Separation of Variables in Spherical Coordinates

Overview and Motivation: We look at separable solutions to the wave equation in one more coordinate system – spherical (polar) coordinates. These coordinates are most useful for solving problems with spherical symmetry.

Key Mathematics: Spherical coordinates, the chain rule, and associated Legendre functions (including Legendre polynomials).

I. Spherical Coordinates and the Wave Equation

As in the case of the cylindrical-coordinates version of the wave equation, our first job will be to express the Laplacian ∇^2 in spherical coordinates (r,θ,ϕ), which are defined in terms of Cartesian coordinates (x,y,z) as

$$r = \sqrt{x^2 + y^2 + z^2}\,, \tag{1a}$$

$$\theta = \arccos\left(\frac{z}{\sqrt{x^2 + y^2 + z^2}}\right), \tag{1b}$$

$$\phi = \arctan\left(\frac{y}{x}\right). \tag{1c}$$

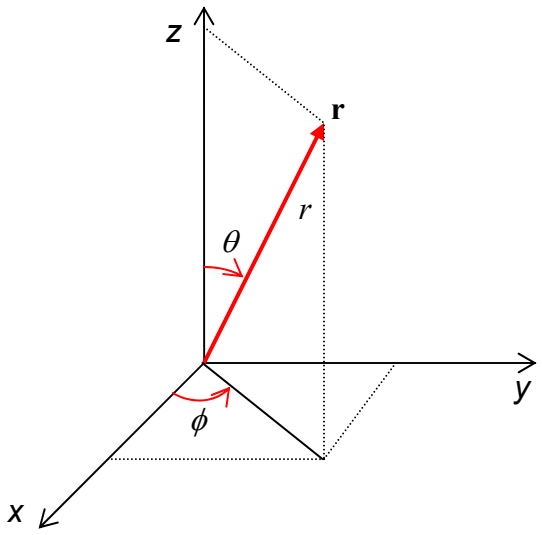
The diagram at the top of the next page graphically illustrates these coordinates for the vector $\mathbf{r}$. The coordinate r is the length of $\mathbf{r}$; the coordinate θ (known as the **polar angle**) is the angle of the vector $\mathbf{r}$ from the z axis; the coordinate ϕ (known as the **azimuthal angle**) is the angle of the xy-plane projection of $\mathbf{r}$ from the x axis to the y axis. Notice that the coordinate ϕ is also used in cylindrical coordinates.

To write $\nabla^2 f$ (where f is some function of r, θ, and ϕ) in spherical coordinates we go through the same procedure as we did for cylindrical coordinates. We think of f as a function of x, y, and z through the new coordinates r, θ, and ϕ

$$f = f\left[r(x,y,z),\theta(x,y,z),\phi(x,y,z)\right]$$

and then re-express

$$\nabla^2 f = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2} \tag{2}$$



in terms of the new coordinates using the chain rule. For example, to re-express the x-derivative term we first use the chain rule to write

$$\frac{\partial f}{\partial x}=\frac{\partial f}{\partial r}\frac{\partial r}{\partial x}+\frac{\partial f}{\partial \theta}\frac{\partial \theta}{\partial x}+\frac{\partial f}{\partial \phi}\frac{\partial \phi}{\partial x}. \tag{3}$$

Using Eq. (3) we can then express the second derivative as

$$\frac{\partial^2 f}{\partial x^2}=\frac{\partial}{\partial x}\left(\frac{\partial f}{\partial x}\right)=\frac{\partial}{\partial x}\left(\frac{\partial f}{\partial r}\frac{\partial r}{\partial x}+\frac{\partial f}{\partial \theta}\frac{\partial \theta}{\partial x}+\frac{\partial f}{\partial \phi}\frac{\partial \phi}{\partial x}\right), \tag{4}$$

