{\hbar\omega_n}{2}, \tag{14.296}$$

where g_n stands for the degeneracy of the nth eigenstate. For the one-dimensional box problem, $\overline{E}_0$ becomes

$$\overline{E}_0 = \frac{2\pi c\hbar}{L} \sum_{n=0}^{\infty} n, \tag{14.297}$$

which diverges. Because the high frequencies are the reason for the divergence of the vacuum energy, we have to suppress them for a finite result. Let us multiply Eq. (14.297) with a **cutoff function** like $e^{-\alpha\omega_n}$ and write

$$\overline{E}_0 = \frac{2\pi c\hbar}{L} \sum_{n=0}^{\infty} n e^{-2\pi cn\alpha/L}, \tag{14.298}$$

where α is the **cutoff parameter**. This sum is now convergent and can be evaluated easily using the geometric series as

$$\overline{E}_0 = \frac{2\pi}{L} e^{-2\pi\alpha/L} \left[1 - e^{-2\pi\alpha/L}\right]^{-2}, \quad \text{we set } \hbar = c = 1. \tag{14.299}$$

The final and the finite result is naturally going to be obtained in the limit where the effects of the cutoff function disappear, that is, when $\alpha \to 0$. We now expand

Eq. (14.299) in terms of the cutoff parameter, α, to write

$$\overline{E}_0 = \frac{L}{2\pi\alpha^2} - \frac{\pi}{6L} + (\text{terms in positive powers of } \alpha). \tag{14.300}$$

Note that in the limit as $\alpha \to 0$, the vacuum energy is still divergent; however, the cutoff function has helped us to **regularize** the divergent expression so that the divergent piece can be identified explicitly as $L/2\pi\alpha^2$. The second term in $\overline{E}_0$ is finite and independent of α, while the remaining terms are all proportional to the positive powers of α, which disappear in the limit $\alpha \to 0$.

The second part of the process is **renormalization**, which is subtracting the divergent piece by a physical argument. We now look at the case where the walls are absent, or taken to infinity. In this case, the eigenfrequencies are continuous; hence we write the vacuum energy in terms of an integral as

$$\overline{E}_0 \to \tilde{E}_0 = \frac{L}{2\pi}\int_0^\infty \omega d\omega. \tag{14.301}$$

This integral is also divergent. We regularize it with the same cutoff function and evaluate its value as

$$\tilde{E}_0 = \frac{L}{2\pi}\int_0^\infty \omega e^{-\alpha\omega} d\omega \tag{14.302}$$

$$= \frac{L}{2\pi\alpha^2}, \tag{14.303}$$

which is identical to the divergent term in the series [Eq. (14.300)].

To be consistent with our expectations, we now argue that in the absence of walls, or as $L \to \infty$, the quantum vacuum energy should be zero. Thus we define the **renormalized** quantum vacuum energy, E_0, by subtracting the divergent piece [Eq. (14.303)] from the unrenormalized energy, $\overline{E}_0$, and then by taking the limit $\alpha \to 0$ as

$$E_0 = \lim_{\alpha\to 0}[\overline{E}_0 - \tilde{E}_0]. \tag{14.304}$$

For the renormalized quantum vacuum energy between the walls, this prescription gives

$$E_0 = \lim_{\alpha\to 0}\left[\frac{L}{2\pi\alpha^2} - \frac{\pi}{6L} + (\text{terms in positive powers of } \alpha) - \frac{L}{2\pi\alpha^2}\right] \tag{14.305}$$

$$= -\frac{\pi}{6L}. \tag{14.306}$$

The minus sign means that the force between the walls is attractive. In three dimensions, this method gives the renormalized electromagnetic vacuum energy between two perfectly conducting neutral plates held at absolute zero and separated by a distance L as

$$E_0 = -\frac{c\hbar\pi^2}{720L^3}S, \tag{14.307}$$

where S is the surface area of the plates and we have inserted c and $\hbar$. This gives the attractive force per unit area between the plates as

$$F_0 = -\frac{\partial E_0}{\partial L} = -\frac{\pi^2 c\hbar}{240L^4}. \tag{14.308}$$

In quantum field theory, this interesting effect is known as the **Casimir effect** and it has been verified experimentally. The Casimir effect has also been calculated for plates with different geometries and also in curved background spacetimes. More powerful and covariant techniques like the point splitting method, which are independent of cutoff functions, have confirmed the results obtained by the simple mode sum method used here. Since in the classical limit, $\hbar \to 0$, the Casimir effect disappears, it is a pure quantum effect.

One should keep in mind that in the regularization and renormalization process we have not cured the divergence problem of the quantum vacuum energy. In the absence of gravity only the energy differences are observable; hence all we have done is to define the renormalized quantum vacuum energy in the absence of plates as zero and then scaled all the other energies with respect to it.

14.14.2 Casimir Effect and MEMS

The Casimir force between two neutral metal plates is very small and goes as A/d^4. For plates with a surface area of 1 cm^2 and a separation of 1 μm, the Casimir force is around $10^{-7}N$. This is roughly the weight of a water drop. When we reduce the separation to 1 nm, roughly 100 times the size of a typical atom, pressure on the plates becomes 1 atm. The Casimir effect plays an important role in **microelectromechanical devices** (**MEMS**). These are systems with moving mechanical parts embedded in silicon chips at micro- and submicroscales. Examples of MEMS are microrefrigerators, actuators, sensors, and switches. In the production of MEMS, the Casimir effect can sometimes produce unwanted effects like sticking between parts, but it can also be used to produce mechanical effects like bending and twisting. A practical use for the Casimir effect in our everyday lives is the pressure sensors of airbags in cars. Casimir energy is bound to make significant changes in our concept of vacuum.

14.15 Infinite Products

Infinite products are closely related to infinite series. Most of the known functions can be written as infinite products, which are also useful in calculating some of the transcendental numbers. We define the Nth partial product of an infinite product of positive terms as

$$P_N = f_1 \cdot f_2 \cdot f_3 \cdots f_N = \prod_{n=1}^{N} f_n. \tag{14.309}$$

If the limit

$$\lim_{N\to\infty} \prod_{n=1}^{N} f_n \to P \tag{14.310}$$

exists, then we say the infinite product converges and write

$$\prod_{n=1}^{\infty} f_n = P. \tag{14.311}$$

Infinite products satisfying the condition $\lim_{n\to\infty} f_n > 1$ are divergent. When the condition $0 < \lim_{n\to\infty} f_n < 1$ is satisfied, it is advantageous to write the product as

$$\prod_{n=1}^{\infty} (1 + a_n). \tag{14.312}$$

The condition $a_n \to 0$ as $n \to \infty$ is necessary, but not sufficient, for convergence. Using the ln function, we can write an infinite product as an infinite sum as

$$\ln \prod_{n=1}^{\infty} (1 + a_n) = \sum_{n=1}^{\infty} \ln(1 + a_n). \tag{14.313}$$

Theorem 14.2 When the inequality $0 \le a_n < 1$ is true, then the infinite products

$$\prod_{n=1}^{\infty} (1 + a_n) \text{ and } \prod_{n=1}^{\infty} (1 - a_n) \tag{14.314}$$

converge or diverge with the infinite series $\sum_{n=1}^{\infty} a_n$.

Proof: Since $1 + a_n \le e^{a_n}$, we write

$$e^{a_n} = 1 + a_n + \frac{a_n^2}{2!} + \cdots, \tag{14.315}$$

which means the inequality

$$P_N = \prod_{n=1}^{N} (1 + a_n) \le \prod_{n=1}^{N} e^{a_n} = \exp\left\{\sum_{n=1}^{N} a_n\right\} = e^{S_N} \tag{14.316}$$

is true. Since in the limit as $N \to \infty$ we can write

$$\prod_{n=1}^{\infty} (1 + a_n) \le \exp\left\{\sum_{n=1}^{\infty} a_n\right\}, \tag{14.317}$$

we obtain an upper bound to the infinite product. For a lower bound, we write the Nth partial sum as

$$P_N = 1 + \sum_{i=1}^{N} a_i + \sum_{i=1}^{N} \sum_{j=1}^{N} a_i a_j + \cdots \tag{14.318}$$

and since $a_i \geq 0$, we obtain the lower bound as

$$\prod_{n=1}^{\infty} (1 + a_n) \geq \sum_{n=1}^{\infty} a_n. \tag{14.319}$$

Both the upper and the lower bounds to the infinite product $\Pi_{n=1}^{\infty}(1 + a_n)$ depend on the series $\sum_{n=1}^{\infty} a_n$; thus both of them converge or diverge together. Proof for the product $\Pi_{n=1}^{\infty}(1 - a_n)$ is done similarly.

14.15.1 Sine, Cosine, and the Gamma Functions

An nth-order polynomial with n real roots can be written as a product:

$$P_n(x) = (x - x_1)(x - x_2) \cdots (x - x_n) = \prod_{i=1}^{n} (x - x_i). \tag{14.320}$$

Naturally, a function with infinitely many roots can be expressed as an infinite product. We can find the infinite product representations of the sine and cosine functions using complex analysis:

In the z-plane a function, $h(z)$, with simple poles at $z = a_n$, $0 < |a_1| < |a_2| < \cdots$, can be written as

$$h(z) = h(0) + \sum_{n=1}^{\infty} b_n \left[\frac{1}{(z - a_n)} + \frac{1}{a_n} \right], \tag{14.321}$$

where b_n is the residue of the function at the pole a_n. This is also known as the **Mittag-Leffler theorem**. We have seen that a function analytic on the entire z-plane is called an entire function. For such a function its logarithmic derivative, f'/f, has poles and its Laurent expansion must be given about the poles. If an entire function $f(z)$ has a simple zero at $z = a_n$, then we can write

$$f(z) = (z - a_n) g(z), \tag{14.322}$$

where $g(z)$ is again an analytic function satisfying $g(z) \neq g(a_n)$. Using the above equation, we can write

$$\frac{f'}{f} = \frac{1}{(z - a_n)} + \frac{g'(z)}{g(z)}. \tag{14.323}$$

Since a_n is a simple pole of f'/f, we can take $b_n = 1$ and $h(z) = f'/f$ in Eq. (14.321) to write

$$\frac{f'(z)}{f(z)} = \frac{f'(0)}{f(0)} + \sum_{n=1}^{\infty} \left[\frac{1}{(z - a_n)} + \frac{1}{a_n} \right]. \tag{14.324}$$

Integrating Eq. (14.324) gives

$$\ln\frac{f(z)}{f(0)} = z\frac{f'(0)}{f(0)} + \sum_{n=1}^{\infty}\left[\ln(z-a_n) - \ln(-a_n) + \frac{z}{a_n}\right], \tag{14.325}$$

and finally the general expression is obtained as

$$f(z) = f(0)\exp\left[z\frac{f'(0)}{f(0)}\right]\prod_{n=1}^{\infty}\left(1-\frac{z}{a_n}\right)\exp\left(\frac{z}{a_n}\right). \tag{14.326}$$

Applying this formula with $z = x$ to the sine and cosine functions, we obtain

$$\boxed{\sin x = x\prod_{n=1}^{\infty}\left(1-\frac{x^2}{n^2\pi^2}\right)} \tag{14.327}$$

and

$$\boxed{\cos x = \prod_{n=1}^{\infty}\left(1-\frac{4x^2}{(2n-1)^2\pi^2}\right).} \tag{14.328}$$

These products are finite for all the finite values of x. For $\sin x$, this can easily be seen by taking $a_n = x^2/n^2\pi^2$. Since the series $\sum_{n=1}^{\infty} a_n$ is convergent, the infinite product is also convergent:

$$\sum_{n=1}^{\infty} a_n = \frac{x^2}{\pi^2}\sum_{n=1}^{\infty}\frac{1}{n^2} = \frac{x^2}{\pi^2}\zeta(2) = \frac{x^2}{6}. \tag{14.329}$$

In the $\sin x$ expression, if we take $x = \frac{\pi}{2}$, we obtain

$$1 = \frac{\pi}{2}\prod_{n=1}^{\infty}\left(1-\frac{1}{(2n)^2}\right) = \frac{\pi}{2}\prod_{n=1}^{\infty}\left(\frac{(2n)^2-1}{(2n)^2}\right).$$

Writing this as

$$\frac{\pi}{2} = \prod_{n=1}^{\infty}\left(\frac{(2n)^2}{(2n-1)(2n+1)}\right) = \frac{2\cdot 2}{1\cdot 3}\cdot\frac{4\cdot 4}{3\cdot 5}\cdot\frac{6\cdot 6}{5\cdot 7}\cdots, \tag{14.330}$$

we obtain the **Wallis' formula** for $\pi/2$.

Infinite products can also be used to write the Γ function as

$$\boxed{\Gamma(x) = \left[xe^{\gamma x}\prod_{r=1}^{\infty}(1+\frac{x}{r})e^{-x/r}\right]^{-1},} \tag{14.331}$$

where γ is the **Euler–Masheroni constant**:

$$\gamma = 0.577216\ldots. \tag{14.332}$$

Using Eq. (14.331), we can write

$$\Gamma(-x)\Gamma(x) = \left[-xe^{-\gamma x}\prod_{r=1}^{\infty}\left(1-\frac{x}{r}\right)e^{x/r}\right]^{-1}\cdot\left[xe^{\gamma x}\prod_{r=1}^{\infty}\left(1+\frac{x}{r}\right)e^{-x/r}\right]^{-1} \tag{14.333}$$

$$= -\left[x^2\prod_{r=1}^{\infty}\left(1-\frac{x^2}{r^2}\right)\right]^{-1}, \tag{14.334}$$

which is also equal to

$$\boxed{\Gamma(x)\Gamma(-x) = -\frac{\pi}{x\sin\pi x}.} \tag{14.335}$$

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Problems

1 Show that the sum of the series

$$\overline{E}_0 = \frac{2\pi}{L}\sum_{n=0}^{\infty} ne^{-2\pi n\alpha/L}$$

is given as

$$\overline{E}_0 = \frac{2\pi}{L}e^{-2\pi\alpha/L}[1-e^{-2\pi\alpha/L}]^{-2}.$$

Expand the result in powers of α to obtain

$$\overline{E}_0 = \frac{L}{2\pi\alpha^2} - \frac{\pi}{6L} + (\text{terms in positive powers of } \alpha).$$

2 Using the Euler–Maclaurin sum formula, find the sum of the series given in Problem 1:

$$\overline{E}_0 = \frac{2\pi}{L}\sum_{n=0}^{\infty} ne^{-2\pi n\alpha/L},$$

and then show that it agrees with the expansion given in the same problem.

3 Find the Casimir energy for the massless conformal scalar field on the surface of a sphere (S-2) with constant radius R_0. The divergent vacuum energy is given as (we set $c = \hbar = 1$)

$$\overline{E}_0 = \frac{1}{2}\sum_{l=0}^{\infty} g_l\omega_l,$$

where the degeneracy, g_n, and the eigenfrequencies, ω_n, are given as

$$g_l = (2l+1), \quad \omega_l = \frac{(l+\frac{1}{2})}{R_0}.$$

Note: Interested students can obtain the eigenfrequencies and the degeneracy by solving the wave equation for the massless conformal scalar field:

$$\Box\Phi(\vec{r},t) + \frac{1}{4}\frac{(n-2)}{(n-1)}R\Phi(\vec{r},t) = 0,$$

where n is the dimension of spacetime, R is the scalar curvature, and $\Box$ is the d'Alembert (wave) operator:

$$\Box = g_{\mu\nu}\partial^\mu\partial_\nu,$$

where ∂_ν stands for the covariant derivative. Use the separation of variables method and impose the boundary condition

$$\Phi = \text{finite}$$

on the sphere. For this problem, spacetime dimension n is 3 and for a sphere of constant radius, R_0, the curvature scalar is $2/R_0^2$.

4 Using asymptotic series, evaluate the logarithmic integral

$$I = \int_0^x \frac{dt}{\ln t}, \quad 0 < x < 1.$$

Hint: Use the substitutions, $t = e^{-u}$ and $a = -\ln x$, $a > 0$, and integrate by parts successively to write the series

$$I = -x\left[\frac{1}{a} - \frac{1!}{a^2} + \frac{2!}{a^3} - \cdots + (-1)^{n-1}\frac{(n-1)!}{a^n}\right] + R_n,$$

where

$$R_n = (-1)^{n+1}n!\int_a^{\infty}\frac{e^{-t}}{t^{n+1}}dt,$$

so that

$$|R_n| < \frac{n!e^{-a}}{a^{n+1}}.$$

5 In a closed Einstein universe, the renormalized energy density of a massless conformal scalar field with thermal spectrum can be written as

$$\langle\rho\rangle_{\text{ren.}} = \frac{1}{2\pi^2 R_0^3}\left[\frac{\hbar c}{R_0}\sum_{n=1}^{\infty}\frac{n^3}{\exp\left(\frac{n\hbar c}{kR_0 T}\right) - 1} + \frac{\hbar c}{240R_0}\right],$$

where R_0 is the constant radius of the universe, T is the temperature of the radiation, and $(2\pi^2 R_0^3)$ is the volume of the universe. The second term:

$$\frac{\hbar c}{240R_0},$$

inside the square brackets is the well-known renormalized quantum vacuum energy, that is, the Casimir energy for the Einstein universe.
First, find the high and low temperature limits of $\langle\rho\rangle_{\text{ren.}}$ and then obtain the flat spacetime limit $R_0 \to \infty$.

6 Without using a calculator evaluate the following sum to five decimal places:

$$\sum_{n=6}^{\infty}\frac{1}{n^2}.$$

How many terms did you have to add?

7 Check the convergence of the following series:
(a) $\sum_{n=1}^{\infty} \dfrac{(\ln n)^2}{n}$,
(b) $\sum_{n=1}^{\infty} n^2 \exp(-n^2)$,
(c) $\sum_{n=1}^{\infty} \ln\left(1 + \frac{1}{n}\right)$,
(d) $\sum_{n=1}^{\infty} \dfrac{(-1)^n n^2}{(2n+1)^2}$,
(e) $\sum_{n=1}^{\infty} \dfrac{\sqrt{n}}{\sqrt{n^4+1}}$,
(f) $\sum_{n=1}^{\infty} \dfrac{\sin^2(nx)}{n^4}$.

8 Find the interval of convergence for the series
(a) $\sum_{n=1}^{\infty} \frac{x^n}{\ln(n+2)}$,
(b) $\sum_{n=1}^{\infty} \frac{(x+1)^n}{\sqrt{n}}$.

9 Evaluate the following sums:
(a) $\sum_{n=0}^{\infty} a^n \cos n\theta$,
(b) $\sum_{n=0}^{\infty} a^n \sin n\theta$, a is a constant.
Hint: Try using complex variables.

10 Verify the following Taylor series:

$$e^x = \sum_{n=0}^{\infty} \frac{x^n}{n!} \quad \text{for all } x,$$

and

$$\frac{1}{1+x^2} = 1 - x^2 + \cdots + (-1)^n x^{2n} + \cdots \quad \text{for } |x| < 1.$$

11 Find the first three nonzero terms of the following Taylor series:
(a) $f(x) = x^3 + 2x + 2$ about $x = 2$,
(b) $f(x) = e^{2x} \cos x$ about $x = 0$.

12 Another important consequence of the Lorentz transformation is the formula for the addition of velocities, where the velocities measured in the K and $\overline{K}$ frames are related by the formula

$$u^1 = \frac{\overline{u}^1 + v}{1 + \overline{u}^1 v/c^2},$$

where

$$u^1 = \frac{dx^1}{dt} \quad \text{and} \quad \overline{u}^1 = \frac{d\overline{x}^1}{d\overline{t}}$$

are the velocities measured in the K and $\overline{K}$ frames, respectively, and $\overline{K}$ is moving with respect to K with velocity v along the common direction of the x- and $\overline{x}$-axes. Using the binomial formula, find an appropriate expansion of the above formula and show that in the limit of small velocities this formula reduces to the well-known Galilean result

$$u^1 = \overline{u}^1 + v.$$

13 In Chapter 9, we have obtained the formulas for the Doppler shift as

$$\omega = \gamma\omega'(1 - \beta\cos\theta),$$
$$\tan\theta' = \sin\theta/\gamma(\cos\theta - \beta),$$

where θ, θ' are the angles of the wave vectors $\vec{k}$ and $\vec{\overline{k}}$ with respect to the relative velocity $\vec{v}$ of the source and the observer. Find the nonrelativistic limit of these equations and interpret your results.

14 Given a power series

$$g(x) = \sum_{n=0}^{\infty} a_n x^n, \quad |x| < R,$$

show that the differentiated and integrated series will have the same radius of convergence.

15 Expand

$$h(x) = \tanh x - \frac{1}{x}$$

as a power series of x.

16 Find the sum

$$g(x) = \frac{1}{1\cdot 2} + \frac{x}{2\cdot 3} + \frac{x^2}{3\cdot 4} + \frac{x^4}{4\cdot 5} + \cdots$$

Hint: First try to convert into geometric series.
Answer: $\left[g(x) = \frac{1}{x} + \frac{1-x}{x^2}\ln(1-x)\right]$.

17 Using the geometric series, evaluate the sum

$$\sum_{n=1}^{\infty} n^3 x^n$$

exactly for the interval $|x| < 1$, then expand your answer in powers of x.

18 Using the Euler–Maclaurin sum formula, evaluate the sum

$$\sum_{n=1}^{\infty} n^3 x^n.$$

Show that it agrees with the expansion found in Problem 14.17.

15

Integral Transforms

Integral transforms are among the most versatile mathematical tools. Their applications range from solutions of differential and integral equations to evaluation of definite integrals. They can even be used to define fractional derivatives and integrals. In this chapter, after a general introduction, we discuss the two of the most frequently used integral transforms, the Fourier and the Laplace transforms and introduce their properties and techniques. We also discuss discrete Fourier transforms and the fast Fourier transform in detail. We finally introduce the Mellin and the Radon transforms, where the latter has some interesting applications to medical technology and CAT scanning.

15.1 Some Commonly Encountered Integral Transforms

Commonly encountered integral transforms allow us to relate two functions through the integral

$$\boxed{g(\alpha) = \int_a^b \kappa(\alpha, t) f(t) dt,} \tag{15.1}$$

where $g(\alpha)$ is called the **integral transform** of $f(t)$ with respect to the **kernel** $\kappa(\alpha, t)$. These transformations are **linear**, that is, if the transforms $g_1(\alpha)$ and $g_2(\alpha)$:

$$g_1(\alpha) = \int_a^b f_1(t)\kappa(\alpha, t)dt, \quad g_2(\alpha) = \int_a^b f_2(t)\kappa(\alpha, t)dt \tag{15.2}$$

exist, then one can write

$$g_1(\alpha) + g_2(\alpha) = \int_a^b [f_1(t) + f_2(t)]\kappa(\alpha, t)dt \tag{15.3}$$

Mathematical Methods in Science and Engineering, Second Edition. Selçuk Ş. Bayın.

and

$$cg_1(\alpha) = \int_a^b [cf_1(t)]\kappa(\alpha, t)dt, \tag{15.4}$$

where c is a constant. Integral transforms can also be shown as an operator:

$$g(\alpha) = \pounds(\alpha, t)f(t), \tag{15.5}$$

where the operator $\pounds(\alpha, t)$ is defined as

$$\pounds(\alpha, t) = \int_a^b dt\ \kappa(\alpha, t). \tag{15.6}$$

We can now show the inverse transform as

$$f(t) = \pounds^{-1}(t, \alpha)g(\alpha). \tag{15.7}$$

Fourier transforms are among the most commonly encountered integral transforms. The Fourier transform, $g(\alpha)$, of a function, $f(x)$, is defined as

$$\boxed{g(\alpha) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} f(t)e^{i\alpha t}dt.} \tag{15.8}$$

Since the kernel of the Fourier transform is also used in defining waves, they are generally used in the study of wave phenomena. Scattering of X-rays from atoms is a typical example, where the Fourier transform of the amplitude of the scattered waves gives the electron distribution. The **Fourier-cosine** and the **Fourier-sine transforms** are defined, respectively, as

$$\boxed{g(\alpha) = \sqrt{\frac{2}{\pi}}\int_0^{\infty} f(t)\cos(\alpha t)dt,} \tag{15.9}$$

$$\boxed{g(\alpha) = \sqrt{\frac{2}{\pi}}\int_0^{\infty} f(t)\sin(\alpha t)dt.} \tag{15.10}$$

Other frequently used kernels are $e^{-\alpha t}$, $tJ_n(\alpha t)$, and $t^{\alpha-1}$. The **Laplace transform** is defined as

$$\boxed{g(\alpha) = \int_0^{\infty} f(t)e^{-\alpha t}dt} \tag{15.11}$$

and it is very useful in finding solutions of systems of ordinary differential equations by converting them into a system of algebraic equations. **Hankel** or **Fourier–Bessel transform** is defined as

$$\boxed{g(\alpha) = \int_0^{\infty} f(t)tJ_n(\alpha t)dt,} \tag{15.12}$$

which is usually encountered in potential energy calculations in cylindrical coordinates. Another useful integral transform is the **Mellin transform**:

$$g(\alpha) = \int_0^{\infty} f(t)t^{\alpha-1}dt. \tag{15.13}$$

The Mellin transform is useful in the reconstruction of "Weierstrass-type" functions from power series expansions. The **Weierstrass function** is defined as

$$f_W(x) = \sum_{n=0}^{\infty} b^n \cos[a^n \pi x], \tag{15.14}$$

where a and b are constants. It has been proven that, provided $0 < b < 1$, $a > 1$, and $ab > 1$, the Weierstrass function has the interesting property of being continuous everywhere but nowhere differentiable. These interesting functions have found widespread use in the study of earthquakes, rupture, and financial crashes.

15.2 Derivation of the Fourier Integral

15.2.1 Fourier Series

Fourier series are very useful in representing a function in a finite interval like $[0, 2\pi]$ or $[-L, L]$, or a periodic function in the infinite interval $(-\infty, \infty)$. We now consider a nonperiodic function in the infinite interval $(-\infty, \infty)$. Physically this corresponds to expressing an arbitrary signal in terms of sine and cosine waves. We first consider the **trigonometric Fourier expansion** of a sufficiently smooth function in the finite interval $[-L, L]$ as

$$f(x) = \frac{1}{2L}\int_{-L}^{L} f(t)dt + \sum_{n=1}^{\infty} a_n \cos\frac{n\pi x}{L} + \sum_{n=1}^{\infty} b_n \sin\frac{n\pi x}{L}, \tag{15.15}$$

where the expansion coefficients, a_n and b_n, are given as

$$a_n = \frac{1}{L}\int_{-L}^{L} f(t)\cos\frac{n\pi t}{L}dt, \tag{15.16}$$

$$b_n = \frac{1}{L}\int_{-L}^{L} f(t)\sin\frac{n\pi t}{L}dt. \tag{15.17}$$

Substituting a_n and b_n explicitly into the Fourier series and using the trigonometric identity $\cos(a-b) = \cos a \cos b + \sin a \sin b$, we get

$$f(x) = \frac{1}{2L}\int_{-L}^{L} f(t)dt + \frac{1}{L}\sum_{n=1}^{\infty}\int_{-L}^{L} f(t)\cos\left[\frac{n\pi}{L}(t-x)\right]dt. \tag{15.18}$$

Since the eigenfrequencies are given as

$$\omega = \frac{n\pi}{L}, \quad n = 0, 1, 2, \dots, \tag{15.19}$$

the difference between two neighboring eigenfrequencies is $\triangle\,\omega = \frac{\pi}{L}$. Using this, we can write $f(x)$ as

$$f(x) = \frac{1}{2L}\int_{-L}^{L} f(t)dt + \frac{1}{\pi}\sum_{n=1}^{\infty}\triangle\,\omega\int_{-\infty}^{\infty} f(t)\cos\omega(t-x)dt. \tag{15.20}$$

We now take the continuum limit, $L \to \infty$, and make the replacement

$$\sum_{n=1}^{\infty}\triangle\,\omega \to \int_{0}^{\infty} d\omega, \tag{15.21}$$

to obtain the **Fourier integral**:

$$\boxed{f(x) = \frac{1}{\pi}\int_{0}^{\infty} d\omega\int_{-\infty}^{\infty} f(t)\cos\omega(t-x)dt,} \tag{15.22}$$

where we have assumed the existence of the integral $\int_{-\infty}^{\infty} f(t)dt$. For the Fourier integral of a function to exist, it is **sufficient** for the integral $\int_{-\infty}^{\infty}|f(t)|dt$ to be convergent.

We can also write the Fourier integral in exponential form. Using the fact that $\sin\omega(t-x)$ is an odd function with respect to ω, we have

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\int_{-\infty}^{\infty} f(t)\sin\omega(t-x)dt = 0. \tag{15.23}$$

Since $\cos\omega(t-x)$ is an even function with respect to ω, we can extend the range of the ω integral in the Fourier integral to $(-\infty, \infty)$:

$$f(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\int_{-\infty}^{\infty} f(t)\cos\omega(t-x)dt. \tag{15.24}$$

We now multiply Eq. (15.23) by i and then add Eq. (15.24) to obtain the **exponential form** of the **Fourier integral** as

$$\boxed{f(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega e^{-i\omega x}\int_{-\infty}^{\infty} f(t)e^{i\omega t}dt.} \tag{15.25}$$

15.2.2 Dirac-Delta Function

Let us now write the Fourier integral as

$$f(x) = \int_{-\infty}^{\infty} f(t) \left\{ \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\omega(t-x)} d\omega \right\} dt, \tag{15.26}$$

where we have interchanged the order of integration. The expression inside the curly brackets is nothing but the **Dirac-delta function**:

$$\boxed{\delta(t-x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\omega(t-x)} d\omega,} \tag{15.27}$$

which has the following properties:

$$\delta(x-a) = 0, \quad x \neq a, \tag{15.28}$$

$$\int_{-\infty}^{\infty} \delta(x-a) dx = 1, \tag{15.29}$$

$$\int_{-\infty}^{\infty} \delta(x-a) f(x) dx = f(a), \tag{15.30}$$

where $f(x)$ is continuous at $x = a$.

15.3 Fourier and Inverse Fourier Transforms

We write the Fourier integral theorem [Eq. (15.25)] as

$$f(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} d\omega e^{-i\omega t} \left[\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(t') e^{i\omega t'} dt' \right] \tag{15.31}$$

and define the **Fourier transform**, $g(\omega)$, of $f(t)$ as

$$\boxed{g(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(t) e^{i\omega t} dt,} \tag{15.32}$$

where the inverse transform is written as

$$\boxed{f(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} g(\omega) e^{-i\omega t} d\omega.} \tag{15.33}$$

15.3.1 Fourier-Sine and Fourier-Cosine Transforms

For an even function, $f_c(-t) = f_c(t)$, using the identity $e^{i\omega t} = \cos\omega t + i\sin\omega t$, we write

$$g_c(\omega) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} f_c(t)(\cos\omega t + i\sin\omega t)dt. \tag{15.34}$$

Since $\sin\omega t$ is an odd function with respect to t, we have the **Fourier-cosine transform**:

$$\boxed{g_c(\omega) = \sqrt{\frac{2}{\pi}}\int_0^{\infty} f_c(t)\cos\omega t dt,} \tag{15.35}$$

$$\boxed{f_c(t) = \sqrt{\frac{2}{\pi}}\int_0^{\infty} g_c(\omega)\cos\omega t d\omega.} \tag{15.36}$$

Similarly, for an odd function, $f_s(-x) = -f_s(x)$, we have the **Fourier-sine transform**:

$$\boxed{g_s(\omega) = \sqrt{\frac{2}{\pi}}\int_0^{\infty} f_s(t)\sin\omega t dt,} \tag{15.37}$$

$$\boxed{f_s(x) = \sqrt{\frac{2}{\pi}}\int_0^{\infty} g_s(\omega)\sin\omega x d\omega.} \tag{15.38}$$

Example 15.1 ***Fourier-sine and Fourier-cosine transform***
Show that the Fourier-sine and the Fourier-cosine transforms satisfy

$$\mathcal{F}_c\{f'(t)\} = \omega\mathcal{F}_s\{f(t)\} - \sqrt{\frac{2}{\pi}}f(0), \tag{15.39}$$

$$\mathcal{F}_s\{f'(t)\} = -\omega\mathcal{F}_c\{f(t)\}, \tag{15.40}$$

where

$$\mathcal{F}_s\{f(t)\} = \sqrt{\frac{2}{\pi}}\int_0^{\infty} f(t)\sin\omega t\, dt, \tag{15.41}$$

$$\mathcal{F}_c\{f(t)\} = \sqrt{\frac{2}{\pi}}\int_0^{\infty} f(t)\cos\omega t\, dt \tag{15.42}$$

and $f(t) \to 0$ as $t \to \pm\infty$. Using these results also find

$$\mathcal{F}_c\{f''(t)\} \text{ and } \mathcal{F}_s\{f''(t)\}. \tag{15.43}$$

Solution
Using integration by parts, we obtain the first relation:

$$\mathcal{F}_c\{f'(t)\} = \sqrt{\frac{2}{\pi}} \int_0^{\infty} \frac{df(t)}{dt} \cos \omega t \, dt \tag{15.44}$$

$$= \sqrt{\frac{2}{\pi}} \left[f(t) \cos \omega t|_0^{\infty} - \int_0^{\infty} f(t) \frac{d \cos \omega t}{dt} dt \right] \tag{15.45}$$

$$= \sqrt{\frac{2}{\pi}} \left[-f(0) + \omega \int_0^{\infty} f(t) \sin \omega t \, dt \right] \tag{15.46}$$

$$= \omega \mathcal{F}_s\{f(t)\} - \sqrt{\frac{2}{\pi}} f(0). \tag{15.47}$$

For the second relation, we follow similar steps. For the remaining two relations, we obtain

$$\mathcal{F}_c\{f''(t)\} = -\omega^2 \mathcal{F}_c\{f(t)\} - \sqrt{\frac{2}{\pi}} f'(0), \tag{15.48}$$

$$\mathcal{F}_s\{f''(t)\} = -\omega^2 \mathcal{F}_s\{f(t)\} + \omega \sqrt{\frac{2}{\pi}} f(0). \tag{15.49}$$

Example 15.2 ***Fourier-sine and Fourier-cosine transform***
Using the results established in the above example, evaluate the Fourier-sine transform $\mathcal{F}_s\{e^{-at}\}$.

Solution
Since

$$f(t) = e^{-at}, \quad f'(t) = -af(t), \quad f''(t) = a^2 f(t), \tag{15.50}$$

we write

$$\mathcal{F}_s\{f''(t)\} = \mathcal{F}_s\{a^2 f(t)\} = a^2 \mathcal{F}_s\{f(t)\}. \tag{15.51}$$

We now write the Fourier-sine transform of the second derivative of $f(t)$ [Eq. (15.49)] as

$$\mathcal{F}_s\{f''(t)\} = -\omega^2 \mathcal{F}_s\{f(t)\} + \omega \sqrt{\frac{2}{\pi}} f(0), \tag{15.52}$$

which when combined with equation (15.51) gives

$$\mathcal{F}_s\{e^{-at}\} = \sqrt{\frac{2}{\pi}} \frac{\omega}{a^2 + \omega^2}. \tag{15.53}$$

15.4 Conventions and Properties of the Fourier Transforms

We have defined the Fourier transform as

$$g(\omega) = \mathcal{F}\{f(t)\} = \frac{1}{(2\pi)^{1/2}} \int_{-\infty}^{\infty} f(t)e^{i\omega t}dt, \tag{15.54}$$

where the inverse Fourier transform is defined as

$$f(t) = \mathcal{F}^{-1}\{g(\omega)\} = \frac{1}{(2\pi)^{1/2}} \int_{-\infty}^{\infty} g(\omega)e^{-i\omega t}d\omega. \tag{15.55}$$

In some books, the sign of $i\omega t$ in the exponential is reversed. However, in applications the final result is not affected. For the coefficients of the integrals, sometimes the following **asymmetric convention** is adopted:

$$g(\omega) = \mathcal{F}\{f(t)\} = \frac{1}{2\pi} \int_{-\infty}^{\infty} f(t)e^{i\omega t}dt, \tag{15.56}$$

$$f(t) = \mathcal{F}^{-1}\{g(\omega)\} = \int_{-\infty}^{\infty} g(\omega)e^{-i\omega t}d\omega, \tag{15.57}$$

where the factor of $1/2\pi$ can also be taken to be in front of the second integral [Eq. (15.57)]:

$$g(\omega) = \mathcal{F}\{f(t)\} = \int_{-\infty}^{\infty} f(t)e^{i\omega t}dt, \tag{15.58}$$

$$f(t) = \mathcal{F}^{-1}\{g(\omega)\} = \frac{1}{2\pi} \int_{-\infty}^{\infty} g(\omega)e^{-i\omega t}d\omega. \tag{15.59}$$

In spectral analysis, instead of the angular frequency, ω, we usually prefer to use the frequency, $\nu = \omega/2\pi$, to write

$$g(\nu) = \mathcal{F}\{f(t)\} = \int_{-\infty}^{\infty} f(t)e^{2\pi i\nu t}dt, \tag{15.60}$$

$$f(t) = \mathcal{F}^{-1}\{g(\nu)\} = \int_{-\infty}^{\infty} g(\nu)e^{-2\pi i\nu t}d\nu. \tag{15.61}$$

Note that the factors in front of the integrals have disappeared all together.

We have already mentioned that both the Fourier transform and its inverse are **linear**:

$$\mathcal{F}\{c_1f_1(t) + c_2f_2(t)\} = c_1\mathcal{F}\{f_1(t)\} + c_2\mathcal{F}\{f_2(t)\}, \tag{15.62}$$

$$\mathcal{F}^{-1}\{c_1g_1(\omega) + c_2g_2(\omega)\} = c_1\mathcal{F}^{-1}\{g_1(\omega)\} + c_2\mathcal{F}^{-1}\{g_2(\omega)\}, \tag{15.63}$$

where c_1 and c_2 are in general complex constants. In addition to linearity, the following properties, which can be proven by direct substitution, are very useful.

15.4.1 Shifting

If the time parameter t is shifted by a positive real constant, a, we get

$$\mathcal{F}\{f(t-a)\} = e^{i\omega a} g(\omega). \tag{15.64}$$

Note that shifting changes only the phase, not the magnitude of the transformation. Similarly, if the frequency is shifted by a, we obtain

$$\mathcal{F}^{-1}\{g(\omega-a)\} = e^{-iat} f(t). \tag{15.65}$$

15.4.2 Scaling

If we rescale the time variable as $t \to at$, $a > 0$, we get

$$\mathcal{F}\{f(at)\} = \frac{1}{a} g\left(\frac{\omega}{a}\right). \tag{15.66}$$

Rescaling ω as $\omega \to a\omega$ gives

$$\mathcal{F}^{-1}\{g(a\omega)\} = \frac{1}{a} f\left(\frac{t}{a}\right). \tag{15.67}$$

15.4.3 Transform of an Integral

Given the integral $\int_{-\infty}^{t} f(t')dt'$, we can write its Fourier transform as

$$\mathcal{F}\left\{\int_{-\infty}^{t} f(t')dt'\right\} = -\frac{1}{i\omega}\mathcal{F}\{f(t)\}. \tag{15.68}$$

15.4.4 Modulation

For a given real number, ω_0, we have [Eq. (15.65)]

$$\mathcal{F}\{f(t)e^{-i\omega_0 t}\} = g(\omega-\omega_0), \tag{15.69}$$

$$\mathcal{F}\{f(t)e^{i\omega_0 t}\} = g(\omega+\omega_0), \tag{15.70}$$

which allows us to write

$$\mathcal{F}\{f(t)\cos(\omega_0 t)\} = \frac{1}{2} g(\omega-\omega_0) + \frac{1}{2} g(\omega+\omega_0), \tag{15.71}$$

$$\mathcal{F}\{f(t)\sin(\omega_0 t)\} = \frac{1}{2i} g(\omega+\omega_0) - \frac{1}{2i} g(\omega-\omega_0). \tag{15.72}$$

These are called the **modulation relations**.

Example 15.3 ***Fourier analysis of finite wave train***
We now find the Fourier transform of a finite wave train, which is given as

$$f(t) = \begin{cases} \sin\omega_0 t, & |t| < \dfrac{N\pi}{\omega_0}, \\ 0, & |t| > \dfrac{N\pi}{\omega_0}. \end{cases} \tag{15.73}$$

For $N = 5$, this wave train is shown in Figure 15.1.

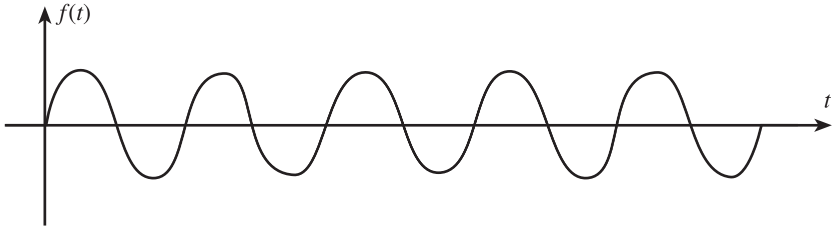


Figure 15.1 Wave train with $N = 5$.

Since $f(t)$ is an odd function, we find its Fourier sine transform as

$$g_s(\omega) = \sqrt{\frac{2}{\pi}}\left[\frac{\sin(\omega_0 - \omega)\frac{N\pi}{\omega_0}}{2(\omega_0 - \omega)} - \frac{\sin(\omega_0 + \omega)\frac{N\pi}{\omega_0}}{2(\omega_0 + \omega)}\right]. \tag{15.74}$$

For frequencies $\omega \sim \omega_0$, only the first term in Eq. (15.74) dominates. Thus $g_s(\omega)$ is given as in Figure 15.2. This is the diffraction pattern for a single slit, which has zeroes at

$$\frac{\omega_0 - \omega}{\omega_0} = \frac{\triangle\omega}{\omega_0} = \pm\frac{1}{N}, \pm\frac{2}{N}, \ldots . \tag{15.75}$$

Because the contribution coming from the central maximum dominates the others, to form the wave train [Eq. (15.73)] it is sufficient to take waves with the spread in their frequency distribution as $\triangle\omega = \frac{\omega_0}{N}$. For a longer wave train, naturally the spread in frequency is less.

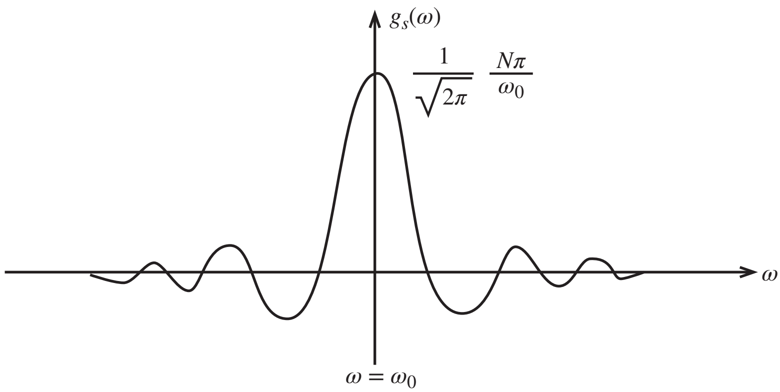


Figure 15.2 $g_s(\omega)$ function.

15.4.5 Fourier Transform of a Derivative

First we write the Fourier transform of $\frac{df(t)}{dt}$:

$$g_1(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \frac{df(t)}{dt} e^{i\omega t} dt, \tag{15.76}$$

and then integrate by parts to obtain

$$g_1(\omega) = \frac{e^{i\omega t}}{\sqrt{2\pi}} f(t)|_{-\infty}^{\infty} - \frac{i\omega}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(t) e^{i\omega t} dt. \tag{15.77}$$

Assuming that

$$f(t) \to 0 \text{ as } t \to \pm\infty, \tag{15.78}$$

we obtain the Fourier transform of the first derivative as

$$g_1(\omega) = -i\omega g(\omega). \tag{15.79}$$

Assuming that all the derivatives

$$f^{n-1}(t),\ f^{n-2}(t),\ f^{n-3}(t), \ldots, f(t) \tag{15.80}$$

go to zero as $t \to \pm\infty$, we write the Fourier transform of the nth derivative as

$$\boxed{g_n(\omega) = (-i\omega)^n g(\omega).} \tag{15.81}$$

Example 15.4 ***Partial differential equations and Fourier transforms***
One of the many uses of integral transforms is solving partial differential equations. Consider vibrations of an infinitely long wire. The equation to be solved is the wave equation:

$$\frac{\partial^2 y(x,t)}{\partial x^2} = \frac{1}{v^2} \frac{\partial^2 y(x,t)}{\partial t^2}, \tag{15.82}$$

where v is the velocity of the wave and $y(x, t)$ is the displacement of the wire from its equilibrium position as a function of position and time. As the initial condition, we take the shape of the wire at $t = 0$:

$$y(x, 0) = f(x). \tag{15.83}$$

We now take the Fourier transform of the wave equation with respect to x:

$$\int_{-\infty}^{\infty} \frac{d^2 y(x,t)}{dx^2} e^{i\alpha x} dx = \frac{1}{v^2} \int_{-\infty}^{\infty} \frac{d^2 y(x,t)}{dt^2} e^{i\alpha x} dx, \tag{15.84}$$

$$(-i\alpha)^2 Y(\alpha, t) = \frac{1}{v^2} \frac{d^2 Y(\alpha, t)}{dt^2}, \tag{15.85}$$

where $Y(\alpha, t)$ represents the Fourier transform of $y(x, t)$:

$$Y(\alpha, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} y(x, t) e^{i\alpha x} dx. \tag{15.86}$$

From Eq. (15.85), we see that the effect of the integral transform on the partial differential equation is to reduce the number of independent variables. Thus the differential equation to be solved for $Y(a, t)$ is now an ordinary differential equation, the solution of which can be written easily as

$$Y(\alpha, t) = F(\alpha) e^{\pm iv\alpha t}, \tag{15.87}$$

where $F(\alpha)$ is the Fourier transform of the initial condition:

$$F(\alpha) = Y(\alpha, 0) \tag{15.88}$$

$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{i\alpha x} dx. \tag{15.89}$$

To be able to interpret this solution, we must go back to $y(x, t)$ by taking the inverse Fourier transform of $Y(a, t)$ as

$$y(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} Y(\alpha, t) e^{-i\alpha x} d\alpha \tag{15.90}$$

$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F(\alpha) e^{-i\alpha(x \mp vt)} d\alpha. \tag{15.91}$$

Because the last expression is nothing but the inverse Fourier transform of $F(\alpha)$, we can write the final solution as

$$y(x, t) = f(x \mp vt). \tag{15.92}$$

This represents a wave moving to the right or left with the velocity v and with its shape unchanged.

15.4.6 Convolution Theorem

Let $F(\omega)$ and $G(\omega)$ be the Fourier transforms of two functions, $f(t)$ and $g(t)$, respectively. The **convolution** $f * g$ is defined as

$$\boxed{f * g = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dt' g(t') f(t - t').} \tag{15.93}$$

Using the shifting property of the Fourier transform [Eq. (15.64)], we can write

$$\int_{-\infty}^{\infty} dt' g(t') f(t-t') = \int_{-\infty}^{\infty} dt' g(t') \left[\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F(\omega) e^{-i\omega(t-t')} d\omega \right] \tag{15.94}$$

$$= \int_{-\infty}^{\infty} d\omega e^{-i\omega t} F(\omega) \left[\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dt' g(t') e^{i\omega t'} \right], \tag{15.95}$$

which is

$$\boxed{\int_{-\infty}^{\infty} g(t') f(t-t') dt' = \int_{-\infty}^{\infty} d\omega F(\omega) G(\omega) e^{-i\omega t'}.} \tag{15.96}$$

In other words, the convolution of $f(t)$ and $g(t)$ is nothing but the inverse Fourier transform of the product of their Fourier transforms:

$$\boxed{f * g = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} d\omega F(\omega) G(\omega) e^{-i\omega t}.} \tag{15.97}$$

For the special case with $t = 0$, we get

$$\int_{-\infty}^{\infty} F(\omega) G(\omega) d\omega = \int_{-\infty}^{\infty} g(t') f(-t') dt'. \tag{15.98}$$

15.4.7 Existence of Fourier Transforms

We can show the Fourier transform of $f(t)$ in terms of an integral operator $\mathfrak{F}$ as

$$F(\omega) = \mathfrak{F}\{f(t)\}, \tag{15.99}$$

$$\mathfrak{F} = \int_{-\infty}^{+\infty} dt e^{i\omega t}. \tag{15.100}$$

For the existence of the Fourier transform of $f(t)$, a **sufficient** but not necessary **condition** [2] is the convergence of the integral $\int_{-\infty}^{\infty} |f(t)| dt$.

15.4.8 Fourier Transforms in Three Dimensions

Fourier transform can also be defined in three dimensions as

$$\boxed{\phi(\overrightarrow{k}) = \frac{1}{\sqrt[3]{2\pi}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} d^3\overrightarrow{r} f(\overrightarrow{r}) e^{i\overrightarrow{k}\cdot\overrightarrow{r}},} \tag{15.101}$$

$$\boxed{f(\overrightarrow{r}) = \frac{1}{\sqrt[3]{2\pi}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} d^3k \phi(\overrightarrow{k}) e^{-i\overrightarrow{k}\cdot\overrightarrow{r}}.} \tag{15.102}$$

Substituting Eq. (15.101) back in Eq. (15.102) and interchanging the order of integration, we obtain the three-dimensional **Dirac-delta function**:

$$\boxed{\delta(\vec{r}-\vec{r}\,')=\frac{1}{(2\pi)^3}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}d^3k e^{i\vec{k}\cdot(\vec{r}-\vec{r}\,')}.} \tag{15.103}$$

These formulas can easily be extended to n dimensions.

15.4.9 Parseval Theorems

Parseval Theorem I

$$\boxed{\int_{-\infty}^{\infty}|F(k)|^2dk=\int_{-\infty}^{\infty}|f(x)|^2dx,} \tag{15.104}$$

Parseval Theorem II

$$\boxed{\int_{-\infty}^{\infty}F(k)G(-k)dk=\int_{-\infty}^{\infty}g(x)f(x)dx.} \tag{15.105}$$

Here, $F(k)$ and $G(k)$ are the Fourier transforms of $f(x)$ and $g(x)$, respectively.

Proof: To prove these theorems, we make the $k\to-k$ change in the Fourier transform of $g(x)$:

$$G(-k)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}g(x)e^{-ikx}dx. \tag{15.106}$$

Multiplying the integral in Eq. (15.106) with $F(k)$ and integrating over k in the interval $(-\infty,\infty)$, we get

$$\int_{-\infty}^{\infty}dkF(k)G(-k)=\int_{-\infty}^{\infty}dkF(k)\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}dxg(x)e^{-ikx}. \tag{15.107}$$

Assuming that the integrals

$$\int_{-\infty}^{\infty}|f(x)|dx \quad \text{and} \quad \int_{-\infty}^{\infty}|g(x)|dx \tag{15.108}$$

converge, we can change the order of the k and x integrals as

$$\int_{-\infty}^{\infty}F(k)G(-k)dk=\int_{-\infty}^{\infty}dxg(x)\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}dkF(k)e^{-ikx}. \tag{15.109}$$

In addition, assuming that the inverse Fourier transform of $F(k)$ exists, the second Parceval theorem is proven.

If we take $f(x) = g(x)$ in Eq. (15.105) and remembering that $G(-k) = G(k)^*$, we can write

$$\int_{-\infty}^{\infty} |G(k)|^2 dk = \int_{-\infty}^{\infty} |g(x)|^2 dx, \tag{15.110}$$

which is the first Parceval theorem. From this proof, it is seen that pointwise existence of the inverse Fourier transform is not necessary; that is, as long as the value of the integral $\int_{-\infty}^{\infty} g(x)f(x)dx$ does not change, the value of the integral $(1/\sqrt{2\pi})\int_{-\infty}^{\infty} dkF(k)e^{-ikx}$ can be different from the value of $f(x)$ at some isolated singular points. In quantum mechanics, wave functions in position and momentum spaces are Fourier transforms of each other. The significance of Parseval's theorems is that normalization in one space ensures normalization in the other.

Example 15.5 ***Diffusion problem in one dimension***
Let us consider a long, thin pipe with cross section A, filled with water and with M amount of salt put at $x = x_0$. We would like to find the concentration of salt as a function of position and time. Because we have a thin pipe, we can neglect the change in concentration across the width of the pipe. The density, $\rho = \rho(x,t)$ g/cm^3 (concentration × mass) satisfies the diffusion equation:

$$\frac{\partial \rho(x,t)}{\partial t} = D\frac{\partial^2 \rho(x,t)}{\partial x^2}. \tag{15.111}$$

At $t = 0$, the density is zero everywhere except at x_0; hence, we write our initial condition as

$$\rho(x,0) = \left(\frac{M}{A}\right)\delta(x - x_0). \tag{15.112}$$

In addition, for all times, the density satisfies $\lim_{x\to\pm\infty}\rho(x,t) = 0$. Because we have an infinite pipe and the density vanishes at the end points, we have to use the Fourier transforms rather than the Fourier series. Since the total amount of salt is conserved, we have

$$\int_{-\infty}^{\infty} \rho(x,t)A dx = M, \tag{15.113}$$

which is sufficient for the existence of the Fourier transform. Taking the Fourier transform of the diffusion equation with respect to x, we get

$$\frac{dR(k,t)}{dt} = -Dk^2 R(k,t). \tag{15.114}$$

This is an ordinary differential equation, where $R(k,t)$ is the Fourier transform of the density. The initial condition for $R(k,t)$ is the Fourier transform of the initial condition for the density:

$$R(k,0) = \mathcal{F}\left\{\left(\frac{M}{A}\right)\delta(x-x_0)\right\} \tag{15.115}$$

$$= \frac{M}{A}\frac{1}{\sqrt{2\pi}}e^{ikx_0}. \tag{15.116}$$

Eq. (15.114) can be solved immediately as

$$R(k,t) = R(k,0)e^{-Dk^2t}, \tag{15.117}$$

$$= \frac{1}{\sqrt{2\pi}}\frac{M}{A}e^{ikx_0}e^{-Dk^2t}. \tag{15.118}$$

For the density, we have to find the inverse Fourier transform of $R(k,t)$:

$$\rho(x,t) = \frac{M}{A2\pi}\int_{-\infty}^{\infty} e^{ikx_0}e^{-Dk^2t}e^{-ikx}dk \tag{15.119}$$

$$= \frac{M}{A2\pi}\int_{-\infty}^{\infty} e^{-Dk^2t-ik(x-x_0)}dk \tag{15.120}$$

$$= \frac{M}{A2\pi}\int_{-\infty}^{\infty} e^{-Dt(k^2+ik\frac{(x-x_0)}{Dt})}dk. \tag{15.121}$$

Completing the square and integrating, we get

$$\rho(x,t) = \frac{M}{A2\pi}\int_{-\infty}^{\infty} e^{-Dt\left[k^2+ik\frac{(x-x_0)}{Dt}-\left(\frac{(x-x_0)}{2Dt}\right)^2+\left(\frac{(x-x_0)}{2Dt}\right)^2\right]}dk \tag{15.122}$$

$$= \frac{M}{A2\pi}\int_{-\infty}^{\infty} e^{-Dt\left[k+\frac{i(x-x_0)}{2Dt}\right]^2}e^{-\frac{(x-x_0)^2}{4Dt}}dk \tag{15.123}$$

$$= \frac{M}{A2\pi}e^{-\frac{(x-x_0)^2}{4Dt}}\int_{-\infty}^{\infty} e^{-Dt\left[k+\frac{i(x-x_0)}{2Dt}\right]^2}dk \tag{15.124}$$

$$= \frac{M}{A2\pi}e^{-\frac{(x-x_0)^2}{4Dt}}\int_{-\infty}^{\infty} e^{-Dtu^2}du \tag{15.125}$$

$$= \frac{M}{A2\pi}e^{-\frac{(x-x_0)^2}{4Dt}}\sqrt{\frac{\pi}{Dt}}. \tag{15.126}$$

Finally, we write the density as

$$\rho(x,t) = \frac{M}{A}\frac{1}{\sqrt{4\pi Dt}}e^{-\frac{(x-x_0)^2}{4Dt}}. \tag{15.127}$$

Check that this solution satisfies the diffusion equation with the initial condition

$$\lim_{t\to 0}\rho(x,t) = \left(\frac{M}{A}\right)\delta(x-x_0). \tag{15.128}$$

Example 15.6 ***Fourier transform of a spherically symmetric function***
Fourier transformation in three dimensions is defined as [Eqs. (15.101) and (15.102)]:

$$\Phi(\overrightarrow{k}) = \frac{1}{\sqrt[3]{2\pi}} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} d^3\overrightarrow{r}\, f(\overrightarrow{r})\, e^{i\overrightarrow{k}\cdot\overrightarrow{r}}, \tag{15.129}$$

$$f(\overrightarrow{r}) = \frac{1}{\sqrt[3]{2\pi}} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} d^3\overrightarrow{k}\, \Phi(\overrightarrow{k})\, e^{-i\overrightarrow{k}\cdot\overrightarrow{r}}. \tag{15.130}$$

We now write the Fourier transform of a spherically symmetric function, $f(\overrightarrow{r}) = f(r)$. In the presence of spherical symmetry, we write $\overrightarrow{k}\cdot\overrightarrow{r} = kr\cos\theta$ and use the volume element $d^3\overrightarrow{r} = r^2 \sin\theta\ drd\theta d\phi$, to obtain the Fourier transform $\mathcal{F}\{f(\overrightarrow{r})\}$ as

$$\mathcal{F}\{f(\overrightarrow{r})\} = \frac{1}{(2\pi)^{3/2}} \int_0^{2\pi} d\phi \int_0^{\infty} f(r) \left[\int_0^{\pi} e^{-ikr\cos\theta} \sin\theta\ d\theta\right] r^2 dr \tag{15.131}$$

$$= \frac{1}{(2\pi)^{3/2}} \int_0^{\infty} f(r) \left[\int_0^{\pi} \frac{1}{ikr} e^{-ikr\cos\theta}\right]_0^{\pi} r^2 dr \tag{15.132}$$

$$= \sqrt{\frac{2}{\pi}}\frac{1}{k} \int_0^{\infty} f(r) r \sin kr\ dr, \tag{15.133}$$

which is now a one-dimensional integral.

Example 15.7 ***Fourier transforms and definite integrals***
To evaluate the integral

$$I = \int_{-\infty}^{\infty} \frac{\sin^2 x}{x^2} dx, \tag{15.134}$$

we first write the Fourier transform of a square wave:

$$\Pi(t) = \begin{cases} 1, & |t| \le 1, \\ 0, & |t| > 1, \end{cases} \tag{15.135}$$

as

$$g(\omega) = \mathcal{F}\{\Pi(t)\} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Pi(t) e^{i\omega t} dt \tag{15.136}$$

$$= \frac{1}{\sqrt{2\pi}} \int_{-1}^{1} e^{i\omega t} dt \tag{15.137}$$

$$= \frac{1}{\sqrt{2\pi}} \frac{2\sin\omega}{\omega}. \tag{15.138}$$

Since $\int_{-\infty}^{\infty} |\Pi(t)|^2 dt = 2$, we now write

$$\int_{-\infty}^{\infty} |g(\omega)|^2 d\omega = \frac{4}{2\pi} \int_{-\infty}^{\infty} \frac{\sin^2\omega}{\omega^2} d\omega \tag{15.139}$$

and use Parceval's first theorem (15.104):

$$\int_{-\infty}^{\infty} |\Pi(t)|^2 dt = \int_{-\infty}^{\infty} |g(\omega)|^2 d\omega, \tag{15.140}$$

to obtain

$$2 = \frac{4}{2\pi} \int_{-\infty}^{\infty} \frac{\sin^2\omega}{\omega^2} d\omega, \tag{15.141}$$

which yields the desired result as

$$\int_{-\infty}^{\infty} \frac{\sin^2\omega}{\omega^2} d\omega = \pi. \tag{15.142}$$

Example 15.8 ***Fourier transforms and differential equations***
Solve the inhomogeneous Helmholtz equation,

$$y'' - k_0^2 y'(t) = f(t), \tag{15.143}$$

with the following boundary conditions:

$$y(t) \to 0 \text{ and } f(t) \to 0 \text{ as } t \to \pm\infty. \tag{15.144}$$

Solution
We first take the Fourier transform of the differential equation:

$$\mathcal{F}\{y'' - k_0^2 y'(t)\} = \mathcal{F}\{f(t)\}, \tag{15.145}$$

$$\mathcal{F}\{y''(t)\} - k_0^2 \mathcal{F}\{y(t)\} = \mathcal{F}\{f(t)\}. \tag{15.146}$$

Utilizing the formula [Eq. (15.81)], which gives the transformation of a derivative, we write

$$-(\omega^2 + k_0^2)\mathcal{F}\{y(t)\} = \mathcal{F}\{f(t)\}. \tag{15.147}$$

Assuming that the Fourier transforms, $\hat{y}(\omega)$ and $\hat{f}(\omega)$, of $y(t)$ and $f(t)$, respectively, exist, we obtain

$$\hat{y}(\omega) = -\frac{\hat{f}(\omega)}{(\omega^2 + k_0^2)}. \tag{15.148}$$

This is the Fourier transform of the needed solution. For the solution, we need to find the inverse transform:

$$y(t) = \mathcal{F}^{-1}\{\hat{y}(\omega)\} \tag{15.149}$$

$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \hat{y}(\omega) e^{-i\omega t} d\omega \tag{15.150}$$

$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} -\frac{\hat{f}(\omega)}{(\omega^2 + k_0^2)} e^{-i\omega t} d\omega. \tag{15.151}$$

In the above expression, the inverse Fourier transforms of $\hat{f}(\omega)$ and $-1/(\omega^2 + k_0^2)$ can be written immediately as

$$\mathcal{F}^{-1}\{\hat{f}(\omega)\} = f(t) \tag{15.152}$$

and

$$\mathcal{F}^{-1}\left\{-\frac{1}{(\omega^2 + k_0^2)}\right\} = -\frac{\sqrt{2\pi}}{2k_0} e^{-k_0|t|}. \tag{15.153}$$

To find the inverse Fourier transform of their product, we utilize the convolution Theorem [Eq. (15.93)] as

$$\int_{-\infty}^{\infty} a(t')b(t - t')dt' = \int_{-\infty}^{\infty} A(\omega)B(\omega)e^{-i\omega t} d\omega, \tag{15.154}$$

where $A(\omega)$ and $B(\omega)$ are the Fourier transforms of $a(t)$ and $b(t)$, respectively, and take

$$B(\omega) = -\frac{1}{(\omega^2 + k_0^2)}, \tag{15.155}$$

$$A(\omega) = \hat{f}(\omega), \tag{15.156}$$

along with their inverses:

$$b(t) = -\frac{\sqrt{2\pi}}{2k_0} e^{-k_0|t|}, \tag{15.157}$$

$$a(t) = f(t), \tag{15.158}$$

to write

$$-\frac{\sqrt{2\pi}}{2k_0} \int_{-\infty}^{\infty} f(t') e^{-k_0|t-t'|} dt' = \int_{-\infty}^{\infty} -\frac{\hat{f}(\omega)}{(\omega^2 + k_0^2)} e^{-i\omega t} d\omega. \tag{15.159}$$

Finally, using Eq. (15.151), we write the solution in terms of an integral which can be evaluated for a given $f(t)$ as

$$y(t) = -\frac{1}{2k_0} \int_{-\infty}^{\infty} f(t') e^{-k_0|t-t'|} dt'. \tag{15.160}$$

15.5 Discrete Fourier Transform

The **Fourier series**, also called the **trigonometric Fourier series**, are extremely useful in analyzing a given signal, $f(x)$, in terms of sinusoidal waves. In exponential form, the Fourier series are written as

$$\boxed{f(x) = \sum_{n=-\infty}^{\infty} c_n e^{2\pi inx/l}, \quad 0 < x < l,} \tag{15.161}$$

where the expansion coefficients, c_n, also called the **Fourier coefficients**, are given as

$$\boxed{c_n = \frac{1}{l}\int_0^l f(x)e^{-2\pi inx/l}dx.} \tag{15.162}$$

This series can be used to represent either a piecewise continuous function in the bounded interval $[0, l]$ or a periodic function with the period l. From the above equations, everything looks straight forward. Given a signal, $f = f(x)$, we first evaluate the definite integral in Eq. (15.162) to find the Fourier coefficients, c_n, which are then used to construct the Fourier series in Eq. (15.161). This gives us the composition of the signal in terms of its sinusoidal components. However, in realistic situations there are many difficulties. First of all, in most cases, the input signal, $f(x)$, can only be given as a finite sequence of numbers with N terms,

$$f = \{f_1, f_2, \dots, f_N\}, \tag{15.163}$$

which may not always be possible to express in terms of a smooth function. Besides, even if we could find a smooth function, $f(x)$, to represent the data, the definite integral in Eq. (15.162) may not be possible to evaluate analytically. In any case, to crunch out a solution, we need to develop a numerical theory of Fourier analysis so that we can feed the problem into a digital computer.

We now divide the interval $[0, l]$ by introducing N evenly spaced points, x_k, as

$$x_k = \frac{kl}{N}, \quad 0 \le k \le N-1, \tag{15.164}$$

where each subinterval has the length

$$\Delta x_k = \frac{l}{N}\Delta k \tag{15.165}$$

$$= \frac{l}{N}. \tag{15.166}$$

We approximate the integral in Eq. (15.162) by the Riemann sum:

$$\tilde{f}_n = \frac{1}{l}\sum_{k=0}^{N-1} f(x_k)e^{-2\pi i n x_k/l}\Delta x_k \tag{15.167}$$

$$= \frac{1}{l}\sum_{k=0}^{N-1} f\left(\frac{kl}{N}\right)e^{-2\pi i k n/N}\Delta x_k, \tag{15.168}$$

where we have written the left-hand side as $\tilde{f}_n$. In general, we can define the **discrete Fourier transform** of any sequence of N terms,

$$f = \{f_j\}, \quad j = 0, 1, \dots, N-1 \tag{15.169}$$

$$= \{f_0, f_1, \dots, f_{N-1}\}, \tag{15.170}$$

as the set

$$\tilde{f} = \{\tilde{f}_j\}, \quad j = 0, 1, \dots, N-1 \tag{15.171}$$

$$= \{\tilde{f}_0, \tilde{f}_1, \dots, \tilde{f}_{N-1}\}, \tag{15.172}$$

where

$$\boxed{\tilde{f}_j = \frac{1}{N}\sum_{k=0}^{N-1} f_k e^{-2\pi i k j/N}, \quad j = 0, 1, \dots, N-1.} \tag{15.173}$$

The **inverse discrete Fourier transform** can be written similarly as

$$\boxed{f_k = \sum_{j=0}^{N-1} \tilde{f}_j e^{2\pi i k j/N}, \quad k = 0, 1, \dots, N-1.} \tag{15.174}$$

To prove the inverse discrete Fourier transform, we substitute $\tilde{f}_j$ [Eq. (15.173)] into Eq. (15.174):

$$f_k = \sum_{j=0}^{N-1} \left[\frac{1}{N}\sum_{l=0}^{N-1} f_l e^{-2\pi i l j/N}\right] e^{2\pi i k j/N} \tag{15.175}$$

$$= \frac{1}{N}\sum_{j=0}^{N-1}\sum_{l=0}^{N-1} f_l e^{2\pi i (k-l) j/N} \tag{15.176}$$

$$= \frac{1}{N}\sum_{l=0}^{N-1} f_l \left[\sum_{j=0}^{N-1} \left(e^{2\pi i (k-l)/N}\right)^j\right]. \tag{15.177}$$

For the inverse discrete transform to be true, we need

$$f_k = \sum_{l=0}^{N-1} f_l \left[\frac{1}{N} \sum_{j=0}^{N-1} \quad (e^{2\pi i(k-l)/N})^j \right] \tag{15.178}$$

$$= \sum_{k=0}^{N-1} f_l \delta_{lk}, \tag{15.179}$$

where

$$\delta_{lk} = \frac{1}{N} \sum_{j=0}^{N-1} (e^{2\pi i(k-l)/N})^j. \tag{15.180}$$

When $l = k$, we have

$$\delta_{kk} = \frac{1}{N} \sum_{j=0}^{N-1} (1)^j. \tag{15.181}$$

Since the sum in the above equation is the sum of N 1's, we obtain the desired result, that is, $\delta_{lk} = 1, l = k$. When $k \neq l$, since k and l are integers, $k - l$ is also an integer satisfying $|k - l| < 1$, hence $|e^{2\pi i(k-l)/N}| < 1$, thus we can use the geometric sum formula:

$$\sum_{n=0}^{M} x^n = \frac{x^{M+1} - 1}{x - 1}, \quad |x| < 1, \tag{15.182}$$

to write

$$\delta_{lk} = \frac{1}{N} \sum_{j=0}^{N-1} \frac{e^{2\pi i(k-l)N/N} - 1}{e^{2\pi i(k-l)/N} - 1}, \quad l \neq k, \tag{15.183}$$

$$= \frac{1}{N} \sum_{j=0}^{N-1} \frac{e^{2\pi i(k-l)} - 1}{e^{2\pi i(k-l)/N} - 1} \tag{15.184}$$

$$= 0, \tag{15.185}$$

thus proving the inverse discrete Fourier transform formula.

In the discrete Fourier transform, the set $\{f_0, f_1, \ldots, f_{N-1}\}$ defines a function, $f(x)$, whose domain is the set of integers $\{0, 1, 2, \ldots, N - 1\}$, and the range of which is $\{f(0) = f_0, f(1) = f_1, \ldots, f(N - 1) = f_{N-1}\}$. In other words, in the discrete Fourier transform, we either describe a function in terms of its **discretization**:

$$f(x) = \left\{ f\left(0 \cdot \frac{l}{N}\right), f\left(1 \cdot \frac{l}{N}\right), \ldots, f\left((N-1) \cdot \frac{l}{N}\right) \right\}, \tag{15.186}$$

or deal with phenomena that can only be described by a sequence of numbers:

$$f(j) = \{f_j\} = \{f_0, f_1, \ldots, f_{N-1}\}. \tag{15.187}$$

The discrete Fourier transform can also be viewed as an operation that maps the set of numbers, $\{f_0, f_1, \dots, f_{N-1}\}$, onto the set $\{\tilde{f}_0, \tilde{f}_1, \dots, \tilde{f}_{N-1}\}$, which is composed of the transformed variables.

For example, consider the set composed of two numbers ($N = 2$):

$$f(i) = \{3, 1\}, \quad i = 0, 1. \tag{15.188}$$

The discrete Fourier transform of this set can be found as

$$\tilde{f}(0) = \frac{1}{2}[f(0)e^{-2\pi i0.0/2} + f(1)e^{-2\pi i1.0/2}] = 2, \tag{15.189}$$

$$\tilde{f}(1) = \frac{1}{2}[f(0)e^{-2\pi i0.1/2} + f(1)e^{-2\pi i1.1/2}] = 1, \tag{15.190}$$

that is,

$$\tilde{f}(j) = \{2, 1\}, \quad j = 0, 1. \tag{15.191}$$

Using the inverse discrete Fourier transform [Eq. (15.174)], we can recover the original set as

$$f(0) = [\tilde{f}(0)e^{2\pi i0.0/2} + \tilde{f}(1)e^{2\pi i0.1/2}] = 3, \tag{15.192}$$

$$f(1) = [\tilde{f}(0)e^{2\pi i1.0/2} + \tilde{f}(1)e^{2\pi i1.1/2}] = 1. \tag{15.193}$$

This result is true in general for arbitrary N and it is usually quoted as the **reciprocity theorem**. In other words, the discrete Fourier transform possesses a **unique inverse**.

With the discrete Fourier transform, we now have an **algorithm** that can be handled by a computer. If we store the numbers

$$f(j), \quad j = 0, 1, \dots, N-1, \tag{15.194}$$

and

$$e^{-2\pi ikj/N}, \quad k = 0, 1, \dots, N-1, \tag{15.195}$$

into two separate registrars, R_1 and R_2, as

$$R_1 = \overline{\underline{|\ f_0\ |\ f_1\ |\ \cdots\ |\ f_{N-1}\ |}} \tag{15.196}$$

and

$$R_2 = \overline{\underline{\left|e^{-2\pi i0j/N}\right|\ e^{-2\pi i1j/N}\left|\ \cdots\ \right|e^{-2\pi i(N-1)j/N}\right|}}, \tag{15.197}$$

so that they can be recalled as needed, we can find how many basic operations, such as additions, multiplications, and divisions, that a computer has to do to compute a discrete Fourier transform, that is, to completely fill a third register R_3 with the Fourier transformed values:

$$R_3 = \overline{\underline{|\ \tilde{f}_0\ |\ \tilde{f}_1\ |\ \cdots\ |\ \tilde{f}_{N-1}\ |}}. \tag{15.198}$$

From Eq. (15.173), it is seen that to find the jth element, $\tilde{f}_j$, we recall the kth entry, f_k, of R_1 and then multiply it with the kth entry, $e^{-2\pi ikj/N}$, of the second registrar R_2. This establishes only one of the terms in the sum [Eq. (15.173)]. This means one multiplication for each term in the sum. Since there are N terms in the sum, the computer performs N multiplications. Then we add these N terms, which requires $N-1$ additions. Finally, we divide the result by N, that is, one more operation. All together, to evaluate the jth term, we need $N+(N-1)+1=2N$ basic operations. There are N such terms to be calculated, hence the computer has to perform $2N^2$ basic operations to find the discrete Fourier transform of a set with N terms. Since each basic operation takes a certain amount of time for a given computer, this is also a measure of how fast the computation will be carried out.

15.6 Fast Fourier Transform

We start with a sequence of N terms, $\{f(j)\}$, with the discrete Fourier transform, $\{\tilde{f}(j)\}$, where $j=0,1,\ldots,N-1$. Let us assume that N is even so that we can write $\frac{N}{2}=M$, where M is an integer. We now split $\{f(j)\}$ into two new sequences

$$\{f_1(j)\} = \{f(2j)\}, \tag{15.199}$$

$$\{f_2(j)\} = \{f(2j+1)\}, \tag{15.200}$$

where $j=0,1,\ldots,M-1$. Note that both $\{f_1(j)\}$ and $\{f_2(j)\}$ are periodic sequences with the period M. We can now use Eq. (15.173) to write their discrete Fourier transforms as

$$\{\tilde{f}_1(j)\} = \frac{1}{M}\sum_{k=0}^{M-1} f_1(k)e^{-2\pi ikj/M}, \quad j=0,1,\ldots,M-1, \tag{15.201}$$

$$\{\tilde{f}_2(j)\} = \frac{1}{M}\sum_{k=0}^{M-1} f_2(k)e^{-2\pi ikj/M}, \quad j=0,1,\ldots,M-1. \tag{15.202}$$

We now return to the discrete Fourier transform of the full set $\{f(j)\}$ and write

$$\{\tilde{f}(j)\} = \frac{1}{N}\sum_{k=0}^{N-1} f(k)e^{-2\pi ikj/N}, \tag{15.203}$$

which can be rearranged as

$$\{\tilde{f}(j)\} = \frac{1}{N}\sum_{k=0}^{M-1} f(2k)e^{-2\pi i(2k)j/N} + \frac{1}{N}\sum_{k=0}^{M-1} f(2k+1)e^{-2\pi i(2k+1)j/N}. \tag{15.204}$$

Using the relations

$$e^{-2\pi i(2k)j/N} = e^{-2\pi ikj/M}, \tag{15.205}$$

$$e^{-2\pi i(2k+1)j/N} = e^{-2\pi ikj/M} e^{-2\pi ij/N}, \tag{15.206}$$

we write Eq. (15.204) as

$$\{\tilde{f}(j)\} = \frac{1}{N} \sum_{k=0}^{M-1} f_1(k) e^{-2\pi ikj/M} + \frac{e^{-2\pi ij/N}}{N} \sum_{k=0}^{M-1} f_2(k) e^{-2\pi ikj/M}, \tag{15.207}$$

where $j = 0, 1, \ldots, N-1$. This is nothing but

$$\{\tilde{f}(j)\} = \frac{\{\tilde{f}_1(j)\}}{2} + \frac{e^{-2\pi ij/N}\{\tilde{f}_2(j)\}}{2}, \quad j = 0, 1, \ldots, N-1. \tag{15.208}$$

Since both $\{\tilde{f}_1(j)\}$ and $\{\tilde{f}_2(j)\}$ are periodic with the period M, that is,

$$\{\tilde{f}_{1 \text{ or } 2}(j+M)\} = \{\tilde{f}_{1 \text{ or } 2}(j)\}, \tag{15.209}$$

we have extended the range of the index j to $N-1$.

We have seen that the sum in Eq. (15.173) requires $2N^2$ basic operations to yield the discrete Fourier transform $\{\tilde{f}(j)\}$. All we have done in Eq. (15.208) is to split the original sum into two parts. Let us see what advantage comes out of this. In order to compute the discrete Fourier transform, $\{\tilde{f}(j)\}$, via the rearranged expression [Eq. (15.208)], we first have to construct the transforms $\{\tilde{f}_1(j)\}$ and $\{\tilde{f}_2(j)\}$, each of which requires $2M^2$ basic operations. Next, we need N multiplications to establish the product of the elements of $\{\tilde{f}_2(j)\}$ with $e^{-2\pi ij/N}$, which will be followed by the $N-1$ additions of the elements of the sets $\{\tilde{f}_1(j)\}$ and $e^{-2\pi ij/N}\{\tilde{f}_2(j)\}$, each of which has N elements. Finally, the sum

$$\{\tilde{f}_1(j)\} + e^{-2\pi ij/N}\{\tilde{f}_2(j)\} \tag{15.210}$$

has to be divided by 2, that is, 1 division to yield the final result:

$$\{\tilde{f}(j)\} = \frac{1}{2}\left[\{\tilde{f}_1(j)\} + e^{-2\pi ij/N}\{\tilde{f}_2(j)\}\right], \quad j = 0, 1, \ldots, N-1. \tag{15.211}$$

All together, this means

$$2M^2 + 2M^2 + N + (N-1) + 1 = N^2 + 2N \tag{15.212}$$

operations, where we have substituted $N = M/2$ in the last step.

In summary, calculating $\{\tilde{f}(j)\}, j = 0, 1, \ldots, N-1$, directly requires $2N^2$ basic operations, while the new approach, granted that N is even, requires $N^2 + 2N$ operations. The fractional reduction in the number of operations is

$$\frac{N^2 + 2N}{2N^2} = \frac{1}{2} + \frac{1}{N}, \tag{15.213}$$

which approaches to $1/2$ as N gets very large. Since each operation takes a certain time in a computer, a reduction in the number of operations by half implies a significant reduction in the overall operation time of the computer.

Wait! we can do even better with this **divide and conquer** strategy. If N is divisible by 4, we can further subdivide the sequences $\{f_1(j)\}$ and $\{f_2(j)\}$ into four new sequences with $M/2$ terms each. Furthermore, if $N = 2^p$, $p > 0$ integer, which is the case of complete reduction, it can be shown that for large N we can achieve a reduction factor of $\log_2 p/N$. Compared to $2N^2$, this is remarkably small and will result in significant reduction of the running time of our computer. We should also add that the actual execution speed of a computer is only proportional to the number of operations and depends also on a number of other critical technical parameters. Note that in cases where our sequence does not have the desired number of terms, we can always add sufficient number of zeros to match the required number. This procedure which tremendously shortens the number of operations needed to compute a discrete Fourier transform was first introduced by Tukey and Cooley in 1965. It is now called the **fast Fourier transform**, and it is considered to be one of the most significant contributions to the field of numerical analysis.

15.7 Radon Transform

Radon transforms were introduced by an Austrian mathematician Johann Radon in 1917. They are extremely useful in medical technology and establish the mathematical foundations of computational axial tomography, that is, CAT scanning. Radon transforms are also very useful in electron microscopy and reflection seismology.

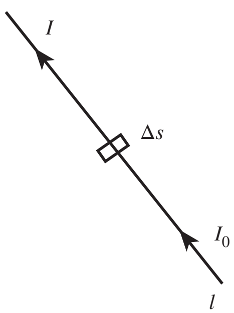


Figure 15.3 A narrow beam going through a homogeneous material of thickness Δs.

To introduce the basic properties of the two-dimensional Radon transforms, consider a narrow beam of X-ray travelling along a straight line (Figure 15.3). As the beam passes through a homogeneous material of length Δs, the initial intensity I_0 will decrease exponentially according to the formula

$$I = I_0 e^{-\alpha\rho\Delta s}, \tag{15.214}$$

where ρ is the linear density along the direction of propagation and α is a positive constant depending on other physical parameters of the medium. If the beam is going through a series of parallel layers described by α_i, ρ_i, and Δs_i, where the index $i = 1, 2, \ldots, n$, denotes the ith layer, we can write the final intensity as

$$I = I_0 e^{-[\alpha_1\rho_1\Delta s_1 + \alpha_2\rho_2\Delta s_2 + \cdots + \alpha_n\rho_n\Delta s_n]}. \tag{15.215}$$

In the continuum limit, we can write this as

$$I = I_0 e^{-\int_l \alpha(\vec{x})\rho(\vec{x})ds_{(x,y)}}, \tag{15.216}$$

where (x, y) is a point on the ray l, and

$$\int_l \alpha(\vec{x})\rho(\vec{x})ds_{(x,y)} \tag{15.217}$$

is a line integral taken over a straight line representing the path of the X-ray. We usually write

$$f(x, y) = \alpha(\vec{x})\rho(\vec{x}), \tag{15.218}$$

where $f(x, y)$ represents the attenuation coefficient of the object, hence Eq. (15.216) becomes

$$\boxed{-\ln\left(\frac{I}{I_0}\right) = \int_l f(x, y)ds_l.} \tag{15.219}$$

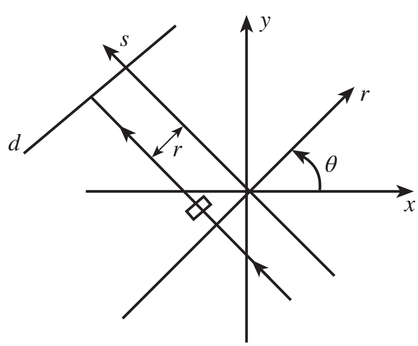
The line integral on the right-hand side is called the **Radon transform** of $f(x, y)$. Along the path of the X-ray, which is a straight line with the equation $y_l = y_l(x), f(x, y_l(x))$ represents the attenuation coefficient along the path of the X-ray.

The method used in the first scanners was to use a system of parallel lines that represents the X rays that scan a certain slice of a three-dimensional object, where $f(x, y)$ represents the attenuation coefficient of the slice. For a mathematical description of the problem, we parametrize the parallel rays in terms of their perpendicular distances to a reference line s and the projection angle θ (Figure 15.4). Now the scanning data consists of a series of Radon transforms of the attenuation coefficient, $f(x, y)$, projected onto the plane of the detector (Figure 15.5). The **projection-slice theorem** says that given an infinite number of one-dimensional projections of an object taken from infinitely many directions, one could perfectly reconstruct the original object, that is, $f(x, y)$.

The Radon transform for a family of parallel lines, l, is shown as

$$R_2[f](l) = \int_l f(x, y_l)ds_l, \tag{15.220}$$

Figure 15.4 Reference axes s and r, projection angle θ and the detector plane d.



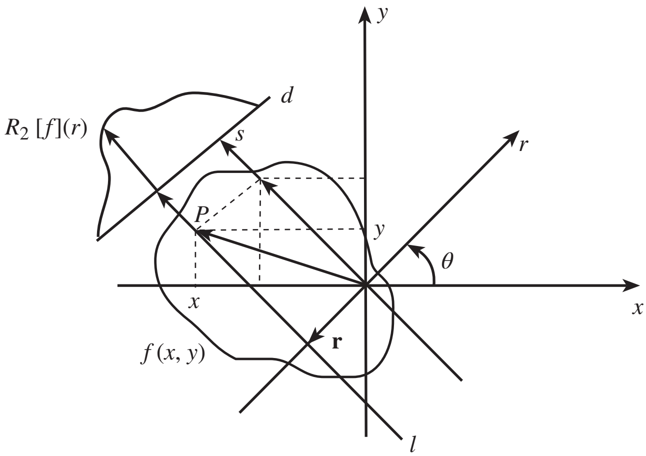


Figure 15.5 Projection of $f(x, y)$ onto the detector surface d.

where the subscript 2 indicates that this is a two-dimensional Radon transform and $R_2[f]$ is a function of lines. In general, $f(x, y)$ is a continuous function on the plane that vanishes outside a finite region. For a given ray, l, we parametrize a point P on the ray as (Figure 15.5)

$$x = s\cos(\pi/2 + \theta) + r\cos(\pi + \theta), \tag{15.221}$$

$$y = s\sin(\pi/2 + \theta) + r\sin(\pi + \theta), \tag{15.222}$$

or as

$$x = -s\sin\theta - r\cos\theta, \tag{15.223}$$

$$y = s\cos\theta - r\sin\theta. \tag{15.224}$$

Hence, we can write Eq. (15.220) as

$$R_2[f](\theta, r) = \int_{-\infty}^{\infty} f(-s\sin\theta - r\cos\theta, s\cos\theta - r\sin\theta)ds. \tag{15.225}$$

Note that on a given ray, that is, a straight line in the family of parallel lines, r is fixed and s is the variable.

