4 Legendre Functions

In order to investigate the solutions of Legendre's differential equation

$$\frac{d}{d\mu}\left[(1-\mu^2)\frac{d\Theta}{d\mu}\right]+\left[\ell(\ell+1)-\frac{m^2}{1-\mu^2}\right]\Theta=0\,. \tag{4.1}$$

consider first the case of $m=0$ where there is no azimuthal dependence on the angle ϕ.

$$\frac{d}{d\mu}\left[(1-\mu^2)\frac{d\Theta}{d\mu}\right]+\ell(\ell+1)\,\Theta=0\,. \tag{4.2}$$

Special case of $\ell=0$

We actually start with the even simpler case that we can treat by A-level methods. For $\ell=0$,

$$\frac{d}{d\mu}\left[(1-\mu^2)\frac{d\Theta}{d\mu}\right]=0\,.$$

This means that the quantity inside the square bracket must be some constant C;

$$(1-\mu^2)\frac{d\Theta}{d\mu}=C\,.$$

This equation separates as

$$\int d\Theta=\int\frac{C}{(1-\mu^2)}\,d\mu\,,$$

giving the solution

$$\Theta=C\,\tfrac{1}{2}\ell n\left(\frac{1+\mu}{1-\mu}\right)+D\,. \tag{4.3}$$

The Legendre equation is an ordinary second order differential equation and so the solution contained two arbitrary integration constants, written here as C and D. There are two independent solutions of the equation, which we can call

$$P_0(\mu) = 1\,, \tag{4.4}$$

$$Q_0(\mu) = \tfrac{1}{2}\ell n\left(\frac{1+\mu}{1-\mu}\right)\,, \tag{4.5}$$

where the subscript denotes the value of ℓ.

Since the Legendre equation is homogeneous, the most general solution is a linear superposition of P_0 and Q_0,

$$\Theta(\mu)=C\,Q_0(\mu)+D\,P_0(\mu)\,.$$

Note that $Q_0(\mu)$ diverges at $\theta=0$, *i.e.* $\mu=\cos\theta=+1$.

Away from $\ell=m=0$, the solutions are rather more complicated. In general though, one of the solutions will be finite at $\mu=\pm1$, whereas the other one blows up there. To find such solutions, we must apply series methods to the differential equation.

4.1 Series solution

The first thing to note is that the equation remains unchanged if we let $\mu\to-\mu$. As we saw previously, this means that we can choose to write the independent solutions as either odd or even functions of μ. This condition was satisfied by the solutions that we obtained for $\ell=m=0$;

$$\begin{aligned}P_0(\mu) &= 1\,,\\ Q_0(\mu) &= \tfrac{1}{2}\ell n\left(\frac{1+\mu}{1-\mu}\right)\,.\end{aligned} \tag{4.6}$$

Carrying out a differentiation, the equation becomes

$$(1-\mu^2)\frac{d^2\Theta}{d\mu^2} - 2\mu\,\frac{d\Theta}{d\mu} + \ell(\ell+1)\,\Theta = 0\,, \tag{4.7}$$

which has regular singularities at $\mu = \pm 1$.

We now look for solutions in the series form

$$\begin{aligned}
\Theta &= \mu^k \sum_{n=0}^{\infty} a_n\,\mu^n\,, \\
\Theta' &= \mu^k \sum_{n=0}^{\infty} (n+k)\,a_n\,\mu^{n-1}\,, \\
\Theta'' &= \mu^k \sum_{n=0}^{\infty} (n+k)(n+k-1)\,a_n\,\mu^{n-2}\,.
\end{aligned} \tag{4.8}$$

The differential equation has regular singularities at $\mu = \pm 1$ and so we can expect that the series solutions will converge for $|\mu| < 1$.

Inserting the expressions for Θ, Θ' and Θ'' into Eq. (4.7), we find

$$\sum_{n=0}^{\infty}(n+k)(n+k-1)\,a_n\,\left[\mu^{n-2}-\mu^n\right] - 2\sum_{n=0}^{\infty}(n+k)\,a_n\,\mu^n + \ell(\ell+1)\sum_{n=0}^{\infty} a_n\,\mu^n = 0\,. \tag{4.9}$$

Grouping together all the similar powers of μ simplifies things a bit:

$$\sum_{n=0}^{\infty}(n+k)(n+k-1)\,a_n\,\mu^{n-2} = \sum_{n=0}^{\infty}\{(n+k)(n+k+1)-\ell(\ell+1)\}\;a_n\,\mu^n\,. \tag{4.10}$$

The indicial equation is derived by examining the coefficient of the lowest power which, in this case corresponds to $n = 0$ on the left hand side. Since $a_0 \neq 0$, this term can only vanish if

$$k(k-1) = 0\,, \tag{4.11}$$

so that the index is either $k = 0$ or $k = 1$.