and then using the chain rule again we can write

$$\begin{aligned}\frac{\partial^2 f}{\partial x^2}=&\left(\frac{\partial^2 f}{\partial r^2}\frac{\partial r}{\partial x}+\frac{\partial^2 f}{\partial \theta \partial r}\frac{\partial \theta}{\partial x}+\frac{\partial^2 f}{\partial \phi \partial r}\frac{\partial \phi}{\partial x}\right)\frac{\partial r}{\partial x}+\frac{\partial f}{\partial r}\frac{\partial^2 r}{\partial x^2}\\&+\left(\frac{\partial^2 f}{\partial r\partial \theta}\frac{\partial r}{\partial x}+\frac{\partial^2 f}{\partial \theta^2}\frac{\partial \theta}{\partial x}+\frac{\partial^2 f}{\partial \phi \partial \theta}\frac{\partial \phi}{\partial x}\right)\frac{\partial \theta}{\partial x}+\frac{\partial f}{\partial \theta}\frac{\partial^2 \theta}{\partial x^2}\\&+\left(\frac{\partial^2 f}{\partial r\partial \phi}\frac{\partial r}{\partial x}+\frac{\partial^2 f}{\partial \theta \partial \phi}\frac{\partial \theta}{\partial x}+\frac{\partial^2 f}{\partial \phi^2}\frac{\partial \phi}{\partial x}\right)\frac{\partial \phi}{\partial x}+\frac{\partial f}{\partial \phi}\frac{\partial^2 \phi}{\partial x^2}\end{aligned}. \tag{5}$$

Pretty ugly, eh? Actually, if you scrutinize Eq. (5) you will see that there is a bit of symmetry present: switching any of the spherical coordinates results in the same equation.

Although we will not go through the rest of the procedure, you should recall that there are two types of terms in Eq. (5). There are derivatives of f with respect to the new variable (which remain unchanged) and there are derivatives of the new variables with respect to the old variable x. We must calculate these second type of derivatives and then express them in terms of the new variables using Eq. (1). If we go through this procedure for all three terms in the Laplacian and sum everything up, we end up with the spherical-coordinates expression for the wave equation

$$\frac{1}{c^2}\frac{\partial^2 q}{\partial t^2} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial q}{\partial r}\right) + \frac{1}{r^2\sin(\theta)}\frac{\partial}{\partial\theta}\left[\sin(\theta)\frac{\partial q}{\partial\theta}\right] + \frac{1}{r^2\sin^2(\theta)}\frac{\partial^2 q}{\partial\phi^2} \tag{6}$$

II. Separation of Variable in Spherical Coordinates

As before we look for separable solutions to the wave equation by assuming that we can write $q(r,\theta,\phi,t)$ as a product solution

$$q(r,\theta,\phi,t) = R(r)\Theta(\theta)\Phi(\phi)T(t). \tag{7}$$

Substituting this into Eq. (6) and dividing the result by $R(r)\Theta(\theta)\Phi(\phi)T(t)$ yields

$$\frac{1}{c^2}\frac{T''}{T} = \frac{1}{r^2R}\left(r^2R'\right)' + \frac{1}{r^2\sin(\theta)}\frac{1}{\Theta}\left[\sin(\theta)\Theta'\right]' + \frac{1}{r^2\sin^2(\theta)}\frac{\Phi''}{\Phi}. \tag{8}$$

A. Dependence on Time

As with Cartesian and cylindrical coordinates, we again make the argument that the rhs of Eq. (8) is independent of t, and so the lhs of this equation must be constant. As with cylindrical coordinates we call this constant $-k^2$ (where we are thinking of k as real) and so we again have

$$T'' + c^2k^2T = 0, \tag{9}$$

which has the two linearly independent solutions,

$$T_k^{\pm}(t) = T_0e^{\pm ikct}. \tag{10}$$

B. Dependence on ϕ

Equating the rhs of Eq. (8) to $-k^2$, multiplying by $r^2\sin^2(\theta)$, and doing some rearranging of terms gives us

$$\frac{\Phi''}{\Phi} = -k^2 r^2 \sin^2(\theta) - \frac{\sin^2(\theta)}{R}\left(r^2 R'\right)' - \frac{\sin(\theta)}{\Theta}\left[\sin(\theta)\Theta'\right]', \tag{11}$$