To find the desired quantity that represents the physical characteristics of the object, $f(x, y)$, we need to find the inverse Radon transform. This corresponds to integrating the Radon transform at (x, y) for all angles:

$$f(x, y) = \int_0^{2\pi} R_2[f](\theta, -x\cos\theta + y\sin\theta)d\theta, \tag{15.226}$$

where using Figure 15.5, we have substituted $r = -x\cos\theta + y\sin\theta$. This method of inversion is proven to be rather unstable with respect to noisy data; hence in applications, an efficient algorithm in terms of its discretized version, called the **filtered back-projection**, is preferred. A lot of research has been done in improving the performance of CAT scanners and improving the practical means of inverting Radon transforms. Radon transforms can also be defined in dimensions higher than two [6]. Besides medicine, electron microscopy of small objects like viruses, and reflection seismography, Radon transforms have also interesting applications in nondestructive testing, stress analysis, astronomy, nuclear magnetic resonance, and optics.

15.8 Laplace Transforms

The Laplace transform of a function is defined as the limit

$$\lim_{a\to\infty}\int_0^a e^{-st}F(t)dt, \quad s>0, \tag{15.227}$$

where s is real. When the limit exists, we simply write

$$\boxed{f(s)=\pounds\{F(t)\}=\int_0^\infty e^{-st}F(t)dt, \quad s>0.} \tag{15.228}$$

For this transformation to exist, we do not need the existence of the integral $\int_0^\infty F(t)dt$. In other words, $F(t)$, could diverge exponentially for large values of t. However, if there exists a constant s_0 and a positive constant C, such that for sufficiently large t, that is, $t>t_0$, the inequality

$$|e^{-s_0t}F(t)|\le C \tag{15.229}$$

is satisfied, then the Laplace transform of this function exists for $s>s_0$. An example is $F(t)=e^{2t^2}$. For this function, we cannot find a suitable s_0 and a C value that satisfies Eq. (15.229); hence, its Laplace transform does not exist. The Laplace transform may also fail to exist if the function $F(t)$ has a sufficiently strong singularity as $t\to 0$. The Laplace transform of t^n:

$$\pounds\{t^n\}=\int_0^\infty e^{-st}t^n dt, \tag{15.230}$$

does not exist for $n\le -1$, because it has a singular point at the origin. On the other hand, for $s>0$ and $n>-1$, the Laplace transform is given as

$$\pounds\{t^n\}=\frac{n!}{s^{n+1}}. \tag{15.231}$$

15.9 Inverse Laplace Transforms

Using operator language, we can show the Laplace transform of a function as

$$f(s)=\pounds\{F(t)\}. \tag{15.232}$$

The inverse transform of $f(s)$ is now shown with $£^{-1}$ as

$$£^{-1}\{f(s)\} = F(t). \tag{15.233}$$

In principle, the inverse transform is not unique. Two functions, $F_1(t)$ and $F_2(t)$, could have the same Laplace transform; however, in such cases the difference of these functions is

$$F_1(t) - F_2(t) = N(t), \tag{15.234}$$

where for all t_0 values $N(t)$ satisfies

$$\int_0^{t_0} N(t)dt = 0. \tag{15.235}$$

In other words, $N(t)$ is a **null function**. This result is also known as the **Lerch theorem**. In practice, we can take $N(t)$ as zero, thus making the inverse Laplace transform unique. In Figure 15.6, we show a null function.

15.9.1 Bromwich Integral

A formal expression for the inverse Laplace transform is given in terms of the **Bromwich integral**:

$$\boxed{F(t) = \lim_{\alpha\to\infty} \frac{1}{2\pi i} \int_{\gamma-i\alpha}^{\gamma+i\alpha} e^{st} f(s)ds,} \tag{15.236}$$

where γ is real and s is a complex variable. The contour for the above integral is an infinite straight line passing through the point γ and parallel to the imaginary axis in the complex s-plane. Here, γ is chosen such that all the singularities of $e^{st}f(s)$ are to the left of the straight line. For $t > 0$, we can close the contour with an infinite semicircle to the left-hand side of the line. The above integral

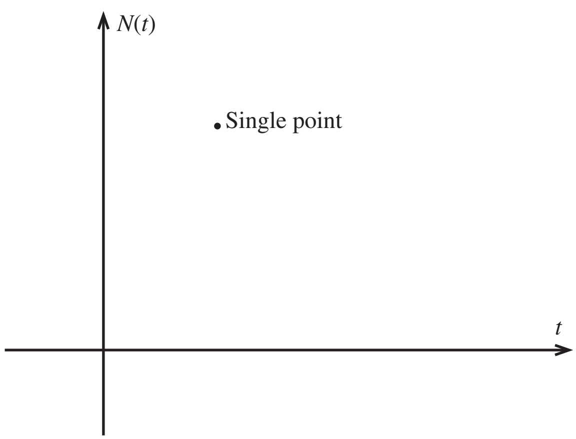


Figure 15.6 Null function.

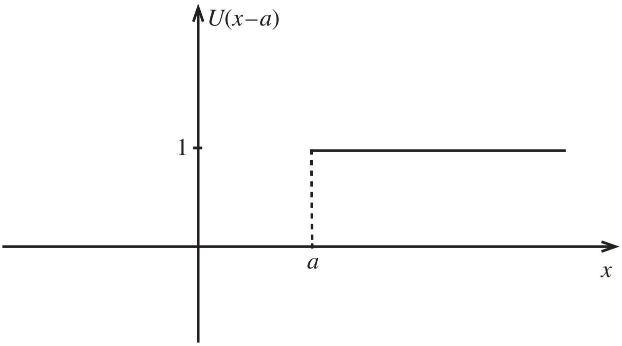


Figure 15.7 Heaviside step function.

can now be evaluated by using the residue theorem to find the inverse Laplace transform.

The Bromwich integral is a powerful tool for inverting complicated Laplace transforms when other means prove inadequate. However, in practice using the fact that Laplace transforms are linear, and with the help of some basic theorems, we can generate many of the inverses needed from a list of elementary Laplace transforms.

15.9.2 Elementary Laplace Transforms

1. Many of the discontinuous functions can be expressed in terms of the Heaviside step function (Figure 15.7):

$$U(t-a) = \begin{cases} 0 & t < a \\ 1 & t > a \end{cases}, \tag{15.237}$$

   the Laplace transform of which is given as

$$\pounds\{U(t-a)\} = \frac{e^{-as}}{s}, \quad s > 0. \tag{15.238}$$

2. For $F(t) = 1$, the Laplace transform is given as

$$\pounds\{1\} = \int_0^\infty e^{-st} dt = \frac{1}{s}, \quad s > 0. \tag{15.239}$$

3. The Laplace transform of $F(t) = e^{kt}$ for $t > 0$ is

$$\pounds\{e^{kt}\} = \int_0^\infty e^{kt} e^{-st} dt = \frac{1}{s-k}, \quad s > k. \tag{15.240}$$

4. Laplace transforms of hyperbolic functions:

$$F(t) = \cosh kt = \frac{1}{2}(e^{kt} + e^{-kt}), \tag{15.241}$$

$$F(t) = \sinh kt = \frac{1}{2}(e^{kt} - e^{-kt}), \tag{15.242}$$

can be found by using the fact that $\pounds$ is a linear operator as

$$\pounds\{\cosh kt\} = \frac{1}{2}\left(\frac{1}{s-k} + \frac{1}{s+k}\right) = \frac{s}{s^2-k^2}, \quad s > k, \tag{15.243}$$

$$\pounds\{\sinh kt\} = \frac{k}{s^2-k^2}, \quad s > k. \tag{15.244}$$

5. Using the relations

$$\cos kt = \cosh ikt \quad \text{and} \quad \sin kt = -i \sinh kt,$$

we can find the Laplace transforms of the cos and the sin functions as

$$\pounds\{\cos kt\} = \frac{s}{s^2+k^2}, \quad s > 0, \tag{15.245}$$

$$\pounds\{\sin kt\} = \frac{k}{s^2+k^2}, \quad s > 0. \tag{15.246}$$

6. For $F(t) = t^n$, we have

$$\pounds\{t^n\} = \frac{n!}{s^{n+1}}, \quad s > 0,\ n > -1. \tag{15.247}$$

15.9.3 Theorems About Laplace Transforms

By using the entries in a list of transforms, the following theorems are very useful in finding inverses of unknown transforms:

Theorem 15.1 ***First Translation Theorem*** If the function $f(t)$ has the Laplace transform

$$\pounds\{f(t)\} = F(s), \tag{15.248}$$

then the Laplace transform of $e^{at}f(t)$ is given as

$$\pounds\{e^{at}f(t)\} = F(s-a). \tag{15.249}$$

Similarly, if $\pounds^{-1}\{F(s)\} = f(t)$ is true, then we can write

$$\pounds^{-1}\{F(s-a)\} = e^{at}f(t). \tag{15.250}$$

Proof:

$$\pounds\{e^{at}f(t)\} = \int_0^\infty e^{at}f(t)e^{-st}dt \tag{15.251}$$

$$= \int_0^\infty e^{-(s-a)t}f(t)dt \tag{15.252}$$

$$= F(s-a). \tag{15.253}$$

Theorem 15.2 ***Second Translation Theorem*** If $F(s)$ is the Laplace transform of $f(t)$ and the Heaviside step function is shown as $U(t-a)$, we can write

$$£\{U(t-a)f(t-a)\} = e^{-as}F(s). \tag{15.254}$$

Similarly, if $£^{-1}\{F(s)\} = f(t)$ is true, then we can write

$$£^{-1}\{e^{-as}F(s)\} = U(t-a)f(t-a). \tag{15.255}$$

Proof: Since the Heaviside step function is defined as

$$U(t-a) = \begin{cases} 0 & t < a \\ 1 & t > a \end{cases}, \tag{15.256}$$

we can write

$$£\{U(t-a)f(t-a)\} = \int_0^\infty e^{-st}U(t-a)f(t-a)dt \tag{15.257}$$

$$= \int_a^\infty e^{-st}f(t-a)dt. \tag{15.258}$$

Changing the integration variable to $v = t - a$, we obtain

$$£\{U(t-a)f(t-a)\} = \int_0^\infty e^{-s(v+a)}f(v)dv \tag{15.259}$$

$$= e^{-as}\int_0^\infty e^{-sv}f(v)dv \tag{15.260}$$

$$= e^{-as}F(s). \tag{15.261}$$

Theorem 15.3 If $£\{f(t)\} = F(s)$ is true, then we can write

$$£\{f(at)\} = \frac{1}{a}F\left(\frac{s}{a}\right). \tag{15.262}$$

If $£^{-1}\{F(s)\} = f(t)$ is true, then we can write the inverse as

$$£^{-1}\left\{F\left(\frac{s}{a}\right)\right\} = af(at). \tag{15.263}$$

Proof: Using the definition of the Laplace transform, we write

$$£\{f(at)\} = \int_0^\infty e^{-st}f(at)dt. \tag{15.264}$$

Changing the integration variable to $v = at$, we find

$$£\{f(at)\} = \frac{1}{a}\int_0^\infty e^{-sv/a}f(v)dv \tag{15.265}$$

$$= \frac{1}{a}F\left(\frac{s}{a}\right). \tag{15.266}$$

Theorem 15.4 ***Derivative of a Laplace Transform*** If the Laplace transform of $f(t)$ is $F(s)$, then the Laplace transform of $t^n f(t)$ is given as

$$£\{t^n f(t)\} = (-1)^n \frac{d^n F(s)}{dt^n} = (-1)^n F^{(n)}(s), \tag{15.267}$$

where $n = 0, 1, 2, 3 \dots$.

Similarly, if $£^{-1}\{F(s)\} = f(t)$ is true, then we can write

$$£^{-1}\{F^{(n)}(s)\} = (-1)^n t^n f(t). \tag{15.268}$$

Proof: Since $£\{f(t)\} = F(s)$, we write

$$F(s) = \int_0^\infty e^{-st} f(t) dt. \tag{15.269}$$

Taking the derivative of both sides with respect to s, we get

$$\int_0^\infty e^{-st} t f(t) dt = -F'(s). \tag{15.270}$$

If we keep on differentiating, we find

$$\int_0^\infty e^{-st} t^2 f(t) dt = F''(s), \tag{15.271}$$

$$\int_0^\infty e^{-st} t^3 f(t) dt = -F'''(s), \tag{15.272}$$

and eventually the nth derivative as

$$\int_0^\infty e^{-st} t^n f(t) dt = (-1)^n F^{(n)}(s). \tag{15.273}$$

Theorem 15.5 ***Laplace Transform of Periodic Functions*** If $f(t)$ is a periodic function with the period $p > 0$, that is, $f(t+p) = f(t)$, then we can write

$$£\{f(t)\} = \frac{\int_0^p e^{-st} f(t) dt}{1 - e^{-sp}}. \tag{15.274}$$

On the other hand, if $£^{-1}\{F(s)\} = f(t)$ is true, then we can write

$$£^{-1}\left\{ \frac{\int_0^p e^{-st} f(t) dt}{1 - e^{-sp}} \right\} = f(t). \tag{15.275}$$

Proof: We first write

$$£\{f(t)\} = \int_0^\infty e^{-st} f(t)dt \tag{15.276}$$

$$= \int_0^p e^{-st} f(t)dt + \int_p^{2p} e^{-st} f(t)dt + \int_{2p}^{3p} e^{-st} f(t)dt + \cdots \tag{15.277}$$

$$= \int_0^p e^{-st} f(t)dt + \int_0^p e^{-s(v+p)} f(v+p)dv \tag{15.278}$$

$$+ \int_0^p e^{-s(v+2p)} f(v+2p)dv + \cdots .$$

Making the variable change $v \to t$ and using the fact that $f(t)$ is periodic we get

$$\int_0^\infty e^{-st} f(t)dt = \int_0^p e^{-st} f(t)dt + e^{-sp} \int_0^p e^{-st} f(t)dt \tag{15.279}$$

$$+ e^{-s2p} \int_0^p e^{-st} f(t)dt + \cdots$$

$$= (1 + e^{-sp} + e^{-s2p} + e^{-s3p} + \cdots) \int_0^p e^{-st} f(t)dt \tag{15.280}$$

$$= \frac{\int_0^p e^{-st} f(t)dt}{1 - e^{-sp}}, \quad s > 0. \tag{15.281}$$

Theorem 15.6 ***Laplace Transform of an Integral*** If the Laplace transform of $f(t)$ is $F(s)$, then we can write

$$£\left\{ \int_0^t f(u)du \right\} = \frac{F(s)}{s}. \tag{15.282}$$

Similarly, if $£^{-1}\{F(s)\} = f(t)$ is true, then the inverse will be given as

$$£^{-1}\left\{ \frac{F(s)}{s} \right\} = \int_0^t f(u)du. \tag{15.283}$$

Proof: Let us define the $G(t)$ function as

$$G(t) = \int_0^t f(u)du. \tag{15.284}$$

Now we have $G'(t) = f(t)$ and $G(0) = 0$; thus we can write

$$£\{G'(t)\} = s£\{G(t)\} - G(0) \tag{15.285}$$

$$= s£\{G(t)\}, \tag{15.286}$$

which gives

$$£\{G(t)\} = £\left\{\int_0^t f(u)du\right\} = \frac{1}{s}£\{f(t)\} = \frac{F(s)}{s}. \tag{15.287}$$

Theorem 15.7 If the limit $\lim_{t\to 0}\frac{f(t)}{t}$ exists and if the Laplace transform of $f(t)$ is $F(s)$, then we can write

$$£\left\{\frac{f(t)}{t}\right\} = \int_s^\infty F(u)du. \tag{15.288}$$

Similarly, if $£^{-1}\{F(s)\} = f(t)$ is true, then we can write

$$£^{-1}\left\{\int_s^\infty F(u)du\right\} = \frac{f(t)}{t}. \tag{15.289}$$

Proof: If we write $g(t) = \frac{f(t)}{t}$, we can take $f(t) = tg(t)$. Hence, we can write

$$F(s) = £\{f(t)\} \tag{15.290}$$

$$= £\{tg(t)\} = -\frac{d}{ds}£\{g(t)\} = -\frac{dG(s)}{ds}, \tag{15.291}$$

where we have used Theorem 15.6. Thus we can write

$$G(s) = -\int_c^s F(u)du. \tag{15.292}$$

From the limit $\lim_{s\to\infty} G(s) = 0$, we conclude that $c = \infty$. Hence, we obtain

$$G(s) = £\left\{\frac{f(t)}{t}\right\} = \int_s^\infty F(u)du. \tag{15.293}$$

Theorem 15.8 ***Convolution Theorem*** If the Laplace transforms of $f(t)$ and $g(t)$ are given as $F(s)$ and $G(s)$, respectively, we can write

$$£\left\{\int_0^t f(u)g(t-u)du\right\} = F(s)G(s). \tag{15.294}$$

Similarly, if the inverses $£^{-1}\{F(s)\} = f(t)$ and $£^{-1}\{G(s)\} = g(t)$ exist, then we can write

$$£^{-1}\{F(s)G(s)\} = \int_0^t f(u)g(t-u)du. \tag{15.295}$$

The above integral is called the **convolution** of $f(t)$ and $g(t)$, and it is shown as $f * g$:

$$\boxed{f * g = \int_0^t f(u)g(t-u)du.} \tag{15.296}$$

The convolution operation has the following properties:

$$\begin{aligned} f * g &= g * f, \\ f * (g + h) &= f * g + f * h, \\ f * (g * h) &= (f * g) * h. \end{aligned} \tag{15.297}$$

Proof: We first write the product of $F(s)$ and $G(s)$:

$$F(s)G(s) = \left[\int_0^{\infty} e^{-su} f(u) du\right]\left[\int_0^{\infty} e^{-sv} g(v) dv\right] \tag{15.298}$$

$$= \int_0^{\infty}\int_0^{\infty} e^{-s(v+u)} g(v) f(u) du dv. \tag{15.299}$$

Using the transformation $v = t - u$, we obtain

$$F(s)G(s) = \int_{t=0}^{\infty}\int_{u=0}^{t} e^{-st} g(t-u) f(u) du dt \tag{15.300}$$

$$= \int_{t=0}^{\infty} e^{-st}\left[\int_{u=0}^{t} g(t-u) f(u) du\right] dt \tag{15.301}$$

$$= £\left\{\int_0^{t} f(u) g(t-u) du\right\}. \tag{15.302}$$

Note that with the $t = u + v$ transformation, we have gone from the uv-plane to the ut-plane.

Example 15.9 ***Inverse Laplace transforms***

1. We now find the function with the Laplace transform

$$\frac{se^{-2s}}{s^2 + 16}. \tag{15.303}$$

Since

$$£\left\{\frac{s}{s^2 + 16}\right\} = \cos 4t, \tag{15.304}$$

we can use Theorem 15.2, which says

$$£\{U(t-a) f(t-a)\} = e^{-as} F(s). \tag{15.305}$$

Using the inverse

$$£^{-1}\{e^{-as} F(s\} = U(t-a) f(t-a), \tag{15.306}$$

we find

$$£^{-1}\left\{e^{-2s}\left(\frac{s}{s^2 + 16}\right)\right\} = U(t-2)\cos 4(t-2) \tag{15.307}$$

$$= \begin{cases} 0, & t < 2, \\ \cos 4(t-2), & t > 2. \end{cases} \tag{15.308}$$

2. To find the inverse Laplace transform of

$$F(s) = \ln\left(1 + \frac{1}{s}\right), \tag{15.309}$$

we first write its derivative:

$$F'(s) = \frac{1}{s+1} - \frac{1}{s}, \tag{15.310}$$

and then using Theorem 15.4:

$$\pounds^{-1}\{F^{(n)}(s)\} = (-1)^n t^n f(t), \tag{15.311}$$

we write

$$\pounds^{-1}\{F'(s)\} = -t\pounds^{-1}\left\{\ln\left(1 + \frac{1}{s}\right)\right\},$$

which yields the inverse as

$$\pounds^{-1}\left\{\ln\left(1 + \frac{1}{s}\right)\right\} = -\frac{1}{t}\pounds^{-1}\left\{\frac{1}{s+1} - \frac{1}{s}\right\} \tag{15.312}$$

$$= \frac{1 - e^{-t}}{t}. \tag{15.313}$$

3. The inverse Laplace transform of $1/s\sqrt{s+1}$ can be found by making use of Theorem 15.6. Since

$$\pounds^{-1}\left\{\frac{1}{\sqrt{s+1}}\right\} = \frac{t^{-\frac{1}{2}}e^{-t}}{\sqrt{\pi}}, \tag{15.314}$$

Theorem 15.6 allows us to write

$$\pounds^{-1}\left\{\frac{F(s)}{s}\right\} = \int_0^t f(u)du, \tag{15.315}$$

hence

$$\pounds^{-1}\left\{\frac{1}{s\sqrt{s+1}}\right\} = \int_0^t \frac{u^{-\frac{1}{2}}e^{-u}}{\sqrt{\pi}}du, \tag{15.316}$$

$$= \frac{2}{\sqrt{\pi}} \int_0^{\sqrt{t}} e^{-v^2}dv. \tag{15.317}$$

We now make the transformation $u = v^2$ to write the result in terms of the error function as

$$\pounds^{-1}\left\{\frac{1}{s\sqrt{s+1}}\right\} = \text{erf}(\sqrt{t}). \tag{15.318}$$

15.9.4 Method of Partial Fractions

We frequently encounter Laplace transforms that are expressed in terms of rational functions as

$$f(s) = g(s)/h(s), \tag{15.319}$$

where $g(s)$ and $h(s)$ are two polynomials with no common factor, and the order of $g(s)$ is less than $h(s)$.

We have the following cases:

(i) When all the factors of $h(s)$ are linear and distinct, we can write $f(s)$ as

$$f(s) = \frac{c_1}{s-a_1} + \frac{c_2}{s-a_2} + \cdots + \frac{c_n}{s-a_n}, \tag{15.320}$$

where c_i are constants independent of s.

(ii) When one of the roots of $h(s)$ is mth order, we write $f(s)$ as

$$f(s) = \frac{c_{1,m}}{(s-a_1)^m} + \frac{c_{1,m-1}}{(s-a_1)^{m-1}} + \cdots + \frac{c_{1,1}}{(s-a_1)} + \sum_{i=2}^{n} \frac{c_i}{s-a_i}. \tag{15.321}$$

(iii) When one of the factors of $h(s)$ is quadratic like $(s^2 + ps + q)$, we add a term to the partial fractions with two constants as

$$\frac{as+b}{(s^2+ps+q)}. \tag{15.322}$$

To find the constants, we usually compare equal powers of s. In the first case, we can also use the limit

$$\lim_{s\to a_i}(s-a_i)f(s) = c_i \tag{15.323}$$

to evaluate the constants.

Example 15.10 ***Method of partial fractions***

We can use the method of partial fractions to find the inverse Laplace transform of

$$f(s) = \frac{k^2}{(s+2)(s^2+2k^2)}. \tag{15.324}$$

We write $f(s)$ as

$$f(s) = \frac{c}{s+2} + \frac{as+b}{s^2+2k^2} \tag{15.325}$$

and equate both expressions:

$$\frac{k^2}{(s+2)(s^2+2k^2)} = \frac{c\left(s^2+2k^2\right) + (s+2)(as+b)}{(s+2)(s^2+2k^2)}. \tag{15.326}$$

Comparing the equal powers of s, we obtain three equations to be solved for $a, b,$ and c as

$$\left.\begin{aligned} c + a &= 0 \\ b + 2a &= 0 \\ 2b + 2ck^2 &= k^2 \end{aligned}\right\} \begin{aligned} &\text{coefficient of } s^2, \\ &\text{coefficient of } s, \\ &\text{coefficient of } s^0, \end{aligned} \tag{15.327}$$

which gives

$$c = -a, \quad b = -2a, \quad a = -k^2/(2k^2 + 4). \tag{15.328}$$

We now have

$$f(s) = -\frac{2}{(s+2)} + \frac{a(s-2)}{s^2 + 2k^2}, \tag{15.329}$$

the inverse Laplace transform of which can be found easily as

$$£^{-1}\{f(s)\} = -a\left[e^{-2t} + \cos\sqrt{2}kt - \frac{\sqrt{2}}{k}\sin\sqrt{2}kt\right], \quad a = -k^2/((2k^2 + 4). \tag{15.330}$$

Example 15.11 ***Definite integrals and Laplace transforms***
We can also use integral transforms to evaluate some definite integrals. Let us consider

$$F(t) = \int_0^\infty \frac{\sin tx}{x} dx. \tag{15.331}$$

Taking the Laplace transform of $F(t)$, we write

$$£\left\{\int_0^\infty \frac{\sin tx}{x} dx\right\} = \int_0^\infty e^{-st} \int_0^\infty \frac{\sin tx}{x} dxdt \tag{15.332}$$

$$= \int_0^\infty \frac{1}{x}\left[\int_0^\infty dte^{-st}\sin(tx)\right]dx. \tag{15.333}$$

The quantity inside the square brackets is the Laplace transform of $\sin tx$. Thus we find

$$£\left\{\int_0^\infty \frac{\sin tx}{x} dx\right\} = \int_0^\infty \frac{1}{s^2 + x^2} dx \tag{15.334}$$

$$= \frac{1}{s}\tan^{-1}\left(\frac{x}{s}\right)\Big|_0^\infty \tag{15.335}$$

$$= \frac{\pi}{2s}. \tag{15.336}$$

Finding the inverse Laplace transform gives the value of the definite integral as

$$F(t) = \frac{\pi}{2}, \quad t > 0. \tag{15.337}$$

15.10 Laplace Transform of a Derivative

One of the main applications of Laplace transforms is to differential equations. In particular, systems of ordinary linear differential equations with constant coefficients can be converted into systems of linear algebraic equations, which are a lot easier to solve both analytically and numerically. The Laplace transform of a derivative is found as

$$\pounds\{F'(t)\} = \int_0^\infty e^{-st}\frac{dF(t)}{dt}dt \tag{15.338}$$

$$= e^{-st}F(t)|_0^\infty + s\int_0^\infty e^{-st}F(t)dt, \tag{15.339}$$

hence

$$\boxed{\pounds\{F'(t)\} = s\pounds\{F(t)\} - F(0).} \tag{15.340}$$

To be precise, we mean that $F(0) = F(+0)$ and $dF(t)/dt$ is piecewise continuous in the interval $0 \leq t < \infty$. Similarly, the Laplace transform of a second-order derivative is given as

$$\pounds\{F^{(2)}(t)\} = s^2\pounds\{F(t)\} - sF(+0) - F'(+0). \tag{15.341}$$

In general, we can write

$$\boxed{\pounds\{F^{(n)}(t)\} = s^n\pounds\{F(t)\} - s^{n-1}F(+0) - s^{n-2}F'(+0) - \cdots - F^{(n-1)}(+0).} \tag{15.342}$$

Example 15.12 ***Laplace transforms and differential equations***
We start with a simple case; the simple harmonic oscillator equation of motion:

$$m\frac{d^2x(t)}{dt^2} + kx(t) = 0, \tag{15.343}$$

with the following initial conditions:

$$x(0) = x_0 \quad \text{and} \quad \left.\frac{dx}{dt}\right|_0 = 0. \tag{15.344}$$

We take the Laplace transform of the equation of motion, which yields the Laplace transform of the solution, $X(s)$, as

$$m\pounds\left\{\frac{d^2x(t)}{dt^2}\right\} + k\pounds\{x(t)\} = 0, \tag{15.345}$$

$$ms^2X(s) - msx_0 + kX(s) = 0, \tag{15.346}$$

$$X(s) = x_0\frac{s}{s^2+\omega_0^2}, \quad \omega_0^2 = k/m. \tag{15.347}$$

Next, we find the inverse Laplace transform of $X(s)$ to obtain the solution as

$$x(t) = \pounds^{-1}\left\{x_0 \frac{s}{s^2+\omega_0^2}\right\} = x_0 \pounds^{-1}\left\{\frac{s}{s^2+\omega_0^2}\right\} = x_0 \cos\omega_0 t. \qquad (15.348)$$

Example 15.13 ***Nutation of Earth***

For the force-free rotation of Earth (Figure 15.8), Euler equations are given as

$$\begin{cases} \dfrac{dX}{dt} = -aY, \\ \dfrac{dY}{dt} = aX. \end{cases} \qquad (15.349)$$

This is a system of two coupled linear ordinary differential equations with constant coefficients, where

$$a = \left[\frac{I_z - I_x}{I_z}\right]\omega_z \qquad (15.350)$$

and

$$X = \omega_x, \quad Y = \omega_y. \qquad (15.351)$$

Here, I_z is the moment of inertia about the z-axis; and because of axial symmetry, we have set $I_x = I_y$. Taking the Laplace transform of this system, we obtain a set of two coupled linear algebraic equations:

$$sx(s) - X(0) = -ay(s), \qquad (15.352)$$

$$sy(s) - Y(0) = ax(s), \qquad (15.353)$$

which can be decoupled easily to yield $x(s)$ as

$$x(s) = X(0)\frac{s}{s^2+a^2} - Y(0)\frac{a}{s^2+a^2}. \qquad (15.354)$$

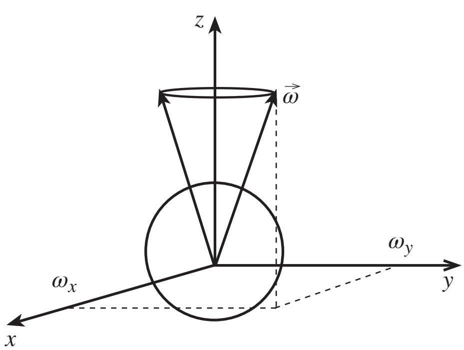


Figure 15.8 Nutation of Earth.

Taking the inverse Laplace transform, we find the solution:

$$X(t) = X(0)\cos at - Y(0)\sin at. \tag{15.355}$$

Similarly, the $Y(t)$ solution is found as

$$Y(t) = X(0)\sin at + Y(0)\cos at. \tag{15.356}$$

Example 15.14 ***Damped harmonic oscillator***
Equation of motion for the damped harmonic oscillator is given as

$$m\ddot{x}(t) + b\dot{x}(t) + kx(t) = 0. \tag{15.357}$$

Let us solve this equation with the initial conditions $x(0) = x_0$, $\dot{x}(0) = 0$. Taking the Laplace transform of the equation of motion:

$$m[s^2X(s) - sx_0] + b[sX(s) - x_0] + kX(s) = 0, \tag{15.358}$$

we obtain the Laplace transform of the solution as

$$X(s) = x_0\frac{ms + b}{ms^2 + bs + k}. \tag{15.359}$$

Completing the square in the denominator, we write

$$s^2 + \frac{b}{m}s + \frac{k}{m} = \left(s + \frac{b}{2m}\right)^2 + \left(\frac{k}{m} - \frac{b^2}{4m^2}\right). \tag{15.360}$$

For weak damping, $b^2 < 4km$, the last term is positive. Calling this ω_1^2, we find

$$X(s) = x_0\frac{s + \frac{b}{m}}{\left(s + \frac{b}{2m}\right)^2 + \omega_1^2} \tag{15.361}$$

$$= x_0\frac{s + \frac{b}{2m} + \frac{b}{2m}}{\left(s + \frac{b}{2m}\right)^2 + \omega_1^2} \tag{15.362}$$

$$= x_0\frac{s + \frac{b}{2m}}{\left(s + \frac{b}{2m}\right)^2 + \omega_1^2} + x_0\frac{\frac{b\omega_1}{2m\omega_1}}{\left(s + \frac{b}{2m}\right)^2 + \omega_1^2}. \tag{15.363}$$

Taking the inverse Laplace transform of $X(s)$, we find the final solution as

$$x(t) = x_0e^{-\left(\frac{b}{2m}\right)t}\left[\cos\omega_1 t + \frac{b}{2m\omega_1}\sin\omega_1 t\right]. \tag{15.364}$$

Check that this solution satisfies the given initial conditions.

Example 15.15 ***Laplace transform of the*** te^{kt} ***function***
Using the elementary Laplace transform

$$£\{e^{kt}\} = \int_0^\infty e^{-st}e^{kt}dt = \frac{1}{s-k}, \quad s > k, \tag{15.365}$$

and Theorem 15.4, we can obtain the desired transform by differentiation with respect to s as

$$£\{te^{kt}\} = \frac{1}{(s-k)^2}, \quad s > k. \tag{15.366}$$

Example 15.16 ***Electromagnetic waves***
For a transverse electromagnetic wave propagating along the x-axis, $E = E_x$ or E_y, satisfies the wave equation

$$\frac{\partial^2 E(x,t)}{\partial x^2} - \frac{1}{v^2}\frac{\partial^2 E(x,t)}{\partial t^2} = 0. \tag{15.367}$$

We take the initial conditions as

$$E(x,0) = 0 \quad \text{and} \quad \left.\frac{\partial E(x,t)}{\partial t}\right|_{t=0} = 0. \tag{15.368}$$

Taking the Laplace transform of the wave equation with respect to t, we obtain

$$\frac{\partial^2}{\partial x^2}£\{E(x,t)\} - \frac{s^2}{v^2}£\{E(x,t)\} + \frac{s}{v^2}E(x,0) + \frac{1}{v^2}\left.\frac{\partial E(x,t)}{\partial t}\right|_{t=0} = 0. \tag{15.369}$$

Using the initial conditions, this becomes

$$\frac{d^2}{dx^2}£\{E(x,t)\} = \frac{s^2}{v^2}£\{E(x,t)\}, \tag{15.370}$$

which is an ordinary differential equation for $£\{E(x,t)\}$ and can be solved immediately as

$$£\{E(x,t)\} = c_1e^{-(s/v)x} + c_2e^{(s/v)x}, \tag{15.371}$$

where c_1 and c_2 are constants independent of x but could depend on s. In the limit as $x \to \infty$, we expect the wave to be finite; hence, we choose c_2 as zero. If we are also given the initial shape of the wave as $E(0,t) = F(t)$, we determine c_1 as

$$£\{E(0,t)\} = c_1 = f(s). \tag{15.372}$$

Thus, with the given initial conditions, the Laplace transform of the solution is given as

$$£\{E(x,t)\} = e^{-(s/v)x}f(s). \tag{15.373}$$

Using Theorem 15.2 we can find the inverse Laplace transform, and the final solution is obtained as

$$E(x,t) = \begin{cases} F\left(t - \frac{x}{v}\right), & t \geq x/v, \\ 0, & t < x/v. \end{cases} \tag{15.374}$$

This is a wave moving along the positive x-axis with velocity v without distortion. Note that the wave still has not reached the region $x > vt$.

Example 15.17 ***Bessel's equation***

We now consider Bessel's equation, which is an ordinary differential equation with variable coefficients:

$$x^2 y''(x) + xy'(x) + x^2 y(x) = 0. \tag{15.375}$$

Dividing this by x, we get

$$xy''(x) + y'(x) + xy(x) = 0. \tag{15.376}$$

Using Laplace transforms, we can find a solution satisfying the boundary condition $y(0) = 1$. From Eq. (15.376), this also means that $y'(+0) = 0$. Assuming that the Laplace and the inverse Laplace transforms of the unknown function exist:

$$£\{y(x)\} = f(s), \quad £^{-1}\{f(s)\} = y(x), \tag{15.377}$$

we write the Laplace transform of Eq. (15.376) as

$$-\frac{d}{ds}[s^2 f(s) - s] + sf(s) - 1 - \frac{d}{ds}f(s) = 0 \tag{15.378}$$

$$(s^2+1)f'(s) + sf(s) = 0 \tag{15.379}$$

$$\frac{df}{f} = -\frac{s}{s^2+1}ds. \tag{15.380}$$

After integration, we find $f(s)$ as

$$\ln\frac{f(s)}{c} = -\frac{1}{2}\ln(s^2+1), \tag{15.381}$$

$$f(s) = \frac{c}{\sqrt{s^2+1}}. \tag{15.382}$$

To find the inverse, we write the binomial expansion of $f(s)$:

$$f(s) = \frac{c}{s\sqrt{1+\frac{1}{s^2}}}, \tag{15.383}$$

$$= \frac{c}{s}\left[1 - \frac{1}{2s^2} + \frac{1.3}{2^2 2! s^4} - \cdots \right.$$
$$\left. \cdots + \frac{(-1)^n (2n)!}{(2^n n!)^2 s^{2n}} + \cdots \right]. \tag{15.384}$$

Since Laplace transforms are linear, we find the inverse as

$$y(x) = c\sum_{n=0}^{\infty} \frac{(-1)^n x^{2n}}{(2^n n!)^2}. \tag{15.385}$$

Using the condition $y(0) = 1$, we determine the constant c as 1. This solution is nothing but the zeroth-order Bessel function $J_0(x)$. Thus, we have determined the Laplace transform of $J_0(x)$ as

$$£\{J_0(x)\} = \frac{1}{\sqrt{s^2+1}}. \tag{15.386}$$

In general, one can show

$$£\{J_n(ax)\} = \frac{a^{-n}(\sqrt{s^2+a^2}-s)^n}{\sqrt{s^2+a^2}}. \tag{15.387}$$

In this example, we see that the Laplace transform can also be used for finding solutions of ordinary differential equations with variable coefficients; however, there is no guarantee that it will work in general.

Example 15.18 ***Solution of*** $y'' + (1/2)y = (a_0/2)\sin t - (1/2)y^{(iv)}$
This could be interpreted as a harmonic oscillator with a driving force depending on the fourth derivative of displacement as

$$(a_0/2)\sin t - (1/2)y^{(iv)}. \tag{15.388}$$

We rewrite this equation as

$$y^{(iv)} + 2y'' + y = a_0 \sin t, \tag{15.389}$$

where a_0 is a constant, and use the following boundary conditions:

$$y(0) = 1, \quad y'(0) = -2, \quad y''(0) = 3, \quad y'''(0) = 0.$$

Taking the Laplace transform and using partial fractions, we write

$$\begin{aligned} &[s^4 Y - s^3(1) - s^2(-2) - s(3) - 0] \\ &+ 2[s^2 Y(s) - s(1) - (-2)] + Y(s) = \frac{a_0}{s^2+1}, \end{aligned} \tag{15.390}$$

where $Y(s)$ is the Laplace transform of $y(x)$. We first write this as

$$(s^4 + 2s^2 + 1)Y(s) = \frac{a_0}{s^2+1} + s^3 - 2s^2 + 5s - 4, \tag{15.391}$$

and then solve for $Y(s)$ to obtain

$$Y(s) = \frac{a_0}{(s^2+1)^3} + \frac{s^3 - 2s^2 + 5s - 4}{(s^2+1)^2}, \tag{15.392}$$

$$= \frac{a_0}{(s^2+1)^3} + \frac{(s^3+s) - 2(s^2+1) + 4s - 2}{(s^2+1)^2}, \tag{15.393}$$

$$= \frac{a_0}{(s^2+1)^3} + \frac{s}{(s^2+1)} - \frac{2}{(s^2+1)} + \frac{4s-2}{(s^2+1)^2}. \tag{15.394}$$

Using the Theorems, we have introduced, the following inverses can be found:

$$\pounds^{-1}\left\{\frac{a_0}{(s^2+1)^3}\right\} = a_0\left[\frac{3}{8}\sin t - \frac{3}{8}t\cos t - \frac{t^2}{8}\sin t\right], \tag{15.395}$$

$$\pounds^{-1}\left\{\frac{4s-2}{(s^2+1)^2}\right\} = 2t\sin t - \sin t + t\cos t. \tag{15.396}$$

Finally, the solution is obtained as

$$y(t) = \left[t\left(1 - \frac{3}{8}a_0\right) + 1\right]\cos t + \left[\frac{a_0}{8}(3 - t^2) - 3 + 2t\right]\sin t. \tag{15.397}$$

Note that the solution is still oscillatory but the amplitude changes with time.

Example 15.19 ***Two Pendlums interacting through a spring***
Consider two pendulums connected by a spring as shown in Figure 15.9. We investigate small oscillations of this system.

As our initial conditions, we take

$$x_1(0) = x_2(0) = 0, \quad \dot{x}_1|_0 = v, \ \dot{x}_1|_0 = 0. \tag{15.398}$$

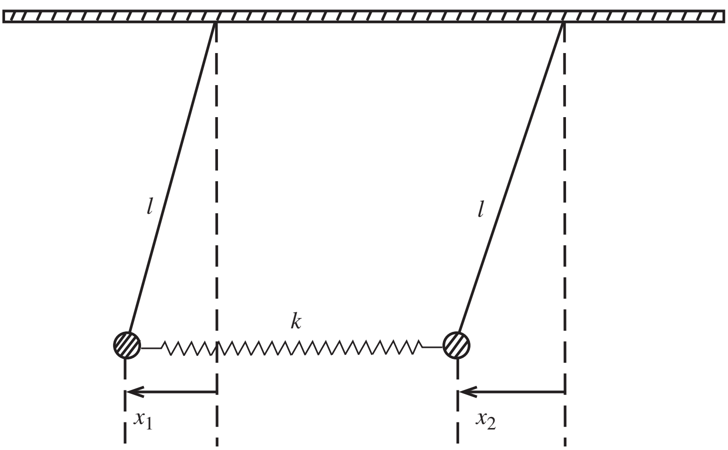


Figure 15.9 Pendulums connected by a spring.

For this system and for small oscillations, equations of motion are written as

$$m\ddot{x}_1 = -\frac{mg}{l}x_1 + k(x_2 - x_1), \tag{15.399}$$

$$m\ddot{x}_2 = -\frac{mg}{l}x_2 + k(x_1 - x_2). \tag{15.400}$$

Showing the Laplace transforms of $x_1(t)$ and $x_2(t)$ as

$$\pounds\{x_i(t)\} = X_i(s), \quad i = 1, 2, \tag{15.401}$$

we take the Laplace transform of both equations:

$$m(s^2X_1(s) - v) = -\frac{mg}{l}X_1(s) + k(X_2(s) - X_1(s)), \tag{15.402}$$

$$ms^2X_2(s) = -\frac{mg}{l}X_2(s) + k(X_1(s) - X_2(s)). \tag{15.403}$$

This gives two coupled linear algebraic equations. We first solve them for $X_1(s)$ to get

$$X_1(s) = \frac{v}{2}[(s^2 + g/l + 2k/m)^{-1} + (s^2 + g/l)^{-1}]. \tag{15.404}$$

Taking the inverse Laplace transform of $X_1(s)$ gives $x_1(t)$ as

$$x_1(t) = \frac{v}{2}\left[\frac{\sin\sqrt{\left(\frac{g}{l} + 2\frac{k}{m}\right)}t}{\sqrt{\left(\frac{g}{l} + 2\frac{k}{m}\right)}} + \frac{\sin\sqrt{\left(\frac{g}{l}\right)}t}{\sqrt{\left(\frac{g}{l}\right)}}\right]. \tag{15.405}$$

In this solution

$$\sqrt{\left(\frac{g}{l} + 2\frac{k}{m}\right)} \quad \text{and} \quad \sqrt{\left(\frac{g}{l}\right)} \tag{15.406}$$

are the normal modes of the system. The solution for $x_2(t)$ can be obtained similarly.

15.10.1 Laplace Transforms in *n* Dimensions

Laplace transforms are defined in two dimensions as

$$F(u, v) = \int_0^\infty \int_0^\infty f(x, y)e^{-ux-vy}dxdy. \tag{15.407}$$

This can also be generalized to n dimensions:

$$F(u_1, u_2, \dots, u_n) \tag{15.408}$$
$$= \int_0^\infty \int_0^\infty \cdots \int_0^\infty f(x_1, x_2, \dots, x_n)e^{-u_1x_1-u_2x_2-\cdots-u_nx_n}dx_1dx_2 \dots dx_n.$$

15.11 Relation Between Laplace and Fourier Transforms

The Laplace transform of a function is defined as

$$F(p) = \pounds\{f(x)\} = \int_0^\infty f(x)e^{-px}dx. \tag{15.409}$$

We now use $f(x)$ to define another function:

$$f_+(x) = \begin{cases} f(x), & x > 0, \\ 0, & x < 0. \end{cases} \tag{15.410}$$

The Fourier transform of this function is given as

$$F_+(k) = \frac{1}{\sqrt{2\pi}} \int_0^\infty f(x)e^{ikx}dx. \tag{15.411}$$

Thus we can write the relation between the Fourier and Laplace transforms as

$$\boxed{F(p) = \sqrt{2\pi}F_+(ip).} \tag{15.412}$$

15.12 Mellin Transforms

Another frequently encountered integral transform is the **Mellin transform**:

$$\boxed{F_m(s) = \int_0^\infty f(x)x^{s-1}dx.} \tag{15.413}$$

The Mellin transform of $\exp(-x)$ is the gamma function. We write $x = e^z$ in the Mellin transform to get

$$F_m(s) = \int_{-\infty}^\infty f(e^z)\, e^{sz}\, dz \tag{15.414}$$

$$= \int_{-\infty}^\infty g(z)\, e^{sz}\, dz, \quad g(z) = f(e^z). \tag{15.415}$$

Comparing this with

$$G(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^\infty g(z)e^{ikz}dz, \tag{15.416}$$

we get the relation between the Fourier and Mellin transforms as

$$\boxed{F_m(s) = \sqrt{2\pi}G(-is).} \tag{15.417}$$

Now all the properties we have discussed for the Fourier transforms can also be adopted to the Mellin transforms.

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Problems

1 Show that the Fourier transform of a Gaussian:

$$f(\vec{r}) = \left(\frac{2}{\pi a^2}\right)^{3/4} e^{-r^2/a^2},$$

is again a Gaussian.

2 Show that the Fourier transform of

$$f(t) = \begin{cases} \sin\omega_0 t, & |t| < \dfrac{N\pi}{\omega_0}, \\ 0, & |t| > \dfrac{N\pi}{\omega_0}, \end{cases}$$

is given as

$$g_s(\omega) = \sqrt{\frac{2}{\pi}}\left[\frac{\frac{N\pi}{\omega_0}\sin(\omega_0-\omega)}{2(\omega_0-\omega)} - \frac{\frac{N\pi}{\omega_0}\sin(\omega_0+\omega)}{2(\omega_0+\omega)}\right].$$

3 Show the following integral by using Fourier transforms:

$$\int_0^\infty \frac{\sin^3 x}{x} dx = \frac{\pi}{4}.$$

4 Using the Laplace transform technique, find the solution of the following second-order inhomogeneous differential equation:

$$y'' - 3y' + 2y = 2e^{-t},$$

with the following boundary conditions:

$$y(0) = 2 \quad \text{and} \quad y'(0) = -1.$$

5 Solve the following system of differential equations:

$$2x(t) - y(t) - y'(t) = 4(1 - \exp(-t)),$$
$$2x'(t) + y(t) = 2(1 + 3\exp(-2t)),$$

with the boundary conditions

$$x(0) = y(0) = 0.$$

6 One end of an insulated semi-infinite rod is held at temperature

$$T(t, 0) = T_0$$

with the initial conditions

$$T(0, x) = 0 \quad \text{and} \quad T(t, \infty) = 0.$$

Solve the heat transfer equation:

$$\frac{\partial T(t,x)}{\partial t} = (k/c\rho)\frac{\partial^2 T(t,x)}{\partial x^2}, \quad k > 0,$$

where k is the thermal conductivity, c is the heat capacity, and ρ is the density.
Hint: The solution is given in terms of erf$c$ as

$$T(t,x) = T_0 \text{ erf } c\left[\frac{x}{2}\frac{\sqrt{c\rho/k}}{\sqrt{t}}\right],$$

where the erf$c$ is defined in terms of erf as

$$\text{erf}c(x) = 1 - \text{erf } x$$
$$= 1 - \frac{2}{\sqrt{\pi}}\int_0^x e^{-u^2} du = \frac{2}{\sqrt{\pi}}\int_x^\infty e^{-u^2} du.$$

7 Find the current, I, for the IR circuit represented by the differential equation

$$L\frac{dI}{dt} + RI = E$$

with the initial condition

$$I(0) = 0.$$

E is the electromotive force and $L, R,$ and E are constants.

8 Using Laplace transforms, find the solution of the following system of differential equations

$$\frac{dx}{dt} + y = 3e^{2t},$$
$$\frac{dy}{dt} + x = 0,$$

subject to the initial conditions

$$x(0) = 2, \quad y(0) = 0.$$

9 Using the Fourier-sine transform, show the integral

$$e^{-x}\cos x = \frac{2}{\pi}\int_0^{\infty} \frac{s^3 \sin sx}{s^4 + 4} ds, \quad x > 0.$$

10 Using the Fourier-cosine transform, show the integral

$$e^{-x}\cos x = \frac{2}{\pi}\int_0^{\infty} \frac{s^2 + 2}{s^4 + 4}(\cos sx) ds, \quad x \geq 0.$$

11 Let a semi-infinite string be extended along the positive x-axis with the end at the origin fixed. The shape of the string at $t = 0$ is given as

$$y(x, 0) = f(x),$$

where $y(x, t)$ represents the displacement of the string perpendicular to the x-axis and satisfies the wave equation

$$\frac{\partial^2 y}{\partial t^2} = a^2 \frac{\partial^2 y}{\partial x^2}, \quad a \text{ is a constant.}$$

Show that the solution is given as

$$y(x, t) = \frac{2}{\pi}\int_0^{\infty} ds \cos(sat) \sin(sx) \int_0^{\infty} d\xi\, f(\xi) \sin(s\xi).$$

12 Establish the Fourier-sine integral representation

$$\frac{x}{x^2+k^2} = \frac{2}{\pi}\int_0^\infty dy \sin(xy) \int_0^\infty dz \frac{z\sin(yz)}{z^2+k^2}.$$

Hint: First show that

$$e^{-ky} = \frac{2}{\pi}\int_0^\infty \frac{z\sin(yz)}{z^2+k^2}dz, \quad x>0,\ k>0.$$

13 Show that the Fourier-sine transform of

$$xe^{-ax}$$

is given as

$$\sqrt{\frac{2}{\pi}}\frac{a^2-k^2}{(a^2+k^2)^2}.$$

14 Establish the result

$$£\left\{\frac{1-\cos at}{t}\right\} = \frac{1}{2}\log\left(1+\frac{a^2}{s^2}\right).$$

15 Use the convolution theorem to show that

$$£^{-1}\left\{\frac{s^2}{(s^2+b^2)^2}\right\} = \frac{t}{2}\cos bt + \frac{1}{2b}\sin bt.$$

16 Use Laplace transforms to find the solution of the following system of differential equations:

$$\frac{dy_1}{dx} = -\alpha_1 y_1,$$
$$\frac{dy_2}{dx} = -\alpha_1 y_1 - \alpha_2 y_2,$$
$$\frac{dy_3}{dx} = -\alpha_2 y_2 - \alpha_3 y_3,$$

with the boundary conditions

$$y_1(0) = C_0,\ y_2(0) = y_3(0) = 0.$$

17 Laguerre polynomials satisfy

$$xL_n'' + (1-t)L_n' + nL_n(x) = 0.$$

Show that

$$£\{L_n(ax)\} = (s-a)^n/s^{n+1}, \quad s>0.$$

16

Variational Analysis

The variational analysis is basically the study of changes. We are often interested in how a system will react to small changes in its parameters. Variational analysis constitutes a powerful tool for determining in which direction a process will go. It is for this reason that it has found a wide range of applications not just in physics and engineering but also in financial mathematics and economics. In applications, we frequently encounter cases where the desired quantity is the one that extremizes a certain integral. Compared to ordinary calculus, where one deals with functions of numbers, these integrals are functions of some unknown function and its derivatives, hence they are called functionals. Search for the extremum of a function yields the points at which the function takes its extremum values. In the case of functionals, the variational analysis gives a differential equation that needs to be solved for the desired function that makes the functional an extremum. After Newton's formulation of mechanics, Lagrange developed a new formalism where the equations of motion are obtained from a variational integral called the action. This new formulation made applications of Newton's theory to many-body problems and continuous systems possible. Today, in making the transition to quantum mechanics and to quantum field theories, a Lagrangian formulation is a must. Geodesics are the shortest paths between two points in a given space and constitute one of the main applications of variational analysis. In Einstein's theory of gravitation, geodesics play a central role as the paths of freely moving particles in curved spacetime. Variational techniques also form the mathematical basis for the finite elements method, which constitutes a powerful tool for solving complex boundary value problems in stability analysis. Variational analysis and the Rayleigh–Ritz method allows us to find approximate eigenvalues and eigenfunctions of a Sturm–Liouville system. A special section of this chapter is on optimum control theory, where we discuss the basics of controlled dynamics and its connections with variational dynamics.

16.1 Presence of One Dependent and One Independent Variable

16.1.1 Euler Equation

Majority of the variational problems encountered in physics and engineering are expressed in terms of an integral:

$$\boxed{J[y(x)] = \int_{x_1}^{x_2} f(y, y_x, x)\, dx,} \tag{16.1}$$

where $y(x)$ is the desired function and $f(y, y_x, x)$ is a known function of $y(x)$ and its derivative y_x and x. Because the unknown of this problem is a function, $y(x)$, J is called a **functional**, hence we write it as $J[y(x)]$. Usually, the purpose of these problems is to find a function, which is a path in the xy-plane between the points (x_1, y_1) and (x_2, y_2), which makes the functional $J[y(x)]$ an extremum. In Figure 16.1, we show potentially possible paths that connects the points (x_1, y_1) and (x_2, y_2). The difference of these paths from the desired path is called the variation, δy, of y. Because δy depends on position, we use $\eta(x)$ for its position dependence and use a scalar parameter α as a measure of its magnitude. Paths close to the desired path can now be parameterized in terms of α as

$$y(x, \alpha) = y(x, 0) + \alpha\eta(x) + 0(\alpha^2), \tag{16.2}$$

where $y(x, \alpha = 0)$ is the desired path, which extremizes the functional $J[y(x)]$. We can now express δy as

$$\delta y = y(x, \alpha) - y(x, 0) = \alpha\eta(x) \tag{16.3}$$

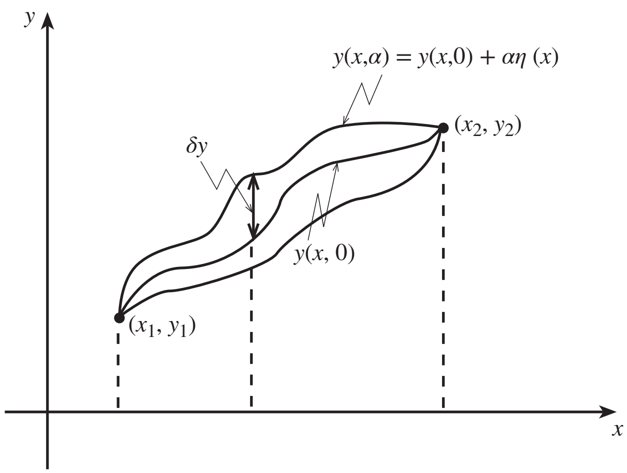

Figure 16.1 Variation of paths.

and write $J[y(x)]$ as a function of α:

$$J(\alpha) = \int_{x_1}^{x_2} f[y(x,\alpha), y_x(x,\alpha), x]\,dx. \tag{16.4}$$

Now the extremum of $J[y(x)]$ can be found as in ordinary calculus by imposing the condition

$$\left|\frac{\partial J(\alpha)}{\partial \alpha}\right|_{\alpha=0} = 0. \tag{16.5}$$

In this analysis, we assume that $\eta(x)$ is a differentiable function and take the variations at the end points as zero:

$$\eta(x_1) = \eta(x_2) = 0. \tag{16.6}$$

Now the derivative of $J(\alpha)$ with respect to α is

$$\frac{\partial J(\alpha)}{\partial \alpha} = \int_{x_1}^{x_2} \left[\frac{\partial f}{\partial y}\frac{\partial y}{\partial \alpha} + \frac{\partial f}{\partial y_x}\frac{\partial y_x}{\partial \alpha}\right] dx. \tag{16.7}$$

Using Eq. (16.2), we can write

$$\frac{\partial y(x,\alpha)}{\partial \alpha} = \eta(x), \tag{16.8}$$

$$\frac{\partial y_x(x,\alpha)}{\partial \alpha} = \frac{d\eta(x)}{dx}, \tag{16.9}$$

which when substituted in Eq. (16.7) gives

$$\left.\frac{\partial J(\alpha)}{\partial \alpha}\right|_{\alpha=0} = \int_{x_1}^{x_2} \left[\frac{\partial f}{\partial y}\eta(x) + \frac{\partial f}{\partial y_x}\frac{d\eta(x)}{dx}\right] dx. \tag{16.10}$$

Integrating the second term by parts:

$$\int_{x_1}^{x_2} \frac{\partial f}{\partial y_x}\frac{d\eta(x)}{dx}dx = \left|\frac{\partial f}{\partial y_x}\eta(x)\right|_{x_1}^{x_2} - \int_{x_1}^{x_2} \eta(x)\left(\frac{d}{dx}\frac{\partial f}{\partial y_x}\right) dx, \tag{16.11}$$

and using the fact that the variation at the end points are zero, we can write Eq. (16.10) as

$$\int_{x_1}^{x_2} \left(\frac{\partial f}{\partial y} - \frac{d}{dx}\frac{\partial f}{\partial y_x}\right)\eta(x)dx = 0. \tag{16.12}$$

Because the variation $\eta(x)$ is arbitrary, the only way to satisfy this equation is by setting the expression inside the brackets to zero:

$$\boxed{\frac{\partial f}{\partial y} - \frac{d}{dx}\frac{\partial f}{\partial y_x} = 0.} \tag{16.13}$$

In conclusion, variational analysis has given us a second-order differential equation to be solved for the path that extremizes the functional $J[y(x)]$. This differential equation is called the **Euler equation**.

16.1.2 Another Form of the Euler Equation

To find another version of the Euler equation, we write the total derivative of the function $f(y, y_x, x)$ as

$$\frac{df}{dx} = \frac{\partial f}{\partial y} y_x + \frac{\partial f}{\partial y_x}\frac{dy_x}{dx} + \frac{\partial f}{\partial x}. \tag{16.14}$$

Using the Euler equation [Eq. (16.13)], we write $\frac{\partial f}{\partial y} = \frac{d}{dx}\frac{\partial f}{\partial y_x}$ and substitute in Eq. (16.14) to get

$$\frac{df}{dx} = y_x \frac{d}{dx}\frac{\partial f}{\partial y_x} + \frac{\partial f}{\partial y_x}\frac{dy_x}{dx} + \frac{\partial f}{\partial x}. \tag{16.15}$$

This can also be written as

$$\boxed{\frac{\partial f}{\partial x} - \frac{d}{dx}\left[f - y_x \frac{\partial f}{\partial y_x}\right] = 0.} \tag{16.16}$$

This is another version of the Euler equation, which is extremely useful when $f(y, y_x, x)$ does not depend on the independent variable, x, explicitly. In such cases, we can immediately write the first integral as

$$\boxed{f - y_x \frac{\partial f}{\partial y_x} = \text{constant},} \tag{16.17}$$

which reduces the problem to the solution of a first-order differential equation.

16.1.3 Applications of the Euler Equation

Example 16.1 ***Shortest path between two points***
To find the shortest path between two points on a plane, we write the line element as

$$ds = [(dx)^2 + (dy)^2]^{\frac{1}{2}} = dx[1 + y_x^2]^{\frac{1}{2}}. \tag{16.18}$$

The distance between two points is now given as a functional of the path and in terms of the integral

$$J[y(x)] = \int_{(x_1,y_1)}^{(x_2,y_2)} ds = \int_{x_1}^{x_2} [1 + y_x^2]^{\frac{1}{2}}\, dx. \tag{16.19}$$

To find the shortest path, we must solve the Euler equation for

$$f(y, y_x, x) = [1 + y_x^2]^{\frac{1}{2}}.$$

Since $f(y, y_x, x)$ does not depend on the independent variable explicitly, we use the second form of the Euler equation [Eq. (16.17)] to write

$$\frac{1}{[1 + y_x^2]^{\frac{1}{2}}} = c, \tag{16.20}$$

where c is a constant. This is a first-order differential equation for $y(x)$ and its solution can be found as $y = ax + b$. This is the equation of a straight line, where the integration constants a and b are to be determined from the coordinates of the end points. The shortest paths between two points in a given geometry are called geodesics. Geodesics in spacetime play a crucial role in Einstein's theory of gravitation as the paths of free particles in curved spacetime.

Example 16.2 ***Shape of a soap film between two rings***
Let us find the shape of a soap film between two rings separated by a distance of $2x_0$. Rings pass through the points (x_1, y_1) and (x_2, y_2) as shown in Figure 16.2. Ignoring gravitation, the shape of the film is a surface of revolution; thus, it is sufficient to find the equation of a curve, $y(x)$, between two points (x_1, y_1) and (x_2, y_2). Because the energy of a soap film is proportional to its surface area, $y(x)$ should be the one that makes the area a minimum. We write the infinitesimal area element of the soap film as

$$dA = 2\pi y ds = 2\pi y[1 + y_x^2]^{\frac{1}{2}}\, dx. \tag{16.21}$$

The area, aside from a factor of 2π, is given by the integral

$$J = \int_{x_1}^{x_2} y[1 + y_x^2]^{\frac{1}{2}}\, dx. \tag{16.22}$$

Since $f(y, y_x, x)$ is given as

$$f(y, y_x, x) = y[1 + y_x^2]^{\frac{1}{2}}, \tag{16.23}$$

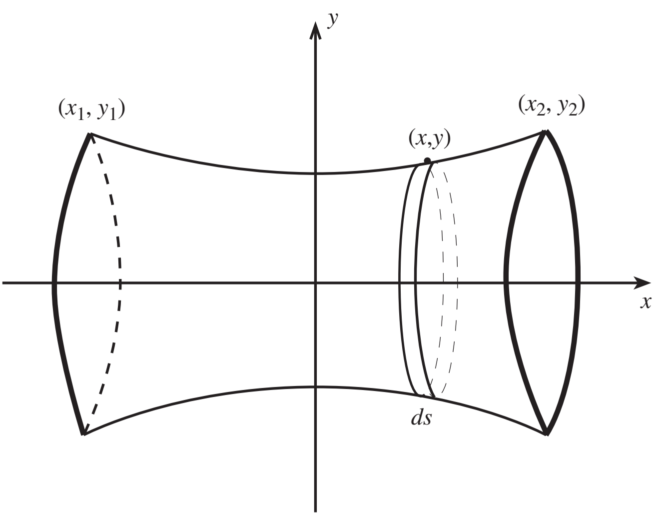

Figure 16.2 Soap film between two rings.

which does not depend on x explicitly, we write the Euler equation as

$$y/[1+y_x^2]^{\frac{1}{2}} = c_1, \tag{16.24}$$

where c_1 is a constant. Taking the square of both sides, we write $y^2/[1+y_x^2] = c_1^2$. This leads us to a first-order differential equation:

$$(y_x)^{-1} = \frac{dx}{dy} = \frac{c_1}{\sqrt{y^2 - c_1^2}}, \quad c_1^2 \leq y_{\min}^2, \tag{16.25}$$

which up on integration gives $x = c_1 \cosh^{-1} \frac{y}{c_1} + c_2$. Thus, the function $y(x)$ is determined as

$$y(x) = c_1 \cosh\left(\frac{x - c_2}{c_1}\right). \tag{16.26}$$

Integration constants c_1 and c_2 are to be determined so that $y(x)$ passes through the points (x_1, y_1) and (x_2, y_2). Symmetry of the problem gives $c_2 = 0$. For two rings with unit radius and $x_0 = 1/2$, we obtain

$$1 = c_1 \cosh\left(\frac{1}{2c_1}\right) \tag{16.27}$$

as the equation to be solved for c_1. This equation has two solutions: $c_1 = 0.2350$, which is known as the **deep curve** and $c_1 = 0.8483$, which is known as the **flat curve**. To find the correct shape, we have to check which one of these makes the area, and hence the energy, a minimum. Using Eqs. (16.22) and (16.24), we write the surface area as

$$A = \frac{4\pi}{c_1} \int_0^{x_0} y^2(x)\, dx. \tag{16.28}$$

Substituting the solution in Eq. (16.26) in Eq. (16.28) we get

$$A = \pi c_1^2 \left[\sinh\left(\frac{2x_0}{c_1}\right) + \frac{2x_0}{c_1}\right]. \tag{16.29}$$

For $x_0 = \frac{1}{2}$ this gives

$$\left.\begin{matrix} c_1 = 0.2350 \\ c_1 = 0.8483 \end{matrix}\right\} \to \left\{\begin{matrix} A = 6.8456, \\ A = 5.9917, \end{matrix}\right. \tag{16.30}$$

This means that the correct value of c_1 is 0.8483. If we increase the separation between the rings beyond a certain point, we expect the film to break. In fact, the transcendental equation

$$1 = c_1 \cosh\left(\frac{x_0}{c_1}\right) \tag{16.31}$$

does not have a solution for $x_0 \geq 1$.

Example 16.3 ***Newton's bucket experiment***
In *Principia* (1689) Newton describes a simple experiment with a bucket half-filled with water and suspended with a rope from a fixed point in space. In this experiment, first the rope is twisted tightly and after the water has settled with a flat surface, the rope is released. Initially the bucket spins rapidly with the water remaining at rest with its surface flat. Eventually, the friction between the water and the bucket communicates the motion of the bucket to the water and the water begins to rotate. As the water rotates, it also rises along the sides of the bucket. Slowly the relative motion between the bucket and the water ceases and the surface of the water assumes a concave shape. Finally, the rope unwinds completely and begins to twist in the other direction, thus slowing and eventually stopping the bucket. Shortly after the bucket has stopped, the water continues its rotation with its surface still concave. The question is; what causes this concave shape of the surface of the water?

At first, the bucket is spinning but the water is at rest and its surface is flat. Eventually, when there is no relative motion between the bucket and the water, the surface is concave. Finally, when the water is spinning but the bucket is at rest, the surface is still concave. From these it is clear that the relative rotation of the water and the bucket is not what determines the shape of the surface.

The crucial question is; what is spinning and with respect to what? Let us try to understand the shape of the surface in terms of interactions. Since the bucket and the water, and the rest of the universe are on the average neutral, electromagnetic forces cannot be the reason. The gravitational interaction between the bucket and the water is surely negligible, hence it cannot be the reason either. Besides, in Newton's theory gravity is a scalar interaction, thus the force between two masses depends only on their separation and not on their relative motion. In this regard, Newton could not have used the gravitational interaction of water with other matter. This lead Newton reluctantly to explain the concave shape as due to rotation with respect to **absolute space**. In other words, the surface of the water is flat when the water is not rotating with respect to absolute space and when there is rotation with respect to absolute space, the surface is concave.

A satisfactory solution to this problem comes only with Einstein's general theory of relativity, where the gravitational force between two masses depends not just on their separation but also on their relative velocity as well. This is analogous to Maxwell's theory, where the electromagnetic interactions are described by a vector potential. Hence, the force between two charged particles has a velocity dependent part aside from the usual Coulomb force. In the general theory of relativity, gravity is described by a tensor potential; the metric tensor. Therefore in Einstein's theory, the velocity dependence is even more complicated. In this regard, in Einstein's theory not just the shape of the surface of the water in the Newton's bucket experiment but also all fictitious forces in Newton's dynamic theory, in principle, can be explained as the gravitational

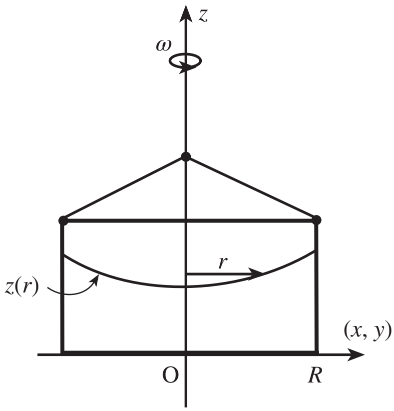

Figure 16.3 Newton's bucket experiment with a cylindrical container.

interaction of matter with other matter, that is, the mean matter distribution of the universe.

Let us now find the equation of the concave shape that the surface of the water assumes. For simplicity, we assume a cylindrical container (Figure 16.3) with the radius R and rotating with uniform angular velocity ω about its axis. We determine the surface height, $z(r)$, of the water by minimizing the potential energy. For a given mass element of the water, we can write the infinitesimal potential energy as

$$dE = \left(\rho g z - \frac{1}{2}\rho\omega^2 r^2\right) dv, \tag{16.32}$$

where ρ is the uniform density of the water and g is the acceleration of gravity. We now write the functional, $I[z(r)]$, that needs to be minimized for $z(r)$ as

$$I[z(r)] = \iiint_V dE = \int_0^{2\pi}\int_0^R\int_0^{z(r)} \left(\rho g z - \frac{1}{2}\rho\omega^2 r^2\right) r \times dz\, dr\, d\theta \tag{16.33}$$

$$= \pi\rho\int_0^R (gz^2 - \omega^2 r^2 z) r dr. \tag{16.34}$$

Note that the integrand in the above functional does not involve any derivatives of $z(r)$, hence the boundary conditions $z(0)$ and $z(R)$ are not needed in the derivation of the Euler equation [Eq. (16.13)], which becomes:

$$\frac{\partial[(gz^2 - \omega^2 r^2 z)r]}{dz} = 0, \tag{16.35}$$

thus, yielding the surface of revolution, $z(r)$, representing the free surface of the water as

$$z(r) = \frac{\omega^2 r^2}{2g}. \tag{16.36}$$

One final remark that needs to be made is that this result is only partially true, since we have not defined the optimization problem correctly. For a proper description of the problem we have to take into account the fact that water is incompressible, that is, its volume is fixed. Now the functional in Eq. (16.34) has to be extremized subject to the constraint

$$J[z(r)] = \iiint_V dv = \int_0^{2\pi} \int_0^R \int_0^{z(r)} r\, dz\, dr\, d\theta \tag{16.37}$$

$$= 2\pi \int_0^R z(r)dr = V_0, \tag{16.38}$$

thus, making the problem one of isoperimetric type and can be solved by using the method discussed in Section 16.6.

Example 16.4 ***Drag force on a surface of revolution***
Consider an axially symmetric object moving in a perfect incompressible fluid with constant velocity. Assuming that at any point on the surface the drag force per unit area is proportional to the square of the normal component of the velocity, find the shape that minimizes the drag force on the object.

Solution
Since the object is axially symmetric, we consider the surface of revolution shown in Figure 16.4, where θ is the angle that the tangent at point P makes with the plane perpendicular to the z-axis. Since the normal component of the velocity at P is

$$v_\perp = v_0 \cos(\pi - \theta) = -v_0 \cos\theta, \tag{16.39}$$

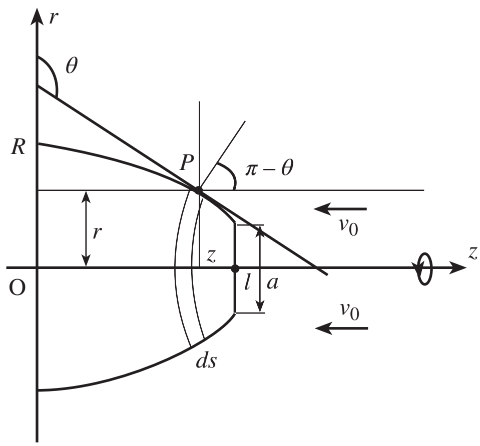

Figure 16.4 Drag force on a surface of revolution.

we write the drag force on the infinitesimal strip with the area $2\pi r ds$ and projected along the z-axis as (Figure 16.4)

$$\alpha(v_0^2\cos^2\theta)\cos\theta\ 2\pi r ds, \tag{16.40}$$

where α is the drag coefficient. Since $ds = dr/\cos\theta$, the total drag on the body is the integral

$$J = 2\pi\alpha v_0^2 \int_0^R r\cos^2\theta\ dr. \tag{16.41}$$

Using the definition of the surface of revolution, $z(r)$, we can write $\frac{dz}{dr} = \tan\theta$, hence

$$\cos\theta = \frac{1}{[1+z'^2]^{1/2}}. \tag{16.42}$$

Now the functional to be minimized for $z(r)$ becomes

$$J[z(r)] = 2\pi\alpha v_0^2 \int_0^R \frac{r\,dr}{1+z'^2}, \tag{16.43}$$

which yields the Euler equation

$$\frac{rz'}{[1+z'^2]^2} = c_0, \tag{16.44}$$

where c_0 is an integration constant. Note that since the integrand does not depend on z explicitly, we have written the first integral [Eq. (16.13)] immediately. For the solution we call $z' = p$ and solve the above equation for r to write

$$r = \frac{c_0}{p}(1+p^2)^2, \tag{16.45}$$

which when differentiated gives

$$dr = c_0\left(-\frac{1}{p^2} + 2 + 3p^2\right)dp. \tag{16.46}$$

Using $dz/dr = p$, we also obtain

$$\int dz = \int p\ dr = c_0 \int p\left(-\frac{1}{p^2} + 2 + 3p^2\right)dp, \tag{16.47}$$

$$z = c_0\left(-\ln p + p^2 + \frac{3p^4}{4}\right) + c_1. \tag{16.48}$$

Equations (16.45) and (16.48) represent the parametric expression of the needed surface of revolution. To determine the integration constants, we can use the values $z(a/2) = z_1$ and $z(R) = z_2$. For a complete treatment of this problem, which was originally discussed by Newton and which still has engineering interest, see Bryson and Ho [2].

16.2 Presence of More than One Dependent Variable

In the variational integral [Eq. (16.1)], if the function f depends on more than one dependent variable:

$$y_1(x), y_2(x), y_3(x), \dots , y_n(x), \tag{16.49}$$

and one independent variable, x, then the functional J is written as

$$J = \int_{x_1}^{x_2} f[y_1(x), y_2(x), \dots , y_n(x), y_{1x}(x), y_{2x}(x), \dots , y_{nx}(x), x]\, dx, \tag{16.50}$$

where $y_{ix} = \partial y_i/\partial x$, $i = 1, 2, \dots , n$. We can now write small deviations from the desired paths, $y_i(x, 0)$, which make the functional J an extremum as

$$y_i(x, \alpha) = y_i(x, 0) + \alpha\eta_i(x) + 0(\alpha^2), \quad i = 1, 2, \dots , n, \tag{16.51}$$

where α is again a small parameter and the functions $\eta_i(x)$ are independent of each other. We again take the variation at the end points as zero:

$$\eta_i(x_1) = \eta_i(x_2) = 0. \tag{16.52}$$

Taking the derivative of $J(\alpha)$ with respect to α and setting α to zero we get

$$\int_{x_1}^{x_2} \sum_i \left(\frac{\partial f}{\partial y_i}\eta_i(x) + \frac{\partial f}{\partial y_{ix}} \frac{d\eta_i(x)}{dx} \right) dx = 0. \tag{16.53}$$

Integrating the second term by parts and using the fact that at the end points variations are zero, we write Eq. (16.53) as

$$\int_{x_1}^{x_2} \sum_i \left(\frac{\partial f}{\partial y_i} - \frac{d}{dx}\frac{\partial f}{\partial y_{ix}} \right) \eta_i(x) dx = 0. \tag{16.54}$$

Because the variations $\eta_i(x)$ are independent, this equation can only be satisfied if all the coefficients of $\eta_i(x)$ vanish simultaneously, that is,

$$\boxed{\frac{\partial f}{\partial y_i} - \frac{d}{dx}\frac{\partial f}{\partial y_{ix}} = 0, \quad i = 1, 2, \dots , n.} \tag{16.55}$$

We now have a system of n Euler equations to be solved simultaneously for the n dependent variables. An important example for this type of variational problems is the Lagrangian formulation of classical mechanics.

16.3 Presence of More than One Independent Variable

Sometimes the unknown functions u and f in the functional J depend on more than one independent variable. For example, in three-dimensional problems J

may be given as

$$J = \iiint_V f[u, u_x, u_y, u_z, x, y, z]\, dxdydz, \tag{16.56}$$

where $u = u(x, y, z)$ and u_x, u_y, and u_z are the partial derivatives with respect to x, y, and z, respectively. We now have to find a function $u(x, y, z)$ such that J is an extremum. We again let $u(x, y, z, \alpha = 0)$ be the function that extremizes J and write the variation about this function as

$$u(x, y, z, \alpha) = u(x, y, z, \alpha = 0) + \alpha\eta(x, y, z) + O(\alpha^2), \tag{16.57}$$

where $\eta(x, y, z)$ is a differentiable function. We take the derivative of Eq. (16.56) with respect to α and set $\alpha = 0$: $\left(\frac{\partial J}{\partial \alpha}\right)_{\alpha=0} = 0$. We then integrate terms like $\frac{\partial f}{\partial u_x}\eta_x$ by parts and use the fact that variation at the end points are zero to write

$$\iiint \left(\frac{\partial f}{\partial u} - \frac{\partial}{\partial x}\frac{\partial f}{\partial u_x} - \frac{\partial}{\partial y}\frac{\partial f}{\partial u_y} - \frac{\partial}{\partial z}\frac{\partial f}{\partial u_z}\right) \eta(x, y, z) dxdydz = 0. \tag{16.58}$$

Because the variation $\eta(x, y, z)$ is arbitrary, the expression inside the parentheses must be zero; thus, yielding

$$\boxed{\frac{\partial f}{\partial u} - \frac{\partial}{\partial x}\frac{\partial f}{\partial u_x} - \frac{\partial}{\partial y}\frac{\partial f}{\partial u_y} - \frac{\partial}{\partial z}\frac{\partial f}{\partial u_z} = 0.} \tag{16.59}$$

This is the Euler equation for one dependent and three independent variables.

Example 16.5 ***Laplace equation***

In electrostatics energy density is given as $\rho = \frac{1}{2}\varepsilon E^2$, where E is the magnitude of the electric field. Because the electric field can be obtained from a scalar potential, Φ, as $\vec{E} = -\vec{\nabla}\Phi$, we can also write $\rho = \frac{1}{2}\varepsilon(\vec{\nabla}\Phi)^2$. Ignoring the $\varepsilon/2$ factor, let us find the Euler equation for the functional

$$J = \iiint_V (\vec{\nabla}\Phi)^2\, dxdydz. \tag{16.60}$$

Since $(\vec{\nabla}\Phi)^2 = \Phi_x^2 + \Phi_y^2 + \Phi_z^2$, f is given as

$$f[\Phi, \Phi_x, \Phi_y, \Phi_z, x, y, z] = \Phi_x^2 + \Phi_y^2 + \Phi_z^2. \tag{16.61}$$

Writing the Euler equation [Eq. (16.59)] for this f, we obtain

$$-2(\Phi_{xx} + \Phi_{yy} + \Phi_{zz}) = 0, \tag{16.62}$$

which is the Laplace equation $\vec{\nabla}^2\Phi(x, y, z) = 0$. A detailed investigation will show that this extremum is actually a minimum.

16.4 Presence of Multiple Dependent and Independent Variables

In general, if the f function depends on three dependent (p, q, r) and three independent variables (x, y, z) as

$$f = f[p, p_x, p_y, p_z, q, q_x, q_y, q_z, r, r_x, r_y, r_z, x, y, z], \tag{16.63}$$

we can parameterize the variation in terms of three scalar parameters α, β, and γ as

$$p(x, y, z; \alpha) = p(x, y, z, \alpha = 0) + \alpha\xi(x, y, z) + 0(\alpha^2), \tag{16.64}$$

$$q(x, y, z; \beta) = q(x, y, z, \beta = 0) + \beta\eta(x, y, z) + 0(\beta^2), \tag{16.65}$$

$$r(x, y, z; \gamma) = r(x, y, z, \gamma = 0) + \gamma\psi(x, y, z) + 0(\gamma^2). \tag{16.66}$$

Now, the p, q, and the r functions that extremize

$$J = \iiint f dxdydz \tag{16.67}$$

will be obtained from the solutions of the following system of three Euler equations:

$$\frac{\partial f}{\partial p} - \frac{\partial}{\partial x}\frac{\partial f}{\partial p_x} - \frac{\partial}{\partial y}\frac{\partial f}{\partial p_y} - \frac{\partial}{\partial z}\frac{\partial f}{\partial p_z} = 0, \tag{16.68}$$

$$\frac{\partial f}{\partial q} - \frac{\partial}{\partial x}\frac{\partial f}{\partial q_x} - \frac{\partial}{\partial y}\frac{\partial f}{\partial q_y} - \frac{\partial}{\partial z}\frac{\partial f}{\partial q_z} = 0, \tag{16.69}$$

$$\frac{\partial f}{\partial r} - \frac{\partial}{\partial x}\frac{\partial f}{\partial r_x} - \frac{\partial}{\partial y}\frac{\partial f}{\partial r_y} - \frac{\partial}{\partial z}\frac{\partial f}{\partial r_z} = 0. \tag{16.70}$$

If we have m dependent and n independent variables, then we can use y_i to denote the dependent variables and x_j for the independent variables and write the Euler equations as

$$\boxed{\frac{\partial f}{\partial y_i} - \sum_{j=1}^{n} \frac{\partial}{\partial x_j}\frac{\partial f}{\partial y_{ij}} = 0, \quad i = 1, 2, \ldots, m,} \tag{16.71}$$

where $y_{ij} = \frac{\partial y_i}{\partial x_j}$, $j = 1, 2, \ldots, n$.

16.5 Presence of Higher-Order Derivatives

Sometimes in engineering problems, we encounter functionals given as

$$J[y(x)] = \int_a^b F(x, y, y', \ldots, y^{(n)})\, dx, \tag{16.72}$$

where $y^{(n)}$ stands for the nth-order derivative, the independent variable x takes values in the closed interval $[a, b]$ and the dependent variable $y(x)$ satisfies the boundary conditions

$$\begin{aligned} &y(a) = y_0, y'(a) = y'_0, \quad \ldots, y^{(n-1)}(a) = y_0^{(n-1)}, \\ &y(b) = y_1, y'(b) = y'_1, \quad \ldots, y^{(n-1)}(b) = y_1^{(n-1)}. \end{aligned} \tag{16.73}$$

Using the same method that we have used for the other cases, we can show that the Euler equation that $y(x)$ satisfies is

$$\boxed{F_y - \frac{d}{dx}F_{y'} + \frac{d^2}{dx^2}F_{y''} - \cdots + (-1)^n \frac{d^n}{dx^n}F_{y^{(n)}} = 0, \quad F_{y^{(n)}} = \frac{\partial F}{\partial y^{(n)}}.} \tag{16.74}$$

This equation is also known as the **Euler–Poisson** equation.