To get the recurrence relation, change the dummy variable $n \to n+2$ on the left of Eq. (4.10):

$$\sum_{n=-2}^{\infty}(n+k+1)(n+k)\,a_{n+2}\,\mu^n = \sum_{n=0}^{\infty}\{(n+k)(n+k+1)-\ell(\ell+1)\}\;a_n\,\mu^n\,. \tag{4.12}$$

Comparing coefficients of powers of μ then gives the recurrence relation

$$a_{n+2} = \frac{(n+k+1)(n+k)-\ell(\ell+1)}{(n+k+1)(n+k+2)}\,a_n\,. \tag{4.13}$$

Notice that the recurrence relation links together terms which differ by two units in n. As for the harmonic oscillator equation, this is a direct consequence of the differential operator being even under $\mu \to -\mu$, which means that there can be odd and even solutions of Legendre's equation.

k =0: Even solutions

$$a_{n+2} = \frac{n(n+1)-\ell(\ell+1)}{(n+1)(n+2)}\,a_n = \frac{(n-\ell)(n+\ell+1)}{(n+1)(n+2)}\,a_n\,. \tag{4.14}$$

The solution is therefore

$$p_\ell(\mu) = a_0\left[1 - \frac{\ell(\ell+1)}{2!}\,\mu^2 + \frac{(\ell-2)(\ell)(\ell+1)(\ell+3)}{4!}\,\mu^4 + \cdots\right]\,. \tag{4.15}$$

k **=1: Odd solutions**

$$a_{n+2} = \frac{(n+2)n(n+1) - \ell(\ell+1)}{(n+2)(n+3)}\, a_n = \frac{(n-\ell+1)(n+\ell+2)}{(n+2)(n+3)}\, a_n\,. \tag{4.16}$$

The solution is then

$$q_\ell(\mu) = a_0 \left[\mu - \frac{(\ell-1)(\ell+2)}{3!}\,\mu^3 + \frac{(\ell-3)(\ell-1)(\ell+2)(\ell+4)}{5!}\,\mu^5 + \cdots\right]\,. \tag{4.17}$$

It is clear from the way we derived them (by putting $a_1 = 0$) that $p_\ell(\mu)$ is an even function of μ whereas $q_\ell(\mu)$ is an odd function. The most general solution of the equation is

$$f_\ell(\mu) = A\,p_\ell(\mu) + B\,q_\ell(\mu)\,. \tag{4.18}$$

Now in an earlier lecture, where we separated the Laplacian operator in polar coordinates, we found the explicit forms of the solutions for $\ell = 0$, *viz*

$$P_0(\mu) = 1 \qquad \text{and} \qquad Q_0 = \tfrac{1}{2}\ell n\left(\frac{1+\mu}{1-\mu}\right)\,.$$

Since $P_0(\mu)$ is even and $Q_0(\mu)$ is odd, we should like to identify P_0 with p_0 and Q_0 with q_0.

Putting $\ell = 0$ in Eq. (4.15),

$$p_0(\mu) = a_0\left[1 - \frac{0(1)}{2!}\,\mu^2 + \frac{(-2)(0)(1)(3)}{4!}\,\mu^4 + \cdots\right] = a_0\,P_0(\mu)\,. \tag{4.19}$$

Every term (except the first one) has an ℓ factor which kills it.

In the case of the odd solution of Eq. (4.17), the situation is a little bit more complicated:

$$q_0(\mu) = a_0\left[\mu - \frac{(-1)(2)}{3!}\,\mu^3 + \frac{(-3)(-1)(2)(4)}{5!}\,\mu^5 + \cdots\right] = a_0\left[\mu + \frac{1}{3}\,\mu^3 + \frac{1}{5}\,\mu^5 + \cdots\right]\,, \tag{4.20}$$

which you recognise as the series expansion of $\tfrac{1}{2}\ell n\left(\dfrac{1+\mu}{1-\mu}\right)$.

This shows that we are not (yet) doing anything obviously stupid since we got the right answer for $\ell = 0$. In this case we got an infinite series for $q_0(\mu)$ but one which <u>terminates</u> for $p_0(\mu)$.

The nasty question that we have to ask now is whether such infinite series converge. These problems were looked at in the 1B21 course where the lecturer generally applied the D'Alembert ratio test to investigate. This is what we must do here for real!

4.2 Range of Convergence

The series goes up by steps of two in n. In the D'Alembert ratio test we have then to compare the $(n+2)$'nd term with the n'th

$$R = \left|\frac{a_{n+2}\,\mu^{n+2}}{a_n\,\mu^n}\right| = \left|\frac{(n+k+1)(n+k) - \ell(\ell+1)}{(n+k+1)(n+k+2)}\,\mu^2\right|\,. \tag{4.21}$$

Convergence only depends upon what happens for large n, where

$$R \longrightarrow \left[1 - \frac{2}{n}\right]\mu^2 \longrightarrow \mu^2\,. \tag{4.22}$$

We need $R < 1$ to guarantee convergence and this is true if $|\mu| < 1$. This is exactly as expected because of the regular singular points of the Legendre equation at $\mu = \pm 1$.

