Orthogonal functions

Given a real variable over the interval (a, b) and a set of real or complex functions $U_n(\xi)$, $n = 1, 2, \ldots$, which are square integrable and orthonormal

$$\int_a^b U_n^*(\xi) U_m(\xi) d\xi = \delta_{n,m} \tag{1}$$

if the set of of functions is complete an arbitrary square integrable function $f(\xi)$ can be expanded as

$$f(\xi) = \sum_{n=1}^{\infty} a_n U_n(\xi) \tag{2}$$

where

$$a_n = \int_a^b U_n^*(\xi') f(\xi') d\xi' \ . \tag{3}$$

Substituting the expressions for a_n back into f we find

$$f(\xi) = \int_a^b \sum_{n=1}^{\infty} U_n^*(\xi') U_n(\xi) f(\xi') d\xi' \tag{4}$$

but this is the definition of the Dirac delta-function and so we have

$$\sum_{n=1}^{\infty} U_n^*(\xi') U_n(\xi) = \delta(\xi - \xi') \tag{5}$$

which is known as the completeness relation.

1 Fourier Series

A familiar example is Fourier series, where the function is a periodic function on the interval $(-L/2, L/2)$. The complete set of functions are labelled by $m \in \mathbb{Z}$ with $m \neq 0$

$$\sqrt{\frac{2}{L}} \sin\left(\frac{2\pi m x}{L}\right) \ , \quad \sqrt{\frac{2}{L}} \cos\left(\frac{2\pi m x}{L}\right) \tag{6}$$

and $m = 0$ $1/\sqrt{L}$. We can expand an arbitrary function as

$$f(x) = \frac{1}{2} A_0 + \sum_{m=1}^{\infty} A_m \cos\left(\frac{2\pi m x}{L}\right) + B_m \sin\left(\frac{2\pi m x}{L}\right) \tag{7}$$

where

$$\begin{aligned} A_m &= \frac{2}{L} \int_{-L/2}^{L/2} dx\ f(x) \cos\left(\frac{2\pi m x}{L}\right) \\ B_m &= \frac{2}{L} \int_{-L/2}^{L/2} dx\ f(x) \sin\left(\frac{2\pi m x}{L}\right) \ . \end{aligned} \tag{8}$$

If we take the interval to be infinite we require a continuum of functions. That is for $f(x)$ defined on the real line

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A(k) e^{ikx} dk \tag{9}$$

where

$$A(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{-ikx} dx \tag{10}$$

and the orthonormality and completeness relations are

$$\begin{aligned} \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i(k-k')x} dx &= \delta(k-k') \\ \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ik(x-x')} dk &= \delta(x-x') \ . \end{aligned} \tag{11}$$

2 Laplace's Equation in two-dimensions

If we consider Laplace's equation in two-dimensions

$$\frac{\partial^2 \Phi}{\partial x^2} + \frac{\partial^2 \Phi}{\partial y^2} = 0 \tag{12}$$

we can look for solutions by separation of variables i.e we take an ansatz $\Phi(x, y) = X(x)Y(y)$ and we find that

$$\frac{1}{X(x)} \frac{d^2 X(x)}{dx^2} + \frac{1}{Y(y)} \frac{d^2 Y(y)}{dy^2} = 0 \tag{13}$$

or equivalently

$$\frac{1}{X(x)} \frac{d^2 X(x)}{dx^2} = -\alpha^2 \ , \qquad \frac{1}{Y(y)} \frac{d^2 Y(y)}{dy^2} = \alpha^2 \ , \tag{14}$$

for an arbitrary constant (possibly complex) α. The solutions of these equations are

$$X = Ae^{\pm i\alpha x} \ , \quad Y = A'e^{\pm \alpha y} \ . \tag{15}$$

Now consider the problem in Fig. 1. We want to find the potential Φ for $0 \leq x \leq a$ and $y \geq 0$ with the boundary conditions as in the figure. We can see that the potential must oscillate in the x-direction and fall off in the y-direction. Hence we take α to be real. We also see that we want the solution to be of the form $\sin(\alpha x)$ as $\Phi = 0$ at $x = 0$. Thus $\Phi \propto e^{-\alpha y} \sin \alpha x$. The boundary condition at $x = a$ sets $\alpha = \pi n/a$. Hence the potential can be written as