which separates out the ϕ dependence from r and θ. Equating the lhs of Eq. (11) to the constant $-m^2$ gives us the equation for Φ,[1]

$$\Phi'' + m^2\Phi = 0, \tag{12}$$

which, yet again, is the harmonic oscillator equation. Equation (12) has the solutions

$$\Phi_m^{\pm}(\phi) = \Phi_0 e^{\pm im\phi}. \tag{13}$$

Again, because we require continuous solutions as a function of ϕ, we must restrict m to integer values, $m = 0, \pm 1, \pm 2, \ldots$. Note that the dependence on ϕ is exactly the same as in the cylindrical-coordinates case.

C. Dependence on θ.

The last variable that we will deal with today is the polar angle θ. If we now equate the rhs of Eq. (11) to $-m^2$, divide by $\sin^2(\theta)$, and do a bit of rearranging, we end up with

$$\frac{1}{\sin(\theta)\Theta}\left[\sin(\theta)\Theta'\right]' - \frac{m^2}{\sin^2(\theta)} = -\frac{1}{R}\left(r^2 R'\right)' - k^2 r^2, \tag{14}$$

which separates the θ and r variables. Each side of this equation is a constant, which by convention is taken to be $-l(l+1)$. This results in the differential equation for $\Theta(\theta)$

$$\frac{1}{\sin(\theta)}\left[\sin(\theta)\Theta'\right]' + \left[l(l+1) - \frac{m^2}{\sin^2(\theta)}\right]\Theta = 0 \tag{15}$$

This is definitely not the harmonic oscillator equation! It is however, close to the standard form of another well known equation. To put Eq. (15) in this standard form we make the change of variables $s(\theta) = \cos(\theta)$. We now think of Θ as a function of θ through the variable s as $\Theta = \Theta[s(\theta)]$, and we write the derivatives of Θ as

[1] You may ask why we do we use $-m^2$ for spherical coordinates when we used $-n^2$ for cylindrical coordinates? I have no idea.

$$\frac{d\Theta}{d\theta}=\frac{d\Theta}{ds}\frac{ds}{d\theta}=\frac{d\Theta}{ds}\left[-\sin(\theta)\right]=\frac{d\Theta}{ds}\left[-\sqrt{1-s^2}\right] \tag{16a}$$