What happens on the boundaries $\mu = \pm 1$? The behaviour at these limits was not pursued very much in the 1B21 course but it is quite easy to see what happens in this case. The 1B21 lecturer showed that the harmonic series $\dfrac{1}{n}$ diverges. Hence the restricted harmonic series,

$$\sum_{n\text{ even}} \frac{1}{n} = \frac{1}{2} + \frac{1}{4} + \frac{1}{6} + \cdots = \tfrac{1}{2}\sum_{m=1}^{\infty}\frac{1}{m}\,, \tag{4.23}$$

also diverges. For this series

$$\frac{a_{n+2}}{a_n} \longrightarrow 1 - \frac{2}{n}\,. \tag{4.24}$$

But this is the identical behaviour to the ratio in Eq. (4.22) in the case of $\mu = 1$. Hence the series solutions of the Legendre equation must **diverge** at $\mu = 1$. This is true for both the $k = 0$ and $k = 1$ solutions. This actually comes about because the differential equation has regular singularities at $\mu = \pm 1$.

It is easy to see that $Q_0(\mu) = \frac{1}{2}\ell n\left(\frac{1+\mu}{1-\mu}\right)$ does indeed blow up at $\mu = \pm 1$; just put it into your calculator and see the error message flashing! The important point to note now is that $\mu = \cos\theta = \pm 1$ corresponds to $\theta = 0^\circ$ and 180°, and we would not like any answer to be infinite at these two points. Why should the electrostatic potential be infinite at the top and bottom of a sphere?

We avoided this problem with $P_0(\mu) = 1$ because the series *terminated* with a finite number of terms (in this case just a single one). The question of convergence did not have to be addressed then. This is the only way out; in order to get finite answers at $\mu = \pm 1$ the series must terminate so that we end up with a polynomial rather than an infinite series.

Going back to the recurrence relation of Eq. (4.13),

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

the series will terminate if the numerator on the right hand side vanishes for some value of n;

$$(n+k+1)(n+k) - \ell(\ell+1) = (n+k-\ell)(n+k+1+\ell) = 0\,. \tag{4.25}$$

The convention that $Re\{\ell\} \geq -\frac{1}{2}$ means that we need

$$\ell = n + k\,. \tag{4.26}$$

Since n is an even integer:
For $k = 0$ we need ℓ to be any positive <u>even</u> integer,
For $k = 1$ we need ℓ to be any positive <u>odd</u> integer.

As you will see in the 2B22 Quantum Mechanics course, the condition that ℓ be an integer corresponds to the quantisation of orbital angular momentum in integral units of $\hbar$. The results obtained in this lecture are therefore utterly fundamental to this, Atomic and countless other branches of Physics.

For any (non-negative) integer N, $p_{2N}(\mu)$ and $q_{2N+1}(\mu)$ are polynomials in μ, but that $p_{2N+1}(\mu)$ and $q_{2N}(\mu)$ are infinite series which diverge at $\mu = 1$. We clearly are mainly interested in the solutions which are finite at $\theta = 0^\circ$ and so it makes sense to group them together with a common notation. Let

$$P_\ell(\mu) = \begin{cases} p_\ell(\mu) & \ell \text{ even}\,, \\ q_\ell(\mu) & \ell \text{ odd}\,, \end{cases}$$
$$Q_\ell(\mu) = \begin{cases} p_\ell(\mu) & \ell \text{ odd}\,, \\ q_\ell(\mu) & \ell \text{ even}\,. \end{cases} \tag{4.27}$$

As a consequence of this definition, $P_\ell(\mu)$ is a polynomial but $Q_\ell(\mu)$ is an infinite series which blows up at $\mu = 1$. Furthermore

$$\begin{aligned} P_\ell(-\mu) &= (-1)^\ell\, P_\ell(\mu)\,, \\ Q_\ell(-\mu) &= (-1)^{\ell+1}\, Q_\ell(\mu)\,. \end{aligned} \tag{4.28}$$

SUMMARY

Only for non-negative integers ℓ do we have solutions of Legendre's equation which are finite at $\mu = \pm 1$. These are the Legendre polynomials $P_\ell(\mu)$. There are also Legendre functions of the second kind, $Q_\ell(\mu)$, but these blow up at $\mu = \pm 1$. The Q_ℓ are far less important in Physics and will be largely neglected throughout the rest of this course.