$$\Phi(x, y) = \sum_{n=1}^{\infty} A_n \sin\left(\frac{n\pi x}{a}\right) e^{-n\pi y/a} \tag{16}$$

where

$$\begin{aligned} A_n &= \frac{2}{a} \int_0^a \Phi(x, 0) \sin\left(\frac{n\pi x}{a}\right) dx \\ &= \frac{2}{a} \int_0^a V \sin\left(\frac{n\pi x}{a}\right) dx \\ &= \begin{cases} 4V/\pi n & n \text{ odd} \ , \\ 0 & n \text{ even} \ . \end{cases} \end{aligned} \tag{17}$$

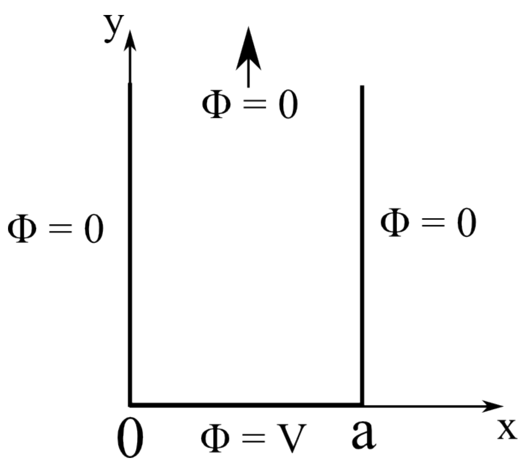

Figure 1: Potential on a two-dimensional semi-infinite strip.

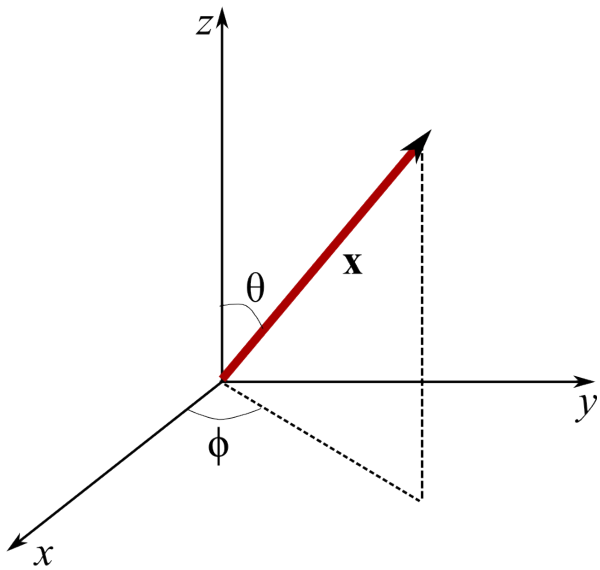

Figure 2: Potential on a two-dimensional semi-infinite strip.

Hence

$$\Phi(x,y) = \frac{4V}{\pi}\sum_{n\ \mathrm{odd}} \frac{1}{n} e^{-\frac{n\pi y}{a}} \sin\left(\frac{n\pi x}{a}\right) \ . \tag{18}$$

This can actually be resumed (see Jackson 2.10)

$$\Phi(x,y) = \frac{2V}{\pi}\tan^{-1}\left(\frac{\sin\frac{\pi x}{a}}{\sinh\frac{\pi y}{a}}\right) \ . \tag{19}$$

3 Laplace's Equation in Spherical coordinates

Now let us consider the three-dimensional problem however rather than using cartesian coordinates we will consider the usual spherical coordinates in three-dimensions (r,θ,ϕ), see Fig. 2, in terms of which the Cartesian coordinates (x,y,z) are given as

$$x = r\sin\theta\cos\phi \ , \quad y = r\sin\theta\sin\phi \ , \quad z = r\cos\theta \ . \tag{20}$$

