Spherical Coordinates and Legendre Functions

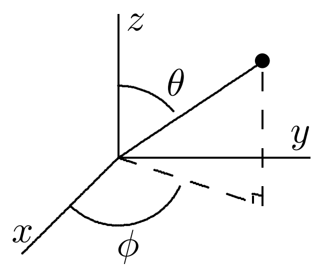
Spherical coordinates

Let's adopt the notation for spherical coordinates that is standard in physics:

$$\phi = \text{longitude or azimuth},$$

$$\theta = \text{colatitude } \left(\tfrac{\pi}{2} - \text{latitude}\right) \text{ or polar angle.}$$

$$x = r \sin\theta \cos\phi,$$
$$y = r \sin\theta \sin\phi,$$
$$z = r \cos\theta.$$



The ranges of the variables are: $0 < r < \infty$, $0 < \theta < \pi$, and ϕ is a periodic coordinate with period 2π.

The Laplacian operator is found to be

$$\nabla^2 u = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial u}{\partial r}\right) + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta\,\frac{\partial u}{\partial \theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2 u}{\partial \phi^2}\,.$$

The term with the r-derivatives can also be written

$$\frac{1}{r}\frac{\partial^2}{\partial r^2}(ru) \quad \text{or} \quad \frac{\partial^2 u}{\partial r^2} + \frac{2}{r}\frac{\partial u}{\partial r}\,.$$

As usual, we try to separate variables by writing

$$u_{\text{sep}} = R(r)\Theta(\theta)\Phi(\phi).$$

We get

$$\frac{r^2\nabla^2 u}{u} = \frac{(r^2 R')'}{R} + \frac{1}{\sin\theta}\,\frac{(\sin\theta\,\Theta')'}{\Theta} + \frac{1}{\sin^2\theta}\,\frac{\Phi''}{\Phi}\,.$$

(Here the primes in the first term indicate derivatives with respect to r, those in the second term derivatives with respect to θ, etc. There is no ambiguity, since each function depends on only one variable.) We have arranged things so that the first term depends only on r, and the others depend on r not at all. Therefore, we can introduce a separation constant (eigenvalue) into Laplace's equation:

$$-\frac{(r^2 R')'}{R} = -K = \frac{1}{\sin\theta}\,\frac{(\sin\theta\,\Theta')'}{\Theta} + \frac{1}{\sin^2\theta}\,\frac{\Phi''}{\Phi}\,.$$

Put the r equation aside for later study. The other equation is

$$\frac{\sin\theta\,(\sin\theta\Theta')'}{\Theta} + K\sin^2\theta + \frac{\Phi''}{\Phi} = 0.$$

We can introduce a second separation constant:

$$-\frac{\Phi''}{\Phi} = m^2 = \frac{\sin\theta\,(\sin\theta\Theta')'}{\Theta} + K\sin^2\theta.$$

Remark: In quantum mechanics, K has the physical interpretation of the square of the total angular momentum of a particle, while m is the component of angular momentum about the z axis.

Just as in two dimensions, problems involving the whole sphere will be different from those involving just a sector. If the region involves a complete sphere, then $\Phi(\phi)$ must be 2π-periodic. Therefore, m is an integer, and Φ is $A\cos(m\phi) + B\sin(m\phi)$ (or $C_+e^{i\phi} + C_-e^{-i\phi}$). Then we can write the θ equation as

$$\frac{1}{\sin\theta}(\sin\theta\,\Theta')' + \left[K - \frac{m^2}{\sin^2\theta}\right]\Theta = 0.$$

This is an eigenvalue problem for K. Recall that the proper interval (for the whole sphere) is $0 < \theta < \pi$. We have a Sturm–Liouville problem, singular at both endpoints, 0 and π, with weight function $r(\theta) = \sin\theta$.

Introduce a new variable by $x \equiv \cos\theta$ and $\Theta(\theta) \equiv Z(x) = Z(\cos\theta)$. (This is not the same as the Cartesian coordinate x.) Then the equation transforms to the purely algebraic form

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

on the interval $-1 < x < 1$. The first two terms can be combined into

$$\frac{d}{dx}\left[(1 - x^2)\,\frac{dZ}{dx}\right].$$

Since $dx = -\sin\theta\,d\theta$, the weight factor is now unity.