Although the choice is arbitrary, it is standard to normalise the Legendre polynomials such that

$$P_\ell(1) = 1\,. \tag{4.29}$$

From the series representation of Eqs. (4.15) and (4.17), we then see that

$$\begin{aligned} P_0(\mu) &= 1\,, \\ P_1(\mu) &= \mu\,, \\ P_2(\mu) &= \tfrac{1}{2}(3\mu^2 - 1)\,. \end{aligned} \tag{4.30}$$

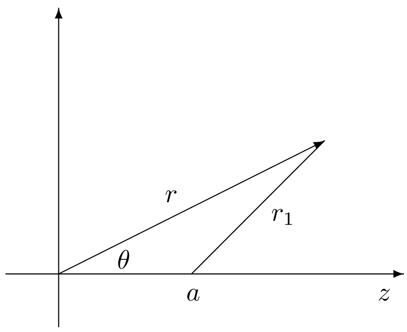
Going back to Eq. (2.30), the original Laplace equation in spherical coordinates, the most general solution which has <u>no</u> ϕ dependence is

$$V(r\,,\,\theta) = \sum_{\ell=0}^{\infty} \left[\alpha_\ell\, r^\ell + \beta_\ell\, r^{-\ell-1}\right]\, P_\ell(\cos\theta)\,, \tag{4.31}$$

where the sum is over discrete integers ℓ, and α_ℓ and β_ℓ are constants to be fixed by the boundary conditions.

4.3 Generating Function for Legendre Polynomials

Consider the physical problem of working out the electrostatic potential due to a point charge q at $z = a$.



In terms of the distance from the point $z = a$, the potential is simply

$$V = \frac{q}{4\pi\varepsilon_0}\,\frac{1}{r_1}\,. \tag{4.32}$$

To evaluate it in terms of r and θ, use the cosine rule to obtain

$$r_1^2 = r^2 + a^2 - 2r\,a\cos\theta\,, \tag{4.33}$$

which leads to a potential of

$$V(r\,,\,\theta) = \frac{q}{4\pi\varepsilon_0}\left[r^2 + a^2 - 2r\,a\cos\theta\right]^{-\frac{1}{2}}\,. \tag{4.34}$$

There is no ϕ dependence because the charge was placed on the z-axis.

If we are interested in the potential in the region $r > a$, then we can expand Eq. (4.34) in powers of a/r,

$$V(r\,,\,\theta) = \frac{q}{4\pi\varepsilon_0\, r}\left[1 + \left(\frac{a}{r}\right)^2 - 2\left(\frac{a}{r}\right)\cos\theta\right]^{-\frac{1}{2}}\,.$$

$$\approx \frac{q}{4\pi\varepsilon_0\, r}\left[1 - \frac{a^2}{2r^2} + \frac{a}{r}\cos\theta + \frac{3a^2}{2r^2}\cos^2\theta + \cdots\right]$$

$$= \frac{q}{4\pi\varepsilon_0\, r}\left[1 + \frac{a}{r}\cos\theta + \frac{a^2}{r^2}\,\tfrac{1}{2}\,(3\cos^2\theta - 1) + \cdots\right] \qquad (4.35)$$

But we already know the general solution for Laplace's equation in any region where there is no charge. If the potential is to remain finite at large r, all the α_ℓ coefficients in Eq. (4.31) must vanish and so

$$V(r\,,\,\theta) = \frac{1}{r}\sum_{\ell=0}^{\infty}\frac{\beta_\ell}{r^\ell}\,P_\ell(\cos\theta)\,. \qquad (4.36)$$

To determine the values of the β_ℓ, look what happens at $\theta = 0$ where, by definition, $P_\ell(\cos\theta) = 1$. In the forward direction $r = r_1 - a$, and so

$$V(r\,,\,\theta) = \frac{1}{r}\sum_{\ell=0}^{\infty}\frac{\beta_\ell}{r^\ell} = \frac{q}{4\pi\varepsilon_0\, r}\,\frac{1}{(1-a/r)} = \frac{q}{4\pi\varepsilon_0\, r}\sum_{\ell=0}^{\infty}\frac{a^\ell}{r^\ell}\,. \qquad (4.37)$$

Comparing different powers of r in the two sums, one can read off immediately that

$$\beta_\ell = \frac{q}{4\pi\varepsilon_0}\,a^\ell\,. \qquad (4.38)$$

The final solution at all angles is therefore

$$V(r\,,\,\theta) = \frac{q}{4\pi\varepsilon_0}\,\frac{1}{\sqrt{r^2 + a^2 - 2r\,a\cos\theta}} = \frac{q}{4\pi\varepsilon_0\, r}\sum_{\ell=0}^{\infty}\frac{a^\ell}{r^\ell}\,P_\ell(\cos\theta)\,. \qquad (4.39)$$

Though we have solved a problem in electrostatics, the result gives us a general method to derive the Legendre polynomials. Comparing the two expressions for the potential in Eq. (4.39), and dropping the funny elecrostatics factor outside, we see that

$$\frac{1}{r}\,\frac{1}{\sqrt{1 + a^2/r^2 - 2\,(a/r)\,\cos\theta}} = \frac{1}{r}\sum_{\ell=0}^{\infty}\frac{a^\ell}{r^\ell}\,P_\ell(\cos\theta)\,. \qquad (4.40)$$

Change to notation where $t = a/r$ and $x = \cos\theta$, we see that

$$g(x,t) \equiv \frac{1}{\sqrt{1 - 2x\,t + t^2}} = \sum_{\ell=0}^{\infty} P_\ell(x)\,t^\ell\,. \qquad (4.41)$$

This is the generating function for the Legendre polynomials. It is only valid if $\mid t \mid < 1$, which corresponds to $r > a$, or otherwise there are convergence problems.