In these coordinates Laplace's equation, $\nabla^2\Phi = 0$, is

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\Phi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Phi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\Phi}{\partial\phi^2} = 0\ . \tag{21}$$

We look for solutions of the form $\Phi(r,\theta,\phi) = \frac{U(r)}{r}Y(\theta,\phi)$; substituting this Ansatz into (21) and dividing by Φ/r^2 we find

$$\frac{r^2}{U(r)}\frac{d^2}{dr^2}U(r) + \frac{1}{Y(\theta,\phi)}\nabla_{\theta,\phi}Y(\theta,\phi) = 0 \tag{22}$$

where

$$\nabla_{\theta,\phi}Y = \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2} \tag{23}$$

which depends only on coordinates (θ,ϕ). Thus we can set [1]

$$\begin{aligned} &r^2U''(r) = \ell(\ell+1)U(r) \\ &\frac{1}{Y(\theta,\phi)}\nabla_{\theta,\phi}Y(\theta,\phi) = -\ell(\ell+1)\ . \end{aligned} \tag{24}$$

We can make the further ansatz $Y(\theta,\phi) = P(\theta)Q(\phi)$, which substituting into (24) and multiplying by $\sin^2\theta$ we find

$$\frac{\sin\theta}{P(\theta)}\frac{d}{d\theta}\left(\sin\theta\frac{d}{d\theta}P\right) + \frac{1}{Q(\phi)}\frac{d^2}{d\phi^2}Q = -\ell(\ell+1)\sin^2\theta$$

which in turn implies that

$$\frac{1}{Q(\phi)}\frac{d^2}{d\phi^2}Q = -m^2\ , \quad \text{and} \tag{25}$$

$$\frac{1}{\sin\theta P(\theta)}\frac{d}{d\theta}\left(\sin\theta\frac{d}{d\theta}P\right) - \frac{m^2}{\sin^2\theta} + \ell(\ell+1) = 0\ . \tag{26}$$

We can immediately write down the solutions to (25): $Q = e^{\pm im\phi}$. It is important to note that because we require $\Phi(\phi+2\pi) = \Phi(\phi)$ this implies $m \in \mathbb{Z}$. In (26) we define $x = \cos\theta$ (which is conventional and has nothing to do with the Cartesian coordinate x) and divide by $\sin^2\theta$ to find,

$$\frac{d}{dx}\left((1-x^2)\frac{d}{dx}P\right) + \left(\ell(\ell+1) - \frac{m^2}{1-x^2}\right)P = 0\ . \tag{27}$$

Equation (27) is the associated Legendre equation.

4 Legendre Equation

When $m = 0$ equation (27) simplifies to the Legendre equation which we can write as

$$P'' - \frac{2x}{(1-x^2)}P' + \frac{\ell(\ell+1)}{(1-x^2)}P = 0\ . \tag{28}$$

[1] Here and below we will use Lagrange's prime notation $f'(x) = \frac{df(x)}{dx}$.

This is an ODE with singular points at $x = \pm 1$ as the coefficients of P' and P diverge at these points. They are regular singular points as they diverge as $\sim (x \pm 1)^{-1}$. The point at $x \to \infty$ requires a little more effort (see [1] section 8.4 for example) but is also a regular singular point.

One can find a solution to such an ODE by making a series expansion about a point as long as the behaviour is no worse than that of a regular singular point; this is also known as the Frobenius method. We thus write

$$P(x) = \sum_{n\geq 0} a_n x^{n+\alpha} \tag{29}$$

with α arbitrary and a_0 the lowest non-vanishing coefficient of the series. Substituting into (28) (and multiplying by $(1-x^2)$) we find

$$\sum_{n\geq 0}(1-x^2)a_n(\alpha+n)(\alpha+n-1)x^{\alpha+n-2} - 2\sum_{n\geq 0} a_n(\alpha+n)x^{\alpha+n} + \ell(\ell+1)\sum_{n\geq 0} a_n x^{\alpha+n} = 0$$

and we can determine the coefficients by demanding the each term in the $x^{n+\alpha}$ expansion vanishes. Starting with

$$\begin{aligned} n=0 &\qquad a_0\alpha(\alpha-1) = 0 \\ n=1 &\qquad a_1\alpha(\alpha+1) = 0 \end{aligned} \tag{30}$$

while for general n we find

$$a_{n+2} = a_n \frac{(\alpha+n)(\alpha+n+1) - \ell(\ell+1)}{(\alpha+n+2)(\alpha+n+1)} \ . \tag{31}$$

