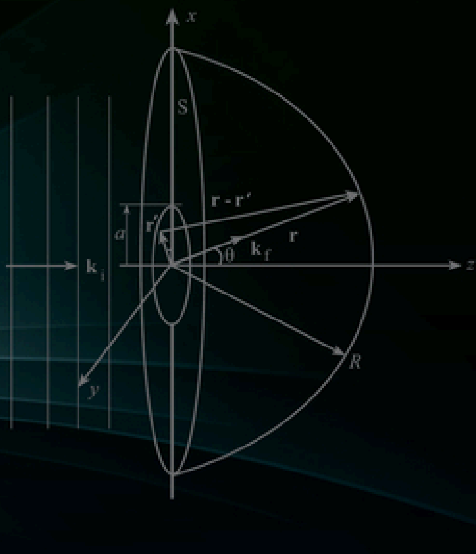
SECOND EDITION

# MATHEMATICAL METHODS IN SCIENCE AND ENGINEERING

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WILEY

**Mathematical Methods in Science and Engineering**

# Mathematical Methods in Science and Engineering

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Second Edition

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# 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:

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

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 $(\theta, \phi)$ 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 $(\theta,\phi)$ 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 $(\theta,\phi)$ are independent variables, this equation can be satisfied for all $r$ and $(\theta,\phi)$ only when both sides of the equation are equal to the same constant. We show this constant with $\lambda$, 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 $\theta$ and the $\phi$ 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, $\lambda$ 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: $0, \pm 1, \pm 2, \dots$ . 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 $\alpha$ 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 $\alpha$ 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, $\alpha_2$ 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 $\lambda$ to integer values:

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

With this restriction on $\lambda$, 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 $\lambda$ 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

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

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

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

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

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

### 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

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

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 $\phi$ dependence. Therefore, in the $\phi$-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

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