1.6 Spherical Harmonics

Physicists are familiar with many special functions that arise over and over again in solutions to various problems. The analysis of problems with spherical symmetry in $\mathbb{R}^3$ often appeal to the *spherical harmonic functions*, often called simply *spherical harmonics*. Spherical harmonics are the restrictions of homogeneous harmonic polynomials of three variables to the sphere S^2. In this section we will give a typical physics-style introduction to spherical harmonics. Here we state, but do not prove, their relationship to homogeneous harmonic polynomials; a formal statement and proof are given Proposition A.2 of Appendix A.

Physics texts often introduce spherical harmonics by applying the technique of *separation of variables* to a differential equation with spherical symmetry. This technique, which we will apply to Laplace's equation, is a method physicists use to find solutions to many differential equations. The technique is often successful, so physicists tend to keep it in the top drawer of their toolbox. In fact, for many equations, separation of variables is guaranteed to find all nice solutions, as we prove in Proposition A.3.

Faced with a partial differential equation (i.e., an equation involving derivatives with respect to more than one independent variable), one can often construct some solutions by looking for solutions that are the product of functions of one variable. We will apply this technique, called *separation of variables*, to find harmonic functions of three variables. Recall from Section 1.5 that a function is harmonic if and only if it satisfies Laplace's equation, which we write in spherical coordinates (see Exercise 1.12):

$$0 = \left(\partial_r^2 + \frac{2}{r}\partial_r + \frac{1}{r^2}\partial_\theta^2 + \frac{\cos\theta}{r^2\sin\theta}\partial_\theta + \frac{1}{r^2\sin^2\theta}\partial_\phi^2\right)\psi, \tag{1.7}$$

where ψ is an unknown function of (r, θ, ϕ). To apply the technique of separation of variables to this equation, suppose that there is a solution of the form

$$\psi(r, \theta, \phi) = R(r)\Theta(\theta)\Phi(\phi), \tag{1.8}$$

where R, Θ and Φ are differentiable functions of one variable. On the face of it, this is quite a bold supposition: in general such a solution might not exist. But when such solutions do exist, our supposition will help us find them. Such a supposition is called an *ansatz*.[8] For example, the equation $\nabla^2\psi = 0$ gives

[8] From the German word *Ansatz*, which means something close to "hypothesis" or "setup" but does not have an exact English equivalent.

enough information about the functions R, Θ and Ψ that we will be able to find them. To this end we multiply Equation 1.7 by r^2/ψ (why? because it ends up working), plug in Equation 1.8 and calculate:

$$\begin{aligned} 0 &= \frac{r^2}{\psi}\left(\partial_r^2 + \frac{2}{r}\partial_r + \frac{1}{r^2}\partial_\theta^2 + \frac{\cos\theta}{r^2\sin\theta}\partial_\theta + \frac{1}{r^2\sin^2\theta}\partial_\phi^2\right) R(r)\Theta(\theta)\Phi(\phi) \\ &= \left(\frac{r^2 R''(r)}{R(r)} + \frac{2r R'(r)}{R(r)}\right) + \left(\frac{\Theta''(\theta)}{\Theta(\theta)} + \frac{\cos\theta}{\sin\theta}\frac{\Theta'(\theta)}{\Theta(\theta)} + \frac{1}{\sin^2\theta}\frac{\Phi''(\phi)}{\Phi(\phi)}\right). \end{aligned}$$

The crucial observation is that the first parenthesis in the last expression depends only on r, while the second parenthesis depends only on θ and ϕ. Because the sum of the two parentheses is 0, each one must be constant in r, θ and ϕ. Let us repeat the argument in a slightly different form. Rearranging the equation above we find

$$\left(-\frac{r^2 R''(r)}{R(r)} - \frac{2r R'(r)}{R(r)}\right) = \left(\frac{\Theta''(\theta)}{\Theta(\theta)} + \frac{\cos\theta}{\sin\theta}\frac{\Theta'(\theta)}{\Theta(\theta)} + \frac{1}{\sin^2\theta}\frac{\Phi''(\phi)}{\Phi(\phi)}\right). \tag{1.9}$$

The right-hand side is constant in r, so the left-hand side must also be constant in r. Contrariwise, both sides are constant in θ and ϕ. In other words, the variables are separated into different terms, a happy accident that we can exploit. We started with one differential equation involving three variables, and ended up with two separate equations, one involving one variable, and one involving two variables. Thus we have reduced the problem (finding solutions to the original equation) to two simpler problems. Of course, this simplification works only if our supposition (that there are solutions of the given form) turns out to be true.