Example 16.6 ***Deformation of an elastic beam***
Let us consider a homogeneous elastic beam supported from its end points at $(-l_1, 0)$ and $(0, l_1)$ as shown in Figure 16.5. Let us find the shape of the centerline of this beam. From the elasticity theory, the potential energy, E, of the beam is given as

$$E = \int_{-l_1}^{l_1} \left[\frac{1}{2}\mu \frac{(y'')^2}{(1 + y'^2)} + \rho y \sqrt{1 + y'^2}\right] dx, \tag{16.75}$$

where μ and ρ are parameters that characterize the physical properties of the beam. Assuming that the deformation is small, we can take $1 + y'^2 \approx 1$. Now the energy becomes

$$E = \int_{-l_1}^{l_1} \left[\frac{1}{2}\mu(y'')^2 + \rho y\right] dx. \tag{16.76}$$

For stable equilibrium, the energy of the beam must be a minimum, hence we have to minimize the energy integral with the conditions

$$y(l_1) = y(-l_1) = 0 \text{ and } y'(l_1) = y'(-l_1) = 0. \tag{16.77}$$

Using

$$F(x, y, y', y'') = \frac{1}{2}\mu(y'')^2 + \rho y, \tag{16.78}$$

we write the Euler–Poisson equation as

$$\mu y^{(4)} + \rho = 0, \tag{16.79}$$

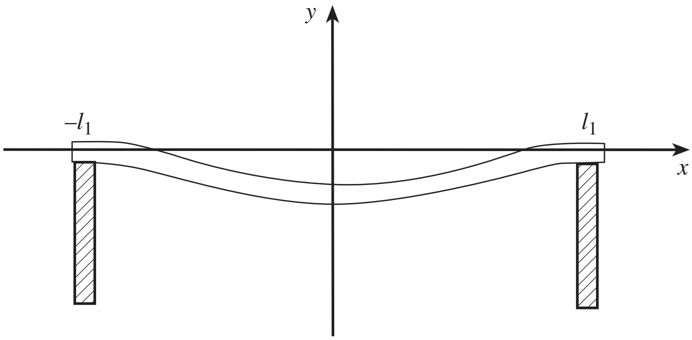

Figure 16.5 Deformation of an elastic beam.

the solution of which is easily obtained as

$$y = \alpha x^3 + \beta x^2 + \gamma x + \delta - \frac{\rho}{24\mu}x^4. \tag{16.80}$$

Using the boundary conditions given in Eq. (16.77), we can determine $\alpha, \beta, \gamma, \delta$ and find $y(x)$ as

$$y = \frac{\rho}{24\mu}[-x^4 + 2l_1^2x^2 - l_1^4]. \tag{16.81}$$

For the cases where there are m dependent variables, we can generalize the variational problem in Eq. (16.74) as

$$\boxed{I(y_1, \dots, y_m, x) = \int F\left(x, y_1, y_1', \dots, y_1^{(n_1)}, y_2, y_2', \dots, y_2^{(n_2)}, \dots, y_m, y_m', \dots, y_m^{(n_m)}\right) dx.} \tag{16.82}$$

The boundary conditions are now given as

$$\boxed{\begin{gathered} y_i^{(k)}(a) = y_{i0}^{(k)}, \;\; y_i^{(k)}(b) = y_{i1}^{(k)}, \\ k = 0, 1, \dots, n_i - 1, \;\; i = 1, 2, \dots, m, \end{gathered}} \tag{16.83}$$

and the **Euler–Poisson equations** become

$$\boxed{\sum_{k=0}^{n_i} (-1)^k \frac{d^k}{dx^k} F_{y_i}(k) = 0, \quad i = 1, 2, \dots, m.} \tag{16.84}$$

16.6 Isoperimetric Problems and the Presence of Constraints

In some applications we search for a function that not only extremizes a given functional:

$$\boxed{I = \int_{x_A}^{x_B} f(x, y, y')\, dx,} \tag{16.85}$$

but also keeps another functional:

$$\boxed{J = \int_{x_A}^{x_B} g(x, y, y')\, dx,} \tag{16.86}$$

at a fixed value. To find the Euler equation for such a function satisfying the boundary conditions

$$\boxed{y(x_A) = y_A, \quad y(x_B) = y_B,} \tag{16.87}$$

we parameterize the possible paths in terms of two parameters ε_1 and ε_2 as $\bar{y}(x, \varepsilon_1, \varepsilon_2)$. These paths also have the following **properties**:

(i) For all values of ε_1 and ε_2, they satisfy the boundary conditions $\bar{y}(x_A, \varepsilon_1, \varepsilon_2) = y_A$ and $\bar{y}(x_B, \varepsilon_1, \varepsilon_2) = y_B$.
(ii) $\bar{y}(x, 0, 0) = y(x)$ is the desired path.
(iii) $\bar{y}(x, \varepsilon_1, \varepsilon_2)$ has continuous derivatives with respect to all variables to second order.

We now substitute these paths into Eqs. (16.85) and (16.86) to get two integrals depending on two parameters ε_1 and ε_2 as

$$I(\varepsilon_1, \varepsilon_2) = \int_{x_A}^{x_B} f(x, \bar{y}, \bar{y}')\, dx, \tag{16.88}$$

$$J(\varepsilon_1, \varepsilon_2) = \int_{x_A}^{x_B} g(x, \bar{y}, \bar{y}')\, dx. \tag{16.89}$$

While we are extremizing $I(\varepsilon_1, \varepsilon_2)$ with respect to ε_1 and ε_2, we are also going to ensure that $J(\varepsilon_1, \varepsilon_2)$ takes a fixed value; thus, ε_1 and ε_2 cannot be independent. Using Lagrange undetermined multiplier λ, we introduce $K(\varepsilon_1, \varepsilon_2)$:

$$K(\varepsilon_1, \varepsilon_2) = I(\varepsilon_1, \varepsilon_2) + \lambda J(\varepsilon_1, \varepsilon_2). \tag{16.90}$$

The condition for $K(\varepsilon_1, \varepsilon_2)$ to be an extremum is now written as

$$\left[\frac{\partial K}{\partial \varepsilon_1}\right]_{\substack{\varepsilon_1=0\\ \varepsilon_2=0}} = \left[\frac{\partial K}{\partial \varepsilon_2}\right]_{\substack{\varepsilon_1=0\\ \varepsilon_2=0}} = 0. \tag{16.91}$$

In integral form this becomes

$$K(\varepsilon_1, \varepsilon_2) = \int_{x_A}^{x_B} h(x, \bar{y}, \bar{y}')\, dx, \tag{16.92}$$

where the h function is defined as

$$\boxed{h = f + \lambda g.} \tag{16.93}$$

Differentiating with respect to these parameters and integrating by parts, and using the boundary conditions we get

$$\left[\frac{\partial K}{\partial \varepsilon_j}\right] = \int_{x_A}^{x_B} \left[\frac{\partial h}{\partial \bar{y}} - \frac{d}{dx}\frac{\partial h}{\partial \bar{y}'}\right] \frac{\partial \bar{y}}{\partial \varepsilon_j} dx, \quad j = 1, 2. \tag{16.94}$$

Taking the variations as

$$\eta_j(x) = \left(\frac{\partial \bar{y}}{\partial \varepsilon_j}\right)_{\substack{\varepsilon_1 = 0 \\ \varepsilon_2 = 0}} \tag{16.95}$$

and using Eq. (16.91), we write

$$\int_{x_A}^{x_B} \left[\frac{\partial h}{\partial y} - \frac{d}{dx}\frac{\partial h}{\partial y'}\right] \eta_j(x)\, dx = 0, \;\; j = 1, 2. \tag{16.96}$$

Because the variations, η_j, are arbitrary, we set the quantity inside the square brackets to zero and obtain the differential equation

$$\frac{\partial h}{\partial y} - \frac{d}{dx}\frac{\partial h}{\partial y'} = 0. \tag{16.97}$$

Solutions of this differential equation contain two integration constants and a Lagrange undetermined multiplier λ. The two integration constants come from the boundary conditions [Eq. (16.87)], and λ comes from the constraint that fixes the value of J, thus completing the solution of the problem.

Another way to reach this conclusion is to consider the variation of the two functionals [Eqs. (16.85) and (16.86)] as

$$\delta I = \int \frac{\delta f}{\delta y} \delta y dx, \tag{16.98}$$

$$\delta J = \int \frac{\delta g}{\delta y} \delta y dx. \tag{16.99}$$

We now require that for all δy that makes $\delta J = 0$, δI should also vanish. This is possible if and only if $\frac{\delta f}{\delta y}$ and $\frac{\delta g}{\delta y}$ are constants independent of x, that is,

$$\left(\frac{\delta f}{\delta y}\right) \Big/ \left(\frac{\delta g}{\delta y}\right) = -\lambda(\text{constant}). \tag{16.100}$$

This is naturally equivalent to extremizing the functional $\int(f + \lambda g)dx$ with respect to arbitrary variations δy.

When we have m constraints like $J_1, \ldots, J_m$, the above method is easily generalized by taking h as

$$\boxed{h = f + \sum_{i=1}^{m} \lambda_i g_i} \tag{16.101}$$

with m Lagrange undetermined multipliers. Constraining integrals now become

$$\boxed{J_i = \int_{x_A}^{x_B} g_i(x, y, y')\, dx = c_j, \quad i = 1, 2, \ldots, m.} \tag{16.102}$$

If we also have n dependent variables, we have a system of n Euler equations given as

$$\boxed{\frac{\partial h}{\partial y_j} - \frac{d}{dx}\frac{\partial h}{\partial y'_j} = 0, \quad j = 1, \ldots, n,} \tag{16.103}$$

where h is given by Eq. (16.93).

Example 16.7 ***Isoperimetric problems***
Let us find the maximum area that can be enclosed by a closed curve of fixed perimeter L on a plane. We can define a curve on a plane in terms of a parameter t by giving a pair of functions as $(x(t), y(t))$. Now the enclosed area becomes

$$A = \frac{1}{2}\int_{t_A}^{t_B} (xy' - x'y)\, dt \tag{16.104}$$

while the fixed perimeter condition is expressed as

$$L = \int_{A}^{B} ds = \int_{t_A}^{t_B} \sqrt{x'^2 + y'^2}\, dt. \tag{16.105}$$

where the prime denotes differentiation with respect to the independent variable t, and x and y are the two dependent variables. Our only constraint is given by Eq. (16.105); thus, we have a single Lagrange undetermined multiplier and the h function is written as

$$h = \frac{1}{2}(xy' - x'y) + \lambda\sqrt{x'^2 + y'^2}. \tag{16.106}$$

Writing the Euler equation for $x(t)$ we get

$$\frac{\partial h}{\partial x} - \frac{d}{dt}\frac{\partial h}{\partial x'} = 0, \tag{16.107}$$

$$\frac{1}{2}y' - \frac{d}{dt}\left(-\frac{1}{2}y + \lambda\frac{x'}{\sqrt{x'^2 + y'^2}}\right) = 0, \tag{16.108}$$

$$y' - \frac{d}{dt}\left(\lambda\frac{x'}{\sqrt{x'^2 + y'^2}}\right) = 0 \tag{16.109}$$

and similarly for $y(t)$:

$$x' + \frac{d}{dt}\left(\lambda\frac{y'}{\sqrt{x'^2 + y'^2}}\right) = 0. \tag{16.110}$$

The first integral of this system of equations [Eqs. (16.109) and (16.110)] can easily be obtained as

$$y - \lambda\frac{x'}{\sqrt{x'^2 + y'^2}} = y_0, \quad x + \lambda\frac{y'}{\sqrt{x'^2 + y'^2}} = x_0. \tag{16.111}$$

Solutions of these are given as

$$y - y_0 = \lambda\frac{x'}{\sqrt{x'^2 + y'^2}}, \; x - x_0 = -\lambda\frac{y'}{\sqrt{x'^2 + y'^2}}, \tag{16.112}$$

which can be combined to obtain the equation of the closed curve as $(x - x_0)^2 + (y - y_0)^2 = \lambda^2$. This is the equation of a circle with its center at (x_0, y_0) and radius λ. Because the circumference is L, we determine λ as $\lambda = \frac{L}{2\pi}$.

Example 16.8 ***Shape of a freely hanging wire with fixed length***
We now find the shape of a wire with length L and fixed at both ends at (x_A, y_A) and (x_B, y_B). The potential energy of the wire is

$$I = \rho g \int_{x_A}^{x_B} y ds = \rho g \int_{x_A}^{x_B} y\sqrt{1 + y'^2}dx. \tag{16.113}$$

Because we take its length as fixed, we take our constraint as

$$L = \int_{x_A}^{x_B} \sqrt{1 + y'^2}dx. \tag{16.114}$$

For simplicity, we use a Lagrange undetermined multiplier defined as $\lambda = -\rho g y_0$ and write the h function:

$$h = \rho g(y - y_0)\sqrt{1 + y'^2}, \tag{16.115}$$

where g is the acceleration of gravity and ρ is the density of the wire. We change our dependent variable to $y \to \eta = y - y_0$, which changes our h function to

$$h = \rho g \eta(x)\sqrt{1 + \eta'^2}. \tag{16.116}$$

After we write the Euler equation, we find the solution as

$$y = y_0 + b\cosh\left(\frac{x - x_0}{b}\right). \tag{16.117}$$

Using the fact that the length of the wire is L and the end points are at (x_A, y_A) and (x_B, y_B), we can determine the Lagrange multiplier y_0 and the other constants x_0 and b.

16.7 Applications to Classical Mechanics

With the mathematical techniques developed in the previous sections, we can conveniently express a fairly large part of classical mechanics as a variational problem. If a classical system is described by the generalized coordinates $q_i(t)$, $i = 1, 2, \ldots, n$ and has a potential $V(q_i, t)$, then its **Lagrangian** can be written as

$$\boxed{L(q_i, \dot{q}_i, t) = T(q_i, \dot{q}_i) - V(q_i, t),} \tag{16.118}$$

where T is the kinetic energy and a dot denotes differentiation with respect to time. We now show that Newton's equations of motion follow from Hamilton's principle:

16.7.1 Hamilton's Principle

As a system moves from some initial time t_1 to t_2, with prescribed initial values $q_i(t_1)$ and $q_i(t_2)$, the actual path followed by the system is the one that makes the integral

$$\boxed{I = \int_{t_1}^{t_2} L(q_i, \dot{q}_i, t)dt} \tag{16.119}$$

an extremum. I is called the **action**.

From the conclusions of Section 16.1, the desired path comes from the solutions of

$$\boxed{\frac{\partial L}{\partial q_i} - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right) = 0, \quad i = 1, 2, \ldots, n,} \tag{16.120}$$

which are now called the **Lagrange** equations or the **Euler–Lagrange** equations. They are n simultaneous second-order differential equations to be solved simultaneously for $q_i(t)$, where the $2n$ arbitrary integration constants are determined from the initial conditions $q_i(t_1)$ and $q_i(t_2)$.

For a particle of mass m and moving in an arbitrary potential $V(x_1, x_2, x_3)$ the Lagrangian is written as

$$L = \frac{1}{2}m\left(\dot{x}_1^2 + \dot{x}_2^2 + \dot{x}_3^2\right) - V(x_1, x_2, x_3) \tag{16.121}$$

and the Lagrange equations become

$$m\dot{x}_i = -\frac{\partial V}{\partial x_i}, \quad i = 1, 2, 3, \tag{16.122}$$

which are nothing but Newton's equations of motion.

The main advantage of the Lagrangian formulation of classical mechanics is that it makes applications to many particle systems and continuous systems possible. It is also a must in making the transition to quantum mechanics and quantum field theories. For continuous systems we define a **Lagrangian density**, £, as

$$\boxed{L = \int_V £ d^3\vec{r},} \tag{16.123}$$

where V is the volume. Now the action in Hamilton's principle becomes

$$I = \int_{t_1}^{t_2} L dt = \int_{t_1}^{t_2} \left[\int_V £\, d^3\vec{r}\right] dt. \tag{16.124}$$

For a continuous time-dependent system with n independent fields, $\phi_i(\vec{r}, t)$, $i = 1, 2, \ldots, n$, the Lagrangian density is given as

$$£(\phi_i, \phi_{it}, \phi_{ix}, \phi_{iy}, \phi_{iz}, \vec{r}, t), \tag{16.125}$$

where $\phi_{it} = \frac{\partial \phi_i}{\partial t}$, $\phi_{ix} = \frac{\partial \phi_i}{\partial x}$, $\phi_{iy} = \frac{\partial \phi_i}{\partial y}$, $\phi_{iz} = \frac{\partial \phi_i}{\partial z}$. We can now use the conclusions of Section 16.4 to write the n Lagrange equations as

$$\frac{\partial £}{\partial \phi_i} - \frac{\partial}{\partial t}\frac{\partial £}{\partial \phi_{it}} - \frac{\partial}{\partial x}\frac{\partial £}{\partial \phi_{ix}} - \frac{\partial}{\partial y}\frac{\partial £}{\partial \phi_{iy}} - \frac{\partial}{\partial z}\frac{\partial £}{\partial \phi_{iz}} = 0. \tag{16.126}$$

For time-independent fields, $\phi_i(\vec{r})$, $i = 1, 2, \ldots, n$, the **Lagrange equations** become

$$\boxed{\frac{\partial £}{\partial \phi_i} - \sum_{j=1}^{3} \frac{\partial}{\partial x_j}\frac{\partial £}{(\partial \phi_i/\partial x_j)} = 0, \quad i = 1, 2, \ldots, n.} \tag{16.127}$$

As an example, consider the Lagrange density

$$£ = \frac{1}{2}\vec{\nabla}\phi(\vec{r}) \cdot \vec{\nabla}\phi(\vec{r}) + \frac{1}{2}m^2\phi(\vec{r})^2 \tag{16.128}$$

$$= \frac{1}{2}\left[\left(\frac{\partial\phi}{\partial x}\right)^2 + \left(\frac{\partial\phi}{\partial y}\right)^2 + \left(\frac{\partial\phi}{\partial y}\right)^2\right] + \frac{1}{2}m^2\phi^2, \tag{16.129}$$

where the corresponding Lagrange equation is

$$\vec{\nabla}^2\phi(\vec{r}) = m^2\phi(\vec{r}). \tag{16.130}$$

16.8 Eigenvalue Problems and Variational Analysis

For the variational problems, we have considered the end product that was a differential equation to be solved for the desired function. We are now going to approach the problem from the other direction and ask the question: Given a differential equation, is it always possible to obtain it as the Euler equation of a variational integral such as

$$\delta J = \delta \int_a^b f\, dt = 0\ ? \tag{16.131}$$

When the differential equation is an equation of motion, then this question becomes: Can we drive it from a Lagrangian? This is a rather subtle point. Even though it is possible to write theories that do not follow from a variational principle, they eventually run into problems.

We have seen that solving the Laplace equation within a volume V is equivalent to extremizing the functional

$$I[\phi(\vec{r})] = \frac{1}{2}\int_V (\vec{\nabla}\phi)^2 d^3\vec{r} \tag{16.132}$$

with the appropriate boundary conditions. Another frequently encountered differential equation in science and engineering is the **Sturm–Liouville equation:**

$$\boxed{\frac{d}{dx}\left[p(x)\frac{du(x)}{dx}\right] - q(x)u(x) + \lambda\rho(x)u(x) = 0, \quad x \in [a, b],} \tag{16.133}$$

which can be obtained by extremizing the functional

$$\boxed{I[u(x)] = \int_a^b [pu'^2 + (q - \lambda\rho)u^2]\, dx.} \tag{16.134}$$

However, because the eigenvalues λ are not known a priori, this form is not very useful. It is better to extremize

$$\boxed{I[u(x)] = \int_a^b [pu'^2 + qu^2]dx,} \tag{16.135}$$

subject to the constraint

$$\boxed{J[u(x)] = \int_a^b \rho u^2 dx = \text{constant.}} \tag{16.136}$$

In this formulation, eigenvalues appear as the Lagrange multipliers. Note that the constraint [Eq. (16.136)] is the normalization condition of $u(x)$; thus, we can also extremize

$$\boxed{K[u(x)] = \frac{I[u(x)]}{J[u(x)]}.} \tag{16.137}$$

If we multiply the Sturm–Liouville equation by $u(x)$ and then integrate by parts from a to b, we see that the extremums of $K[u(x)]$ correspond to the eigenvalues λ. In a Sturm–Liouville problem [7, Section 6.3]

1) There exists a minimum eigenvalue.
2) $\lambda_n \to \infty$ as $n \to \infty$.
3) To be precise, $\lambda_n \sim n^2$ as $n \to \infty$.

Thus, the minimums of Eq. (16.137) give the eigenvalues λ_n. In fact, from the first property, the absolute minimum of K is the lowest eigenvalue λ_0. This is very useful in putting an upper bound to the lowest eigenvalue. To estimate the lowest eigenvalue we choose a trial function, $u(x)$, and expand in terms of the exact eigenfunctions, $u_i(x)$, which are not known:

$$u(x) = u_0(x) + c_1 u_1(x) + c_2 u_2(x) + \cdots. \tag{16.138}$$

Depending on how close our trial function is to the exact eigenfunction, the coefficients $c_1, c_2, \ldots$ will be small numbers. Before we evaluate $K[u(x)]$, let us substitute our trial function into Eq. (16.135):

$$\int_a^b [p(x)(u_0' + c_1 u_1' + c_2 u_2' + \cdots)^2 + q(x)(u_0 + c_1 u_1 + c_2 u_2 + \cdots)^2]\, dx. \tag{16.139}$$

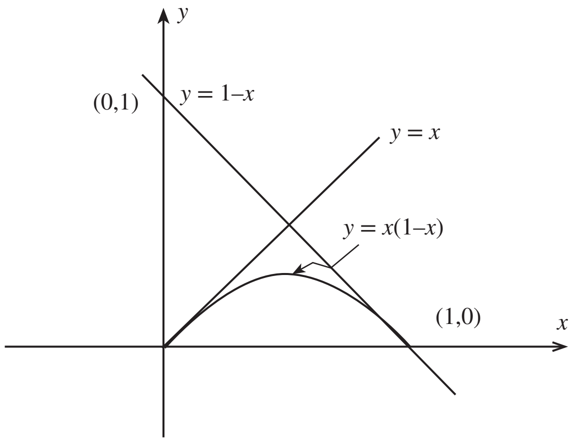

Figure 16.6 sin(πx) could be approximated by $x(1-x)$.

Since the set $\{u_i\}$ is orthonormal, using the following relations:

$$\int_a^b [pu_i'^2 + qu_i^2]\, dx = \lambda_i, \tag{16.140}$$

$$\int_a^b [pu_i'u_j' + qu_iu_j]\, dx = 0, \quad i \neq j, \tag{16.141}$$

we can write

$$K[u(x)] = \frac{\int_a^b [pu'^2 + qu^2]\, dx}{\int_a^b \rho u^2 dx} \tag{16.142}$$

$$\simeq \frac{\lambda_0 + c_1^2\lambda_1 + c_2^2\lambda_2 + \cdots}{1 + c_1^2 + c_2^2 + \cdots}. \tag{16.143}$$

Because $c_1, c_2, \ldots$ are small numbers, K gives us the approximate value of the lowest eigenvalue as

$$K \simeq \lambda_0 + c_1^2(\lambda_1 - \lambda_0) + c_2^2(\lambda_2 - \lambda_0) + \cdots. \tag{16.144}$$

What is significant here is that even though our trial function is good to the first order, our estimate of the lowest eigenvalue is good to the second order. This is also called the **Hylleraas–Undheim theorem**. Because the eigenvalues are monotonic increasing, this estimate is also an **upper bound** to the **lowest eigenvalue**.

Example 16.9 ***How to estimate lowest eigenvalue***
Let us estimate the lowest eigenvalue of

$$\frac{d^2u}{dx^2} + \lambda u = 0 \tag{16.145}$$

with the boundary conditions $u(0) = 0$, $u(1) = 0$. As shown in Figure 16.6 we can take our trial function as

$$u = x(1 - x). \tag{16.146}$$

This gives

$$\lambda_0 \leq \frac{\int_0^1 u'^2 dx}{\int_0^1 u^2 dx} = \frac{\frac{1}{3}}{\frac{1}{30}} = 10. \tag{16.147}$$

This is already close to the exact eigenvalue π^2. For a better upper bound we can improve our trial function as

$$u = x(1 - x)(1 + c_1 x + \cdots) \tag{16.148}$$

and determine c_i by extremizing K. For this method to work, our trial function:

1. must satisfy the boundary conditions.
2. should reflect the general features of the exact eigenfunction.
3. should be sufficiently simple to allow analytic calculations.

Example 16.10 ***Vibrations of a drumhead***
We now consider the wave equation:

$$\vec{\nabla}^2 u + k^2 u = 0, \quad k^2 = \frac{\omega^2}{c^2}, \tag{16.149}$$

in two dimensions and in spherical polar coordinates. We take the radius as a and use $u(a) = 0$ as our boundary condition. This suggests the trial function

$$u = 1 - \frac{r}{a}. \tag{16.150}$$

Now the upper bound for the lowest eigenvalue, k_0^2, is obtained from

$$k_0^2 \leq \frac{\int_0^a \int_0^{2\pi} (\vec{\nabla} u)^2 \, r dr d\theta}{\int_0^a \int_0^{2\pi} u^2 r dr d\theta} \tag{16.151}$$

as

$$k_0^2 \leq \frac{\pi}{\pi a^2/6} = \frac{6}{a^2}. \tag{16.152}$$

Compare this with the exact eigenvalue $k_0^2 = 5.78/a^2$.

Example 16.11 ***Harmonic oscillator problem***
The Schrödinger equation can be driven from the functional

$$\frac{\Psi \cdot H\Psi}{\Psi \cdot \Psi}, \tag{16.153}$$

where $\Psi_1 \cdot \Psi_2 = \int_{-\infty}^{\infty} \Psi_1^* \Psi_2 dx$. For the harmonic oscillator problem the Schrödinger equation is written as

$$H\Psi = -\frac{d^2\Psi}{dx^2} + x^2\Psi = E\Psi, \quad x \in (-\infty, \infty). \tag{16.154}$$

For the lowest eigenvalue we take our trial function as

$$\Psi = (1 + \alpha x^2)e^{-x^2}. \tag{16.155}$$

For an upper bound this gives

$$E_0 \leq \frac{\Psi \cdot H\Psi}{\Psi \cdot \Psi} = \frac{\frac{5}{4} - \frac{\alpha}{8} + \frac{43\alpha^2}{64}}{1 + \frac{\alpha}{2} + \frac{3\alpha^2}{16}}. \tag{16.156}$$

To find its minimum, we solve

$$23\alpha^2 + 56\alpha - 48 = 0 \tag{16.157}$$

and find $\alpha = 0.6718$. Thus, the upper bound to the lowest energy is obtained as $E_0 \leq 1.034$, where the exact eigenvalue is 1.0. This method can also be used for the higher-order eigenvalues. However, one must make sure that the chosen trial function is orthogonal to the eigenfunctions corresponding to the lower eigenvalues.

16.9 Rayleigh–Ritz Method

In this method we aim to find an approximate solution to a differential equation satisfying certain boundary conditions. We first write the solution in terms of suitably chosen functions, $\phi_i(x)$, $i = 0, \ldots, n$, as

$$y(x) \simeq \phi_0(x) + c_1\phi_1(x) + c_2\phi_2(x) + c_3\phi_3(x) + \cdots + c_n\phi_n(x), \tag{16.158}$$

where $c_1, c_2, \ldots, c_n$ are constants to be determined. Here, $\phi_i(x)$, $i = 0, \ldots, n$, are chosen functions so that $y(x)$ satisfies the boundary conditions for any choice of the c values. In general, $\phi_0(x)$ is chosen such that it satisfies the boundary conditions at the end points of our interval and $\phi_1(x), \phi_2(x), \ldots, \phi_n(x)$ are chosen such that they vanish at the end points.

Example 16.12 ***Loaded cable fixed between two points***
We consider a cable fixed between the points $(0, 0)$ and (l, h). The cable carries a load along the y-axis distributed as $f(x) = -q_0\frac{x}{l}$.

To find the shape of this cable, we have to solve the variational problem

$$\delta \int_0^l \left(\frac{1}{2}T_0 y'^2 + q_0\frac{x}{l}y\right) dx = 0 \tag{16.159}$$

with the boundary conditions $y(0) = 0$ and $y(l) = h$, where T_0 and q_0 are constants. Using the Rayleigh–Ritz method, we choose $\phi_0(x)$ such that it satisfies the above boundary conditions and choose $\phi_1, \ldots, \phi_n$ such that they vanish at both end points:

$$\phi_0 = \frac{h}{l}x, \tag{16.160}$$

$$\phi_1 = x(x-l), \tag{16.161}$$

$$\phi_2 = x^2(x-l), \tag{16.162}$$

$$\vdots$$

$$\phi_n = x^n(x-l). \tag{16.163}$$

Now the approximate solution $y(x)$ becomes

$$y(x) \simeq \frac{h}{l}x + x(x-l)(c_1 + c_2x + \cdots + c_nx^{n-1}). \tag{16.164}$$

For simplicity, we choose $n = 1$ so that $y(x)$ becomes

$$y(x) \simeq \frac{h}{l}x + x(x-l)c_1. \tag{16.165}$$

Substituting this into the variational integral we get

$$\delta \int_0^l \left[\frac{1}{2}T_0\left(\frac{h}{l} + (2x-l)c_1\right)^2 + q_0\frac{x}{l}\left(\frac{h}{l}x + x(x-l)c_1\right)\right] dx = 0, \tag{16.166}$$

$$\delta\left[\frac{1}{2}T_0\left(\frac{h^2}{l} + \frac{1}{3}l^3c_1^2\right) + q_0\left(\frac{1}{3}hl - \frac{1}{12}c_1l^3\right)\right] = 0, \tag{16.167}$$

$$\frac{1}{3}T_0l^3c_1\delta c_1 - \frac{1}{12}q_0l^3\delta c_1 = 0, \tag{16.168}$$

$$\frac{1}{3}T_0l^3\left(c_1 - \frac{q_0}{4T_0}\right)\delta c_1 = 0. \tag{16.169}$$

Because the variation δc_1 is arbitrary, the quantity inside the brackets must vanish, thus giving $c_1 = q_0/4T_0$ and

$$y(x) \simeq \frac{h}{l}x + \frac{q_0}{4T_0}x(x-l). \tag{16.170}$$

The Euler equation for the variational problem [Eq. (16.159)] can easily be written as

$$T_0y'' - \frac{q_0x}{l} = 0, \tag{16.171}$$

where the exact solution of this problem is

$$y(x) = \frac{h}{l}x + \frac{q_0}{6T_0l}x(x^2 - l^2). \tag{16.172}$$

As we will see in the next example, an equivalent approach is to start with the Euler equation (16.171), which results from the variational integral

$$\int_0^l \left[T_0 y'' - \frac{q_0 x}{l}\right] \delta y dx = 0. \tag{16.173}$$

Substituting Eq. (16.165) into the above equation, we write

$$\int_0^l \left[2c_1 T_0 - \frac{q_0 x}{l}\right] x(x-l)\delta c_1 dx = 0, \tag{16.174}$$

which after integration yields

$$\left[-\frac{1}{3}c_1 T_0 l^3 + \frac{1}{12}q_0 l^3\right] \delta c_1 = 0. \tag{16.175}$$

Since δc_1 is arbitrary, we again obtain $c_1 = q_0/4T_0$.

Example 16.13 ***Rayleigh–Ritz Method***
We now find the solution of the differential equation

$$\frac{d^2y}{dx^2} + xy = -x, \tag{16.176}$$

with the boundary conditions $y(0) = 0$ and $y(1) = 0$ by using the Rayleigh–Ritz method. The variational problem corresponding to this differential equation can be written as

$$\int_0^1 (y'' + xy + x)\delta y dx = 0. \tag{16.177}$$

We take the approximate solution as

$$y(x) \simeq x(1-x)(c_1 + c_2 x + \cdots), \tag{16.178}$$

and substitute this in Eq. (16.177) to obtain

$$\int_0^1 [(-2 + x^2 - x^3)\, c_1 + (2 - 6x + x^3 - x^4)\, c_2 + \cdots + x] \times [\delta c_1 (x - x^2) + \delta c_2 (x^2 - x^3) + \cdots]\, dx = 0. \tag{16.179}$$

Solution with one term is given as

$$y^{(1)} = c_1 x(1-x), \quad c_1 = \frac{5}{19}, \tag{16.180}$$

while the solution with two terms is given as

$$y^{(2)} = c_1 x(1-x) + c_2 x^2(1-x), \tag{16.181}$$

where $c_1 = 0.177$ and $c_2 = 0.173$.

Example 16.14 ***Rayleigh–Ritz method (first order)***
Consider the differential equation

$$y'' + \lambda a(x)y(x) = 0, \ y(0) = y(1) = 0, \tag{16.182}$$

which could represent the vibrations of a rod with nonuniform cross-section given by $a(x)$. By choosing a suitable trial function, estimate the lowest eigenvalue for $a(x) = x$.

Solution
Using the trial functions

$$y(x) = \sin \pi x \text{ and } y(x) = x(1 - x), \tag{16.183}$$

we can estimate the lowest eigenvalue, λ_0, by

$$\lambda_0 \leq \frac{\int_0^1 |y'(x)|^2 dx}{\int_0^1 a(x)|y(x)|^2 \, dx}. \tag{16.184}$$

For the two trial functions, this yields the λ_0 values, respectively, as

$$\lambda_0 \leq 19.74, \ \lambda_0 \leq 20.0. \tag{16.185}$$

One can show that for $a(x) = \alpha + \beta x$, Eq. (16.182) can be reduced to Bessel's equation, where for $\alpha = 0$, $\beta = 1$, the exact lowest eigenvalue is given as $\lambda_0 = 18.956$. We can improve our approximation by choosing the trial function as

$$y(x) = \sin \pi x + c \sin 2\pi x, \tag{16.186}$$

which leads to the inequality

$$\lambda_0 \leq \frac{2\pi^2(1 + 4c^2)}{1 + c^2 - 64c/9\pi^2}. \tag{16.187}$$

Minimizing the right-hand side gives $c = -0.11386$ and the improved estimate becomes $\lambda_0 \leq 18.961$.

Example 16.15 ***Rayleigh–Ritz method (second order)***
For the previous problem, we now find an upper bound to the second-order eigenvalue. In Example 16.11, we have said that the method we use to estimate the lowest eigenvalue can also be used for the higher-order eigenvalues, granted that the trial function is chosen orthogonal to the lower eigenfunctions. In the previous problem, we have estimated the lowest eigenvalue via the test function [Eq. (16.186)]

$$y_0 = \sin \pi x - 0.11386 \ \sin \ 2\pi x. \tag{16.188}$$

For the second-order trial function we can use

$$y_1 = \sin \pi x + d \sin\ 2\pi x, \tag{16.189}$$

where d is determined such that y_0 and y_1 are orthogonal. A simple calculation yields

$$d = \frac{9\pi^2(-0.11386) - 32}{32(-0.11386) - 9\pi^2} = 2.1957, \tag{16.190}$$

which gives the estimate $\lambda_1 \leq 94.45$. An exact calculation in terms of Bessel functions gives $\lambda_1 = 81.89$. Note and also show that the estimates for λ_0 and λ_1 are both upper bounds to the exact eigenvalues.

Example 16.16 ***Variational analysis***

If $y(x)$ extremizes $J[y(x)]$, then regardless of the prescribed end conditions, show that the first variation must vanish:

$$\delta J[y(x)] = 0. \tag{16.191}$$

Solution

Using the variational notation, we write the variation of the functional

$$J[y(x)] = \int_1^2 F(y, y', x)dx \tag{16.192}$$

as

$$J[y(x) + \delta y] - J[y(x)] = \delta J + \delta^2 J + \delta^3 J + \cdots , \tag{16.193}$$

where the second variation is given as

$$\delta^2 J = \frac{1}{2!} \int_1^2 [F_{yy}\delta y^2 + 2F_{yy'}\delta y \delta y' + F_{y'y'}\delta y'^2]\, dx. \tag{16.194}$$

Since [Eq. (16.3)] $\delta y = \varepsilon\eta(x)$, $\delta y' = \varepsilon\eta'(x), \ldots$, where ε is a small parameter, $\delta^2 J$ is smaller in magnitude by at least one power of ε than δJ and so are the higher-order variations. On the other hand, $\delta J[\delta y]$ can be written as

$$\delta J[\delta y] = \varepsilon \int_1^2 [F_y \eta(x) + F_{y'}\eta'(x)]\, dx, \tag{16.195}$$

which can be made to be positive or negative for the positive or the negative choices of the small parameter ε, respectively, hence $\delta J[y(x)]$ must vanish for any $y(x)$ that extremizes the functional in Eq. (16.192).

16.10 Optimum Control Theory

Let us now discuss a slightly different problem, where we have to produce a certain amount, say by weight, of goods to meet a certain order at time $t = T$. The problem is to determine the best strategy to follow so that our cost is minimum. One obvious strategy is to produce at a constant rate determined by the amount of goods to be delivered at time T. To see whether this actually minimizes our cost or not, let us formulate this as a variational problem. We first let $x(t)$ be the total amount of goods accumulated at $t \geq 0$, hence its derivative, $x'(t)$, gives the production rate. For the cost there are mainly two sources, one of which is the **production cost per unit item**, c_P, which can be taken as proportional to the production rate:

$$c_P = k_1 x'(t), \tag{16.196}$$

Naturally, producing faster while maintaining the quality of the product increases the cost per item. Besides, producing the goods faster will increase our inventory unnecessarily before the delivery time, thus increasing the **holding cost**, c_H, which is defined as the **cost per unit item per unit time**. As a first approximation, we can take c_H to be proportional to $x(t)$:

$$c_H = k_2 x(t). \tag{16.197}$$

We can now write the **total cost of production** over the time interval

$$(t, t + \Delta t) \tag{16.198}$$

as

$$\delta J = c_P \delta x + c_H \delta t \tag{16.199}$$

$$= [c_P x'(t) + c_H]\, \delta t \tag{16.200}$$

$$= [k_1 x'(t)^2 + k_2 x(t)]\, \delta t. \tag{16.201}$$

We also assume that production starts at $t = 0$ with **zero inventory**:

$$x(0) = x_0 = 0, \tag{16.202}$$

and we need

$$x(T) = x_T, \tag{16.203}$$

where x_T is the amount of goods to be delivered at $t = T$. We can know write the total cost of the entire process as the functional

$$\boxed{J[x(t)] = \int_0^T [k_1 x'(t)^2 + k_2 x(t)]\, dt.} \tag{16.204}$$

The problem is to find a production strategy, $x(t)$, that minimizes the functional $J[x(t)]$, subject to the initial conditions

$$x(0) = 0, \quad x(T) = x_T. \tag{16.205}$$

An acceptable solution should also satisfy the conditions

$$x(t) \geq 0 \text{ and } x'(t) \geq 0. \tag{16.206}$$

Solution of the **unconstrained problem** with the given initial equations [Eq. (16.205)] is

$$\boxed{x(t) = \left(x_T - \frac{k_2}{4k_1}T\right)\frac{t}{T} + \frac{k_2}{4k_1}t^2.} \tag{16.207}$$

The uniform rate of production,

$$x(t) = \frac{x_T t}{T}, \tag{16.208}$$

even though satisfies the end conditions [Eq. (16.205)] and the inequalities in Eq. (16.206), does not minimize $J[x(t)]$ for $k_2 \neq 0$. Besides, for realistic problems due to finite capacity we also have an upper and a lower bound for the production rate, hence we also need to satisfy the inequalities

$$x'_M \geq x'(t) \geq x'_m \geq 0, \tag{16.209}$$

where x'_M and x'_M represent the possible maximum and the minimum production rates, respectively. The unconstrained solution is valid only for the times that the inequalities in Eqs. (16.206) and (16.209) are satisfied. Variational problems with constraints on $x(t)$ and/or $x'(t)$, expressed either as equalities, or inequalities, are handled by the **optimal control theory**, which is a derivative of the variational analysis. In the minimum cost production schedule, to obtain the desired result we need to control the production rate, $x'(t)$, hence the optimal control theory is needed to determine the correct strategy.

16.11 Basic Theory: Dynamics versus Controlled Dynamics

In physics a **dynamic system** is described by the second law of Newton as

$$\vec{F} = m\vec{a}, \tag{16.210}$$

where $\vec{F}$ represents the net force acting on the mass, m, and $\vec{a}$ is the acceleration. For example, for the one-dimensional motion of a mass falling in uniform gravity, g, under the influence of a restoring force, $-kx$, and a friction force, $-\mu\dot{x}$, the second law of Newton becomes

$$m\ddot{x} = -\mu\dot{x} - kx - mg, \tag{16.211}$$

where k and μ are constants. With the appropriate initial conditions, $x(0)$ and $\dot{x}(0)$, we can solve this differential equation to find the position, $x(t)$, at a later time. If we also attach a thrust mechanism that allows us to apply force, $f(t)$, to the mass m, then we can control its dynamics so that it arrives at a specific point at a specific time and with a predetermined velocity. Equation (16.211) is now written as

$$\ddot{x} = -\frac{\mu}{m}\dot{x} - \frac{k}{m}x - g + \frac{f(t)}{m}. \tag{16.212}$$

We now define two new variables, y_1 and y_2, that define the **state of the system**:

$$y_1(t) = x(t),\ \ y_2(t) = \dot{x}(t), \tag{16.213}$$

and introduce u_1 and u_2, called the **control variables** or parameters as

$$u_1(t) = 0,\ \ u_2(t) = \frac{f(t)}{m}. \tag{16.214}$$

We can write them as the column vectors

$$\mathbf{y} = \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} \text{ and } \mathbf{u} = \begin{pmatrix} u_1 \\ u_2 \end{pmatrix}. \tag{16.215}$$

Controlled dynamics of this system is now governed by the differential equation

$$\boxed{\dot{\mathbf{y}} = \mathbf{f}(\mathbf{y}, \mathbf{u}, t),} \tag{16.216}$$

where $\mathbf{f}(\mathbf{y}, \mathbf{u}, t)$ is given as

$$\mathbf{f}(\mathbf{y}, \mathbf{u}, t) = \begin{pmatrix} y_2 \\ -\frac{k}{m}y_1 - \frac{\mu}{m}y_2 - g + u_2 \end{pmatrix} \tag{16.217}$$

$$= \begin{pmatrix} 0 & 1 \\ -\frac{k}{m} & -\frac{\mu}{m} \end{pmatrix}\mathbf{y} + \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}\mathbf{u} + \begin{pmatrix} 0 \\ -g \end{pmatrix}. \tag{16.218}$$

Introducing the matrices

$$\mathbf{A} = \begin{pmatrix} 0 & 1 \\ -\frac{k}{m} & -\frac{\mu}{m} \end{pmatrix}, \tag{16.219}$$

$$\mathbf{B} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \tag{16.220}$$

$$\mathbf{f}_0 = \begin{pmatrix} 0 \\ -g \end{pmatrix}. \tag{16.221}$$

we can write the above equation as

$$\mathbf{f}(\mathbf{y}, \mathbf{u}, t) = \mathbf{A}\mathbf{y} + \mathbf{B}\mathbf{u} + \mathbf{f}_0. \tag{16.222}$$

Note that Eq. (16.216) gives two differential equations:

$$\dot{y}_1 = y_2 \tag{16.223}$$

and

$$\dot{y}_2 = -\frac{k}{m}y_1 - \frac{\mu}{m}y_2 - g + u_2, \tag{16.224}$$

to be solved simultaneously, which are coupled and linear. However, in general they are nonlinear and cannot be decoupled. For a realistic solution of the **fuel-optimal** horizontal motion of a **rocket problem**, one also has to consider the loss of mass due to thrusting [4].

General Statement of a Controlled Dynamics Problem
A general optimal control problem involves the following features:

(I) **State variables and Controls:**
State of the system is described by the state variable, $\mathbf{y}$, written as the column $(n \times 1)$ vector

$$\mathbf{y}(t) = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix} \tag{16.225}$$

while all the admissible controls are described by the $(m \times 1)$ column vector

$$\mathbf{u}(t) = \begin{pmatrix} u_1 \\ \vdots \\ u_m \end{pmatrix}. \tag{16.226}$$

(II) **Vector differential equation of state:**
Dynamical evolution of the system is described by the ordinary differential equation

$$\boxed{\dot{y} = \mathbf{f}(\mathbf{y}, \mathbf{u}, t),} \tag{16.227}$$

also called the **equation of state**, where $\mathbf{f}(\mathbf{y}, \mathbf{u}, t)$ is a known $(n \times 1)$ continuously differentiable column vector, with the usual **initial condition**

$$\boxed{\mathbf{y}(t_0) = \mathbf{y}_0.} \tag{16.228}$$

Depending on the problem, the terminal state, $\mathbf{y}(T)$, is either fixed or left free.

(III) **Constraints:**

(a) Some constraints on the controls, which are of the form

$$\mathbf{u}(t_1) = \mathbf{u}_1, \tag{16.229}$$

for some t_1 in the time domain.

(b) Some constraints on the controls in the form of inequalities, such as

$$\mathbf{u}_m \leq \mathbf{u} \leq \mathbf{u}_M. \tag{16.230}$$

(c) Some constraints on the state variables, which are either expressed as equality:

$$\Phi(\mathbf{y}, t) = 0, \tag{16.231}$$

or as inequality:

$$\Theta(\mathbf{y}, t) \geq 0. \tag{16.232}$$

(d) One could also have constraints mixing the state variables and the controls and expressed in various forms.

(IV) **Solution:**

For a given choice of an admissible control, $\mathbf{u}(t)$, we solve the initial value problem [Eq. (16.227)] for $\mathbf{y}(t)$. In other cases, we seek for an admissible $\mathbf{u}(t)$ that steers $\mathbf{y}(t)$ to a target value $\mathbf{y}(T)$ at some terminal time T. In optimal control problems, we look for the admissible control variables, $\mathbf{u}(t)$, such that the functional,

$$\boxed{J[u(t)] = \int_{t_0}^{T} F(\mathbf{y}, \mathbf{u}, t)dt + \Psi(T, \mathbf{y}(T)), m} \tag{16.233}$$

where $F(\mathbf{y}(t), \mathbf{u}(t), t)$ and $\Psi(T, \mathbf{y}(T))$ are known functions, is minimized or maximized. Note that $F(\mathbf{y}, \mathbf{u}, t)$ in Eq. (16.233) is different from $f(\mathbf{y}, \mathbf{u}, t)$ in Eq. (16.227). In certain type of problems we look for the maximum of $J[u(t)]$, where it is called the **payoff functional**, while $F(\mathbf{y}, \mathbf{u}, t)$ is the **running payoff** and $\Psi(T, \mathbf{y}(T))$ is called the **terminal payoff**. In certain other problems, the minimum of $J[u(t)]$ is desired, where it is called the **cost functional.**

16.11.1 Connection with Variational Analysis

There is a definite connection between optimal control theory and variational analysis. If we set $\dot{x} = u$ in the action:

$$J[x(t)] = \int_{1}^{2} \pounds(x, \dot{x}, t)dt, \tag{16.234}$$

and write

$$J[x(t)] = \int_1^2 \pounds(x, u, t)dt, \tag{16.235}$$

and take the constraint as the entire real axis for u, we transform a variational problem to an optimal control one with

$$\dot{x} = u \tag{16.236}$$

representing the equation of state [Eq. (16.227)]. Similarly, if we solve the equation of state [Eq. (16.227)] for u in terms of $\dot{y}, y$, and t, and substitute the result into the payoff functional in Eq. (16.233), we can convert an optimal control problem into a variational problem.

However, it should be kept in mind that there is a philosophical difference between the two approaches. In Lagrangian mechanics nature does the optimization and hence controls the entire process. All we can do is to adjust the initial conditions. For example, when firing a cannon ball controlling the system through initial conditions helps to achieve a simple goal like having the ball drop to a specific point. However, if we are sending astronauts to the moon, to assure that they land on the moon safely we have to steer the process all the way. Among other things, we have to assure that the fuel is used efficiently, that is, we have to make sure that the accelerations involved and the cabin conditions stay within certain limits and the rocket lands softly on the moon with enough fuel left to return. Optimum control theory basically allows us to develop the most advantageous strategy to achieve the desired result through some control variables that we build into the system, like the thrust system. In optimal control theory, we are basically **steering the system** to achieve a certain goal.

16.11.2 Controllability of a System

A major concern in optimal control theory is the controllability of a given system. Landing a rocket safely on the moon is a difficult problem, but if we insist on landing it at a specific point at a specific time, that is, if we also fix the terminal state, it becomes a much more difficult problem. In general, it is not clear that a system can be steered from an initial state to a predetermined final state with an admissible choice of the control variables. To demonstrate some of the basic ideas, we confine ourselves to linear systems where the equation of state can be written as

$$\dot{\mathbf{y}} = F(\mathbf{y}, \mathbf{u}, t) \tag{16.237}$$

$$= \mathbf{A}\mathbf{y} + \mathbf{B}\mathbf{u}. \tag{16.238}$$

Here, **A** and **B** are $(n \times n)$ and $(n \times m)$ matrices, respectively. To simplify the matter further, consider time-invariant, that is, **autonomous**, systems. For such systems the **A** and **B** matrices are constant matrices, hence the controllability of such a system does not depend on the initial time. Let us now consider that **A** has a complete set of eigenvectors and let **M** be the matrix, columns of which are composed of the eigenvectors of **A**. We also define the column vector **z** as

$$\mathbf{z} = \mathbf{M}^{-1}\mathbf{y}, \tag{16.239}$$

and write Eq. (16.239) as

$$\dot{\mathbf{z}} = \mathbf{M}^{-1}\dot{\mathbf{y}} \tag{16.240}$$
$$= \mathbf{M}^{-1}[\mathbf{A}\mathbf{y} + \mathbf{B}\mathbf{u}] \tag{16.241}$$
$$= \mathbf{M}^{-1}\mathbf{A}\mathbf{M}\mathbf{M}^{-1}\mathbf{y} + \mathbf{M}^{-1}\mathbf{B}\mathbf{u} \tag{16.242}$$
$$= (\mathbf{M}^{-1}\mathbf{A}\mathbf{M})\mathbf{M}^{-1}\mathbf{y} + \mathbf{M}^{-1}\mathbf{B}\mathbf{u} \tag{16.243}$$
$$= (\mathbf{M}^{-1}\mathbf{A}\mathbf{M})\mathbf{z} + (\mathbf{M}^{-1}\mathbf{B})\mathbf{u}, \tag{16.244}$$

where $\mathbf{M}^{-1}\mathbf{A}\mathbf{M}$ is a diagonal $(n \times n)$ matrix, $\boldsymbol{\lambda}$, with its diagonal terms being the eigenvalues:

$$\mathbf{M}^{-1}\mathbf{A}\mathbf{M} = \boldsymbol{\lambda} = \begin{pmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_n \end{pmatrix}. \tag{16.245}$$

From here it is seen that if the matrix $\mathbf{M}^{-1}\mathbf{B}$ has a zero row, say, the kth row, then the kth component of $\dot{\mathbf{z}}$ satisfies

$$\dot{z}_k = \lambda_k z_k. \tag{16.246}$$

That is, $z_k(t)$ is determined entirely by the initial conditions at t_0. In general, for a linear autonomous system, if **A** has a complete set of eigenfunctions, a necessary and sufficient condition for its controllability is that $\mathbf{M}^{-1}\mathbf{B}$ has no zero rows. For linear autonomous systems, where the constant matrix **A** does not necessarily has a complete set of eigenvectors, then the following theorem is more useful:

Theorem 16.1 A linear autonomous system is controllable, if and only if the $(n \times m)$ matrix

$$\mathbf{C} = [\mathbf{B}, \mathbf{A}\mathbf{B}, \mathbf{A}^2\mathbf{B}, \ldots, \mathbf{A}^{n-1}\mathbf{B}] \tag{16.247}$$

is of rank n. Proof of this theorem can be found in Wan [8]. There exists a set of conditions that the optimal solution of an optimal control theory problem should satisfy. This set of conditions is called the **Pontryagin's Minimum Principle,** which can also be used to solve several optimal control problems. For a formulation of the optimal control problem via the Pontryagin's minimum principal see Geering [4].

Example 16.17 ***Inventory control model***
A firm has an inventory of y_1 amount (by weight) of goods produced at the rate of $u_1 = u(t)$. If the rate of sales, which could be taken from the past records is y_2, we can write the rate of change of the inventory as

$$\dot{y}_1 = u - y_2. \tag{16.248}$$

It is natural to think that the firm will try harder to sell when the inventory increases, hence we can take $\dot{y}_2$ as proportional to the inventory:

$$\dot{y}_2 = \alpha^2 y_1, \tag{16.249}$$

where α, real and positive, is a known number. If C_P is the price per unit sale, c_p is the cost per unit produced, and c_h is the holding cost per unit item per unit time, we can write the **total revenue** over a period of time T as the integral

$$J[\mathbf{u}] = \int_0^T F(\mathbf{y}, \mathbf{u}, t)dt \tag{16.250}$$

$$= \int_0^T [C_P y_2 - c_p u - c_h y_1]dt. \tag{16.251}$$

Note that we have only one control variable, hence we take

$$u_2 = 0 \tag{16.252}$$

in this problem. We now look for the control variable, $u(t)$, that maximizes the revenue, $J[\mathbf{u}]$, subject to the initial conditions:

$$y_1(0) = y_{10}, \tag{16.253}$$

$$y_2(0) = y_{20}. \tag{16.254}$$

We now write the two conditions [Eqs. (16.248) and (16.249)] as

$$\dot{y}_1 - u + y_2 = 0, \tag{16.255}$$

$$\dot{y}_2 - \alpha^2 y_1 = 0 \tag{16.256}$$

and incorporate them into the problem through two Lagrange multipliers, $\lambda_1(t)$, $\lambda_2(t)$, by defining a new *Lagrangian*, H, as

$$H = F - \lambda_1[\dot{y}_1 - u + y_2] - \lambda_2[\dot{y}_2 - \alpha^2 y_1] \tag{16.257}$$

and consider the variation of

$$I[\mathbf{u}] = \int_0^T Hdt \tag{16.258}$$

$$= \int_0^T [F - \lambda_1(\dot{y}_1 - u + y_2) - \lambda_2(\dot{y}_2 - \alpha^2 y_1)]dt \tag{16.259}$$

$$= -[\lambda_1 y_1 + \lambda_2 y_2]_0^T$$

$$+ \int_0^T [(C_P y_2 - c_p u - c_h y_1) + (\dot{\lambda}_1 + \alpha^2 \lambda_2) y_1 + (\dot{\lambda}_2 - \lambda_1) y_2 + \lambda_1 u] dt. \tag{16.260}$$

Note that the stationary values of $J[\mathbf{u}]$ are also the stationary values of $I[\mathbf{u}]$ [8, p. 345]. However, we also have to take into account that in any realistic business the rate of production is always limited, that is,

$$0 \leq u_m \leq u \leq u_M, \tag{16.261}$$

where u_m and u_M represent the possible minimum and the maximum production rates possible. In this regard, we cannot insist on the optimal strategy to be a stationary value of $J[\mathbf{u}]$. We can at most ask for $\delta I[\mathbf{u}]$ be nonincreasing, that is, $\delta I[\mathbf{u}] \leq 0$, for a maximum of $J[\mathbf{u}]$:

$$\begin{aligned} \delta I[\mathbf{u}] = & -[\lambda_1(T)\delta y_1(T) + \lambda_2(T)\delta y_2(T)] \\ & + \int_0^T [(\dot{\lambda}_1 + \alpha^2 \lambda_2 - c_h)\delta y_1 + (\dot{\lambda}_2 - \lambda_1 + C_P)\delta y_2 \\ & + (\lambda_1 - c_p)\delta u] dt \leq 0. \end{aligned} \tag{16.262}$$

Since we have fixed the initial conditions [Eqs. (16.253) and (16.254)], we have taken

$$\delta y_1(0) = \delta y_2(0) = 0. \tag{16.263}$$

For simplicity, we also choose the Lagrange multipliers such that

$$\lambda_1(T) = 0, \tag{16.264}$$

$$\lambda_2(T) = 0, \tag{16.265}$$

$$\dot{\lambda}_1(t) + \alpha^2 \lambda_2(t) - c_h = 0, \tag{16.266}$$

$$\dot{\lambda}_2(t) - \lambda_1(t) + C_P = 0. \tag{16.267}$$

The first two terms eliminate the surface term in Eq. (16.262), which is needed, since we are not given the terminal values $y_1(T)$ and $y_2(T)$, and the last two equations are needed to avoid the need for a relation between δy_1 and δy_2 in the integrand, thus reducing Eq. (16.262) to

$$\delta I[\mathbf{u}] = \int_0^T (\lambda_1 - c_p)\delta u dt \leq 0. \tag{16.268}$$

The two coupled linear equations for $\lambda_1(t)$ and $\lambda_2(t)$ [Eqs. (16.266) and (16.267)] can be solved immediately. After incorporating the end conditions [Eqs. (16.264) and (16.265)] we obtain

$$\lambda_1(t) = C_P\{1 - \cos(\alpha[T - t])\} - \frac{c_h}{\alpha} \sin(\alpha[T - t]), \tag{16.269}$$

$$\lambda_2(t) = \frac{c_h}{\alpha^2}\{1 - \cos(\alpha[T - t])\} + \frac{C_p}{\alpha} \sin(\alpha[T - t]). \tag{16.270}$$

With $\lambda_1(t)$ determined as in Eq. (16.269), we cannot in general have

$$\lambda_1(t) - c_p = 0, \tag{16.271}$$

obviously not when c_p is a constant, hence we cannot use

$$\delta I = 0. \tag{16.272}$$

We now turn to $I[u]$ in Eq. (16.260) and substitute the expressions found for $\lambda_1(t)$ and $\lambda_2(t)$ to get

$$I[\mathbf{u}] = -[\lambda_1(0)y_{10} + \lambda_2(0)y_{20}] + \int_0^T (\lambda_1 - c_p)u\, dt. \tag{16.273}$$

In conclusion, for a maximum of $J[u]$ we need to pick the largest possible value of u that makes the above integral a maximum. In other words, we need

$$u(t) = \begin{cases} u_M & \text{when} \quad (\lambda_1(t) - c_p) > 0, \\ u_m & \text{when} \quad (\lambda_1(t) - c_p) < 0. \end{cases} \tag{16.274}$$

We now check the inequality in Eq. (16.268). Since $\lambda_1(T) = 0$, we have

$$\lambda_1(T) - c_p = -c_p \leq 0, \tag{16.275}$$

and by continuity

$$\lambda_1(t) \leq c_p, \quad t' \leq t \leq T, \tag{16.276}$$

for some $t' \geq 0$, hence it is also satisfied. In practice, during the course of time the sign of $(\lambda_1(t) - c_p)$ could alternate. Optimum control models, where the control variables alternate between two extreme values are called the **bang-bang** models. For the limitations of this simple control model see Wan [8]. What is depicted here is a very brief introduction to the interesting field of optimal control theory. For the interested reader who wants to explore this subject further, we recommend the books in our references.

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Problems

1 For the variational problem

$$\delta \int_a^b F(x, y, y', \ldots, y^{(n)})\, dx = 0,$$

show that the Euler equation is given as

$$F_y - \frac{d}{dx}F_{y'} + \frac{d^2}{dx^2}F_{y''} - \cdots + (-1)^n \frac{d^n}{dx^n}F_{y^{(n)}} = 0.$$

Assume that the variation at the end points is zero.

2 For the Sturm–Liouville system

$$y''(x) = -\lambda y(x), \quad y(0) = y(1) = 0,$$

find the approximate eigenvalues to first and second order.
Compare your results with the exact eigenvalues.

3 Given the variational problem for the massive scalar field with the potential $V(\vec{r})$ as

$$\delta \int \pounds d^3\vec{r}\, dt = 0,$$

where

$$\pounds(\vec{r}, t) = \frac{1}{2}(\dot{\Phi}^2 - (\vec{\nabla}\Phi)^2 - m^2\Phi^2) - V(\vec{r}).$$

Find the equation of motion for

$$\Phi(\vec{r}, t).$$

4 Treat $\Psi(\vec{r},t)$ and $\Psi^*(\vec{r},t)$ as independent fields in the Lagrangian density:

$$£ = \frac{\hbar^2}{2m}\vec{\nabla}\Psi\vec{\nabla}\Psi^* + V\Psi\Psi^* - \frac{i\hbar}{2}\left(\Psi^* \quad \frac{\partial\Psi}{\partial t} - \Psi\frac{\partial\Psi^*}{\partial t}\right),$$

where

$$\int £ d^3\vec{r}\, dt = 0.$$

Show that the corresponding Euler equations are the Schrödinger equations:

$$H\Psi = \left(-\frac{\hbar^2}{2m}\vec{\nabla}^2 + V\right)\Psi = i\hbar \quad \frac{\partial\Psi}{\partial t}$$

and

$$H\Psi^* = \left(-\frac{\hbar^2}{2m}\vec{\nabla}^2 + V\right)\Psi^* = -i\hbar\frac{\partial\Psi^*}{\partial t}.$$

5 Consider a cable fixed at the points $(0, 0)$ and (l, h). It carries a load along the y-axis distributed as

$$f(x) = -q\frac{x}{l}.$$

To find the shape of this cable we have to solve the variational problem

$$\delta\int_0^l \left(\frac{1}{2}T_0 y'^2 + q\frac{x}{l}y\right) dx = 0$$

with the boundary conditions

$$y(0) = 0 \text{ and } y(l) = h.$$

Find the shape of the wire accurate to second order.

6 Show that the exact solution in Problem 5 is given as

$$y(x) = \frac{h}{l}x + \frac{q}{6T_0 l}x(x^2 - l^2).$$

7 Find an upper bound for the lowest eigenvalue of the differential equation

$$\frac{d^2y}{dx^2} + \lambda xy = 0$$

with the boundary conditions

$$y(0) = y(1) = 0.$$

8 For a flexible elastic string with constant tension and fixed at the end points:

$$y(0,t) = y(L,t) = 0,$$

Show that the Lagrangian density is given as

$$£ = \frac{1}{2}\rho(x)\left[\frac{\partial y(x,t)}{\partial t}\right]^2 - \frac{1}{2}\tau\left[\frac{\partial y(x,t)}{\partial x}\right]^2,$$

where ρ is the density and τ is the tension. Show that the Lagrange equation is

$$\frac{\partial^2 y(x,t)}{\partial x^2} - \frac{\rho}{\tau}\frac{\partial^2 y(x,t)}{\partial t^2} = 0.$$

9 For a given Lagrangian representing a system with n degrees of freedom, show that adding a total time derivative to the Lagrangian does not effect the equations of motion, that is, L and L' related by

$$L' = L + \frac{dF(q_1, q_2, \ldots, q_n, t)}{dt},$$

where F is an arbitrary function, have the same Lagrange equations.

10 For a given Lagrangian $L(q_i, \dot{q}_i, t)$, where $i = 1, 2, \ldots, n$, show that

$$\frac{d}{dt}\left[\sum_{i=1}^{n} \dot{q}_i \frac{\partial L}{\partial \dot{q}_i} - L\right] + \frac{\partial L}{\partial t} = 0.$$

This means that if the Lagrangian does not depend on time explicitly, then the quantity, H, defined as

$$H\left(q_i, \frac{\partial L}{\partial \dot{q}_i}, t\right) = \sum_{i=1}^{n} \dot{q}_i \frac{\partial L}{\partial \dot{q}_i} - L$$

is conserved. Using Cartesian coordinates, interpret H.

11 **The brachistochrone problem**: Find the shape of the curve joining two points, along which a particle, initially at rest, falls freely under the influence of gravity from the higher point to the lower point in the least amount of time.

12 In an expanding flat universe the metric is given as

$$\begin{aligned} ds^2 &= -dt^2 + a^2(t)(dx^2 + dy^2 + dz^2) \\ &= -dt^2 + a^2(t)\delta_{ij}dx^i dx^j, \end{aligned}$$

where $i = 1, 2, 3$, and $a(t)$ is the scale factor. Given this metric, consider the following variational integral for the geodesics:

$$\delta I = \frac{1}{2} \int \left[-\left(\frac{dt}{d\tau} \right)^2 + a^2(t)\delta_{ij} \frac{dx^i}{d\tau} \frac{dx^j}{d\tau} \right] d\tau,$$

where τ is the proper time. For the dependent variables, $t(\tau)$ and $x^i(\tau)$, show that the Euler equations for the geodesics are:

$$\frac{d^2t}{d\tau^2} + a\dot{a}\delta_{ij} \frac{dx^i}{d\tau} \frac{dx^j}{d\tau} = 0$$

and

$$\frac{d^2x^i}{d\tau^2} + 2\frac{\dot{a}}{a} \frac{dt}{d\tau} \frac{dx^i}{d\tau} = 0,$$

where $\dot{a} = \partial a / \partial t$.

13 Using cylindrical coordinates, find the geodesics on a cone.

14 Write the Lagrangian and the Lagrange equations of motion for a double pendulum in uniform gravitational field.

15 Consider the following Lagrangian density for the massive scalar field in curved background spacetimes:

$$\pounds(x) = \frac{1}{2}[g(x)]^{\frac{1}{2}} \{g^{\mu\nu}(x)\partial_\mu \Phi(x)\partial_\nu \Phi(x) - [m^2 + \xi R(x)]\Phi^2(x)\},$$

where $\Phi(x)$ is the scalar field, m is the mass of the field quanta, x stands for (x^0, x^1, x^2, x^3), and

$$g(x) = |\det g_{\alpha\beta}|.$$

Coupling between the scalar field and the background geometry is represented by the term

$$\xi R(x)\Phi^2(x),$$

where ξ is called the coupling constant and $R(x)$ is the Ricci curvature scalar. The corresponding action is

$$S = \int \pounds(x) d^4x, \quad d^4x = dx^0 dx^1 dx^2 dx^3.$$

By setting the variation of the action with respect to $\Phi(x)$ to zero, show that the scalar field equation is given as

$$[\Box + m^2 + \xi R(x)]\Phi(x) = 0,$$

where $\Box = \partial_\mu \partial^\mu$ is the d'Alembert wave operator, ∂_μ stands for the covariant derivative. Take the signature of the metric as $(+ - - -)$.

16 Find the extremals of the problem

$$\delta \int_{x_1}^{x_2} [a(x)y''^2 - p(x)y'^2 + q(x)y^2]dx = 0$$

subject to the constraint

$$\int_{x_1}^{x_2} r(x)y^2(x)dx = 1,$$

where $y(x_1)$, $y'(x_1)$, $y(x_2)$, and $y'(x_2)$ are prescribed.

17

Integral Equations

Differential equations have been extremely useful in describing physical processes. They are composed of the derivatives of the unknown function. Since derivatives are defined in terms of the ratios of differences in the neighborhood of a point, differential equations are local equations. In our mathematical toolbox, there are also integral equations, where the unknown function appears under an integral sign. Since the integral equations involve integrals of the unknown function over a domain, they are global or nonlocal equations. In general, integral equations are much more difficult to solve. An important property of the differential equations is that to describe a physical process completely, they must be supplemented with boundary conditions. Integral equations, on the other hand, constitute a complete description of a given problem where extra conditions are neither needed nor could be imposed. Because the boundary conditions can be viewed as a convenient way of including global effects into a system, a connection between differential and integral equations is to be expected. In fact, under certain conditions integral and differential equations can be transformed into each other. Whether an integral or a differential equation is more suitable for expressing laws of nature is still an interesting problem, with some philosophical overtones that Einstein himself once investigated. Sometimes the integral equation formulation of a given problem may offer advantages over its differential equation description. At other times, when the physical processes involve nonlocal effects or the system has memory, we may have no choice but to use integral equations. In this chapter, we discuss the basic properties of linear integral equations and introduce some techniques for obtaining their solutions. We also discuss the Hilbert–Schmidt theory, where an eigenvalue problem is defined in terms of linear integral operators.

Mathematical Methods in Science and Engineering, Second Edition. Selçuk Ş. Bayın.

17.1 Classification of Integral Equations

Linear integral equations are classified under two general categories. Equations that can be written as

$$\boxed{\alpha(x)y(x) = F(x) + \lambda \int_a^b \kappa(x,\xi)\, y(\xi)\, d\xi} \tag{17.1}$$

are called **Fredholm equations**. Here, $\alpha(x)$, $F(x)$, and $\kappa(x,\xi)$ are known functions, $y(x)$ is the unknown function and λ, a, and b are known constants. $\kappa(x,\xi)$ is called the **kernel**, which is closely related to Green's functions. When the upper limit of the integral is variable, we have the **Volterra equation**:

$$\boxed{\alpha(x)y(x) = F(x) + \lambda \int_a^x \kappa(x,\xi)\, y(\xi)\, d\xi.} \tag{17.2}$$

The Fredholm and Volterra equations also have the following kinds:

$\alpha \neq 0$ kind I

$\alpha = 1$ kind II

$\alpha = \alpha(x)$ kind III

When $F(x)$ is zero, the integral equation is called **homogeneous**. Integral equations can also be defined in higher dimensions. For example, in two dimensions we can write a linear integral equation as

$$\alpha(x,y)\omega(x,y) = F(x,y) + \lambda \iint_R \kappa(x,y;\xi,\eta)\omega(\xi,\eta)d\xi\, d\eta. \tag{17.3}$$

17.2 Integral and Differential Equations

Some integral equations can be obtained from differential equations. To see this connection we derive a useful formula. First consider the integral

$$I_n(x) = \int_a^x (x-\xi)^{n-1} f(\xi) d\xi, \tag{17.4}$$

where $n > 0$ integer and a is a constant. Using the formula:

$$\boxed{\begin{aligned}\frac{d}{dx}\int_{A(x)}^{B(x)} F(x,\xi)d\xi = \int_{A(x)}^{B(x)} \frac{\partial F(x,\xi)}{\partial x} d\xi + F(x,B(x))\frac{dB(x)}{dx} \\ - F(x,A(x))\frac{dA(x)}{dx},\end{aligned}} \tag{17.5}$$

we take the derivative of $I_n(x)$ as

$$\frac{dI_n}{dx} = (n-1)\int_a^x (x-\xi)^{n-2} f(\xi)\, d\xi + [(x-\xi)^{n-1} f(\xi)]_{\xi=x}, \tag{17.6}$$

which for $n > 1$ gives

$$\frac{dI_n}{dx} = (n-1)I_{n-1}. \tag{17.7}$$

For $n = 1$, Eq. (17.4) can be used to write $\frac{dI_1}{dx} = f(x)$. K-fold differentiation of $I_n(x)$ gives

$$\frac{d^k I_n}{dx^k} = (n-1)(n-2)\cdots(n-k)I_{n-k}, \tag{17.8}$$

which can be written as

$$\frac{d^{n-1} I_n}{dx^{n-1}} = (n-1)!\, I_1(x), \tag{17.9}$$

or as

$$\frac{d^n I_n}{dx^n} = (n-1)!\, f(x). \tag{17.10}$$

Since $I_n(a) = 0$ for $n \geq 1$, Eq. (17.9) implies that $I_n(x)$ and all of its derivatives up to order $(n-1)$ are zero at $x = a$. Thus,

$$I_1(x) = \int_a^x f(x_1)\, dx_1, \tag{17.11}$$

$$I_2(x) = \int_a^x I_1(x_2)\, dx_2 = \int_a^x \int_a^{x_2} f(x_1)\, dx_1 dx_2, \tag{17.12}$$

$$\vdots$$

$$I_n(x) = (n-1)! \int_a^x \int_a^{x_n} \cdots \int_a^{x_3} \int_a^{x_2} f(x_1)\, dx_1\, dx_2 \ldots dx_{n-1} dx_n. \tag{17.13}$$

Using Eq. (17.13), we can now write the following useful formula, which is also known as the **Cauchy formula**:

$$\int_a^x \int_a^{x_n} \cdots \int_a^{x_3} \int_a^{x_2} f(x_1)\, dx_1\; dx_2 \ldots dx_{n-1}\; dx_n = \frac{1}{(n-1)!} \int_a^x (x-\xi)^{n-1} f(\xi)\, d\xi. \tag{17.14}$$

17.2.1 Converting Differential Equations into Integral Equations

We now consider the following second-order ordinary differential equation with variable coefficients:

$$\boxed{\frac{d^2y}{dx^2} + A(x)\frac{dy}{dx} + B(x)y = f(x),} \tag{17.15}$$

which is frequently encountered in physics and engineering applications. Let the **boundary conditions** be given as $y(a) = y_0$, $y'(a) = y'_0$. Integrating this differential equation once gives

$$y'(x) - y'_0 = -\int_a^x A(x_1)\, y'(x_1)\, dx_1 - \int_a^x B(x_1)\, y(x_1)\, dx_1 + \int_a^x f(x_1)\, dx_1.$$

We integrate the first term on the right-hand side by parts and then solve for $y'(x)$ to write

$$y'(x) = -A(x)y(x) - \int_a^x [B(x_1) - A'(x_1)]y(x_1)dx_1 + \int_a^x f(x_1)dx_1 + A(a)y_0 + y'_0. \tag{17.16}$$

We integrate again to obtain

$$y(x) - y_0 = -\int_a^x A(x_1)y(x_1)\, dx_1 - \int_a^x\int_a^{x_2} [B(x_1) - A'(x_1)]\, y(x_1)\, dx_1 dx_2 + \int_a^x\int_a^{x_2} f(x_1)\, dx_1 dx_2 + [A(a)y_0 + y'_0](x - a). \tag{17.17}$$

Using the Cauchy formula [Eq. (17.14)], we can write this as

$$y(x) = -\int_a^x \{A(\xi) + (x - \xi)[B(\xi) - A'(\xi)]\}y(\xi)d\xi + \int_a^x (x - \xi)f(\xi)\, d\xi + [A(a)y_0 + y'_0](x - a) + y_0, \tag{17.18}$$

or as

$$\boxed{y(x) = \int_a^x \kappa(x, \xi)y(\xi)d\xi + F(x),} \tag{17.19}$$

where $\kappa(x, \xi)$ and $F(x)$ are given as

$$\kappa(x, \xi) = -(x - \xi)[B(\xi) - A'(\xi)] - A(\xi), \tag{17.20}$$

$$F(x) = \int_a^x (x - \xi)f(\xi)\, d\xi + [A(a)y_0 + y'_0](x - a) + y_0. \tag{17.21}$$

This is an inhomogeneous Volterra equation of the second kind. This integral equation [Eqs. (17.19)–(17.21)] is equivalent to the differential equation [Eq. (17.15)] plus the boundary conditions $y(a) = y_0$ and $y'(a) = y'_0$.

Example 17.1 ***Converting differential into integral equations***
Using Eqs. (17.15), (17.19)–(17.21), we can convert the differential equation

$$\frac{d^2y}{dx^2} + \lambda y = f(x) \tag{17.22}$$

and the boundary conditions $y(0) = 1$ and $y'(0) = 0$, into an integral equation as

$$y(x) = \lambda \int_0^x (\xi - x)y(\xi)\, d\xi - \int_0^x (\xi - x)f(\xi)\, d\xi + 1. \tag{17.23}$$

Example 17.2 ***Converting differential into integral equations***
In the previous example we had a **single-point** boundary condition. We now consider the differential equation

$$\frac{d^2y}{dx^2} + \lambda y = 0 \tag{17.24}$$

with a **two-point** boundary condition $y(0) = 0$ and $y(l) = 0$. Integrating equation [Eq. (17.24)] between $(0, x)$ we get

$$\frac{dy}{dx} = -\lambda \int_0^x y(\xi)\, d\xi + C, \tag{17.25}$$

where C is an integration constant that is equal to $y'(0)$, which is not given. A second integration gives

$$y(x) = -\lambda \int_0^x (x - \xi)y(\xi)\, d\xi + Cx, \tag{17.26}$$

where we have used the Cauchy formula [Eq. (17.14)] and the boundary condition at $x = 0$. We now use the remaining boundary condition, $y(l) = 0$, to determine C as

$$C = \frac{\lambda}{l} \int_0^l (l - \xi)y(\xi)\, d\xi. \tag{17.27}$$

Substituting this back in Eq. (17.26) we write the result as

$$y(x) = -\lambda \int_0^x (x - \xi)y(\xi)\, d\xi + \frac{x\lambda}{l} \int_0^l (l - \xi)y(\xi)\, d\xi, \tag{17.28}$$

or as

$$y(x) = \lambda \int_0^x \frac{\xi}{l}(l - x)y(\xi)\, d\xi + \lambda \int_x^l \frac{x}{l}(l - \xi)y(\xi)\, d\xi. \tag{17.29}$$

This is a homogeneous Fredholm equation of the second kind:

$$y(x) = \lambda \int_0^l \kappa(x, \xi)y(\xi) d\xi, \tag{17.30}$$

where the kernel is given as

$$\kappa(x,\xi) = \begin{cases} \frac{\xi}{l}(l - x), & \xi < x, \\ \frac{x}{l}(l - \xi), & \xi > x. \end{cases} \tag{17.31}$$

17.2.2 Converting Integral Equations into Differential Equations

Volterra equations can sometimes be converted into differential equations. Consider the following integral equation:

$$y(x) = x^2 - 2\int_0^x ty(t)\,dt. \tag{17.32}$$

We define $f(x)$ as $f(x) = \int_0^x ty(t)dt$, where the derivative of $f(x)$ is

$$\frac{df(x)}{dx} = xy(x). \tag{17.33}$$

Using $f(x)$ in Eq. (17.32), we can also write $y(x) = x^2 - 2f(x)$, which when substituted back into Eq. (17.33) gives a differential equation to be solved for $f(x)$:

$$\frac{df(x)}{dx} = x^3 - 2xf(x), \tag{17.34}$$

the solution of which is

$$f(x) = \frac{1}{2}(Ce^{-x^2} + x^2 - 1). \tag{17.35}$$

Finally, substituting this into Eq. (17.33) gives us the solution for the integral equation:

$$y(x) = 1 - Ce^{-x^2}. \tag{17.36}$$

Because an integral equation also contains the boundary conditions, the constant of integration, C, is found by substituting this solution into the integral equation [Eq. (17.32)] as 1.

We now consider the Volterra equation:

$$y(x) = g(x) + \lambda\int_0^x e^{x-t}y(t)dt \tag{17.37}$$

and differentiate it with respect to x as

$$y'(x) = g'(x) + \lambda y(x) + \lambda\int_0^x e^{x-t}y(t)dt, \tag{17.38}$$

where we have used Eq. (17.5). Eliminating the integral between these two formulas we obtain

$$y'(x) - (\lambda + 1)y(x) = g'(x) - g(x). \tag{17.39}$$

The boundary condition to be imposed on this differential equation follows from integral equation [Eq. (17.37)] as $y(0) = g(0)$.

17.3 Solution of Integral Equations

Because the unknown function appears under an integral sign, integral equations are in general more difficult to solve than differential equations. However, there are also quite a few techniques that one can use in finding their solutions. In this section, we introduce some of the most commonly used techniques.

17.3.1 Method of Successive Iterations: Neumann Series

Consider a Fredholm equation given as

$$f(x) = g(x) + \lambda \int_a^b K(x,t) f(t)\, dt. \tag{17.40}$$

We start the Neumann sequence by taking the first term as $f_0(x) = g(x)$. Using this as the approximate solution of Eq. (17.40), we write

$$f_1(x) = g(x) + \int_a^b K(x,t) f_0(t)\, dt. \tag{17.41}$$

We keep iterating like this to construct the **Neumann sequence** as

$$f_0(x) = g(x), \tag{17.42}$$

$$f_1(x) = g(x) + \lambda \int_a^b K(x,t) f_0(t)\, dt, \tag{17.43}$$

$$f_2(x) = g(x) + \lambda \int_a^b K(x,t) f_1(t)\, dt, \tag{17.44}$$

$$\vdots$$

$$f_{n+1}(x) = g(x) + \lambda \int_a^b K(x,t) f_n(t)\, dt, \tag{17.45}$$

$$\vdots$$

This gives the **Neumann series** solution as

$$\boxed{\begin{aligned} f(x) &= g(x) + \lambda \int_a^b K(x,x') g(x') dx' \\ &\quad + \lambda^2 \int_a^b dx' \int_a^b dx'' K(x,x') K(x',x'') g(x'') + \cdots . \end{aligned}} \tag{17.46}$$

If we take

$$\int_a^b \int_a^b |K(x,t)|^2 dx\, dt = B^2, \quad B > 0, \tag{17.47}$$

and if the inequality

$$\int_a^b |K(x,t)|^2 dt \leq C \tag{17.48}$$

is true, where $\lambda < \frac{1}{B}$, and if C is a constant the same for all x in the interval $[a, b]$, then the following sequence is **uniformly convergent** in the interval $[a, b]$:

$$\{f_i\} = f_0, f_1, f_2, \dots, f_n, \dots \to f(x). \tag{17.49}$$

The limit of this sequence, that is, $f(x)$, is the solution of Eq. (17.40) and it is unique.

Example 17.3 ***Neumann sequence***
For the integral equation

$$f(x) = x^2 + \frac{1}{2}\int_{-1}^{1} (t - x) f(t)\, dt, \tag{17.50}$$

we start the Neumann sequence by taking $f_0(x) = x^2$ and continue to write:

$$f_1(x) = x^2 + \frac{1}{2}\int_{-1}^{1} (t - x) t^2 dt = x^2 - \frac{x}{3}, \tag{17.51}$$

$$f_2(x) = x^2 + \frac{1}{2}\int_{-1}^{1} (t - x)\left(t^2 - \frac{t}{3}\right) dt = x^2 - \frac{x}{3} - \frac{1}{9}, \tag{17.52}$$

$$f_3(x) = x^2 + \frac{1}{2}\int_{-1}^{1} (t - x)\left(t^2 - \frac{t}{3} - \frac{1}{9}\right) dt = x^2 - \frac{2x}{9} - \frac{1}{9} \tag{17.53}$$

$$\vdots$$

Obviously, in this case the solution is of the form

$$f(x) = x^2 + C_1 x + C_2. \tag{17.54}$$

Substituting this [Eq. (17.54)] into Eq. (17.50) and comparing the coefficients of equal powers of x, we obtain $C_1 = -\frac{1}{4}$ and $C_2 = -\frac{1}{12}$; thus, the exact solution in this case is given as

$$f(x) = x^2 - \frac{1}{4}x - \frac{1}{12}. \tag{17.55}$$

17.3.2 Error Calculation in Neumann Series

By using the nth term of the Neumann sequence as our solution, we will have committed ourselves to the error given by

$$|f(x) - f_n(x)| < D\sqrt{C}\frac{B^n|\lambda|^{n+1}}{1 - B|\lambda|}, \quad D = \sqrt{\int_a^b |g^2(x)|dx}. \tag{17.56}$$

Example 17.4 ***Error calculation in Neumann series***
For the integral equation:

$$f(x) = 1 + \frac{1}{10}\int_0^1 K(x,t)f(t)\,dt, \tag{17.57}$$

$$K(x,t) = \begin{cases} x, & 0 \le x \le t, \\ t, & t \le x \le 1, \end{cases} \tag{17.58}$$

since

$$B = \frac{1}{\sqrt{6}}, \ C = \frac{1}{3}, \ D = 1, \ \lambda = 0.1, \tag{17.59}$$

Eqs. (17.46–17.49) tell us that the Neumann sequence is convergent. Taking $f_0(x) = 1$, we find the first three terms as

$$f_0(x) = 1, \tag{17.60}$$

$$f_1(x) = 1 + (1/10)\,x - (1/20)\,x^2, \tag{17.61}$$

$$f_2(x) = 1 + (31/300)\,x - (1/20)\,x^2 - (1/600)\,x^3 + (1/2400)\,x^4. \tag{17.62}$$

If we take the solution as $f(x) \simeq f_2(x)$, the error in the entire interval will be less than

$$1.\sqrt{\frac{1}{3}}\frac{(1/6)(0.1)^3}{[1 - (0.1/\sqrt{6})]} = 0.0001. \tag{17.63}$$

17.3.3 Solution for the Case of Separable Kernels

When the kernel is given in the form

$$K(x,t) = \sum_{j=1}^{n} M_j(x)N_j(t), \quad n \text{ is a finite number}, \tag{17.64}$$

it is called **separable** or **degenerate**. In such cases, we can reduce the solution of an integral equation to the solution of a linear system of equations. Let us write a Fredholm equation with a separable kernel as

$$y(x) = f(x) + \lambda \sum_{j=1}^{n} M_j(x)\left[\int_a^b N_j(t)\,y(t)\,dt\right]. \tag{17.65}$$

If we define the quantity inside the square brackets as $\int_a^b N_j(t)\, y(t)\, dt = c_j$, Eq. (17.65) becomes

$$y(x) = f(x) + \lambda \sum_{j=1}^{n} c_j M_j(x) \quad . \tag{17.66}$$

After the coefficients, c_j, are evaluated, this will give us the solution $y(x)$. To find these constants, we multiply Eq. (17.66) with $N_i(x)$ and integrate to get

$$c_i = b_i + \lambda \sum_{j=1}^{n} a_{ij} c_j, \tag{17.67}$$

$$b_i = \int_a^b N_i(x) f(x)\, dx, \tag{17.68}$$

$$a_{ij} = \int_a^b N_i(x) M_j(x)\, dx. \tag{17.69}$$

We now write Eq. (17.67) as a matrix equation:

$$\mathbf{b} = \mathbf{c} - \lambda \mathbf{A}\mathbf{c}\,, \ \mathbf{A} = a_{ij}, \tag{17.70}$$

$$\mathbf{b} = (\mathbf{I} - \lambda \mathbf{A})\mathbf{c}\,. \tag{17.71}$$

This gives us a system of n linear equations to be solved for the n coefficients c_j as

$$\boxed{\begin{array}{c} (1 - \lambda a_{11})c_1 - \lambda a_{12} c_2 - \lambda a_{13} c_3 - \cdots - \lambda a_{1n} c_n = b_1, \\ -\lambda a_{21} c_1 + (1 - \lambda a_{22}) c_2 - \lambda a_{23} c_3 - \cdots - \lambda a_{2n} c_n = b_2, \\ \vdots \\ -\lambda a_{n1} c_1 - \lambda a_{n2} c_2 - \lambda a_{n3} c_3 - \cdots + (1 - \lambda a_{nn}) c_n = b_n. \end{array}} \tag{17.72}$$

When the Fredholm equation is **homogeneous**, that is, when $f(x) = 0$, then all b_i are zero; thus, for the solution to exist we must have

$$\boxed{\det[\mathbf{I} - \lambda \mathbf{A}] = 0.} \tag{17.73}$$

Solutions of this equation give the eigenvalues λ_i. Substituting these eigenvalues into Eq. (17.72) we can solve for the values of c_i.