If you expand the square root using the binomial expansion, and compare powers of t, then you get the same answers as we got before, *viz*

$$\begin{aligned} P_0(x) &= 1\,, \\ P_1(x) &= x\,, \\ P_2(x) &= \tfrac{1}{2}(3x^2 - 1)\,. \end{aligned} \qquad (4.42)$$

4.4 Recurrence Relations

Apart from the physical interpretation, one of the big uses of the generating function is to help derive recurrence relations between Legendre polynomials. This is the most efficient way of deriving the polynomials in practice.

Differentiate the generating function of Eq. (4.41) partially with respect to t

$$\frac{\partial g(x,t)}{\partial t} = \frac{x - t}{(1 - 2x\,t + t^2)^{3/2}} = \sum_{n=0}^{\infty} n\,P_n(x)\,t^{n-1}\,. \qquad (4.43)$$

Multiply both sides by $1 - 2x\,t + t^2$ to give

$$(x-t)\,\frac{1}{(1-2x\,t+t^2)^{\frac{1}{2}}} = (1-2x\,t+t^2)\sum_{n=0}^{\infty} n\,P_n(x)\,t^{n-1}\,. \tag{4.44}$$

On the left-hand side we see once again the generating function for the Legendre polynomials, which means that

$$(x-t)\sum_{n=0}^{\infty} P_n(x)\,t^n = (1-2x\,t+t^2)\sum_{n=0}^{\infty} n\,P_n(x)\,t^{n-1}\,. \tag{4.45}$$

This equation is a power series in t which is supposed to be valid for a range of values of t. Consequently it must be valid separately for each power of t. This is exactly the same argument that we used in the series solution of the differential equations. Writing out explicitly all the different powers,

$$x\sum_{n=0}^{\infty} P_n(x)\,t^n - \sum_{m=0}^{\infty} P_m(x)\,t^{m+1} = \sum_{\ell=0}^{\infty} \ell\,P_\ell(x)\,t^{\ell-1} - 2x\sum_{n=0}^{\infty} n\,P_n(x)\,t^n + \sum_{m=0}^{\infty} m\,P_m(x)\,t^{m+1}\,. \tag{4.46}$$

The formula has been written different dummy indices ℓ, m, and n such that we can change a couple of them easily. Let now

$$\begin{aligned} m &\longrightarrow n-1\,,\\ \ell &\longrightarrow n+1\,. \end{aligned}$$

Then all the terms in the sums contain the same t^n factor. Reading off the coefficient we get

$$x\,P_n(x) - P_{n-1}(x) = (n+1)\,P_{n+1}(x) - 2n\,x\,P_n(x) + (n-1)\,P_{n-1}(x)\,.$$

Grouping like terms together, we get the recurrence relation

$$(2n+1)\,x\,P_n(x) = (n+1)\,P_{n+1}(x) + n\,P_{n-1}(x)\,. \tag{4.47}$$

Thus, if you know $P_n(x)$ and $P_{n-1}(x)$, the recurrence relation allows you to obtain the formula for $P_{n+1}(x)$.

For example, putting $n = 1$ in Eq. (4.47), we get

$$3x\,P_1(x) = 2P_2(x) + P_0(x)\,. \tag{4.48}$$

Since $P_0(x) = 1$ and $P_1(x) = x$, this then immediately gives $P_2(x) = \frac{1}{2}\,(3x^2 - 1)$.

Using instead $n = 2$, we obtain

$$5x\,P_2(x) = 3P_3(x) + 2P_1(x)\,, \tag{4.49}$$

which means that

$$P_3(x) = \tfrac{1}{2}\,(5x^3 - 3x)\,.$$

4.5 Orthogonality of Legendre Polynomials

The Legendre differential equations for $P_n(x)$ and $P_m(x)$ are

$$\begin{aligned} &\frac{d}{dx}\left[(1-x^2)\,P_n'(x)\right] + n(n+1)\,P_n(x) = 0\,,\\ &\frac{d}{dx}\left[(1-x^2)\,P_m'(x)\right] + m(m+1)\,P_m(x) = 0\,. \end{aligned} \tag{4.50}$$

Multiply the first of Eqs. (4.50) by $P_m(x)$ and the second by $P_n(x)$ and subtract one from the other to find:

$$P_m(x)\,\frac{d}{dx}\left[(1-x^2)\,P_n'(x)\right] - P_n(x)\,\frac{d}{dx}\left[(1-x^2)\,P_m'(x)\right] = \left[m(m+1) - n(n+1)\right]\,P_m(x)P_n(x)\,.$$