If $m = 0$, this equation is called *Legendre's equation* and the solutions are *Legendre functions*. Solutions of the equation with $m \neq 0$ are *associated Legendre functions*.

We concentrate first on $m = 0$. (This means that we are looking only at solutions of the original PDE that are rotationally symmetric about the z axis — i.e., independent of ϕ.) We now get the payoff from a problem that you may have studied in differential equations or in linear algebra or both. When the equation is solved by power series (method of Frobenius), one finds that if $K = l(l+1)$, where l is a nonnegative integer, then there is one solution (of the two independent ones) that is a *polynomial* — the Frobenius series terminates. These are called the *Legendre polynomials*, $P_l(x)$, and a totally different way of stumbling upon them is to apply the Gram–Schmidt orthogonalization procedure to the sequence of powers, $\{1, x, x^2, \ldots\}$, regarded as functions on the interval $[-1, 1]$ with the usual inner product. The first few of them (normalized so that $P(\cos 0) = P(1) = 1$) are

$$P_0(x) = 1$$

$$P_1(x) = x; \qquad \Theta_1(\theta) = \cos\theta$$

$$P_2(x) = \tfrac{1}{2}(3x^2 - 1); \qquad \Theta_2(\theta) = \tfrac{1}{2}(3\cos^2\theta - 1)$$

$P_l(x)$ is a polynomial of degree l. It is given explicitly by *Rodrigues's formula*,

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

Just as we required solutions in polar coordinates to be bounded at the origin, we must require solutions in spherical coordinates to be bounded at the north and south poles ($x = \pm 1$). It is a fact that all solutions except the polynomials P_l behave unacceptably at one or the other of the endpoints. In our problem, therefore, the eigenvalues are the numbers $l(l+1)$, and the Legendre polynomials are the eigenvectors. The other solutions become relevant in other PDE problems where the region does not contain the whole sphere (a cone, for instance). When $K = l(l+1)$ (so that P_l exists), another, linearly independent, solution can be found by the method of *reduction of order* or the general Frobenius theory [review your ODE textbook]. It is called Q_l .

$$Q_0(x) = \frac{1}{2} \ln\left(\frac{1+x}{1-x}\right), \qquad Q_1(x) = \frac{x}{2} \ln\left(\frac{1+x}{1-x}\right) - 1.$$

It's clear that any linear combination of P and Q with a nonzero Q component is singular at the endpoints.

The orthogonality and normalization properties of the Legendre polynomials are

$$\int_{-1}^{1} P_l(x)\, P_k(x)\, dx = 0 \quad \text{if } l \neq k,$$

$$\int_{-1}^{1} P_l(x)^2\,dx = \frac{2}{2l+1}\,.$$

Note that $\int_{-1}^{1}[\ldots x\ldots]\,dx$ is the same as $\int_0^\pi[\ldots\cos\theta\ldots]\,\sin\theta\,d\theta$. The factor $\sin\theta$ is to be expected on geometrical grounds; it appears naturally in the volume element in spherical coordinates,

$$dV = dx\,dy\,dz = r^2\,\sin\theta\,dr\,d\theta\,d\phi,$$

and the surface area element on a sphere,

$$dS = r_0^2\,\sin\theta\,d\theta\,d\phi.$$

Now let's return to the radial equation,

$$r(rR)'' = l(l+1)R,$$

that came out of Laplace's equation. Its solutions are

$$R(r) = Ar^l + Br^{-l-1}.$$

(Except for the -1 in the second exponent, this is just like the two-dimensional case.) We note that one of the basis solutions vanishes as $r \to 0$, the other as $r \to \infty$.