Example 17.5 ***The case of separable kernels***
Consider the homogeneous Fredholm equation given as

$$y(x) = \lambda \int_{-1}^{1} (2t + x) y(t)\, dt, \tag{17.74}$$

where

$$\begin{aligned} M_1(x) &= 1, \quad M_2(x) = x, \\ N_1(t) &= 2t, \quad N_2(t) = 1 \end{aligned} \tag{17.75}$$

and with **A** written as

$$\mathbf{A} = \begin{bmatrix} 0 & 4/3 \\ 2 & 0 \end{bmatrix}. \tag{17.76}$$

Using Eq. (17.73), we write

$$\det \begin{vmatrix} 1 & -\frac{4\lambda}{3} \\ -2\lambda & 1 \end{vmatrix} = 0, \tag{17.77}$$

and find the eigenvalues as $\lambda_{1,2} = \pm\frac{1}{2}\sqrt{3/2}$. Substituting these into Eq. (17.72) we find two relations between c_1 and c_2:

$$c_1 \mp c_2\sqrt{\frac{2}{3}} = 0. \tag{17.78}$$

As in the eigenvalue problems in linear algebra, we have only obtained the ratio, c_1/c_2, of these constants. Because Eq. (17.74) is homogeneous, normalization is arbitrary. Choosing c_1 as 1, we can write the solutions of Eq. (17.74) as

$$y_1(x) = \frac{1}{2}\sqrt{\frac{3}{2}}\left(1 + \sqrt{\frac{3}{2}}x\right) \quad \text{for} \quad \lambda_1 = \frac{1}{2}\sqrt{\frac{3}{2}}, \tag{17.79}$$

$$y_2(x) = -\frac{1}{2}\sqrt{\frac{3}{2}}\left(1 - \sqrt{\frac{3}{2}}x\right) \quad \text{for} \quad \lambda_2 = -\frac{1}{2}\sqrt{\frac{3}{2}}. \tag{17.80}$$

When the equations in Eq. (17.72) are inhomogeneous, then the solution can still be found by using the techniques of linear algebra [1]. We will come back to the subject of integral equations and eigenvalue problems shortly.

17.3.4 Solution by Integral Transforms

Sometimes using integral transforms it may be possible to free the unknown function under the integral sign, thus making the solution possible.

17.3.4.1 Fourier Transform Method

When the kernel is a function of $(x - t)$ and the range of the integral is from $-\infty$ to $+\infty$, we can use the Fourier transform method. For example, consider the integral equation

$$y(x) = \phi(x) + \lambda \int_{-\infty}^{\infty} K(x - t)y(t)\,dt. \tag{17.81}$$

We take the Fourier transform of this equation to write

$$\widetilde{y}(k) = \widetilde{\phi}(k) + \lambda\widetilde{K}(k)\widetilde{y}(k). \tag{17.82}$$

Aside from constant scale factors, Fourier transform is defined as

$$\tilde{y}(k) = \int_{-\infty}^{\infty} y(x)e^{ikx}dx. \tag{17.83}$$

In writing Eq. (17.82), we have also used the convolution theorem:

$$f * g = \int_{-\infty}^{\infty} g(y)f(x-y)dy = \int_{-\infty}^{\infty} \tilde{f}(k)\tilde{g}(k)e^{-ikx}dk,$$

which indicates that the Fourier transform of the convolution of two functions, $f * g$, is the product of their Fourier transforms. We now solve Eq. (17.82) for $\tilde{y}(k)$ to find

$$\tilde{y}(k) = \frac{\tilde{\phi}(k)}{1 - \lambda\tilde{K}(k)}, \tag{17.84}$$

which after taking the inverse transform will give the solution in terms of a definite integral:

$$y(x) = \int_{-\infty}^{\infty} \frac{\tilde{\phi}(k)e^{-ikx}dk}{1 - \lambda\tilde{K}(k)}. \tag{17.85}$$

17.3.4.2 Laplace Transform Method

The Laplace transform method is useful when the kernel is a function of $(x-t)$ and the range of the integral is from 0 to x. For example, consider the integral equation

$$y(x) = 1 + \int_0^x y(u)\sin(x-u)du. \tag{17.86}$$

We take the Laplace transform of this equation to write

$$£[y(x)] = £[1] + £\left[\int_0^x y(u)\sin(x-u)du\right]. \tag{17.87}$$

After using the convolution theorem:

$$F(s)G(s) = £\left[\int_0^x f(u)g(x-u)du\right], \tag{17.88}$$

where $F(s)$ and $G(s)$ indicate the Laplace transforms of $f(x)$ and $g(x)$, respectively, we obtain the Laplace transform of the solution as

$$Y(s) = \frac{1}{s} + \frac{Y(s)}{s^2+1}, \tag{17.89}$$

$$Y(s) = \frac{1+s^2}{s^3}. \tag{17.90}$$

Taking the inverse Laplace transform, we obtain the solution:

$$y(x) = 1 + \frac{x^2}{2}. \tag{17.91}$$

17.4 Hilbert–Schmidt Theory

In the Sturm–Liouville theory, we have defined eigenvalue problems using linear differential operators. We are now going to introduce the Hilbert–Schmidt theory, where an eigenvalue problem is defined in terms of linear integral operators.

17.4.1 Eigenvalues for Hermitian Operators

Using the Fredholm equation of the second kind, we can define an **eigenvalue problem** as

$$\boxed{y(x) = \lambda \int_a^b K(x,t)y(t)\,dt,} \tag{17.92}$$

where for the ith eigenvalue λ_i, and the eigenfunction $y_i(t)$, we can write

$$y_i(x) = \lambda_i \int_a^b K(x,t)y_i(t)\,dt, \tag{17.93}$$

Similarly, we write Eq. (17.92) for another eigenvalue, λ_j, and take its complex conjugate as

$$y_j^*(x) = \lambda_j^* \int_a^b K^*(x,t)y_j^*(t)\,dt. \tag{17.94}$$

Multiplying Eq. (17.93) by $\lambda_j^* y_j^*(x)$ and Eq. (17.94) by $\lambda_i y_i(x)$, and integrating over x in the interval $[a,b]$ we obtain two equations:

$$\lambda_j^* \int_a^b y_j^*(x)y_i(x)\,dx = \lambda_i\lambda_j^* \int_a^b \int_a^b K(x,t)y_j^*(x)y_i(t)\,dt\;dx \tag{17.95}$$

and

$$\lambda_i \int_a^b y_j^*(x)y_i(x)\,dx = \lambda_i\lambda_j^* \int_a^b \int_a^b K^*(x,t)y_j^*(t)y_i(x)\,dt\;dx. \tag{17.96}$$

If the kernel satisfies the relation

$$\boxed{K^*(x,t) = K(t,x),} \tag{17.97}$$

Eq. (17.96) becomes

$$\lambda_i \int_a^b y_j^*(x)y_i(x)\,dx = \lambda_i\lambda_j^* \int_a^b \int_a^b K(t,x)y_j^*(t)y_i(x)\,dt\;dx. \tag{17.98}$$

Subtracting Eqs. (17.95) and (17.98), we obtain

$$\boxed{(\lambda_j^* - \lambda_i) \int_a^b y_j^*(x)y_i(x)\,dx = 0.} \tag{17.99}$$

Kernels satisfying relation (17.97) are called **Hermitian**.

For $i = j$ Eq. (17.99) becomes

$$(\lambda_i^* - \lambda_i) \int_a^b |y_i(x)|^2 dx = 0. \tag{17.100}$$

Since $\int_a^b |y_i(x)|^2 dx \neq 0$, we conclude that Hermitian operators have **real eigenvalues**.

17.4.2 Orthogonality of Eigenfunctions

Using the fact that eigenvalues are real, for $i \neq j$ Eq. (17.99) becomes

$$(\lambda_j - \lambda_i) \int_a^b y_j^*(x) y_i(x)\, dx = 0. \tag{17.101}$$

For distinct (nondegenerate) eigenvalues this gives

$$\int_a^b y_j^*(x) y_i(x)\, dx = 0, \quad \lambda_j \neq \lambda_i. \tag{17.102}$$

This means that the eigenfunctions for the distinct eigenvalues are **orthogonal**. In the case of degenerate eigenvalues, using the Gram–Schmidt orthogonalization method we can always choose the eigenvectors as orthogonal. Thus, we can write

$$\int_a^b y_j^*(x) y_i(x)\, dx = 0, \quad i \neq j. \tag{17.103}$$

Summary: For a linear integral operator

$$£ = \int_a^b dt K(x,t), \tag{17.104}$$

we can define an eigenvalue problem as

$$y_i(x) = \lambda_i \int_a^b K(x,t) y_i(t)\, dt. \tag{17.105}$$

For Hermitian kernels satisfying $K^*(x,t) = K(t,x)$, eigenvalues are real and the eigenfunctions are orthogonal; hence after a suitable normalization we can write:

$$\int_a^b y_i^*(x) y_j(x)\, dx = \delta_{ij}. \tag{17.106}$$

17.4.3 Completeness of the Eigenfunction Set

Proof of the completeness of the eigenfunction set is rather technical for our purposes and can be found in Courant and Hilbert [2, Chapter 3, vol. 1, p. 136]. We simply quote the following theorem:

Expansion theorem: Every continuous function, $F(x)$, which can be represented as the integral transform of a piecewise continuous function, $G(x)$, and with respect to the real and symmetric kernel $K(x, x')$ as

$$F(x) = \int K(x, x')G(x')dx', \tag{17.107}$$

can be expanded in a series in the eigenfunctions of $K(x, x')$; this series converges uniformly and absolutely.

This conclusion is also true for Hermitian kernels. We can now write

$$F(x) = \sum_{m=0}^{\infty} a_m y_m(x), \tag{17.108}$$

where the coefficients, a_m, are found by using the orthogonality relation:

$$\begin{aligned} \int_a^b F(x)y_m^*(x)dx &= \sum_n \int_a^b a_n y_n(x) y_m^*(x)dx \\ &= \sum_n a_n \int_a^b y_n(x)y_m^*(x)dx \\ &= \sum_n a_n \delta_{nm} \\ &= a_m. \end{aligned} \tag{17.109}$$

Substituting these coefficients back into Eq. (17.108), we get

$$F(x) = \sum_{m=0}^{\infty} \int_a^b F(x')y_m^*(x')y_m(x)dx', \tag{17.110}$$

$$= \int_a^b F(x') \left[\sum_{m=0}^{\infty} y_m^*(x')y_m(x)\right] dx'. \tag{17.111}$$

This gives us a formal expression for the **completeness** of $\{y_m(x)\}$ as

$$\boxed{\sum_{m=0}^{\infty} y_m^*(x')y_m(x) = \delta(x' - x).} \tag{17.112}$$

Keep in mind that in general $\{y_i(x)\}$ do not form a complete set. Not just any function, but only the functions that can be generated by the integral transform [Eq. (17.107)] can be expanded in terms of them.

Let us now assume that a given Hermitian kernel can be expanded in terms of the eigenfunction set $\{y_i(x)\}$ as

$$K(x, x') = \sum_i c_i(x)y_i(x'), \tag{17.113}$$

where the expansion coefficients, c_i, carry the x dependence. Using Eq. (17.109), $c_i(x)$ are written as

$$c_i(x) = \int K(x, x')y_i^*(x')dx', \tag{17.114}$$

which after multiplying by λ_i becomes

$$\lambda_i c_i(x) = \lambda_i \int K(x, x')y_i^*(x')dx'. \tag{17.115}$$

We now take the Hermitian conjugate of the eigenvalue equation:

$$y_i(x) = \lambda_i \int K(x, x')y_i(x')dx', \tag{17.116}$$

to write

$$y_i^*(x) = \lambda_i \int y_i^*(x')K^*(x', x)dx' \tag{17.117}$$

$$= \lambda_i \int y_i^*(x')K(x, x')dx' \tag{17.118}$$

$$= \lambda_i \int K(x, x')y_i^*(x')dx'. \tag{17.119}$$

Substituting Eq. (17.119) to Eq. (17.115) we solve for $c_i(x)$:

$$c_i(x) = \frac{y_i^*(x)}{\lambda_i}. \tag{17.120}$$

Finally, substituting Eq. (17.120) to Eq. (17.113) we obtain an elegant expression for the Hermitian kernels in terms of the eigenfunctions as

$$\boxed{K(x, x') = \sum_i \frac{y_i^*(x)y_i(x')}{\lambda_i}.} \tag{17.121}$$

17.5 Neumann Series and the Sturm–Liouville Problem

We often encounter cases where a given second-order linear differential operator

$$£ = \frac{d}{dx}\left[p(x)\frac{d}{dx}\right] + q^{(0)}(x) + q^{(1)}(x), \quad x \in [a, b], \tag{17.122}$$

differs from an exactly solvable Sturm–Liouville operator

$$£_0 = \frac{d}{dx}\left[p(x)\frac{d}{dx}\right] + q^{(0)}(x), \tag{17.123}$$

by a small term $q^{(1)}(x)$ compared to $q^{(0)}(x)$. Since the eigenvalue problem for $£_0$ is exactly solvable, it yields a complete and orthonormal set of eigenfunctions, u_i, which satisfy the eigenvalue equation

$$£_0 u_i + \lambda_i u_i = 0, \tag{17.124}$$

where λ_i are the eigenvalues. We now consider the eigenvalue equation for the general operator $£$:

$$£\Psi(x) + \lambda\Psi(x) = 0, \tag{17.125}$$

and write it as

$$£_0\Psi(x) + \lambda\Psi(x) = -q^{(1)}\Psi(x). \tag{17.126}$$

In general, the above equation is given as

$$£_0\Psi(x) + \lambda\Psi(x) = f(x, \Psi(x)), \tag{17.127}$$

where the inhomogeneous term usually corresponds to sources or interactions. We confine our discussion to cases where $f(x, \Psi)$ is separable:

$$f(x, \Psi(x)) = h(x)\Psi(x). \tag{17.128}$$

This covers a wide range of physically interesting cases. For example, in scattering problems the time independent Schrödinger equation is written as

$$\vec{\nabla}^2\Psi(\vec{r}) + \frac{2mE}{\hbar^2}\Psi(\vec{r}) = \frac{2m}{\hbar^2}V(\vec{r})\Psi(\vec{r}), \tag{17.129}$$

where $V(\vec{r})$ is the scattering potential.

The general solution of Eq. (17.127) with Eq. (17.128) can be written as

$$\Psi(x) = \Psi^{(0)}(x) + \int dx' G(x, x')h(x')\Psi(x') \tag{17.130}$$

$$= \Psi^{(0)}(x) + \int dx' K(x, x')\Psi(x'), \tag{17.131}$$

where $G(x, x')$ is the **Green's function**, while

$$K(x, x') = G(x, x')h(x') \tag{17.132}$$

is the **kernel** of the integral equation and $\Psi^{(0)}(x)$ is the known solution of the homogeneous equation:

$$£_0\Psi(x) + \lambda\Psi(x) = 0. \tag{17.133}$$

Introducing the linear integral operator $\mathbb{K}$:

$$\mathbb{K} = \int_a^b dx' K(x, x'), \tag{17.134}$$

$$\mathbb{K}(\alpha\Psi_1 + \beta\Psi_2) = \alpha\mathbb{K}\Psi_1 + \beta\mathbb{K}\Psi_2, \tag{17.135}$$

where α, β are constants, we can write Eq. (17.131) as

$$(\mathbf{I} - \mathbb{K})\Psi(x) = \Psi^{(0)}(x), \tag{17.136}$$

where $\mathbf{I}$ is the identity operator. Assuming that $K(x, x')$ is small, we can write

$$\Psi(x) = \frac{\Psi^{(0)}(x)}{(\mathbf{I} - \mathbb{K})} \tag{17.137}$$

$$= (\mathbf{I} + \mathbb{K} + \mathbb{K}^2 + \cdots)\Psi^{(0)}(x). \tag{17.138}$$

A similar expansion can be written for $\Psi(x)$ as

$$\Psi(x) = \Psi^{(0)}(x) + \Psi^{(1)}(x) + \cdots , \tag{17.139}$$

which when substituted into Eq. (17.138) yields the zeroth-order term of the approximation as $\Psi(x) \simeq \Psi^{(0)}(x)$, and the subsequent terms of the expansion as

$$\Psi^{(1)}(x) = \int dx' K(x, x')\Psi^{(0)}(x), \tag{17.140}$$

$$\Psi^{(2)}(x) = \mathbb{K}\Psi^{(1)}(x) = \mathbb{K}^2\Psi^{(0)}(x) = \int dx'' K(x, x'') \int dx' K(x'', x')\Psi^{(0)}(x'), \tag{17.141}$$

$$\vdots$$

We can now write the following Neumann series [Eq. (17.46)]:

$$\Psi(x) = \Psi^{(0)}(x) + \int dx' K(x, x')\Psi^{(0)}(x') + \int dx' K(x, x')\Psi^{(1)}(x') + \cdots , \tag{17.142}$$

that is,

$$\begin{aligned}\Psi(x) = {} & \Psi^{(0)}(x) \\ & + \int dx' K(x, x')\Psi^{(0)}(x') \\ & + \int dx' K(x, x') \int dx'' K(x', x'')\Psi^{(0)}(x'') \\ & + \int dx' K(x, x') \int dx'' K(x', x'') \int dx'' K(x', x'')\Psi^{(0)}(x'') \\ & + \cdots .\end{aligned} \tag{17.143}$$

If we approximate $\Psi(x)$ with the first N terms,

$$\Psi(x) \simeq \Psi^{(0)}(x) + \Psi^{(1)}(x) + \cdots + \Psi^{(N)}(x), \tag{17.144}$$

we can write Eq. (17.136) as

$$(\mathbf{I} - \mathbb{K})(\Psi^{(0)} + \Psi^{(1)} + \cdots + \Psi^{(N)}) \simeq \Psi^{(0)}, \tag{17.145}$$

$$\Psi^{(0)} - \Psi^{(N+1)} \simeq \Psi^{(0)}. \tag{17.146}$$

For the **convergence** of Neumann series, for a given small positive number, ε_0, we should be able to find a number, N_0, independent of x, such that for $N+1 > N_0$, we have $|\Psi^{(N+1)}| < \varepsilon_0$. To obtain the **sufficient condition** for convergence let $\max|K(x,x')| = M$ for $x, x' \in [a,b]$ and take $\int_a^b dx' |\Psi^{(0)}(x)| = C$. We can now write the inequality

$$\left|\Psi^{(n+1)}(x)\right| < CM^{N+1}(b-a)^N = CM[M(b-a)]^N, \tag{17.147}$$

which yields the error committed by approximating $\Psi(x)$ with the first $N+1$ terms of the Neumann series [Eq. (17.19)] as

$$\left|\Psi(x) - \sum_{n=0}^{N} \Psi^{(n)}(x)\right| \le |\Psi^{N+1}(x)| + |\Psi^{N+2}(x)| + \cdots \tag{17.148}$$

$$\le CM[M(b-a)]^N\{1 + M(b-a) + M^2(b-a)^2 + \cdots\}. \tag{17.149}$$

If $M(b-a) < 1$, which is **sufficient** but not necessary, we can write

$$\boxed{\left|\Psi(x) - \sum_{n=0}^{N} \Psi^{(n)}(x)\right| \le \frac{CM[M(b-a)]^N}{[1-M(b-a)]} < \varepsilon_0,} \tag{17.150}$$

which is true for all $N > N_0$ independent of x.

In scattering problems, **Schrödinger equation**:

$$\vec{\nabla}\Psi(\vec{r}) + k^2\Psi(\vec{r}) = \frac{2m}{\hbar^2} V(\vec{r})\Psi(\vec{r}), \tag{17.151}$$

can be written as the integral equation [Eq. (17.131)]:

$$\Psi(\vec{r}) = e^{i\vec{k}_0\cdot\vec{r}} - \frac{2m}{4\pi\hbar^2}\int d^3\vec{r}\, \frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} V(\vec{r}')\Psi(\vec{r}'), \tag{17.152}$$

where $e^{i\vec{k}_0\cdot\vec{r}}$ is the solution of the homogeneous equation representing the incident plane wave and $k^2 = k_0^2 = 2mE/\hbar^2$. Wave vector of the incident wave is $\vec{k}_0$ while $\vec{k}$ is the wave vector of the outgoing wave as $\vec{r} \to \infty$. The first two terms of Eq. (17.143) already gives the important result

$$\boxed{\Psi(\vec{r}) \simeq e^{i\vec{k}_0\cdot\vec{r}} - \frac{2m}{4\pi\hbar^2}\int d^3\vec{r}\, \frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} V(\vec{r}')e^{i\vec{k}_0\cdot\vec{r}},} \tag{17.153}$$

which is called the **Born approximation**.

17.6 Eigenvalue Problem for the Non-Hermitian Kernels

In most of the important cases a **non-Hermitian kernel,** $K(x,t)$, in Eq. (17.93) can be written as

$$y_i(x) = \lambda_i \int_a^b [\overline{K}(x,t)w(t)]y_i(t)\,dt, \tag{17.154}$$

where $\overline{K}(x,t)$ satisfies the relation $\overline{K}(x,t) = \overline{K}^*(t,x)$. We multiply Eq. (17.92) by $\sqrt{w(x)}$ and define

$$\sqrt{w(x)}y(x) = \psi(x), \tag{17.155}$$

to write

$$\psi_i(x) = \lambda_i \int_a^b [\overline{K}(x,t)\sqrt{w(x)w(t)}]\psi_i(t)\,dt. \tag{17.156}$$

Now the kernel, $\overline{K}(x,t)\sqrt{w(x)w(t)}$, in this equation is Hermitian and the eigenfunctions, $\psi_i(x)$, are orthogonal with respect to the weight function $w(x)$ as

$$\int_a^b w(x)\psi_i^*(x)\psi_i(x)\,dx = \delta_{ij}. \tag{17.157}$$

Bibliography

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Problems

1 Find the solution of the following integral equation:

$$y(t) = 1 + \int_0^t y(u)\sin(t-u)du.$$

Check your answer by substituting into the above integral equation.

2 Show that the following differential equation and boundary conditions:

$$y''(x) - y(x) = 0,$$

$$y(0) = 0 \text{ and } y'(0) = 1,$$

are equivalent to the integral equation

$$y(x) = x + \int_0^x (x - x')y(x')dx'.$$

3 Write the following differential equation and boundary conditions as an integral equation:

$$y''(x) - y(x) = 0,$$
$$y(1) = 0 \text{ and } y(-1) = 1.$$

4 Using the Neumann series method solve the integral equation

$$y(x) = x + \int_0^x (x' - x)y(x')\, dx.$$

5 For the following integral equation find the eigenvalues and the eigenfunctions:

$$y(x) = \lambda \int_0^{2\pi} \cos(x - x')y(x')dx'.$$

6 To show that the solution of the integral equation

$$y(x) = 1 + \lambda^2 \int_0^x (x - x')y(x')dx'$$

is given as

$$y(x) = \cosh \lambda x.$$

(i) First convert the integral equation into a differential equation and then solve.
(ii) Solve by using Neumann series.
(iii) Solve by using the integral transform method.

7 By using different methods of your choice find the solution of the integral equation

$$y(x) = x + \lambda \int_0^1 xx'y(x')dx'.$$

Answer: $y(x) = 3x/(3 - \lambda)$.

8 Consider the damped harmonic oscillator problem, where the equation of motion is given as

$$\frac{d^2x(t)}{dt^2} + 2\varepsilon\frac{dx(t)}{dt} + \omega_0^2 x(t) = 0.$$

(i) Using the boundary conditions

$$x(0) = x_0 \text{ and } \dot{x}(0) = 0$$

show that $x(t)$ satisfies the integral equation

$$x(t) = x_0 \cos\omega_0 t + \frac{2x_0\varepsilon}{\omega_0}\sin\omega_0 t + 2\varepsilon\int_0^t x(t')\cos\omega_0(t-t')dt'.$$

(ii) Iterate this equation several times and show that it agrees with the exact solution expanded to the appropriate order.

9 Obtain an integral equation for the anharmonic oscillator, where the equation of motion and the boundary conditions are given as

$$\frac{d^2x(t)}{dt^2} + \omega_0^2 x(t) = -bx^3(t),$$
$$x(0) = x_0 \text{ and } \dot{x}(0) = 0.$$

10 Consider the integral equation

$$y(x) = x + 2\int_0^1 [x\theta(x'-x) + x'\theta(x-x')]y(x')dx'.$$

First show that a Neumann series solution exists and then find it.

11 Using the Neumann series method find the solution of

$$y(x) = x^2 + 6\int_0^1 (x+t)y(t)\,dt.$$

18

Green's Functions

Green's functions are among the most versatile tools in applied mathematics. They provide a powerful alternative to solving differential equations. They are also very useful in transforming differential equations into integral equations, which are preferred in certain cases like the scattering problems. Propagator interpretation of the Green's functions is also very useful in quantum field theory, and with their path integral representation, they are the starting point of modern perturbation theory. In this chapter, we introduce the basic features of both the time-dependent and the time-independent Green's functions, which have found a wide range of applications in science and engineering. We also introduce the time-independent perturbation theory.

18.1 Time-Independent Green's Functions in One Dimension

We start with the differential equation

$$\boxed{\pounds y(x) = \phi(x),} \tag{18.1}$$

where $\pounds$ is the **Sturm–Liouville operator**:

$$\pounds = \frac{d}{dx}\left(p(x)\frac{d}{dx}\right) + q(x), \tag{18.2}$$

with $p(x)$ and $q(x)$ as continuous functions defined in the interval $[a, b]$. Along with this differential equation, we use the **homogeneous boundary conditions**:

$$\begin{aligned} \alpha y(x) + \beta \frac{dy(x)}{dx}\bigg|_{x=a} &= 0, \\ \alpha y(x) + \beta \frac{dy(x)}{dx}\bigg|_{x=b} &= 0, \end{aligned} \tag{18.3}$$

Mathematical Methods in Science and Engineering, Second Edition. Selçuk Ş. Bayın.

where α and β are constants. Because $\phi(x)$ could also depend on the unknown function explicitly, we will also write

$$\phi(x, y(x)).$$

Note that even though the differential operator $\pounds$ is linear, the differential equation [Eq. (18.1)] could be nonlinear.

We now define a function $G(x, \xi)$, which for a given $\xi \in [a, b]$ reduces to $G_1(x)$ when $x < \xi$ and to $G_2(x)$ when $x > \xi$, and also has the following properties:

i) Both $G_1(x)$ and $G_2(x)$, in their intervals of definition, satisfy $\pounds G(x) = 0$:

$$\begin{aligned} \pounds G_1(x) &= 0, \quad x < \xi, \\ \pounds G_2(x) &= 0, \quad x > \xi. \end{aligned} \tag{18.4}$$

ii) $G_1(x)$ satisfies the boundary condition at $x = a$ and $G_2(x)$ satisfies the boundary condition at $x = b$.

iii) $G(x, \xi)$ is continuous at $x = \xi$:

$$G_2(\xi) = G_1(\xi). \tag{18.5}$$

iv) $G'(x, \xi)$ is discontinuous by the amount $1/p(\xi)$ at $x = \xi$:

$$G_2'(\xi) - G_1'(\xi) = 1/p(\xi). \tag{18.6}$$

We also assume that $p(x)$ is finite in the interval (a, b); thus the discontinuity is of finite order.

We are now going to prove that if such a function can be found, then the problem defined by the differential equation plus the boundary conditions [Eqs. (18.1–18.3)] is equivalent to the equation

$$\boxed{y(x) = \int_a^b G(x, \xi)\phi(\xi, y(\xi))\, d\xi,} \tag{18.7}$$

where $G(x, \xi)$ is called the **Green's function**. If $\phi(x, y(\xi))$ does not depend on $y(x)$ explicitly, then finding the Green's function is tantamount to solving the problem. For the cases where $\phi(x, y(\xi))$ depends explicitly on $y(x)$, then Eq. (18.7) becomes the integral equation version of the problem defined by the differential equation plus the homogeneous boundary conditions [Eqs. (18.1–18.3)]. Before we prove the equivalence of Eq. (18.7) and the Eqs. (18.1–18.3), we show how a Green's function can be constructed. We first drive a useful result called **Abel's formula**.

18.1.1 Abel's Formula

Let $u(x)$ and $v(x)$ be two linearly independent solutions of $£y(x) = 0$, so that we can write, respectively,

$$\frac{d}{dx}\left(p(x)\frac{d}{dx}\right)u(x) + q(x)u(x) = 0, \tag{18.8}$$

$$\frac{d}{dx}\left(p(x)\frac{d}{dx}\right)v(x) + q(x)v(x) = 0, \tag{18.9}$$

Multiplying the first equation by v and the second by u and then subtracting gives

$$v(x)\frac{d}{dx}\left(p(x)\frac{d}{dx}\right)u(x) - u(x)\frac{d}{dx}\left(p(x)\frac{d}{dx}\right)v(x) = 0. \tag{18.10}$$

After expanding and rearranging, we can write $\frac{d}{dx}[p(x)(uv' - vu')] = 0$, which implies

$$\boxed{(uv' - vu') = \frac{A}{p(x)},} \tag{18.11}$$

where A is a constant. This result is known as **Abel's formula**.

18.1.2 Constructing the Green's Function

Let $y = u(x)$ be a nontrivial solution of $£y = 0$ satisfying the boundary condition at $x = a$ and let $y = v(x)$ be another nontrivial solution of $£y = 0$ satisfying the boundary condition at $x = b$. We now define a **Green's function** as

$$G(x,\xi) = \begin{cases} c_1 u(x), & x < \xi, \\ c_2 v(x), & x > \xi. \end{cases} \tag{18.12}$$

This Green's function satisfies conditions (i) and (ii). For conditions (iii) and (iv), we require c_1 and c_2 to satisfy the following equations:

$$c_2 v(\xi) - c_1 u(\xi) = 0, \tag{18.13}$$

$$c_2 v'(\xi) - c_1 u'(\xi) = 1/p(\xi). \tag{18.14}$$

For a unique solution of these equations, we have to satisfy the condition

$$W[u,v] = \begin{vmatrix} u(\xi) & v(\xi) \\ u'(\xi) & v'(\xi) \end{vmatrix} = u(\xi)v'(\xi) - v(\xi)u'(\xi) \neq 0, \tag{18.15}$$

where $W[u,v]$ is called the Wronskian of the solutions $u(x)$ and $v(x)$. When these solutions are linearly independent, $W[u,v]$ is different from zero and according to Abel's formula, $W[u,v]$ is equal to $A/p(\xi)$, where A is a constant independent of ξ. Eqs. (18.13) and (18.14) can now be solved for c_1 and c_2 to yield $c_1 = v(\xi)/A$ and $c_2 = u(\xi)/A$. Now the Green's function becomes

$$G(x,\xi) = \begin{cases} (1/A)u(x)v(\xi), & x < \xi, \\ (1/A)u(\xi)v(x), & x > \xi. \end{cases} \tag{18.16}$$

Evidently, this Green's function is symmetric and unique. We now show that the integral

$$y(x) = \int_a^b G(x,\xi)\phi(\xi)\, d\xi \tag{18.17}$$

is equivalent to the differential equation [Eq. (18.1)] plus the boundary conditions [Eq. (18.3)]. We first write equation Eq. (18.17) explicitly as

$$y(x) = \frac{1}{A}\left[\int_a^x v(x)u(\xi)\phi(\xi)d\xi + \int_x^b v(\xi)u(x)\phi(\xi)d\xi\right] \tag{18.18}$$

and evaluate its first- and second-order derivatives:

$$y'(x) = \frac{1}{A}\left[\int_a^x v'(x)u(\xi)\phi(\xi)\, d\xi + \int_x^b v(\xi)u'(x)\phi(\xi)\, d\xi\right], \tag{18.19}$$

$$y''(x) = \frac{1}{A}\left[\int_a^x v''(x)u(\xi)\phi(\xi)\, d\xi + \int_x^b v(\xi)u''(x)\phi(\xi)\, d\xi\right] + \frac{1}{A}[v'(x)u(x) - v(x)u'(x)]\phi(x), \tag{18.20}$$

where we have used the formula

$$\frac{d}{dx}\int_{A(x)}^{B(x)} F(x,\xi)\, d\xi = \int_{A(x)}^{B(x)} \frac{\partial F(x,\xi)}{\partial x}\, d\xi + F(x,B(x))\frac{dB(x)}{dx} - F(x,A(x))\frac{dA(x)}{dx}. \tag{18.21}$$

Substituting these derivatives into $£y(x) = p(x)y''(x) + p'(x)y'(x) + q(x)y(x)$, we get

$$£y(x) = \frac{1}{A}\left\{\int_a^x [£v(x)]u(\xi)\phi(\xi)\, d\xi + \int_x^b v(\xi)[£u(x)]\phi(\xi)\, d\xi\right\} + \frac{1}{A}\left[p(x)\frac{A}{p(x)}\phi(x)\right]. \tag{18.22}$$

Since $u(x)$ and $v(x)$ satisfy $£u(x) = 0$ and $£v(x) = 0$, respectively, we obtain $£y(x) = \phi(x)$. To see which boundary conditions $y(x)$ satisfies, we write

$$\left\{\begin{aligned} y(a) &= (1/A)u(a)\int_a^b v(\xi)\phi(\xi)\, d\xi \\ y'(a) &= (1/A)u'(a)\int_a^b v(\xi)\phi(\xi)\, d\xi \end{aligned}\right\}, \tag{18.23}$$

$$\left.\begin{cases} y(b) = (1/A)v(b) \displaystyle\int_a^b u(\xi)\phi(\xi)\, d\xi \\ y'(b) = (1/A)v'(b) \displaystyle\int_a^b u(\xi)\phi(\xi)\, d\xi \end{cases}\right\}. \tag{18.24}$$

It is easily seen that $y(x)$ satisfies the same boundary condition with $u(x)$ at $x = a$ and with $v(x)$ at $x = b$.

In some cases, it is convenient to write $\phi(x)$ as $\phi(x) = \lambda r(x)y(x) + f(x)$, thus Eq. (18.1) becomes $\pounds y(x) - \lambda r(x)y(x) = f(x)$. With the homogeneous boundary conditions, this is equivalent to the integral equation

$$y(x) = \lambda \int_a^b G(x,\xi)r(\xi)y(\xi)\, d\xi + \int_a^b G(x,\xi)f(\xi)\, d\xi. \tag{18.25}$$

18.1.3 Differential Equation for the Green's Function

To find the differential equation that the Green's function satisfies, we operate on $y(x)$ in Eq. (18.17) with $\pounds$ to write $\pounds y(x) = \int_a^b \pounds G(x,\xi)\phi(\xi)\, d\xi$. Because the operator $\pounds$ [Eq. (18.2)] acts only on x, we can write this as

$$\phi(x) = \int_a^b [\pounds G(x,\xi)]\phi(\xi)\, d\xi, \tag{18.26}$$

which is the defining equation for the Dirac-delta function $\delta(x - \xi)$. Hence, we obtain the differential equation for the Green's function as

$$\boxed{\pounds G(x,\xi) = \delta(x - \xi).} \tag{18.27}$$

Along with the homogeneous boundary conditions:

$$\begin{aligned} \alpha G(x,\xi) + \beta \frac{dG(x,\xi)}{dx}\bigg|_{x=a} &= 0, \\ \alpha G(x,\xi) + \beta \frac{dG(x,\xi)}{dx}\bigg|_{x=b} &= 0, \end{aligned} \tag{18.28}$$

Equation (18.27) is the defining equation for $G(x,\xi)$.

18.1.4 Single-Point Boundary Conditions

We have so far used the boundary conditions in Eq. (18.3), which are also called the **two-point** boundary conditions. In mechanics, we usually encounter **single-point** boundary conditions, where the position and the velocity are given at some initial time. We now write the Green's function satisfying the homogeneous single-point boundary conditions, $G(x_0, x') = 0$ and $G'(x_0, x') = 0$, as

$$\begin{aligned} G(x,x') &= c_1 y_1(x) + c_2 y_2(x), \quad x > x', \\ G(x,x') &= 0, \quad x < x', \end{aligned} \tag{18.29}$$

where $y_1(x)$ and $y_2(x)$ are two linearly independent solutions of $\pounds y(x) = 0$. Following the steps of the method used for two-point boundary conditions (see Problem 4), we can find the constants c_1 and c_2, and construct the Green's function as

$$\boxed{G(x,x') = -\frac{y_1(x)y_2(x') - y_2(x)y_1(x')}{p(x')W[y_1(x'), y_2(x')]}\theta(x - x'),} \tag{18.30}$$

where $W[y_1(x'), y_2(x')]$ is the Wronskian.

Now the differential equation $\pounds y(x) = \phi(x)$ with the given single-point boundary conditions, $y(x_0) = y_0$ and $y'(x_0) = y'_0$, is equivalent to the integral equation

$$y(x) = C_1 y_1(x) + C_2 y_2(x) + \int_{x_0}^{x} G(x,x')\phi(x')\,dx'. \tag{18.31}$$

The first two terms come from the solutions of the homogeneous equation. Because the integral term and its derivative vanish at $x = x_0$, we use C_1 and C_2 to satisfy the single-point boundary conditions.

18.1.5 Green's Function for the Operator d^2/dx^2

Consider the following differential equation:

$$\boxed{\frac{d^2y}{dx^2} = -k_0^2 y,} \tag{18.32}$$

where k_0 is a constant. Using the homogeneous boundary conditions, $y(0) = 0$ and $y(L) = 0$, we integrate Eq. (18.32) between $(0, x)$ to write

$$\frac{dy}{dx} = -k_0^2 \int_0^x y(\xi)\,d\xi + C, \tag{18.33}$$

where C is an integration constant corresponding to the unknown value of the derivative at $x = 0$. A second integration yields

$$y(x) = -k_0^2 \int_0^x (x - \xi)y(\xi)\,d\xi + Cx, \tag{18.34}$$

where we have used one of the boundary conditions, that is, $y(0) = 0$. Using the second boundary condition, we can now evaluate C as

$$C = \frac{k_0^2}{L}\int_0^L (L - \xi)y(\xi)\,d\xi. \tag{18.35}$$

This leads us to the following integral equation for $y(x)$:

$$y(x) = -k_0^2 \int_0^x (x-\xi)y(\xi)\,d\xi + \frac{xk_0^2}{L}\int_0^L (L-\xi)y(\xi)\,d\xi. \tag{18.36}$$

To identify the Green's function for the operator $\pounds = d^2/dx^2$, we rewrite this as

$$y(x) = -k_0^2 \int_0^x (x-\xi)y(\xi)\,d\xi + \frac{xk_0^2}{L}\int_0^x (L-\xi)y(\xi)\,d\xi$$
$$+\frac{xk_0^2}{L}\int_x^L (L-\xi)y(\xi)\,d\xi, \tag{18.37}$$
$$= k_0^2 \int_0^x \frac{\xi}{L}(L-x)y(\xi)\,d\xi + k_0^2\int_x^L \frac{x}{L}(L-\xi)y(\xi)\,d\xi. \tag{18.38}$$

Comparing with

$$y(x) = \int_0^L G(x,\xi)[-k_0^2 y(\xi)]\,d\xi, \tag{18.39}$$

we obtain the Green's function for the $\pounds = d^2/dx^2$ operator as

$$\boxed{G(x,\xi) = \begin{cases} -(x/L)(L-\xi), & x<\xi, \\ -(x/L)(L-x), & x>\xi. \end{cases}} \tag{18.40}$$

Now the integral equation (18.39) is equivalent to the differential equation $d^2y(x)/dx^2 = -k_0^2 y(x)$ with the boundary conditions $y(0) = y(L) = 0$. As long as the boundary conditions remain the same, we can use this Green's function to express the solution of the differential equation $d^2y(x)/dx^2 = \phi(x,y)$ as

$$y(x) = \int_0^L G(x,\xi)\phi(\xi, y(\xi))\,d\xi. \tag{18.41}$$

For a different set of boundary conditions, one must construct a new Green's function.

Example 18.1 ***Green's function for the $\pounds = d^2/dx^2$ operator***
We have obtained the Green's function [Eq. (18.40)] for the operator $\pounds = d^2/dx^2$ with the boundary conditions $y(0) = y(L) = 0$. Transverse waves on a uniform string of fixed length L with both ends clamped rigidly are described by

$$\frac{d^2}{dx^2}y(x) + k_0^2 y(x) = f(x,y), \tag{18.42}$$

where $f(x,y)$ represents external forces acting on the string. Using the Green's function for the d^2/dx^2 operator, we can convert this into an integral equation:

$$y(x) = -k_0^2\int_0^L G(x,\xi)y(\xi)\,d\xi + \int_0^L G(x,\xi)f(\xi,y(\xi))\,d\xi. \tag{18.43}$$

18.1.6 Inhomogeneous Boundary Conditions

In the presence of inhomogeneous boundary conditions, we can still use the Green's function obtained for the homogeneous boundary conditions and modify the solution [Eq. (18.7)] as

$$\boxed{y(x) = P(x) + \int_a^b G(x,\xi)\phi(\xi)\, d\xi,} \tag{18.44}$$

where $y(x)$ now satisfies $£y(x) = \phi(x)$ with the **inhomogeneous** boundary conditions. Operating on Eq. (18.44) with $£$ and using the relation between the Green's functions and the Dirac-delta function [Eq. (18.27)], we obtain a differential equation to be solved for $P(x)$:

$$\phi(x) = £[P(x)] + \int_a^b [£G(x,\xi)]\phi(\xi)\, d\xi, \tag{18.45}$$

$$\phi(x) = £P(x) + \phi(x), \tag{18.46}$$

$$\boxed{£P(x) = 0.} \tag{18.47}$$

Because the second term in Eq. (18.44) satisfies the homogeneous boundary conditions, $P(x)$ must satisfy the inhomogeneous boundary conditions. Existence of $P(x)$ is guaranteed by the existence of $G(x,\xi)$. The equivalence of this approach with our previous method can easily be seen by defining a new unknown function $\bar{y}(x) = y(x) - P(x)$, which satisfies the homogeneous boundary conditions.

Example 18.2 ***Inhomogeneous boundary conditions***
Equation of motion of a simple plane pendulum of length l is given as

$$\frac{d^2\theta(t)}{dt^2} = -\omega_0^2 \sin\theta, \quad \omega_0^2 = g/l, \tag{18.48}$$

where g is the acceleration of gravity and θ represents the angle from the equilibrium position. We use the inhomogeneous boundary conditions:

$$\theta(0) = 0 \quad \text{and} \quad \theta(t_1) = \theta_1. \tag{18.49}$$

We have already obtained the Green's function for the d^2/dx^2 operator for the homogeneous boundary conditions [Eq. (18.40)]. We now solve $d^2P(t)/dt^2 = 0$ with the inhomogeneous boundary conditions $P(0) = 0$ and $P(t_1) = \theta_1$, to find $P(t) = \theta_1 t/t_1$. Because $\phi(t)$ is $\phi(t) = -\omega_0^2 \sin\theta(t)$, we can write the differential equation [Eq. (18.48)] plus the inhomogeneous boundary conditions [Eq. (18.49)] as an integral equation:

$$\theta(t) = \frac{\theta_1 t}{t_1} + \omega_0^2 \left[\frac{(t_1 - t)}{t_1}\int_0^t \xi \sin\theta(\xi)\, d\xi + \frac{t}{t_1}\int_t^{t_1} (t_1 - \xi)\sin\theta(\xi)\, d\xi\right]. \tag{18.50}$$

Example 18.3 ***Green's function***
We now consider the differential equation

$$x^2\frac{d^2y}{dx^2}+x\frac{dy}{dx}+(k^2x^2-1)y=0 \tag{18.51}$$

with the following homogeneous boundary conditions:

$$y(0)=0, \quad y(L)=0. \tag{18.52}$$

We write this differential equation in the form

$$\left[\frac{d}{dx}\left(x\frac{dy}{dx}\right)-\frac{y}{x}\right]=-k^2xy(x) \tag{18.53}$$

and define the £ operator as

$$£=\frac{d}{dx}\left(x\frac{d}{dx}\right)-\frac{1}{x}, \tag{18.54}$$

where $p(x)=x$, $q(x)=-1/x$, and $r(x)=x$. The general solution of $£y=0$ is given as $y=c_1x+c_2x^{-1}$. Using the first boundary condition $y(0)=0$, we find $u(x)$ as $y(x)=u(x)=x$. Similarly, using the second boundary condition $y(L)=0$, we find $v(x)$ as $v(x)=\frac{L^2}{x}-x$. We now evaluate the Wronskian of the u and the v solutions as

$$W[u,v]=u(x)v'(x)-v(x)u'(x)=-\frac{2L^2}{x} \tag{18.55}$$

$$=\frac{A}{p(x)}=\frac{A}{x}, \tag{18.56}$$

which determines A as $-2L^2$. Putting all these together, we obtain the Green's function as

$$G(x,\xi)=\begin{cases}-\dfrac{x}{2L^2\xi}(L^2-\xi^2), & x<\xi,\\[2ex] -\dfrac{\xi}{2L^2x}(L^2-x^2), & x>\xi.\end{cases} \tag{18.57}$$

Using this Green's function, we can now write the integral equation

$$y(x)=-k^2\int_0^L G(x,\xi)\xi y(\xi)\,d\xi, \tag{18.58}$$

which is equivalent to the differential equation plus the boundary conditions in Eqs. (18.51) and (18.52).

Note that the differential equation in this example is the Bessel equation and the only useful solutions are those with the eigenvalues, k_n, satisfying the characteristic equation $J_1(k_nL)=0$. In this case, the solution is given as $y(x)=CJ_1(k_nx)$, where C is a constant. The same conclusion is valid for the integral equation (18.58). In addition, note that we could have arranged the differential equation (18.51) as

$$\left[\frac{d}{dx}\left(x\frac{dy}{dx}\right)\right] = \left(\frac{y}{x} - k^2xy\right), \tag{18.59}$$

where the operator £ is now defined as

$$£ = \frac{d}{dx}\left(x\frac{d}{dx}\right). \tag{18.60}$$

If the new operator, £, and the corresponding Green's function are compatible with the boundary conditions, then the final answer, $y(x, k_n)$, will be the same. In the above example, Green's function for the new operator [Eq. (18.60)] has a logarithmic singularity at the origin. We will explore these points in Problems 11 and 12. In physical applications, the form of the operator £ is usually dictated by the physics of the problem. For example, in quantum mechanics £ represents physical properties with well-defined expressions with their eigenvalues corresponding to observables like angular momentum and energy.

18.1.7 Green's Functions and Eigenvalue Problems

Consider the differential equation

$$£y(x) = f(x), \quad x \in [a, b], \tag{18.61}$$

with the appropriate boundary conditions, where £ is the Sturm–Liouville operator:

$$£ = \frac{d}{dx}\left(p(x)\frac{d}{dx}\right) - q(x). \tag{18.62}$$

We have seen that the £ operator has a complete set of eigenfunctions defined by the equation

$$£\phi_n(x) = \lambda_n\phi_n(x), \tag{18.63}$$

where λ_n are the eigenvalues. Eigenfunctions satisfy the orthogonality relation, $\int \phi_n^*(x)\phi_m(x)dx = \delta_{nm}$, and the completeness relation, $\sum_n \phi_n^*(x)\phi_n(x')dx = \delta(x - x')$. In the interval $x \in [a, b]$, we can expand $y(x)$ and $f(x)$ in terms of the set $\{\phi_n(x)\}$ as

$$\begin{aligned} y(x) &= \sum_n^{\infty} \alpha_n\phi_n(x), \\ f(x) &= \sum_n^{\infty} \beta_n\phi_n(x), \end{aligned} \tag{18.64}$$

where α_n and β_n are the expansion coefficients:

$$\alpha_n = \int_a^b \phi_n^*(x) y(x)\, dx,$$
$$\beta_n = \int_a^b \phi_n^*(x) f(x)\, dx. \tag{18.65}$$

Operating on $y(x)$ with $£$, we get

$$£y(x) = £ \sum_n^\infty \alpha_n \phi_n(x) = \sum_n^\infty \alpha_n £\phi_n(x). \tag{18.66}$$

Using Eq. (18.66) with the eigenvalue equation [Eq. (18.63)] and Eq. (18.64), we can write $£y(x) = f(x)$ as $\sum_n^\infty [\alpha_n \lambda_n - \beta_n]\phi_n(x) = 0$. Because ϕ_n are linearly independent, the only way to satisfy this equation for all n is to set the expression inside the square brackets to zero, thus obtaining $\alpha_n = \beta_n / \lambda_n$. We use this in Eq. (18.64) to write

$$y(x) = \sum_n^\infty \frac{\beta_n}{\lambda_n} \phi_n(x). \tag{18.67}$$

After substituting the β_n given in Eq. (18.65), this becomes

$$y(x) = \int \sum_n^\infty \frac{\phi_n(x)\phi_n^*(x')}{\lambda_n} f(x')\, dx'. \tag{18.68}$$

Using the definition of the Green's function, that is, $y(x) = \int G(x, x') f(x')\, dx'$, we obtain

$$G(x, x') = \sum_n^\infty \frac{\phi_n(x)\phi_n^*(x')}{\lambda_n}. \tag{18.69}$$

Usually, we encounter differential equations given as

$$\boxed{£y(x) - \lambda y(x) = f(x),} \tag{18.70}$$

where the Green's function for the operator $(£ - \lambda)$ can be written as

$$\boxed{G(x, x') = \sum_n^\infty \frac{\phi_n(x)\phi_n^*(x')}{\lambda_n - \lambda}.} \tag{18.71}$$

Note that in complex spaces Green's function is **Hermitian**:

$$\boxed{G(x, x') = G^*(x', x).} \tag{18.72}$$

18.1.8 Green's Functions and the Dirac-Delta Function

Let us operate on the Green's function [Eq. (18.69)] with the £ operator:

$$£G(x,x') = £\sum_{n}^{\infty} \frac{\phi_n(x)\phi_n^*(x')}{\lambda_n}. \tag{18.73}$$

Because £ is a linear operator acting on the variable x, we can write

$$£G(x,x') = \sum_{n}^{\infty} \frac{\phi_n^*(x')[£\phi_n(x)]}{\lambda_n}. \tag{18.74}$$

Using the eigenvalue equation, $£\phi_n(x) = \lambda_n\phi_n(x)$, we obtain

$$£G(x,x') = \sum_{n}^{\infty} \phi_n^*(x')\phi_n(x) = I(x,x'). \tag{18.75}$$

For a given function, $f(x)$, we write the integral

$$\int I(x,x')f(x')\,dx' = \sum_{n}^{\infty} \phi_n(x)\int \phi_n^*(x')f(x')\,dx' = \sum_{n}^{\infty} \phi_n(x)(\phi_n,f). \tag{18.76}$$

For a complete and orthonormal set, the right-hand side is the generalized Fourier expansion of $f(x)$; thus we can write $\int I(x,x')f(x')\,dx' = f(x)$. Hence, $I(x,x')$ is nothing but the Dirac-delta function:

$$I(x,x') = £G(x,x') = \delta(x-x'). \tag{18.77}$$

Summary: A differential equation:

$$£y(x) = f(x,y),$$

defined with the Sturm–Liouville operator £ [Eq. (18.2)] and with the homogeneous boundary conditions [Eq. (18.3)] is equivalent to the integral equation

$$y(x) = \int G(x,x')f(x',y(x'))\,dx',$$

where $G(x,x')$ is the Green's function satisfying

$$\boxed{£G(x,x') = \delta(x-x')}$$

with the same boundary conditions.

Example 18.4 ***Eigenfunctions and the Green's function for $£ = d^2/dx^2$***
Let us reconsider the $£ = d^2/dx^2$ operator in the interval $[0,L]$. The corresponding eigenvalue equation is $d^2\phi_n/dx^2 = -k_n^2\phi_n$. Using the boundary

conditions $\phi_n(0) = 0$ and $\phi_n(L) = 0$, we find the eigenfunctions and the eigenvalues as

$$\left\{\begin{array}{c} \phi_n(x) = \sqrt{\frac{2}{L}}\sin(k_n x), \\ -\lambda_n = k_n^2 = \frac{n^2\pi^2}{L^2}, \quad n = 1, 2, 3, \ldots. \end{array}\right\} \tag{18.78}$$

We now construct the Green's function as

$$G(x, x') = \frac{2}{L}\sum_n^{\infty} \frac{\sin\left(\frac{n\pi}{L}x\right)\sin\left(\frac{n\pi}{L}x'\right)}{-n^2\pi^2/L^2}. \tag{18.79}$$

For the same operator, using the Green's function in Eq. (18.40), we have seen that the inhomogeneous equation $d^2y/dx^2 = F(x, y)$, and the boundary conditions $y(0) = y(L) = 0$, can be written as an integral equation:

$$y(x) = \int_0^x (x - x')F(x')\, dx' - \frac{x}{L}\int_0^L (L - x')F(x')\, dx'. \tag{18.80}$$

Using the step function, $\theta(x - x')$, we can write this as

$$y(x) = \int_0^L (x - x')\theta(x - x')F(x')\, dx' - \frac{x}{L}\int_0^L (L - x')F(x')\, dx', \tag{18.81}$$

or as

$$y(x) = \int_0^L \left[(x - x')\theta(x - x') - \frac{x}{L}(L - x')\right] F(x')\, dx'. \tag{18.82}$$

This also gives the Green's function for the $£ = d^2/dx^2$ operator as

$$G(x, x') = \left[(x - x')\theta(x - x') - \frac{x}{L}(L - x')\right]. \tag{18.83}$$

One can easily show that the Green's function given in Eq. (18.79) is the generalized Fourier expansion of Eq. (18.83) in terms of the complete and orthonormal set [Eq. (18.78)].

18.1.9 Helmholtz Equation with Discrete Spectrum

Let us now consider the inhomogeneous Helmholtz equation:

$$\boxed{\frac{d^2y(x)}{dx^2} + k_0^2 y(x) = f(x),} \tag{18.84}$$

with the boundary conditions $y(0) = 0$ and $y(L) = 0$. Using Eqs. (18.70) and (18.71), we can write the Green's function as

$$G(x,x') = \frac{2}{L}\sum_n \frac{\sin k_n x \sin k_n x'}{k_0^2 - k_n^2}. \tag{18.85}$$

Using this Green's function, solution of the inhomogeneous Helmholtz equation [Eq. (18.84)] is written as $y(x) = \int_0^L G(x,x')f(x')\,dx'$, where $f(x)$ represents the driving force in the wave motion. Note that in this case the operator is defined as $£ = d^2/dx^2 + k_0^2$. Green's function for this operator can also be obtained by direct construction, that is, by determining the u and the v solutions in Eq. (18.16) as $\sin k_0 x$ and $\sin k_0(x-L)$, respectively. We can now obtain a closed expression for $G(x,x')$ as

$$G(x,x') = \begin{cases} \dfrac{\sin k_0 x \sin k_0(x'-L)}{k_0 \sin k_0 L}, & x < x', \\[2ex] \dfrac{\sin k_0 x' \sin k_0(x-L)}{k_0 \sin k_0 L}, & x > x'. \end{cases} \tag{18.86}$$

18.1.10 Helmholtz Equation in the Continuum Limit

We now consider the operator $£ = d^2/dx^2 + k_0^2$ in the continuum limit with

$$\frac{d^2y}{dx^2} + k_0^2 y = f(x), \quad x \in (-\infty, \infty). \tag{18.87}$$

Because the eigenvalues are continuous, we use the Fourier transforms of $y(x)$ and $f(x)$ as

$$f(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dk' g(k')e^{ik'x}, \tag{18.88}$$

$$y(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dk' \eta(k')e^{ik'x}. \tag{18.89}$$

Their inverse Fourier transforms are

$$g(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dx' f(x')e^{-ikx'}, \tag{18.90}$$

$$\eta(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dx' y(x')e^{-ikx'}. \tag{18.91}$$

Using these in Eq. (18.87), we get

$$\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dk'\{[-k'^2+k_0^2]\eta(k')-g(k')\}e^{ik'x}=0, \tag{18.92}$$

which gives us

$$\eta(k')=-\frac{g(k')}{(k'^2-k_0^2)}. \tag{18.93}$$

Substituting this in Eq. (18.89), we obtain

$$y(x)=-\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dk'\frac{g(k')}{(k'^2-k_0^2)}e^{ik'x}. \tag{18.94}$$

Writing $g(k')$ explicitly, this becomes

$$y(x)=-\frac{1}{2\pi}\int_{-\infty}^{\infty} dx'f(x')\int_{-\infty}^{\infty} dk'\frac{e^{ik'(x-x')}}{(k'-k_0)(k'+k_0)}, \tag{18.95}$$

which allows us to define the Green's function as $y(x)=\int_{-\infty}^{\infty} dx'f(x')\,G(x,x')$, where

$$\boxed{G(x,x')=-\frac{1}{2\pi}\int_{-\infty}^{\infty} dk'\frac{e^{ik'(x-x')}}{(k'-k_0)(k'+k_0)}.} \tag{18.96}$$

Using one of the representations of the Dirac-delta function:

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ik(x-x')}dk=\delta(x-x'), \tag{18.97}$$

it is easy to see that $G(x,x')$ satisfies the equation $\pounds G(x,x')=\delta(x-x')$.

The integral in Eq. (18.96) is undefined at $k'=\pm k_0$. However, we can use the Cauchy principal value, $P\int_{-\infty}^{\infty} dx\ \frac{f(x)}{(x-a)}=\pm i\pi f(a)$, to make it well defined. The + or − signs depend on whether the contour is closed in the upper or the lower z-planes, respectively. There are also other ways to treat these singular points in the complex plane, thus giving us a collection of Green's functions each satisfying a different boundary condition, which we study in the following example.

Example 18.5 ***Helmholtz equation in the continuum limit***
We now evaluate the Green's function given in Eq. (18.96) by using the Cauchy principal value and the complex contour integral techniques.

Case I. Using the contours in Figures 18.1 and 18.2, we can evaluate the integral

$$G(x,x')=-\frac{1}{2\pi}P\int_{-\infty}^{\infty} dk'\frac{e^{ik'(x-x')}}{(k'-k_0)(k'+k_0)}. \tag{18.98}$$

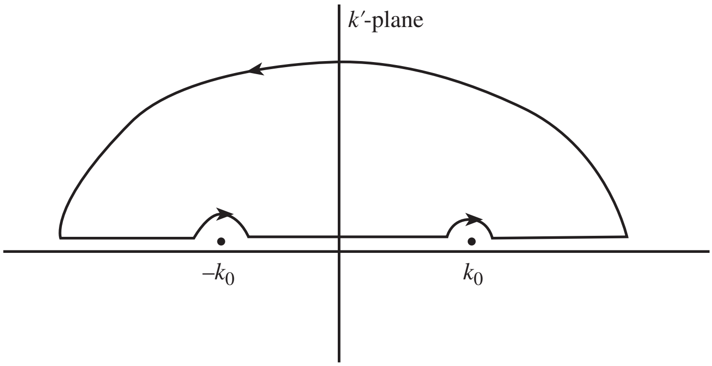

Figure 18.1 Contour for Case I: $(x - x') > 0$.

For $(x - x') > 0$, we use the contour in Figure 18.1 to find

$$G(x, x') = -\frac{i\pi}{2\pi}\left[\frac{e^{ik_0(x-x')}}{2k_0} - \frac{e^{-ik_0(x-x')}}{2k_0}\right] = \frac{1}{2k_0}\sin k_0(x - x'). \tag{18.99}$$

For $(x - x') < 0$, we use the contour in Figure 18.2 to find

$$G(x, x') = -\frac{1}{2k_0}\sin k_0(x - x') = \frac{1}{2k_0}\sin k_0(x' - x). \tag{18.100}$$

Note that for the $(x - x') < 0$ case, the Cauchy principal value is $-i\pi f(a)$, where a is the pole on the real axis. In the following cases, we add small imaginary pieces, $\pm i\varepsilon$, to the two roots, $+k_0$ and $-k_0$, of the denominator in Eq. (18.96), thus moving them away from the real axis. We can now use the Cauchy integral theorems to evaluate the integral (18.96) and then obtain the Green's function in the limit $\varepsilon \to 0$.

Case II: Using the contours shown in Figure 18.3, we obtain the following Green's function:
For $(x - x') > 0$, we use the contour in the upper half complex k'-plane to find

$$G(x, x') = -\lim_{\varepsilon\to 0}\frac{1}{2\pi}\int_{-\infty}^{\infty} dk' \frac{e^{ik'(x-x')}}{(k' - k_0 + i\varepsilon)(k' + k_0 - i\varepsilon)} \tag{18.101}$$

$$= -\lim_{\varepsilon\to 0}\frac{2\pi i}{2\pi}\frac{e^{i(-k_0+i\varepsilon)(x-x')}}{2(-k_0 + i\varepsilon)} = -\frac{e^{-ik_0(x-x')}}{2k_0 i}. \tag{18.102}$$

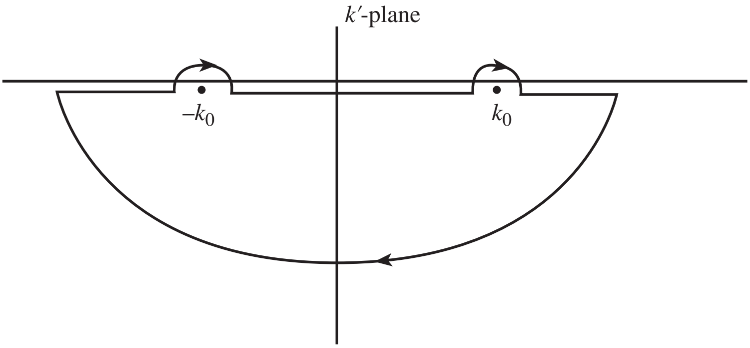

Figure 18.2 Contour for Case I: $(x - x') < 0$.

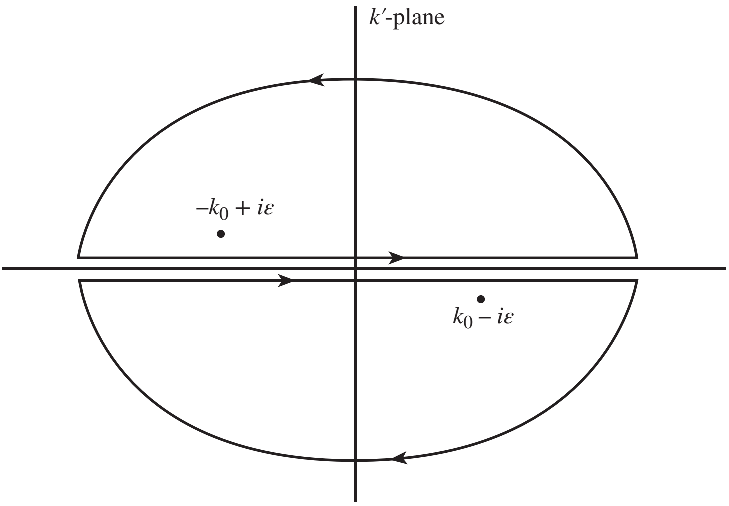

Figure 18.3 Contours for Case II.

For $(x - x') < 0$, we use the contour in the lower half-plane to get

$$G(x, x') = -\frac{e^{ik_0(x-x')}}{2k_0 i}. \tag{18.103}$$

Note that there is an extra minus sign coming from the fact that the contour for the $(x - x') < 0$ case is clockwise; thus we obtain the Green's function as

$$G(x, x') = -\frac{e^{-ik_0(x-x')}}{2k_0 i}\theta(x - x') - \frac{e^{ik_0(x-x')}}{2k_0 i}\theta(x' - x). \tag{18.104}$$

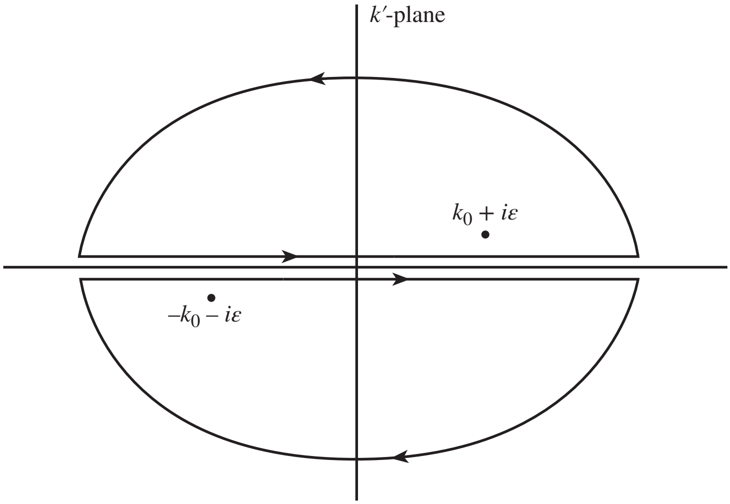

Figure 18.4 Contours for Case III.

Case III: Using the contours shown in Figure 18.4, the Green's function is now given as the integral

$$G(x,x') = -\lim_{\varepsilon\to 0}\frac{1}{2\pi}\int_{-\infty}^{\infty} dk' \frac{e^{ik'(x-x')}}{(k'-k_0-i\varepsilon)(k'+k_0+i\varepsilon)}. \tag{18.105}$$

For $(x-x') > 0$, we use the upper contour in Figure 18.4 to find

$$G(x,x') = -\frac{1}{2\pi}2\pi i \lim_{\varepsilon\to 0}\left[\frac{e^{i(k_0+i\varepsilon)(x-x')}}{2(k_0+i\varepsilon)}\right] = \frac{e^{ik_0(x-x')}}{2k_0 i} \tag{18.106}$$

and for $(x-x') < 0$, we use the lower contour to find

$$G(x,x') = -(-)\frac{2\pi i}{2\pi}\frac{e^{-ik_0(x-x')}}{-2k_0} = \frac{e^{-ik_0(x-x')}}{2k_0 i}. \tag{18.107}$$

Combining these, we write the Green's function as

$$G(x,x') = \frac{e^{ik_0(x-x')}}{2k_0 i}\theta(x-x') + \frac{e^{-ik_0(x-x')}}{2k_0 i}\theta(x'-x). \tag{18.108}$$

Case IV: Green's function for the contours in Figure 18.5:
For $(x-x') > 0$, we use the upper contour to find

$$G(x,x') = 0. \tag{18.109}$$

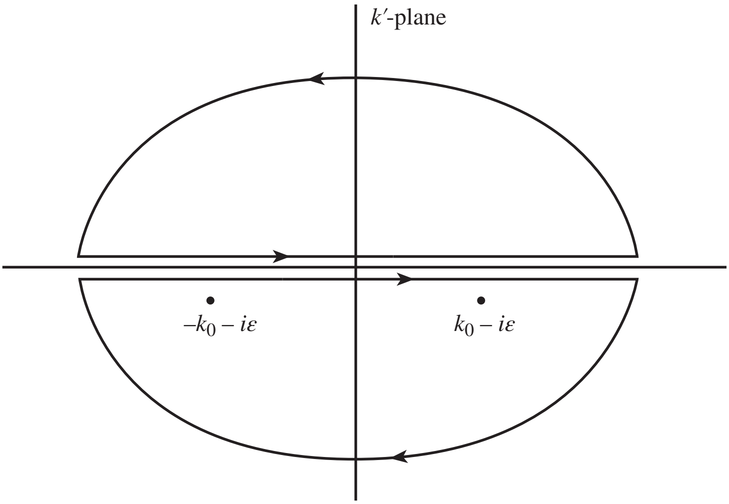

Figure 18.5 Contours for Case IV.

Similarly, for $(x - x') < 0$, we use the lower contour to obtain

$$G(x, x') = -\frac{1}{2\pi}(-)2\pi i \lim_{\varepsilon \to 0} \left[\frac{e^{i(k_0 - i\varepsilon)(x - x')}}{2(k_0 - i\varepsilon)} + \frac{e^{i(-k_0 - i\varepsilon)(x - x')}}{2(-k_0 - i\varepsilon)} \right] \tag{18.110}$$

$$= i \left[\frac{e^{ik_0(x-x')}}{2k_0} + \frac{e^{-ik_0(x-x')}}{2k_0} \right] = -\frac{\sin k_0(x - x')}{k_0}. \tag{18.111}$$

The combined result becomes

$$G(x, x') = -\frac{\sin k_0(x - x')}{k_0} \theta(x' - x). \tag{18.112}$$

This Green's function is good for the boundary conditions given as

$$\lim_{x \to \infty} \left\{ \begin{array}{c} G(x, x') \to 0 \\ G'(x, x') \to 0 \end{array} \right\}. \tag{18.113}$$

Case V: Green's function using the contours in Figure 18.6:
For $(x - x') > 0$, we use the upper contour to find

$$G(x, x') = \frac{1}{i} \left[\frac{e^{ik_0(x-x')}}{2k_0} - \frac{e^{-ik_0(x-x')}}{2k_0} \right] = \frac{\sin k_0(x - x')}{k_0}. \tag{18.114}$$

For $(x - x') < 0$, we use the lower contour to find $G(x, x') = 0$. The combined result becomes

$$G(x, x') = \frac{\sin k_0(x - x')}{k_0} \theta(x - x'), \tag{18.115}$$

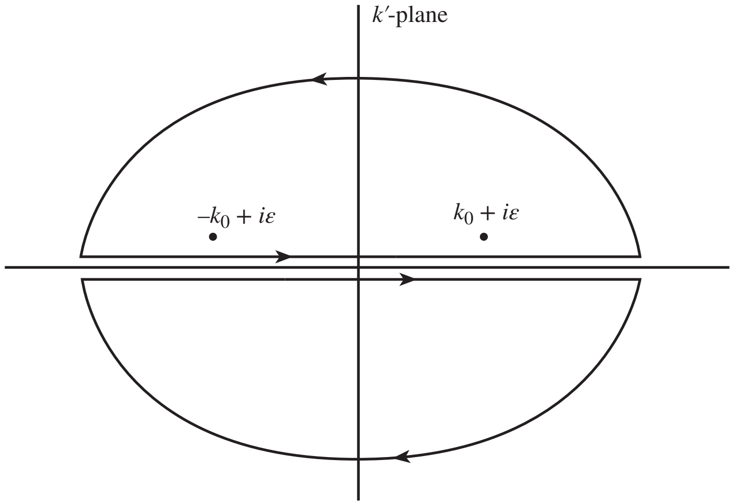

Figure 18.6 Contours for Case V.

which is useful for the cases where

$$\lim_{x\to-\infty} \left\{ \begin{matrix} G(x,x') \to 0 \\ G'(x,x') \to 0 \end{matrix} \right\}. \tag{18.116}$$

Example 18.6 ***Green's function for the harmonic oscillator***

For the damped driven harmonic oscillator, the equation of motion is written as

$$\frac{d^2x}{dt^2} + 2\varepsilon\frac{dx}{dt} + \omega_0^2 x(t) = f(t), \quad \varepsilon > 0. \tag{18.117}$$

In terms of a Green's function, the solution can be written as

$$x(t) = C_1x_1(t) + C_2x_2(t) + \int_{-\infty}^{\infty} G(x,x')f(t')\,dt', \tag{18.118}$$

where $x_1(t)$ and $x_2(t)$ are the solutions of the homogeneous equation. Assuming that all the necessary Fourier transforms and their inverses exist, we take the Fourier transform of the equation of motion to write the Green's function as

$$G(t,t') = -\frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega' \frac{e^{i\omega'(t-t')}}{(\omega'^2 - 2i\varepsilon\omega' - \omega_0^2)}. \tag{18.119}$$

Since the denominator has zeroes at

$$\omega'_{1,2} = \frac{2i\varepsilon \mp \sqrt{-4\varepsilon^2 + 4\omega_0^2}}{2} = \mp\sqrt{\omega_0^2 - \varepsilon^2} + i\varepsilon, \tag{18.120}$$

we can write $G(t,t')$ as

$$G(t,t') = -\frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega' \frac{e^{i\omega'(t-t')}}{(\omega'-\omega'_1)(\omega'-\omega'_2)}. \tag{18.121}$$

We can evaluate this integral by going to the complex ω-plane. For $(t-t')>0$, we use the upper contour in Figure 18.7 to write the Green's function as

$$G(t,t') = -\frac{2\pi i}{2\pi}\left[\frac{e^{i\omega'_1(t-t')}}{(\omega'_1-\omega'_2)} + \frac{e^{i\omega'_2(t-t')}}{(\omega'_2-\omega'_1)}\right] \tag{18.122}$$

$$= \frac{1}{i}\left[\frac{e^{-\varepsilon(t-t')}}{2\sqrt{\omega_0^2-\varepsilon^2}}\left(e^{i\sqrt{\omega_0^2-\varepsilon^2}(t-t')} - e^{-i\sqrt{\omega_0^2-\varepsilon^2}(t-t')}\right)\right] \tag{18.123}$$

$$= \frac{1}{i}\left[\frac{e^{-\varepsilon(t-t')}}{2\sqrt{\omega_0^2-\varepsilon^2}}2i\ \sin\left(\sqrt{\omega_0^2-\varepsilon^2}(t-t')\right)\right]. \tag{18.124}$$

For $(t-t')<0$, we use the lower contour in Figure 18.7. Because there are no singularities inside the contour, Green's function is now given as $G(t,t')=0$. Combining these results, we write the Green's function as

$$G(t,t') = \begin{cases} \dfrac{e^{-\varepsilon(t-t')}}{\sqrt{\omega_0^2-\varepsilon^2}} \sin\sqrt{\omega_0^2-\varepsilon^2}(t-t'), & t-t'>0, \\ 0, & t-t'<0, \end{cases} \tag{18.125}$$

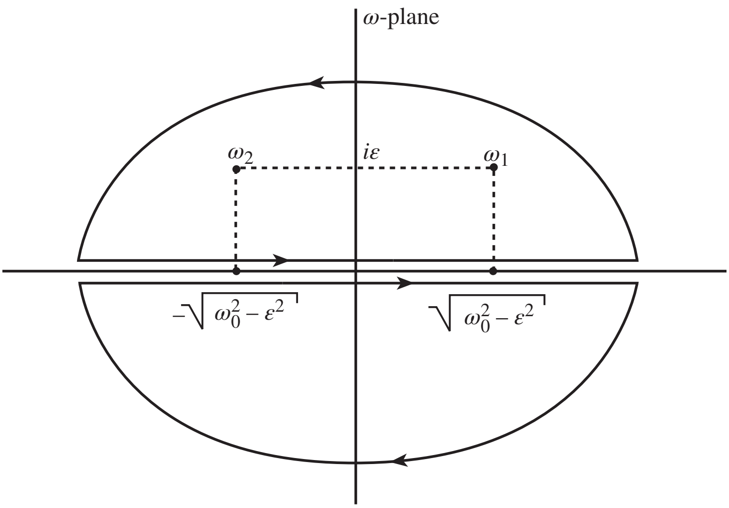

Figure 18.7 Contours for the harmonic oscillator.

or as

$$G(t,t') = \frac{e^{-\varepsilon(t-t')}}{\sqrt{\omega_0^2-\varepsilon^2}}\left[\sin\sqrt{\omega_0^2-\varepsilon^2}(t-t')\right]\theta(t-t'). \tag{18.126}$$

It is easy to check that this Green's function satisfies the equation

$$\left[\frac{d^2}{dt^2}+2\varepsilon\frac{d}{dt}+\omega_0^2\right]G(t,t') = \delta(t-t'). \tag{18.127}$$

Example 18.7 ***Damped driven harmonic oscillator***
In the previous example, let us take the driving force as $f(t) = F_0e^{-\alpha t}$, where α is a constant. For sinosoidal driving forces, we could take α as $i\omega_1$, where ω_1 is the frequency of the driving force. If we start the system with the initial conditions $x(0) = \dot{x}(0) = 0$, C_1 and C_2 in Eq. (18.118) are zero; hence, the solution will be written as

$$x(t) = F_0e^{-\varepsilon t}\int_0^t \frac{dt'}{\sqrt{\omega_0^2-\varepsilon^2}}\sin\left[\sqrt{\omega_0^2-\varepsilon^2}(t-t')\right]e^{(\varepsilon-\alpha)t'} \tag{18.128}$$

$$= \frac{F_0}{\sqrt{\omega_0^2-\varepsilon^2}}\frac{\sin\left[\sqrt{\omega_0^2-\varepsilon^2}t-\eta\right]}{\sqrt{\omega_0^2+\alpha^2-2\alpha\varepsilon}}e^{-\varepsilon t}+\frac{F_0}{\omega_0^2+\alpha^2-2\alpha\varepsilon}e^{-\alpha t}, \tag{18.129}$$

where we have defined $\tan\eta = \sqrt{\omega_0^2-\varepsilon^2}/(\alpha-\varepsilon)$. One can easily check that $x(t)$ satisfies the differential equation

$$\frac{d^2x(t)}{dt^2}+2\varepsilon\frac{dx(t)}{dt}+\omega_0^2x(t) = F_0e^{-\alpha t}. \tag{18.130}$$

For weak damping, the solution reduces to

$$x(t) = \frac{F_0}{\omega_0}\frac{\sin[\omega_0t-\eta]}{\sqrt{\omega_0^2+\alpha^2}}+\frac{F_0}{\omega_0^2+\alpha^2}e^{-\alpha t}. \tag{18.131}$$

As expected, in the $t\to\infty$ limit, this becomes

$$x(t) = \left(F_0/\omega_0\sqrt{\omega_0^2+\alpha^2}\right)\sin\,[\omega_0t-\eta]. \tag{18.132}$$

18.1.11 Another Approach for the Green's function

Let us start with the most general second-order differential equation:

$$£y(x) = f(x, y(x)), \quad x \in [a, b], \tag{18.133}$$

$$£ = p_0(x)\frac{d^2}{dx^2} + p_1(x)\frac{d}{dx} + p_2(x), \tag{18.134}$$

where for self-adjoint operators $p_1(x) = p_0'(x)$. Green's function, $G(x, x')$, allows us to convert the differential equation [Eq. (18.133)] into an integral equation:

$$y(x) = \int_a^b dx' G(x, x') f(x', y(x')), \tag{18.135}$$

where the Green's function satisfies the differential equation $£G(x, x') = \delta(x - x')$ with the same boundary conditions that $y(x)$ is required to satisfy. These boundary conditions are usually one of the following two types:

(1) **Single point boundary condition:**

$$G(a, x') = 0, \tag{18.136}$$

$$\frac{\partial G(a, x')}{\partial x} = 0. \tag{18.137}$$

(2) **Two point boundary condition:**

$$G(a, x') = 0, \tag{18.138}$$

$$G(b, x') = 0. \tag{18.139}$$

From the differential equation that the Green's function satisfies:

$$p_0(x)\frac{d^2G(x, x')}{dx^2} + p_1(x)\frac{dG(x, x')}{dx} + p_2(x)G(x, x') = \delta(x - x'), \tag{18.140}$$

we can deduce that $G(x, x')$ must be continuous at $x = x'$. Otherwise, $G(x, x')$ would be proportional to the unit step function and since the derivative of the unit step function is a Dirac-delta function, the first term on the left would be proportional to the derivative of the Dirac-delta function, which would make it incompatible with the Dirac-delta function on the right-hand side. Let us now integrate the differential equation [Eq. (18.140)] between $x' \in (x' - \epsilon, x' + \epsilon)$ and take the limit $\epsilon \to 0$:

$$\int_{x'-\epsilon}^{x'+\epsilon} dx' \, p_0(x')\frac{d^2G(x, x')}{dx'^2} + \int_{x'-\epsilon}^{x'+\epsilon} dx' \, p_1(x')\frac{dG(x, x')}{dx'} + \int_{x'-\epsilon}^{x'+\epsilon} dx' \, p_2(x')G(x, x') = \int_{x'-\epsilon}^{x'+\epsilon} dx' \, \delta(x - x'). \tag{18.141}$$

We now analyze this equation term by term. From the definition of the Dirac-delta function, the term on the right-hand side is $\int_{x'-\epsilon}^{x'+\epsilon} dx' \, \delta(x - x') = 1$.

In the integrals on the left-hand side, since p_0, p_1, p_2 are continuous functions, in the limit as $\epsilon \to 0$, we can replace them with their values at $x = x'$:

$$p_0(x') \lim_{\epsilon\to 0} \int_{x'-\epsilon}^{x'+\epsilon} dx' \frac{d^2G(x,x')}{dx'^2} + p_1(x') \lim_{\epsilon\to 0} \int_{x'-\epsilon}^{x'+\epsilon} dx' \frac{dG(x,x')}{dx'} + p_2(x') \lim_{\epsilon\to 0} \int_{x'-\epsilon}^{x'+\epsilon} dx' G(x,x') = 1. \tag{18.142}$$

Since $G(x,x')$ is continuous at $x = x'$, in the limit as $\epsilon \to 0$, the last term on the left-hand side vanishes, $\lim_{\epsilon\to 0} \int_{x'-\epsilon}^{x'+\epsilon} dx' G(x,x') = 0$, thus leaving

$$p_0(x') \lim_{\epsilon\to 0} \int_{x'-\epsilon}^{x'+\epsilon} dx' \frac{d^2G(x,x')}{dx'^2} + p_1(x') \lim_{\epsilon\to 0} \int_{x'-\epsilon}^{x'+\epsilon} dG(x,x') = 1 \tag{18.143}$$

or

$$p_0(x') \lim_{\epsilon\to 0} \left[\frac{dG(x,x'+\epsilon)}{dx'} - \frac{dG(x,x'-\epsilon)}{dx'} \right] + p_1(x') \lim_{\epsilon\to 0} [G(x,x'+\epsilon) - G(x,x'-\epsilon)] = 1. \tag{18.144}$$

From the continuity of $G(x,x')$, in the limit as $\epsilon \to 0$, the second term on the left-hand side vanishes, thus leaving us with the fact that the derivative of $G(x,x')$ has a finite discontinuity by the amount $1/p_0(x')$ at $x = x'$.

Using these results, we now construct the Green's function under more general conditions than used in Section 18.1.2. Let the general solution of $£y(x) = 0$ be given as $y(x) = ay_1(x) + by_2(x)$, where $£y_1(x) = 0$ and $£y_2(x) = 0$. We write the general form of the Green's function as

$$\begin{aligned} G(x,x') &= Ay_1(x) + By_2(x), \quad x - x' > 0, \\ G(x,x') &= Cy_1(x) + Dy_2(x), \quad x - x' < 0. \end{aligned} \tag{18.145}$$

At $x = x'$, the two functions must match and their derivatives differ by $1/p_0(x)$:

$$Ay_1(x') + By_2(x') = Cy_1(x') + Dy_2(x'), \tag{18.146}$$

$$Ay_1'(x') + By_2'(x') = Cy_1'(x') + Dy_2'(x') + \frac{1}{p_0(x')}. \tag{18.147}$$

We first write these equations as

$$(A - C)y_1(x') + (B - D)y_2(x') = 0, \tag{18.148}$$

$$(A - C)y_1'(x') + (B - D)y_2'(x') = \frac{1}{p_0(x')}, \tag{18.149}$$

so that

$$(A - C) = \frac{\begin{vmatrix} 0 & y_2(x') \\ 1/p_0(x') & y_2'(x') \end{vmatrix}}{\begin{vmatrix} y_1(x') & y_2(x') \\ y_1'(x') & y_2'(x') \end{vmatrix}} = -\frac{y_2(x')}{p_0(x')W(x')}, \tag{18.150}$$

where the Wronskian, $W(y_1, y_2)$, is defined as

$$W(x') = y_1(x')y_2'(x') - y_2(x')y_1'(x'). \tag{18.151}$$

Similarly,

$$(B - D) = \frac{y_1(x')}{p_0(x')W(x')}. \tag{18.152}$$

We can now write the Green's function as

$$G(x', x) = Cy_1(x) + Dy_2(x) - \frac{[y_1(x)y_2(x') - y_2(x)y_1(x')]}{p_0(x')W(x')}, \quad x - x' > 0, \tag{18.153}$$

$$G(x - x') = Cy_1(x) + Dy_2(x), \quad x - x' < 0. \tag{18.154}$$

Let us now impose the **boundary conditions**.