If we choose $\alpha = 1$ we must take $a_1 = 0$ and, from the general formula (31), we find a series of odd powers of x

$$P_{(1)} = a_0 x + a_2 x^3 + a_4 x^5 + \dots \ . \tag{32}$$

while if we take $\alpha = 0$ and choose $a_1 = 0$ then we find a series with even terms only

$$P_{(2)} = a_0 + a_2 x^2 + a_4 x^4 + \dots \ . \tag{33}$$

In both cases the coefficients $a_2, a_4, \dots$ are related to a_0 by the general formula (31). This gives us two linearly independent solutions

$$\begin{aligned} P_{(1)} &= a_0\Big[x + \tfrac{1}{6}(2-\ell(\ell+1))x^3 + \tfrac{1}{120}(2-\ell(\ell+1))(12-\ell(\ell+1))x^5 + \dots\Big] \\ P_{(2)} &= a_0\Big[1 - \tfrac{1}{2}\ell(\ell+1)x^2 - \tfrac{1}{24}\ell(\ell+1)(6-\ell(\ell+1))x^4 + \dots\Big] \ , \end{aligned}$$

which as we are considering a second order differential equation gives us a complete basis of solutions. We can naturally consider $\alpha = 0$ and $a_1 \neq 0$ this will give us a linear combination of the above solutions. [2]

In general (i.e. for arbitrary ℓ) these solutions are infinite series and it is important to question whether they converge. In fact for $|x| < 1$ they do, however they will not for $x = \pm 1$ unless the series terminates at some value of n; that is to say $a_n = 0$ for all $n > N$. This will be the case if ℓ is some positive integer. For example, $a_{\ell+2} = 0$ (and hence all $a_n = 0$ for all $n > \ell$) when $\alpha = 0$ and $\ell = n$ as $(\alpha+n)(\alpha+n+1) - \ell(\ell+1) = 0$. Thus the even series terminates when ℓ is an even integer and the odd series terminates when ℓ is an odd integer. For each ℓ we will call this solution $P_\ell(x)$. We fix the overall constant by choosing to normalise $P_\ell(1) = 1$. The first few Legendre functions are

$$P_0(x) = 1 \ , \quad P_1(x) = x \ , \quad P_2(x) = \tfrac{1}{2}(3x^2-1) \ , \quad P_3(x) = \tfrac{1}{2}(5x^3-3x) \ . \tag{34}$$

Note that from the construction it is immediately apparent that $P_\ell(-x) = (-1)^\ell P_\ell(x)$.

[2] Jackson allows $a_0 = 0$ and for the $\alpha = 0$ case considers $a_1 \neq 0$. This is, by a simple relabelling, our second solution.

Useful Properties These functions are orthogonal and normalised such that

$$\int_{-1}^{1} P_{\ell'}(x) P_\ell(x) dx = \frac{2}{2\ell+1}\delta_{\ell'\ell} \ . \tag{35}$$

A compact and useful expression for the Legendre functions is given by Rodrigues equation

$$P_\ell(x) = \frac{1}{2^\ell \ell!}\frac{d^\ell}{dx^\ell}(x^2-1)^\ell \ . \tag{36}$$

Moreover these functions satisfy various recursion relations e.g.

$$(\ell+1)P_{\ell+1} - (2\ell+1)xP_\ell + \ell P_{\ell-1} = 0 \ . \tag{37}$$

See for example [1] for a more complete discussion of their many properties.