Now we can put all the pieces together to solve a boundary value problem with no ϕ dependence. (If the problem has this axial symmetry and the solution is unique, then the solution must also have that symmetry. Clearly, this will require axially symmetric boundary data.) If the region in question is a ball (the interior of a sphere), then the form of the general axially symmetric solution is

$$u(r, \theta) = \sum_{l=0}^{\infty} b_l \, r^l \, P_l(\cos\theta).$$

If Dirichlet boundary data are given on the sphere, then

$$f(\theta) \equiv u(r_0, \theta) = \sum_{l=0}^{\infty} b_l \, r_0{}^l \, P_l(\cos\theta)$$

for all θ between 0 and π. Therefore, by the orthogonality and normalization formulas previously stated,

$$b_l = \frac{2l+1}{2r_0{}^l} \int_0^{\pi} f(\theta)\, P_l(\cos\theta)\, \sin\theta \, d\theta.$$

If the region is the exterior of a sphere, we would use $r^{-(l+1)}$ instead of r^l. For the shell between two spheres, we would use both, and would need data on both surfaces to determine the coefficients. As always, Neumann or Robin data instead of Dirichlet might be appropriate, depending on the physics of the individual problem.

What if the boundary data do depend on ϕ as well as θ? We must generalize the sum to

$$\sum_{l=0}^{\infty} \sum_{m=-l}^{l} b_{lm} \, r^l \, P_l^m(\cos\theta) \, e^{im\phi},$$

where the functions P_l^m, called *associated Legendre functions*, are solutions of

$$[(1-x^2)P']' + \left[l(l+1) - \frac{m^2}{1-x^2} \right] P = 0.$$

The condition of regularity at the poles forces $|m| \le l$, and this constraint has been taken into account by writing the sum over m from $-l$ to l. There is a generalized Rodrigues formula,

$$P_l^m(x) = \frac{(-1)^m}{2^l l!} (1-x^2)^{m/2} \frac{d^{l+m}}{dx^{l+m}} (x^2-1)^l.$$

These provide a *complete, orthogonal set of functions* on (the surface of) a sphere. The basis functions most commonly used are called *spherical harmonics*, defined by

$$Y_l^m(\theta,\phi) = \left[\frac{2l+1}{4\pi}\,\frac{(l-m)!}{(l+m)!}\right]^{\frac{1}{2}} P_l^m(\cos\theta)\, e^{im\phi}$$

for $-l < m < l$ and $l = 0,\ 1,\ \ldots$. The purpose of the complicated numerical coefficient is to make them orthonormal. Integration over the sphere is done with respect to the usual area element,

$$\int \ldots\, d\Omega \equiv \int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta\, d\theta \ldots.$$

Then one has the orthonormality relation

$$\int d\Omega\, Y_{l'}^{m'}(\theta,\phi)^*\, Y_l^m(\theta,\phi) = \begin{cases} 1 & \text{if } l' = l \text{ and } m' = m, \\ 0 & \text{otherwise.} \end{cases}$$

The completeness (basis) property is: An arbitrary* function on the sphere (i.e., a function of θ and ϕ as they range through their standard intervals) can be expanded as

$$g(\theta,\phi) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} A_{lm}\, Y_l^m(\theta,\phi),$$

where

$$A_{lm} = \int d\Omega\, Y_l^m(\theta,\phi)^*\, g(\theta,\phi).$$

This, of course, is precisely what we need to solve the potential equation with arbitrary boundary data on a spherical boundary. But such a way of decomposing functions on a sphere may be useful even when no PDE is involved, just as the Fourier series and Fourier transform have many applications outside differential

* sufficiently well-behaved, say square-integrable

A table of the first few spherical harmonics

$$Y_0^0 = \frac{1}{\sqrt{4\pi}}$$

$$Y_1^1 = -\sqrt{\frac{3}{8\pi}}\,\sin\theta\, e^{i\phi}$$

$$Y_1^0 = \sqrt{\frac{3}{4\pi}}\,\cos\theta$$

$$Y_1^{-1} = \sqrt{\frac{3}{8\pi}}\,\sin\theta\, e^{-i\phi}$$

$$Y_2^2 = \frac{1}{4}\sqrt{\frac{15}{2\pi}}\,\sin^2\theta\, e^{2i\phi}$$

$$Y_2^1 = -\sqrt{\frac{15}{8\pi}}\,15\,\sin\theta\cos\theta\, e^{i\phi}$$

$$Y_2^0 = \sqrt{\frac{5}{4\pi}}\,\left(\frac{3}{2}\,\cos^2\theta - \frac{1}{2}\right)$$

equations. For example, the shape of the earth (as measured by the gravitational attraction on satellites) is represented by a sum of spherical harmonics, where the first (constant) term is by far the largest (since the earth is nearly round). The three terms with $l = 1$ can be removed by moving the origin of coordinates to the right spot; this defines the "center" of a nonspherical earth. Thus the first interesting terms are the five with $l = 2$; their nonzero presence is called the *quadrupole moment* of the earth. Similar remarks apply to the analysis of any approximately spherical object, force field, etc.*