Now integrate both sides of this expression over x from -1 to $+1$:

$$\int_{-1}^{+1} dx \left\{ P_m(x) \frac{d}{dx} \left[(1-x^2)\, P_n'(x)\right] - P_n(x) \frac{d}{dx} \left[(1-x^2)\, P_m'(x)\right] \right\}$$

$$= [m(m+1) - n(n+1)] \int_{-1}^{+1} P_m(x) P_n(x)\, dx\,. \tag{4.51}$$

What we have to do now is show that the left hand side of Eq. (4.51) vanishes. This we do through integrating by parts.

$$\int_{-1}^{+1} dx\, P_m(x) \frac{d}{dx} \left[(1-x^2)\, P_n'(x)\right] = \left[P_m(x)\,(1-x^2)\, P_n'(x)\right]_{-1}^{+1} - \int_{-1}^{+1} dx\, (1-x^2)\, P_n'(x) P_m'(x)\,. \tag{4.52}$$

Now the first term on the RHS of Eq. (4.52) equals zero because $(1-x^2) = 0$ at both the limits. On the other hand, the second term is cancelled by an identical one coming from the second term in Eq.(4.51) where $m \Leftrightarrow n$. Hence

$$[m(m+1) - n(n+1)] \int_{-1}^{+1} P_m(x) P_n(x)\, dx = 0\,, \tag{4.53}$$

which means that, if $n \neq m$,

$$\int_{-1}^{+1} P_m(x) P_n(x)\, dx = 0\,. \tag{4.54}$$

This is called the *Orthogonality relation*. It is analogous to the orthogonality of two vectors except that we have an integral over a continuous variable rather than a summation over components.

To construct the equivalent of a unit vector, we have to work out the integral when $m = n$:

$$I_n = \int_{-1}^{+1} \left[P_n(x)\right]^2\, dx\,. \tag{4.55}$$

There are many ways of working this out, but one of the easiest ways uses the generating function of Eq. (4.41). Writing this down twice gives

$$\frac{1}{\sqrt{1-2x\,t+t^2}} = \sum_{n=0}^{\infty} P_n(x)\, t^n\,,$$

$$\frac{1}{\sqrt{1-2x\,t+t^2}} = \sum_{n=0}^{\infty} P_m(x)\, t^m\,. \tag{4.56}$$

Multiply these two expressions together to give a double summation over n and m.

$$\frac{1}{1-2x\,t+t^2} = \sum_{n=0}^{\infty}\sum_{m=0}^{\infty} P_n(x)\, P_m(x)\, t^{n+m}\,. \tag{4.57}$$

Now integrate over x from -1 to $+1$:

$$\int_{-1}^{+1} \frac{dx}{1-2x\,t+t^2} = \sum_{n=0}^{\infty}\sum_{m=0}^{\infty} \int_{-1}^{+1} P_n(x)\, P_m(x)\, t^{n+m}\,. \tag{4.58}$$

The integral on the left is simple, so that

$$\frac{1}{2t}\, \ell n \left(\frac{(1+t)^2}{(1-t)^2}\right) = \frac{1}{t}\, \ell n \left(\frac{1+t}{1-t}\right) = 2 \sum_{n=0}^{\infty} \frac{t^{2n}}{2n+1}\,. \tag{4.59}$$

But we have already shown that the integral on the RHS vanishes unless $n = m$ and so we really only have a single summation to worry about:

$$\text{RHS} = \sum_{n=0}^{\infty} I_n \, t^{2n} \,. \tag{4.60}$$

Comparing coefficients of t^{2n} on the left and right hand sides, we see that

$$I_n = \int_{-1}^{+1} \left[P_n(x)\right]^2 \, dx = \frac{2}{2n+1} \,. \tag{4.61}$$

The orthogonality and normalisation of the Legendre polynomials can be written neatly in one equation as

$$\int_{-1}^{+1} P_\ell(x) \, P_n(x) \, dx = \frac{2}{2\ell+1} \, \delta_{\ell\, n} \,, \tag{4.62}$$

where the Kronecker delta symbol for two integers m and n is defined by

$$\delta_{m\,n} = \begin{cases} 1 & \text{for } m = n \\ 0 & \text{for } m \neq n \,. \end{cases} \tag{4.63}$$

4.6 Expansion in series of Legendre polynomials

You learned in the 1B21 course how to expand a function $f(x)$ in a Maclaurin series:

$$f(x) = \sum_{n=0}^{\infty} \alpha_n \, x^n \,.$$

Also, in the first year Waves and Optics course, you learned about expanding functions in series of sine and cosine functions. Such Fourier expansions will be the topic of the next section. What we want to do here is expand $f(x)$ in an infinite series of Legendre polynomials:

$$f(x) = \sum_{n=0}^{\infty} a_n \, P_n(x) \,. \tag{4.64}$$

Let us start off with a simple example:

$$f(x) = \frac{15}{2}x^2 - \frac{3}{2} = \frac{15}{2} \cdot \frac{1}{3} \left(2P_2(x) + P_0(x)\right) - \frac{3}{2} \, P_0(x) = P_0(x) + 5P_2(x) \,.$$

