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:

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

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

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: $0, \pm1, \pm2, \ldots$. 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

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

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

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

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

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

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

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

   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

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

One can also show the useful integral

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

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

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

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

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

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

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

are simultaneously satisfied. The first inequality gives $\lambda \geq l' - m$, while the second one gives $\lambda \leq l - m$. For $m \geq 0$, 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

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

$$= 2(-1)^l \int_{0}^{\pi/2} (\sin\theta)^{2l+1} d\theta \tag{1.149}$$

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

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

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

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

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

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

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:

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

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:

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

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

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

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:

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

where in spherical polar coordinates

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

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 $\overrightarrow{L}^2$ 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

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

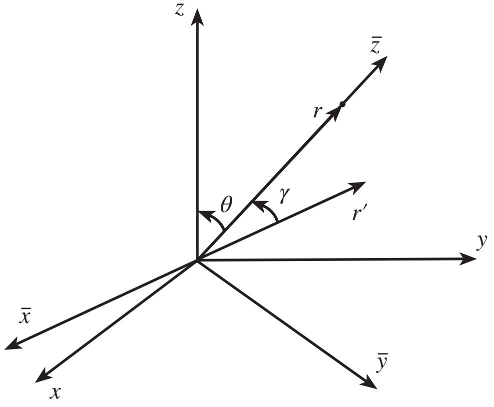
Substituting the definition of spherical harmonics, this also becomes

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

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

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 $\bar{z}$-axis of the new coordinates. Hence, θ in the new coordinates is 0 and the angle θ' that $\overrightarrow{r}'$ makes with the $\bar{z}$-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 $\overrightarrow{r}$ and $\overrightarrow{r}'$ 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 $\overrightarrow{r}'$. 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 $\overrightarrow{r}$ and $\overrightarrow{r}'$. 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

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

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

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

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, $\vec{\nabla}^2 = \vec{\nabla} \cdot \vec{\nabla}$, is invariant under rotations. That is, $\vec{\nabla}^2 = \vec{\nabla}'^2$. 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

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