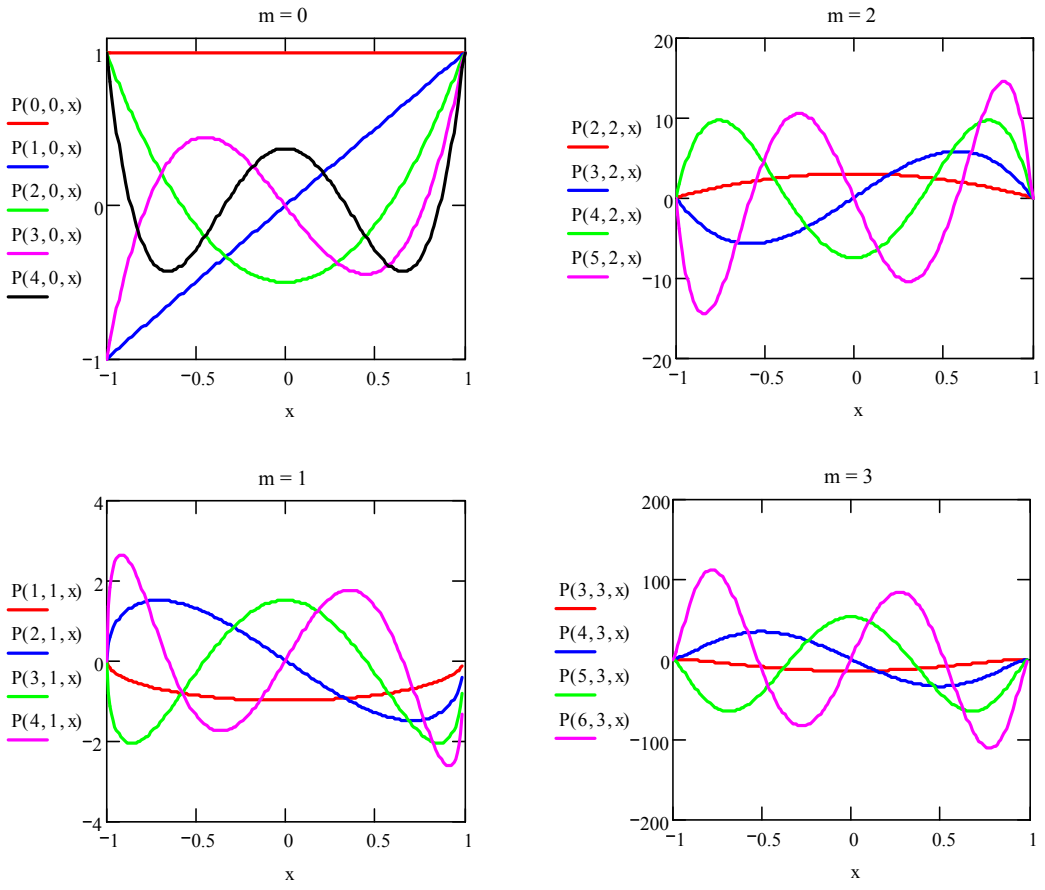
and

$$\begin{aligned}\frac{d^2\Theta}{d\theta^2}&=\frac{d}{d\theta}\left(\frac{d\Theta}{ds}\frac{ds}{d\theta}\right)=\frac{d^2\Theta}{ds^2}\left(\frac{ds}{d\theta}\right)^2+\frac{d\Theta}{ds}\frac{d^2s}{d\theta^2}\\&=\frac{d^2\Theta}{ds^2}\left(1-s^2\right)+\frac{d\Theta}{ds}\left[-s\right]\end{aligned}. \tag{16b}$$

Substituting Eq. (16) into Eq. (15) yields, after a bit of algebra,

$$\left(1-s^2\right)\Theta''(s)-2s\,\Theta'(s)+\left[l(l+1)-\frac{m^2}{1-s^2}\right]\Theta(s)=0\,. \tag{17}$$

This equation is known as the **associated Legendre equation**. As with all second-order linear, ordinary differential equations, there are two linearly independent solutions. These solutions are know as **associated Legendre functions of the first**



and second kind, which are denoted $P_l^m(s)$ and $Q_l^m(s)$, respectively. Usually we are interested in only the $P_l^m(s)$ solutions because the $Q_l^m(s)$ solutions diverge as $s \to \pm 1$.

The figure on the previous page plots some of the $P_l^m(s)$ functions for various values of l and m. Notice that these functions are plotted for $-1 \le s \le 1$ because this corresponds to $0 \le \theta \le \pi$, the range of the polar angle θ. The following statements summarize some key feature of the associate Legendre functions, some of which are evident in the figure.

(*i*) For the $P_l^m(s)$ solutions to Eq. (17) to remain finite, the parameter l must be an integer and m, which is already an integer, must satisfy $|m| \le l$. (You are already likely familiar with this result from quantum mechanics, where the angular parts of the separable solutions of the Schrödinger in spherical coordinates are identical to the solutions here.)

(*ii*) For $m = 0$ (azimuthal symmetry) the solutions $P_l(s) \equiv P_l^0(s)$ are known as **Legendre polynomials**. These functions are polynomials in s of order l. The first four Legendre polynomials are

$$P_0(s) = 1, \qquad P_1(s) = s, \qquad P_2(s) = \frac{1}{2}\left(3s^2 - 1\right), \qquad P_3(s) = \frac{1}{2}\left(5s^3 - 3s\right) \qquad \text{(18a)} - \text{(18d)}$$