Whenever the power series for $f(x)$ only has a finite number of terms, *i.e.* is a polynomial, we can calculate the coefficients by solving a system of algebraic equations. The example above was of this kind. If $f(x)$ is not a polynomial then we can still calculate the coefficients using the orthonormality integral of Eq. (4.63). Multiplying Eq. (4.64) by $P_m(x)$ and integrating from -1 to $+1$ gives

$$\int_{-1}^{+1} f(x) \, P_m(x) \, dx = \sum_{n=0}^{\infty} a_n \int_{-1}^{+1} P_n(x) \, P_m(x) \, dx = \sum_{n=0}^{\infty} a_n \, \frac{2}{2n+1} \, \delta_{m\,n} = \frac{2}{2m+1} \, a_m \,. \tag{4.65}$$

Hence

$$a_m = \frac{2m+1}{2} \int_{-1}^{+1} f(x) \, P_m(x) \, dx \,. \tag{4.66}$$

Example 1. Calculate the Legendre coefficients for $f(x) = \dfrac{15}{2}x^2 - \dfrac{3}{2}$. Putting in the explicit forms for the Legendre polynomials, we have

$$a_0 = \frac{1}{2} \int_{-1}^{+1} \left(\frac{15}{2}x^2 - \frac{3}{2}\right) dx = \frac{1}{2}\left(\frac{15}{3} - 3\right) = 1 \,,$$

$$a_1 = \frac{3}{2}\int_{-1}^{+1}\left(\frac{15}{2}x^2 - \frac{3}{2}\right) x\,dx = 0 \quad \text{(integrand odd)},$$

$$a_2 = \frac{5}{2}\int_{-1}^{+1}\left(\frac{15}{2}x^2 - \frac{3}{2}\right)\left(\frac{3x^2}{2} - \frac{1}{2}\right) dx = \frac{5}{4}\left(\frac{45}{5} - \frac{24}{3} + 3\right) = 5\,.$$

These agree with what we found using direct algebra.

Example 2. Obtain the first two the Legendre coefficients for $f(x) = e^{\alpha x}$.

$$a_0 = \frac{1}{2}\int_{-1}^{+1} e^{\alpha x}\,dx = \frac{1}{2\alpha}\left(e^{\alpha} - e^{-\alpha}\right) = \frac{\sinh\alpha}{\alpha}\,,$$

$$a_1 = \frac{3}{2}\int_{-1}^{+1} x\,e^{\alpha x}\,dx = 3\left(\frac{\cosh\alpha}{\alpha} - \frac{\sinh\alpha}{\alpha^2}\right),$$

where we had to do some integration by parts.

4.7 Return to the Potential Problem

We saw, when separating the Laplace equation in spherical polar coordinates, that the most general solution with axial symmetry (no ϕ dependence) for the electrostatic potential in charge-free space is

$$V(r,\cos\theta) = \sum_{\ell=0}^{\infty}\left(A_\ell r^\ell + \frac{B_\ell}{r^{\ell+1}}\right) P_\ell(\cos\theta)\,. \tag{4.67}$$

Suppose that $V(r) \to 0$ as $r \to \infty$. This means that all the $A_\ell = 0$ and

$$V(r,\cos\theta) = \sum_{\ell=0}^{\infty}\frac{B_\ell}{r^{\ell+1}}\,P_\ell(\cos\theta)\,. \tag{4.68}$$

To fix the values of the B_ℓ coefficients, we need another boundary condition, as in the following case:

Example

Suppose that on an isolated sphere of radius a the electrostatic potential varies like $V(r=a,\theta) = V_0\,e^{\alpha\cos\theta}$. How does the potential behave for large distances?

Using the Legendre series example already worked out,

$$B_0 = V_0 a\,\frac{\sinh\alpha}{\alpha}\,,$$

$$B_1 = 3V_0 a^2\left(\frac{\cosh\alpha}{\alpha} - \frac{\sinh\alpha}{\alpha^2}\right),$$

and

$$V(r,\cos\theta) = V_0\left[\frac{a}{r}\,\frac{\sinh\alpha}{\alpha} + 3\frac{a^2}{r^2}\left(\frac{\cosh\alpha}{\alpha} - \frac{\sinh\alpha}{\alpha^2}\right)\cos\theta + 0\left(\frac{1}{r^3}\right)\right].$$

For those of you familiar with electrostatics, the $\cos\theta$ term corresponds to the electric dipole moment and the discarded next term the quadrupole moment *etc.*