Second solutions Finally we note that for each ℓ this gives us only one solution, the other series does not terminate and is singular at $x = \pm 1$. These solutions can be written as

$$\tilde{P}_n(x) = \tfrac{1}{2} P_n(x) \ln \frac{1+x}{1-x} \ . \tag{38}$$

4.1 Generating function for Legendre functions

There is a nice way to write the Legendre functions: Consider the function

$$G(x,t) = (1 - 2xt + t^2)^{-1/2} \ . \tag{39}$$

It is easy to check that

$$(1-x^2)\frac{\partial^2 G}{\partial x^2} - 2x\frac{\partial G}{\partial x} + t\frac{\partial^2}{\partial t^2}(tG) = 0 \ . \tag{40}$$

Now expand $G(x,t)$ in powers of t

$$G(x,t) = \sum_{\ell \geq 0} t^\ell L_\ell(x) \ , \tag{41}$$

and substituting this into (40) it easy to see that it implies

$$\sum_{\ell \geq 0} t^\ell \big[(1-x)^2 L''_\ell - 2xL'_\ell + \ell(\ell+1)L_\ell\big] = 0 \tag{42}$$

i.e. that each L_ℓ satisfies the Legendre equation i.e. $L_\ell(x) = P_\ell(x)$, and so

$$G(x,t) = \sum_{\ell \geq 0} t^\ell P_\ell(x) \ . \tag{43}$$

This relation can be explicitly checked at low orders by inspection

$$G(x,t) = 1 + xt + \tfrac{1}{2}(3x^2-1)t + \tfrac{1}{2}(5x^3-3x)t^3 + \dots \ . \tag{44}$$

We in fact proved a version of this in class when considering the potential due to a point charge in terms of Legendre functions.

5 Associated Legendre equation

We now return to the more general case of the associated Legendre equation (27). It is in fact straightforward to solve this having already solved the Legendre equation. Let us write $P = (1-x^2)^{m/2}v(x)$, this implies that (27) becomes

$$(1-x^2)v'' - 2x(1+m)v' + v(\ell(\ell+1) - m(m+1))v = 0 \ . \tag{45}$$

Now consider any solution $u(x)$ of the Legendre equation i.e.

$$(1-x^2)u'' - 2xu' + \ell(\ell+1)u = 0 \ . \tag{46}$$

We now differentiate this equation m times w.r.t. x and find

$$(1-x^2)u^{(m+2)} - 2x(m+1)u^{(m+1)} + u^{(m)}(\ell(\ell+1) - m(m+1)) = 0 \ , \tag{47}$$

where we have used the notation $u^{(m)} = \frac{d^m}{dx^m}u(x)$ This implies that $v{=}u^{(m)}$ solves (45) and so

$$P_\ell^m = (-1)^m(1-x^2)^{m/2}\frac{d^m}{dx^m}P_\ell(x) \tag{48}$$

solves the associated Legendre equation (27) and hence we call these associated Legendre functions. $P_\ell^m(x)$ is regular everywhere, including $x = \pm 1$, as P_ℓ is. This derivation also implies $m \le \ell$ as otherwise the function would be zero given that P_ℓ is an ℓ-fold polynomial in x. We can now use Rodrigues formula to find

$$P_\ell^m(x) = \frac{(-1)^m}{2^\ell \ell!}(1-x^2)^{m/2}\frac{d^{m+\ell}}{dx^{m+\ell}}(x^2-1)^\ell \ . \tag{49}$$

This formula is, perhaps surprisingly, also valid for $m < 0$ as long as $\ell + m \ge 0$ i.e. $m \ge -\ell$.

Useful Properties The associated Legendre functions also have many useful properties, here we will mention just two: They are related under change of the sign of m by

$$P_\ell^{-m}(x) = (-1)^m\frac{(\ell-m)!}{(\ell+m)!}P_\ell^m(x) \ . \tag{50}$$

Secondly, for fixed m the associated Legendre functions form an orthogonal set on the interval $-1 \le x \le 1$ and they are normalised so that

$$\int_{-1}^{1} P_{\ell'}^m(x)P_\ell^m(x)dx = \frac{2}{2\ell+1}\frac{(\ell+m)!}{(\ell-m)!}\delta_{\ell'\ell} \ . \tag{51}$$