(*iii*) A nice simple formula for calculating the Legendre polynomials, known as **Rodrigues' formula**, is

$$P_l(s) = \frac{1}{2^l\, l!}\frac{d^l\left(s^2 - 1\right)^l}{ds^l} \tag{19}$$

(*iv*) For the associated Legendre functions Rodrigues' formula generalizes to

$$P_l^m(s) = \frac{1}{2^l\, l!}\left(1 - s^2\right)^{|m|/2}\frac{d^{|m|+l}}{ds^{|m|+l}}\left(s^2 - 1\right)^l. \tag{20}$$

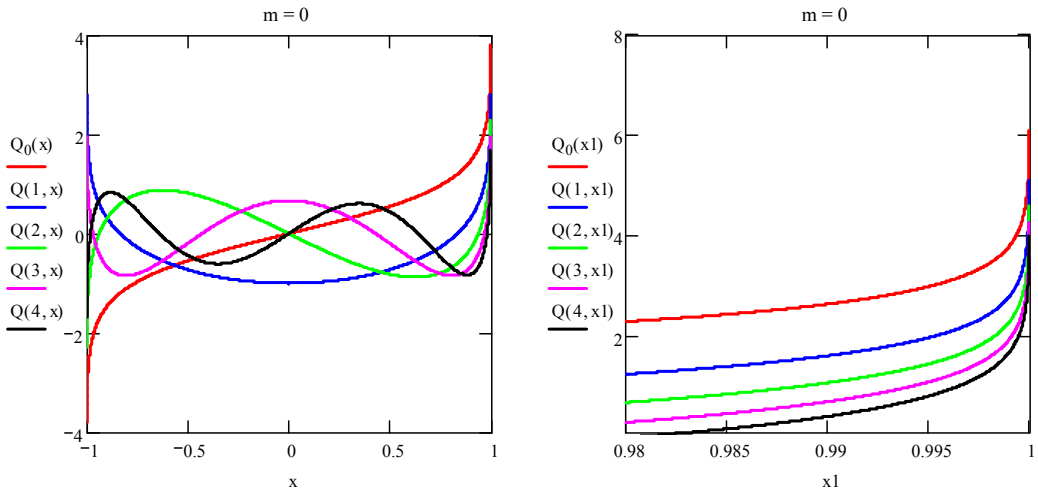
(*v*) The first few $m = 0$ Legendre functions of the second kind can be written as

$$Q_0(s) = \frac{1}{2}\ln\left(\frac{1+s}{1-s}\right), \quad Q_1(s) = \frac{s}{2}\ln\left(\frac{1+s}{1-s}\right) - 1, \quad Q_2(s) = \frac{3s^2 - 1}{4}\ln\left(\frac{1+s}{1-s}\right) - \frac{3s}{2}. \quad \text{(21a)} - \text{(21c)}$$

(*vi*) For $l \geq 1$ the $m = 0$ Legendre functions of the second kind can be expressed in terms of the Legendre functions of the first kind as

$$Q_l(s) = \frac{1}{2} P_l(s) \ln\left(\frac{1+s}{1-s}\right) - \sum_{m=1}^{l} \left[\frac{1}{m} P_{m-1}(s) P_{l-m}(s)\right]. \tag{22}$$

The following figure plots the first few of these functions. Notice that they all diverge as $|s| \to 1$, although because the divergence involves the logarithm function, the divergence is very slow, as the graph on the rhs of the figure illustrates.