Type I. Using

$$G(a, x') = 0, \tag{18.155}$$

$$\frac{\partial G(a, x')}{\partial x'} = 0, \tag{18.156}$$

we write

$$Cy_1(a) + Dy_2(a) = 0, \tag{18.157}$$

$$Cy_1'(a) + Dy_2'(a) = 0. \tag{18.158}$$

Since $W(x') \neq 0$, we get $C = D = 0$, thus the Green's function becomes

$$G(x', x) = -\Theta(x - x')\frac{[y_1(x)y_2(x') - y_2(x)y_1(x')]}{p_0(x')W(x')}, \tag{18.159}$$

where $\Theta(x - x')$ is the unit step function.

As an example, consider

$$\frac{d^2y}{dx^2} + k_0^2 y(x) = f(x), \quad y(0) = y'(0) = 0. \tag{18.160}$$

The two linearly independent solutions are $y_1(x) = \cos(k_0 x)$ and $y_2(x) = \sin(k_0 x)$. With the Wronskian determined as $W(x) = k_0$, Eq. (18.159) allows us to write the Green's function as

$$G(x', x) = \Theta(x - x')\frac{\sin[k_0(x - x')]}{k_0}, \tag{18.161}$$

which agrees with our earlier result [Eq. (18.115)].

Type II. We now use the two point boundary condition:

$$G(a, x') = 0, \tag{18.162}$$

$$G(b, x') = 0 \tag{18.163}$$

to write

$$Cy_1(a) + Dy_2(a) = 0, \tag{18.164}$$

$$Cy_1(b) + Dy_2(b) - \frac{[y_1(b)y_2(x') - y_2(b)y_1(x')]}{p_0(x')W(x')} = 0. \tag{18.165}$$

Simultaneous solution of these yield the Green's function

$$G(x, x') = \frac{[y_1(x')y_2(a) - y_1(a)y_2(x')][y_1(b)y_2(x) - y_2(b)y_1(x)]}{[y_1(b)y_2(a) - y_1(a)y_2(b)]p_0(x')W(x')}, \quad x - x' > 0, \tag{18.166}$$

$$G(x, x') = \frac{[y_1(x)y_2(a) - y_1(a)y_2(x)][y_1(b)y_2(x') - y_2(b)y_1(x')]}{[y_1(b)y_2(a) - y_1(a)y_2(b)]p_0(x')W(x')}, \quad x - x' < 0. \tag{18.167}$$

The second solution: In constructing Green's functions by using the above formulas, we naturally need two linearly independent solutions and also the Wronskian of the solutions. The nice thing about the Wronskian in these cases is that it can be obtained from the differential operator:

$$\pounds = p_0(x)\frac{d^2}{dx^2} + p_1(x)\frac{d}{dx} + p_2(x), \quad x \in [a, b]. \tag{18.168}$$

Let us now write the derivative of the Wronskian:

$$\frac{dW(x)}{dx} = \frac{d}{dx}[y_1(x)y_2'(x) - y_2(x)y_1'(x)] = y_1(x)y_2''(x) - y_1''(x)y_2(x), \tag{18.169}$$

where

$$\left[p_0(x)\frac{d^2}{dx^2} + p_1(x)\frac{d}{dx} + p_2(x)\right] y_i(x) = 0, \quad i = 1 \text{ or } 2. \tag{18.170}$$

We rewrite the differential equation, $\pounds y(x) = 0$, as

$$\frac{d^2 y_i}{dx^2} + P(x)\frac{dy_i}{dx} + Q(x)y_i(x) = 0, \quad i = 1 \text{ or } 2, \tag{18.171}$$

to get

$$y_1 y_2'' - y_1'' y_2 = -P(x)[y_1 y_2' - y_2 y_1'] = -P(x)W(x), \tag{18.172}$$

thus $dW/dx = -P(x)W(x)$. Hence, the Wronskian can be obtained from the differential operator, $\pounds$, by the integral

$$W(x) = e^{-\int_a^x dx' P(x')}. \tag{18.173}$$

Furthermore, by using the Wronskian and a special solution, we can also obtain a second solution. If we write $W(x)$ as

$$W(x) = y_1 y_2' - y_2 y_1' = y_1^2 \frac{d}{dx}\left(\frac{y_2}{y_1}\right), \tag{18.174}$$

we obtain

$$y_2(x) = y_1(x) \int_a^x \frac{W(x')}{y_1^2(x')}\, dx'. \tag{18.175}$$

In other words, a second solution, y_2, can be obtained from a given solution, y_1, and the Wronskian, W.

18.2 Time-Independent Green's Functions in Three Dimensions

18.2.1 Helmholtz Equation in Three Dimensions

The Helmholtz equation in three dimensions is given as

$$\boxed{(\vec{\nabla}^2 + k_0^2)\psi(\vec{r}) = F(\vec{r}).} \tag{18.176}$$

We now look for a Green's function satisfying

$$(\vec{\nabla}^2 + k_0^2)G(\vec{r}, \vec{r}') = \delta(\vec{r} - \vec{r}'). \tag{18.177}$$

We multiply the first equation by $G(\vec{r}, \vec{r}')$ and the second by $\psi(\vec{r})$ and then subtract, and integrate the result over the volume V to get

$$\begin{aligned} -\psi(\vec{r}') = &\iiint_V [G(\vec{r}, \vec{r}')\vec{\nabla}^2 \psi(\vec{r}) - \psi(\vec{r})\vec{\nabla}^2 G(\vec{r}, \vec{r}')]\, d^3\vec{r} \\ &- \iiint_V F(\vec{r})G(\vec{r}, \vec{r}')\, d^3\vec{r}. \end{aligned} \tag{18.178}$$

Using the **Green's theorem**:

$$\boxed{\iiint_V (F\vec{\nabla}^2 G - G\vec{\nabla}^2 F)\, d^3\vec{r} = \iint_S (F\vec{\nabla} G - G\vec{\nabla} F) \cdot \hat{\mathbf{n}}\, ds,} \tag{18.179}$$

where S is a closed surface enclosing the volume V with the outward unit normal $\hat{\mathbf{n}}$, we obtain

$$\psi(\vec{r}\,') = \iiint_V F(\vec{r})G(\vec{r},\vec{r}\,')\, d^3\vec{r} + \iint_S [\psi(\vec{r})\vec{\nabla}G(\vec{r},\vec{r}\,') - G(\vec{r},\vec{r}\,')\vec{\nabla}\psi(\vec{r})] \cdot \hat{\mathbf{n}}\, ds. \tag{18.180}$$

Interchanging the primed and the unprimed variables and assuming that the Green's function is symmetric in anticipation of the corresponding boundary conditions to be imposed later, we obtain the following remarkable formula:

$$\boxed{\begin{aligned}\psi(\vec{r}) = &\iiint_{V'} G(\vec{r},\vec{r}\,')F(\vec{r}\,')\, d^3\vec{r}\,' \\ &+ \iint_{S'} [\vec{\nabla}' G(\vec{r},\vec{r}\,')\psi(\vec{r}\,')] \cdot \hat{\mathbf{n}}\, ds' \\ &- \iint_{S'} G(\vec{r},\vec{r}\,')\vec{\nabla}'\psi(\vec{r}\,') \cdot \hat{\mathbf{n}}\, ds'.\end{aligned}} \tag{18.181}$$

Boundary conditions: The most frequently used boundary conditions are:

i) Dirichlet boundary conditions, where G is zero on the boundary.
ii) Neumann boundary conditions, where the normal gradient of G on the surface is zero:

$$\vec{\nabla}G \cdot \hat{\mathbf{n}}|_{\text{boundary}} = 0. \tag{18.182}$$

iii) General boundary conditions:

$$\vec{\nabla}G + \vec{v}(\vec{r}\,')G|_{\text{boundary}} = 0, \tag{18.183}$$

where $\vec{v}(\vec{r}\,')$ is a function of the boundary point $\vec{r}\,'$.

For any one of these cases, the Green's function is symmetric and the surface term in the above equation vanishes, thus giving

$$\boxed{\psi(\vec{r}) = \iiint_V G(\vec{r},\vec{r}\,')F(\vec{r}\,')\, d^3\vec{r}\,'.} \tag{18.184}$$

18.2.2 Green's Functions in Three Dimensions

Consider the inhomogeneous equation

$$\mathbf{H}\psi(\vec{r}) = F(\vec{r}), \tag{18.185}$$

where **H** is a linear differential operator. **H** has a complete set $\{\boldsymbol{\phi}_\lambda(\overrightarrow{r})\}$ of orthonormal eigenfunctions, which are determined by the eigenvalue equation $\mathbf{H}\phi_\lambda(\overrightarrow{r}) = \lambda\boldsymbol{\phi}_\lambda(\overrightarrow{r})$, where λ stands for the eigenvalues and the eigenfunctions satisfy the homogeneous boundary conditions given in the previous section. We need a Green's function satisfying the equation $\mathbf{H}G(\overrightarrow{r}, \overrightarrow{r}') = \delta(\overrightarrow{r} - \overrightarrow{r}')$. Expanding $\Psi(\overrightarrow{r})$ and $F(\overrightarrow{r})$ in terms of this complete set of eigenfunctions, we write

$$\Psi(\overrightarrow{r}) = \sum_\lambda a_\lambda \boldsymbol{\phi}_\lambda(\overrightarrow{r}), \quad a_\lambda = \iiint_V \boldsymbol{\phi}^*_\lambda(\overrightarrow{r})\Psi(\overrightarrow{r})\, d^3\overrightarrow{r}, \tag{18.186}$$

$$F(\overrightarrow{r}) = \sum_\lambda c_\lambda \boldsymbol{\phi}_\lambda(\overrightarrow{r}), \quad c_\lambda = \iiint_V \boldsymbol{\phi}^*_\lambda(\overrightarrow{r})F(\overrightarrow{r})\, d^3\overrightarrow{r}. \tag{18.187}$$

Substituting these into Eq. (18.185), we obtain $a_\lambda = c_\lambda/\lambda$. Using a_λ and the explicit form of c_λ [Eqs. (18.186) and (18.187)], we can write $\Psi(\overrightarrow{r})$ as

$$\Psi(\overrightarrow{r}) = \iiint_V \left[\sum_\lambda \frac{\boldsymbol{\phi}_\lambda(\overrightarrow{r})\boldsymbol{\phi}^*_\lambda(\overrightarrow{r}')}{\lambda}\right] F(\overrightarrow{r}')\, d^3\overrightarrow{r}', \tag{18.188}$$

which gives the Green's function

$$G(\overrightarrow{r}, \overrightarrow{r}') = \sum_\lambda \frac{\boldsymbol{\phi}_\lambda(\overrightarrow{r})\boldsymbol{\phi}^*_\lambda(\overrightarrow{r}')}{\lambda}. \tag{18.189}$$

This Green's function can easily be generalized to the equation

$$\boxed{(\mathbf{H} - \lambda_0)\Psi(\overrightarrow{r}) = F(\overrightarrow{r}),} \tag{18.190}$$

for the operator $(\mathbf{H} - \lambda_0)$ as

$$\boxed{G(\overrightarrow{r}, \overrightarrow{r}') = \sum_\lambda \frac{\boldsymbol{\phi}_\lambda(\overrightarrow{r})\boldsymbol{\phi}^*_\lambda(\overrightarrow{r}')}{\lambda - \lambda_0}.} \tag{18.191}$$

As an example, we find the Green's function for the three-dimensional Helmholtz equation

$$(\overrightarrow{\nabla}^2 + k_0^2)\psi(\overrightarrow{r}) = F(\overrightarrow{r}) \tag{18.192}$$

in a rectangular region bounded by six planes:

$$\left\{\begin{matrix} x = 0, & x = a, \\ y = 0, & y = b, \\ z = 0, & z = c \end{matrix}\right\} \tag{18.193}$$

and with the homogeneous Dirichlet boundary conditions. The corresponding eigenvalue equation is $\vec{\nabla}^2 \boldsymbol{\phi}_{lmn}(\vec{r}) + k^2_{lmn}\boldsymbol{\phi}_{lmn}(\vec{r}) = 0$. The normalized eigenfunctions are easily obtained as

$$\boldsymbol{\phi}_{lmn}(\vec{r}) = \frac{8}{abc} \sin\left(\frac{l\pi x}{a}\right) \sin\left(\frac{m\pi y}{b}\right) \sin\left(\frac{n\pi z}{c}\right), \tag{18.194}$$

where the eigenvalues are

$$k^2_{lmn} = \frac{l^2\pi^2}{a^2} + \frac{m^2\pi^2}{b^2} + \frac{n^2\pi^2}{c^2}, \quad l, m, n = \text{positive integer.} \tag{18.195}$$

Using these eigenfunctions [Eq. (18.194)], we can now write the Green's function as

$$G(\vec{r}, \vec{r}') = \sum_{lmn} \frac{\boldsymbol{\phi}_{lmn}(\vec{r})\boldsymbol{\phi}^*_{lmn}(\vec{r}')}{k_0^2 - k^2_{lmn}}. \tag{18.196}$$

18.2.3 Green's Function for the Laplace Operator

Green's function for the Laplace operator, $\vec{\nabla}^2$, satisfies the differential equation $\vec{\nabla}^2 G(\vec{r}, \vec{r}') = \delta(\vec{r}, \vec{r}')$. Using spherical polar coordinates, this can be written as

$$\vec{\nabla}^2 G(\vec{r}, \vec{r}') = \frac{\delta(r - r')}{r'^2}\delta(\cos\theta - \cos\theta')\delta(\phi - \phi') \tag{18.197}$$

$$= \frac{\delta(r - r')}{r'^2} \sum_{l=0}^{\infty} \sum_{m=-l}^{m=l} Y_l^{*m}(\theta', \phi')Y_l^m(\theta, \phi), \tag{18.198}$$

where we have used the completeness relation of the spherical harmonics. For the Green's function inside a sphere, we use the boundary conditions $G(0, \vec{r}') =$ finite and $G(a, \vec{r}') = 0$. In spherical polar coordinates, we can separate the radial and the angular parts of the Green's function as

$$\boxed{G(\vec{r}, \vec{r}') = \sum_{l=0}^{\infty} \sum_{m=-l}^{m=l} g_l(r, r')Y_l^{*m}(\theta', \phi')Y_l^m(\theta, \phi).} \tag{18.199}$$

We now substitute Eq. (18.199) into Eq. (18.198) to find the differential equation that $g_l(r, r')$ satisfies:

$$\frac{1}{r}\frac{d^2}{dr^2}[rg_l(r, r')] - \frac{l(l+1)}{r^2}g_l(r, r') = \frac{1}{r'^2}\delta(r - r'). \tag{18.200}$$

A general solution of the homogeneous equation:

$$\frac{1}{r}\frac{d^2}{dr^2}[rg_l(r, r')] - \frac{l(l+1)}{r^2}g_l(r, r') = 0, \tag{18.201}$$

can be obtained by trying a solution as $c_0 r^l + c_1 r^{-(l+1)}$. We can now construct the radial part of the Green's function for the inside of a sphere by finding the appropriate u and the v solutions [Eq. (18.16)] as

$$g_l(r,r') = \frac{r^l r'^l}{(2l+1)a^{2l+1}} \begin{cases} [1-(a/r')^{2l+1}], & r < r', \\ [1-(a/r)^{2l+1}], & r > r'. \end{cases} \tag{18.202}$$

Now the complete Green's function can be written by substituting this result to Eq. (18.199).

18.2.4 Green's Functions for the Helmholtz Equation

We now consider the operator $\mathbf{H}_0 = \vec{\nabla}^2 + \lambda$ in the **continuum limit**. Using $\mathbf{H}_0$, we can write the following differential equation:

$$\mathbf{H}_0 \Psi(\vec{r}) = F(\vec{r}). \tag{18.203}$$

Let us assume that the Fourier transforms of $\Psi(\vec{r})$ and $F(\vec{r})$ exist:

$$\hat{F}(\vec{k}) = \frac{1}{(2\pi)^{3/2}} \iiint_V e^{-i\vec{k}\cdot\vec{r}} F(\vec{r})\, d^3\vec{r}, \tag{18.204}$$

$$\hat{\Psi}(\vec{k}) = \frac{1}{(2\pi)^{3/2}} \iiint_V e^{-i\vec{k}\cdot\vec{r}} \Psi(\vec{r})\, d^3\vec{r}. \tag{18.205}$$

Taking the Fourier transform of Eq. (18.203), we get

$$\frac{1}{(2\pi)^{3/2}} \iiint_V e^{-i\vec{k}\cdot\vec{r}} \vec{\nabla}^2 \Psi(\vec{r})\, d^3\vec{r} + \lambda\hat{\Psi}(\vec{k}) = \hat{F}(\vec{k}). \tag{18.206}$$

Using the Green's theorem [Eq. (18.179)], we can write the first term in Eq. (18.206) as

$$\begin{aligned} \frac{1}{(2\pi)^{3/2}} \iiint_V e^{-i\vec{k}\cdot\vec{r}} \vec{\nabla}^2 \Psi(\vec{r})\, d^3\vec{r} &= \frac{1}{(2\pi)^{3/2}} \iiint_V \Psi(\vec{r}) \vec{\nabla}^2 e^{-i\vec{k}\cdot\vec{r}}\, d^3\vec{r} \\ &+ \frac{1}{(2\pi)^{3/2}} \iint_S (e^{-i\vec{k}\cdot\vec{r}} \vec{\nabla}\Psi(\vec{r}) - \Psi(\vec{r})\vec{\nabla} e^{-i\vec{k}\cdot\vec{r}}) \cdot \hat{\mathbf{n}}\, ds, \end{aligned} \tag{18.207}$$

where S is a surface with an outward unit normal $\hat{\mathbf{n}}$ enclosing the volume V. We now take our region of integration as a sphere of radius R and consider the limit $R \to \infty$. In this limit, the **surface term** becomes

$$\begin{aligned} &\frac{1}{(2\pi)^{3/2}} \lim_{R\to\infty} \iint_S (e^{-i\vec{k}\cdot\vec{r}} \vec{\nabla}\Psi(\vec{r}) - \Psi(\vec{r})\vec{\nabla} e^{-i\vec{k}\cdot\vec{r}}) \cdot \hat{\mathbf{n}}\, ds \\ &= \frac{1}{(2\pi)^{3/2}} \lim_{R\to\infty} R^2 \left\{ \iint_S \left[e^{-i\vec{k}\cdot\vec{r}} \frac{d\Psi}{dr} - \Psi \frac{d(e^{-i\vec{k}\cdot\vec{r}})}{dr} \right] d\Omega \right\}_{r=R}, \end{aligned} \tag{18.208}$$

where $\hat{\mathbf{n}} = \hat{\mathbf{e}}_r$ and $d\Omega = \sin\theta d\theta d\phi$. If the function $\Psi(\vec{r})$ goes to zero sufficiently rapidly as $|\vec{r}| \to \infty$, that is, when $\Psi(\vec{r})$ goes to zero faster than $1/r$, the surface term vanishes, thus Eq. (18.207) reduces to

$$\frac{1}{(2\pi)^{3/2}} \iiint_V e^{-i\vec{k}\cdot\vec{r}} \vec{\nabla}^2 \Psi(\vec{r})\, d^3\vec{r} = -k^2 \hat{\Psi}(\vec{k}). \tag{18.209}$$

Consequently, Eq. (18.206) becomes

$$\hat{\Psi}(\vec{k}) = \frac{\hat{F}(\vec{k})}{(-k^2 + \lambda)}. \tag{18.210}$$

In this equation, we have to treat the cases $\lambda > 0$ and $\lambda \leq 0$ separately.

Case I. $\lambda \leq 0$:

In this case, we can write $\lambda = -\kappa^2$; thus the denominator in

$$\hat{\Psi}(\vec{k}) = -\frac{\hat{F}(\vec{k})}{k^2 + \kappa^2} \tag{18.211}$$

never vanishes. Taking the inverse Fourier transform of this, we write the general solution of Eq. (18.203) as

$$\Psi(\vec{r}) = \xi(\vec{r}) - \frac{1}{(2\pi)^{3/2}} \iiint \frac{\hat{F}(\vec{k})}{k^2 + \kappa^2} e^{i\vec{k}\cdot\vec{r}}\, d^3\vec{k}, \tag{18.212}$$

where $\xi(\vec{r})$ denotes the solution of the homogeneous equation, $\mathbf{H}_0\xi(\vec{r}) = (\vec{\nabla}^2 - \kappa^2)\xi(\vec{r}) = 0$. Defining a Green's function $G(\vec{r}, \vec{r}\,')$ as

$$G(\vec{r}, \vec{r}\,') = -\frac{1}{(2\pi)^3} \iiint \frac{e^{i\vec{k}\cdot(\vec{r}-\vec{r}\,')}}{k^2 + \kappa^2}\, d^3\vec{k}, \tag{18.213}$$

we can express the general solution of Eq. (18.203) as

$$\Psi(\vec{r}) = \xi(\vec{r}) + \iiint_V G(\vec{r}, \vec{r}\,') F(\vec{r}\,')\, d^3\vec{r}, \tag{18.214}$$

The integral in the Green's function can be evaluated by using complex contour integral techniques. Taking the $\vec{k}$ vector as

$$\vec{k} = k\hat{\mathbf{r}}, \quad \hat{\mathbf{r}} = \frac{\vec{r} - \vec{r}\,'}{|\vec{r} - \vec{r}\,'|}, \tag{18.215}$$

we write

$$I = \iiint \frac{e^{i\vec{k}\cdot(\vec{r}-\vec{r}\,')}}{k^2 + \kappa^2}\, d^3\vec{k}, \tag{18.216}$$

where $d^3\overrightarrow{k} = k^2 \sin\theta dk d\theta d\phi$. We can take the ϕ and the θ integrals immediately, thus obtaining

$$I = 2\pi \int_0^\infty \frac{kdk}{k^2+\kappa^2} . \left[\frac{e^{ik|\overrightarrow{r}-\overrightarrow{r}'|} - e^{-ik|\overrightarrow{r}-\overrightarrow{r}'|}}{i|\overrightarrow{r}-\overrightarrow{r}'|} \right] \tag{18.217}$$

$$= \frac{2\pi}{i|\overrightarrow{r}-\overrightarrow{r}'|} \int_{-\infty}^{\infty} dk \frac{ke^{ik|\overrightarrow{r}-\overrightarrow{r}'|}}{k^2+\kappa^2}. \tag{18.218}$$

Using Jordan's lemma (Section 12.7), we can show that the integral over the circle in the upper half complex k-plane goes to zero as the radius goes to infinity; thus we obtain I as

$$I = \frac{2\pi}{i|\overrightarrow{r}-\overrightarrow{r}'|} 2\pi i \sum_{k>0} \text{residues of} \left\{ \frac{ke^{ik|\overrightarrow{r}-\overrightarrow{r}'|}}{k^2+\kappa^2} \right\} \tag{18.219}$$

$$= \frac{4\pi^2}{|\overrightarrow{r}-\overrightarrow{r}'|} . \frac{i\kappa e^{-\kappa|\overrightarrow{r}-\overrightarrow{r}'|}}{2i\kappa} = \frac{2\pi^2}{|\overrightarrow{r}-\overrightarrow{r}'|} e^{-\kappa|\overrightarrow{r}-\overrightarrow{r}'|}. \tag{18.220}$$

Using this in Eq. (18.213), we obtain the **Green's function** as

$$\boxed{G(\overrightarrow{r}, \overrightarrow{r}') = -\frac{1}{4\pi} \frac{e^{-\kappa|\overrightarrow{r}-\overrightarrow{r}'|}}{|\overrightarrow{r}-\overrightarrow{r}'|}.} \tag{18.221}$$

To complete the solution [Eq. (18.214)], we also need $\xi(\overrightarrow{r})$, which is easily obtained as

$$\xi(\overrightarrow{r}) = C_0 e^{\pm\kappa_1 x} e^{\pm\kappa_2 y} e^{\pm\kappa_3 z}, \quad \kappa^2 = \kappa_1^2 + \kappa_2^2 + \kappa_3^2. \tag{18.222}$$

Because this solution diverges for $|r| \to \infty$, for a finite solution everywhere we set $C_0 = 0$ and write the general solution as

$$\boxed{\Psi(\overrightarrow{r}) = -\frac{1}{4\pi} \iiint_V \frac{e^{-\kappa|\overrightarrow{r}-\overrightarrow{r}'|}}{|\overrightarrow{r}-\overrightarrow{r}'|} F(\overrightarrow{r}')\, d^3\overrightarrow{r}'.} \tag{18.223}$$

In this solution, if $F(\overrightarrow{r}')$ goes to zero sufficiently rapidly as $|r'| \to \infty$, or if $F(\overrightarrow{r}')$ is zero beyond some $|r'| = r_0$, we see that for large r, $\Psi(\overrightarrow{r})$ decreases exponentially as

$$\Psi(\overrightarrow{r}) \to C \frac{e^{-\kappa r}}{r}. \tag{18.224}$$

This is consistent with the neglect of the surface term in our derivation in Eq. (18.208).

Example 18.8 ***Green's function for the Poisson equation***
Using the above Green's function [Eq. (18.221)] with $\kappa = 0$, we can now convert the Poisson equation, $\vec{\nabla}^2 \phi(\vec{r}) = -4\pi\rho(\vec{r})$, into an integral equation. In this case, $\lambda = 0$; thus the solution is given as

$$\phi(\vec{r}) = -4\pi \iiint_V G(\vec{r}, \vec{r}')\rho(\vec{r}')\, d^3\vec{r}', \tag{18.225}$$

where

$$G(\vec{r}, \vec{r}') = \frac{1}{4\pi} \frac{1}{|\vec{r} - \vec{r}'|}. \tag{18.226}$$

Example 18.9 ***Green's function for the Schrödinger equation – −E < 0***
Another application for Green's functions [Eq. (18.221)] is the time-independent Schrödinger equation:

$$\left(\vec{\nabla}^2 + \frac{2mE}{\hbar^2}\right)\Psi(\vec{r}) = \frac{2m}{\hbar^2} V(\vec{r})\Psi(\vec{r}). \tag{18.227}$$

For central potentials and bound states, ($E < 0$) κ^2 is given as $\kappa^2 = -2m|E|/\hbar^2$. Thus the solution of Eq. (18.227) can be written as

$$\Psi(\vec{r}) = -\frac{m}{2\pi\hbar^2} \iiint_V \frac{e^{-\kappa|\vec{r}-\vec{r}'|}}{|\vec{r} - \vec{r}'|} V(\vec{r}')\Psi(\vec{r}')\, d^3\vec{r}'. \tag{18.228}$$

This is also the integral equation version of the time-independent Schrödinger equation for bound states.

Case II. $\lambda > 0$ In this case, the denominator in the definition [Eq. (18.210)] of $\hat{\Psi}(\vec{k})$ has zeroes at $k = \pm\sqrt{\lambda}$. To eliminate this problem, we add a small imaginary piece, $i\varepsilon$, to λ as $\lambda = (q \pm i\varepsilon)$, $\varepsilon > 0$. Substituting this in Eq. (18.210), we get

$$\hat{\Psi}_{\pm}(\vec{k}) = -\frac{\hat{F}(\vec{k})}{k^2 - (q \pm i\varepsilon)^2}, \tag{18.229}$$

which is now well defined everywhere on the real k-axis. Taking the inverse Fourier transform of this, we get

$$\Psi(\vec{r}) = \xi(\vec{r}) + \iiint_V G_{\pm}(\vec{r}, \vec{r}')F(\vec{r}')\, d^3\vec{r}', \tag{18.230}$$

$$G_{\pm}(\vec{r}, \vec{r}') = -\frac{1}{(2\pi)^3} \iiint \frac{e^{i\vec{k}\cdot(\vec{r}-\vec{r}')}}{k^2 - (q \pm i\varepsilon)^2}\, d^3\vec{k}. \tag{18.231}$$

We can now evaluate this integral in the complex k-plane using the complex contour integral theorems and take the limit $\varepsilon \to 0$ to obtain the final result.

Because our integrand has two isolated simple poles at $k = (q \pm i\varepsilon)$, we use the Cauchy integral theorem (Chapter 12). However, as before, we first take the θ and the ϕ integrals to write

$$G_{\pm}(\vec{r}, \vec{r}\,') = -\frac{1}{8\pi^2 i|\vec{r} - \vec{r}\,'|} \int_{-\infty}^{\infty} k\, dk \left[\frac{e^{ik|\vec{r}-\vec{r}\,'|}}{(k - q \mp i\varepsilon)(k + q \pm i\varepsilon)} - \frac{e^{-ik|\vec{r}-\vec{r}\,'|}}{(k - q \mp i\varepsilon)(k + q \pm i\varepsilon)} \right]. \tag{18.232}$$

For the first integral, we close the contour in the upper half complex k-plane and get

$$\int_{-\infty}^{\infty} k\, dk \frac{e^{ik|\vec{r}-\vec{r}\,'|}}{(k - q \mp i\varepsilon)(k + q \pm i\varepsilon)} = \pi i e^{\pm iq|\vec{r}-\vec{r}\,'| - \varepsilon|\vec{r}-\vec{r}\,'|}. \tag{18.233}$$

Similarly, for the second integral, we close our contour in the lower half complex k-plane to get

$$\int_{-\infty}^{\infty} k\, dk \frac{e^{-ik|\vec{r}-\vec{r}\,'|}}{(k - q \mp i\varepsilon)(k + q \pm i\varepsilon)} = -\pi i e^{\pm iq|\vec{r}-\vec{r}\,'| - \varepsilon|\vec{r}-\vec{r}\,'|}. \tag{18.234}$$

Combining these, we obtain the Green's function:

$$G_{\pm}(\vec{r}, \vec{r}\,') = -\frac{1}{4\pi} \frac{e^{\pm iq|\vec{r}-\vec{r}\,'|}}{|\vec{r} - \vec{r}\,'|} e^{-\varepsilon|\vec{r}-\vec{r}\,'|}, \tag{18.235}$$

and the solution as

$$\Psi_{\pm}(\vec{r}) = \xi(\vec{r}) - \frac{1}{4\pi} \iiint_V \frac{e^{i(\pm q + i\varepsilon)|\vec{r}-\vec{r}\,'|}}{|\vec{r} - \vec{r}\,'|} F(\vec{r}\,')\, d^3\vec{r}\,'. \tag{18.236}$$

The choice of the $\pm$ sign is very important. In the limit as $|\vec{r}| \to \infty$, this solution behaves as

$$\Psi_{\pm}(\vec{r}) \to \xi(\vec{r}) + C\frac{e^{\pm iqr}}{r}, \tag{18.237}$$

where C is a constant independent of r, but it could depend on θ and ϕ. The $\pm$ signs physically correspond to the incoming and outgoing waves. We now look at the solutions of the homogeneous equation $(\vec{\nabla}^2 + q^2)\xi(\vec{r}) = 0$, which are now given as plane waves, $e^{i\vec{q}\cdot\vec{r}}$; thus the general solution becomes

$$\Psi_{\pm}(\vec{r}) = \frac{A}{(2\pi)^{3/2}} e^{i\vec{q}\cdot\vec{r}} - \frac{1}{4\pi} \iiint_V \frac{e^{i(\pm q + i\varepsilon)|\vec{r}-\vec{r}\,'|}}{|\vec{r} - \vec{r}\,'|} F(\vec{r}\,')\, d^3\vec{r}\,'. \tag{18.238}$$

The constant A and the direction of the $\vec{q}$ vector come from the initial conditions.

Example 18.10 ***Green's function for the Schrödinger equation – –$E \geq 0$***
An important application of the $\lambda > 0$ case is the Schrödinger equation for the scattering problems, that is, for states with $E \geq 0$. Using the Green's function, we have found [Eq. (18.235)] and we can write the Schrödinger equation,

$$\left(\vec{\nabla}^2 + \frac{2mE}{\hbar^2}\right)\Psi(\vec{r}) = \frac{2m}{\hbar^2}V(\vec{r})\Psi(\vec{r}), \tag{18.239}$$

as an integral equation for the scattering states as

$$\Psi_\pm(\vec{r}) = \frac{A}{(2\pi)^{3/2}}e^{i\vec{q}_i\cdot\vec{r}} - \frac{m}{2\pi\hbar^2}\iiint_V \frac{e^{\pm iq_i|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|}V(\vec{r}')\Psi_\pm(\vec{r}')\,d^3\vec{r}'. \tag{18.240}$$

The magnitude of $\vec{q}_i$ is given as $q_i = \sqrt{2mE/\hbar^2}$. Equation (18.240) is known as the **Lippmann–Schwinger equation**. For bound state problems, it is easier to work with the differential equation version of the Schrödinger equation; hence, it is preferred. However, for the scattering problems, the Lippmann–Schwinger equation is the starting point of modern quantum mechanics. Note that we have written the result free of ε in anticipation that the $\varepsilon \to 0$ limit will not cause any problems.

18.2.5 General Boundary Conditions and Electrostatics

In the problems we have discussed so far, the Green's function and the solution were required to satisfy the same homogeneous boundary conditions (Section 18.2.2). However, in electrostatics we usually deal with cases in which we are interested in finding the potential of a charge distribution in the presence of conducting surfaces held at constant potentials. The question we now ask is: Can we still use the Green's function found from the solution of

$$£G(\vec{r},\vec{r}') = \delta(\vec{r}-\vec{r}') \tag{18.241}$$

with the homogeneous boundary conditions? To answer this question, we start with a general second-order linear operator of the form

$$£ = \vec{\nabla}\cdot[p(\vec{r})\vec{\nabla}] + q(r), \tag{18.242}$$

which covers a wide range of interesting cases. The corresponding inhomogeneous differential equation is now given as

$$£\Phi(\vec{r}) = F(\vec{r}), \tag{18.243}$$

where the solution, $\Phi(\vec{r})$, is required to satisfy more complex boundary conditions than the usual homogeneous boundary conditions that the Green's function is required to satisfy. Let us first multiply Eq. (18.243) with $G(\vec{r},\vec{r}')$ and

Eq. (18.241) with $\Phi(\overrightarrow{r})$, and then subtract and integrate the result over V to write

$$\Phi(\overrightarrow{r}') = \iiint_V F(\overrightarrow{r})G(\overrightarrow{r},\overrightarrow{r}')d^3\overrightarrow{r} \tag{18.244}$$
$$+ \iiint_V [\Phi(\overrightarrow{r})£G(\overrightarrow{r},\overrightarrow{r}') - G(\overrightarrow{r},\overrightarrow{r}')£\Phi(\overrightarrow{r})]\, d^3\overrightarrow{r}.$$

We now write $£$ explicitly and use the following property of the $\overrightarrow{\nabla}$ operator:

$$\overrightarrow{\nabla}\cdot[f(\overrightarrow{r})\overrightarrow{v}(\overrightarrow{r})] = \overrightarrow{\nabla}f(\overrightarrow{r})\cdot\overrightarrow{v}(\overrightarrow{r}) + f(\overrightarrow{r})\overrightarrow{\nabla}\cdot\overrightarrow{v}(\overrightarrow{r}), \tag{18.245}$$

to write

$$\Phi(\overrightarrow{r}') = \iiint_V F(\overrightarrow{r})G(\overrightarrow{r},\overrightarrow{r}')\, d^3\overrightarrow{r} \tag{18.246}$$
$$+ \iiint_V \overrightarrow{\nabla}\cdot[p(\overrightarrow{r})\Phi(\overrightarrow{r})\overrightarrow{\nabla}G(\overrightarrow{r},\overrightarrow{r}') - G(\overrightarrow{r},\overrightarrow{r}')p(\overrightarrow{r})\overrightarrow{\nabla}\Phi(\overrightarrow{r})]d^3\overrightarrow{r}.$$

Using the fact that for homogeneous boundary conditions the Green's function is symmetric, we interchange $\overrightarrow{r}'$ and $\overrightarrow{r}$:

$$\Phi(\overrightarrow{r}) = \iiint_V F(\overrightarrow{r}')G(\overrightarrow{r},\overrightarrow{r}')\, d^3\overrightarrow{r}' \tag{18.247}$$
$$+ \iiint_V \overrightarrow{\nabla}'\cdot[p(\overrightarrow{r}')\Phi(\overrightarrow{r}')\overrightarrow{\nabla}'G(\overrightarrow{r},\overrightarrow{r}') - G(\overrightarrow{r},\overrightarrow{r}')p(\overrightarrow{r}')\overrightarrow{\nabla}'\Phi(\overrightarrow{r}')]\, d^3\overrightarrow{r}.$$

We finally use the Gauss theorem to write

$$\Phi(\overrightarrow{r}) = \iiint_V F(\overrightarrow{r}')G(\overrightarrow{r},\overrightarrow{r}')\, d^3\overrightarrow{r}' \tag{18.248}$$
$$+ \iint_S p(\overrightarrow{r}')[\Phi(\overrightarrow{r}')\overrightarrow{\nabla}'G(\overrightarrow{r},\overrightarrow{r}') - G(\overrightarrow{r},\overrightarrow{r}')\overrightarrow{\nabla}'\Phi(\overrightarrow{r}')]\cdot\hat{\mathbf{n}}\,ds',$$

where $\hat{\mathbf{n}}$ is the outward unit normal to the surface S bounding the volume V. If we impose the same homogeneous boundary conditions on $\Phi(\overrightarrow{r})$ and $G(\overrightarrow{r},\overrightarrow{r}')$, the surface term vanishes and we reach the conclusions of Section 18.2.2.

In general, in order to evaluate the surface integral, we have to know the function $\Phi(\overrightarrow{r})$ and its normal derivative on the surface. As boundary conditions, we can fix the value of $\Phi(\overrightarrow{r})$, its normal derivative, or even their linear combination on the surface S, but not $\Phi(\overrightarrow{r})$ and its normal derivative at the same time. In practice, this difficulty is circumvented by choosing the Green's function such that it vanishes on the surface. In such cases, the solution becomes

$$\boxed{\Phi(\vec{r}) = \iiint_V F(\vec{r}\,')G(\vec{r},\vec{r}\,')d^3\vec{r} + \iint_S [p(\vec{r}\,')\Phi(\vec{r}\,')\vec{\nabla}' G(\vec{r},\vec{r}\,')] \cdot \hat{\mathbf{n}} ds'.} \tag{18.249}$$

As an example, consider **electrostatics problems** where we have

$$\begin{Bmatrix} F(\vec{r}) = -4\pi\rho(\vec{r}), \\ p(\vec{r}) = 1, \\ q(\vec{r}) = 0. \end{Bmatrix} \tag{18.250}$$

The potential inside a region bounded by a conducting surface held at constant potential V_0 is now given as

$$\boxed{\Phi(\vec{r}) = -\int_V 4\pi\rho(\vec{r})G(\vec{r},\vec{r}\,')\, d^3\vec{r}\,' + V_0 \oint_S \vec{\nabla}' G(\vec{r},\vec{r}\,') \cdot \hat{\mathbf{n}}\, ds',} \tag{18.251}$$

where $G(\vec{r},\vec{r}\,')$ comes from the solution of Eq. (18.241) subject to the (homogeneous) boundary condition, which requires it to vanish on the surface. The geometry of the surface bounding the volume V could in principle be rather complicated and $\Phi(\vec{r}\,')$ in the surface integral does not have to be a constant.

Similarly, if we fix the value of the normal derivative $\vec{\nabla}\Phi(\vec{r}) \cdot \hat{\mathbf{n}}$ on the surface, then we use a Green's function with a normal derivative vanishing on the surface. Now the solution becomes

$$\boxed{\begin{aligned} \Phi(\vec{r}) = & \iiint_V F(\vec{r}\,')G(\vec{r},\vec{r}\,')\, d^3\vec{r}\,' \\ & - \iint_S p(\vec{r}\,')[G(\vec{r},\vec{r}\,')\vec{\nabla}'\Phi(\vec{r}\,')] \cdot \hat{\mathbf{n}}\, ds'. \end{aligned}} \tag{18.252}$$

18.2.6 Helmholtz Equation in Spherical Coordinates

We now consider the open problem for the Helmholtz equation in spherical coordinates with an inhomogeneous term:

$$\vec{\nabla}^2\Psi(r,\theta,\phi) + k^2\Psi(r,\theta,\phi) = F(r), \quad r \in [0,\infty]. \tag{18.253}$$

In terms of spherical harmonics, the **general solution** can be written as $\Psi(r,\theta,\phi) = \sum_{lm} R_l(kr)Y_{lm}(\theta,\phi)$. Substituting this into the **homogeneous** Helmholtz equation, we obtain the differential equation that $R_l(kr)$ satisfies as

$$\frac{d^2R_l}{dr^2} + \frac{2}{r}\frac{dR_l}{dr} + \left[k^2 - \frac{l(l+1)}{r^2}\right] R_l(kr) = 0. \tag{18.254}$$

Substituting $R_l(kr) = y_l(kr)/kr$, we obtain

$$y_l''(x) + \left[1 - \frac{l(l+1)}{x^2}\right] y_l(x) = 0, \tag{18.255}$$

where $x = kr$. The two linearly independent solutions can be written in terms of Bessel functions, J_n, N_n, as

$$R_l(kr) = \frac{y_l(kr)}{kr} = \begin{cases} j_l(kr) = \sqrt{\frac{\pi}{2}}\frac{J_{l+1/2}(kr)}{\sqrt{kr}}, \\ \\ n_l(kr) = \sqrt{\frac{\pi}{2}}\frac{N_{l+1/2}(kr)}{\sqrt{kr}}. \end{cases} \tag{18.256}$$

For large r, these solutions behave as

$$R_l(kr) = \lim_{r\to\infty} \begin{cases} j_l(kr) \xrightarrow{r\to\infty} \dfrac{\cos(kr - (l+1)\frac{\pi}{2})}{kr}, \\ \\ n_l(kr) \xrightarrow{r\to\infty} \dfrac{\sin(kr - (l+1)\frac{\pi}{2})}{kr}. \end{cases} \tag{18.257}$$

Using Eqs. (18.153) and (18.154), we can now construct the **radial Green's function** as

$$g_l(r,r') = Cj_l(kr) + Dn_l(kr) - \frac{j_l(kr)n_l(kr') - n_l(kr)j_l(kr')}{p_0(r)W(r')}, \quad r - r' > 0, \tag{18.258}$$

$$g_l(r,r') = Cj_l(kr) + Dn_l(kr), \quad r - r' < 0. \tag{18.259}$$

For a regular solution at the origin, we set $D = 0$. We evaluate the Wronskian, $W(r)$, by using Eq. (18.173) as $dW/W = -P(r)\,dr = -(2/r)\,dr$, which yields $W(r) = \text{constant}\,/r^2$. To evaluate the constant, we use the asymptotic forms of the Bessel functions:

$$\lim_{r\to\infty} W(kr) = \lim_{r\to\infty} \begin{vmatrix} j_l(kr) & n_l(kr) \\ j_l'(kr) & n_l'(kr) \end{vmatrix} \tag{18.260}$$

$$= \begin{vmatrix} \dfrac{\cos(kr-(l+1)\frac{\pi}{2})}{kr} & \dfrac{\sin(kr-(l+1)\frac{\pi}{2})}{kr} \\ \dfrac{-k\sin(kr-(l+1)\frac{\pi}{2})}{kr} & \dfrac{k\cos(kr-(l+1)\frac{\pi}{2})}{kr} \end{vmatrix} \tag{18.261}$$

$$= \frac{k}{(kr)^2} = \frac{1}{kr^2}, \tag{18.262}$$

thus $W(r) = 1/kr^2$. Since $p_0(x) = 1$ [Eq. (18.254)], we write

$$g_l(r,r') = Cj_l(kr) + Dn_l(kr) - \frac{j_l(kr)n_l(kr') - n_l(kr)j_l(kr')}{(1/kr'^2)}, \quad r - r' > 0, \tag{18.263}$$

$$g_l(r,r') = Cj_l(kr) + Dn_l(kr), \quad r - r' < 0. \tag{18.264}$$

For a solution regular at the origin, we set $D = 0$:

$$g_l(r,r') = Cj_l(kr) - \frac{j_l(kr)n_l(kr') - n_l(kr)j_l(kr')}{(1/kr'^2)}, \quad r - r' > 0, \tag{18.265}$$

$$g_l(r,r') = Cj_l(kr), \quad r - r' < 0. \tag{18.266}$$

To determine the remaining constant, we demand that as $r \to \infty$, we have a spherically outgoing wave, that is,

$$\lim_{r\to\infty} g_l(r,r') \to \frac{e^{ikr}}{r}. \tag{18.267}$$

This implies the relation

$$\frac{kr'^2 j_l(kr')}{[C - kr'^2 n_l(kr')]} = i, \tag{18.268}$$

which gives $C = -ikr'^2 h^{(1)}(kr')$. Substituting this into the expression for the Green's function [Eqs. (18.265) and (18.266)], we obtain, after some algebra,

$$g_l(r,r') = -ikr'^2 h_l^{(1)}(kr) j_l(kr'), \quad r - r' > 0, \tag{18.269}$$

$$g_l(r,r') = -ikr'^2 h_l^{(1)}(kr') j_l(kr), \quad r - r' < 0. \tag{18.270}$$

We usually write this as

$$g_l(r,r') = -ikr'^2 h_l^{(1)}(kr_>) j_l(kr_<). \tag{18.271}$$

In Section 18.2.4, using Fourier transforms, we have solved the Helmholtz equation:

$$\vec{\nabla}^2 \Psi(\vec{r}) + k^2 \Psi(\vec{r}) = F(\vec{r}), \quad r \in [0,\infty] \tag{18.272}$$

as

$$\Psi(\vec{r}) = \xi(\vec{r}) + \int d\vec{r}\, G(\vec{r}, \vec{r}')F(\vec{r}'), \tag{18.273}$$

where $\xi(\vec{r})$ is the solution of the homogeneous equation $\vec{\nabla}^2\Psi(\vec{r}) + k^2\Psi(\vec{r}) = 0$ and the Green's function $G(\vec{r}, \vec{r}')$ is given as

$$G(\vec{r}, \vec{r}') = -\frac{1}{4\pi}\frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|}. \tag{18.274}$$

We now expand $F(\vec{r}')$ as $F(\vec{r}') = \sum_{l,m} F_l(r')Y_{lm}(\theta', \phi')$, where the angular part is separated and then expanded in terms of spherical harmonics. Since $G(\vec{r}, \vec{r}')$ depends only on $|\vec{r} - \vec{r}'|$, we can write its expansion as

$$G(\vec{r}, \vec{r}') = \sum_{l''=0}^{\infty} C_{l''}(r, r')P_{l''}(\cos\theta_{12}), \tag{18.275}$$

where θ_{12} is the angle between $\vec{r}$ and $\vec{r}'$. Using the addition theorem of spherical harmonics [Eq. (10.360)]:

$$\sum_{m=-l}^{m=l} Y^*_{lm}(\theta_1, \phi_1)Y_{lm}(\theta_2, \phi_2) = \frac{2l+1}{4\pi}P_l(\cos\theta_{12}), \tag{18.276}$$

we can write this as

$$G(\vec{r}, \vec{r}') = \sum_{l''=0}^{\infty} C_{l''}(r, r') \sum_{m''=-l''}^{l''} \frac{4\pi}{(2l''+1)} Y^*_{l''m''}(\theta', \phi')Y_{l''m''}(\theta, \phi), \tag{18.277}$$

which allows us to write the solution as

$$\Psi(\vec{r}) = \xi(\vec{r}) + \left[\int_0^{2\pi}\int_0^{\pi} d\Omega' \int_0^{\infty} dr'\, r'^2 \right. \tag{18.278}$$

$$\left. \times \sum_{l'',m'',l,m} \frac{4\pi}{(2l''+1)} C_{l''}(r, r')Y^*_{l''m''}(\theta', \phi')F_l(r')Y_{lm}(\theta', \phi')\right] Y_{l''m''}(\theta, \phi).$$

We can also expand the solution $\Psi(\vec{r})$ and $\xi(\vec{r})$ to write

$$\sum_{l,m} R_l(kr)Y_{lm}(\theta, \phi) = \sum_{l,m} \xi(r)Y_{lm}(\theta, \phi) \tag{18.279}$$

$$+ \sum_{l,m} \left[\frac{4\pi}{(2l+1)}\int_0^{\infty} dr'\, r'^2 C_l(r, r')F_l(r')\right] Y_{lm}(\theta, \phi),$$

where the orthogonality relation, $\int_0^{2\pi} d\varphi \int_0^{\pi} d\theta \sin\theta Y^{m'*}_{l'}(\theta, \phi)Y^m_l(\theta, \phi) = \delta^{m'}_m \delta^{l'}_l$, of spherical harmonics [Eq. (1.201)] have been used. Comparing both sides of Eq. (18.279) gives

$$R_l(kr) = \xi(r) + \frac{4\pi}{(2l+1)} \int_0^\infty dr' \ r'^2 C_l(r,r') F_l(r'). \tag{18.280}$$

To get the relation between $C_l(r,r')$ and $g_l(r,r')$, we now compare this with

$$R_l(kr) = \xi(r) + \int_0^\infty dr' g_l(r,r') F_l(r') \tag{18.281}$$

to get

$$\frac{4\pi}{(2l+1)} r'^2 C_l(r,r') = g_l(r,r'). \tag{18.282}$$

Using Eq. (18.271), this becomes

$$\frac{4\pi}{(2l+1)} r'^2 C_l(r,r') = -ikr'^2 h_l^{(1)}(kr_>) j_l(kr_<). \tag{18.283}$$

Finally, substituting this into Eq. (18.280) and with Eqs. (18.274) and (18.277), we obtain a formula extremely useful in applications:

$$\boxed{-\frac{1}{4\pi}\frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} = -ik \sum_{l=0}^{\infty} h_l^{(1)}(kr_>) j_l(kr_<) \sum_{m=-l}^{l} Y_{lm}^*(\theta',\phi') Y_{lm}(\theta,\phi).} \tag{18.284}$$

18.2.7 Diffraction from a Circular Aperture

In the previous problems, we have considered the entire space. If there are some black surfaces that restrict the region available to us, we use the formula [Eq. (18.248)]:

$$\Psi(\vec{r}) = \int_V d\vec{r}' G(\vec{r},\vec{r}') F(\vec{r}') + \sum_{i=1}^{k} \int ds_i' \, \hat{\mathbf{n}}_i' \cdot [\Psi(\vec{r}')\vec{\nabla}' G(\vec{r},\vec{r}') - G(\vec{r},\vec{r}')\vec{\nabla}'\Psi(\vec{r}')]. \tag{18.285}$$

Let us now apply this formula to diffraction from a circular aperture, where a plane wave, $\Psi(\vec{r}) = Ae^{ikz}$, moving in the z-direction is incident upon a screen lying in the xy-plane with a circular aperture. Our region of integration is the inside of the hemisphere as the radius R goes to infinity (Figure 18.8). The surfaces that bound our region are the screen S which lies in the xy-plane and which has a circular aperture of radius a, and the surface of the hemisphere

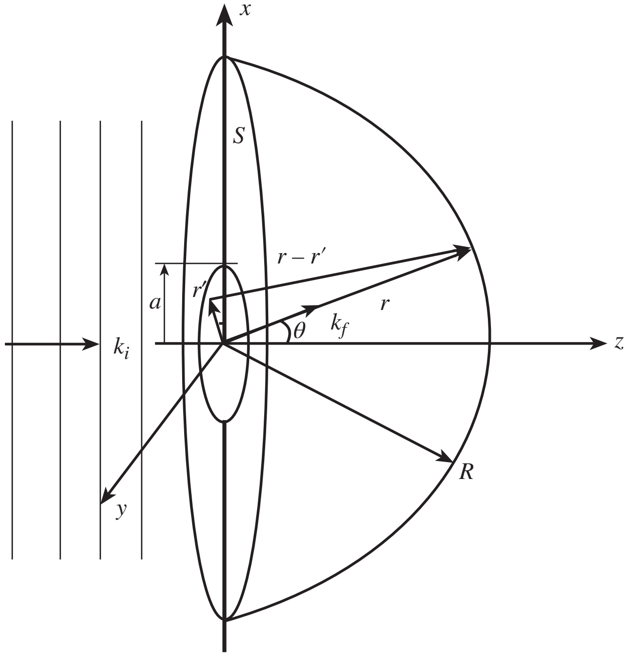

Figure 18.8 Diffraction from a circular aperture.

as $R \to \infty$. Inside the hemisphere, there are no sources, $F(\overrightarrow{r}') = 0$; hence, the Green's function in this region is

$$G(\overrightarrow{r}, \overrightarrow{r}') = -\frac{1}{4\pi}\frac{e^{ik|\overrightarrow{r}-\overrightarrow{r}'|}}{|\overrightarrow{r}-\overrightarrow{r}'|}. \tag{18.286}$$

The solution is now written entirely in terms of surface integrals as

$$\begin{aligned}\Psi(\overrightarrow{r}) = &\int_{xy\text{-plane}} ds'\ \hat{\mathbf{e}}_z \cdot [\Psi(\overrightarrow{r}')\overrightarrow{\nabla}' G(\overrightarrow{r}, \overrightarrow{r}') - G(\overrightarrow{r}, \overrightarrow{r}')\overrightarrow{\nabla}'\Psi(\overrightarrow{r}')] \\ &+ \int_{R\to\infty} ds'\ \hat{\mathbf{e}}_r \cdot [\Psi(\overrightarrow{r}')\overrightarrow{\nabla}' G(\overrightarrow{r}, \overrightarrow{r}') - G(\overrightarrow{r}, \overrightarrow{r}')\overrightarrow{\nabla}'\Psi(\overrightarrow{r}')],\end{aligned} \tag{18.287}$$

where $\overrightarrow{r}'$ is a vector on the aperture. We use $\overrightarrow{k}_i$ to denote wave vector of the incident plane wave moving in the direction of $\hat{\mathbf{e}}_z$, and use $\overrightarrow{k}_f$ for the diffracted wave propagating in the direction of $\overrightarrow{r}$. Both vectors have the same magnitude: $|\overrightarrow{k}_i| = |\overrightarrow{k}_f| = k$. We impose the following boundary conditions: On the hemisphere and in the limit as R goes to infinity, we have an outgoing spherical wave,

$\Psi(\overrightarrow{r}) \rightarrow^{r\rightarrow\infty} f(\theta,\phi)\frac{e^{ikr}}{r}$. On the **screen**, we have

$$\Psi(\overrightarrow{r})|_{z=0} = 0, \tag{18.288}$$

$$\overrightarrow{\nabla}\Psi(\overrightarrow{r})|_{z=0} = 0, \tag{18.289}$$

and on the **aperture**:

$$\Psi = Ae^{ikz'}|_{z'=0} = A, \tag{18.290}$$

$$\frac{d\Psi}{dz'} = Aike^{ikz'}|_{z'=0} = Aik. \tag{18.291}$$

Let us first look at the integral over the hemisphere, which we can write as

$$\iint_{R\rightarrow\infty} r'^2\, d\Omega' f(\theta',\phi') \left[\frac{e^{ikr'}}{r'}\frac{\partial}{\partial r'}\left(-\frac{1}{4\pi}\frac{e^{ik|\overrightarrow{r}-\overrightarrow{r}'|}}{|\overrightarrow{r}-\overrightarrow{r}'|}\right) + \frac{1}{4\pi}\frac{e^{ik|\overrightarrow{r}-\overrightarrow{r}'|}}{|\overrightarrow{r}-\overrightarrow{r}'|}\frac{\partial}{\partial r'}\left(\frac{e^{ikr'}}{r'}\right)\right]. \tag{18.292}$$

In the limit as $R \rightarrow \infty$, the quantity inside the square brackets goes to zero as $1/r'^3$; hence, the above integral goes to zero as $1/r'$. This leaves us with the first term in Eq. (18.287):

$$\Psi(\overrightarrow{r}) = \int_{xy\text{-plane}} ds'\ \hat{\mathbf{e}}_n \cdot [\Psi(\overrightarrow{r}')\overrightarrow{\nabla}' G(\overrightarrow{r},\overrightarrow{r}') - G(\overrightarrow{r},\overrightarrow{r}')\overrightarrow{\nabla}'\Psi(\overrightarrow{r}')]. \tag{18.293}$$

From the boundary conditions on the screen [Eqs. (18.288) and (18.289)], we see that the only contribution to this integral comes from the aperture, where the boundary conditions are given by Eqs. (18.290) and (18.291); hence, we write

$$\Psi(\overrightarrow{r}) = -\int_{\text{Aperture}} ds'\ A\left[\frac{\partial}{\partial z'}\left(-\frac{1}{4\pi}\frac{e^{ik|\overrightarrow{r}-\overrightarrow{r}'|}}{|\overrightarrow{r}-\overrightarrow{r}'|}\right) - ik\left(-\frac{1}{4\pi}\frac{e^{ik|\overrightarrow{r}-\overrightarrow{r}'|}}{|\overrightarrow{r}-\overrightarrow{r}'|}\right)\right]. \tag{18.294}$$

The extra **minus sign** in front of the integral comes from the fact that the outward normal to the aperture is in the **negative** z direction. Let

$$\overrightarrow{R} = \overrightarrow{r} - \overrightarrow{r}' = (X,Y,Z);\quad X = x - x',\quad Y = y - y',\quad Z = z - z', \tag{18.295}$$

thus

$$\Psi(\vec{r}) = -\frac{A}{4\pi}\int_{\text{Aperture}} ds' \left[-\frac{\partial}{\partial z'}\left(\frac{e^{ikR}}{R}\right) + ik\frac{e^{ikR}}{R}\right] \tag{18.296}$$

$$= -\frac{A}{4\pi}\int_{\text{Aperture}} ds' \left[-\frac{d}{dR}\left(\frac{e^{ikR}}{R}\right)\frac{\partial R}{\partial z'} + ik\frac{e^{ikR}}{R}\right] \tag{18.297}$$

$$= -\frac{A}{4\pi}\int_{\text{Aperture}} ds' \left[-\left(\frac{ike^{ikR}}{R} - \frac{e^{ikR}}{R^2}\right)\left(-\frac{Z}{R}\right) + ik\frac{e^{ikR}}{R}\right]. \tag{18.298}$$

We now write $|\vec{r} - \vec{r}'|$ as

$$|\vec{r} - \vec{r}'|^2 = (\vec{r} - \vec{r}')\cdot(\vec{r} - \vec{r}') = r^2 + r'^2 - 2\vec{r}\cdot\vec{r}' \tag{18.299}$$

$$= r^2\left(1 - 2\frac{\vec{r}}{r}\cdot\frac{\vec{r}'}{r} + \frac{r'^2}{r^2}\right), \tag{18.300}$$

hence

$$R = |\vec{r} - \vec{r}'| = r\left(1 - 2\frac{\vec{r}}{r}\cdot\frac{\vec{r}'}{r} + \frac{r'^2}{r^2}\right)^{1/2}. \tag{18.301}$$

For $\frac{r'}{r} \ll 1$, we use the approximation $|\vec{r} - \vec{r}'| \simeq 1 - \hat{\mathbf{n}}\cdot\frac{\vec{r}'}{r} + 0(1/r^2)$, where $\hat{\mathbf{n}}$ is a unit vector in the direction of $\vec{r}$. For large r, we also use the approximation $\frac{Z}{R} \simeq \frac{z}{R} = \cos\theta$, to write the solution as

$$\Psi(\vec{r}) \simeq -\frac{Aik}{4\pi}\int_{\text{Aperture}} ds' \left[(\cos\theta + 1)\frac{e^{ikr\left(1-\hat{\mathbf{n}}\cdot\frac{\vec{r}'}{r}\right)}}{r} + 0\left(\frac{1}{r^2}\right)\right] \tag{18.302}$$

$$\simeq -\frac{Aik}{4\pi}\int_{\text{Aperture}} ds' \left[(\cos\theta + 1)\frac{e^{ikr}}{r}e^{-ik\hat{\mathbf{n}}\cdot\vec{r}'}\right] \tag{18.303}$$

$$\simeq -\frac{Aik}{4\pi}\int_{\text{Aperture}} ds' \left[(\cos\theta + 1)\frac{e^{ikr}}{r}e^{-i\vec{k}_f\cdot\vec{r}'}\right], \tag{18.304}$$

where $\vec{k}_f$ is in the direction of $\vec{r}$. For a circular aperture, we can write this integral as

$$\Psi(\vec{r}) \simeq -\frac{ikA}{4\pi}(\cos\theta + 1)\frac{e^{ikr}}{r}\left[\int_0^{2\pi} d\phi' \int_0^a dr'\ r'e^{-i\vec{k}_f\cdot\vec{r}'}\right]. \tag{18.305}$$

To evaluate this integral, we have to find the cosine of the angle between $\vec{k}_f$ and $\vec{r}'$. The angular coordinates of $\vec{r}$ and $\vec{r}'$ are given by (θ, ϕ) and

(θ', ϕ'), respectively. Using the trigonometric relation $\cos\gamma = \cos\theta\cos\theta' + \sin\theta\sin\theta'\cos(\phi - \phi')$, where γ is the angle between the two vectors, $\overrightarrow{r}$ and $\overrightarrow{r}'$, and since $\overrightarrow{r}'$ is a vector on the aperture, $\theta' = \pi/2$, we get $\cos\gamma = \sin\theta\cos(\phi - \phi')$. Equation (18.305) now becomes

$$\Psi(\overrightarrow{r}) \simeq -\frac{ikA}{4\pi}\frac{e^{ikr}}{r}(\cos\theta + 1)\left[\int_0^{2\pi} d\phi' \int_0^a dr'\ r' e^{-ikr'\cos\gamma}\right] \tag{18.306}$$

$$\simeq -\frac{ikA}{4\pi}\frac{e^{ikr}}{r}(\cos\theta + 1)\left[\int_0^{2\pi} d\phi' \int_0^a dr'\ r' e^{-ikr'\sin\theta\cos(\phi-\phi')}\right]. \tag{18.307}$$

We define two new variables, $x = kr'\sin\theta$ and $\beta = \phi - \phi'$, to write the above integrals as

$$\Psi(\overrightarrow{r}) \simeq -\frac{ikA}{2}\left(\frac{e^{ikr}}{r}\right)\frac{(\cos\theta + 1)}{k^2\sin^2\theta}\left[\frac{1}{2\pi}\int_0^{ka\sin\theta} dx\, x \int_0^{2\pi} d\beta\ e^{-ix\cos\beta}\right]. \tag{18.308}$$

We now concentrate on the integral:

$$I = \int_0^{ka\sin\theta} dx\, x \left[\frac{1}{2\pi}\int_0^{2\pi} d\beta\ e^{-ix\cos\beta}\right]. \tag{18.309}$$

Using the integral definition of Bessel functions [Eq. (5.61)]:

$$J_n(x) = \frac{(x/2)^n}{\sqrt{\pi}\Gamma(n + 1/2)}\int_{-1}^{1}(1 - t^2)^{n-\frac{1}{2}}\cos xtdt, \quad n > -\frac{1}{2}, \tag{18.310}$$

we can show that the expression inside the square brackets [Eq. (18.309)] is nothing but $J_0(x)$, hence $I = \int_0^{ka\sin\theta} dx\ xJ_0(x)$. Using the recursion relation [Eq. (5.64)], $J_{m-1}(x) = \frac{m}{x}J_m(x) + J'_m(x)$, we write $xJ_0(x) = \frac{d}{dx}[xJ_1(x)]$ and evaluate the final integral in I to get $I = ka\sin\theta J_1(ka\sin\theta)$. Substituting this into Eq. (18.308) gives us the solution as

$$\Psi(\overrightarrow{r}) \simeq -\frac{iAa}{2}\left(\frac{e^{ikr}}{r}\right)\frac{(\cos\theta + 1)}{\sin\theta}J_1(ka\sin\theta). \tag{18.311}$$

Since the intensity is $|\Psi(r)|^2 r^2$, we obtain

$$\boxed{\text{Intensity} = \frac{A^2a^2(\cos\theta + 1)^2}{4r^2\sin^2\theta}J_1^2(ka\sin\theta).} \tag{18.312}$$

Problems in diffraction theory are usually very difficult and exact solutions are quite rare. For a detailed treatment of the subject, we refer the reader to *Classical Electrodynamics* by Jackson [4].

18.3 Time-Independent Perturbation Theory

18.3.1 Nondegenerate Perturbation Theory

We now consider the following problem:

$$\{\pounds_0 + \lambda\}\Psi(x) = \varepsilon h(x)\Psi(x), \tag{18.313}$$

where $\pounds_0$ is an exactly solvable Sturm–Liouville operator and ε is a small parameter that allows us to keep track of the order of the terms in our equations. In the limit as $\varepsilon \to 0$ and assuming that $h(x)$ is bounded, the solution $\Psi(x)$ and the parameter λ reduce to the exact eigenfunctions $\Phi_n(x)$ and the exact eigenvalues λ_n of the unperturbed operator $\pounds_0$:

$$\{\pounds_0 + \lambda_n\}\Phi_n(x) = 0. \tag{18.314}$$

As $\varepsilon \to 0$,

$$\Psi(x) \to \Psi^{(0)}(x) = \Phi_n(x), \tag{18.315}$$

$$\lambda \to \lambda_n. \tag{18.316}$$

We now write the perturbed eigenvalues as $\lambda = \lambda_n + \Delta\lambda$, thus Eq. (18.313) becomes

$$\{\pounds_0 + \lambda_n\}\Psi(x) = [\varepsilon h(x) - \Delta\lambda]\Psi(x) = f(x, \Psi(x)), \tag{18.317}$$

Since the eigenfunctions of the unperturbed operator $\pounds_0$ form a complete and orthonormal set, $\int_a^b dx\, \Phi_n(x)\Phi_m(x) = \delta_{nm}$, we can write the expansions

$$f(x) = \sum_k c_k\Phi_k(x), \quad c_k = \int_a^b dx'\Phi_k^*(x')f(x'), \tag{18.318}$$

and

$$\Psi(x) = \sum_k a_k\Phi_k(x), \quad a_k = \int_a^b dx'\Phi_k^*(x')\Psi(x'). \tag{18.319}$$

Using these in Eq. (18.317):

$$\sum_k a_k(\lambda_n - \lambda_k)\Phi_k = \sum_k c_k\Phi_k, \tag{18.320}$$

we obtain

$$a_k = \frac{c_k}{(\lambda_n - \lambda_k)}. \tag{18.321}$$

When $n = k$, we insist that $c_k = 0$. We now substitute a_k [Eq. (18.321)] and c_k [Eq. (18.318)] into the expansion of $\Psi(x)$ [Eq. (18.319)] to get

$$\Psi(x) = \sum_k \frac{1}{(\lambda_n - \lambda_k)} \int_a^b dx'\Phi_k^*(x')\Phi_k(x)f(x'), \tag{18.322}$$

which after rearranging becomes

$$\Psi(x) = \int_a^b dx' \left[\sum_k \frac{\Phi_k(x)\Phi_k^*(x')}{(\lambda_n - \lambda_k)} \right] [\varepsilon h(x') - \Delta\lambda]\Psi(x'). \tag{18.323}$$

The quantity inside the square brackets is the **Green's function**:

$$\boxed{G(x, x') = \left[\sum_k \frac{\Phi_k(x)\Phi_k^*(x')}{(\lambda_n - \lambda_k)} \right].} \tag{18.324}$$

For the general solution of the differential equation [Eq. (18.317)], we also add the solution of the homogeneous equation, that is, the unperturbed solution, to write

$$\Psi(x) = \Phi_n(x) + \int_a^b dx' \left[\sum_k \frac{\Phi_k(x)\Phi_k^*(x')}{(\lambda_n - \lambda_k)} \right] [\varepsilon h(x') - \Delta\lambda]\Psi(x'). \tag{18.325}$$

Comparing with

$$\Psi(x) = \Phi_n(x) + \int_a^b dx' K(x, x')\Psi(x'), \tag{18.326}$$

we obtain the **kernel** as

$$K(x, x') = G(x, x')[\varepsilon h(x') - \Delta\lambda]. \tag{18.327}$$

This is an integral equation, where the unknown $\Psi(x)$ appears on both sides of the equation. To obtain the perturbed solution in terms of known quantities, we expand $\Psi(x)$ and $\Delta\lambda$ in terms of the small parameter ε as

$$\Psi(x) = \Phi_n(x) + \varepsilon\Psi^{(1)}(x) + \varepsilon^2\Psi^{(2)}(x) + \cdots , \tag{18.328}$$

$$\lambda = \lambda_n + \varepsilon[\Delta\lambda^{(1)} + \varepsilon\Delta\lambda^{(2)} + \varepsilon^2\Delta\lambda^{(3)} + \cdots], \tag{18.329}$$

which gives

$$\Delta\lambda = \varepsilon[\Delta\lambda^{(1)} + \varepsilon\Delta\lambda^{(2)} + \varepsilon^2\Delta\lambda^{(3)} + \cdots]. \tag{18.330}$$

We now substitute these expansions into Eq. (18.325) and simplify:

$$\Psi(x) = \Phi_n(x) + \int_a^b dx' \left[\sum_k \frac{\Phi_k(x)\Phi_k^*(x')}{(\lambda_n - \lambda_k)} \right] \times \left[(\varepsilon h(x') - \varepsilon \Delta\lambda^{(1)}) - \varepsilon^2 \Delta\lambda^{(2)} + \cdots \right] \times \left[\Phi_n(x') + \varepsilon \Psi^{(1)}(x') + \varepsilon^2 \Psi^{(2)}(x') + \cdots \right], \tag{18.331}$$

$$\Psi(x) = \Phi_n(x) + \varepsilon \int_a^b dx' \left[\sum_k \frac{\Phi_k(x)\Phi_k^*(x')}{(\lambda_n - \lambda_k)} \right] \times \left[(h(x') - \Delta\lambda^{(1)}) - \varepsilon \Delta\lambda^{(2)} + \cdots \right] \times \left[\Phi_n(x') + \varepsilon \Psi^{(1)}(x') + \varepsilon^2 \Psi^{(2)}(x') + \cdots \right], \tag{18.332}$$

$$\Psi(x) = \Phi_n(x) + \varepsilon \int_a^b dx' \left[\sum_k \frac{\Phi_k(x)\Phi_k^*(x')}{(\lambda_n - \lambda_k)} \right] [h(x') - \Delta\lambda^{(1)}]\Phi_n(x') + \varepsilon \int_a^b dx' \left[\sum_j \frac{\Phi_j(x)\Phi_j^*(x')}{(\lambda_n - \lambda_j)} \right] \times [-\varepsilon \Delta\lambda^{(2)}\Phi_n(x') + (h(x') - \Delta\lambda^{(1)})\varepsilon \Psi^{(1)}(x')] + 0(\varepsilon^3). \tag{18.333}$$

Collecting terms with equal powers of ε, we get

$$\Psi(x) = \Phi_n(x) + \varepsilon \int_a^b dx' \left[\sum_k \frac{\Phi_k(x)\Phi_k^*(x')}{(\lambda_n - \lambda_k)} \right] [h(x') - \Delta\lambda^{(1)}]\Phi_n(x') + \varepsilon^2 \int_a^b dx' \left[\sum_j \frac{\Phi_j(x)\Phi_j^*(x')}{(\lambda_n - \lambda_j)} \right] \times [-\Delta\lambda^{(2)}\Phi_n(x') + (h(x') - \Delta\lambda^{(1)})\Psi^{(1)}(x')] + 0(\varepsilon^3). \tag{18.334}$$

Comparing the right-hand side with the expansion of the left-hand side, $\Psi(x) = \Psi^{(0)}(x) + \varepsilon \Psi^{(1)}(x) + \varepsilon^2 \Psi^{(2)}(x) + \cdots$, we obtain

$$\Psi^{(0)}(x) = \Phi_n(x), \tag{18.335}$$

$$\Psi^{(1)}(x) = \int_a^b dx' \left[\sum_k \frac{\Phi_k(x)\Phi_k^*(x')}{(\lambda_n - \lambda_k)} \right] [h(x') - \Delta\lambda^{(1)}]\Phi_n(x'), \tag{18.336}$$

$$\Psi^{(2)}(x) = \int_a^b dx' \sum_j \left[\frac{\Phi_j(x)\Phi_j^*(x')}{(\lambda_n - \lambda_j)} \right] \times [-\Delta\lambda^{(2)}\Phi_n(x') + (h(x') - \Delta\lambda^{(1)})\Psi^{(1)}(x')], \tag{18.337}$$

$$\vdots$$

In the first-order term [Eq. (18.336)], the numerator has to vanish for $k = n$, thus

$$\Phi_n(x)\int_a^b dx'\Phi_n^*(x')[h(x') - \Delta\lambda^{(1)}]\Phi_n(x') = 0, \tag{18.338}$$

$$\Phi_n(x)\int_a^b dx'\Phi_n^*(x')h(x')\Phi_n(x') = \Phi_n(x)\Delta\lambda^{(1)}\int_a^b dx'\Phi_n^*(x')\Phi_n(x'), \tag{18.339}$$

$$\int_a^b dx'\Phi_n^*(x')h(x')\Phi_n(x') = \Delta\lambda^{(1)}\int_a^b dx'\Phi_n^*(x')\Phi_n(x'). \tag{18.340}$$

Using the orthogonality relation:

$$\int_a^b dx'\Phi_k^*(x')\Phi_n(x') = \delta_{kn}, \tag{18.341}$$

we obtain the **first-order** correction to the nth eigenvalue λ_n as

$$\boxed{\Delta\lambda^{(1)} = h_{nn} = \int_a^b dx'\Phi_n^*(x')h(x')\Phi_n(x').} \tag{18.342}$$

We can now write the first-order correction to the eigenfunction as

$$\Psi^{(1)}(x) = \sum_{k\neq n}\int_a^b dx'\frac{\Phi_k(x)\Phi_k^*(x')}{(\lambda_n - \lambda_k)}\left[h(x') - \Delta\lambda^{(1)}\right]\Phi_n(x') \tag{18.343}$$

$$= \sum_{k\neq n}\frac{\Phi_k(x)}{(\lambda_n - \lambda_k)} \tag{18.344}$$

$$\times\left[\int_a^b dx'\Phi_k^*(x')h(x')\Phi_n(x') - \Delta\lambda^{(1)}\int_a^b dx'\Phi_k^*(x')\Phi_n(x')\right].$$

We again use the orthogonality relation [Eq. (18.341)] to write

$$\boxed{\Psi^{(1)}(x) = \sum_{k\neq n}\frac{\Phi_k(x)\quad h_{kn}}{(\lambda_n - \lambda_k)},} \tag{18.345}$$

where h_{kn} is the Hermitian matrix

$$\boxed{h_{kn} = \int_a^b dx'\Phi_k^*(x')h(x')\Phi_n(x').} \tag{18.346}$$

Let us now turn to the **second-order** term. Substituting $\Psi^{(1)}(x)$ [Eq. (18.345)] into $\Psi^{(2)}(x)$ [Eq. (18.337)]:

$$\Psi^{(2)}(x) = \int_a^b dx' \left[\sum_j \frac{\Phi_j(x)\Phi_j^*(x')}{(\lambda_n - \lambda_j)} \right] \times [-\Delta\lambda^{(2)}\Phi_n(x') + (h(x') - \Delta\lambda^{(1)})\Psi^{(1)}(x')], \tag{18.347}$$

we obtain

$$\Psi^{(2)}(x) = \int_a^b dx' \left[\sum_j \frac{\Phi_j(x)\Phi_j^*(x')}{(\lambda_n - \lambda_j)} \right] \times \left[-\Delta\lambda^{(2)}\Phi_n(x') + (h(x') - \Delta\lambda^{(1)}) \sum_{k\neq n} \frac{\Phi_k(x')\ h_{kn}}{(\lambda_n - \lambda_k)} \right], \tag{18.348}$$

which also becomes

$$\Psi^{(2)}(x) = \sum_j \frac{\Phi_j(x)}{(\lambda_n - \lambda_j)} \left[\int_a^b dx'\Phi_j^*(x')(-\Delta\lambda^{(2)})\Phi_n(x') + \int_a^b dx'\Phi_j^*(x')[h(x') - \Delta\lambda^{(1)}] \sum_{k\neq n} \frac{\Phi_k(x')h_{kn}}{(\lambda_n - \lambda_k)} \right], \tag{18.349}$$

where $h_{kn} = \int_a^b dx''\Phi_k^*(x'')h(x'')\Phi_n(x'')$. For $j = n$, we again set the numerator to zero:

$$\int_a^b dx'\Phi_n^*(x')\Delta\lambda^{(2)}\Phi_n(x') = \int_a^b dx'\Phi_n^*(x')[h(x') - \Delta\lambda^{(1)}] \sum_{k\neq n} \frac{\Phi_k(x')h_{kn}}{(\lambda_n - \lambda_k)}, \tag{18.350}$$

$$\Delta\lambda^{(2)} \int_a^b dx'\Phi_n^*(x')\Phi_n(x') = \sum_{k\neq n} \left[\frac{\left[\int_a^b dx'\Phi_n^*(x')h(x')\Phi_k(x')\right] h_{kn}}{(\lambda_n - \lambda_k)} - \Delta\lambda^{(1)} \frac{\left[\int_a^b dx'\Phi_n^*(x')\Phi_k(x')\right] h_{kn}}{(\lambda_n - \lambda_k)} \right]. \tag{18.351}$$

Using the orthogonality relation [Eq. (18.341)], we obtain

$$\boxed{\Delta\lambda^{(2)} = \sum_{k\neq n} \frac{h_{nk}h_{kn}}{(\lambda_n - \lambda_k)}.} \tag{18.352}$$

Substituting this in Eq. (18.337), we obtain $\Psi^{(2)}(x)$ as

$$\Psi^{(2)}(x) = \sum_{j\neq n} \frac{\Phi_j(x)}{(\lambda_n - \lambda_j)} \left[(-\Delta\lambda^{(2)}) \int_a^b dx' \Phi_j^*(x') \;\; \Phi_n(x') \right.$$
$$+ \sum_{k\neq n} \frac{\left[\int_a^b dx' \Phi_j^*(x') h(x') \Phi_k(x')\right] \quad h_{kn}}{(\lambda_n - \lambda_k)}$$
$$\left. -(\Delta\lambda^{(1)}) \int_a^b dx' \Phi_j^*(x') \Phi_k(x') \sum_{k\neq n} \frac{h_{kn}}{(\lambda_n - \lambda_k)} \right]. \tag{18.353}$$

Using the orthogonality relation [Eq. (18.341)], this also becomes

$$\Psi^{(2)}(x) = \sum_{j\neq n} \frac{\Phi_j(x)}{(\lambda_n - \lambda_j)} [(-\Delta\lambda^{(2)})\delta_{jn}$$
$$\left. + \sum_{k\neq n} \frac{h_{jk} \;\; h_{kn}}{(\lambda_n - \lambda_k)} - (\Delta\lambda^{(1)})\delta_{jk} \sum_{k\neq n} \frac{h_{kn}}{(\lambda_n - \lambda_k)} \right]. \tag{18.354}$$

Finally, using $\Delta\lambda^{(1)} = h_{nn}$, we obtain

$$\boxed{\Psi^{(2)}(x) = \sum_{j\neq n} \Phi_j(x) \left[\sum_{k\neq n} \frac{[h_{jk} - \delta_{jk} h_{nn}] \;\; h_{kn}}{(\lambda_n - \lambda_j)(\lambda_n - \lambda_k)} \right].} \tag{18.355}$$

18.3.2 Slightly Anharmonic Oscillator in One Dimension

We now consider the slightly anharmonic oscillator problem in quantum mechanics with the potential

$$V(x) = \frac{1}{2} k_2 x^2 - k_3 x^3, \tag{18.356}$$

where k_2 and k_3 are constants such that $k_3 \ll k_1$. We have already solved the Schrödinger equation for the harmonic oscillator potential, $V(x) = \frac{1}{2} k_2 x^2$, in Chapter 3 that leads to the eigenvalue equation $d^2\Psi_n/dx^2 - x^2\Psi_n + \epsilon\Psi_n(x) = 0$, where $x = x_{\text{physical}}/\sqrt{\hbar/m\omega}$, $\epsilon = E/\hbar\omega/2$. We rewrite the exactly solvable case as

$$£_0 \Phi_n + \epsilon_n \Phi_n(x) = 0, \quad £_0 = \frac{d^2}{dx^2} - x^2, \tag{18.357}$$

where the solution is given in terms of the Hermite polynomials [Eq. (3.35)]:

$$\Phi_n(x) = \frac{e^{-x^2/2} H_n(x)}{\sqrt{2^n n! \sqrt{\pi}}}, \quad n = 0, 1, \ldots \;. \tag{18.358}$$

We are now looking for the solution of the slightly anharmonic oscillator that satisfies the equation

$$(\pounds_0 + \lambda)\Psi(x) = \alpha x^3\Psi, \tag{18.359}$$

where $\alpha \ll 1$. The perturbed energy eigenvalues are written as

$$\lambda = \epsilon_n + \alpha\Delta\lambda^{(1)} + \alpha^2\Delta\lambda^{(2)} + \cdots, \tag{18.360}$$

where $\epsilon_n = 2n + 1$ are the exact eigenvalues. We can easily verify that

$$\Delta\lambda^{(1)} = h_{nn} = \int_{-\infty}^{\infty} dx'\Phi_n^2(x')x'^3 = 0. \tag{18.361}$$

For $\Psi^{(1)}(x)$, we need to evaluate the integral

$$h_{kn} = \int_{-\infty}^{\infty} dx' \frac{e^{-x'^2}H_n(x')x'^3H_k(x')}{\sqrt{2^n n!}\sqrt{2^k k!}\sqrt{\pi}}. \tag{18.362}$$

Using the recursion relation [Eq. (3.27)] $xH_n = \frac{1}{2}H_{n+1} + nH_{n-1}$, we write

$$x^2H_n = \frac{1}{2}\left(\frac{1}{2}H_{n+2} + (n+1)H_n\right) + n\left(\frac{1}{2}H_n + (n-1)H_{n-2}\right), \tag{18.363}$$

$$= \frac{1}{4}H_{n+2} + \frac{2n+1}{2}H_n + n(n-1)H_{n-2}. \tag{18.364}$$

Similarly,

$$x^3H_n = \frac{1}{8}H_{n+3} + \frac{3}{4}(n+1)H_{n+1} + \frac{3}{2}n^2H_{n-1} + n(n-1)(n-2)H_{n-3}. \tag{18.365}$$

Using Eq. (18.365) in Eq. (18.362), along with the orthogonality relation $\int_{-\infty}^{\infty} dxe^{-x^2/2}H_n(x)H_k(x) = 0,\ \ n \neq k,$ we obtain $h_{kn} = 0,$ unless $k = (n+3),$ $(n+1), (n-1), (n-3)$. We evaluate the component $h_{n(n+3)}$ as

$$h_{n(n+3)} = h_{(n+3)n} = \frac{1}{8}\int_{-\infty}^{\infty} dx' e^{-x'^2/2}\frac{H_{n+3}(x')}{\sqrt{2^n n!}}\ \frac{H_{n+3}(x')}{\sqrt{2^{n+3}(n+3)!}\sqrt{\pi}} \tag{18.366}$$

$$= \frac{1}{8}\frac{\sqrt{2^{n+3}(n+3)!}}{\sqrt{2^n n!}}\left\{\int_{-\infty}^{\infty} dx' \frac{e^{-x'^2H_{n+3}^2(x')}}{[\sqrt{2^{n+3}(n+1)!\sqrt{\pi}}]^2}\right\} \tag{18.367}$$

$$= \frac{1}{8}\sqrt{8}\sqrt{\frac{(n+3)!}{n!}} = \sqrt{\frac{(n+3)(n+2)(n+1)}{8}}. \tag{18.368}$$

Similarly, we evaluate the other nonzero components:

$$h_{(n-3)n} = \sqrt{\frac{n(n-1)(n-2)}{8}}, \tag{18.369}$$

$$h_{n(n+1)} = 3(n+1)\sqrt{\frac{n+1}{8}}, \tag{18.370}$$

$$h_{n(n-1)} = 3n\sqrt{\frac{n}{8}}. \tag{18.371}$$

Using these results, we now write

$$\Delta\lambda^{(2)} = \sum_k \frac{h_{nk}h_{kn}}{2(n-k)} \tag{18.372}$$

$$= \frac{\frac{1}{8}(n+3)(n+2)(n+1)}{-6} + \frac{\frac{1}{8}n(n-1)(n-2)}{6} + \frac{9(n+1)^2(n+1)}{-2(8)} + \frac{9n^2n}{2(8)}, \tag{18.373}$$

to obtain λ as

$$\lambda = (2n+1) - \alpha^2\frac{[30n^2+30n+11]}{16} + 0(\alpha^3). \tag{18.374}$$

Similarly, we evaluate the first nonzero term of the perturbed wave function as

$$\Psi(x) = \Phi_n(x) + \alpha\left[\frac{\sqrt{n(n-1)(n-2)}}{12\sqrt{2}}\Phi_{n-3}(x) - \frac{\sqrt{(n+3)(n+2)(n+1)}}{12\sqrt{2}}\Phi_{n+3}(x) + \frac{3n\sqrt{n}}{4\sqrt{2}}\Phi_{n-1}(x) - \frac{3(n+1)\sqrt{n+1}}{4\sqrt{2}}\Phi_{n+1}(x)\right] + 0(\alpha^2). \tag{18.375}$$

18.3.3 Degenerate Perturbation Theory

The preceding formalism works fine as long as the eigenvalues are distinct, that is, $\lambda_i \neq \lambda_j$ when $i \neq j$. In the event that multiple eigenvalues turn out to be equal, the method can still be rescued with a simple procedure. We first remember that the first-order correction to $\Psi(x)$ [Eq. (18.345)] is written as

$$\Psi^{(1)}(x) = \sum_{k\neq n}\Phi_k(x)\left[\frac{h_{kn}(x)}{(\lambda_n-\lambda_k)}\right]. \tag{18.376}$$

In the above series, the expansion coefficients, $[h_{kn}/(\lambda_n-\lambda_k)]$, diverge for the degenerate eigenvalues, where $\lambda_n = \lambda_k$ for $n \neq k$. This would be okay, if somehow the corresponding matrix elements, h_{kn}, $k \neq n$, also vanished. In other words, if the submatrix h_{kn} corresponding to the degenerate eigenvalues is diagonal. From the Sturm–Liouville theory, we know that for Hermitian operators and for distinct eigenvalues, the corresponding eigenfunctions are mutually orthogonal. However, for the degenerate eigenvalues, there is an ambiguity. All vectors that are perpendicular to the eigenvectors corresponding to the distinct eigenvalues are legitimate eigenvectors for the degenerate eigenvalues. For example, if $\lambda_1 = \lambda_2 \neq \lambda_3$, then all vectors that lie on a plane perpendicular to the third eigenvector for λ_3 are good eigenvectors for λ_1 and λ_2. Normally, we would pick any two perpendicular vectors on this plane as the eigenvectors of λ_1 and λ_2, thus obtaining a mutually orthogonal eigenvector set for $(\lambda_1, \lambda_2, \lambda_3)$. In the presence of a perturbation, we use this freedom to find an appropriate orientation for the eigenvectors of λ_1 and λ_2, such that the 2×2 submatrix, $h_{kn} = \int_a^b dx' \Phi_k^*(x') h(x') \Phi_n(x')$, corresponding to the degenerate eigenvalues is diagonal. In other words, perturbation removes the degeneracy and picks a particular orientation for the orthogonal eigenvectors of λ_1 and λ_2 on the plane perpendicular to the third eigenvector corresponding to the distinct eigenvalue. This procedure is called **diagonalization**. For an l-fold degenerate eigenvalue, the corresponding submatrix to be diagonalized is an $l \times l$ square matrix. This procedure, albeit being cumbersome, can be extended to higher order terms in the perturbation expansion and to any number of multiply degenerate eigenvalues.