6 Spherical Harmonics

We had decomposed the function $Y(\theta,\phi) = P(\theta)Q(\phi)$, now recombining them we can define our spherical harmonics (after choosing an overall constant)

$$Y_{\ell m}(\theta,\phi) = \sqrt{\frac{2\ell+1}{4\pi}\frac{(\ell-m)!}{(\ell+m)!}}P_\ell^m(\cos\theta)e^{im\phi} \ . \tag{52}$$

From (50) we can see that $Y_{\ell(-m)}(\theta,\phi) = (-1)^m Y_{\ell m}^*(\theta,\phi)$ and, from the normalisation, that the spherical harmonics are orthonormal

$$\int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta d\theta \ Y_{\ell' m'}^*(\theta,\phi)Y_{\ell m}(\theta,\phi) = \delta_{\ell,\ell'}\delta_{m,m'} \ . \tag{53}$$

Furthermore the spherical harmonics form a complete set of functions and hence satisfy the completeness relation

$$\sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell} Y^*_{\ell m}(\theta',\phi')Y_{\ell m}(\theta,\phi) = \delta(\phi-\phi')\delta(\cos\theta-\cos\theta') \ . \tag{54}$$

Some simple examples are,

$$\begin{aligned}
Y_{00} &= \frac{1}{\sqrt{4\pi}} \ , \\
Y_{11} &= -\sqrt{\frac{3}{8\pi}}\sin\theta e^{i\phi} \ , \\
Y_{10} &= \sqrt{\frac{3}{4\pi}}\cos\theta \ , \\
Y_{22} &= \frac{1}{4}\sqrt{\frac{15}{2\pi}}\sin^2\theta e^{2i\phi} \ , \\
Y_{21} &= -\sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta e^{i\phi} \ , \\
Y_{20} &= \sqrt{\frac{5}{4\pi}}(\tfrac{3}{2}\cos^2\theta-\tfrac{1}{2}) \ .
\end{aligned}$$

Given this completeness and orthogonality we can expand an arbitrary function, $g(\theta,\phi)$, in spherical harmonics

$$g(\theta,\phi) = \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell} A_{\ell m}Y_{\ell m}(\theta,\phi) \tag{55}$$

where the coefficients are given by

$$A_{lm} = \int d\Omega \ Y^*_{lm}(\theta,\phi)g(\theta,\phi) \ . \tag{56}$$

Finally let us recall that an arbitrary potential which satisfies Laplace's equation can thus be expanded as

$$\Phi(r,\theta,\phi) = \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell}\left[A_{\ell m}r^{\ell}+B_{\ell m}r^{-\ell-1}\right]Y_{\ell m}(\theta,\phi) \ . \tag{57}$$

Addition Theorem for Spherical Harmonics An important property of spherical harmonics is encoded in the theorem (see Jackson sec. 3.6): Given two vectors $\mathbf{x}$ and $\mathbf{x}'$ with coordinates (r,θ,ϕ) and (r',θ',ϕ') with the angle between them being γ

$$\cos\gamma = \cos\theta\cos\theta' + \sin\theta\sin\theta'\cos(\phi-\phi') \tag{58}$$

one can write

$$P_\ell(\cos\gamma) = \frac{4\pi}{2\ell+1}\sum_{m=-\ell}^{\ell} Y^*_{\ell m}(\theta',\phi')Y_{\ell m}(\theta,\phi) \ . \tag{59}$$

Recalling the expansion of $1/|\mathbf{x}-\mathbf{x}'|$ in terms of $P_\ell(\cos\gamma)$ from class notes or Jackson equation (3.38),

$$\frac{1}{|\mathbf{x}-\mathbf{x}'|} = \sum_{\ell=0}^{\infty} \frac{r_<^\ell}{r_>^{\ell+1}} P_\ell(\cos\gamma) \tag{60}$$

this can be used to write

$$\frac{1}{|\mathbf{x}-\mathbf{x}'|} = 4\pi \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \frac{1}{2\ell+1} \frac{r_<^\ell}{r_>^{\ell+1}} Y_{\ell m}^*(\theta',\phi') Y_{\ell m}(\theta,\phi) \ . \tag{61}$$