4.8 Associated Legendre Functions

We saw that in general the ϕ dependence of the solutions to Laplace's equation is of the form $e^{im\phi}$, where m is an integer. To get the θ dependence, we have to solve

$$\frac{d}{dx}\left[(1-x^2)\frac{dP_\ell^m}{dx}\right] + \left[\ell(\ell+1) - \frac{m^2}{1-x^2}\right] P_\ell^m = 0\,. \tag{4.69}$$

[N.B. Have here replaced $\mu \to x$ and called $\Theta(\mu) \to P_\ell^m(x)$.] Only for $m = 0$ do we get the Legendre polynomials $P_\ell(x)$. To solve the equation for $m \neq 0$ is even more tedious than for $m = 0$. Only a summary will be presented of results which are very important for Quantum Mechanics, where ℓ is known as the angular momentum quantum number and m the magnetic quantum number.

Well behaved solutions of Legendre's equation are only possible if

- ℓ is a non-negative integer.
- m is an integer with $-\ell \le m \le \ell$.

The solutions for m and $-m$ are the same since only m^2 occurs in Legendre's equation. For $m > 0$ the associated Legendre functions can be derived from the Legendre polynomials using

$$P_\ell^m(x) = (1-x^2)^{m/2}\left(\frac{d}{dx}\right)^m P_\ell(x)\,. \tag{4.70}$$

The orthogonality relation is also a bit more complicated than that of Eq. (4.62):

$$\int_{-1}^{+1} P_\ell^m(x)\,P_n^m(x)\,dx = \frac{2}{2\ell+1}\,\frac{(\ell+m)!}{(\ell-m)!}\,\delta_{\ell\,n}\,. \tag{4.71}$$

Specific cases

$\ell = 1$, $m = 1$:

$$P_1^1(x) = (1-x^2)^{1/2}\,\frac{d}{dx}\,x = (1-x^2)^{1/2} = \sin\theta\,.$$

$\ell = 2$, $m = 1$:

$$P_2^1(x) = (1-x^2)^{1/2}\,\frac{d}{dx}\,\tfrac{1}{2}(3x^2-1) = 3x\,(1-x^2)^{1/2} = 3\sin\theta\cos\theta\,.$$

$\ell = 2$, $m = 2$:

$$P_2^2(x) = (1-x^2)\,\frac{d^2}{dx^2}\,\tfrac{1}{2}(3x^2-1) = 3(1-x^2) = 3\sin^2\theta\,.$$

As a couple of examples to check the orthogonality relations, consider

$$\int_{-1}^{+1} P_2^1(x)\,P_1^1(x)\,dx = \int_{-1}^{+1} 3x(1-x^2)\,dx = 0\,.$$

$$\int_{-1}^{+1} \left[P_2^1(x)\right]^2\,dx = \int_{-1}^{+1} 9x^2(1-x^2)\,dx = 2\,\frac{9}{3} - 2\,\frac{9}{5} = \frac{12}{5}\,.$$

The last one agrees with the $\frac{2}{5}\,3!$ of Eq. (4.71).

4.9 Spherical Harmonics

In Quantum Mechanics, one often gets the θ and ϕ dependence packaged together as one function called a spherical harmonic $Y_\ell^m(\theta,\phi)$. Thus

$$Y_\ell^m(\theta,\phi) = c_{\ell,m}\,P_\ell^m(\cos\theta)\,e^{im\phi} \tag{4.72}$$

is a solution of Legendre equation. Here the constants $c_{\ell,m}$ could be chosen in any way we want. However, it is conventional to choose them such that the orthogonality/normalisation relation becomes

$$\int_{-1}^{+1} d(\cos\theta)\int_0^{2\pi} d\phi\,Y_\ell^{m\,*}(\theta,\phi)\,Y_{\ell'}^{m'}(\theta,\phi) = \delta_{\ell,\ell'}\,\delta_{m,m'}\,. \tag{4.73}$$

Using Eq. (4.71), this is achieved with

$$c_{\ell,m} = (-1)^m\sqrt{\frac{(\ell-m)!\,(2\ell+1)}{(\ell+m)!\,4\pi}}\,. \tag{4.74}$$

In Quantum Mechanics you will at some stage need to remember the orthogonality/normalisation relation of Eq. (4.73) but you will NOT be required to remember the actual algebraic form of Eq. (4.73).

The first few spherical harmonics are

$$\begin{aligned}
Y_0^0(\theta,\phi) &= \frac{1}{\sqrt{4\pi}}\,, \\
Y_1^1(\theta,\phi) &= -\sqrt{\frac{3}{8\pi}}\,\sin\theta\, e^{i\phi}\,, \\
Y_1^0(\theta,\phi) &= \sqrt{\frac{3}{4\pi}}\,\cos\theta\,, \\
Y_1^{-1}(\theta,\phi) &= \sqrt{\frac{3}{8\pi}}\,\sin\theta\, e^{-i\phi}\,.
\end{aligned} \tag{4.75}$$