A sensible person does not try to memorize all the formulas about spherical harmonics (or any other class of special functions). The point is to understand

* See, for example, M. T. Zuber et al., "The Shape of 433 Eros from the NEAR-Shoemaker Laser Rangefinder," *Science* **289**, 2097–2101 (2000), and adjacent articles, for an analysis of a potato-shaped asteroid. There the harmonics with factors $e^{\pm im\phi}$ are combined into real functions with factors $\cos m\phi$ and $\sin m\phi$, so the five coefficients for $l = 2$ are named C_{20}, C_{21}, S_{21}, C_{22}, S_{22}.

that they exist and why they are useful. The details when needed are looked up in handbooks or obtained from computer software. Complicated formulas should not obscure the beauty and power of our march from a basis of eigenvectors in $\mathbf{R}^2$, through Fourier series in one dimension, to this basis of eigenfunctions on a sphere!

Spherical Bessel functions

Instead of the potential equation, $\nabla^2 u = 0$, consider now the Helmholtz equation,

$$\nabla^2 u = -\omega^2 u.$$

This will arise from the separation of variables in the wave or heat equation in three dimensions. When we continue the separation in spherical coordinates, the angular part is exactly the same as before, so the angular dependence of solutions of the Helmholtz equation is still given by the spherical harmonics (or Legendre polynomials, in the axially symmetric case). The radial equation, however, becomes

$$\frac{d^2R}{dr^2} + \frac{2}{r}\frac{dR}{dr} + \left[\omega^2 - \frac{l(l+1)}{r^2}\right] R = 0.$$

Thus the radial solutions are no longer just powers of r.

Let $z \equiv \omega r$, $Z(z) \equiv \sqrt{z}\, R$. Then (another exercise)

$$\frac{d^2Z}{dz^2} + \frac{1}{z}\frac{dZ}{dz} + \left[1 - \frac{l(l+1) + \frac{1}{4}}{z^2}\right] Z = 0.$$

This is Bessel's equation, with $\mu = l + \frac{1}{2}$ (since $(l + \frac{1}{2})^2 = l(l+1) + \frac{1}{4}$). The consequent solutions

$$R(r) = \frac{1}{\sqrt{\omega r}}\, J_{l+\frac{1}{2}}(\omega r)$$

are called *spherical Bessel functions*, with the notation

$$j_l(z) \equiv \sqrt{\frac{\pi}{2z}}\, J_{l+\frac{1}{2}}(z).$$

Similarly, the other types of Bessel functions have their spherical counterparts, y_l , $h_l^{(1)}$, etc.

The surprising good news is that these fractional-order Bessel functions are not an entirely new family of functions. They can all be expressed in terms of sines and cosines. One has

$$j_0(z) = \frac{\sin z}{z}\,, \qquad y_0(z) = -\frac{\cos z}{z}$$

(note that j_0 is regular at 0 and y_0 is not, as expected from their definitions),

$$j_1(z) = \frac{\sin z}{z^2} - \frac{\cos z}{z}\,,$$

and, in general,

$$j_l(z) = z^l \left(-\frac{1}{z}\frac{d}{dz}\right)^l \frac{\sin z}{z}\,,$$

$$y_l(z) = -z^l \left(-\frac{1}{z}\frac{d}{dz}\right)^l \frac{\cos z}{z}\,.$$

Notice that for large l they contain many terms, if all the derivatives are worked out.

We would naturally want to use these to solve a PDE with a homogeneous boundary condition on a sphere. As in the case of integer-order Bessel functions, there will be a normal mode corresponding to each value of z for which $j_l(z)$ vanishes (or its derivative vanishes, if the boundary condition is of the Neumann type). To find these roots one needs to solve a trigonometric equation, as in the classic Sturm–Liouville problems; many of the small roots can be looked up in tables, and there are approximate asymptotic formulas for the large ones. The resulting normal modes form a complete, orthogonal set for expanding functions in the interior of a ball.