7 Multipole Expansion

Let us consider a distribution of charge with some charge density, $\rho(\mathbf{x}')$, localised about the origin. The potential at a position $\mathbf{x}$ outside of the charge distribution is given by

$$\Phi(\mathbf{x}) = \frac{1}{4\pi\epsilon_0} \int \frac{\rho(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|} d^3x' \ . \tag{62}$$

We can now use the expansion (61), with $r_< = r'$ and $r_> = r$, so that

$$\Phi(\mathbf{x}) = \frac{1}{\epsilon_0} \sum_{\ell,m} \frac{1}{2\ell+1} \Big[\int Y_{\ell m}^*(\theta',\phi') \rho(\mathbf{x}') r'^\ell d^3x' \Big] \frac{Y_{\ell m}(\theta,\phi)}{r^{\ell+1}} \ . \tag{63}$$

That is to say we can write the potential as an expansion, called the multipole expansion, in spherical harmonics

$$\Phi(\mathbf{x}) = \frac{1}{4\pi\epsilon_0} \sum_{\ell,m} \frac{4\pi}{2\ell+1} q_{lm} \frac{Y_{\ell m}(\theta,\phi)}{r^{\ell+1}} \ ,$$

where the coefficients

$$q_{lm} = \int Y_{\ell m}^*(\theta',\phi') \rho(\mathbf{x}') r'^\ell d^3x'$$

are called the multipole moments of the charge distribution. Note that because of the properties of the spherical harmonics $q_{\ell,(-m)} = (-1)^m q_{\ell m}^*$. The first few terms in the expansion are called:
$\ell = 0$ term is called the monopole term
$\ell = 1$ term is called the dipole term
$\ell = 2$ term is called the quadrupole term etc.
Explicitly they are given by:

$$q_{00} = \frac{1}{\sqrt{4\pi}} \int \rho(\mathbf{x}') \ d^3x' = \frac{1}{\sqrt{4\pi}} q \tag{64}$$

where q is the total charge. The dipole terms are

$$q_{11} = -\sqrt{\frac{3}{8\pi}} (p_x - ip_y) \ , \quad q_{10} = \sqrt{\frac{3}{4\pi}} p_z \tag{65}$$

where $p_{x,y,z}$ are the components of the electric dipole moment

$$\mathbf{p} = \int \mathbf{x}' \rho(\mathbf{x}') \ d^3x' \ . \tag{66}$$

The quadrupole terms are

$$
\begin{aligned}
q_{22} &= \frac{1}{12}\sqrt{\frac{15}{2\pi}}(Q_{11} - 2iQ_{12} - Q_{22}) \\
q_{21} &= -\frac{1}{3}\sqrt{\frac{15}{8\pi}}(Q_{13} - iQ_{23}) \ , \quad q_{20} = \frac{1}{2}\sqrt{\frac{5}{4\pi}}Q_{33}
\end{aligned} \tag{67}
$$

where the quadrupole moments are given by

$$
Q_{ij} = \int (3x'_i x'_j - r'^2 \delta_{ij}) \rho(\mathbf{x}') \ d^3x' \tag{68}
$$

which are traceless tensors of rank two. In rectangular coordinates, by directly making a Taylor expansion of the $\frac{1}{|\mathbf{x}-\mathbf{x}'|}$ potential, one can find

$$
\Phi(\mathbf{x}) = \frac{1}{4\pi\epsilon_0}\Big[\frac{q}{r} + \frac{\mathbf{p}\cdot\mathbf{x}}{r^3} + \frac{1}{2}\sum_{i,j} Q_{ij}\frac{x_i x_j}{r^5} + \dots\Big] \tag{69}
$$

where as usual $r = |\mathbf{x}|$. Of course one can make a similar expansion for the electric field.

References

[1] G. Arfken, and H. Weber, Mathematical Methods for Physicists, 5th edition, Academic Press.