18.4 First-Order Time-Dependent Green's Functions

We now consider differential equations that could be written as

$$\boxed{H\Psi(\overrightarrow{r}, \tau) + \frac{\partial \Psi(\overrightarrow{r}, \tau)}{\partial \tau} = 0,} \tag{18.377}$$

where τ is a timelike variable and H is a linear differential operator independent of τ with a complete set of orthonormal eigenfunctions. In applications, we frequently encounter differential equations of this type. For the heat transfer equation: $\overrightarrow{\nabla}^2 T(\overrightarrow{r}, t) = (c/k)\frac{\partial T(\overrightarrow{r}, t)}{\partial t}$, where T is temperature, c is specific heat per unit volume, and k is conductivity, we have

$$H = -\overrightarrow{\nabla}^2, \quad \tau = \frac{kt}{c}. \tag{18.378}$$

In quantum mechanics, the Schrödinger equation is written as $H\Psi(\overrightarrow{r}, t) = i\hbar\frac{\partial \Psi(\overrightarrow{r}, t)}{\partial t}$, where H is the Hamiltonian operator. For a particle moving under the influence of a central potential $V(\overrightarrow{r})$, the Hamiltonian operator becomes $H = -(\hbar^2/2m)\overrightarrow{\nabla}^2 + V(\overrightarrow{r})$, hence in Eq. (18.377)

$$H = -\overrightarrow{\nabla}^2 + \frac{2m}{\hbar^2}V(\overrightarrow{r}), \quad \tau = \left(\frac{i\hbar}{2m}\right)t. \tag{18.379}$$

In the diffusion equation: $\overrightarrow{\nabla}^2 \rho = (1/a^2)\frac{\partial \rho}{\partial t}$, where ρ is the density, or concentration, and a is the diffusion coefficient, we have

$$H = -\overrightarrow{\nabla}^2, \quad \tau = a^2 t. \tag{18.380}$$

Since H has a complete and orthonormal set of eigenfunctions, we can write the corresponding eigenvalue equation as

$$\boxed{H\phi_m = \lambda_m \phi_m,} \tag{18.381}$$

where λ_m are the eigenvalues and ϕ_m are the eigenfunctions. We now write the solution of Eq. (18.377) as

$$\boxed{\Psi(\overrightarrow{r}, \tau) = \sum_m A_m(\tau)\phi_m(\overrightarrow{r}),} \tag{18.382}$$

where the time dependence is carried in the expansion coefficients, $A_m(\tau)$. Operating on $\Psi(\overrightarrow{r}, \tau)$ with H and remembering that H is independent of τ, we obtain

$$H\Psi = H\left[\sum_m A_m(\tau)\phi_m(\overrightarrow{r})\right] \tag{18.383}$$

$$= \sum_m A_m(\tau) H\phi_m(\overrightarrow{r}) \tag{18.384}$$

$$= \sum_m \lambda_m A_m(\tau)\phi_m(\overrightarrow{r}). \tag{18.385}$$

Using Eq. (18.385) and the time derivative of Eq. (18.382) in Eq. (18.377), we get

$$\sum_m \left[\lambda_m A_m(\tau) + \frac{dA_m(\tau)}{d\tau}\right] \phi_m(\overrightarrow{r}) = 0. \tag{18.386}$$

Because $\{\phi_m\}$ is a set of linearly independent functions, this equation cannot be satisfied unless all the coefficients of ϕ_m vanish simultaneously, that is,

$$\frac{dA_m(\tau)}{d\tau} + \lambda_m A_m(\tau) = 0, \quad \text{for all } m. \tag{18.387}$$

Solution of this differential equation can be written immediately:

$$A_m(\tau) = A_m(0)e^{-\lambda_m \tau}, \tag{18.388}$$

thus giving $\Psi(\overrightarrow{r},\tau)$ as

$$\Psi(\overrightarrow{r},\tau)=\sum_m A_m(0)\phi_m(\overrightarrow{r})e^{-\lambda_m\tau}. \tag{18.389}$$

To complete the solution, we need an initial condition. Assuming that the solution at $\tau=0$ is given as $\Psi(\overrightarrow{r},0)$, we write

$$\Psi(\overrightarrow{r},0)=\sum_m A_m(0)\phi_m(\overrightarrow{r}). \tag{18.390}$$

Because the eigenfunctions satisfy the **orthogonality relation**:

$$\iiint_V \phi_m^*(\overrightarrow{r})\phi_n(\overrightarrow{r})\,d^3\overrightarrow{r}=\delta_{mn} \tag{18.391}$$

and the **completeness relation**:

$$\sum_m \phi_m^*(\overrightarrow{r}')\phi_m(\overrightarrow{r})=\delta(\overrightarrow{r}-\overrightarrow{r}'), \tag{18.392}$$

we can solve Eq. (18.389) for $A_m(0)$ as

$$A_m(0)=\iiint_V \phi_m^*(\overrightarrow{r}')\Psi(\overrightarrow{r}',0)\,d^3\overrightarrow{r}'. \tag{18.393}$$

Substituting these $A_m(0)$ functions back to Eq. (18.389), we obtain

$$\Psi(\overrightarrow{r},\tau)=\sum_m e^{-\lambda_m\tau}\phi_m(\overrightarrow{r})\iiint_V \phi_m^*(\overrightarrow{r}')\Psi(\overrightarrow{r}',0)\,d^3\overrightarrow{r}'. \tag{18.394}$$

Rearranging this expression as

$$\boxed{\Psi(\overrightarrow{r},\tau)=\iiint_V G_1(\overrightarrow{r},\overrightarrow{r}',\tau)\Psi(\overrightarrow{r}',0)\,d^3\overrightarrow{r}',} \tag{18.395}$$

we obtain a function

$$\boxed{G_1(\overrightarrow{r},\overrightarrow{r}',\tau)=\sum_m e^{-\lambda_m\tau}\phi_m(\overrightarrow{r})\phi_m^*(\overrightarrow{r}'),} \tag{18.396}$$

where the subscript 1 denotes the fact that we have first-order time dependence. Note that $G_1(\overrightarrow{r},\overrightarrow{r}',\tau)$ satisfies the relation

$$G_1(\overrightarrow{r},\overrightarrow{r}',0)=\sum_m \phi_m(\overrightarrow{r})\phi_m^*(\overrightarrow{r}')=\delta^3(\overrightarrow{r}-\overrightarrow{r}') \tag{18.397}$$

and the differential equation

$$\boxed{\left(H+\frac{\partial}{\partial\tau}\right)G_1(\overrightarrow{r},\overrightarrow{r}',\tau)=0.} \tag{18.398}$$

Because $G_1(\overrightarrow{r}, \overrightarrow{r}', \tau)$ does not satisfy the basic equation,

$$\left(H + \frac{\partial}{\partial \tau}\right) G(\overrightarrow{r}, \overrightarrow{r}', \tau) = \delta^3(\overrightarrow{r} - \overrightarrow{r}')\delta(\tau), \tag{18.399}$$

for the Green's functions, it is not yet the Green's function for this problem. However, as we shall see shortly, it is very closely related to it. Note that if we take the initial condition as $\Psi(\overrightarrow{r}, 0) = \delta^3(\overrightarrow{r} - \overrightarrow{r}_0)$, which is called the **point source initial condition**, G_1 becomes the solution of Eq. (18.377): $\Psi(\overrightarrow{r}, \tau) = G_1(\overrightarrow{r}, \overrightarrow{r_0}, \tau)$, $\tau \geq 0$.

18.4.1 Propagators

Because our choice of initial time as $\tau' = 0$ was arbitrary, for a general initial time τ', the $\Psi(\overrightarrow{r}, \tau)$ and the G_1 functions become

$$\Psi(\overrightarrow{r}, \tau) = \iiint G_1(\overrightarrow{r}, \overrightarrow{r}', \tau, \tau')\Psi(\overrightarrow{r}', \tau')\, d^3\overrightarrow{r}', \tag{18.400}$$

$$G_1(\overrightarrow{r}, \overrightarrow{r}', \tau, \tau') = \sum_m e^{-\lambda_m(\tau - \tau')}\phi_m(\overrightarrow{r})\phi_m^*(\overrightarrow{r}'). \tag{18.401}$$

From Eq. (18.400), it is seen that, given the solution at $(\overrightarrow{r}', \tau')$ as $\Psi(\overrightarrow{r}', \tau')$, we can find the solution at a later time, $\Psi(\overrightarrow{r}, \tau > \tau')$, by using $G_1(\overrightarrow{r}, \overrightarrow{r}', \tau, \tau')$. It is for this reason that $G_1(\overrightarrow{r}, \overrightarrow{r}', \tau, \tau')$ is also called the **propagator**. In quantum field theory and perturbation calculations, propagator interpretation of G_1 is very useful in the interpretation of Feynman diagrams.

18.4.2 Compounding Propagators

Given a solution at τ_0, let us propagate it first to $\tau_1 > \tau_0$ and then to $\tau_2 > \tau_1$:

$$\Psi(\overrightarrow{r}, \tau_1) = \int G_1(\overrightarrow{r}, \overrightarrow{r}'', \tau_1, \tau_0)\Psi(\overrightarrow{r}'', \tau_0)\, d^3\overrightarrow{r}'', \tag{18.402}$$

$$\Psi(\overrightarrow{r}, \tau_2) = \int G_1(\overrightarrow{r}, \overrightarrow{r}', \tau_2, \tau_1)\Psi(\overrightarrow{r}', \tau_1)\, d^3\overrightarrow{r}', \tag{18.403}$$

where we used $\int d^3\overrightarrow{r}$ instead of $\iiint d^3\overrightarrow{r}$. Using Eq. (18.402), we can write the second equation as

$$\Psi(\overrightarrow{r}, \tau_2) = \int\int G_1(\overrightarrow{r}, \overrightarrow{r}', \tau_2, \tau_1)G_1(\overrightarrow{r}', \overrightarrow{r}'', \tau_1, \tau_0)\Psi(\overrightarrow{r}'', \tau_0)\, d^3\overrightarrow{r}'\, d^3\overrightarrow{r}''. \tag{18.404}$$

Using the definition of propagator [Eq. (18.401)], we can also write

$$\int G_1(\vec{r},\vec{r}',\tau_2,\tau_1)G_1(\vec{r}',\vec{r}'',\tau_1,\tau_0)\,d^3\vec{r}' \tag{18.405}$$

$$= \int \sum_m e^{-\lambda_m(\tau_2-\tau_1)}\phi_m(\vec{r})\phi_m^*(\vec{r}')\sum_n e^{-\lambda_n(\tau_1-\tau_0)}\phi_n(\vec{r}')\phi_n^*(\vec{r}'')\,d^3\vec{r}'$$

$$= \sum_m e^{-\lambda_m(\tau_2-\tau_1)}\phi_m(\vec{r})\left[\int \phi_m^*(\vec{r}')\phi_n(\vec{r}')d^3\vec{r}'\right]\sum_n e^{-\lambda_n(\tau_1-\tau_0)}\,\phi_n^*(\vec{r}''). \tag{18.406}$$

Using the orthogonality relation, $\int \phi_m^*(\vec{r}')\phi_n(\vec{r}')\,d^3\vec{r}' = \delta_{nm}$, Eq. (18.406) becomes

$$\int G_1(\vec{r},\vec{r}',\tau_2,\tau_1)G_1(\vec{r}',\vec{r}'',\tau_1,\tau_0)\,d^3\vec{r}' \tag{18.407}$$

$$= \sum_m e^{-\lambda_m(\tau_2-\tau_1)}\phi_m(\vec{r})\phi_m^*(\vec{r}'')e^{-\lambda_m(\tau_1-\tau_0)} \tag{18.408}$$

$$= \sum_m \phi_m(\vec{r})\phi_m^*(\vec{r}'')e^{-\lambda_m(\tau_2-\tau_0)} \tag{18.409}$$

$$= G_1(\vec{r},\vec{r}'',\tau_2,\tau_0). \tag{18.410}$$

Using this in Eq. (18.404), we obtain the propagator, $G_1(\vec{r},\vec{r}'',\tau_2,\tau_0)$, that takes us from τ_0 to τ_2 in a single step in terms of the propagators that take us from τ_0 to τ_1 and then from τ_1 to τ_2 as

$$\Psi(\vec{r},\tau_2) = \int G_1(\vec{r},\vec{r}'',\tau_2,\tau_0)\Psi(\vec{r}'',\tau_0)d^3\vec{r}'', \tag{18.411}$$

$$G_1(\vec{r},\vec{r}'',\tau_2,\tau_0) = \int G_1(\vec{r},\vec{r}',\tau_2,\tau_1)G_1(\vec{r}',\vec{r}'',\tau_1,\tau_0)\,d^3\vec{r}', \tag{18.412}$$

18.4.3 Diffusion Equation with Discrete Spectrum

As an important example of the first-order time-dependent equations, we now consider the diffusion or the heat transfer equations, which are both in the form

$$\vec{\nabla}^2\Psi(\vec{x},\tau) = \frac{\partial\Psi(\vec{x},\tau)}{\partial\tau}. \tag{18.413}$$

To simplify the problem, we consider only one dimension with $-\frac{L}{2} \le x \le \frac{L}{2}$ and use the periodic boundary condition $\Psi\left(-\frac{L}{2},\tau\right) = \Psi\left(\frac{L}{2},\tau\right)$. Because the

H operator for this problem is $H = -d^2/dx^2$, we easily write the eigenvalues and the eigenfunctions as

$$-\frac{d^2\phi_m}{dx^2} = \lambda_m \phi_m, \tag{18.414}$$

$$\phi_m(x) = \frac{1}{\sqrt{L}} e^{i\sqrt{\lambda_m}x}, \quad \lambda_m = \left(\frac{2\pi m}{L}\right)^2, \qquad m = \pm\text{integer}. \tag{18.415}$$

If we define $k_m = 2\pi m/L$, we obtain $G_1(x, x', \tau)$ as

$$\boxed{G_1(x, x', \tau) = \sum_{m=-\infty}^{\infty} \frac{1}{L} e^{ik_m(x-x')} e^{-k_m^2 \tau}.} \tag{18.416}$$

18.4.4 Diffusion Equation in the Continuum Limit

We now consider the continuum limit of the propagator [Eq. (18.416)]. Because the difference of two neighboring eigenvalues is $\Delta k_m = 2\pi/L$, we can write $G_1(x, x', \tau)$ as

$$G_1(x, x', \tau) = \frac{1}{2\pi} \sum_{m=-\infty}^{\infty} \Delta k_m e^{ik_m(x-x')} e^{-k_m^2 \tau}. \tag{18.417}$$

In the continuum limit, $L \to \infty$, the difference between two neighboring eigenvalues becomes infinitesimally small; thus we may replace the summation with an integral as

$$\lim_{L\to\infty} \sum_m \Delta k_m f(k_m) \to \int f(k)\, dk. \tag{18.418}$$

This gives us the propagator as

$$G_1(x, x', \tau) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk e^{ik(x-x')} e^{-k^2\tau}. \tag{18.419}$$

Completing the square:

$$ik(x - x') - k^2\tau = -\tau\left(k - \frac{i(x - x')}{2\tau}\right)^2 - \frac{(x - x')^2}{4\tau} \tag{18.420}$$

and defining $\delta = (x - x')/2\tau$, we can write $G_1(x, x', \tau)$ as

$$G_1(x, x', \tau) = \frac{1}{2\pi} e^{-(x-x')^2/4\tau} \int_{-\infty}^{\infty} dk e^{-\tau(k-i\delta)^2}. \tag{18.421}$$

This integral can be taken easily, thus yielding the propagator

$$\boxed{G_1(x, x', \tau) = \frac{1}{\sqrt{4\pi\tau}} e^{-(x-x')^2/4\tau}.} \tag{18.422}$$

Note that G_1 is symmetric with respect to x and x'. In the limit $\tau \to 0$, it becomes

$$\lim_{\tau\to 0} G_1(x, x', \tau) = \lim_{\tau\to 0} \frac{1}{\sqrt{4\pi\tau}} e^{-(x-x')^2/4\tau} = I(x, x'), \tag{18.423}$$

which is one of the definitions of the Dirac-delta function, hence $I(x, x') = \delta(x - x')$. Plotting Equation (18.422), we see that it is a Gaussian (Figure 18.9).

Because the area under a Gaussian is constant:

$$\int_{-\infty}^{\infty} G_1(x, x')\, dx = \frac{1}{\sqrt{4\pi\tau}} \int_{-\infty}^{\infty} e^{-(x-x')^2/4\tau}\, dx = 1, \tag{18.424}$$

the total amount of the diffusing material is conserved. Using $G_1(x, x', \tau)$ and given the initial concentration, $\Psi(x', 0)$, we can find the concentration at subsequent times as $\Psi(x, \tau) = \int_{-\infty}^{\infty} G_1(x, x', \tau)\Psi(x', 0)\, dx'$:

$$\boxed{\Psi(x, \tau) = \frac{1}{\sqrt{4\pi\tau}} \int_{-\infty}^{\infty} e^{-(x-x')^2/4\tau}\Psi(x', 0)\, dx'.} \tag{18.425}$$

Note that our solution satisfies the relation $\int_{-\infty}^{\infty} \Psi(x, \tau)dx = \int_{-\infty}^{\infty} \Psi(x', 0)dx'$.

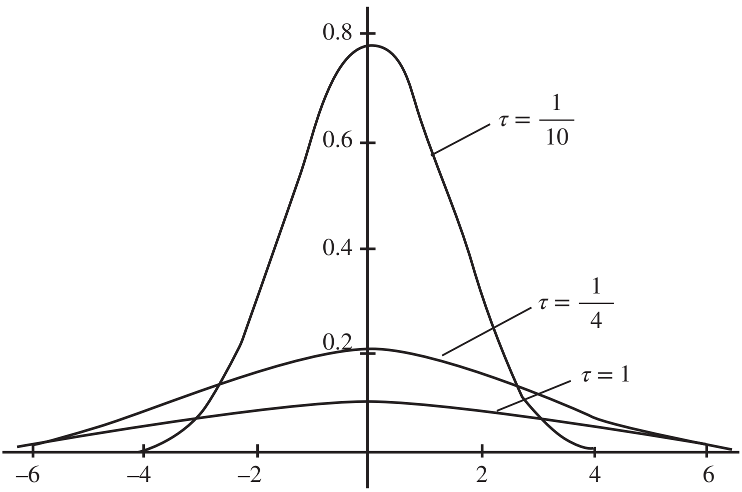

Figure 18.9 Gaussian.

18.4.5 Presence of Sources or Interactions

First-order time-dependent equations frequently appear with an inhomogeneous term:

$$\boxed{H\Psi(\vec{r},\tau) + \frac{\partial\Psi(\vec{r},\tau)}{\partial\tau} = F(\vec{r},\tau),} \tag{18.426}$$

where $F(\vec{r},\tau)$ represents sources or interactions in the system; thus we need a Green's function which allows us to express the solution as

$$\Psi(\vec{r},\tau) = \Psi_0(\vec{r},\tau) + \int G(\vec{r},\vec{r}\,',\tau,\tau')F(\vec{r}\,',\tau')\, d^3\vec{r}\,'\, d\tau', \tag{18.427}$$

where $\Psi_0(\vec{r},\tau)$ represents the solution of the homogeneous part of Eq. (18.426). We have seen that the propagator $G_1(\vec{r},\vec{r}\,',\tau,\tau')$ satisfies the equation

$$\left(H + \frac{\partial}{\partial\tau}\right) G_1(\vec{r},\vec{r}\,',\tau,\tau') = 0. \tag{18.428}$$

However, the Green's function that we need in Eq. (18.427) satisfies

$$\left(H + \frac{\partial}{\partial\tau}\right) G(\vec{r},\vec{r}\,',\tau,\tau') = \delta^3(\vec{r} - \vec{r}\,')\delta(\tau - \tau'). \tag{18.429}$$

It is clear that even though $G_1(\vec{r},\vec{r}\,',\tau,\tau')$ is not the Green's function, it is closely related to it. After all, except for the point $\vec{r} = \vec{r}\,'$, it satisfies the differential Eq. (18.429). Considering that $G_1(\vec{r},\vec{r}\,',\tau,\tau')$ satisfies the relation

$$\lim_{\tau\to\tau'} G_1(\vec{r},\vec{r}\,',\tau,\tau') = \delta^3(\vec{r} - \vec{r}\,'), \tag{18.430}$$

we can expect to satisfy Eq. (18.429) by introducing a discontinuity at $\tau = \tau'$. Let us start with

$$G(\vec{r},\vec{r}\,',\tau,\tau') = G_1(\vec{r},\vec{r}\,',\tau,\tau')\theta(\tau - \tau'), \tag{18.431}$$

so that

$$\left\{\begin{matrix} G = G_1, & \tau > \tau', \\ G = 0, & \tau < \tau'. \end{matrix}\right\} \tag{18.432}$$

Substituting this in Eq. (18.429), we get

$$\left(H+\frac{\partial}{\partial\tau}\right)G(\vec{r},\vec{r}',\tau,\tau')$$
$$= HG_1(\vec{r},\vec{r}',\tau,\tau')\theta(\tau-\tau') + \frac{\partial}{\partial\tau}[G_1(\vec{r},\vec{r}',\tau,\tau')\theta(\tau-\tau')] \tag{18.433}$$
$$= \theta(\tau-\tau')HG_1(\vec{r},\vec{r}',\tau,\tau') + \theta(\tau-\tau')\frac{\partial}{\partial\tau}G_1(\vec{r},\vec{r}',\tau,\tau') \tag{18.434}$$
$$+ G_1(\vec{r},\vec{r}',\tau,\tau')\frac{\partial}{\partial\tau}\theta(\tau-\tau')$$
$$= \theta(\tau-\tau')\left(H+\frac{\partial}{\partial\tau}\right)G_1(\vec{r},\vec{r}',\tau,\tau') + G_1(\vec{r},\vec{r}',\tau,\tau')\delta(\tau-\tau'). \tag{18.435}$$

We have used the relation $\frac{d}{d\tau}\theta(\tau-\tau') = \delta(\tau-\tau')$. Considering the fact that G_1 satisfies Eq. (18.428), we obtain

$$\left(H+\frac{\partial}{\partial\tau}\right)G(\vec{r},\vec{r}',\tau,\tau') = G_1(\vec{r},\vec{r}',\tau,\tau')\delta(\tau-\tau'). \tag{18.436}$$

Because the Dirac-delta function is zero except at $\tau=\tau'$, we only need the value of G_1 at $\tau=\tau'$, which is equal to $\delta^3(\vec{r}-\vec{r}')$ [Eq. (18.430)]; thus we can write Eq. (18.436) as

$$\left(H+\frac{\partial}{\partial\tau}\right)G(\vec{r},\vec{r}',\tau,\tau') = \delta^3(\vec{r}-\vec{r}')\delta(\tau-\tau'). \tag{18.437}$$

From here, we see that the Green's function for Eq. (18.426) is

$$\boxed{G(\vec{r},\vec{r}',\tau,\tau') = G_1(\vec{r},\vec{r}',\tau,\tau')\theta(\tau-\tau')} \tag{18.438}$$

and the general solution of Eq. (18.426) can now be written as

$$\Psi(\vec{r},\tau) = \Psi_0(\vec{r},\tau) + \int d^3\vec{r}'\int d\tau' G(\vec{r},\vec{r}',\tau,\tau')F(\vec{r}',\tau') \tag{18.439}$$
$$= \Psi_0(\vec{r},\tau) + \int d^3\vec{r}'\int_{-\infty}^{\tau} d\tau' G_1(\vec{r},\vec{r}',\tau,\tau')F(\vec{r}',\tau'). \tag{18.440}$$

18.4.6 Schrödinger Equation for Free Particles

To write the Green's function for the Schrödinger equation for a free particle, we can use the similarity between the Schrödinger and the diffusion equations. Making the replacement $\tau \to i\hbar t/2m$ in Eq. (18.422) gives us the propagator for a free particle as

$$G_1(x, x', t) = \frac{1}{\sqrt{2\pi i\hbar t/m}} e^{-m(x-x')^2/2i\hbar t}. \tag{18.441}$$

Now the solution of the Schrödinger equation,

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x, t) = i\hbar\frac{\partial}{\partial t}\Psi(x, t), \tag{18.442}$$

with the initial condition $\Psi(x', 0)$, can be written as

$$\Psi(x, t) = \int G_1(x, x', t)\Psi(x', 0)\, dx'. \tag{18.443}$$

18.4.7 Schrödinger Equation with Interactions

When a particle is moving under the influence of a potential, $V(x)$, the Schrödinger equation becomes

$$-\frac{\partial^2}{\partial x^2}\Psi(x, t) + \frac{2m}{i\hbar}\frac{\partial}{\partial t}\Psi(x, t) = -\frac{2m}{\hbar^2}V(x)\Psi(x, t), \tag{18.444}$$

For an arbitrary initial time, t', Green's function is given as $G(x, x', t, t') = G_1(x, x', t, t')\theta(t - t')$ and the solution becomes

$$\Psi(x, t) = \Psi_0(x, t) - \frac{i}{\hbar}\int dx' \int_{-\infty}^{t} dt' G(x, x', t, t')\, V(x')\Psi(x', t'). \tag{18.445}$$

18.5 Second-Order Time-Dependent Green's Functions

Most of the frequently encountered time-dependent equations with second-order time dependence can be written as

$$\boxed{\left[H + \frac{\partial^2}{\partial \tau^2}\right]\Psi(\vec{r}, \tau) = 0,} \tag{18.446}$$

where τ is a timelike variable and H is a linear differential operator independent of τ. We again assume that H has a complete set of orthonormal eigenfunctions satisfying $H\phi_n(\vec{r}) = \lambda_n\phi_n(\vec{r})$, where λ_n are the eigenvalues. We expand $\Psi(\vec{r}, \tau)$ in terms of this complete and orthonormal set as

$$\Psi(\vec{r}, \tau) = \sum_n A_n(\tau)\phi_n(\vec{r}), \tag{18.447}$$

where the coefficients, $A_n(\tau)$, carry the τ dependence. Substituting this in Eq. (18.446), we obtain

$$\sum_n [\ddot{A}_n(\tau) + \lambda_n A_n(\tau)]\phi_n(\vec{r}) = 0. \tag{18.448}$$

Since ϕ_n are linearly independent, we set the quantity inside the square brackets to zero and obtain the differential equation that the coefficients, $A_n(\tau)$, satisfy as

$$\ddot{A}_n(\tau) + \lambda_n A_n(\tau) = 0. \tag{18.449}$$

The solution of this equation can be written immediately:

$$A_n(\tau) = a_n e^{i\sqrt{\lambda_n}\tau} + b_n e^{-i\sqrt{\lambda_n}\tau}, \tag{18.450}$$

which when substituted in Eq. (18.447) gives $\Psi(\vec{r}, \tau)$:

$$\Psi(\vec{r}, \tau) = \sum_n [a_n e^{i\sqrt{\lambda_n}\tau} + b_n e^{-i\sqrt{\lambda_n}\tau}]\phi_n(\vec{r}). \tag{18.451}$$

Integration constants, a_n and b_n, are to be determined from the initial conditions. Assuming that $\Psi(\vec{r}, 0)$ and $\dot{\Psi}(\vec{r}, 0)$ are given, we write

$$\Psi(\vec{r}, 0) = \sum_n [a_n + b_n]\phi_n(\vec{r}), \tag{18.452}$$

$$\dot{\Psi}(\vec{r}, 0) = i \sum_n \sqrt{\lambda_n}[a_n - b_n]\phi_n(\vec{r}). \tag{18.453}$$

Using the orthogonality relation of $\phi_n(\vec{r})$ [Eq. (18.391)], we obtain two relations between a_n and b_n:

$$[a_n + b_n] = \int \phi_n^*(\vec{r}')\Psi(\vec{r}', 0)\, d^3\vec{r}', \tag{18.454}$$

$$[a_n - b_n] = \frac{-i}{\sqrt{\lambda_n}} \int \phi_n^*(\vec{r}')\dot{\Psi}(\vec{r}', 0)\, d^3\vec{r}'. \tag{18.455}$$

These equations can be solved easily for a_n and b_n to yield

$$a_n = \frac{1}{2}\left[\int \phi_n^*(\vec{r}')\Psi(\vec{r}', 0)\, d^3\vec{r}' + \frac{1}{i\sqrt{\lambda_n}} \int \phi_n^*(\vec{r}')\dot{\Psi}(\vec{r}', 0)\, d^3\vec{r}'\right], \tag{18.456}$$

$$b_n = \frac{1}{2}\left[\int \phi_n^*(\vec{r}')\Psi(\vec{r}', 0)\, d^3\vec{r}' - \frac{1}{i\sqrt{\lambda_n}} \int \phi_n^*(\vec{r}')\dot{\Psi}(\vec{r}', 0)\, d^3\vec{r}'\right]. \tag{18.457}$$

Substituting the above a_n and b_n into $\Psi(\vec{r},\tau)$ gives

$$\Psi(\vec{r},\tau) = \int \sum_n \cos(\sqrt{\lambda_n}\tau)\phi_n(\vec{r})\phi_n^*(\vec{r}')\Psi(\vec{r}',0)\, d^3\vec{r}' + \int \sum_n \sin(\sqrt{\lambda_n}\tau)\frac{1}{\sqrt{\lambda_n}}\phi_n(\vec{r})\phi_n^*(\vec{r}')\dot{\Psi}(\vec{r}',0)\, d^3\vec{r}'. \tag{18.458}$$

We now rewrite $\Psi(\vec{r},\tau)$ as

$$\boxed{\Psi(\vec{r},\tau) = \int G_2(\vec{r},\vec{r}',\tau)\Psi(\vec{r}',0)\, d^3\vec{r}' + \int \tilde{G}_2(\vec{r},\vec{r}',\tau)\dot{\Psi}(\vec{r}',0)\, d^3\vec{r}'} \tag{18.459}$$

and define two new functions, G_2 and $\tilde{G}_2$:

$$\boxed{G_2(\vec{r},\vec{r}',\tau) = \sum_n \cos(\sqrt{\lambda_n}\tau)\phi_n(\vec{r})\phi_n^*(\vec{r}'),} \tag{18.460}$$

$$\boxed{\tilde{G}_2(\vec{r},\vec{r}',\tau) = \sum_n \frac{\sin(\sqrt{\lambda_n}\tau)}{\sqrt{\lambda_n}}\phi_n(\vec{r})\phi_n^*(\vec{r}').} \tag{18.461}$$

Among these functions, G_2 acts on $\Psi(\vec{r}',0)$ and $\tilde{G}_2$ acts on $\dot{\Psi}(\vec{r}',0)$. They both satisfy the homogeneous equation

$$\left[H + \frac{\partial^2}{\partial\tau^2}\right]\left\{\begin{matrix} G_2(\vec{r},\vec{r}',\tau) \\ \tilde{G}_2(\vec{r},\vec{r}',\tau) \end{matrix}\right\} = 0. \tag{18.462}$$

Thus, $\Psi(\vec{r},\tau)$ is a solution of the differential Eq. (18.446). Note that G_2 and $\tilde{G}_2$ are related by

$$G_2(\vec{r},\vec{r}',\tau) = \frac{d}{d\tau}\tilde{G}_2(\vec{r},\vec{r}',\tau), \tag{18.463}$$

hence, we can obtain $G_2(\vec{r},\vec{r}',\tau)$ from $\tilde{G}_2(\vec{r},\vec{r}',\tau)$ by differentiation with respect to τ. Using Eq. (18.460) and the completeness relation, we can write

$$G_2(\vec{r},\vec{r}',0) = \sum_n \phi_n(\vec{r})\phi_n^*(\vec{r}') = \delta^3(\vec{r}-\vec{r}'). \tag{18.464}$$

Using the completeness relation (18.392) in Eq. (18.458), one can easily check that $\Psi(\vec{r},\tau)$ satisfies the initial conditions.

For an arbitrary initial time, τ', we write $\Psi(\overrightarrow{r},\tau)$, $\tilde{G}_2(\overrightarrow{r},\overrightarrow{r}',\tau,\tau')$, and $G_2(\overrightarrow{r},\overrightarrow{r}',\tau,\tau')$ as

$$\boxed{\begin{aligned}\Psi(\overrightarrow{r},\tau) = &\int G_2(\overrightarrow{r},\overrightarrow{r}',\tau,\tau')\Psi(\overrightarrow{r}',\tau')\, d^3\overrightarrow{r}' \\ &+\int \tilde{G}_2(\overrightarrow{r},\overrightarrow{r}',\tau,\tau')\dot{\Psi}(\overrightarrow{r}',\tau')\, d^3\overrightarrow{r}',\end{aligned}} \tag{18.465}$$

$$\boxed{\tilde{G}_2(\overrightarrow{r},\overrightarrow{r}',\tau,\tau') = \sum_n \frac{\sin[\sqrt{\lambda_n}(\tau-\tau')]}{\sqrt{\lambda_n}}\phi_n(\overrightarrow{r})\phi_n^*(\overrightarrow{r}'),} \tag{18.466}$$

$$\boxed{\begin{aligned}G_2(\overrightarrow{r},\overrightarrow{r}',\tau,\tau') &= \frac{d}{dt}\tilde{G}_2(\overrightarrow{r},\overrightarrow{r}',\tau,\tau') \\ &= \sum_n \cos[\sqrt{\lambda_n}(\tau-\tau')]\phi_n(\overrightarrow{r})\phi_n^*(\overrightarrow{r}').\end{aligned}} \tag{18.467}$$

18.5.1 Propagators for the Scalar Wave Equation

An important example of the second-order time-dependent equations is the scalar wave equation, $\square\Psi(\overrightarrow{r},t)=0$, where the wave, or the d'Alembert, operator is defined as $\square = -\overrightarrow{\nabla}^2 + \frac{1}{c^2}\frac{\partial^2}{\partial t^2}$. Comparing with Eq. (18.446), we have $H = -\overrightarrow{\nabla}^2$, $\tau = ct$. Considering a rectangular region with the dimensions (L_1, L_2, L_3) and using periodic boundary conditions, eigenfunctions and the eigenvalues of the H operator are written as

$$H\phi_{n_1,n_2,n_3}(\overrightarrow{r}) = \lambda_{n_1,n_2,n_3}\phi_{n_1,n_2,n_3}(\overrightarrow{r}), \tag{18.468}$$

$$\phi_{n_1,n_2,n_3}(\overrightarrow{r}) = \frac{1}{\sqrt{L_1L_2L_3}}e^{ik_xx}e^{ik_yy}e^{ik_zz}, \tag{18.469}$$

$$k_x = \frac{2\pi n_1}{L_1},\ k_y = \frac{2\pi n_2}{L_2},\ k_z = \frac{2\pi n_3}{L_3}, \tag{18.470}$$

where $n_i = \pm$ integer and $\neq 0$. Eigenvalues satisfy the relation

$$\lambda_{n_1,n_2,n_3} = k_x^2 + k_y^2 + k_z^2. \tag{18.471}$$

Using these eigenfunctions, we can construct $\tilde{G}_2(\overrightarrow{r},\overrightarrow{r}',\tau)$ as

$$\tilde{G}_2(\overrightarrow{r},\overrightarrow{r}',\tau) = \frac{1}{L_1L_2L_3}\sum_{n_1,n_2,n_3}^{\infty} \frac{\sin\left(\sqrt{k_x^2+k_y^2+k_z^2}\right)\tau}{\sqrt{k_x^2+k_y^2+k_z^2}} e^{ik_x(x-x')}e^{ik_y(y-y')}e^{ik_z(z-z')}. \tag{18.472}$$

We now consider the continuum limit, where we make the replacements

$$\lim_{L_1\to\infty} \frac{1}{L_1} \sum_{n_1=-\infty}^{\infty} \to \frac{1}{2\pi} \int_{-\infty}^{\infty} dk_x, \tag{18.473}$$

$$\lim_{L_2\to\infty} \frac{1}{L_2} \sum_{n_2=-\infty}^{\infty} \to \frac{1}{2\pi} \int_{-\infty}^{\infty} dk_y, \tag{18.474}$$

$$\lim_{L_3\to\infty} \frac{1}{L_3} \sum_{n_3=-\infty}^{\infty} \to \frac{1}{2\pi} \int_{-\infty}^{\infty} dk_z. \tag{18.475}$$

Thus $\tilde{G}_2(\vec{r}, \vec{r}', \tau)$ becomes

$$\tilde{G}_2(\vec{r}, \vec{r}', \tau) = \frac{1}{(2\pi)^3} \int_{-\infty}^{\infty} dk_x \int_{-\infty}^{\infty} dk_y \int_{-\infty}^{\infty} dk_z \frac{\sin k\tau}{k} e^{i\vec{k}\cdot\vec{\rho}}, \tag{18.476}$$

where $\vec{\rho} = (\vec{r} - \vec{r}')$. Defining a wave vector, $\vec{k} = (k_x, k_y, k_z)$, and using polar coordinates, we can write

$$\tilde{G}_2(\vec{r}, \vec{r}', \tau) = \frac{1}{(2\pi)^3} \int_0^{\infty} dk k^2 \frac{\sin k\tau}{k} \int_0^{2\pi} d\phi_k \int_{-1}^{1} d(\cos\theta_k) e^{i\vec{k}\cdot\vec{\rho}}. \tag{18.477}$$

Choosing the direction of the $\vec{\rho}$ vector along the z-axis, we write $\vec{k}\cdot\vec{\rho} = k\rho\cos\theta_k$ and define x as $x = \cos\theta_k$. After taking the θ_k and ϕ_k integrals, $\tilde{G}_2(\vec{r}, \vec{r}', \tau)$ becomes

$$\tilde{G}_2(\vec{r}, \vec{r}', \tau) = \frac{2\pi}{(2\pi)^3} \int_0^{\infty} dk k^2 \frac{\sin k\tau}{k} \int_{-1}^{1} d(\cos\theta_k) e^{ik\rho\cos\theta_k} \tag{18.478}$$

$$= \frac{1}{2\pi^2\rho} \int_0^{\infty} dk \sin k\tau \cdot \sin k\rho \tag{18.479}$$

$$= \frac{1}{4\pi^2\rho} \int_{-\infty}^{\infty} dk \sin k\tau \cdot \sin k\rho \tag{18.480}$$

$$= \frac{1}{8\pi^2\rho} \int_{-\infty}^{\infty} dk[\cos k(\rho - \tau) - \cos k(\rho + \tau)]. \tag{18.481}$$

Using one of the definitions of the Dirac-delta function:

$$\delta(x - x') = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk e^{ik(x-x')} = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk \cos k(x - x'), \tag{18.482}$$

we can write $\tilde{G}_2(\vec{r}, \vec{r}', \tau)$ as

$$\tilde{G}_2(\vec{r}, \vec{r}', \tau) = \frac{1}{4\pi\rho}[\delta(\rho - \tau) - \delta(\rho + \tau)]. \tag{18.483}$$

Going back to our original variables, $\tilde{G}_2(\overrightarrow{r}, \overrightarrow{r}', t)$ becomes

$$\tilde{G}_2(\overrightarrow{r}, \overrightarrow{r}', t) = \frac{1}{4\pi|\overrightarrow{r} - \overrightarrow{r}'|}[\delta(|\overrightarrow{r} - \overrightarrow{r}'| - ct) - \delta(|\overrightarrow{r} - \overrightarrow{r}'| + ct)]. \tag{18.484}$$

We write this for an arbitrary initial time t' to obtain the final form of the propagator as

$$\begin{aligned} &\tilde{G}_2(\overrightarrow{r}, \overrightarrow{r}', t, t') \\ &= \frac{1}{4\pi|\overrightarrow{r} - \overrightarrow{r}'|}[\delta(|\overrightarrow{r} - \overrightarrow{r}'| - c(t - t')) - \delta(|\overrightarrow{r} - \overrightarrow{r}'| + c(t - t'))]. \end{aligned} \tag{18.485}$$

18.5.2 Advanced and Retarded Green's Functions

In the presence of a source, $\rho(\overrightarrow{r}, \tau)$, Eq. (18.446) becomes

$$H\Psi(\overrightarrow{r}, \tau) + \frac{\partial^2 \Psi(\overrightarrow{r}, \tau)}{\partial \tau^2} = \rho(\overrightarrow{r}, \tau). \tag{18.486}$$

To solve this equation, we need a Green's function satisfying the equation

$$\left(H + \frac{\partial^2}{\partial \tau^2}\right) G(\overrightarrow{r}, \overrightarrow{r}', \tau, \tau') = \delta^3(\overrightarrow{r} - \overrightarrow{r})\delta(\tau - \tau'). \tag{18.487}$$

However, the propagators $G_2(\overrightarrow{r}, \overrightarrow{r}', \tau, \tau')$ and $\tilde{G}_2(\overrightarrow{r}, \overrightarrow{r}', \tau, \tau')$ both satisfy

$$\left[H + \frac{\partial^2}{\partial \tau^2}\right] \begin{pmatrix} G_2 \\ \tilde{G}_2 \end{pmatrix} = 0. \tag{18.488}$$

Guided by our experience in G_1, to find the Green's function, we start by introducing a discontinuity in either G_2 or $\tilde{G}_2$ as

$$G_R(\overrightarrow{r}, \overrightarrow{r}', \tau, \tau') = G_\zeta(\overrightarrow{r}, \overrightarrow{r}', \tau, \tau')\theta(\tau - \tau'). \tag{18.489}$$

G_ζ stands for G_2 or $\tilde{G}_2$, while the subscript R will be explained later. Operating on $G_R(\overrightarrow{r}, \overrightarrow{r}', \tau, \tau')$ with $H + \frac{\partial^2}{\partial \tau^2}$, we get

$$\left[H + \frac{\partial^2}{\partial \tau^2}\right] G_R(\overrightarrow{r}, \overrightarrow{r}', \tau, \tau') \tag{18.490}$$

$$= \theta(\tau - \tau')HG_\zeta + \frac{\partial^2}{\partial \tau^2}[G_\zeta(\overrightarrow{r}, \overrightarrow{r}', \tau, \tau')\theta(\tau - \tau')] \tag{18.491}$$

$$= \theta(\tau - \tau')\left[H + \frac{\partial^2}{\partial \tau^2}\right] G_\zeta + 2\left[\frac{\partial}{\partial \tau}\theta(\tau - \tau')\right] \frac{\partial}{\partial \tau} G_\zeta + G_\zeta \frac{\partial^2}{\partial \tau^2}\theta(\tau - \tau'). \tag{18.492}$$

Since $G_2(\overrightarrow{r}, \overrightarrow{r}', \tau, \tau')$ and $\tilde{G}_2(\overrightarrow{r}, \overrightarrow{r}', \tau, \tau')$ both satisfy

$$\left[H + \frac{\partial^2}{\partial \tau^2}\right] G_\zeta = 0, \tag{18.493}$$

this becomes

$$\left[H + \frac{\partial^2}{\partial \tau^2}\right] G_R = 2\left[\frac{\partial}{\partial \tau}\theta(\tau - \tau')\right]\frac{\partial}{\partial \tau}G_\zeta + G_\zeta \frac{\partial^2}{\partial \tau^2}\theta(\tau - \tau'). \tag{18.494}$$

Using the fact that the derivative of a step function is a Dirac-delta function, we can write

$$\left[H + \frac{\partial^2}{\partial \tau^2}\right] G_R(\vec{r}, \vec{r}', \tau, \tau') \tag{18.495}$$
$$= 2\delta(\tau - \tau')\frac{\partial}{\partial \tau}G_\zeta(\vec{r}, \quad \vec{r}', \tau, \tau') + \left[\frac{\partial}{\partial \tau}\delta(\tau - \tau')\right] G_\zeta(\vec{r}, \vec{r}', \tau, \tau').$$

Using the following properties of the Dirac-delta function:

$$\delta(\tau - \tau')\frac{\partial}{\partial \tau}G_\zeta(\vec{r}, \vec{r}', \tau, \tau') = \left[\frac{\partial}{\partial \tau}G_\zeta(\vec{r}, \vec{r}', \tau, \tau')\right]_{\tau=\tau'}\delta(\tau - \tau'), \tag{18.496}$$

$$\left[\frac{\partial}{\partial \tau}\delta(\tau - \tau')\right] G_\zeta(\vec{r}, \vec{r}', \tau, \tau') = -\left[\frac{\partial}{\partial \tau}G_\zeta(\vec{r}, \vec{r}', \tau, \tau')\right]_{\tau=\tau'}\delta(\tau - \tau'), \tag{18.497}$$

we can write Eq. (18.495) as

$$\left[H + \frac{\partial^2}{\partial \tau^2}\right] G_R(\vec{r}, \vec{r}', \tau, \tau') = \delta(\tau - \tau')\left[\frac{\partial}{\partial \tau}G_\zeta(\vec{r}, \vec{r}', \tau, \tau')\right]_{\tau=\tau'}. \tag{18.498}$$

If we take G_2 as G_ζ, the right-hand side becomes zero; thus it is not useful for our purposes. However, taking $\tilde{G}_2$, we find

$$\left[H + \frac{\partial^2}{\partial \tau^2}\right] G_R(\vec{r}, \vec{r}', \tau, \tau') = \delta(\tau - \tau')\delta^3(\vec{r} - \vec{r}'), \tag{18.499}$$

which means that the Green's function that we need is

$$\boxed{G_R(\vec{r}, \vec{r}', \tau, \tau') = \tilde{G}_2(\vec{r}, \vec{r}', \tau, \tau')\theta(\tau - \tau').} \tag{18.500}$$

The **general solution** can now be expressed as

$$\boxed{\Psi_R(\vec{r}, \tau) = \Psi_0(\vec{r}, \tau) + \int d^3\vec{r}' \int_{-\infty}^{\tau} d\tau' \tilde{G}_2(\vec{r}, \vec{r}', \tau, \tau')\rho(\vec{r}', \tau').} \tag{18.501}$$

There is also another choice for the Green's function, which is given as

$$\boxed{G_A(\vec{r}, \vec{r}', \tau, \tau') = -\tilde{G}_2(\vec{r}, \vec{r}', \tau, \tau')\theta(\tau' - \tau).} \tag{18.502}$$

Following similar steps:

$$\left[H+\frac{\partial^2}{\partial\tau^2}\right]G_A$$
$$= -\theta(\tau'-\tau)H\tilde{G}_2 - \frac{\partial^2}{\partial\tau^2}[\tilde{G}_2(\overrightarrow{r},\overrightarrow{r}',\tau,\tau')\theta(\tau'-\tau)] \tag{18.503}$$
$$= -\theta(\tau'-\tau)\left[H+\frac{\partial^2}{\partial\tau^2}\right]\tilde{G}_2 - 2\frac{\partial}{\partial\tau}\theta(\tau'-\tau)\ \frac{\partial}{\partial\tau}\tilde{G}_2 - \tilde{G}_2\frac{\partial^2}{\partial\tau^2}\theta(\tau'-\tau) \tag{18.504}$$
$$= -\left[\frac{\partial}{\partial\tau}\tilde{G}_2\right]\frac{\partial}{\partial\tau}\theta(\tau'-\tau) = \left[\frac{\partial}{\partial\tau}\tilde{G}_2\right]\frac{\partial}{\partial\tau'}\theta(\tau'-\tau) \tag{18.505}$$
$$= \left[\frac{\partial}{\partial\tau}\tilde{G}_2(\overrightarrow{r},\overrightarrow{r}',\tau,\tau')\right]\delta(\tau'-\tau) \tag{18.506}$$
$$= \left[\frac{\partial}{\partial\tau}\tilde{G}_2(\overrightarrow{r},\overrightarrow{r}',\tau,\tau')\right]_{\tau'=\tau}\delta(\tau'-\tau), \tag{18.507}$$

we see that $G_A(\overrightarrow{r},\overrightarrow{r}',\tau,\tau')$ also satisfies the defining equation for the Green's function as

$$\left[H+\frac{\partial^2}{\partial\tau^2}\right]G_A(\overrightarrow{r},\overrightarrow{r}',\tau,\tau') = \delta(\tau-\tau')\delta^3(\overrightarrow{r}-\overrightarrow{r}'). \tag{18.508}$$

Now the **general solution** of Eq. (18.486) can be written as

$$\boxed{\Psi_A(\overrightarrow{r},\tau) = \Psi_0(\overrightarrow{r},\tau) - \int d^3\overrightarrow{r}'\int_\tau^\infty d\tau'\tilde{G}_2(\overrightarrow{r},\overrightarrow{r}',\tau,\tau')\rho(\overrightarrow{r}',\tau').} \tag{18.509}$$

From Eq. (18.501), it is seen that the solution $\Psi_R(\overrightarrow{r},\tau)$ is determined by the past behavior of the source, that is, with source times $\tau' < \tau$, while $\Psi_A(\overrightarrow{r},\tau)$ is determined by the behavior of the source in the future, that is, with source times $\tau' > \tau$. We borrowed the subscripts from relativity, where R and A stand for the "**retarded**" and the "**advanced**" solutions, respectively. These terms acquire their true meaning with the relativistic wave equation discussed in the next section.

18.5.3 Scalar Wave Equation

In the presence of sources or sinks, the scalar wave equation is given as

$$\overrightarrow{\nabla}^2\Psi(\overrightarrow{r},t) - \frac{1}{c^2}\frac{\partial^2\Psi(\overrightarrow{r},t)}{\partial t^2} = \rho(\overrightarrow{r},t). \tag{18.510}$$

We have already found the propagator $\tilde{G}_2$ for the scalar wave equation [Eq. (18.485)]:

$$\tilde{G}_2(\vec{r}, \vec{r}', t, t') = \frac{1}{4\pi|\vec{r} - \vec{r}'|}[\delta(|\vec{r} - \vec{r}'| - c(t-t')) - \delta(|\vec{r} - \vec{r}'| + c(t-t'))]. \tag{18.511}$$

Using Eq. (18.500), we now write the Green's function for $t > t'$ as

$$G_R(\vec{r}, \vec{r}', t, t') = \frac{[\delta(|\vec{r} - \vec{r}'| - c(t-t')) - \delta(|\vec{r} - \vec{r}'| + c(t-t'))]}{4\pi|\vec{r} - \vec{r}'|}\theta(t-t'). \tag{18.512}$$

For $t < t'$, the Green's function is $G_R = 0$. For $t > t'$, the argument of the second Dirac-delta function never vanishes; thus the Green's function becomes

$$G_R(\vec{r}, \vec{r}', t, t') = \frac{1}{4\pi|\vec{r} - \vec{r}'|}\delta[|\vec{r} - \vec{r}'| - c(t-t')]. \tag{18.513}$$

Now the general solution with this Green's function is expressed as

$$\Psi_R(\vec{r}, t) = \Psi_0(\vec{r}, t) + \frac{1}{4\pi}\int d^3\vec{r}' \int_{-\infty}^{\infty} dt' \frac{\delta[|\vec{r} - \vec{r}'| - c(t-t')]}{|\vec{r} - \vec{r}'|}\rho(\vec{r}', t'), \tag{18.514}$$

where $\Psi_0(\vec{r}, \tau)$ is the solution of the homogeneous equation. Taking the t' integral, we find

$$\Psi_R(\vec{r}, t) = \Psi_0(\vec{r}, t) + \frac{1}{4\pi}\int d^3\vec{r}' \frac{[\rho(\vec{r}', t')]_R}{|\vec{r} - \vec{r}'|}, \tag{18.515}$$

where $[\rho(\vec{r}', t')]_R$ means that the solution Ψ_R at $(\vec{r}, t)$ is found by using the values of the source $\rho(\vec{r}', t')$ evaluated at **retarded times** $t' = t - |\vec{r} - \vec{r}'|/c$. We show the source at retarded times as $[\rho(\vec{r}', t')]_R = \rho(\vec{r}', t - |\vec{r} - \vec{r}'|/c)$, and the solution found by using $[\rho(\vec{r}', t')]_R$ is shown as $\Psi_R(\vec{r}, t)$. The physical interpretation of this solution is that whatever happens at the source point shows its effect at the field point later by the amount of time that signals (light) take to travel from the source to the field point. In other words, causes precede their effects.

Retarded solutions are of basic importance in electrodynamics, where the scalar potential $\Phi(\vec{r}, t)$ and the vector potential $\vec{A}(\vec{r}, t)$ satisfy the following equations:

$$\left[\overrightarrow{\nabla}^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right]\Phi(\overrightarrow{r},t) = -4\pi\rho(\overrightarrow{r},t), \tag{18.516}$$

$$\left[\overrightarrow{\nabla}^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right]\overrightarrow{A}(\overrightarrow{r},t) = -\frac{4\pi}{c}\overrightarrow{J}(\overrightarrow{r},t). \tag{18.517}$$

Here, $\rho(\overrightarrow{r},t)$ and $\overrightarrow{J}(\overrightarrow{r},t)$ stand for the charge and the current densities, respectively.

In search of a Green's function for Eq. (18.510), we have added a discontinuity to $\tilde{G}_2$ as $\tilde{G}_2(\overrightarrow{r},\overrightarrow{r}',\tau,\tau')\theta(\tau-\tau')$. However, there is also another alternative, where we take

$$G_A(\overrightarrow{r},\overrightarrow{r}',\tau,\tau') = -\tilde{G}_2(\overrightarrow{r},\overrightarrow{r}',\tau,\tau')\theta(\tau'-\tau). \tag{18.518}$$

Solution of the wave equation with this Green's function is now given as

$$\Psi_A(\overrightarrow{r},t) = \Psi_0(\overrightarrow{r},t) + \frac{1}{4\pi}\int d^3\overrightarrow{r}' \, \frac{[\rho(\overrightarrow{r}',t')]_A}{|\overrightarrow{r}-\overrightarrow{r}'|}. \tag{18.519}$$

In this solution, A stands for **advanced times**, that is, $t' = t + |\overrightarrow{r}-\overrightarrow{r}'|/c$. In other words, whatever " happens" at the source point shows its effect at the field point before its happening by the amount of time $|\overrightarrow{r}-\overrightarrow{r}'|/c$, which is again equal to the amount of time that light takes to travel from the source to the field point. In summary, in advanced solutions, effects precede their causes.

We conclude this section by saying that the wave equation (18.510) is covariant with c standing for the speed of light; hence, the two solutions $\Psi_R(\overrightarrow{r},t)$ and $\Psi_A(\overrightarrow{r},t)$ are both legitimate solutions of the relativistic wave equation. Thus the general solution is in principle their linear combination:

$$\Psi(\overrightarrow{r},t) = c_1\Psi_A(\overrightarrow{r},t) + c_2\Psi_R(\overrightarrow{r},t). \tag{18.520}$$

However, because we have no evidence of a case where causes precede their effects, as a boundary condition we set c_1 to zero, and take the retarded solution as the physically meaningful solution. This is also called the **principle of causality** [3].

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Problems

1 Given the Bessel equation

$$\frac{d}{dx}\left[x\frac{dy}{dx}\right]+\left(kx-\frac{m^2}{x}\right)y(x)=0$$

and its general solution, $y(x)=A_0J_m(x)+B_0N_m(x)$, find the Green's function satisfying the boundary conditions $y(0)=0$ and $y'(a)=0$.

2 For the operator $£=d^2/dx^2$ and the boundary conditions $y(0)=y(L)=0$, we have found the Green's function as

$$G(x,x')=\left[(x-x')\theta(x-x')-\frac{x}{L}(L-x')\right].$$

Show that the trigonometric Fourier expansion of this is

$$G(x,x')=-\frac{2}{L}\sum_n\frac{\sin k_nx\sin k_nx'}{k_n^2}.$$

3 Show that the Green's function for the differential operator $£=\frac{d^2}{dx^2}+k_0^2$ with the boundary conditions $y(0)=0$ and $y(L)=0$ is given as

$$G(x,x')=\frac{1}{k_0\sin k_0L}\begin{cases}\sin k_0x\sin k_0(x'-L), & x<x',\\ \sin k_0x'\sin k_0(x-L), & x>x'.\end{cases}$$

Show that this is equivalent to the eigenvalue expansion

$$G(x,x')=\frac{2}{L}\sum_{n=1}^{\infty}\frac{\sin\frac{n\pi x}{L}\sin\frac{n\pi x'}{L}}{k_0^2-(n\pi/L)^2}.$$

4 *Single-point boundary condition:* Consider the differential equation $£y(x)=\phi(x)$, where $£$ is the Sturm–Liouville operator, $£=\frac{d}{dx}\left(p(x)\frac{d}{dx}\right)+q(x)$. Construct the Green's function satisfying the single-point boundary conditions $y(x_0)=y_0$ and $y'(x_0)=y'_0$.

Hint: First write the Green's function as

$$G(x,x') = Ay_1(x) + By_2(x), \;\; x > x',$$
$$G(x,x') = Cy_1(x) + Dy_2(x), \;\; x < x',$$

where $y_1(x)$ and $y_2(x)$ are two linearly independent solutions of $\pounds y(x) = 0$. Because the Green's function is continuous at $x = x'$ and its derivative has a discontinuity of magnitude $1/p(x)$ at $x = x'$, find the constants A, B, C, and D, thus obtaining the Green's function as

$$G(x,x') = Cy_1(x) + Dy_2(x) - \frac{[y_1(x)y_2(x') - y_2(x)y_1(x')]}{p(x')W[y_1(x'), y_2(x')]}, \;\; x > x',$$
$$G(x,x') = Cy_1(x) + Dy_2(x), \;\; x < x',$$

where $W[y_1(x), y_2(x)]$ is the Wronskian defined as $W[y_1, y_2] = y_1y_2' - y_2y_1'$. Now impose the single-point boundary conditions $G(x_0, x') = 0$ and $G'(x_0, x') = 0$ to show that $C = D = 0$. Finally show that the differential equation $\pounds y(x) = \phi(x)$ with the single-point boundary conditions $y(x_0) = y_0$ and $y'(x_0) = y_0'$ is equivalent to the integral equation

$$y(x) = C_1y_1(x) + C_2y_2(x) + \int_{x_0}^{x} G(x,x')\phi(x')\, dx'.$$

5 Consider the differential operator $\pounds = \frac{d^2}{dt^2} + \omega_0^2$ with the single-point boundary conditions $x(0) = x_0$ and $\dot{x}(0) = 0$. Show that the Green's function is given as

$$G(t,t') = \frac{\sin \omega_0(t - t')}{\omega_0}\theta(t - t')$$

and write the solution for $\ddot{x}(t) + \omega_0^2 x^2(t) = F(t)$.

6 Find the Green's function for the Sturm–Liouville operator:

$$\pounds = a_3(x)\frac{d^3}{dx^3} + a_2(x)\frac{d^2}{dx^2} + a_1(x)\frac{d}{dx} + a_0(x),$$

satisfying the boundary conditions

$$G(x,x')|_{x=a} = 0 \quad \frac{dG(x,x')}{dx}|_{x=a} = 0 \quad \frac{d^2G(x,x')}{dx^2}|_{x=a} = 0,$$

in the interval $[a, b]$.

7 Find the Green's function for the differential equation $\frac{d^4y}{dx^4} = \phi(x,y)$, with the boundary conditions $y(0) = y'(0) = y(1) = y'(1) = 0$.

8 For the scalar wave equation:

$$\vec{\nabla}^2 \Psi(\vec{r}, t) - \frac{1}{c^2}\frac{\partial^2 \Psi(\vec{r}, t)}{\partial t^2} = \rho(\vec{r}, t),$$

take the Green's function as

$$G_A(\vec{r}, \vec{r}', \tau, \tau') = -\tilde{G}_2(\vec{r}, \vec{r}', \tau, \tau')\theta(\tau' - \tau)$$

and show that the solution is given as

$$\Psi_A(\vec{r}, t) = \Psi_0(\vec{r}, t) + \frac{1}{4\pi}\int d^3\vec{r}' \frac{[\rho(\vec{r}', t')]_A}{|\vec{r} - \vec{r}'|}.$$

What does $[\rho(\vec{r}', t')]_A$ stand for? Discuss your answer. (Read chapter 28 of *The Feynman Lectures on Physics* [3].)

9 Consider the partial differential equation $\left(\frac{\partial^2}{\partial x^2} - \frac{\partial}{\partial t}\right) y(x, t) = 0$ with the boundary conditions $y(0, t) = 0$ and $y(L, t) = y_0$. If $y(x, 0)$ represents the initial solution, find the solution at subsequent times.

10 Using the Green's function technique, solve the differential equation $\pounds y(x) = -\lambda x y(x), x \in [0, L]$, where

$$\pounds y(x) = \left[\frac{d}{dx}\left(x\frac{d}{dx}\right) - \frac{n^2}{x}\right] y(x), \quad n = \text{constant},$$

with the boundary conditions $y(0) = 0, y(L) = 0$.
What is the solution of $\pounds y = -\lambda x^n$ with the above boundary conditions?

11 Find the Green's function for the problem $\pounds y(x) = F(x), x \in [0, L]$, where $\pounds = \frac{d}{dx}\left(x\frac{d}{dx}\right)$. Use the boundary conditions $y(0) =$ finite, $y(L) = 0$. Write Green's theorem [Eq. (18.179)] in one dimension. Does the surface term in (18.181) vanish?

12 Given the differential equation $y''(t) - 3y'(t) + 2y(t) = 2e^{-t}$ and the boundary conditions $y(0) = 2, y'(0) = -1$.

i) Defining the operator in $\pounds y(x) = \phi(x)$ as

$$\pounds = \frac{d^2}{dx^2} - 3\frac{d}{dx} + 2$$

find the solution by using the Green's function method.

ii) Confirm your answer by solving the above problem using the Laplace transform technique.

iii) Using a different definition for $\pounds$, show that you get the same answer.

13 Consider the wave equation $\Box y(x,t) = F(x,t)$ with the boundary conditions $y(0,t) = y(L,t) = 0$. Find the Green's functions satisfying $\Box G(x,x') = \delta(x-x')\delta(t-t')$ and the initial conditions:

$$\text{i)} \qquad y(x,0) = y_0(x), \quad \frac{\partial y(x,0)}{\partial t} = 0,$$

$$\text{ii)} \qquad y(x,0) = 0, \quad \frac{\partial y(x,0)}{\partial t} = v_0(x).$$

14 Consider the partial differential equation $\vec{\nabla}^2 \Psi(\vec{r}) = F(\vec{r})$. Show that the Green's function for the inside of a sphere satisfying the boundary conditions that $G(\vec{r}, \vec{r}')$ be finite at the origin and zero on the surface, $r = a$, is given as

$$G(\vec{r}, \vec{r}') = \sum_{l=0}^{\infty} \sum_{m=-l}^{m=l} g_l(r,r') Y_l^{*m}(\theta', \phi') Y_l^m(\theta, \phi),$$

where

$$g_l(r,r') = \frac{r^l r'^l}{(2l+1)a^{2l+1}} \begin{cases} [1-(a/r')^{2l+1}], & r < r', \\ [1-(a/r)^{2l+1}], & r > r'. \end{cases}$$

15 Consider the Helmholtz equation $\vec{\nabla}^2 \Psi(\vec{r}) + k_0^2 \Psi(\vec{r}) = F(\vec{r})$, for the forced oscillations of a two-dimensional circular membrane (drumhead) with radius a and with the boundary conditions $\Psi(0) =$ finite and $\Psi(a) = 0$. Show that the Green's function obeying $\vec{\nabla}^2 G(\vec{r}, \vec{r}') + k_0^2 G(\vec{r}, \vec{r}') = \delta(\vec{r} - \vec{r}')$ is given as

$$G(\vec{r}, \vec{r}') = \sum_{m=0}^{\infty} \cos m(\theta - \theta') \times \begin{cases} \dfrac{J_m(ka)N_m(kr') - N_m(ka)J_m(kr')}{2\epsilon_m J_m(ka)} J_m(kr), & r < r', \\[2ex] \dfrac{J_m(ka)N_m(kr) - N_m(ka)J_m(kr)}{2\epsilon_m J_m(ka)} J_m(kr'), & r > r', \end{cases}$$

where

$$\epsilon_m = \begin{cases} 2, & m = 0, \\ 1, & m = 1, 2, 3, \ldots. \end{cases}$$

Hint: use

$$\delta(\vec{r} - \vec{r}') = \frac{\delta(r-r')}{r} \delta(\theta - \theta') = \frac{\delta(r-r')}{r} \frac{1}{2\pi} \sum_{m=-\infty}^{m=\infty} e^{im(\theta-\theta')}$$

and separate the Green's function as

$$G(\vec{r},\vec{r}\,') = \frac{1}{2\pi}\sum_{m=-\infty}^{m=\infty} g_m(r,r')e^{im(\theta-\theta')}.$$

One also needs the identity $J_m(r)N_m'(r) - J_m'(r)N_m(r) = 2/\pi r$, and ϵ_m is introduced when we combined the $\pm m$ terms to get $\cos m(\theta-\theta')$.

16 In the previous forced drumhead problem (Problem 15), first find the appropriate eigenfunctions and then show that the Green's function can also be written as

$$G(\vec{r},\vec{r}\,') = \sum_{m=0}^{\infty}\sum_{n=1}^{\infty}\frac{N_{mn}^2 J_m(k_{mn}r)J_m(k_{mn}r')\cos m(\theta-\theta')}{k^2-k_{mn}^2},$$

where the normalization constant N_{mn} is given as
$N_{mn} = \left[\sqrt{\frac{\pi\epsilon_m}{2}}aJ_m'(k_{mn}a)\right]^{-1}$. Compare the two results.

17 Consider the differential equation $\pounds\Phi(\vec{r}) = F(\vec{r})$ with the operator $\pounds = \vec{\nabla}\cdot[p(\vec{r})\vec{\nabla}] + q(r)$. Show that the solution

$$\Phi(\vec{r}\,') = \iiint_V F(\vec{r})G(\vec{r},\vec{r}\,')\,d^3\vec{r} + \iiint_V [\Phi(\vec{r})\pounds G(\vec{r},\vec{r}\,') - G(\vec{r},\vec{r}\,')\pounds\Phi(\vec{r}\,')]\,d^3\vec{r}$$

can be expressed as

$$\Phi(\vec{r}) = \int_V F(\vec{r}\,')G(\vec{r},\vec{r}\,')\,d^3\vec{r}\,' + \oint_S p(\vec{r}\,')[\Phi(\vec{r}\,')\vec{\nabla}G(\vec{r},\vec{r}\,') - G(\vec{r},\vec{r}\,')\vec{\nabla}\Phi(\vec{r}\,')]\cdot\hat{\mathbf{n}}\,ds',$$

where $\hat{\mathbf{n}}$ is the outward normal to the surface S bounding V.

18 Find the Green's function, $G(\rho,\phi,\rho',\phi')$, for the two-dimensional Helmholtz equation $[\vec{\nabla}^2 + \kappa^2]\Psi(\rho,\phi) = 0$, for the full region outside a cylindrical surface, $\rho = a$, which is appropriate for the following boundary conditions:

i) Ψ is specified everywhere on $\rho = a$.
ii) As $\rho\to\infty$, $\Psi\to\frac{e^{i\kappa\rho}}{\sqrt{\rho}}f(\phi)$; outgoing cylindrical wave. Note that Ψ is independent of z.

19 Find the solution of the following eigenvalue problem:

$$\frac{d^2\Psi}{d\theta^2} + \cot\theta\frac{d\Psi}{d\theta} + \lambda\Psi = \alpha\cos^2\theta\Psi,$$

where $\Psi = \Psi(\theta)$ is defined over the interval $0 \leq \theta \leq \pi$ and must be square-integrable with the weight function $\sin\theta$. The parameter α is $\ll 1$; hence, the solution can be expanded in terms of the positive powers of α. Find the solution, which in the limit as $\alpha \to 0$, has the eigenvalue $\lambda^{(0)} = l(l+2)$ with $l = 2$. In addition, for this eigenvalue, find the eigenvalue correct to order α^2 and the solution $\Psi(\theta)$ correct to order α.

20 Find the Green's function for the three-dimensional Helmholtz equation $[\vec{\nabla}^2 + \kappa^2]\Psi(\vec{r}) = 0$, for the region bounded by two spheres of radii a and b $(a > b)$ and which is appropriate for the boundary condition where $\Psi(\vec{r})$ is specified on the spheres of radius $r = a$ and $r = b$.

21 Find the Green's function for the Helmholtz equation outside a spherical boundary with the radius a and satisfying the boundary conditions $R(a) =$ finite and $R(r) \xrightarrow{r\to\infty} e^{ikr}/kr$.

22 Find the Green's function for the operator

$$£ = \frac{d}{dx}\left(x\frac{d}{dx}\right) - \frac{n^2}{x}, \quad n = \text{integer},$$

with the boundary conditions $y(0) = 0$ and $y(L) = y_L$.

23 In Example 18.2, show that the solution for small oscillations is $\theta = \theta_1 \sin\omega_0 t / \sin\omega_0 t_1$. Show that this result satisfies the integral Eq. (18.50) in the small oscillations limit.

19

Green's Functions and Path Integrals

In 1827, Brown investigates the random motions of pollen suspended in water under a microscope. The irregular movements of the pollen particles are due to their random collisions with the water molecules. Later, it becomes clear that many small objects interacting randomly with their environment behave the same way. Today, this motion is known as the Brownian motion and forms the prototype of many different phenomena in diffusion, colloid chemistry, polymer physics, quantum mechanics, and finance. During the years 1920–1930, Wiener approaches Brownian motion in terms of path integrals. This opens up a whole new avenue in the study of many classical systems. In 1948, Feynman gives a new formulation of quantum mechanics in terms of path integrals. In addition to the existing Schrödinger and Heisenberg formulations, this new approach not only makes the connection between quantum and classical physics clearer but also leads to many interesting applications in field theory. In this chapter, we introduce the basic features of this intriguing technique, which not only has many interesting existing applications but also has tremendous potential for future uses. In conjunction with the anomalous diffusion phenomena and the path integrals over Lévy paths, we also introduce the Fox's H-functions; a versatile and an elegant tool of applied mathematics.

19.1 Brownian Motion and the Diffusion Problem

Starting with the principle of conservation of matter, we write the **diffusion equation** as

$$\frac{\partial \rho(\overrightarrow{r}, t)}{\partial t} = D\overrightarrow{\nabla}^2 \rho(\overrightarrow{r}, t), \tag{19.1}$$

where $\rho(\overrightarrow{r}, t)$ is the density of the diffusing material and D is the diffusion constant depending on the characteristics of the medium. Because the diffusion process is also many particles undergoing **Brownian motion** at the same

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time, division of $\rho(\overrightarrow{r},t)$ by the total number of particles gives the **probability**, $w(\overrightarrow{r},t)$, of finding a particle at $\overrightarrow{r}$ and t as $w(\overrightarrow{r},t)=\rho(\overrightarrow{r},t)/N$. Naturally, $w(\overrightarrow{r},t)$ also satisfies the diffusion equation:

$$\boxed{\frac{\partial w(\overrightarrow{r},t)}{\partial t}=D\overrightarrow{\nabla}^2 w(\overrightarrow{r},t).} \tag{19.2}$$

For a particle starting its motion from $\overrightarrow{r}=0$, we have to solve Eq. (19.2) with the initial condition $\lim_{t\to 0} w(\overrightarrow{r},t)\to\delta(\overrightarrow{r})$. In one dimension, Eq. (19.2):

$$\frac{\partial w(x,t)}{\partial t}=D\frac{\partial^2 w(x,t)}{\partial x^2}, \tag{19.3}$$

can be solved using the Fourier transform technique as

$$w(x,t)=\frac{1}{\sqrt{4\pi Dt}}\exp\left\{-\frac{x^2}{4Dt}\right\}. \tag{19.4}$$

This is consistent with the probability interpretation of $w(x,t)$, which is always positive. Because it is certain that the particle is somewhere in the interval $(-\infty,\infty)$, $w(x,t)$ also satisfies the normalization condition

$$\int_{-\infty}^{\infty} dx w(x,t)=\int_{-\infty}^{\infty} dx\frac{1}{\sqrt{4\pi Dt}}\exp\left\{-\frac{x^2}{4Dt}\right\}=1. \tag{19.5}$$

For a particle starting its motion from an arbitrary point (x_0,t_0), we write the probability distribution as

$$W(x,t,x_0,t_0)=\frac{1}{\sqrt{4\pi D(t-t_0)}}\exp\left\{-\frac{(x-x_0)^2}{4D(t-t_0)}\right\}, \tag{19.6}$$

where $W(x,t,x_0,t_0)$ is the solution of

$$\frac{\partial W(x,t,x_0,t_0)}{\partial t}=D\frac{\partial^2 W(x,t,x_0,t_0)}{\partial x^2} \tag{19.7}$$

satisfying the initial condition $\lim_{t\to t_0} W(x,t,x_0,t_0)\to\delta(x-x_0)$ and the normalization condition $\int_{-\infty}^{\infty} dx W(x,t,x_0,t_0)=1$.

From our discussion of Green's functions in Chapter 18, we recall that $W(x,t,x_0,t_0)$ is also the **propagator** of the operator

$$£=\frac{\partial}{\partial t}-D\frac{\partial^2}{\partial x^2}. \tag{19.8}$$

Thus, given the probability at some initial point and time, $w(x_0,t_0)$, we can find the probability at subsequent times, $w(x,t)$, using $W(x,t,x_0,t_0)$ as

$$w(x,t)=\int_{-\infty}^{\infty} dx_0 W(x,t,x_0,t_0)w(x_0,t_0),\quad t>t_0. \tag{19.9}$$

Combination of propagators gives us the **Einstein-Smoluchowski-Kolmogorov–Chapman** equation (ESKC):

$$\boxed{W(x,t,x_0,t_0) = \int_{-\infty}^{\infty} dx'\, W(x,t,x',t')W(x',t',x_0,t_0), \quad t > t' > t_0.} \tag{19.10}$$

The significance of this equation is that it gives the causal connection of events in Brownian motion as in the Huygens–Fresnel equation.

19.1.1 Wiener Path Integral and Brownian Motion

In Eq. (19.9), we have seen how to find the probability of finding a particle at (x, t) from the probability at (x_0, t_0) using the propagator $W(x, t, x_0, t_0)$. We now divide the interval between t_0 and t into $N + 1$ equal segments:

$$\Delta t_i = t_i - t_{i-1} = \frac{t - t_0}{N + 1}, \tag{19.11}$$

which is covered by the particle in N steps. The propagator of each step is given as

$$W(x_i, t_i, x_{i-1}, t_{i-1}) = \frac{1}{\sqrt{4\pi D(t_i - t_{i-1})}} \exp\left\{-\frac{(x_i - x_{i-1})^2}{4D(t_i - t_{i-1})}\right\}. \tag{19.12}$$

Assuming that each step is taken independently, we combine propagators N times using the ESKC relation to get the propagator that takes us from (x_0, t_0) to (x, t) in a single step as

$$W(x,t,x_0,t_0) = \int \cdots \int \exp\left\{-\sum_{i=1}^{N+1} \frac{(x_i - x_{i-1})^2}{4D(t_i - t_{i-1})}\right\} \prod_{i=1}^{N} \frac{dx_i}{\sqrt{4\pi D(t_i - t_{i-1})}}. \tag{19.13}$$

This equation is valid for $N > 0$. Assuming that it is also valid in the limit as $N \to \infty$, that is, as $\Delta t_i \to 0$, we write

$$W(x,t,x_0,t_0) = \lim_{\substack{N\to\infty,\\ \Delta t_i \to 0}} \int \cdots \int \exp\left\{-\frac{1}{4D} \sum_{i=1}^{N+1} \left(\frac{x_i - x_{i-1}}{t_i - t_{i-1}}\right)^2 \Delta t_i\right\} \prod_{i=1}^{N} \frac{dx_i(\tau)}{\sqrt{4\pi D \Delta t_i}}, \tag{19.14}$$

$$W(x,t,x_0,t_0) = \int \cdots \int \exp\left\{-\frac{1}{4D} \int_{t_0}^{t} \dot{x}^2(\tau)\, d\tau\right\} \prod_{\tau=t_0}^{t} \frac{dx(\tau)}{\sqrt{4\pi D d\tau}}. \tag{19.15}$$

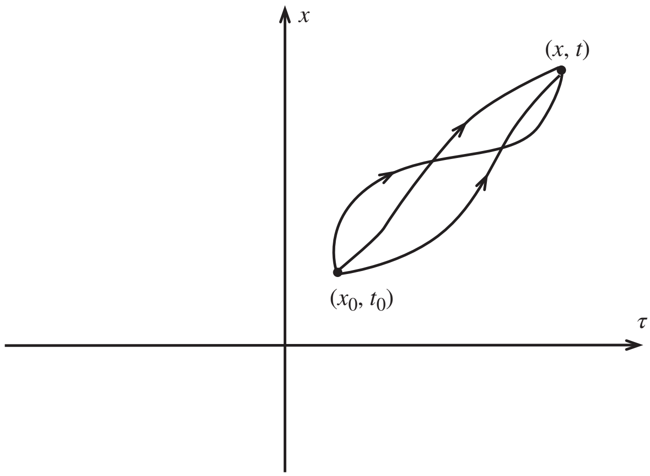

Figure 19.1 Paths $C[x_0, t_0; x, t]$ for the pinned Wiener measure.

Here, τ is a time parameter (Figure 19.1) introduced to parametrize the paths as $x(\tau)$. We can also write $W(x, t, x_0, t_0)$ in short as

$$W(x, t, x_0, t_0) = \check{N} \int \exp\left\{-\frac{1}{4D}\int_{t_0}^{t} \dot{x}^2(\tau)\, d\tau\right\} \check{D}x(\tau), \tag{19.16}$$

where $\check{N}$ is a normalization constant and $\check{D}x(\tau)$ indicates that the integral should be taken over all paths starting from (x_0, t_0) and end at (x, t). This expression can also be written as

$$\boxed{W(x, t, x_0, t_0) = \int_{C[x_0, t_0; x, t]} d_w x(\tau),} \tag{19.17}$$

where $d_w x(\tau)$ is called the **Wiener measure**. Because $d_w x(\tau)$ is the measure for all paths starting from (x_0, t_0) and ending at (x, t), it is called the **pinned** or **conditional Wiener measure** (Figure 19.1). It is important to note that for $N + 1$ segments, when N is finite, there are $N + 1$ propagators connected by N variables x_i, hence there is one more factor of the square root in Eq. (19.14) [see Eqs. (19.168) and (19.169)].

Summary: For a particle starting its motion from (x_0, t_0) and ending at (x, t) the **propagator**, $W(x, t, x_0, t_0)$, is given as

$$\boxed{W(x, t, x_0, t_0) = \frac{1}{\sqrt{4\pi D(t - t_0)}} \exp\left\{-\frac{(x - x_0)^2}{4D(t - t_0)}\right\}.} \tag{19.18}$$

This satisfies the **differential equation**

$$\boxed{\frac{\partial W(x,t,x_0,t_0)}{\partial t} = D\frac{\partial^2}{\partial x^2}W(x,t,x_0,t_0)} \tag{19.19}$$

with the **initial condition** $\lim_{t\to t_0} W(x,t,x_0,t_0) \to \delta(x-x_0)$.

In terms of the **Wiener path integral**, the **propagator** $W(x,t,x_0,t_0)$ is also expressed as

$$\boxed{W(x,t,x_0,t_0) = \int_{C[x_0,t_0;x,t]} d_w x(\tau),} \tag{19.20}$$

whereas $N \to \infty$, the **measure** of this integral is

$$\boxed{d_w x(\tau) = \exp\left\{-\frac{1}{4D}\int_{t_0}^{t} \dot{x}^2(\tau)d\tau\right\}\prod_{i=1}^{N}\frac{dx_i}{\sqrt{4\pi D\, d\tau}}.} \tag{19.21}$$

Because the integral is taken over all continuous paths from (x_0, t_0) to (x, t), which are shown as $C[x_0, t_0; x, t]$, this measure is also called the **pinned Wiener measure** (Figure 19.1).