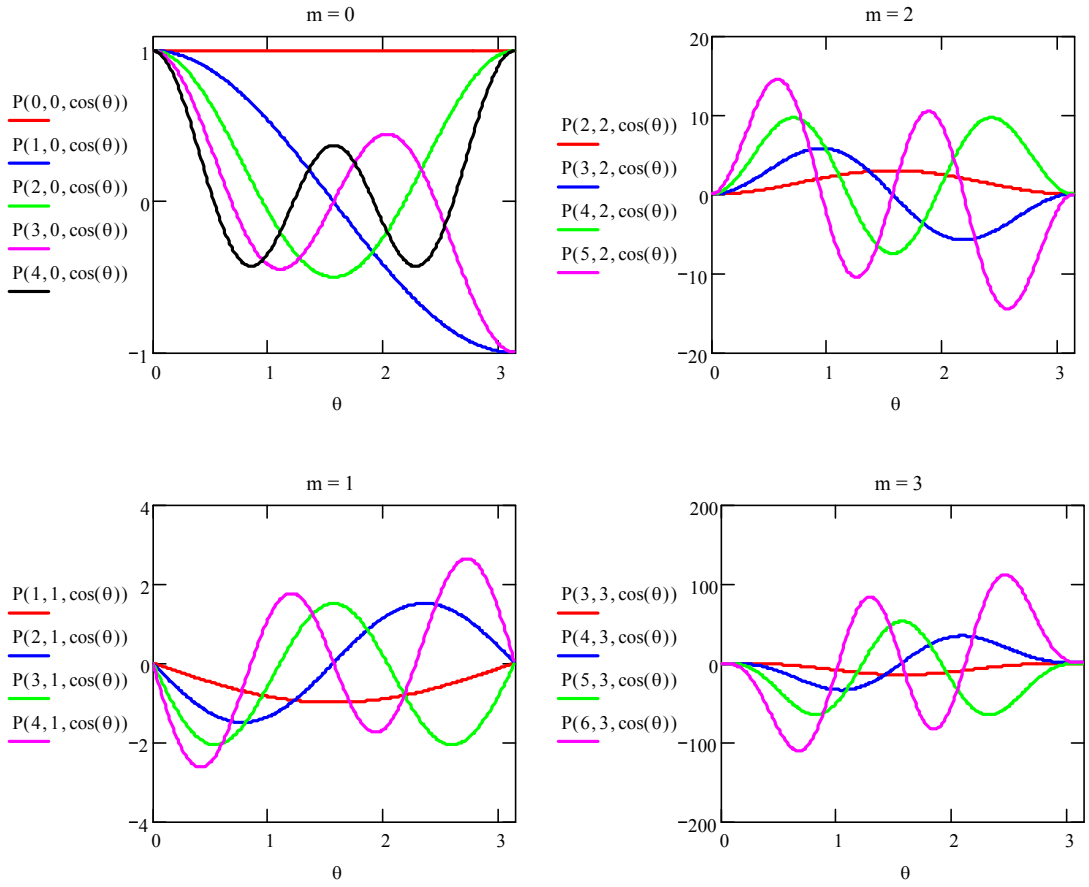


As with the Bessel functions, more entertaining facts about associated Legendre functions can be found in *Handbook of Mathematical Functions* by Abramowitz and Stegun or in the online *NIST Digital Library of Mathematical Functions*.

Now that we have some idea of the behavior of these functions, we can get back to our solution of the wave equation. Because $s = \cos(\theta)$ the solutions to Eq. (15) are

$$\Theta^P_{l,m}(\theta) = \Theta_P P_l^m(\cos(\theta)) \quad \text{and} \quad \Theta^Q_{l,m}(\theta) = \Theta_Q Q_l^m(\cos(\theta)), \tag{23}$$

(or some linear combination of the two solutions) Because they remain finite, we are usually exclusively interested in solutions involving Legendre functions of the first kind. The figure at the top of the next page plots some of the $P_l^m(\cos(\theta))$ functions as a function of θ. Notice that they are similar, but not identical to the functions plotted on p. 5.



Exercises

*__22.1__ Calculate the change-of-coordinates derivatives $\partial r/\partial x$, $\partial\theta/\partial x$, and $\partial\phi/\partial x$ and express them as functions of the new variables.

*__22.2__ Consult the figure on p. 5. For the function $P_l^m(s)$, how many zero crossings of are there for $-1 < s < 1$? That is, deduce the formula for the number of zero crossings as a function of l and m.

*__22.3__ The Legendre polynomials $P_l^0(x)$ can be used as a set of orthogonal basis functions on the interval $-1 \le x \le 1$. Using the standard definition of the inner product, show that P_0, P_1, and P_2 are all orthogonal. Find normalized versions of each of these functions.

*__22.4__ Using Eq. (7), derive Eq. (8) from Eq. (6).