For a particle starting from (x_0, t_0), the probability of finding it in the interval Δx at time t is given by

$$\boxed{\Delta x\int_{C[x_0,t_0;t]} d_w x(\tau).} \tag{19.22}$$

In this integral, because the position of the particle at time t is not fixed, $d_w x(\tau)$ is called the **unpinned,** or **unconditional Wiener measure.** At time t, because it is certain that the particle is somewhere in the interval $x \in [-\infty, \infty]$, we write (Figure 19.2)

$$\int_{C[x_0,t_0;t]} d_w x(\tau) = \int_{-\infty}^{\infty} dx \int_{C[x_0,t_0;x,t]} d_w x(\tau) = 1. \tag{19.23}$$

The average of a functional, $F[x(t)]$, found over all paths $C[x_0, t_0; t]$ at time t is given by the formula

$$\langle F[x(t)]\rangle_C = \int_{C[x_0,t_0;t]} d_w x(\tau)F[x(\tau)] \tag{19.24}$$

$$= \int_{-\infty}^{\infty} dx \int_{C[x_0,t_0;x,t]} d_w x(\tau)F[x(\tau)]. \tag{19.25}$$

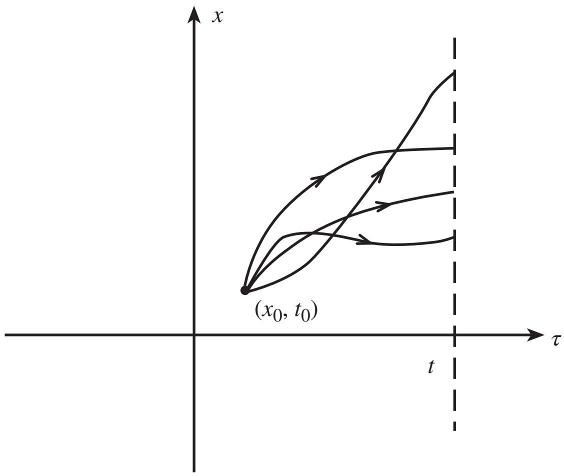

Figure 19.2 Paths $C[x_0, t_0; t]$ for the unpinned Wiener measure.

In terms of the Wiener measure, we can express the **ESKC** relation as

$$\boxed{\int_{C[x_0,t_0;x,t]} d_w x(\tau) = \int_{-\infty}^{\infty} dx' \int_{C[x_0,t_0;x',t']} d_w x(\tau) \int_{C[x',t';x,t]} d_w x(\tau).} \tag{19.26}$$

19.1.2 Perturbative Solution of the Bloch Equation

We have seen that the propagator of the diffusion equation:

$$\frac{\partial w(x,t)}{\partial t} - D\frac{\partial^2 w(x,t)}{\partial x^2} = 0, \tag{19.27}$$

can be expressed as a path integral [Eq. (19.20)]. However, when we have a closed expression as in Eq. (19.18), it is not clear what advantage this new representation has. In this section, we study the diffusion equation in the presence of interactions, where the advantages of the path integral approach begin to appear. In the presence of a potential, $V(x)$, the diffusion equation can be written as

$$\boxed{\frac{\partial w(x,t)}{\partial t} - D\frac{\partial^2 w(x,t)}{\partial x^2} = -V(x,t)w(x,t),} \tag{19.28}$$

which is also known as the **Bloch equation**. We now need a **Green's function**, $W_D(x,t,x',t')$, that satisfies the inhomogeneous equation:

$$\frac{\partial W_D(x,t,x',t')}{\partial t} - D\frac{\partial^2 W_D(x,t,x',t')}{\partial x^2} = \delta(x-x')\delta(t-t'), \tag{19.29}$$

so that we can express the general solution of Eq. (19.28) as

$$\boxed{w(x,t) = w_0(x,t) - \iint W_D(x,t,x',t')V(x',t')w(x',t')\,dx'dt',} \tag{19.30}$$

where $w_0(x,t)$ is the solution of the homogeneous part of Eq. (19.28), that is, Eq. (19.3).

We can construct $W_D(x,t,x',t')$ using the **propagator**, $W(x,t,x',t')$, that satisfies the homogeneous equation (Chapter 18)

$$\frac{\partial W(x,t,x',t')}{\partial t} - D\frac{\partial^2 W(x,t,x',t')}{\partial x^2} = 0, \tag{19.31}$$

as

$$W_D(x,t,x',t') = W(x,t,x',t')\theta(t-t'). \tag{19.32}$$

Because the unknown function also appears under the integral sign, Eq. (19.30) is still not the solution, that is, it is just the integral equation version of Eq. (19.28). On the other hand $W_B(x,t,x',t')$, which satisfies the Bloch equation:

$$\boxed{\frac{\partial W_B(x,t,x',t')}{\partial t} - D\frac{\partial^2 W_B(x,t,x',t')}{\partial x^2} = -V(x,t)W_B(x,t,x',t'),} \tag{19.33}$$

is given as

$$\begin{aligned} W_B(x,t,x_0,t_0) &= W_D(x,t,x_0,t_0) \\ &\quad - \int_{-\infty}^{\infty} dx' \int_{-\infty}^{\infty} dt'\, W_D(x,t,x',t')V(x',t')W_B(x',t',x_0,t_0). \end{aligned} \tag{19.34}$$

The first term on the right-hand side is the solution, $W(x,t,x',t')$, of the homogeneous equation [Eq. (19.31)]. However, since $t > t_0$, Eq. (19.32) allows us to write it as $W_D(x,t,x_0,t_0)$.

A very useful formula called the **Feynman–Kac formula**, or theorem, is given as

$$\boxed{W_B(x,t,x_0,0) = \int_{C[x_0,0;x,t]} d_w x(\tau) \exp\left\{-\int_0^t d\tau\, V[x(\tau),\tau]\right\}.} \tag{19.35}$$

This is a **solution** of Eq. (19.33) with the initial condition

$$\boxed{\lim_{t\to t'} W_B(x,t,x',t') = \delta(x-x').} \tag{19.36}$$

The Feynman-Kac theorem constitutes a very important step in the development of path integrals. We leave its proof to the next section and continue by writing the path integral in Eq. (19.35) as a **Riemann sum**:

$$W_B(x,t,x_0,0) = \lim_{\substack{N\to\infty,\\ \varepsilon\to 0}} (4\pi D\varepsilon)^{-(N+1)/2} \int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dx_2 \cdots \int_{-\infty}^{\infty} dx_N \\ \times \exp\left\{-\frac{1}{4D\varepsilon}\sum_{j=1}^{N+1}(x_j - x_{j-1})^2 - \varepsilon\sum_{j=1}^{N} V(x_j,t_j)\right\}, \quad (19.37)$$

where we have taken

$$\varepsilon = t_i - t_{i-1} = \frac{t-t_0}{N+1}. \quad (19.38)$$

The first exponential factor in Eq. (19.37) is the solution [Eq. (19.13)] of the homogeneous equation. After expanding the second exponential factor as

$$\exp\left\{-\varepsilon\sum_{j=1}^{N} V(x_j,t_j)\right\} \quad (19.39)$$
$$= 1 - \varepsilon\sum_{j=1}^{N} V(x_j,t_j) + \frac{1}{2}\varepsilon^2 \sum_{j=1}^{N}\sum_{k=1}^{N} V(x_j,t_j)V(x_k,t_k) - \cdots,$$

we integrate over the intermediate x variables and rearrange to obtain

$$W_B(x,t,x_0,t_0) = W(x,t,x_0,t_0) \quad (19.40)$$
$$- \varepsilon\sum_{j=1}^{N}\int_{-\infty}^{\infty} dx_j W(x,t,x_j,t_j)V(x_j,t_j)W(x_j,t_j,x_0,t_0)$$
$$+ \frac{1}{2!}\varepsilon^2\sum_{j=1}^{N}\sum_{k=1}^{N}\int_{-\infty}^{\infty} dx_j \int_{-\infty}^{\infty} dx_k W(x,t,x_j,t_j)V(x_j,t_j)W(x_j,t_j,x_k,t_k)$$
$$\times V(x_k,t_k)W(x_k,t_k,x_0,t_0) + \cdots.$$

In the limit as $\varepsilon \to 0$, we now make the replacement $\varepsilon\sum_j \to \int_{t_0}^{t} dt_j$ and suppress the factors of factorials, $1/n!$, since they are multiplied by ε^n, which also goes to zero as $\varepsilon \to 0$. Besides, because the times in Eq. (19.40) are ordered as $t_0 < t_1 < t_2 < \cdots < t$, we replace W with W_D and write W_B as

$$W_B(x,t,x_0,t_0) = W_D(x,t,x_0,t_0) \quad (19.41)$$
$$- \int_{-\infty}^{\infty} dx' \int_{t_0}^{t} dt' W_D(x,t,x',t')V(x',t')W_D(x',t',x_0,t_0)$$
$$+ \int_{-\infty}^{\infty} dx' \int_{t_0}^{t} dt' \int_{-\infty}^{\infty} dx'' \int_{t_0'}^{t'} dt'' W_D(x,t,x',t')V(x',t')W_D(x',t',x'',t'')$$
$$\times V(x'',t'')W_D(x'',t'',x_0,t_0) + \cdots.$$

Now $W_B(x, t, x_0, t_0)$ no longer appears on the right-hand side of this equation. Thus, it is the **perturbative solution** of Eq. (19.34) by the iteration method. Note that $W_B(x, t, x_0, t_0)$ satisfies the initial condition given in Eq. (19.36).

19.1.3 Derivation of the Feynman–Kac Formula

We now show that the Feynman–Kac formula:

$$W_B(x, t, x_0, 0) = \int_{C[x_0,0;x,t]} d_w x(\tau) \exp\left\{ - \int_0^t d\tau V[x(\tau), \tau] \right\}, \tag{19.42}$$

is identical to the iterative solution to all orders of the following integral equation:

$$\begin{aligned} W_B(x, t, x_0, t_0) = {} & W_D(x, t, x_0, t_0) \\ & - \int_{-\infty}^{\infty} dx' \int_0^t dt' W_D(x, t, x', t') V(x', t') W_B(x', t', x_0, t_0), \end{aligned} \tag{19.43}$$

which is equivalent to the differential equation

$$\frac{\partial W_B(x, t, x', t')}{\partial t} - D\frac{\partial^2 W_B(x, t, x', t')}{\partial x^2} = -V(x, t) W_B(x, t, x', t') \tag{19.44}$$

with the initial condition given in Eq. (19.36).

We first show that the Feynman-Kac formula satisfies the ESKC [Eq. (19.10)] relation. Note that we write $V[x(\tau)]$ instead of $V[x(\tau), \tau]$ when there is no room for confusion:

$$\begin{aligned} & \int_{-\infty}^{\infty} dx_s W_B(x, t, x_s, t_s) W_B(x_s, t_s, x_0, 0) \\ & = \int_{-\infty}^{\infty} dx_s \int_{C[x_0,0;x_s,t_s]} d_w x(\tau) \exp\left\{ - \int_0^s d\tau V[x(\tau)] \right\} \\ & \quad \times \int_{C[x_s,t_s;x,t]} d_w x(\tau') \exp\left\{ - \int_{t_s}^t d\tau' V[x(\tau')] \right\}. \end{aligned} \tag{19.45}$$

In this equation, x_s denotes the position at t_s, and x denotes the position at t. Because $C[x_0, 0; x_\tau, t_\tau; x, t]$ denotes all paths starting from $(x_0, 0)$, passing through (x_τ, t_τ) and then ending up at (x, t), we can write the right-hand side of the above equation as

$$\int_{-\infty}^{\infty} dx_s \int_{C[x_0,0;x_s,t_s;x,t]} d_w x(\tau) \exp\left\{ - \int_0^{t_s} d\tau V[x(\tau)] \right\}$$

$$= \int_{C[x_0,0;x,t]} d_w x(\tau) \exp\left\{ - \int_0^t d\tau V[x(\tau)] \right\} \tag{19.46}$$

$$= W_B(x, t, x_0, 0), \tag{19.47}$$

which shows that the Feynman–Kac formula satisfies the ESKC relation:

$$\int_{-\infty}^{\infty} dx_s W_B(x,t,x_s,t_s) W_B(x_s,t_s,x_0,0) = W_B(x,t,x_0,0). \tag{19.48}$$

Using Eqs. (19.17) and (19.18), we also see that the Feynman–Kac formula satisfies the initial condition:

$$\lim_{t\to 0} W_B(x,t,x_0,0) \to \delta(x-x_0). \tag{19.49}$$

The functional in the Feynman–Kac formula satisfies the equality

$$\exp\left\{-\int_0^t d\tau V[x(\tau)]\right\} = 1 - \int_0^t d\tau \left(V[x(\tau)] \exp\left\{-\int_0^\tau ds V[x(s)]\right\}\right), \tag{19.50}$$

which we can easily show by taking the derivative of both sides. Because this equality holds for all continuous paths, $x(s)$, we take the integral of both sides over the paths $C[x_0,0;x,t]$ via the Wiener measure to get

$$\begin{aligned}\int_{C[x_0,0;x,t]} d_w x(\tau) \exp\left\{-\int_0^t d\tau V[x(\tau)]\right\} &= \int_{C[x_0,0;x,t]} d_w x(\tau) \\ &- \int_{C[x_0,0;x,t]} d_w x(\tau) \int_0^t d\tau \left(V[x(\tau)] \exp\left\{-\int_0^\tau ds V[x(s)]\right\}\right).\end{aligned} \tag{19.51}$$

The first term on the right-hand side is the solution of the homogeneous part of Eq. (19.33). Also for $t > 0$, Eq. (19.32) allows us to write $W_D(x_0,0,x,t)$ instead of $W(x_0,0,x,t)$. Since the integral in the second term involves exponentially decaying terms, it converges. Hence, we can interchange the order of the integrals to write

$$\int_{C[x_0,0;x,t]} d_w x(s) \int_0^t ds \left(V[x(s)] \exp\left\{-\int_0^s d\tau V[x(\tau)]\right\}\right)$$

$$= \int_0^t ds \int_{C[x_0,0;x,t]} d_w x(s) \left[V[x(s)] \exp\left\{-\int_0^s d\tau V[x(\tau)]\right\}\right] \tag{19.52}$$

$$= \int_0^t ds \int_{-\infty}^{\infty} dx_s \int_{C[x_0,0;x_s,t_s;x,t]} d_w x(s) \left[V[x(s)] \exp\left\{-\int_0^s d\tau V[x(\tau)]\right\}\right] \tag{19.53}$$

$$= \int_0^t ds \int_{-\infty}^{\infty} dx_s V[x(s)] \int_{C[x_0,0;x_s,t_s]} d_w x(\tau) \left[\exp\left\{-\int_0^s d\tau V[x(\tau)]\right\}\right] \tag{19.54}$$

$$\times \int_{C[x_s,t_s;x,t]} d_w x(\tau)$$

$$= \int_0^t ds \int_{-\infty}^{\infty} dx_s V[x(s)] W_B(x_s,t_s,x_0,0) W_D(x,t,x_s,t_s), \tag{19.55}$$

where we have used the ESKC relation. We now substitute this to Eq. (19.51) and use the result in Eq. (19.42) to obtain

$$W_B(x,t,x_0,0) = \int_{C[x_0,0;x,t]} d_w x(\tau) \exp\left\{-\int_0^t d\tau V[x(\tau),\tau]\right\} \tag{19.56}$$

$$= W_D(x,t,x_0,0) \tag{19.57}$$

$$-\int_{-\infty}^{\infty} dx' \int_0^t dt' W_D(x,t,x',t')V(x',t')W_B(x',t',x_0,0).$$

This is nothing but Eq. (19.34), thus proving the Feynman–Kac formula. Generalization to arbitrary initial time t_0 is obvious.

19.1.4 Interpretation of $V(x)$ in the Bloch Equation

We have seen that the **solution** of the **Bloch equation**:

$$\frac{\partial W_B(x,t,x_{0,}t_0)}{\partial t} - D\frac{\partial^2 W_B(x,t,x_{0,}t_0)}{\partial x^2} = -V(x,t)W_B(x,t,x_{0,}t_0), \tag{19.58}$$

with the initial condition

$$W_B(x,t,x_{0,}t_0)|_{t=t_0} = \delta(x-x_0), \tag{19.59}$$

is given by the **Feynman-Kac formula**:

$$W_B(x,t;x_0,t_0) = \int_{C[x_0,t_0;x,t]} d_w x(\tau) \exp\left\{-\int_{t_0}^t V[x(\tau),\tau]d\tau\right\}. \tag{19.60}$$

In these equations, even though $V(x)$ is not exactly a potential, it is closely related to the external forces acting on the system.

In fluid mechanics, the probability distribution of a particle undergoing Brownian motion and under the influence of an external force satisfies the differential equation

$$\frac{\partial W(x,t;x_0,t_0)}{\partial t} - D\frac{\partial^2 W(x,t;x_0,t_0)}{\partial x^2} = -\frac{1}{\eta}\frac{\partial}{\partial x}[F(x)W(x,t;x_0,t_0)], \tag{19.61}$$

where η is the friction coefficient in the drag force, which is proportional to the velocity. In Eq. (19.61), if we try a solution of the form

$$W(x,t;x_0,t_0) = \exp\left\{\frac{1}{2\eta D}\int_{x_0}^x dx F(x)\right\}\widetilde{W}(x,t;x_0,t_0), \tag{19.62}$$

we obtain a differential equation to be solved for $\widetilde{W}(x,t;x_0,t_0)$:

$$\frac{\partial \widetilde{W}(x,t;x_0,t_0)}{\partial t} - D\frac{\partial^2 \widetilde{W}(x,t;x_0,t_0)}{\partial x^2} = -V(x)\widetilde{W}(x,t;x_0,t_0), \tag{19.63}$$

where we have defined $V(x)$ as

$$V(x) = \frac{1}{4\eta^2 D} F^2(x) + \frac{1}{2\eta}\frac{dF(x)}{dx}. \tag{19.64}$$

Using the Feynman–Kac formula as the solution of Eq. (19.63), we can write the solution of Eq. (19.61) as

$$W(x,t;x_0,t_0) = \exp\left\{\frac{1}{2\eta D}\int_{x_0}^{x} dxF(x)\right\}\int_{C[x_0,t_0;x,t]} d_w x(\tau) \times \exp\left\{-\int_{t_0}^{t} V[x(\tau)]d\tau\right\}. \tag{19.65}$$

With the Wiener measure [Eq. (19.21)], we rewrite this equation as

$$W(x,t;x_0,t_0) = \int_{C[x_0,t_0;x,t]} \prod_{\tau=t_0}^{t} \frac{dx(\tau)}{\sqrt{4\pi D d\tau}} \times \exp\left\{\frac{1}{2\eta D}\int_{x_0}^{x} dxF(x) - \frac{1}{4D}\int_{t_0}^{t} d\tau x^2(\tau) - \int_{t_0}^{t} d\tau V[x(\tau)]\right\}. \tag{19.66}$$

Finally, using the equality $\int_{x_0}^{x} dxF(x) = \int_{t_0}^{t} d\tau \dot{x} F(x)$, we write

$$W(x,t;x_0,t_0) = \int_{C[x_0,t_0;x,t]} \prod_{\tau=t_0}^{t} \frac{dx(\tau)}{\sqrt{4\pi D d\tau}} \times \exp\left\{\frac{1}{2\eta D}\int_{t_0}^{t} d\tau \dot{x} F(x) - \frac{1}{4D}\int_{t_0}^{t} d\tau \dot{x}^2(\tau) - \int_{t_0}^{t} d\tau V[x(\tau)]\right\} \tag{19.67}$$

$$= \int_{C[x_0,t_0;x,t]} \exp\left\{-\frac{1}{4D}\int_{t_0}^{t} d\tau L[x(\tau)]\right\} \prod_{\tau=t_0}^{t} \frac{dx(\tau)}{\sqrt{4\pi D d\tau}}, \tag{19.68}$$

where we have defined

$$L[x(\tau)] = \left(\dot{x} - \frac{F}{\eta}\right)^2 + 2\frac{D}{\eta}\frac{dF}{dx} \tag{19.69}$$

and used Eq. (19.64).

As we see from here, $V(x)$ is not quite the potential, nor is $L[x(\tau)]$ the Lagrangian. In the limit as $D \to 0$, fluctuations in the Brownian motion disappear and the argument of the exponential function goes to infinity. Thus, only the path satisfying the condition

$$\int_{t_0}^{t} d\tau \left(\dot{x} - \frac{F}{\eta}\right)^2 = 0, \tag{19.70}$$

or

$$\frac{dx}{d\tau} - \frac{F}{\eta} = 0, \tag{19.71}$$

contributes to the path integral in Eq. (19.68). Comparing this with

$$mx = -\eta\dot{x} + F(x), \tag{19.72}$$

we see that it is the deterministic equation of motion of a particle with negligible mass, moving under the influence of an external force, $F(x)$, and a friction force $-\eta\dot{x}$ [12, p. 463].

When the diffusion constant differs from zero, the solution is given as the path integral

$$W(x,t,x_0,t_0) = \int_{C[x_0,t_0;x,t]} \exp\left\{-\frac{1}{4D}\int_{t_0}^{t} d\tau L[x(\tau)]\right\} \prod_{\tau=t_0}^{t} \frac{dx(\tau)}{\sqrt{4\pi D d\tau}}. \tag{19.73}$$

In this case, all the continuous paths between (x_0, t_0) and (x, t) will contribute to the integral. It is seen from Eq. (19.73) that each path contributes to the propagator $W(x, t, x_0, t_0)$ with the **weight factor**

$$\exp\left\{-\frac{1}{4D}\int_{t_0}^{t} d\tau L[x(\tau)]\right\}. \tag{19.74}$$

Naturally, majority of the contribution comes from places where the paths with comparable weights cluster. These paths are the ones that make the functional in the exponential an extremum, that is,

$$\delta \int_{t_0}^{t} d\tau L[x(\tau)] = 0. \tag{19.75}$$

These paths are the solutions of the **Euler–Lagrange equation**:

$$\frac{\partial L}{\partial x} - \frac{d}{d\tau}\left[\frac{\partial L}{\partial(dx/d\tau)}\right] = 0. \tag{19.76}$$

At this point, we remind the reader that $L[x(\tau)]$ is not quite the Lagrangian of the particle undergoing Brownian motion. It is intriguing that $V(x)$ and $L[x(\tau)]$ gain their true meaning only when we consider the applications of path integrals to quantum mechanics.

19.2 Methods of Calculating Path Integrals

We have obtained the solution of Eq. (19.28):

$$\frac{\partial w(x,t)}{\partial t} - D\frac{\partial^2 w(x,t)}{\partial x^2} = -V(x,t)w(x,t), \tag{19.77}$$

as

$$W(x,t;x_0,t_0)$$
$$= \check{N} \int_{C[x_0,t_0;x,t]} \exp\left\{-\frac{1}{4D}\int_{t_0}^{t} \dot{x}^2(\tau)\, d\tau - \int_{t_0}^{t} V[x(\tau)]\, d\tau\right\} \check{D}x(\tau). \tag{19.78}$$

In term of the Wiener measure, this can also be written as [Eq. (19.35)]

$$W(x,t;x_0,t_0) = \check{N} \int_{C[x_0,t_0;x,t]} \exp\left\{-\int_{t_0}^{t} V[x(\tau)]\, d\tau\right\} d_w x(\tau), \tag{19.79}$$

where $d_w x(\tau)$ is defined as

$$d_w x(\tau) = \exp\left\{-\frac{1}{4D}\int_{t_0}^{t} \dot{x}^2(\tau)\, d\tau\right\} \prod_{\tau=t_0}^{t} \frac{dx(\tau)}{\sqrt{4\pi D dt}}. \tag{19.80}$$

The average of a functional $F[x(\tau)]$ over the paths $C[x_0,t_0;x,t]$ is defined as

$$\boxed{\langle F[x(\tau)]\rangle_C = \int_{C[x_0,t_0;x,t]} F[x(\tau)] \exp\left\{-\int_{t_0}^{t} V[x(\tau)]\, d\tau\right\} d_w x(\tau),} \tag{19.81}$$

where $C[x_0,t_0;x,t]$ denotes all continuous paths starting from (x_0,t_0) and ending at (x,t). Before we discuss techniques of evaluating path integrals, we should talk about a technical problem that exists in Eq. (19.79). In this expression, even though all the paths in $C[x_0,t_0;x,t]$ are continuous, because of the nature of the Brownian motion they zig zag. The average distance squared covered by a Brown particle is given as

$$\langle x^2\rangle = \int_{-\infty}^{\infty} w(x,t)x^2\, dx \propto t. \tag{19.82}$$

From here, we find the average distance covered during time t as $\sqrt{\langle x^2\rangle} \propto \sqrt{t}$, which gives the velocity of the particle at any point as $\lim_{t\to 0}\sqrt{t}/t \to \infty$. Thus, $\dot{x}$ appearing in the propagator [Eq. (19.78)] is actually undefined for all t values. However, the integrals in Eqs. (19.79) and (19.80) are convergent for $V(x) \geq c$, where c is some constant. In Eq. (19.79), $W(x,t,x_0,t_0)$ is always positive, thus consistent with its probability interpretation and satisfies the ESKC relation [Eq. (19.10)], and the normalization condition $\int_{C[x_0,t_0;x,t]} d_w x(\tau) = 1$. In summary, if we look at Eq. (19.79) as a probability distribution, it is basically Eq. (19.78) written as a path integral evaluated over all Brown paths with a suitable weight factor depending on the potential $V(x)$.

The zig zag motion of the particles in Brownian motion is essential in the fluid exchange process of living cells. In fractal theory, paths of Brown particles are two-dimensional fractal curves. The possible connections between fractals, path integrals, and differintegrals are active areas of research.

19.2.1 Method of Time Slices

Let us evaluate the path integral of the functional $F[x(\tau)]$ with the Wiener measure. We slice a given path $x(\tau)$ into N equal time intervals and approximate the path in each slice with a straight line $l_N(\tau)$ as

$$l_N(t_i) = x(t_i) = x_i, \quad i = 1, 2, 3, \ldots, N. \tag{19.83}$$

This means that for a given path, $x(\tau)$, and a small number ε, we can always find a number $N = N(\varepsilon)$ independent of τ such that $|x(\tau) - l_N(\tau)| < \varepsilon$ is true. Under these conditions, for smooth functionals (Figure 19.3), the inequality $|F[x(\tau)] - F[l_N(\tau)]| < \delta(\varepsilon)$ is satisfied such that in the limit as $\varepsilon \to 0$, the limit $\delta(\varepsilon) \to 0$ is true. Because all the information about $l_N(\tau)$ is contained in the set

$$x_1 = x(t_1), \ldots, x_N = x(t_N), \tag{19.84}$$

we can also describe the functional $F[l_N(\tau)]$ by

$$F[l_N(\tau)] = F_N(x_1, x_2, \ldots, x_N), \tag{19.85}$$

which means that

$$\begin{aligned}
&\left| \int_{C[0,0;t]} d_w x(\tau) F[x(\tau)] - \int_{C[0,0;t]} d_w x(\tau) F_N(x_1, x_2, \ldots, x_N) \right| \\
&\quad \le \int_{C[0,0;t]} d_w x(\tau) |F[x(\tau)] - F_N(x_1, x_2, \cdots, x_N)| &(19.86)\\
&\quad \le \int_{C[0,0;t]} d_w x(\tau) \delta(\varepsilon) &(19.87)\\
&\quad \le \delta(\varepsilon) \int_{C[0,0;t]} d_w x(\tau) &(19.88)\\
&\quad \le \delta(\varepsilon). &(19.89)
\end{aligned}$$

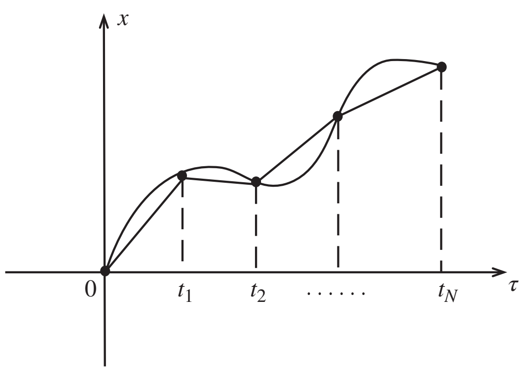

Figure 19.3 Paths for the time slice method.

Because for $N = 1, 2, 3, \dots$, the function set $F_N(x_1, x_2, \dots, x_N)$ forms a Cauchy set approaching $F[x(\tau)]$, for a suitably chosen N, we can use the integral

$$\int_{C[0,0;t]} d_w x(\tau) F_N(x_1, x_2, \dots, x_N) \tag{19.90}$$
$$= \int_{-\infty}^{\infty} \frac{dx_1}{\sqrt{4\pi D t_1}} \cdots \frac{dx_N}{\sqrt{4\pi D(t_N - t_{N-1})}} F_N(x_1, x_2, \dots, x_N)$$
$$\times \exp\left\{ -\frac{1}{4D} \sum_{i=1}^{N} \frac{(x_i - x_{i-1})^2}{t_i - t_{i-1}} \right\}$$

to evaluate the path integral

$$\int_{C[0,0;t]} d_w x(\tau) F[x(\tau)] \tag{19.91}$$
$$= \lim_{N\to\infty} \int_{-\infty}^{\infty} \frac{dx_1}{\sqrt{4\pi D t_1}} \cdots \frac{dx_N}{\sqrt{4\pi D(t_N - t_{N-1})}} F_N(x_1, x_2, \dots, x_N)$$
$$\times \exp\left\{ -\frac{1}{4D} \sum_{i=1}^{N} \frac{(x_i - x_{i-1})^2}{t_i - t_{i-1}} \right\}.$$

For a given ε, the difference between the two approaches can always be kept less than a small number, $\delta(\varepsilon)$, by choosing a suitable $N(\varepsilon)$. In this approach, a Wiener path integral:

$$\int_{C[0,0;t]} d_w x(\tau) F[x(\tau)], \tag{19.92}$$

will be converted to an N-dimensional integral [Eq. (19.90)].

19.2.2 Path Integrals With the ESKC Relation

We introduce this method by evaluating the path integral of a functional

$$F[x(\tau)] = x(\tau), \tag{19.93}$$

in the interval $[0, t]$ via the unpinned Wiener measure. Let τ be any time in the interval $[0, t]$. Using Eq. (19.24) and the ESKC relation, we can write the path integral

$$\int_{C[x_0,0;t]} d_w x(\tau)\, x(\tau) \tag{19.94}$$

as

$$\int_{C[x_0,0;t]} d_w x(\tau) x(\tau)$$
$$= \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dx_\tau x_\tau \int_{C[x_0,0;x_\tau,\tau]} d_w x(\tau) \int_{C[x_\tau,\tau;x,t]} d_w x(\tau) \tag{19.95}$$

$$= \int_{-\infty}^{\infty} dx_\tau x_\tau \int_{C[x_0,0;x_\tau,\tau]} d_w x(\tau) \int_{-\infty}^{\infty} dx \int_{C[x_\tau,\tau;x,t]} d_w x(\tau) \tag{19.96}$$

$$= \int_{-\infty}^{\infty} dx_\tau x_\tau \int_{C[x_0,0;x_\tau,\tau]} d_w x(\tau) \int_{C[x_\tau,\tau;t]} d_w x(\tau). \tag{19.97}$$

From Eq. (19.23), the value of the last integral is 1. Finally, using Eqs. (19.20) and (19.18), we obtain

$$\int_{C[x_0,0;t]} d_w x(\tau) x(\tau)$$

$$= \int_{-\infty}^{\infty} dx_\tau x_\tau W(x_\tau, \tau, x_0, 0) \tag{19.98}$$

$$= \int_{-\infty}^{\infty} dx_\tau x_\tau \frac{1}{\sqrt{4\pi D\tau}} \exp\left\{-\frac{(x_\tau - x_0)^2}{4D\tau}\right\} \tag{19.99}$$

$$= x_0. \tag{19.100}$$

19.2.3 Path Integrals by the Method of Finite Elements

We now evaluate the path integral we have found above for the functional $F[x(\tau)] = x(\tau)$ using the formula [Eq. (19.90)]:

$$\int_{C[x_0,0;t]} d_w x(\tau) x(\tau) = \int dx \int_{C[x_0,0;x,t]} d_w x(\tau) x(\tau) \tag{19.101}$$

$$= \int_{-\infty}^{\infty} \prod_{i=1}^{N} \frac{dx_i}{\sqrt{4\pi D\Delta t_i}} \exp\left\{-\sum_{i=1}^{N} \frac{(x_i - x_{i-1})^2}{4D(t_i - t_{i-1})}\right\} x_k \tag{19.102}$$

$$= \int_{-\infty}^{\infty} \frac{dx_k x_k}{\sqrt{4\pi D\Delta t_k}} \int_{-\infty}^{\infty} \prod_{i=1}^{k-1} \frac{dx_i}{\sqrt{4\pi D\Delta t_i}} \exp\left\{-\sum_{i=1}^{k} \frac{(x_i - x_{i-1})^2}{4D(t_i - t_{i-1})}\right\}$$

$$\times \int_{-\infty}^{\infty} \prod_{i=k+1}^{N} \frac{dx_i}{\sqrt{4\pi D\Delta t_i}} \exp\left\{-\sum_{i=k+1}^{N} \frac{(x_i - x_{i-1})^2}{4D(t_i - t_{i-1})}\right\} \tag{19.103}$$

$$= \int_{-\infty}^{\infty} \frac{dx_k x_k}{\sqrt{4\pi D\Delta t_k}} \exp\left\{-\frac{(x_k - x_0)^2}{4D\Delta t_k}\right\} \tag{19.104}$$

$$= x_0. \tag{19.105}$$

In this calculation, we have assumed that τ lies in the kth time slice, hence $x(t_k) = x_k$. Complicated functionals can be handled by Eq. (19.90).

19.2.4 Path Integrals by the "Semiclassical" Method

We have seen that the solution of the Bloch equation in the presence of a nonzero diffusion constant is given as

$$W(x,t,x_0,t_0) = \int_{C[x_0,t_0;x,t]} \exp\left\{-\frac{1}{4D}\int_{t_0}^{t} d\tau L[x(\tau)]\right\}\prod_{\tau=t_0}^{t}\frac{dx(\tau)}{\sqrt{4\pi D d\tau}}. \tag{19.106}$$

Naturally, the major contribution to this integral comes from the paths that satisfy the Euler–Lagrange equation

$$\frac{\partial L}{\partial x} - \frac{d}{d\tau}\left[\frac{\partial L}{\partial(dx/d\tau)}\right] = 0. \tag{19.107}$$

We show these "classical" paths by $x_c(\tau)$. These paths also make the integral $\int L\, d\tau$ an extremum, that is,

$$\delta \int L d\tau = 0. \tag{19.108}$$

However, we should also remember that in the Bloch equation $V(x)$ is not quite the potential and L is not the Lagrangian. Similarly, $\int L\, d\tau$ in Eq. (19.108) is not the action, $S[x(\tau)]$, of classical physics. These expressions gain their conventional meanings only when we apply path integrals to the Schrödinger equation. It is for this reason that we have used the term "semiclassical."

When the diffusion constant is much smaller than the functional S, that is, $D/S << 1$, we write an approximate solution to Eq. (19.106) as

$$W(x,t;x_0,t_0) \simeq \phi(t-t_0)\exp\left\{-\frac{1}{4D}\int_{t_0}^{t} d\tau L[x_c(\tau)]\right\}, \tag{19.109}$$

where $\phi(t-t_0)$ is called the **fluctuation factor**. Even though methods of finding the fluctuation factor are beyond our scope, we give two examples for its appearance and evaluation [3, 6, 13].

Example 19.1 ***Evaluation of*** $\int_{C[x_0,0;x,t]} d_w x(\tau)$

To find the propagator $W(x,t,x_0,0)$:

$$W(x,t,x_0,0) = \int_{C[x_0,0;x,t]} \exp\left\{-\frac{1}{4D}\int_{0}^{t} d\tau \dot{x}^2\right\}\prod_{\tau=0}^{t}\frac{dx(\tau)}{\sqrt{4\pi D d\tau}}, \tag{19.110}$$

we write the Euler–Lagrange equation

$$x_c(\tau) = 0,\ x_c(0) = x_0,\ x(t) = x \tag{19.111}$$

with the solution

$$x_c(\tau) = x_0 + \frac{\tau}{t}(x - x_0). \tag{19.112}$$

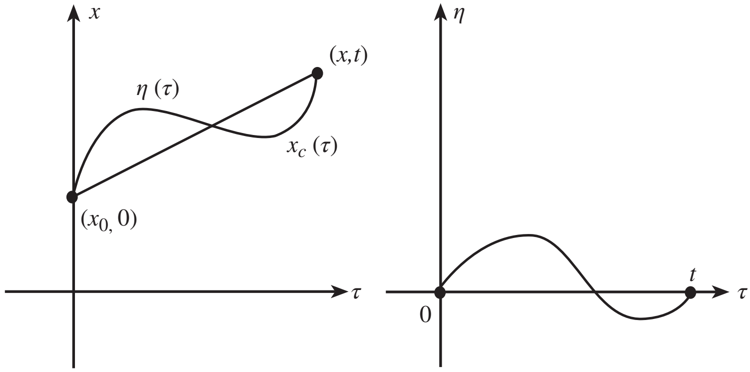

Figure 19.4 Path and deviation in the "semiclassical" method.

We show the deviation from the classical path $x_c(\tau)$ as $\eta(\tau)$ so that we write

$$x(\tau) = x_c(\tau) + \eta(\tau). \tag{19.113}$$

At the end points (Figure 19.4), $\eta(\tau)$ satisfies $\eta(0) = \eta(t) = 0$. In terms of $\eta(\tau)$, $W(x, t, x_0, 0)$ is given as

$$W(x, t, x_0, 0) = \exp\left\{-\frac{1}{4D}\int_0^t d\tau \dot{x}_c^2\right\} \times \int_{C[0,0;0,t]} \exp\left\{-\frac{1}{4D}\int_0^t d\tau(\dot{\eta}^2 + 2\,\dot{x}_c\dot{\eta})\right\}\prod_{\tau=0}^{t}\frac{d\eta(\tau)}{\sqrt{4\pi D d\tau}}. \tag{19.114}$$

We have to remember that the paths $x(\tau)$ do not have to satisfy the Euler–Lagrange equation. Since we can write

$$\int_0^t d\tau \dot{x}_c\dot{\eta} = \frac{(x - x_0)}{t}\eta(\tau)\bigg|_0^t = 0, \tag{19.115}$$

Eq. (19.114) becomes

$$W(x, t, x_0, 0) = \exp\left\{-\frac{1}{4D}\int_0^t d\tau \dot{x}_c^2\right\} \times \int_{C[0,0;0,t]} \exp\left\{-\frac{1}{4D}\int_0^t d\tau\dot{\eta}^2\right\}\prod_{\tau=0}^{t}\frac{d\eta(\tau)}{\sqrt{4\pi D d\tau}}. \tag{19.116}$$

Since $\dot{x}_c = (x - x_0)/t$ is independent of τ, we can evaluate the factor in front of the integral on the right-hand side as

$$\exp\left\{-\frac{1}{4D}\int_0^t d\tau \dot{x}_c^2\right\} = \exp\left\{-\frac{1}{4D}\frac{(x - x_0)^2}{t}\right\}. \tag{19.117}$$

Because the integral

$$\int_{C[0,0;0,t]} \exp\left\{-\frac{1}{4D}\int_{t_0}^{t} d\tau\dot{\eta}^2\right\}\prod_{\tau=0}^{t}\frac{d\eta(\tau)}{\sqrt{4\pi D d\tau}} \tag{19.118}$$

only depends on t, we show it as $\phi(t)$ and write the propagator as

$$W(x,t,x_0,0) = \phi(t)\exp\left\{-\frac{(x-x_0)^2}{4Dt}\right\}. \tag{19.119}$$

The probability density interpretation of the propagator gives us the condition $\int_{-\infty}^{\infty} dx W(x,t,x_0,0) = 1$, which leads us to the $\phi(t)$ function as

$$\phi(t) = \frac{1}{\sqrt{4\pi Dt}}. \tag{19.120}$$

Finally, the propagator is obtained as

$$W(x,t,x_0,0) = \frac{1}{\sqrt{4\pi Dt}}\exp\left\{-\frac{(x-x_0)^2}{4Dt}\right\}. \tag{19.121}$$

In this case, the "semiclassical" method has given us the exact result. For more complicated cases, we could use the method of time slices to find the factor $\phi(t-t_0)$. In this example, we have also given an explicit derivation of Eq. (19.18) for $t_0 = 0$, from Eq. (19.20).

Example 19.2 ***Evaluation of $\varphi(t)$ by the method of time slices***
Because our previous example is the prototype of many path integral applications, we also evaluate the integral

$$\phi(t) = \int_{C[0,0;0,t]} \exp\left\{-\frac{1}{4D}\int_{0}^{t} d\tau\dot{\eta}^2\right\}\prod_{\tau=0}^{t}\frac{d\eta(\tau)}{\sqrt{4\pi D d\tau}} \tag{19.122}$$

using the method of time slices. We divide the interval $[0,t]$ into $(N+1)$ equal segments:

$$t_i - t_{i-1} = \varepsilon = \frac{t}{(N+1)}, \quad i = 1,2,\dots,(N+1). \tag{19.123}$$

Now the integral (19.122) becomes

$$\phi(t) = \lim_{N\to\infty,\varepsilon\to 0}\frac{1}{[\sqrt{4\pi D\varepsilon}]^{N+1}} \tag{19.124}$$

$$\times\int d\eta_1\int d\eta_2\cdots\int d\eta_N \exp\left\{-\frac{1}{4D\epsilon}\sum_{i=0}^{N}(\eta_{i+1}-\eta_i)^2\right\}.$$

The argument of the exponential function, aside from a minus sign, is a quadratic of the form

$$\frac{1}{4D\varepsilon}\sum_{i=0}^{N}(\eta_{i+1}-\eta_i)^2=\sum_{k=1}^{N}\sum_{l=1}^{N}\eta_k A_{kl}\eta_l. \tag{19.125}$$

We can write A_{kl} as an $N \times N$ matrix ($\eta_0 = \eta_{N+1} = 0$):

$$A=\frac{1}{4D\varepsilon}\begin{pmatrix} 2 & -1 & 0 & 0 & \cdots & \cdots & 0 \\ -1 & 2 & -1 & 0 & \cdots & \cdots & 0 \\ 0 & -1 & 2 & -1 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \cdots & 0 & -1 & 2 & -1 & 0 \\ 0 & \cdots & \cdots & 0 & -1 & 2 & -1 \\ 0 & \cdots & \cdots & \cdots & 0 & -1 & 2 \end{pmatrix}. \tag{19.126}$$

Using the techniques of linear algebra, we can evaluate the integral

$$\int d\eta_1\int d\eta_2\cdots\int d\eta_N \exp\left\{-\sum_{k=1}^{N}\sum_{l=1}^{N}\eta_k A_{kl}\eta_l\right\} \tag{19.127}$$

as (Problem 7)

$$\int d\eta_1\int d\eta_2\cdots\int d\eta_N \exp\left\{-\sum_{k=1}^{N}\sum_{l=1}^{N}\eta_k A_{kl}\eta_l\right\} = \frac{\left(\sqrt{4\pi D\varepsilon}\right)^N}{\sqrt{\det A_N}}. \tag{19.128}$$

Using the last column of A, we find a recursion relation that $\det A_N$ satisfies:

$$\det A_N = 2\det A_{N-1} - \det A_{N-2}. \tag{19.129}$$

For the first two values of N, $\det A_N$ is found as $\det A_1 = 2$ and $\det A_2 = 3$. This can be generalized to $N-1$ as $\det A_{N-1} = N$. Using the recursion relation [Eq. (19.129)], this gives $\det A_N = N+1$, which leads us to the $\phi(t)$ function:

$$\phi(t)=\frac{\left(\sqrt{4\pi D\varepsilon}\right)^N}{\left(\sqrt{4\pi D\varepsilon}\right)^{N+1}\sqrt{N+1}}=\frac{1}{\sqrt{4\pi Dt}}. \tag{19.130}$$

Another way to calculate the integral in Eq. (19.122) is to evaluate the η integrals one by one using the formula

$$\int_{-\infty}^{\infty} d\eta \exp\left\{-a(\eta-\eta')^2-b(\eta-\eta'')^2\right\} = \left[\frac{\pi}{a+b}\right]^{1/2}\exp\left\{-\frac{ab}{a+b}(\eta'-\eta'')^2\right\}. \tag{19.131}$$

19.3 Path Integral Formulation of Quantum Mechanics

19.3.1 Schrödinger Equation For a Free Particle

We have seen that the propagator for a particle undergoing Brownian motion with its initial position at (x_0, t_0) is given as

$$W(x,t,x_0,t_0) = \frac{1}{\sqrt{4\pi D(t-t_0)}} \exp\left\{-\frac{(x-x_0)^2}{4D(t-t_0)}\right\}. \tag{19.132}$$

This satisfies the diffusion equation:

$$\frac{\partial W(x,t,x_0,t_0)}{\partial t} = D\frac{\partial^2 W(x,t,x_0,t_0)}{\partial x^2} \tag{19.133}$$

with the initial condition $\lim_{t\to t_0} W(x,t,x_0,t_0) \to \delta(x-x_0)$. We have also seen that this propagator can also be written as a Wiener path integral:

$$W(x,t,x_0,t_0) = \int_{C[x_0,t_0;x,t]} d_w x(\tau). \tag{19.134}$$

In this integral, $C[x_0, t_0; x, t]$ denotes all continuous paths starting from (x_0, t_0) and ending at (x, t), where $d_w x(\tau)$ is called the Wiener measure and is given as

$$d_w x(\tau) = \exp\left\{-\frac{1}{4D}\int_{t_0}^{t} \dot{x}^2(\tau)\, d\tau\right\} \prod_{i=1}^{N} \frac{dx_i}{\sqrt{4\pi D d\tau}}. \tag{19.135}$$

In quantum mechanics, for a free particle of mass m, the **Schrödinger equation** is given as

$$\boxed{\frac{\partial \Psi(x,t)}{\partial t} = \frac{i\hbar}{2m}\frac{\partial^2 \Psi(x,t)}{\partial x^2}.} \tag{19.136}$$

The **propagator** for the Schrödinger equation, $K(x,t,x',t')$, satisfies the equation

$$\frac{\partial K(x,t,x',t')}{\partial t} = \frac{i\hbar}{2m}\frac{\partial^2 K(x,t,x',t')}{\partial x^2}. \tag{19.137}$$

Using this propagator, given the solution at (x', t'), we can find the **solution** at another point (x, t) as

$$\boxed{\Psi(x,t) = \int K(x,t,x',t')\Psi(x',t')dx', \quad t > t'.} \tag{19.138}$$

Since the diffusion equation becomes the Schrödinger equation by the replacement $D \to \frac{i\hbar}{2m}$, we can immediately write the propagator of the Schrödinger equation by making the same replacement in Eq. (19.132):

$$K(x,t,x',t') = \frac{1}{\sqrt{\frac{2\pi i\hbar}{m}(t-t_0)}} \exp\left\{-\frac{m(x-x_0)^2}{2i\hbar(t-t_0)}\right\}. \tag{19.139}$$

Even though this expression is mathematically correct, at this point, we begin to encounter problems and differences between the two cases. For the diffusion phenomena, we have said that the solution of the diffusion equation gives the probability of finding a Brown particle at (x, t). Thus the propagator:

$$W(x,t,x_0,t_0) = \frac{1}{\sqrt{4\pi D(t-t_0)}} \exp\left\{-\frac{(x-x_0)^2}{4D(t-t_0)}\right\}, \tag{19.140}$$

is always positive with the normalization condition $\int_{-\infty}^{\infty} dx W(x,t,x_0,t_0) = 1$. For the Schrödinger equation, the argument of the exponential function is proportional to i, which makes $K(x,t,x',t')$ oscillate violently; hence $K(x,t,x',t')$ cannot be normalized. This is not too surprising, since the **solutions** of the Schrödinger equation are the **probability amplitudes**, which are more fundamental, and thus carry more information than the probability density. In quantum mechanics, the probability density, $\rho(x,t)$, is obtained from the solutions of the Schrödinger equation, $\Psi(x,t)$, as

$$\rho(x,t) = \Psi(x,t)\Psi^*(x,t) = |\Psi(x,t)|^2, \tag{19.141}$$

where $\rho(x,t)$ is now positive definite and normalizable.

Can we also write the propagator of the Schrödinger equation as a path integral? Making the replacement $D \to \frac{i\hbar}{2m}$ in Eq. (19.134), we get

$$K(x,t,x',t') = \int_{C[x',t';x,t]} d_F x(\tau), \tag{19.142}$$

where

$$d_F x(\tau) = \exp\left\{\frac{i}{\hbar}\int_{t_0}^{t} \frac{1}{2} m\dot{x}^2(\tau)\, d\tau\right\} \prod_{i=1}^{N} \frac{dx_i}{\sqrt{\frac{2\pi i\hbar}{m} d\tau}}. \tag{19.143}$$

This definition was given first by Feynman, and $d_F x(\tau)$ is known as the **Feynman measure.** The problem in this definition is again the fact that the argument of the exponential, which is responsible for the convergence of the integral, is proportional to i, and thus the exponential factor oscillates. An elegant solution to this problem comes from noting that the Schrödinger equation is analytic in the lower half complex t-plane. Thus we make a rotation by $-\pi/2$ and write $-it$ instead of t in the Schrödinger equation (Figure 19.5). This reduces the

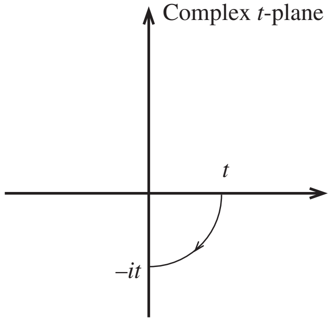

Figure 19.5 Rotation by $-\frac{\pi}{2}$ in the complex-t plane.

Schrödinger equation to the diffusion equation with the diffusion constant $D = \hbar/2m$. Now the path integral in Eq. (19.142) can be taken as a Wiener path integral, and then going back to real time, we can obtain the propagator of the Schrödinger equation as Eq. (19.139).

19.3.2 Schrödinger Equation with a Potential

In the presence of interactions, the **Schrödinger equation** is given as

$$\boxed{\frac{\partial \Psi(x,t)}{\partial t} = \frac{i\hbar}{2m}\frac{\partial^2 \Psi(x,t)}{\partial x^2} - \frac{i}{\hbar}V(x)\Psi(x,t),} \tag{19.144}$$

where $V(x)$ is the potential. Making the transformation $t \to -it$, we obtain the **Bloch equation**:

$$\frac{\partial \Psi(x,t)}{\partial t} = \frac{\hbar}{2m}\frac{\partial^2 \Psi(x,t)}{\partial x^2} - \frac{1}{\hbar}V(x)\Psi(x,t). \tag{19.145}$$

Using the **Feynman–Kac theorem**, we write the propagator and then transforming back to real time gives

$$\boxed{K(x,t,x_0,t_0) = \int_{C[x_0,t_0;x,t]} d_F x(\tau) \exp\left\{-\frac{i}{\hbar}\int_{t_0}^{t} d\tau V[x(\tau)]\right\},} \tag{19.146}$$

or

$$\boxed{\begin{aligned} K(x,t,x_0,t_0) = \int_{C[x_0,t_0;x,t]} \prod_{i=1}^{N} \frac{dx_i}{\sqrt{\frac{2i\hbar}{m}\pi d\tau}} \\ \times \exp\left\{\frac{i}{\hbar}\int_{t_0}^{t}\left[\frac{1}{2}m\dot{x}^2(\tau) - V(x)\right] d\tau\right\}. \end{aligned}} \tag{19.147}$$

This propagator was first given by Feynman. Using the **Feynman propagator**, we can write the solution of the Schrödinger equation as

$$\boxed{\Psi(x,t) = \int K(x,t,x',t')\Psi(x',t')\,dx'.} \tag{19.148}$$

Today the path integral formulation of quantum mechanics, after the Schrödinger and the Heisenberg formulations, has become the foundation of modern quantum mechanics. Writing the propagator [Eq. (19.147)] as

$$\boxed{K(x,t,x_0,t_0) = \int_{C[x_0,t_0;x,t]} \prod_{i=1}^{N} \frac{dx_i}{\sqrt{\frac{2i\hbar}{m}\pi d\tau}} \exp\left\{\frac{i}{\hbar}S[x(\tau)]\right\},} \tag{19.149}$$

we see that, in contrast to the Bloch equation, $S[x(\tau)]$ in the propagator is the **classical action**:

$$S[x(\tau)] = \int_{t_0}^{t} L[x(\tau)]\,d\tau, \tag{19.150}$$

where $L[x(\tau)]$ is the **classical Lagrangian**:

$$L[x(\tau)] = \left[\frac{1}{2}m\dot{x}^2(\tau) - V(x)\right]. \tag{19.151}$$

In the Feynman propagator [Eq. (19.149)], we should note that $C[x_0,t_0;x,t]$ includes not only the paths that satisfy the Euler–Lagrange equation, but also all the continuous paths that start from (x_0,t_0) and end at (x,t). In the classical limit, that is, $\hbar \to 0$, the exponential term, $\exp\left\{\frac{i}{\hbar}S[x(\tau)]\right\}$, in the propagator oscillates violently. In this case, the major contribution to the integral comes from the paths with comparable weights bunched together. These paths are naturally the ones that make $S[x]$ an extremum, that is, the paths that satisfy the Euler–Lagrange equation:

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}}\right) - \frac{\partial L}{\partial x} = 0. \tag{19.152}$$

In most cases, this extremum is a minimum [12, p. 281].

As in the applications of path integrals to neural networks, sometimes a system can have more than one extremum. In such cases, a system could find itself in a local maximum or minimum. Is it then possible for such systems to reach the desired global minimum? If possible, how is this achieved and how long will it take? These are all very interesting questions and potential research topics, indicating that path integral formalism still has a long way to go.

19.3.3 Feynman Phase Space Path Integral

The propagator of the Schrödinger equation expressed as a path integral:

$$K(x,t,x_0,t_0) = \int_{C[x_0,t_0;x,t]} \prod_{i=1}^{N} \frac{dx_i}{\sqrt{\frac{2\pi i\hbar}{m} d\tau}} \times \exp\left\{ \frac{i}{\hbar} \int_{t_0}^{t} \left[\frac{1}{2} m\dot{x}^2(\tau) - V(x) \right] d\tau \right\}, \tag{19.153}$$

is useful if the Lagrangian can be expressed as $T - V$. However, as in the case of the free relativistic particle, where $L(x) = -m_0 c^2 \sqrt{1 - (\dot{x}^2/c^2)}$, sometimes the Lagrangian cannot be written as $T - V$. In such cases, Eq. (19.153) is not much of a help. It is for this reason that in 1951, Feynman introduced the phase space version of the path integral:

$$\boxed{K(q'',t'',q',t') = \check{N} \int \exp\left\{ \frac{i}{\hbar} \int_{t'}^{t''} dt[p\dot{q} - H(p,\dot{q})] \right\} \check{D}p\check{D}q.} \tag{19.154}$$

This integral is to be taken over t, where $t \in [t', t'']$. $\check{D}q$ means that the integral is taken over the paths, $q(t)$, fixed between $q''(t'') = q''$ and $q'(t') = q'$ and which make $S[x]$ an extremum. The integral over momentum p is taken over the same time interval but without any restrictions.

To bring this integral into a form that can be evaluated in practice, we introduce the phase space lattice by dividing the time interval $t \in [t', t'']$ into $N + 1$ slices as

$$\varepsilon = \frac{t'' - t'}{(N+1)}. \tag{19.155}$$

Now the propagator becomes

$$K(q'',t'',q',t') = \lim_{\varepsilon \to 0} \int \cdots \int \times \exp\left\{ \left(\frac{i}{\hbar}\right) \sum_{l=0}^{N} \left[p_{l+1/2}(q_{l+1} - q_l) - \varepsilon H\left(p_{l+1/2}, \frac{1}{2}(q_{l+1} + q_l)\right) \right] \right\} \times \prod_{l=0}^{N} \frac{dp_{l+1/2}}{2\pi\hbar} \prod_{l=1}^{N} dq_l. \tag{19.156}$$

In this expression, except for the points at $q_{N+1} = q''$ and $q_0 = q'$, we have to integrate over all q and p. Because the Heisenberg uncertainty principle forbids us from determining the momentum and position simultaneously at the same point, we have taken the momentum values at the center of the time slices as

$p_{l+1/2}$. In this equation, one extra integral is taken over p. It is easily seen that this propagator satisfies the **ESKC** relation:

$$K(q''', t''', q', t') = \int K(q''', t''', q'', t'')K(q'', t'', q', t')\, dq''. \tag{19.157}$$

19.3.4 The Case of Quadratic Dependence on Momentum

In phase space, the exponential function in the Feynman propagator [Eq. (19.156)] is written as

$$\exp\left\{\left(\frac{i}{\hbar}\right)\sum_{l=0}^{N}\left[p_{l+1/2}(q_{l+1}-q_l) - \varepsilon H\left(p_{l+1/2}, \frac{1}{2}(q_{l+1}+q_l)\right)\right]\right\}.$$

When the **Hamiltonian** has **quadratic dependence** on p as in

$$H(q,p) = \frac{p^2}{2m} + V(q,t), \tag{19.158}$$

this exponential function becomes

$$\exp\left\{\left(\frac{i}{\hbar}\right)\sum_{l=0}^{N}\varepsilon\quad\left[\frac{p_{l+1/2}(q_{l+1}-q_l)}{\varepsilon} - \frac{p_{l+1/2}^2}{2m} - V\left(\frac{1}{2}(q_l+q_{l+1}), t_l\right)\right]\right\}. \tag{19.159}$$

Completing the square in the expression inside the brackets, we can write

$$\exp\left\{\left(\frac{i}{\hbar}\right)\sum_{l=0}^{N}\varepsilon\times\left[-\frac{1}{2m}\left(p_{l+1/2} - \frac{(q_{l+1}-q_l)}{\varepsilon}m\right)^2 + \frac{m}{2}\left(\frac{q_{l+1}-q_l}{\varepsilon}\right)^2 - V\left(\frac{q_l+q_{l+1}}{2}, t_l\right)\right]\right\}. \tag{19.160}$$

Substituting this in Eq. (19.156) and taking the momentum integral, we find the **propagator** as

$$\boxed{K(q'', t'', q', t') = \lim_{\substack{N\to\infty\\ \varepsilon\to 0}} \frac{1}{\sqrt{2\pi i\hbar\frac{\varepsilon}{m}}}\prod_{l=0}^{N}\int_{-\infty}^{\infty}\left[\frac{dq_l}{\sqrt{2\pi i\hbar\frac{\varepsilon}{m}}}\right]\exp\left\{\frac{i}{\hbar}S\right\},} \tag{19.161}$$

where S is given as

$$S = \sum_{l=0}^{N}\varepsilon\left[\frac{m}{2}\left(\frac{(q_{l+1}-q_l)}{\varepsilon}\right)^2 - V\left(\frac{1}{2}(q_l+q_{l+1}), t_l\right)\right]. \tag{19.162}$$

In the **continuum limit**, this becomes

$$S[q] = \lim_{\substack{N\to\infty \\ \varepsilon\to 0}} \sum_{l=0}^{N} \varepsilon \left[\frac{m}{2}\left(\frac{q_{l+1}-q_l}{\varepsilon}\right)^2 - V\left(\frac{1}{2}(q_l+q_{l+1}), t_l\right)\right] = \int_{t'}^{t''} dtL[q,\dot{q},t], \tag{19.163}$$

where

$$L[q,\dot{q},t] = \frac{1}{2}m\dot{q}^2 - V(q,t) \tag{19.164}$$

is the **classical action**. In other words, the phase space path integral reduces to the standard Feynman path integral.

We can write the **free particle propagator** in terms of the phase space path integral as

$$\boxed{K(x,t,x_0,t_0) = \check{N}\int_{C[x_0,t_0;x,t]} \check{D}p\check{D}x \exp\left\{\frac{i}{\hbar}\int_{t_0}^{t} d\tau \left[p\dot{x} - \frac{p^2}{2m}\right]\right\}.} \tag{19.165}$$

After we take the momentum integral and after putting all the new constants coming into $\check{D}$, Eq. (19.165) becomes

$$K(x,t,x_0,t_0) = \check{N}\int_{C[x_0,t_0;x,t]} \check{D}x \exp\left\{\frac{i}{\hbar}\int_{t_0}^{t} d\tau \left(\frac{1}{2}m\dot{x}^2\right)\right\}. \tag{19.166}$$

We can convert this into a Wiener path integral by the $t \to -it$ rotation, and after evaluating it, we return to real time to obtain the propagator as

$$K(x,t,x_0,t_0) = \frac{1}{\sqrt{2\pi i\hbar(t-t_0)/m}} \exp \frac{i}{\hbar}\frac{m(x-x_0)^2}{2(t-t_0)}. \tag{19.167}$$

We conclude by giving the following **useful rules** for **Wiener path integrals** with $N+1$ **segments** [Eq. (19.11)]:

For the pinned Wiener measure:

$$\int d_w x(\tau) = \frac{1}{(4\pi D\varepsilon)^{(N+1)/2}} \int_{-\infty}^{\infty} dx_1 \cdots \int_{-\infty}^{\infty} dx_N \exp\left\{-\frac{1}{4D\varepsilon}\sum_{i=1}^{N+1}(x_i - x_{i-1})^2\right\}$$
$$\times \int \prod_{\tau=0}^{t} \frac{dx(\tau)}{\sqrt{4\pi D d\tau}} = \frac{1}{(4\pi D\varepsilon)^{(N+1)/2}} \int_{-\infty}^{\infty} dx_1 \cdots \int_{-\infty}^{\infty} dx_N. \tag{19.168}$$

For the unpinned Wiener measure:

$$\int d_w x(\tau) = \frac{1}{(4\pi D\varepsilon)^{(N+1)/2}} \int_{-\infty}^{\infty} dx_1 \cdots \int_{-\infty}^{\infty} dx_{N+1} \exp\left\{-\frac{1}{4D\varepsilon}\sum_{i=1}^{N+1}(x_i - x_{i-1})^2\right\}$$
$$\times \int \prod_{\tau=0}^{t} \frac{dx(\tau)}{\sqrt{4\pi D d\tau}} = \frac{1}{(4\pi D\varepsilon)^{(N+1)/2}} \int_{-\infty}^{\infty} dx_1 \cdots \int_{-\infty}^{\infty} dx_{N+1}. \tag{19.169}$$

Also,

$$\int_0^t d\tau \dot{x}^2(\tau) = \frac{1}{\varepsilon}\sum_{i=1}^{N+1}(x_i - x_{i-1})^2, \tag{19.170}$$

$$\int_0^t d\tau V(\tau) = \varepsilon \sum_{i=1}^{N+1} V\left(\frac{1}{2}(x_i + x_{i-1}), t_i\right) \overset{\text{or}}{=} \varepsilon \sum_{i=1}^{N+1} V(x_i, t_i). \tag{19.171}$$

19.4 Path Integrals Over Lévy Paths and Anomalous Diffusion

Wiener path integral approach to Brownian motion can be used to represent a wide range of stochastic processes, where the probability density, $W(x, t, x_0, t_0)$, of finding a random variable at the value x at time t is given by the Gaussian distribution [Eq. (19.6)]:

$$W(x, t, x_0, t_0) = \frac{1}{\sqrt{4\pi D(t - t_0)}} \exp\left\{-\frac{(x - x_0)^2}{4D(t - t_0)}\right\}, \quad t > t_0, \tag{19.172}$$

which satisfies the diffusion equation [Eq. (19.3)]:

$$\frac{\partial W(x, t, x_0, t_0)}{\partial t} = D\frac{\partial^2 W(x, t, x_0, t_0)}{\partial x^2} \tag{19.173}$$

with the initial condition $\lim_{t\to t_0} W(x, t, x_0, t_0) \to \delta(x - x_0)$. An important feature of the **Wiener process** is that at all times the **scaling relation**

$$(x - x_0)^2 \propto (t - t_0), \tag{19.174}$$

where x_0 and t_0 are the initial values of x and t, respectively, are satisfied. To find the **fractal dimension** of the **Brownian motion**, we divide the time interval, T, into N slices, $T = N\Delta t$, which gives the length of the diffusion path as

$$L = N\Delta x = \frac{T}{\Delta t}\Delta x. \tag{19.175}$$

Using the scaling property [Eq. (19.174)], we write

$$L \propto \frac{1}{\Delta x}. \tag{19.176}$$

When the spatial increment Δx goes to zero, the fractal dimension, d_{fractal}, is defined as [8]

$$L \propto (\Delta x)^{1-d_{\text{fractal}}}. \tag{19.177}$$

In the limit as $\Delta x \to 0$, Eqs. (19.176) and (19.177) give the fractal dimension of the Brownian motion as

$$\boxed{\mathrm{d}_{\text{fractal}}^{\text{Brownian}} = 2.} \tag{19.178}$$

In terms of Wiener path integrals, $W(x,t,x_0,t_0)$ is expressed as [Eq. (19.20)]

$$W(x,t,x_0,t_0) = \int_{C[x_0,t_0;x,t]} d_w x(\tau), \tag{19.179}$$

where the Wiener measure, $d_w x(\tau)$, is written as

$$d_w x(\tau) = \exp\left\{-\frac{1}{4D}\int_{t_0}^{t} \dot{x}^2(\tau)d\tau\right\}\prod_{i=1}^{N}\frac{dx_i}{\sqrt{4\pi D d\tau}} \tag{19.180}$$

and the integral is evaluated over all continuous paths from (x_0,t_0) to (x,t) [Eqs. (19.20) and (19.21)].

In the presence of a **potential**, $V(x,t)$, the diffusion equation is written as

$$\boxed{\frac{\partial W_B(x,t,x_0,t_0)}{\partial t} - D\frac{\partial^2 W_B(x,t,x_0,t_0)}{\partial x^2} = -V(x,t)W_B(x,t,x_0,t_0),} \tag{19.181}$$

which is also called the **Bloch equation**. Using the **Feynman–Kac formula** [Eq. (19.35)]:

$$W_B(x,t,x_0,0) = \int_{C[x_0,0;x,t]} d_w x(\tau)\exp\left\{-\int_0^t d\tau V(x(\tau),\tau)\right\}, \tag{19.182}$$

a perturbative solution of the Bloch equation can be given as [Eq. (19.41)]

$$\begin{aligned} W_B(x,t,x_0,t_0) &= W_D(x,t,x_0,t_0) \\ &- \int_{-\infty}^{\infty} dx' \int_{t_0}^{t} dt' W_D(x,t,x',t')V(x',t')W_D(x',t',x_0,t_0) \\ &+ \int_{-\infty}^{\infty} dx' \int_{t_0}^{t} dt' \int_{-\infty}^{\infty} dx'' \int_{t'_0}^{t'} dt'' W_D(x,t,x',t')V(x',t')W_D(x',t',x'',t'') \\ &\times V(x'',t'')W_D(x'',t'',x_0,t_0) + \cdots, \end{aligned} \tag{19.183}$$

where the Green's function $W_D(x,t,x',t')$ [Eq. (19.32)]:

$$W_D(x,t,x',t') = W(x,t,x',t')\theta(t-t'), \tag{19.184}$$

satisfies

$$\frac{\partial W_D(x,t,x',t')}{\partial t} - D\frac{\partial^2 W_D(x,t,x',t')}{\partial x^2} = \delta(x-x')\delta(t-t') \tag{19.185}$$

and $W(x,t,x',t')$ is the solution of the homogeneous equation:

$$\frac{\partial W_D(x,t,x',t')}{\partial t} - D\frac{\partial^2 W_D(x,t,x',t')}{\partial x^2} = 0. \tag{19.186}$$

Even though the Wiener's mathematical theory of the Brownian motion can be used to describe a wide range of stochastic processes in nature, there also exist a lot of interesting phenomenon where the **scaling law** in Eq. (19.174) is violated. The processes that obey the scaling rule

$$(x - x_0)^2 \propto (t - t_0)^q, \quad q \neq 1, \tag{19.187}$$

are in general called **anomalous diffusion**, where the cases with $q < 1$ are called **subdiffusive** and the cases with $q > 1$ are called **superdiffusive**.

One of the ways to study anomalous diffusion is to use the **space fractional diffusion equation**:

$$\boxed{\frac{\partial W_L(x,t,x_0,t_0)}{\partial t} = D_q \nabla^q W_L(x,t,x_0,t_0), \quad q < 2,} \tag{19.188}$$

where ∇^q is the **Riesz derivative**. We will also use the **notation**

$$\nabla^q = \frac{\partial^q}{\partial x^q} = \mathbf{R}_x^q. \tag{19.189}$$

In Eq. (19.188) D_q stands for the fractional diffusion constant, which has the dimension $[D_q] = \mathrm{cm}^q\mathrm{s}^{-1}$. In Chapter 13, we have seen how the **Riesz derivative** is defined. However, in this chapter, all we need is that it is defined with respect to its **Fourier transform** as

$$\boxed{\nabla^q W_L(x,t) = -\frac{1}{2\pi}\int_{-\infty}^{\infty} dk e^{ikx}|k|^q \overline{W}_L(k,t),} \tag{19.190}$$

where $W_L(x,t)$ and its Fourier transform, $\overline{W}_L(k,t)$, are related by the equations

$$W_L(x,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dk e^{ikx}\overline{W}_L(k,t), \tag{19.191}$$

$$\overline{W}_L(k,t) = \int_{-\infty}^{\infty} dx e^{-ikx} W_L(x,t). \tag{19.192}$$

Solution of the fractional diffusion equation [Eq. (19.188)] with the initial condition

$$\lim_{t\to t_0} W_L(x,t,x_0,t_0) = \delta(x - x_0), \tag{19.193}$$

yields the **probability density**

$$W_L(x,t,x_0,t_0) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dk\, e^{ik(x-x_0)} \exp\{-D_q|k|^q(t - t_0)\}. \tag{19.194}$$

To obtain this solution [Eq. (19.194)], we first take the Fourier transform of the fractional diffusion equation:

$$\frac{\partial \overline{W}_L(x,t,x_0,t_0)}{\partial t} = -D_q|k|^q\overline{W}_L(x,t,x_0,t_0), \tag{19.195}$$

which with the initial condition $\overline{W}_L(k, 0) = 1$ can be integrated to yield the solution in the transform space as

$$\overline{W}_L(k, t) = \exp(-D_q t|k|^q). \tag{19.196}$$

For simplicity, we have set $x_0 = t_0 = 0$. Using **Fox's H-functions**, we can also write $\overline{W}_L(k, t)$ as

$$\overline{W}_L(k, t) = \frac{1}{q} H^{1,0}_{0,1} \left((D_q t)^{1/q} |k| \big|_{\left(0, \frac{1}{q}\right)} \right). \tag{19.197}$$

At this point, for our purposes, it is sufficient to say that this rather strange looking mathematical object:

$$H^{a,b}_{c,d} \left(x \big|^{(g,h)}_{(e,f)} \right),$$

is a just a symbolic expression of a function of x in terms of eight parameters, a, b, c, d, e, f, g, h. It is somewhat like the hypergeometric function, $F(a, b, c; x)$, but with more parameters. In the following section, we will give a detailed account of this extremely versatile tool of mathematical physics.

Finally, using the properties of the H-functions, we find the inverse Fourier transform of $\overline{W}_L(k, t)$ to write the solution of the fractional diffusion equation [Eq. (19.188)] in closed form as [7, 16]

$$\boxed{W_L(x, t) = \frac{\pi}{q|x|} H^{1,1}_{2,2} \left(\frac{|x|}{(D_q t)^{1/q}} \Bigg|^{(1,1/q),(1,1/2)}_{(1,1),(1,1/2)} \right).} \tag{19.198}$$

For large arguments, $|x|/(D_q t)^{1/q} \gg 1$, we can write the following series expansion:

$$W_L(x, t) = \sum_{l=1}^{\infty} (-1)^{l+1} \frac{\Gamma(1 + lq)}{l!} \sin\left(\frac{l\pi q}{2}\right) \frac{(D_q t)^l}{|x|^{lq+1}}. \tag{19.199}$$

For $q = 2$, $W_L(x, t)$ reduces to the **Gaussian distribution** [Eq. (19.172)] and for $0 < q < 2$, $W_L(x, t)$ is called the q **-stable Lévy distribution**, which possesses finite moments of order up to $m < q$, where all higher order moments diverge. Lévy processes obey the scaling rule

$$(x - x_0) \propto (t - t_0)^{1/q}, \quad 1 < q \leq 2, \tag{19.200}$$

where $(x - x_0)$ is the length of the Lévy path for the time interval $(t - t_0)$. Dividing a given time interval T into N slices, $T = N\Delta t$, we write

$$L = N\Delta x = \frac{T}{\Delta t}\Delta x, \tag{19.201}$$

where L is the length of the Lévy path and Δx is the length increment for Δt. Substituting the scaling rule [Eq. (19.200)] into the above equation gives $L \propto$

$(\Delta x)^{1-q}$. Considered in the limit as $\Delta x \to 0$, this yields the **fractal dimension** of the **Lévy path** as

$$\boxed{d_{\text{fractal}}^{\text{Lévy}} = q, \quad 1 < q \leq 2.} \tag{19.202}$$

For a **Lévy process** obeying the **fractional Bloch equation**:

$$\boxed{\frac{\partial W_L}{\partial t} - D_q \nabla^q W_L = -V(x,t) W_L,} \tag{19.203}$$

where $V(x,t)$ is the potential, we write the corresponding **Feynman–Kac formula** as [Eq. (19.35)]

$$\boxed{W_L(x,t,x_0,0) = \int_{C[x_0,0;x,t]} d_L x(\tau) \exp\left\{-\int_0^t d\tau V(x(\tau),\tau)\right\},} \tag{19.204}$$

where the **Wiener measure**, $d_w x(\tau)$, is replaced by the **Lévy measure**, $d_L x(\tau)$, defined as

$$\boxed{\begin{aligned} d_L x(\tau) = \lim_{N\to\infty} \Bigg[& dx_1 \cdots dx_N \left(\frac{1}{D_q \Delta\tau}\right)^{\frac{N+1}{q}} \\ & \times \prod_{i=1}^{N+1} L_q \left\{ \left(\frac{1}{D_q \Delta\tau}\right)^{\frac{1}{q}} |x_i - x_{i-1}| \right\} \Bigg]. \end{aligned}} \tag{19.205}$$

We have divided the interval $[t-0]$ into $N+1$ segments [Eq. (19.11)]:

$$\Delta\tau = \frac{t-0}{N+1}, \tag{19.206}$$

covered in N steps and comparing with Eq. (19.18), we have introduced the function $L_q(x,t)$ such that the Lévy distribution function, $W_L(x,t)$, is expressed in terms of the **Fox's H-functions** as

$$W_L(x,t) = (D_q t)^{-1/q} L_q \left\{ \left(\frac{1}{D_q t}\right)^{1/q} |x| \right\} \tag{19.207}$$

$$= \frac{\pi}{q|x|} H_{2,2}^{1,1} \left(\frac{|x|}{(D_q t)^{1/q}} \middle|_{(1,1),(1,1/2)}^{(1,1/q),(1,1/2)} \right). \tag{19.208}$$

Note that $i = 1$ marks the initial point, while $t = N+1$ is the end point of the path. Since the particle is certain to be somewhere in the internal $x \in [-\infty, \infty]$, we have

$$\int_{-\infty}^{\infty} dx \int_{[x_0,t_0;x,t]} d_L x(\tau) = 1. \tag{19.209}$$

In this regard, the dimension of $d_L x(\tau)$ and the propagator

$$W_L(x,t) = \int_{[x_0,t_0;x,t]} d_L x(\tau) \tag{19.210}$$

is 1/cm, a point that will be needed shortly.

19.5 Fox's *H*-Functions

In 1961, Fox introduced the H **-function**, which is a **special function** of very general nature. It represents an elegant and an efficient formalism of mathematical physics that has proven to be very effective in a wide range of physics and engineering problems like anomalous diffusion. H-functions offer an alternate way of expressing a large class of functions in terms of certain parameters. They are generally expressed in one of the following forms:

$$\boxed{H^{m,n}_{p,q}(z) = H^{m,n}_{p,q}\left(z\middle|^{(a_p,A_p)}_{(b_q,B_q)}\right) = H^{m,n}_{p,q}\left(z\middle|^{(a_1,A_1),\ldots,(a_p,A_p)}_{(b_1,B_1),\ldots,(b_q,B_q)}\right).} \tag{19.211}$$

Definition 19.1 H-function is a generalization of the Meijer's G-function and is defined with respect to a Mellin–Barnes type integral as [4, 9, 14, 16]

$$\boxed{H^{m,n}_{p,q}(z) = \frac{1}{2\pi i}\int_C h(s) z^{-s}\, ds,} \tag{19.212}$$

where

$$\boxed{h(s) = \frac{\prod_{j=1}^{m}\Gamma(b_j + B_j s)\prod_{j=1}^{n}\Gamma(1 - a_j - A_j s)}{\prod_{j=n+1}^{p}\Gamma(a_j + A_j s)\prod_{j=m+1}^{q}\Gamma(1 - b_j - B_j s)},} \tag{19.213}$$

m, n, p, q are positive integers satisfying

$$0 \le n \le p, \quad 1 \le m \le q, \tag{19.214}$$

and empty products are taken as 1. Also, $A_j, j = 1,\ldots,p$, and $B_j, j = 1,\ldots,q$, are positive numbers, and $a_j, j = 1,\ldots,p$, and $b_j, j = 1,\ldots,q$, are in general complex numbers satisfying

$$A_j(b_h + \nu) \ne B_h(a_j - \lambda - 1); \quad \nu,\lambda = 0,1,\ldots;\ h = 1,\ldots,m,\ j = 1,\ldots,n. \tag{19.215}$$

C is a suitable contour in the complex plane so that the poles of $\Gamma(b_j + B_j s)$, $j = 1,\ldots,m$, are separated from the poles of $\Gamma(1 - a_j - A_j s)$, $j = 1,\ldots,n$, such that the poles of $\Gamma(b_j + B_j s)$ lie to the left of C and the poles of $\Gamma(1 - a_j - A_j s)$ lie to the right of C. The poles of the integrand are assumed to be simple.

The H-function is an **analytic function** of z for all $|z| \neq 0$, when $\mu > 0$;

$$\mu > 0;\ \ 0 < |z| < \infty \tag{19.216}$$

and analytic for $0 < |z| < 1/\beta$ when $\mu = 0$;

$$\mu = 0;\ \ 0 < |z| < 1/\beta, \tag{19.217}$$

where

$$\mu = \sum_{j=1}^{q} B_j - \sum_{j=1}^{p} A_j \tag{19.218}$$

and

$$\beta = \prod_{j=1}^{p} A_j^{A_j} \prod_{j=1}^{q} B_j^{-B_j}. \tag{19.219}$$

Important. In literature, sometimes the H-function is defined with the sign of s reversed in the integrand [Eq. (19.212)], $h(s)z^{-s}$, and in $h(s)$ [Eq. (19.213)] along with an appropriate orientation of the contour. However, the final expression as $H_{p,q}^{m,n}\left(z\Big|_{(b_q,B_q)}^{(a_p,A_p)}\right)$ is the same in both conventions.

19.5.1 Properties of the *H*-Functions

Some of the frequently used properties of the H-functions are listed below. These are extremely useful in solving fractional differential equations. More can be found in the book by Mathai *et al.* [9]:

1. **Fractional derivative and integral:**
   Remembering the definitions of the Riemann–Liouville fractional integral (Chapter 13):

$$ {}_0D_t^{-q}[f(t)] = {}_0\mathbf{I}_t^{q}[f(t)] = \frac{1}{\Gamma(q)}\int_0^t \frac{f(\tau)d\tau}{(t-\tau)^{1-q}}, \quad q > 0, \tag{19.220}$$

   and the Riemann–Liouville fractional derivative as

$$ {}_0D_t^{q}[f(t)] = \frac{d^n}{dt^n}({}_0\mathbf{I}_t^{n-q}[f(t)]), \quad n > q, \quad q > 0, \tag{19.221}$$

   we can write the following useful differintegral of the H-function for arbitrary α [5]:

$$\boxed{ {}_0D_z^{\alpha}\left[z^a H_{p,q}^{m,n}\left((cz)^b\Big|_{(b_q,B_q)}^{(a_p,A_p)}\right)\right] = z^{a-\alpha} H_{p+1,q+1}^{m,n+1}\left((cz)^b\Big|_{(b_q,B_q),(\alpha-a,b)}^{(-a,b),(a_p,A_p)}\right),} \tag{19.222}$$

where $c, b > 0$ and

$$a + b\min(b_j/B_j) > -1, \quad 1 \le j \le m. \tag{19.223}$$

Solutions of the fractional diffusion equation can be obtained by formally manipulating the parameters in the above formula.

2. **Laplace transform:**
Laplace transform of the H-function is very useful in solving fractional differential equations. They can be obtained using the formula

$$\boxed{£\left\{x^{\rho-1}H^{m,n}_{p,q+1}\left(ax^{\sigma}\Big|^{(a_p,A_p)}_{(b_q,B_q),(1-\rho,\sigma)}\right)\right\} = s^{-\rho}H^{m,n}_{p,q}\left(as^{-\sigma}\Big|^{(a_p,A_p)}_{(b_q,B_q)}\right),} \tag{19.224}$$

where the **inverse transform** is given as

$$\boxed{£^{-1}\left\{s^{-\rho}H^{m,n}_{p,q}\left(as^{\sigma}\Big|^{(a_p,A_p)}_{(b_q,B_q)}\right)\right\} = x^{\rho-1}H^{m,n}_{p+1,q}\left(ax^{-\sigma}\Big|^{(a_p,A_p),(\rho,\sigma)}_{(b_q,B_q)}\right),} \tag{19.225}$$

where

$$\rho, \alpha, s \in \mathbb{C}, \quad \mathrm{Re}(s) > 0, \quad \sigma > 0 \tag{19.226}$$

and

$$\mathrm{Re}(\rho) + \sigma \max_{1\le i\le n}\left[\frac{1}{A_i} + \frac{\mathrm{Re}(a_i)}{A_i}\right] > 0, \quad |\arg a| < \frac{\pi\theta}{2}, \theta = \alpha - \sigma. \tag{19.227}$$

3. **Fourier-sine transform:**

$$\boxed{\begin{aligned}&\int_0^\infty x^{\rho-1}\sin(ax)H^{m,n}_{p,q}\left(bx^{\sigma}\Big|^{(a_p,A_p)}_{(b_q,B_q)}\right)\,dx\\ &\quad = \frac{2^{\rho-1}\sqrt{\pi}}{a^{\rho}}H^{m,n+1}_{p+2,q}\left(b\left(\frac{2}{a}\right)^{\sigma}\Big|^{((1-\rho)/2,\sigma/2),(a_p,A_p),((2-\rho)/2,\sigma/2)}_{(b_q,B_q)}\right),\end{aligned}} \tag{19.228}$$

where

$$a, \alpha, \sigma > 0, \quad \rho, b \in \mathbb{C}; \ |\arg b| < (1/2)\pi\sigma, \tag{19.229}$$

and

$$\mathrm{Re}\rho + \sigma \min_{1\le j\le m}\mathrm{Re}(b_j/B_j) > -1; \ \mathrm{Re}\rho + \sigma\max_{1\le j\le n}((a_j - 1)/A_j) < 1. \tag{19.230}$$

4. **Fourier-cosine transform:**

$$\boxed{\begin{aligned}&\int_0^\infty x^{\rho-1}\cos(ax)H^{m,n}_{p,q}\left(bx^{\sigma}\Big|^{(a_p,A_p)}_{(b_q,B_q)}\right)dx\\ &\quad = \frac{2^{\rho-1}\sqrt{\pi}}{a^{\rho}}H^{m,n+1}_{p+2,q}\left(b\left(\frac{2}{a}\right)^{\sigma}\Big|^{((2-\rho)/2,\sigma/2),(a_p,A_p),((1-\rho)/2,\sigma/2)}_{(b_q,B_q)}\right),\end{aligned}} \tag{19.231}$$

where

$$a, \alpha, \sigma > 0, \rho, b \in \mathbb{C}; \ |\arg b| < (1/2)\pi\alpha, \tag{19.232}$$

and

$$\text{Re } \rho + \sigma \min_{1\le j\le m} \text{Re } (b_j/B_j) > 0; \ \text{Re } \rho + \sigma \max_{1\le j\le n}((a_j - 1)/A_j) < 1. \tag{19.233}$$

19.5.2 Useful Relations of the *H*-Functions

The following relations are extremely useful in manipulations with the parameters of the H-functions and showing the equivalence of solutions expressed in different forms in literature.

1.

$$\boxed{H_{p,q}^{m,n}\left(z\Big|_{(b_q,B_q)}^{(a_p,A_p)}\right) = H_{q,p}^{n,m}\left(\frac{1}{z}\Big|_{(1-a_p,A_p)}^{(1-b_q,B_q)}\right).} \tag{19.234}$$

2.

$$\boxed{\frac{1}{k}H_{p,q}^{m,n}\left(z\Big|_{(b_q,B_q)}^{(a_p,A_p)}\right) = H_{p,q}^{m,n}\left(z^k\Big|_{(b_q,kB_q)}^{(a_p,kA_p)}\right),} \tag{19.235}$$

where $k > 0$.

3.

$$\boxed{z^{\sigma}H_{p,q}^{m,n}\left(z\Big|_{(b_q,B_q)}^{(a_p,A_p)}\right) = H_{p,q}^{m,n}\left(z\Big|_{(b_q+\sigma B_q,B_q)}^{(a_p+\sigma A_p,A_p)}\right),} \tag{19.236}$$

where $\sigma \in \mathbb{C}$.

4.

$$\boxed{H_{p,q}^{m,n}\left(z\Big|_{(b_1,B_1),\ldots,(b_{q-1},B_{q-1}),(a_1,A_1)}^{(a_1,A_1),\ldots,(a_p,A_p)}\right) = H_{p-1,q-1}^{m,n-1}\left(z\Big|_{(b_1,B_1),\ldots,(b_{q-1},B_{q-1})}^{(a_2,A_2),\ldots,(a_p,A_p)}\right),} \tag{19.237}$$

where $n \ge 1, q > m$.

5.

$$\boxed{H_{p,q}^{m,n}\left(z\Big|_{(b_1,B_1),\ldots,(b_q,B_q)}^{(a_1,A_1),\ldots,(a_{p-1},A_{p-1}),(b_1,B_1)}\right) = H_{p-1,q-1}^{m-1,n}\left(z\Big|_{(b_2,B_2),\ldots,(b_q,B_q)}^{(a_1,A_1),\ldots,(a_{p-1},A_{p-1})}\right),} \tag{19.238}$$

where $m \ge 1, p > n$.

6.

$$H_{p,q}^{m,n}\left(z\Big|_{(b_1,B_1),\ldots,(b_q,B_q)}^{(a_1,A_1),\ldots,(a_{p-1},A_{p-1}),(a,0)}\right) = \frac{1}{\Gamma(a)}H_{p-1,q}^{m,n}\left(z\Big|_{(b_1,B_1),\ldots,(b_q,B_q)}^{(a_1,A_1),\ldots,(a_{p-1},A_{p-1})}\right), \quad (19.239)$$

where $a, b \in \mathbb{C}$, Re $a > 0$ and $p > n$.

7.

$$H_{p,q}^{m,n}\left(z\Big|_{(b_q,B_q)}^{(a,0),(a_2,A_2),\ldots,(a_p,A_p)}\right) = \Gamma(1-a)H_{p-1,q}^{m,n-1}\left(z\Big|_{(b_q,B_q)}^{(a_2,A_2),\ldots,(a_p,A_p)}\right), \quad (19.240)$$

where $a, b \in \mathbb{C}$, Re $a < 1$ and $n \geq 1$.

8.

$$H_{p,q}^{m,n}\left(z\Big|_{(b,0),(b_2,B_2),\ldots,(b_q,B_q)}^{(a_1,A_1),\ldots,(a_p,A_p)}\right) = \Gamma(b)H_{p,q-1}^{m-1,n}\left(z\Big|_{(b_2,B_2),\ldots,(b_q,B_q)}^{(a_1,A_1),\ldots,(a_p,A_p)}\right), \quad (19.241)$$

where $a, b \in \mathbb{C}$, Re $b > 0$ and $m \geq 1$.

9.

$$H_{p,q}^{m,n}\left(z\Big|_{(b_1,B_1),\ldots,(b_{q-1},B_{q-1}),(b,0)}^{(a_1,A_1),\ldots,(a_p,A_p)}\right) = \frac{1}{\Gamma(1-b)}H_{p,q-1}^{m,n}\left(z\Big|_{(b_1,B_1),\ldots,(b_{q-1},B_{q-1})}^{(a_1,A_1),\ldots,(a_p,A_p)}\right), \quad (19.242)$$

where $a, b \in \mathbb{C}$, Re $b < 1$ and $q > m$.

19.5.3 Examples of *H*-Functions

1. **Exponential Function:**
   Consider the integral

$$f(z) = \frac{1}{2\pi i}\int_{\gamma-i\infty}^{\gamma+i\infty}\Gamma(s)z^{-s}ds, \quad |\arg z| < \pi/2, \ z \neq 0, \ \gamma \in \mathbb{R} \text{ and } > 0, \quad (19.243)$$

where the contour is a straight line, Re$s = \gamma$, such that all the poles of $\Gamma(s)$:

$$s = -\nu, \quad \nu = 0, 1, 2, \ldots, \quad (19.244)$$

lie to the left of the straight line. Using the residue theorem, we can evaluate this integral:

$$f(z) = 2\pi i \sum_n \text{Residues of } \left[\frac{\Gamma(s)z^{-s}}{2\pi i}\right]_{\text{Poles of } \Gamma(s)} \quad (19.245)$$

$$= \sum_{n=0}^{\infty}\lim_{s\to -n}(s+n)\Gamma(s)z^{-s} \quad (19.246)$$

$$= \sum_{n=0}^{\infty} \lim_{s \to -n} \Gamma(s) \frac{(s+n)(s+n-1)\cdots s}{(s+n-1)\cdots s} z^{-s}, \tag{19.247}$$

which we rewrite as

$$f(z) = \sum_{n=0}^{\infty} \lim_{s \to -n} \frac{\Gamma(s+n+1)}{(s+n-1)\cdots s} z^{-s} \tag{19.248}$$

$$= \sum_{n=0}^{\infty} \lim_{s \to -n} \frac{(-1)^n}{n!} z^{-s}. \tag{19.249}$$

Thus,

$$f(z) = e^{-z}. \tag{19.250}$$

We now compare the integral [Eq. (19.243)] with the definition of the H-function [Eqs. (19.212) and (19.213)] and identify the parameters of the H-function as

$$m = 1,\ n = 0,\ p = 0,\ q = 1, \tag{19.251}$$

$$b_1 = 0,\ B_1 = 1, \tag{19.252}$$

Now, the H-function representation of the **exponential function** is written as

$$\boxed{e^{-z} = H_{0,1}^{1,0}(z|_{(0,1)}).} \tag{19.253}$$

2. The H-function representation of $z^{\alpha} e^{-z}$ can be written as

$$\boxed{z^{\alpha} e^{-z} = H_{0,1}^{1,0}(z|_{(\alpha,1)}).} \tag{19.254}$$

3. **Mittag-Leffler function:**
Consider the following Mellin–Barnes integral:

$$f(z) = \frac{1}{2\pi i} \int_{\gamma - i\infty}^{\gamma + i\infty} \frac{\Gamma(s)\Gamma(1-s)}{\Gamma(1-\alpha s)} (-z)^{-s}\, ds, \quad |\arg z| < \pi, \tag{19.255}$$

where α is positive and real. Using the residue theorem, this integral can be shown to be the integral representation of the Mittag–Leffler function $E_{\alpha}(z)$:

$$f(z) = \sum_{n=0}^{\infty} \lim_{s \to -n} \left\{ (s+n) \frac{\Gamma(s)\Gamma(1-s)}{\Gamma(1-\alpha s)} (-z)^{-s} \right\} \tag{19.256}$$

$$= \sum_{n=0}^{\infty} \frac{z^n}{\Gamma(\alpha n + 1)} \tag{19.257}$$

$$= E_{\alpha}(z). \tag{19.258}$$

Comparing the integral in Eq. (19.255) with the definition of the H-function [Eqs. (19.212) and (19.213)], we determine the parameters as

$$m = 1,\ n = 1,\ p = 1,\ q = 2, \tag{19.259}$$

$$a_1 = 0,\ A_1 = 1, \tag{19.260}$$

$$b_1 = 0,\ B_1 = 1, \tag{19.261}$$

$$b_2 = 0,\ B_2 = \alpha. \tag{19.262}$$

Thus, the H-function representation of the **Mittag–Leffler function** is obtained as

$$\boxed{E_\alpha(z) = H^{1,1}_{1,2}\left(-z\middle|^{(0,1)}_{(0,1),(0,\alpha)}\right).} \tag{19.263}$$

4. **Generalized Mittag–Leffler function:**
Consider the following integral representation of the generalized Mittag-Leffler function:

$$E_{\alpha,\beta}(z) = \frac{1}{2\pi i}\int_{\gamma-i\infty}^{\gamma+i\infty}\frac{\Gamma(s)\Gamma(1-s)}{\Gamma(\beta-\alpha s)}(-z)^{-s}\,ds, \quad |\arg z| < \pi, \tag{19.264}$$

where α is real and positive and β is in general complex. We can evaluate this integral as

$$E_{\alpha,\beta}(z) = \sum_{n=0}^{\infty}\lim_{s\to -n}\left\{(s+n)\frac{\Gamma(s)\Gamma(1-s)}{\Gamma(\beta-\alpha s)}(-z)^{-s}\right\} \tag{19.265}$$

$$= \sum_{n=0}^{\infty}\frac{z^n}{\Gamma(\alpha n+\beta)}. \tag{19.266}$$

The parameters of the H-function are determined by direct comparison with Eqs. (19.212) and (19.213) as

$$m = 1,\ n = 1,\ p = 1,\ q = 2, \tag{19.267}$$

$$a_1 = 0,\ A_1 = 1, \tag{19.268}$$

$$b_1 = 0,\ B_1 = 1, \tag{19.269}$$

$$b_2 = 1-\beta,\ B_2 = \alpha, \tag{19.270}$$

thus yielding

$$\boxed{E_{\alpha,\beta}(z) = H^{1,1}_{1,2}\left(-z\middle|^{(0,1)}_{(0,1),(1-\beta,\alpha)}\right).} \tag{19.271}$$

5. H-**function representation of** $1/(1-z)^a$, $|z| < 1$:
Let us now consider the integral

$$f(z) = \frac{1}{2\pi i\Gamma(a)} \int_{\gamma-i\infty}^{\gamma+i\infty} \Gamma(s)\Gamma(-s+a)(-z)^{-s}\, ds, \tag{19.272}$$

where $|\arg(-z)| < \pi$, $\operatorname{Re} a > \operatorname{Re}\gamma > 0$ and the contour is the straight line $\operatorname{Re} s = \gamma$ that separates the poles of

$$\Gamma(s), \quad s = -n,\ n = 0, 1, \ldots \tag{19.273}$$

and the poles of

$$\Gamma(-s+a), \quad s = a+n,\ n = 0, 1, \ldots . \tag{19.274}$$

Using the residue theorem, we evaluate the above integral:

$$f(z) = 2\pi i \sum_{n=0}^{\infty} \text{Residues} \left[\frac{\Gamma(s)\Gamma(-s+a)(-z)^{-s}}{2\pi i\Gamma(a)}\right]_{\text{poles of } \Gamma(s)} \tag{19.275}$$

$$= \sum_{n=0}^{\infty} \text{Residues} \left[\frac{\Gamma(s)\Gamma(-s+a)(-z)^{-s}}{\Gamma(a)}\right]_{\text{poles of } \Gamma(s)} \tag{19.276}$$

$$= \sum_{n=0}^{\infty} \lim_{s\to -n} \left\{ \begin{array}{c} (s+n)\dfrac{(s+n-1)(s+n-2)\cdots s\Gamma(s)}{(s+n-1)(s+n-2)\cdots s} \\ \times \left[\dfrac{\Gamma(-s+a)}{\Gamma(a)}(-z)^{-s}\right] \end{array} \right\}, \tag{19.277}$$

which we write as

$$f(z) = \sum_{n=0}^{\infty} \lim_{s\to -n} \left\{ \frac{\Gamma(s+n+1)}{(s+n-1)(s+n-2)\cdots s} \left[\frac{\Gamma(-s+a)}{\Gamma(a)}(-z)^{-s}\right] \right\}, \tag{19.278}$$

$$= \sum_{n=0}^{\infty} \lim_{s\to -n} \left\{ \frac{1}{(-1)^s(-s-n+1)(-s-n+2)\cdots(-s)} \frac{\Gamma(-s+a)}{\Gamma(a)}(-z)^{-s} \right\}, \tag{19.279}$$

$$= \sum_{n=0}^{\infty} \frac{\Gamma(n+a)}{\Gamma(a)} \frac{z^n}{n!}. \tag{19.280}$$

This is nothing but $1/(1-z)^a$, thus

$$\sum_{n=0}^{\infty} \frac{\Gamma(n+a)}{\Gamma(a)} \frac{z^n}{n!} = \frac{1}{(1-z)^a}, \quad |z| < 1. \tag{19.281}$$

In other words, Eq. (19.272) is nothing but an integral representation of $1/(1-z)^a$. Comparing with the definition of the H-function [Eqs. (19.212) and (19.213)], we identify the parameters as

$$m = 1,\ n = 1,\ p = 1,\ q = 1, \tag{19.282}$$

$$a_1 = 1 - a,\ A_1 = 1, \tag{19.283}$$

$$b_1 = 0,\ B_1 = 1. \tag{19.284}$$

Thus, obtaining the desired H-function representation as

$$\boxed{\frac{1}{(1-z)^a} = H_{1,1}^{1,1}\left(-z\Big|_{(0,1)}^{(1-a,1)}\right).} \tag{19.285}$$

6. H-**function representation of** $\dfrac{z^\beta}{1+az^\alpha}$ **:**
   Following similar steps, one can also show the following useful result:

$$\boxed{\frac{z^\beta}{1+az^\alpha} = a^{-\beta/\alpha} H_{1,1}^{1,1}\left(az^\alpha\Big|_{(\beta/\alpha,1)}^{(\beta/\alpha,1)}\right).} \tag{19.286}$$

19.5.4 Computable Form of the *H*-Function

Given an H-function, we can compute, plot, and also study its asymptotic forms using the following **series expressions** [2, 5, 9, 14]:

(I) If the poles of

$$\prod_{j=1}^{m} \Gamma(b_j + sB_j) \tag{19.287}$$

are simple, that is, if

$$B_h(b_j + \lambda) \neq B_j(b_h + \nu), \quad j \neq h,\ j,h = 1,\dots,m,\ \lambda,\nu = 0,1,2,\dots, \tag{19.288}$$

then the following expansion can be used:

$$\boxed{\begin{aligned} H_{p,q}^{m,n}(z) &= \sum_{h=1}^{m}\sum_{\nu=0}^{\infty}(-1)^\nu \frac{z^{(b_h+\nu)/B_h}}{\nu! B_h} \\ &\times \frac{\left[\prod_{j=1}^{\prime m} \Gamma(b_j - B_j(b_h+\nu)/B_h)\right]\left[\prod_{j=1}^{n}\Gamma(1-a_j+A_j(b_h+\nu)/B_h)\right]}{\left[\prod_{j=m+1}^{q}\Gamma(1-b_j+B_j(b_h+\nu)/B_h)\right]\left[\prod_{j=n+1}^{p}\Gamma(a_j-A_j(b_h+\nu)/B_h)\right]}, \end{aligned}} \tag{19.289}$$

where a prime in the product means $j \neq h$. This series converges for all $z \neq 0$ if $\mu > 0$ and for $0 < |z| < 1/\beta$ if $\mu = 0$, where μ and β are defined as

$$\mu = \sum_{j=1}^{q} B_j - \sum_{j=1}^{p} A_j, \tag{19.290}$$

$$\beta = \prod_{j=1}^{p} A_j^{A_j} \prod_{j=1}^{q} B_j^{-B_j}. \tag{19.291}$$

(II) If the poles of

$$\prod_{j=1}^{m} \Gamma(1 - a_j - sA_j) \tag{19.292}$$

are simple:

$$A_h(1 - a_j + \nu) \neq A_j(1 - a_h + \lambda), \quad j \neq h,\ j, h = 1, \dots, n,\ \lambda, \nu = 0, 1, 2, \dots, \tag{19.293}$$

then the following expansion can be used:

$$H_{p,q}^{m,n}(z) = \sum_{h=1}^{n} \sum_{\nu=0}^{\infty} (-1)^{\nu} \frac{(1/z)^{(1-a_h+\nu)/A_h}}{\nu! A_h} \times \frac{\left[\prod_{j=1}^{\prime n} \Gamma(1 - a_j - A_j(1 - a_h + \nu)/A_h)\right] \left[\prod_{j=1}^{m} \Gamma(b_j + B_j(1 - a_h + \nu)/A_h)\right]}{\left[\prod_{j=m+1}^{q} \Gamma(1 - b_j - B_j(1 - a_h + \nu)/A_h)\right] \left[\prod_{j=n+1}^{p} \Gamma(a_j + A_j(1 - a_h + \nu)/A_h)\right]}, \tag{19.294}$$

where a prime in the product means $j \neq h$. This series converges for all $z \neq 0$ if $\mu < 0$ and for $|z| > 1/\beta$ if $\mu = 0$, where μ and β are defined as above.

19.6 Applications of *H*-Functions

Before we discuss the applications of H-functions to relaxation and anomalous diffusion phenomena, for the sake of completeness, we review the basic definitions and properties of fractional calculus, where additional details can be found in Chapter 13.

19.6.1 Riemann–Liouville Definition of Differintegral

The basic definition of fractional derivative and integral, that is, **differintegral**, is the Riemann–Liouville (R-L) definition [Eqs. (13.77) and (13.78)]:

For $q < 0$, the **R–L fractional integral** is evaluated using the formula

$$\left[\frac{d^q f}{[d(t-a)]^q}\right] = \frac{1}{\Gamma(-q)} \int_a^t [t-t']^{-q-1} f(t')\, dt', \quad q < 0. \tag{19.295}$$

For the **R–L fractional derivatives**, $q \geq 0$, the above integral is divergent, hence the R–L formula is modified as

$$\left[\frac{d^q f}{[d(t-a)]^q}\right] = \frac{d^n}{dt^n}\left[\frac{1}{\Gamma(n-q)} \int_a^t [t-t']^{-(q-n)-1} f(t') dt'\right], \quad q \geq 0,\ n > q, \tag{19.296}$$

where the integer n must be chosen as the smallest integer satisfying $(q-n) < 0$.

For $0 < q < 1$ and $a = 0$, the Riemann–Liouville fractional derivative becomes

$$\left[\frac{d^q f(t)}{dt^q}\right]_{R-L} = \frac{1}{\Gamma(1-q)} \frac{d}{dx} \int_0^t \frac{f(t')\, d\tau}{(t-t')^q}, \quad 0 < q < 1. \tag{19.297}$$

19.6.2 Caputo Fractional Derivative

In 1960s, Caputo introduced a new definition of fractional derivative:

$$\left[\frac{d^q f(t)}{dt^q}\right]_C = \frac{1}{\Gamma(1-q)} \int_0^t \left(\frac{df(\tau)}{d\tau}\right) \frac{d\tau}{(t-\tau)^q}, \quad 0 < q < 1, \tag{19.298}$$

which was used by him to model dissipation effects in linear viscosity. The two derivatives are related by

$$\left[\frac{d^q f(t)}{dt^q}\right]_C = \left[\frac{d^q f(t)}{dt^q}\right]_{R-L} - \frac{t^{-q} f(0)}{\Gamma(1-q)}, \quad 0 < q < 1. \tag{19.299}$$

Laplace transforms of the Riemann–Liouville and the Caputo derivatives are given, respectively, as

$$\pounds\{{}_0^{R-L}D_t^q f(t)\} = s^q \tilde{f}(s) - \sum_{k=0}^{n-1} s^k \left({}_0^{R-L}D_t^{q-k-1} f(t)\right)|_{t=0}, \quad n-1 < q \leq n, \tag{19.300}$$

$$\pounds\{{}_0^C D_t^q f(t)\} = s^q \tilde{f}(s) - \sum_{k=0}^{n-1} s^{q-k-1} \left.\frac{d^k f(t)}{dt^k}\right|_{t=0}, \quad n-1 < q \leq n, \tag{19.301}$$

where ${}_0D_t^q f(t) \equiv \frac{d^q f}{dt^q}$. Whenever there is need for distinction, we use the abbreviation "R–L" or "C." When there is no abbreviation, it means R–L. Since the

Caputo derivative allows us to impose boundary conditions in terms of the ordinary derivatives, it has found widespread use.

For $0 < q < 1$, the **Laplace transform** of the **Caputo derivative** becomes

$$\boxed{\pounds\left\{{}_0^C D_t^q f(t)\right\} = s^q \tilde{f}(s) - s^{q-1} f(0),} \tag{19.302}$$

while the **R–L derivative** has the Laplace transform

$$\boxed{\pounds\left\{{}_0 D_t^q f(t)\right\} = s^q \tilde{f}(s) - {}_0 D_t^{q-1} f(0).} \tag{19.303}$$

19.6.3 Fractional Relaxation

The **fractional relaxation** equation in terms of the **Caputo derivative** is written as

$$\boxed{{}_0^C D_t^\alpha f(t) = -\frac{1}{\tau^\alpha} f(t), \quad 0 < \alpha < 1,\ t > 0,} \tag{19.304}$$

where τ is a positive constant with the appropriate units. With the initial condition $f(0) = f_0$, the Laplace transform [Eq. (19.302)] of the fractional relaxation equation becomes:

$$s^\alpha \tilde{f}(s) - s^{\alpha-1} f_0 = -\frac{1}{\tau^\alpha} \tilde{f}(s). \tag{19.305}$$

This gives the solution in the transform space as

$$\tilde{f}(s) = \frac{f_0 s^{\alpha-1}}{s^\alpha + (1/\tau^\alpha)} = f_0 \frac{s^{-1}}{1 + (s\tau)^{-\alpha}}. \tag{19.306}$$

Using Eq. (19.286), we can write this in terms of H-functions as

$$\tilde{f}(s) = \frac{f_0}{\tau} H_{1,1}^{1,1}\left(\frac{1}{(\tau s)^\alpha} \bigg|_{(1/\alpha,1)}^{(1/\alpha,1)} \right). \tag{19.307}$$

Using the relations in Eq. (19.234) and (19.235), we rewrite this as

$$\tilde{f}(s) = f_0 \left(\frac{\tau}{\alpha}\right) H_{1,1}^{1,1}\left(\tau s \big|_{(1-1/\alpha,1/\alpha)}^{(1-1/\alpha,1/\alpha)} \right) \tag{19.308}$$

and take its inverse Laplace transform [Eq. (19.225)] to obtain

$$f(t) = \frac{f_0}{\alpha}\left(\frac{\tau}{t}\right) H_{2,1}^{1,1}\left((\tau/t) \big|_{(1-1/\alpha,1/\alpha),}^{(1-1/\alpha,1/\alpha),(0,1)} \right). \tag{19.309}$$

This can also be written as

$$f(t) = \frac{f_0}{\alpha} H_{1,2}^{1,1}\left((t/\tau) \big|_{(0,1/\alpha),(0,1)}^{(0,1/\alpha)} \right), \tag{19.310}$$

or as

$$f(t) = f_0 H_{1,2}^{1,1}\left((t/\tau)^\alpha \big|_{(0,1),(0,\alpha)}^{(0,1)} \right), \tag{19.311}$$

which is nothing but the **Mittag–Leffler** function [Eq. (19.263)]:

$$\boxed{f(t) = f_0 E_\alpha(-(t/\tau)^\alpha).} \tag{19.312}$$

The Mittag–Leffler function gives relaxation between a power law and an exponential. Naturally, as $\alpha \to 1$, the solution becomes an exponential: $f(t) = f_0 \exp(-(t/\tau))$.

19.6.4 Time Fractional Diffusion via *R–L* Derivative

The time fractional diffusion equation with the **Riemann–Liouville** derivative is written as

$$\boxed{{}_0D_t^\alpha u(x,t) = D_\alpha^2 \frac{\partial^2 u(x,t)}{\partial x^2}, \quad t > 0, \ -\infty < x < \infty, \quad 0 < \alpha < 1,} \tag{19.313}$$

where D_α is a constant with the appropriate units. Using the following boundary conditions:

$$\lim_{x \to \pm\infty} u(x,t) \to 0, \tag{19.314}$$

$${}_0D_t^{\alpha-1} u(x,0) = \phi(x), \tag{19.315}$$

we first take the Fourier transform with respect to x and then the Laplace transform with respect to t of Eq. (19.313) to obtain

$$\tilde{\overline{u}}(k,s) = \frac{\overline{\phi}(k)/k^2 D_\alpha^2}{1 + s^2/k^2 D_\alpha^2}, \tag{19.316}$$

where $\tilde{\overline{u}}(k,s) = \int_0^\infty \int_{-\infty}^\infty e^{-st+ikx} u(x,t)\, dxdt$ and $\overline{\phi}(k) = \mathcal{F}\{{}_0D_t^{\alpha-1}\overline{u}(k,0)\}$. Note that "– " denotes the Fourier and "∼" the Laplace transform. Using Eq. (19.286), we can express $\tilde{\overline{u}}(k,s)$ in terms of H-functions as

$$\tilde{\overline{u}}(k,s) = \frac{\overline{\phi}(k)}{k^2 D_\alpha^2} H_{1,1}^{1,1}\left(\frac{s^\alpha}{k^2 D_\alpha^2} \middle|_{(0,1)}^{(0,1)} \right). \tag{19.317}$$

Inverting the Laplace transform [Eq. (19.225)]:

$$\overline{u}(k,t) = \frac{\overline{\phi}(k)}{k^2 D_\alpha^2} \left(\frac{1}{t}\right) H_{2,1}^{1,1}\left(\frac{t^{-\alpha}}{k^2 D_\alpha^2} \middle|_{(0,1)}^{(0,1),(0,\alpha)} \right). \tag{19.318}$$

Using Eqs. (19.234) and then (19.236), we rewrite this as

$$\overline{u}(k,t) = \overline{\phi}(k) t^{\alpha-1} H_{1,2}^{1,1}\left(k^2 D_\alpha^2 t^\alpha \middle|_{(0,1),(1-\alpha,\alpha)}^{(0,1)} \right). \tag{19.319}$$

Finally, taking the inverse Fourier transform:

$$u(x,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dk e^{-ikx}\overline{\phi}(k) t^{\alpha-1} H_{1,2}^{1,1}\left(k^2 D_\alpha^2 t^\alpha \Big|_{(0,1),(1-\alpha,\alpha)}^{(0,1)}\right) \tag{19.320}$$

and substituting $\overline{\phi}(k) = \int_{-\infty}^{\infty} e^{ikx'}\phi(x')\,dx'$, we write

$$u(x,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} t^{\alpha-1} H_{1,2}^{1,1}\left(D_\alpha^2 k^2 t^\alpha \Big|_{(0,1),(1-\alpha,\alpha)}^{(0,1)}\right) e^{-ik(x-x')}\phi(x')\,dx'dk. \tag{19.321}$$

Using symmetry, we can also write this as

$$\boxed{u(x,t) = \int_{-\infty}^{\infty} dx'\phi(x')G(x-x'),} \tag{19.322}$$

where

$$\boxed{G(x-x') = \frac{1}{\pi}\int_0^{\infty} dk t^{\alpha-1} H_{1,2}^{1,1}\left(D_\alpha^2 k^2 t^\alpha \Big|_{(0,1),(1-\alpha,\alpha)}^{(0,1)}\right)\cos k(x-x').} \tag{19.323}$$

We now use the **Fourier-cosine** transform of the H-function in Eq. (19.231) to write the following closed expression for $G(x-x')$:

$$\boxed{G(x-x') = \frac{t^{\alpha-1}}{\sqrt{\pi}|x-x'|} H_{3,2}^{1,2}\left(\frac{4D_\alpha^2 t^\alpha}{|x-x'|^2}\Bigg|_{(0,1),(1-\alpha,\alpha)}^{(1/2,1),(0,1),(0,1)}\right).} \tag{19.324}$$

19.6.5 Time Fractional Diffusion via Caputo Derivative

We now consider the time fractional diffusion equation in terms of the Caputo derivative:

$$\boxed{{}_0^C D_t^\alpha u(x,t) = D_\alpha^2 \frac{\partial^2 u(x,t)}{\partial x^2}, \quad t>0,\ -\infty<x<\infty,\ 0<\alpha<1,} \tag{19.325}$$

with the following boundary conditions:

$$u(x,0) = \delta(x), \tag{19.326}$$

$$\lim_{x\to\pm\infty} u(x,t) \to 0. \tag{19.327}$$

Taking the **Laplace–Fourier** transform:

$$\tilde{\bar{u}}(k,s) = \int_0^{\infty}\int_{-\infty}^{\infty} e^{-st+ikx}u(x,t)\,dxdt, \tag{19.328}$$

and using the fact that

$$\mathcal{F}\{u(x,0)\} = \int_{-\infty}^{\infty} e^{ikx}\delta(x) = 1, \tag{19.329}$$

we write

$$s^{\alpha}\tilde{\bar{u}}(k,s) - s^{\alpha-1} = -D_{\alpha}k^2\tilde{\bar{u}}(k,s), \tag{19.330}$$

hence

$$\boxed{\tilde{\bar{u}}(k,s) = \frac{s^{\alpha-1}}{s^{\alpha}+D_{\alpha}k^2}.} \tag{19.331}$$

As in the previous case, first by inverting the Laplace transform and then by finding the inverse Fourier transform, we obtain the solution as

$$u(x,t) = \frac{1}{|x|}H_{1,1}^{1,0}\left(\frac{|x|^2}{D_{\alpha}t^{\alpha}}\middle|_{(1,2)}^{(1,\alpha)}\right). \tag{19.332}$$

The $\alpha \to 1$ Limit:
For the $\alpha \to 1$ limit, we first write the solution as

$$u(x,t) = \frac{1}{|x|}H_{1,1}^{1,0}\left(\frac{|x|^2}{Dt}\middle|_{(1,2)}^{(1,1)}\right), \tag{19.333}$$

where we have substituted $D_1 = D$ and then express it as a **Mellin–Barnes** type integral:

$$u(x,t) = \frac{1}{|x|}\frac{1}{2\pi i}\int_C \frac{\Gamma(1-2s)}{\Gamma(1-s)}\left(\frac{|x|^2}{Dt}\right)^s ds. \tag{19.334}$$

Using the **duplication**formula of the gamma functions:

$$\Gamma(2x) = \frac{4^x\Gamma(x)\Gamma(x+1/2)}{2\sqrt{\pi}}, \tag{19.335}$$

we write

$$\Gamma(1-2s) = \Gamma(2(1/2-s)) \tag{19.336}$$

$$= \frac{4^{(1/2-s)}\Gamma(1/2-s)\Gamma(1/2-s+1/2)}{2\sqrt{\pi}} \tag{19.337}$$

$$= 2^{-2s}\pi^{-1/2}\Gamma(1/2-s)\Gamma(1-s). \tag{19.338}$$

Now the solution [Eq. (19.334)] becomes

$$u(x,t) = \frac{1}{|x|}\frac{1}{2\pi i}\int_C 2^{-2s}\pi^{-1/2}\Gamma(1/2-s)\left(\frac{|x|^2}{Dt}\right)^s ds, \tag{19.339}$$

where the contour is the straight line

$$s = \gamma, \quad \gamma \in \mathbb{R}, \tag{19.340}$$

that is,

$$u(x,t) = \frac{1}{|x|}\frac{1}{2\pi i}\int_{\gamma-i\infty}^{\gamma+i\infty} \pi^{-1/2}\Gamma(1/2-s)\left(\frac{|x|^2}{4Dt}\right)^s ds. \tag{19.341}$$

We evaluate the integral using the residue theorem:

$$u(x,t) = \frac{1}{|x|}\frac{1}{2\pi i}2\pi i\left[-\sum \text{Residues}\left(\Gamma(1/2-s)\left(\frac{|x|^2}{4Dt}\right)^s\right)\right], \tag{19.342}$$

where the residues are at the poles of the gamma function $\Gamma(1/2-s)$:

$$s_\nu = 1/2+\nu, \quad \nu = 0,1,2,\ldots \tag{19.343}$$

and lies to the right of the contour. Using the relation

$$\frac{\Gamma(-n)}{\Gamma(-N)} = (-1)^{N-n}\frac{N!}{n!}, \tag{19.344}$$

for $N = 0$, we write

$$\Gamma(-n) = (-1)^n\frac{1}{n!}\Gamma(0). \tag{19.345}$$

In other words, each pole acts like $\Gamma(0)$, thus allowing us to write

$$u(x,t) = \frac{1}{|x|\sqrt{\pi}}\left[\sum_{\nu=0}^{\infty}(-1)^\nu\frac{1}{\nu!}\left(\frac{|x|^2}{4Dt}\right)^{1/2+\nu}\right] \tag{19.346}$$

$$= \frac{1}{\sqrt{\pi}}\frac{1}{\sqrt{4Dt}}\sum_{\nu=0}^{\infty}\frac{(-1)^\nu}{\nu!}\left(\frac{|x|^2}{4Dt}\right)^\nu, \tag{19.347}$$

which is the **Gaussian**

$$\boxed{u(x,t) = \frac{1}{\sqrt{4\pi D_\alpha t}}e^{-(|x|^2/4D_\alpha t)}.} \tag{19.348}$$

19.6.6 Derivation of the Lévy Distribution

We are now ready to give the derivation of the Lévy distribution [Eq. (19.198)]:

$$\boxed{W_L(x,t) = \frac{\pi}{q|x|}H_{2,2}^{1,1}\left(\frac{|x|}{(D_q t)^{1/q}}\middle|\begin{matrix}(1,1/q),(1,1/2)\\ \\(1,1),(1,1/2)\end{matrix}\right),} \tag{19.349}$$

in terms of H-functions. The Lévy distribution, $W_L(x,t)$, satisfies the space fractional diffusion equation

$$\frac{\partial W_L(x,t)}{\partial t} = D_q R_x^q W_L(x,t), \tag{19.350}$$

where R_x^q is the fractional Riesz derivative operator and D_q is the fractional diffusion constant. The boundary conditions are given as

$$\lim_{t\to t_0} W_L(x,t,x_0,t_0) = \delta(x-x_0), \tag{19.351}$$

$$\lim_{t\to\infty} W_L(x,t,x_0,t_0) = 0. \tag{19.352}$$

Taking the Fourier transform of Eq. (19.350), we obtain the Fourier transform of the solution [Eq. (19.196)]:

$$\overline{W}_L(k,t) = \exp(-D_q t|k|^q), \tag{19.353}$$

where for simplicity, we have set $x_0 = t_0 = 0$. Using the H-function representation of the exponential function [Eq. (19.253)], we write

$$\overline{W}_L(k,t) = H_{0,1}^{1,0}\left(D_q t|k|^q|_{(0,1)}\right) \tag{19.354}$$

and after using Eq. (19.235), we rewrite this as

$$\overline{W}_L(k,t) = \frac{1}{q}H_{0,1}^{1,0}\left((D_q t)^{1/q}|k||_{(0,1/q)}\right). \tag{19.355}$$

To find the solution, we need the inverse Fourier transform:

$$W_L(x,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dk e^{ikx}\overline{W}_L(k,t) \tag{19.356}$$

$$= \frac{1}{2\pi}\int_{-\infty}^{\infty} dk e^{ikx}\frac{1}{q}H_{0,1}^{1,0}\left((D_q t)^{1/q}|k||_{(0,1/q)}\right), \tag{19.357}$$

which can also be written as

$$W_L(x,t) = \frac{1}{q\pi}\int_0^{\infty} dk \cos kx H_{0,1}^{1,0}\left((D_q t)^{1/q}|k||_{(0,1/q)}\right). \tag{19.358}$$

We now make use of the Fourier–cosine transform formula [Eq. (19.231)] with the substitutions

$$\rho = 1,\ a = |x|,\ x = |k|, \tag{19.359}$$

$$b = (D_q t)^{1/q},\ \sigma = 1, \tag{19.360}$$

$$m = 1,\ n = 0,\ p = 0,\ q = 1, \tag{19.361}$$

$$b_1 = 0,\ B_1 = 1/q, \tag{19.362}$$

to write the solution as

$$W_L(x,t) = \frac{1}{q\pi}\frac{\sqrt{\pi}}{|x|}H_{2,1}^{1,1}\left((D_q t)^{1/q}\frac{2}{|x|}\middle|_{(0,1/q)}^{(1/2,1/2),(0,1/2)}\right). \tag{19.363}$$

Using Eq. (19.234), we rewrite this as

$$\boxed{W_L(x,t) = \frac{1}{\sqrt{\pi}q|x|} H_{1,2}^{1,1}\left(\frac{|x|}{2(D_q t)^{1/q}} \middle|_{(1/2,1/2),(1,1/2)}^{(0,1/q)} \right).} \tag{19.364}$$

To show the equivalence of this with the expression in Eq. (19.349), we first write it as a Mellin–Barnes type integral:

$$W_L(x,t) = \frac{1}{\sqrt{\pi}q|x|} \frac{1}{2\pi i} \int_C \frac{\Gamma\left(\frac{1}{2} - \frac{s}{2}\right)\Gamma\left(\frac{s}{q}\right)}{\Gamma(s/2)} \left(\frac{|x|}{2(D_q t)^{1/q}} \right)^s ds. \tag{19.365}$$

Similarly, we also convert [Eq. (19.349)]:

$$W_L(x,t) = \frac{\pi}{q|x|} H_{2,2}^{1,1}\left(\frac{|x|}{(D_q t)^{1/q}} \middle|_{(1,1),(1,1/2)}^{(1,1/q),(1,1/2)} \right), \tag{19.366}$$

into a Mellin–Barnes type integral as

$$W_L(x,t) = \frac{\pi}{q|x|} \frac{1}{2\pi i} \int_C \frac{\Gamma(b_1 - B_1 s)\Gamma(1 - a_1 + A_1 s)}{\Gamma(a_2 - A_2 s)\Gamma(1 - b_2 + B_2 s)} \left(\frac{|x|}{(D_q t)^{1/q}} \right)^s ds, \tag{19.367}$$

where

$$m = 1,\ n = 1,\ p = 2,\ q = 2, \tag{19.368}$$

$$b_1 = 1,\ B_1 = 1,\ b_2 = 1,\ B_2 = 1/2, \tag{19.369}$$

$$a_1 = 1,\ A_1 = 1/q,\ a_2 = 1,\ A_2 = 1/2. \tag{19.370}$$

Using these values in Eq. (19.367), we write

$$W_L(x,t) = \frac{\pi}{q|x|} \frac{1}{2\pi i} \int_C \frac{\Gamma(1-s)\Gamma(s/q)}{\Gamma(1-s/2)\Gamma(s/2)} \left(\frac{|x|}{(D_q t)^{1/q}} \right)^s ds, \tag{19.371}$$

$$= \frac{\pi}{q|x|} \frac{1}{2\pi i} \int_C \frac{\Gamma(2(1/2 - s/2)\Gamma(s/q)}{\Gamma(1-s/2)\Gamma(s/2)} \left(\frac{|x|}{(D_q t)^{1/q}} \right)^s ds. \tag{19.372}$$

Using the duplication formula:

$$\Gamma(2x) = \frac{4^x \Gamma(x)\Gamma(x+1/2)}{2\sqrt{\pi}}, \tag{19.373}$$

along with the substitution $x = (1/2 - s/2)$, we get

$$W_L(x,t) = \frac{\pi}{q|x|}\frac{1}{2\pi i}\int_C \frac{2^{1-s}\Gamma(1/2 - s/2)\Gamma(1/2 - s/2 + 1/2)\Gamma(s/q)}{2\sqrt{\pi}\Gamma(1 - s/2)\Gamma(s/2)}\left(\frac{|x|}{(D_q t)^{1/q}}\right)^s ds, \tag{19.374}$$

$$= \frac{1}{\sqrt{\pi}q|x|}\frac{1}{2\pi i}\int_C \frac{\Gamma(1/2 - s/2)\Gamma(s/q)}{\Gamma(s/2)}\left(\frac{|x|}{2(D_q t)^{1/q}}\right)^s ds, \tag{19.375}$$

which is identical to Eq. (19.365).

19.6.7 Lévy Distributions in Nature

The **Gaussian,** or the **normal distribution,** describes many important phenomena in nature like the thermal motion of atoms, Brownian motion, and diffusion. Recent experimental results indicate that there are also other interesting phenomena that are better described by the **Lévy distribution** introduced by the, French mathematician, Paul Lévy, in 1937. In Brownian motion, the distribution function is a Gaussian, where the mean distance, $<x>$, is zero but the variance, $<x^2>$, is finite and changes linearly with time as $<x^2> \propto t$. In Brownian motion, particles always take small steps about their initial positions but they slowly drift away with time. This basically follows from the fact that Gaussian distribution decays rapidly as $1/x^3$. On the other hand, the Lévy distribution decays as $1/x^{1+\alpha}$, $0 < \alpha < 2$, thus making much larger steps possible. An interesting example is that researchers from Boston University and the British Antarctic Survey in 1996 found that albatrosses foraging behavior follow the Lévy distribution. That is, first they search for food in their neighborhood with small steps but every now and then they fly off to large distances and continue feeding in a new location before flying off again. This can be understood by the fact that looking for food in the same neighborhood for too long will not only be inefficient but also risk being spotted by predators. Besides anomalous diffusion, there are other interesting examples of Lévy distribution. Among these, we could name the leaky faucet and the erratic heart beats of healthy subjects, which can be described by the Lévy distribution with $\alpha = 1.7$. Data from patients with severe heart failure turns out to be much closer to a Gaussian. Lévy distributions have also found interesting applications to stock markets, where stock prices may stall for a while before making a big move [15].

19.6.8 Time and Space Fractional Schrödinger Equation

To write the most general fractional Schrödinger equation, we use the fact that the Schrödinger equation is analytic in the lower half of the complex t-plane and perform a Wick rotation, $t \to -it$, on the one-dimensional Schrödinger equation:

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} + V(x)\Psi(x,t), \tag{19.376}$$

to obtain

$$-\hbar\frac{\partial\Psi(x,t)}{\partial t} = -\frac{1}{2m}\left(\hbar\frac{\partial}{\partial x}\right)^2\Psi(x,t) + V(x)\Psi(x,t). \tag{19.377}$$

This is nothing but the **Bloch equation** [Eq. (19.33)]:

$$\frac{\partial\Psi(x,t)}{\partial t} = \check{D}\frac{\partial^2\Psi(x,t)}{\partial x^2} - \frac{1}{\hbar}V(x)\Psi(x,t), \quad \check{D} > 0, \tag{19.378}$$

where $\check{D} = \hbar/2m$ is the quantum diffusion constant and $V(x)$ is the potential. We now write the **time** and **space fractional Bloch equation** as

$$\boxed{{}^{C}_{0}D^{\alpha}_{t}\Psi(x,t) = \frac{1}{\hbar}\check{D}_{\alpha,\beta}\hbar^{\beta}R^{\beta}_{x}\Psi(x,t) - \frac{1}{\hbar}V(x)\Psi(x,t), \quad 0 < \alpha < 1,\ 1 < \beta < 2,} \tag{19.379}$$

where ${}^{C}_{0}D^{\alpha}_{t}$ is the **Caputo derivative** [Eq. (19.298)]:

$${}^{C}_{0}D^{\alpha}_{t}\Psi(x,t) = \frac{1}{\Gamma(1-\alpha)}\int_0^t \left(\frac{d\Psi(x,\tau)}{d\tau}\right)\frac{d\tau}{(t-\tau)^{\alpha}}, \quad 0 < \alpha < 1, \tag{19.380}$$

and R^{β}_{x} is the **Riesz derivative** [Eqs. (19.189) and (19.190)]:

$$R^{\beta}_{x}\Psi(x,t) = -\frac{1}{2\pi}\int_{-\infty}^{\infty} dk e^{ikx}|k|^{\beta}\overline{\Psi}(k,t), \tag{19.381}$$

where $\overline{\Psi}(k,t)$ is the Fourier transform of $\Psi(x,t)$. When there is no room for confusion, we will also write

$${}^{C}_{0}D^{\alpha}_{t} = \frac{\partial^{\alpha}}{\partial t^{\alpha}} \text{ and } R^{\beta}_{x} = \nabla^{\beta} = \frac{\partial^{\beta}}{\partial x^{\beta}}. \tag{19.382}$$

In Eq. (19.379), we have introduced a new quantum diffusion constant with the appropriate units as $\check{D}_{\alpha,\beta}$. Performing an inverse Wick rotation, $t \to it$, we obtain the **time** and **space fractional Schrödinger equation**:

$$\boxed{{}^{C}_{0}D^{\alpha}_{t}\Psi(x,t) = \frac{i^{\alpha}}{\hbar}\check{D}_{\alpha,\beta}\left(\hbar\frac{\partial}{\partial x}\right)^{\beta}\Psi(x,t) - \frac{i^{\alpha}}{\hbar}V(x)\Psi(x,t).} \tag{19.383}$$

19.6.8.1 Free Particle Solution

We now consider the free Schrödinger equation with both time and space fractional derivatives [Eq. (19.383)]:

$$ {}_0^C D_t^\alpha \Psi(x,t) = \frac{i^\alpha}{\hbar}\check{D}_{\alpha,\beta}\left(\hbar\frac{\partial}{\partial x}\right)^\beta \Psi(x,t), \quad 0<\alpha<1,\ 1<\beta<2, \tag{19.384} $$

Performing a Wick rotation, $t \to -it$, this becomes:

$$ \frac{\partial^\alpha}{\partial t^\alpha}\Psi(x,t) = \frac{1}{\hbar}\check{D}_{\alpha,\beta}\hbar^\beta \nabla_x^\beta \Psi(x,t), \quad 0<\alpha<1,\ 1<\beta<2, \tag{19.385} $$

where $\check{D}_{1,2} = 1/2m$. Using the boundary conditions as $\Psi(x,0) = \delta(x)$ and $\lim_{x\to\pm\infty}\Psi(x,t) \to 0$, we first take the Fourier transform with respect to space and then the Laplace transform with respect to time to obtain the Fourier-Laplace transform of the solution. Finding the inverse transforms and then performing an inverse Wick rotation, yields the wave function in integral form as

$$ \Psi(x,t) = \frac{\Psi_0}{2\pi}\int_{-\infty}^{+\infty} e^{-ikx}\ E_\alpha\left(-\frac{i^\alpha}{\hbar}\check{D}_{\alpha,\beta}\hbar^\beta k^\beta t^\alpha\right)\ dk, \tag{19.386} $$

where $E_\alpha(z)$ is the Mittag–Leffler function. We can also write $\Psi(x,t)$ as

$$ \Psi(x,t) = \frac{\Psi_0}{\pi}\int_0^{+\infty} \cos kx\ E_\alpha\left(-\frac{i^\alpha}{\hbar}\check{D}_{\alpha,\beta}\hbar^\beta k^\beta t^\alpha\right)\ dk. \tag{19.387} $$

This wave function satisfies both the time and space fractional Schrödinger equation [Eq. (19.384)]

In terms of H-functions, Eq. (19.387) can be written as [Eq. (19.271)]

$$ \Psi(x,t) = \frac{\Psi_0}{\pi}\int_0^{+\infty} \cos kx\ H_{1,2}^{1,1}\left(\frac{i^\alpha}{\hbar}\check{D}_{\alpha,\beta}\hbar^\beta k^\beta t^\alpha \,\middle|\, \begin{matrix}(0,1)\\(0,1),(0,\alpha)\end{matrix}\right)\ dk, \tag{19.388} $$

which can be integrated using the properties of the H-functions as [Eq. (19.231)]

$$ \Psi(x,t) = \frac{\Psi_0}{\sqrt{\pi}|x|}H_{3,2}^{1,2}\left(\frac{i^\alpha}{\hbar}\check{D}_{\alpha,\beta}\hbar^\beta t^\alpha\left(\frac{2}{|x|}\right)^\beta \,\middle|\, \begin{matrix}(1/2,\beta/2),(0,1),(0,\beta/2)\\(0,1),(0,\alpha)\end{matrix}\right). \tag{19.389} $$

To determine Ψ_0, the wave function has to be normalized as $\int |\Psi(x,0)|^2\,dx = 1$.

Solution with $\beta = 2$: This solution becomes the free particle solution of the time fractional Schrödinger equation as

$$ \Psi(x,t) = \frac{\Psi_0}{\sqrt{\pi}|x|}H_{3,2}^{1,2}\left(\frac{4i^\alpha D_\alpha t^\alpha}{|x|^2} \,\middle|\, \begin{matrix}(1/2,1),(0,1),(0,1)\\(0,1),(0,\alpha)\end{matrix}\right), \quad D_\alpha = \check{D}_{\alpha,2}\hbar. \tag{19.390} $$

This can also be shown to be equal to

$$ \Psi(x,t) = \frac{\Psi_0}{\sqrt{\pi}|x|}H_{1,2}^{2,0}\left(\frac{|x|^2}{4i^\alpha D_\alpha t^\alpha} \,\middle|\, \begin{matrix}(1,\alpha)\\(1/2,1),(1,1)\end{matrix}\right), \tag{19.391} $$

or to

$$\Psi(x,t) = \frac{\Psi_0}{|x|} H_{1,1}^{1,0}\left(\frac{|x|^2}{i^\alpha D_\alpha t^\alpha} \middle|_{(1,2)}^{(1,\alpha)} \right). \tag{19.392}$$

In the limit as $\alpha \to 1$, this becomes the well-known solution of the Schrödinger equation:

$$\Psi(x,t) = \frac{\Psi_0}{(4\pi i D_1 t)^{1/2}} \exp\left(-\frac{|x|^2}{4iD_1 t}\right), \tag{19.393}$$

where $D_1 = \hbar/2m$.

Solution with $\alpha = 1$:
We now obtain the wave function as

$$\Psi(x,t) = \frac{\Psi_0}{\sqrt{\pi}|x|} H_{3,2}^{1,2}\left(\frac{i}{\hbar} D_\beta \hbar^\beta t \left(\frac{2}{|x|}\right)^\beta \middle|_{(0,1),(0,1)}^{(1/2,\beta/2),(0,1),(0,\beta/2)} \right), \tag{19.394}$$

which satisfies

$$i\hbar \frac{\partial}{\partial t}\Psi(x,t) = -D_\beta \hbar^\beta R_x^\beta \Psi(x,t), \quad 1 < \beta < 2, \tag{19.395}$$

where $\check{D}_{1,\beta} = D_\beta$. This solution can also be written in the form:

$$\Psi(x,t) = \frac{\pi\Psi_0}{\beta|x|} H_{2,2}^{1,1}\left(\frac{1}{\hbar}\left(\frac{\hbar}{iD_\beta t}\right)^{1/\beta} |x| \middle|_{(1,1),(1,1/2)}^{(1,1/\beta),(1,1/2)} \right). \tag{19.396}$$

19.7 Space Fractional Schrödinger Equation

For $\alpha = 1$, Eq. (19.383) reduces to the space fractional Schrödinger equation:

$$\frac{\partial}{\partial t}\Psi(x,t) = \frac{i}{\hbar}\check{D}_{1,\beta}\left(\hbar\frac{\partial}{\partial x}\right)^\beta \Psi(x,t) - \frac{i}{\hbar}V(x)\Psi(x,t), \quad 1 < \beta < 2, \tag{19.397}$$

which Laskin [7] wrote as

$$\boxed{i\hbar\frac{\partial}{\partial t}\Psi(x,t) = -D_\beta[\hbar\nabla]^\beta\Psi(x,t) + V(x)\Psi(x,t).} \tag{19.398}$$

Here, $[\hbar\nabla]^\beta$ is called the **quantum Riesz derivative** and D_β is the quantum diffusion constant, where $D_\beta \to 1/2m$ as $\beta \to 2$.

19.7.1 Feynman Path Integrals Over Lévy Paths

In the presence of interactions, the space fractional version of the Schrödinger equation:

$$\frac{\partial\Psi(x,t)}{\partial t} = \frac{i}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} - iV(x)\Psi(x,t), \tag{19.399}$$

is written as [Eq. (19.398)]

$$\boxed{\frac{\partial\Psi(x,t)}{\partial t} = i\tilde{D}_q\nabla^q\Psi(x,t) - iV(x)\Psi(x,t), \quad 1 < q < 2,} \tag{19.400}$$

where for time being, we have set $\hbar = 1$ for simplicity. After a Wick rotation, $t \to -it$, this becomes the **space fractional Bloch equation**:

$$\frac{\partial\Psi(x,t)}{\partial t} = \tilde{D}_q\nabla^q\Psi(x,t) - V(x)\Psi(x,t). \tag{19.401}$$

When $q = 2$, the generalized fractional quantum diffusion constant, $\tilde{D}_2$, becomes

$$\tilde{D}_2 = 1/2m. \tag{19.402}$$

We now follow the steps described in Section 19.3 that lead to the Feynman path integral formulation of quantum mechanics and replace D_q with $i\tilde{D}_q$ in $d_L x(\tau)$ [Eq. (19.205)] to write the Feynman measure over Lévy paths as

$$d_L^{\text{Feynman}}x(\tau) = \lim_{N\to\infty}\left[dx_1\cdots dx_N \left(\frac{1}{i\tilde{D}_q\Delta\tau}\right)^{-(N+1)/q} \times \prod_{i=1}^{N+1} L_q\left\{\left(\frac{1}{i\tilde{D}_q\Delta\tau}\right)^{1/q}|x_i - x_{i-1}|\right\}\right]. \tag{19.403}$$

Since the path integrals are to be evaluated over Lévy paths, we replace the Feynman measure, $d_F x(\tau)$, in Eq. (19.143) with the Feynman measure over Lévy paths, $d_L^{\text{Feynman}}x(\tau)$, where $\tilde{D}_q$ is the generalized fractional diffusion constant of the space fractional quantum mechanics.

To convert these equations into proper physical dimensions, we have to introduce suitable powers of $\hbar$ into $d_L^{\text{Feynman}}x(\tau)$. We first note that the physical dimension of $(1/i\tilde{D}_q\Delta\tau)^{1/q}$ is $1/\text{cm}$, hence the dimension of $(i\tilde{D}_q\Delta\tau)^{-(N+1)/q}$ must be cm^{N-1}. We now consider the following expression:

$$\hbar^a\left(\frac{\hbar^b}{i\tilde{D}_q\Delta\tau}\right)^{1/q}, \tag{19.404}$$

where a and b are to be determined. Using $[\hbar] = ergs.\mathrm{s}$, $[\Delta\tau] = \mathrm{s}$, and the fact that

$$\left[\hbar^a\left(\frac{\hbar^b}{i\tilde{D}_q\Delta\tau}\right)^{1/q}\right] = \frac{1}{\mathrm{cm}}, \tag{19.405}$$

we get,

$$[\tilde{D}_q]^{1/q} = erg^{aq+1}\mathrm{cm}^q\mathrm{s}^{aq+b-1}, \tag{19.406}$$

$$= gm^{aq+b}\mathrm{cm}^{2aq+q+2b}\mathrm{s}^{-aq-b-1}. \tag{19.407}$$

Since when $q = 2$, the dimension of $\tilde{D}_2$ is $[\tilde{D}_2] = \left[\frac{1}{2m}\right] = gm^{-1}$ [Eq. (19.402)], we require the following set of equations to be true at $q = 2$:

$$\left.\begin{array}{l} aq + b = -1, \\ 2aq + q + 2b = 0, \\ -aq - b - 1 = 0, \end{array}\right|_{q=2}, \tag{19.408}$$

which yields the values $a = -1$ and $b = 1$. The physical dimension of $\tilde{D}_q$ is now obtained as $[\tilde{D}_q] = ergs^{1-q}\mathrm{cm}^q\mathrm{s}^{-q}$ and the Feynman measure over the Lévy paths with the physical dimensions becomes

$$d_L^{\text{Feynman}}x(\tau) = \lim_{N\to\infty}\left[dx_1\cdots dx_N\frac{1}{\hbar^{N+1}}\left(\frac{\hbar}{i\tilde{D}_q\Delta\tau}\right)^{(N+1)/q} \times \prod_{i=1}^{N+1} L_q\left\{\frac{1}{\hbar}\left(\frac{\hbar}{i\tilde{D}_q\Delta\tau}\right)^{1/q}|x_i - x_{i-1}|\right\}\right]. \tag{19.409}$$

Note that the physical dimension of $d_L^{\text{Feynman}}x(\tau)$ is $1/\mathrm{cm}$.

We now modify the **Feynman–Kac formula** [Eq. (19.35)]:

$$W_B(x, t, x_0, 0) = \int_{C[x_0,0;x,t]} d_w x(\tau)\exp\left\{-\int_0^t d\tau V[x(\tau),\tau]\right\}, \tag{19.410}$$

where the path integral is now to be taken over the **Lévy paths**. This gives the new **propagator**:

$$\boxed{K(x, t, x_0, t_0) = \int_{[x_0,t_0,x,t]} d_L^{\text{Feynman}}x(\tau)\exp\left\{-\frac{i}{\hbar}\int_{t_0}^t d\tau V[x(\tau)]\right\},} \tag{19.411}$$

which can be used to write the solution of the **space fractional Schrödinger equation** [Eq. (19.400)] as

$$\boxed{\Psi(x,t) = \int K(x,t,x',t')\Psi(x',t')\,dx'.} \tag{19.412}$$

With the proper factors of $\hbar$ introduced, the space fractional Schrödinger equation in physical dimensions becomes

$$\boxed{i\hbar\frac{\partial\Psi(x,t)}{\partial t} = -\tilde{D}_q(\hbar\nabla)^q\Psi(x,t) + V(x)\Psi(x,t).} \tag{19.413}$$

19.8 Time Fractional Schrödinger Equation

Substituting $\beta = 2$ in Eq. (19.383), we get

$${}_0^C D_t^\alpha \Psi(x,t) = \frac{i^\alpha}{\hbar}\check{D}_{\alpha,2}\left(\hbar\frac{\partial}{\partial x}\right)^2\Psi(x,t) - \frac{i^\alpha}{\hbar}V(x)\Psi(x,t) \tag{19.414}$$

or,

$${}_0^C D_t^\alpha \Psi(x,t) = i^\alpha\check{D}_{\alpha,2}\hbar\frac{\partial^2}{\partial x^2}\Psi(x,t) - \frac{i^\alpha}{\hbar}V(x)\Psi(x,t). \tag{19.415}$$

By defining a new quantum diffusion constant, $D_\alpha = \check{D}_{\alpha,2}\hbar$, we write the time fractional Schrödinger equation as

$$\boxed{{}_0^C D_t^\alpha \Psi(x,t) = i^\alpha D_\alpha\frac{\partial^2}{\partial x^2}\Psi(x,t) - \frac{i^\alpha}{\hbar}V(x)\Psi(x,t), \quad 0 < \alpha < 1,} \tag{19.416}$$

where $D_\alpha \to \hbar/2m$ as $\alpha \to 1$.

19.8.1 Separable Solutions

We now consider the separable solutions of the time fractional Schrödinger equation [1, 11]. Substituting

$$\boxed{\Psi(x,t) = X(x)T(t),} \tag{19.417}$$

we obtain the equations to be solved for $X(x)$ and $T(t)$, respectively, as

$$D_\alpha\frac{d^2X(x)}{dx^2} - \frac{V(x)}{\hbar}X(x) = \lambda_n X(x), \tag{19.418}$$

$${}_0^C D_t^\alpha T(t) = i^\alpha\lambda_n T(t), \quad 0 < \alpha < 1, \tag{19.419}$$

where the spatial equation [Eq. (19.418)] has to be solved with the appropriate boundary conditions and λ_n is the separation constant. At this point, the index

n is superfluous but we keep it for the cases where λ is discrete. Since in the limit as $\alpha \to 1$, $D_\alpha \to \hbar/2m$, and $\lambda_n \to -E_n/\hbar$, for physically interesting cases $\lambda_n < 0$.

19.8.2 Time Dependence

Taking the Laplace transform of Eq. (19.419):

$$\pounds\left\{{}_0^C D_t^\alpha T(t)\right\} = i^\alpha \lambda_n \pounds\{T(t)\}, \tag{19.420}$$

we write

$$s^\alpha \widetilde{T}(s) - s^{\alpha-1} T(0) = i^\alpha \lambda_n \widetilde{T}(s), \tag{19.421}$$

where $\widetilde{T}(s) = \pounds\{T(t)\}$. This gives the **Laplace transform** of the time dependence of the wave function as

$$\widetilde{T}(s) = T(0)\frac{s^{\alpha-1}}{s^\alpha - i^\alpha \lambda_n}. \tag{19.422}$$

We rewrite this as

$$\boxed{\widetilde{T}(s) = T(0)\frac{s^{-1}}{1 - i^\alpha \lambda_n s^{-\alpha}}.} \tag{19.423}$$

Using the geometric series, $\sum_{n=0}^{\infty} s^n = 1/(1-s)$, we obtain

$$\widetilde{T}(s) = T(0)\sum_{m=0}^{\infty} (i^\alpha \lambda_n s^{-\alpha})^m s^{-1} = T(0)\sum_{m=0}^{\infty} i^{\alpha m} \lambda_n^m s^{-m\alpha-1}, \tag{19.424}$$

which converges for $|i^\alpha \lambda_n s^{-\alpha}| < 1$. The inverse Laplace transform of $\tilde{T}(s)$ can be found easily as

$$T(t) = T(0)\sum_{m=0}^{\infty} \frac{i^{\alpha m}\lambda_n^m t^{\alpha m}}{\Gamma(1+\alpha m)} = T(0)\sum_{m=0}^{\infty} \frac{(i^\alpha \lambda_n t^\alpha)^m}{\Gamma(1+\alpha m)}, \tag{19.425}$$

which yields the **time dependence** of the wave function:

$$\boxed{T(t) = T(0)E_\alpha(i^\alpha \lambda_n t^\alpha),} \tag{19.426}$$

where $E_\alpha(i^\alpha \lambda_n t^\alpha)$ is the **Mittag–Leffler** function with an imaginary argument.

To develop an alternate expression for $T(t)$, in the following two sections, we introduce the fractional differential equation that the Mittag–Leffler function satisfies and the **Euler equation** for the Mittag–Leffler function.

19.8.3 Mittag–Leffler Function and the Caputo Derivative

Consider the following fractional differential equation:

$$\boxed{{}_0^C D_t^\alpha y(t) = \omega y(t), \quad y(0) = 1,\ 0 < \alpha < 1.} \tag{19.427}$$

Taking its Laplace transform:

$$s^\alpha \tilde{y}(s) - s^{\alpha-1} = \omega \tilde{y}(s), \tag{19.428}$$

we obtain the solution in the transform space as

$$\tilde{y}(s) = \frac{s^{\alpha-1}}{s^\alpha - \omega} = \frac{s^{-1}}{1 - \omega s^{-\alpha}}. \tag{19.429}$$

Using the geometric series, we write

$$\tilde{y}(s) = \sum_{n=0}^{\infty} \frac{\omega^n}{s^{1+\alpha n}} \tag{19.430}$$

and find the inverse to obtain the solution as

$$\boxed{y(t) = \sum_{n=0}^{\infty} \frac{(\omega t^\alpha)^n}{\Gamma(\alpha n + 1)}.} \tag{19.431}$$

This is nothing but the **Mittag–Leffler function** with the argument ωt^α:

$$\boxed{y(t) = E_\alpha(\omega t^\alpha),} \tag{19.432}$$

which is a generalization of the exponential function, $e^t = \sum_{n=0}^{\infty} t^n/n!$ Note that we will also use the notation

$$\boxed{y(t) = E_\alpha(\omega; t) = E_\alpha(\omega t^\alpha),} \tag{19.433}$$

$$\boxed{{}_0^C D_t^\alpha E_\alpha(\omega; t) = \omega E_\alpha(\omega; t), \quad E_\alpha(\omega; 0) = 1.} \tag{19.434}$$

19.8.4 Euler Equation for the Mittag–Leffler Function

Euler equation for the trigonometric functions is given as

$$y(t) = e^{i\omega t} = \cos \omega t + i \sin \omega t, \tag{19.435}$$

where $y(t)$ satisfies the differential equation

$$\frac{dy}{dt} = i\omega y(t), \quad y(0) = 1. \tag{19.436}$$

We now consider the following fractional differential equation:

$$ {}_0^C D_t^\alpha y(t) = \omega i^\alpha y(t), \quad y(0) = y_0,\ 0 < \alpha < 1, \tag{19.437} $$

where the solution is written as $y(t) = y_0 E_\alpha(\omega i^\alpha; t)$, or as $y(t) = y_0 E_\alpha(\omega i^\alpha t^\alpha)$. For an alternate expression, we write the Laplace transform of Eq. (19.437):

$$ \tilde{y}(s) = \frac{s^{\alpha-1} y_0}{s^\alpha - \omega i^\alpha}, \tag{19.438} $$

which when inverted yields the solution:

$$ y(t) = \frac{1}{2\pi i} \int_{\gamma - i\infty}^{\gamma + i\infty} \left[\frac{e^{st} s^{\alpha-1} y_0}{s^\alpha - \omega i^\alpha} \right] ds. \tag{19.439} $$

Since the integrand has a branch point at $s = 0$, the **Bromwich contour** has to be modified as in Figure 19.6. We have located the branch cut along the negative real axis and the contour around the branch cut is called the **Hankel contour**. There are two contributions to this integral, one of which is due to the pole at $s = \omega^{1/\alpha} i$ and the other one comes from the straight line segments of the contour above and below the branch cut. We can now write

$$ y(t) = [\text{residue at } s = \omega^{1/\alpha} i] + \frac{y_0}{2\pi i} \int_{\text{Hankel}} \left[\frac{e^{st} s^{\alpha-1}}{s^\alpha - \omega i^\alpha} \right] ds. \tag{19.440} $$

The residue is evaluated easily as

$$ \text{residue} = \lim_{s \to s_0} \frac{(s - s_0) y_0 e^{st} s^{\alpha-1}}{s^\alpha - \omega i^\alpha} = \frac{e^{i\omega^{1/\alpha} t}}{\alpha}, \quad s_0 = \omega^{1/\alpha} i, \tag{19.441} $$

and the remaining integral over the Hankel contour can be written as

$$ -\frac{y_0 \omega i^\alpha}{\pi} \int_0^\infty \frac{(\sin \alpha\pi) e^{-xt} x^{\alpha-1}\, dx}{x^{2\alpha} - 2\omega i^\alpha (\cos \alpha\pi) x^\alpha + (\omega i^\alpha)^2}. \tag{19.442} $$

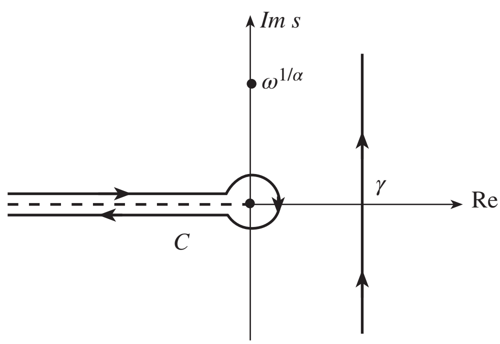

Figure 19.6 Modified Bromwich contour.

Putting these together, the final expression for the solution becomes

$$\boxed{y(t) = y_0 \left[\frac{e^{i\omega^{1/\alpha}t}}{\alpha} - \frac{\omega i^\alpha (\sin \alpha\pi)}{\pi} \int_0^\infty \frac{e^{-xt} x^{\alpha-1}\, dx}{x^{2\alpha} - 2\omega i^\alpha (\cos \alpha\pi) x^\alpha + (\omega i^\alpha)^2} \right].} \tag{19.443}$$

The first term on the right-hand side is oscillatory. As $\alpha \to 1$, the above expression reduces to the Euler equation.

Defining the function $F_\alpha(\sigma; t)$:

$$\boxed{F_\alpha(\sigma; t) = \frac{\sigma(\sin \alpha\pi)}{\pi} \int_0^\infty \frac{e^{-xt} x^{\alpha-1}\, dx}{x^{2\alpha} - 2\sigma(\cos \alpha\pi) x^\alpha + \sigma^2},} \tag{19.444}$$

where

$$\sigma = \omega i^\alpha, \tag{19.445}$$

$$F_\alpha(0; t) = 0, \tag{19.446}$$

$$F_1(\sigma; t) = 0, \tag{19.447}$$

$$F_\alpha(\sigma; 0) = \frac{1-\alpha}{\alpha}, \tag{19.448}$$

$$0 \le F_\alpha(\sigma; t) \le \frac{1-\alpha}{\alpha}, \tag{19.449}$$

we can write the solution of the differential equation:

$${}_0^C D_t^\alpha y(t) = \omega i^\alpha y(t),\ y(0) = y_0, \quad 0 < \alpha < 1, \tag{19.450}$$

as

$$y(t) = y_0 \left[\frac{1}{\alpha} e^{i\omega^{1/\alpha}t} - F_\alpha(\omega i^\alpha; t) \right], \tag{19.451}$$

We now write the **fractional** analogue of the **Euler equation** as

$$\boxed{E_\alpha(\omega i^\alpha; t) = \frac{1}{\alpha} e^{i\omega^{1/\alpha}t} - F_\alpha(\omega i^\alpha; t), \quad 0 < \alpha < 1,} \tag{19.452}$$

which satisfies the differential equation

$$\boxed{{}_0^C D_t^\alpha E_\alpha(\omega i^\alpha; t) = \omega i^\alpha E_\alpha(\omega i^\alpha; t), \quad 0 < \alpha < 1.} \tag{19.453}$$

For $\alpha = 1$, as expected, $E_\alpha(\omega i^\alpha; t)$ reduces to the Euler equation:

$$E_1(i\omega; t) = e^{i\omega t}. \tag{19.454}$$

Note that Eq. (19.439) gives an **integral representation** of the **Mittag-Leffler function** as

$$E_\alpha(\omega i^\alpha; t) = \frac{1}{2\pi i}\int_{\gamma-i\infty}^{\gamma+i\infty}\left[\frac{e^{st}s^{\alpha-1}}{s^\alpha - \omega i^\alpha}\right] ds, \tag{19.455}$$

which with the substitution $x = \omega i^\alpha$, $t = 1$, becomes

$$E_\alpha(x) = \frac{1}{2\pi i}\int_{\gamma-i\infty}^{\gamma+i\infty}\left[\frac{e^{s}s^{\alpha-1}}{s^\alpha - x}\right] ds, \quad \alpha > 0. \tag{19.456}$$

In applications, we frequently need the **asymptotic forms**:

$$E_\alpha(x) \sim \frac{1}{\alpha}e^{x^{1/\alpha}} - \sum_{k=1}^{\infty}\frac{x^{-k}}{\Gamma(1-\alpha k)}, \quad |x| \to \infty,\ 0 < \alpha < 2, \tag{19.457}$$

$$E_\alpha(x) \sim -\sum_{k=1}^{\infty}\frac{x^{-k}}{\Gamma(1-\alpha k)}, \quad |x| \to \infty,\ \alpha < 0, \tag{19.458}$$

$$E_\alpha(x) \sim \frac{1}{\alpha}\sum_{m} e^{(x^{1/2}e^{2\pi i m/\alpha})} - \sum_{k=1}^{\infty}\frac{x^{-k}}{\Gamma(1-\alpha k)}, \quad |x| \to \infty,\ \alpha \geq 2, \tag{19.459}$$

where m takes all the integer values such that $-\alpha\pi/2 < 2\pi m < \alpha\pi/2, x > 0$.

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Problems

1 Show that

$$W(x,t,x_0,t_0) = \frac{1}{\sqrt{4\pi D(t-t_0)}} \exp\left\{-\frac{(x-x_0)^2}{4D(t-t_0)}\right\}$$

satisfies the normalization condition $\int_{-\infty}^{\infty} dx W(x,t,x_0,t_0) = 1$.

2 By differentiating both sides with respect to t show that the following equation is true:

$$\exp\left\{-\int_0^t d\tau V[x(\tau)]\right\} = 1 - \int_0^t d\tau\left(V[x(\tau)]\exp\left\{-\int_0^\tau ds V[x(s)]\right\}\right).$$

3 Show that $V(x)$ in Eq. (19.63):

$$\frac{\partial \widetilde{W}(x,t;x_0,t_0)}{\partial t} - D\frac{\partial^2 \widetilde{W}(x,t;x_0,t_0)}{\partial x^2} = V(x)\widetilde{W}(x,t;x_0,t_0),$$

is defined as

$$V(x) = \frac{1}{4\eta^2 D}F^2(x) + \frac{1}{2\eta}\frac{dF(x)}{dx}.$$

4 Show that the following propagator:

$$W(x,t,x_0,t_0) = \frac{1}{\sqrt{4\pi D(t-t_0)}} \exp\left\{-\frac{(x-x_0)^2}{4D(t-t_0)}\right\},$$

satisfies the ESKC relation [Eq. (19.10)].

5 Derive equation

$$\begin{aligned} W_B(x,t,x_0,t_0) &= W(x,t,x_0,t_0) \\ &-\varepsilon \sum_{j=1}^{N} \int_{-\infty}^{\infty} dx_j W(x,t,x_j,t_j) V(x_j,t_j) W(x_j,t_j,x_0,t_0) \\ &+\frac{1}{2!}\varepsilon^2 \sum_{j=1}^{N}\sum_{k=1}^{N} \int_{-\infty}^{\infty} dx_j \int_{-\infty}^{\infty} dx_k W(x,t,x_j,t_j) V(x_j,t_j) W(x_j,t_j,x_k,t_k) \\ &\times V(x_k,t_k) W(x_k,t_k,x_0,t_0) + \cdots . \end{aligned}$$

given in Section 19.1.2 [Eq. (19.40)].

6 Using the semiclassical method, show that the result of the Wiener integral:

$$W(x,t,x_0,t_0) = \int_{C[x_0,0;x,t]} d_w x(\tau) \exp\left\{ -k^2 \int_{t_0}^{t} d\tau x^2 \right\},$$

is given as

$$W(x,t,x_0,t_0) = \left[\frac{k}{2\pi\sqrt{D}\sinh(2k\sqrt{D}(t-t_0)} \right]^{(1/2)} \times \exp\left\{ -k \frac{(x^2+x_0^2)\cosh(2k\sqrt{D}(t-t_0)) - 2x_0 x}{2\sqrt{D}\sinh(2k\sqrt{D}(t-t_0))} \right\}.$$

7 By diagonalizing the real symmetric matrix, A [Eq. (19.126)], show that

$$\int d\eta_1 \int d\eta_2 \cdots \int d\eta_N \exp\left\{ -\sum_{k=1}^{N}\sum_{l=1}^{N} \eta_k A_{kl} \eta_l \right\} = \frac{(\sqrt{\pi})^N}{\sqrt{\det A}}.$$

8 Use the formula,

$$\begin{aligned} &\int_{-\infty}^{\infty} d\eta \exp\{-a(\eta-\eta')^2 - b(\eta-\eta'')^2\} \\ &= \left[\frac{\pi}{a+b} \right]^{1/2} \exp\left\{ -\frac{ab}{a+b}(\eta'-\eta'')^2 \right\} \end{aligned}$$

to evaluate the integral

$$\phi(t) = \int_{C[0,0;0,t]} \exp\left\{ -\frac{1}{4D} \int_0^t d\tau \dot{\eta}^2 \right\} \prod_{\tau=0}^{t} \frac{d\eta(\tau)}{\sqrt{4\pi D d\tau}}.$$

9 By taking the momentum integral in Eq. (19.156), derive the propagator in Eq. (19.161):

$$K(q'',t'',q',t') = \lim_{\substack{N\to\infty \\ \varepsilon\to 0}} \frac{1}{\sqrt{2\pi i\hbar\frac{\varepsilon}{m}}} \prod_{l=1}^{N} \int_{-\infty}^{\infty} \left[\frac{dq_l}{\sqrt{2\pi i\hbar\frac{\varepsilon}{m}}} \right] \exp\left\{ \frac{i}{\hbar} S \right\},$$

where S is given as

$$S = \sum_{l=0}^{N} \varepsilon \left[\frac{m}{2} \quad \left(\frac{(q_{l+1} - q_l)}{\varepsilon} \right)^2 - V\left(\frac{1}{2}(q_l + q_{l+1}), t_l \right) \right].$$

10 Show that $z^{\alpha} e^{-z}$ can be represented in terms of H-functions as

$$z^{\alpha} e^{-z} = H_{0,1}^{1,0} \left(z|_{(\alpha,1)} \right).$$

11 Prove the following H-function representation:

$$\frac{z^{\beta}}{1 + az^{\alpha}} = a^{-\beta/\alpha} H_{1,1}^{1,1} \left(az^{\alpha} \Big|_{(\beta/\alpha,1)}^{(\beta/\alpha,1)} \right).$$

12 By evaluating the corresponding Mellin–Barnes type integral, show that the $q \to 2$ limit of the Lévy distribution:

$$W_L(x,t) = \frac{1}{\sqrt{\pi} q|x|} H_{1,2}^{1,1} \left(\frac{|x|}{2(D_q t)^{1/q}} \Bigg|_{(1/2,1/2),(0,1/2)}^{(0,1/q)} \right),$$

is a Gaussian.

13 Using the computable form of the H-functions, verify that for large arguments:

$$|x|/(D_q t)^{1/q} \gg 1,$$

one can write the following series expansion [16]:

$$W_L(x,t) = \sum_{l=1}^{\infty} (-1)^{l+1} \frac{\Gamma(1+lq)}{l!} \sin\left(\frac{l\pi q}{2} \right) \frac{(D_q t)^l}{|x|^{lq+1}},$$

for

$$W_L(x,t) = \frac{\pi}{q|x|} H_{2,2}^{1,1} \left(\frac{|x|}{(D_q t)^{1/q}} \Bigg|_{(1,1),(1,1/2)}^{(1,1/q),(1,1/2)} \right).$$

14 Using H-functions, solve the following fractional differential equation given in terms of the $R-L$ derivative:

$$ {}^{R-L}_{0}D^{\alpha}_{t}f(t) - f_0 \frac{t^{-\alpha}}{\Gamma(1-\alpha)} = -\tau^{-\alpha} f(t), \quad f(0) = f_0, $$

where τ is a positive constant. Write the solution you obtained as an H-function in computable form.

15 Using the computable form of the H-function, show that the solution:

$$ f(t) = \frac{f_0}{\alpha} H^{1,1}_{1,2}\left((t/\tau)\Big|^{(0,1/\alpha)}_{(0,1/\alpha),(0,1)} \right), $$

of the fractional relaxation equation:

$$ {}^{C}_{0}D^{\alpha}_{t}f(t) = -\frac{1}{\tau^{\alpha}} f(t), \quad 0 < \alpha < 1, \; t > 0, $$

is the Mittag–Leffler function $f(t) = f_0 E_\alpha(-(t/\tau)^\alpha)$.

16 Find the solution of the following fractional integral equation:

$$ u(t) = u_0 t^{\alpha-1} - c^{\nu} {}_{0}D^{-\nu}_{t} u(t), \quad \nu > 0, \; \mu > 0. $$

17 Solution of the time fractional diffusion equation:

$$ {}_{0}D^{\alpha}_{t} u(x,t) = D^2_\alpha \frac{\partial^2 u(x,t)}{\partial x^2}, \quad t > 0, \; -\infty < x < \infty, \; 0 < \alpha < 1, $$

with the boundary conditions

$$ \lim_{x \to \pm\infty} u(x,t) \to 0 \quad \text{and} \quad {}_{0}D^{\alpha-1}_{t} u(x,0) = \phi(x), $$

can be written as

$$ u(x,t) = \int_{-\infty}^{\infty} dx' \phi(x') G(x-x'), $$

where

$$ G(x-x') = \frac{1}{\pi} \int_0^{\infty} dk t^{\alpha-1} H^{1,1}_{1,2}\left(D^2_\alpha k^2 t^\alpha \Big|^{(0,1)}_{(0,1),(1-\alpha,\alpha)} \right) \cos k(x-x'). $$

Also show that

$$ G(x-x') = \frac{t^{\alpha-1}}{\sqrt{\pi}|x-x'|} H^{1,2}_{3,2}\left(\frac{4D^2_\alpha t^\alpha}{|x-x'|^2} \Bigg|^{(1/2,1),(0,1),(0,1)}_{(0,1),(1-\alpha,\alpha)} \right). $$

18 Show that the solution of the time fractional diffusion equation:

$$ {}^{C}_{0}D^{\alpha}_{t} u(x,t) = D^2_\alpha \frac{\partial^2 u(x,t)}{\partial x^2}, \quad t > 0, \; -\infty < x < \infty, \; 0 < \alpha < 1, $$

with the boundary conditions

$$u(x,0)=\delta(x) \text{ and } \lim_{x\to\pm\infty} u(x,t)\to 0,$$

can be given as

$$u(x,t)=\frac{1}{\pi}\int_0^{\infty} dk\cos(kx)E_\alpha(-D_\alpha k^2t^2).$$

Also show that for $\alpha = 1$, this solution reduces to a Gaussian:

$$u(x,t)=\frac{1}{\sqrt{4\pi D_\alpha t}}e^{-(|x|^2/4D_\alpha t)}.$$

19 Both time and space fractional diffusion equation can be written as

$${}_0^C D_t^\alpha u(x,t)=D_{\alpha,q}R_x^\beta u(x,t),\quad \alpha\in(0,1],\ \beta\in(1,2],$$

where R_x^q is the fractional Riesz derivative operator and $D_{\alpha,q}$ is the fractional diffusion constant. Using the boundary conditions

$$u(x,0)=\delta(x) \text{ and } \lim_{x\to\pm\infty} u(x,t)=0,$$

show that the general solution is given as

$$u(x,t)=\frac{1}{\sqrt{\pi}|x|}H_{3,2}^{1,2}\left(D_{\alpha,q}t^\alpha\left(\frac{2}{|x|}\right)^\beta\Bigg|^{(1/2,\beta/2),(0,1),(0,\beta/2)}_{(0,1),(0,\alpha)}\right).$$

20 Show that the following solution for the time and space fractional diffusion equation:

$$u(x,t)=\frac{1}{\sqrt{\pi}|x|}H_{3,2}^{1,2}\left(D_{\alpha,q}t^\alpha\left(\frac{2}{|x|}\right)^\beta\Bigg|^{(1/2,\beta/2),(0,1),(0,\beta/2)}_{(0,1),(0,\alpha)}\right),$$

reproduces the expected results in the limits as $\alpha\to 1$ and $\beta\to 2$.

21 (i) Verify the following solution given in Section 19.6.6 as the free particle solution of the time and space fractional Schrödinger equation:

$$\Psi(x,t)=\frac{\Psi_0}{\pi}\int_0^{+\infty}\cos kx\ H_{1,2}^{1,1}\left(\frac{i^\alpha}{\hbar}\check{D}_{\alpha,\beta}\hbar^\beta k^\beta t^\alpha\Bigg|^{(0,1)}_{(0,1),(0,\alpha)}\right)dk.$$

(ii) Evaluate the above integral to obtain

$$\Psi(x,t)=\frac{\Psi_0}{\sqrt{\pi}|x|}H_{3,2}^{1,2}\left(\frac{i^\alpha}{\hbar}\check{D}_{\alpha,\beta}\hbar^\beta t^\alpha\left(\frac{2}{|x|}\right)^\beta\Bigg|^{(1/2,\beta/2),(0,1),(0,\beta/2)}_{(0,1),(0,\alpha)}\right)$$

and write the $\alpha\to 1$ and $\beta\to 2$ limits of $\Psi(x,t)$.

(iii) Show that the $\alpha \to 1$ limit of $\Psi(x,t)$ could be expressed as

$$\Psi(x,t) = \frac{\pi\Psi_0}{\beta|x|} H^{1,1}_{2,2}\left(\frac{1}{\hbar}\left(\frac{\hbar}{iD_\beta t}\right)^{1/\beta} |x| \middle|^{(1,1/\beta),(1,1/2)}_{(1,1),(1,1/2)} \right).$$

22 Derive the following formula for the Caputo derivative:

$$\frac{dT(t)}{dt} = {}^C_0 D^{1-\alpha}_t [{}^C_0 D^\alpha_t T(t)] + \frac{\left[{}^C_0 D^\alpha_t T(t)\right]_{t=0}}{\Gamma(\alpha) t^{1-\alpha}}.$$

23 Find the $q \to 2$ limit of Eq. (19.208):

$$W_L(x,t) = (D_q t)^{-1/q} L_q \left\{ \left(\frac{1}{D_q t}\right)^{1/q} |x| \right\}$$
$$= \frac{\pi}{q|x|} H^{1,1}_{2,2}\left(\frac{|x|}{(D_q t)^{1/q}} \middle|^{(1,1/q),(1,1/2)}_{(1,1),(1,1/2)} \right).$$

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Index

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