Let us first find some solutions to the equation for R. We will make another ansatz, i.e., another supposition: we will look for solutions of the form $R(r) = r^\ell$ for some nonnegative integer ℓ. In other words, we will look for homogeneous solutions to Laplace's equation. Then $R'(r) = \ell r^{\ell-1}$ and $R''(r) = \ell(\ell-1)r^{\ell-2}$. Such an ℓ must satisfy

$$\text{constant} = -\frac{r^2\ell(\ell-1)r^{\ell-2}}{r^\ell} - \frac{2r\ell r^{\ell-1}}{r^\ell} = -\ell(\ell+1),$$

which is true for any nonnegative integer ℓ.

Next, we must find corresponding solutions for Θ and Φ. According to Equation 1.9, if $R(r) = r^\ell$, then we must have

$$-\ell(\ell+1) = \left(\frac{\Theta''(\theta)}{\Theta(\theta)} + \frac{\cos\theta}{\sin\theta}\frac{\Theta'(\theta)}{\Theta(\theta)} + \frac{1}{\sin^2\theta}\frac{\Phi''(\phi)}{\Phi(\phi)}\right). \tag{1.10}$$

Functions $\Theta(\theta)\Phi(\phi)$ such that Θ and Φ solve this equation are called *spherical harmonic functions of degree* ℓ. We can find solutions by separating variables again. Multiplying both sides by $\sin^2\theta$ and rearranging we have

$$-\frac{\Phi''(\phi)}{\Phi(\phi)} = \ell(\ell+1)\sin^2\theta + \frac{\Theta''(\theta)}{\Theta(\theta)}\sin^2\theta + \frac{\Theta'(\theta)}{\Theta(\theta)}\sin\theta\cos\theta.$$

Because the left-hand side is constant in θ and the right-hand side is constant in ϕ, both must be constant.

Next we find solutions for Φ. It is known from the theory of ordinary differential equations that the only solutions of $\Phi''/\Phi = \text{constant}$ are of the form $\Phi(\phi) = e^{im\phi}$. In our situation, ϕ is an angular variable, so Φ must satisfy $\Phi(\phi + 2\pi) = \Phi(\phi)$ for all $\phi \in \mathbb{R}$. So a legitimate solution requires $m \in \mathbb{Z}$, and in this case we have

$$-\frac{\Phi''(\phi)}{\Phi(\phi)} = m^2.$$

Finally we must solve the equation

$$\ell(\ell+1)\sin^2\theta + \frac{\Theta''(\theta)}{\Theta(\theta)}\sin^2\theta + \frac{\Theta'(\theta)}{\Theta(\theta)}\sin\theta\cos\theta = m^2$$

for Θ. While the solutions we found before (r^ℓ and $e^{im\phi}$) are probably familiar to most readers, the functions that solve this equation are more obscure. A change of variables will let us rewrite this equation. Define $P\colon [-1,1] \to \mathbb{R}$ by $P(\cos\theta) = \Theta(\theta)$, where $\theta \in [0,\pi]$. Then $\Theta'(\theta) = -P'(\cos\theta)\sin\theta$ and $\Theta''(\theta) = P''(\cos\theta)\sin^2\theta - P'(\cos\theta)\cos\theta$, and so we can rewrite the differential equation as

$$\ell(\ell+1)\sin^2\theta + \frac{P''(\cos\theta)}{P(\cos\theta)}\sin^4\theta - \frac{P'(\cos\theta)}{P(\cos\theta)}(2\cos\theta\sin^2\theta) = m^2.$$

Setting $t := \cos\theta$ and recalling that $\sin^2 + \cos^2 = 1$ we find

$$\ell(\ell+1)(1-t^2) + (1-t^2)^2\frac{P''(t)}{P(t)} + 2t(t^2-1)\frac{P'(t)}{P(t)} = m^2. \qquad (1.11)$$

Equation 1.11 is known as the *Legendre equation* and it has solutions for integers m with $m^2 \leq \ell^2$, as the reader may check in Appendix A. The solutions $\mathbf{P}_{\ell,m}$ to the Legendre equation are called *Legendre functions*. Putting it all together we have a harmonic function

$$R(r)\Theta(\theta)\Phi(\phi) = r^\ell P_{\ell,m}(\cos\theta)e^{im\phi} \qquad (1.12)$$

for some nonnegative integer ℓ, some integer m and a function $P_{\ell,m}$ satisfying the Legendre equation (Equation 1.11).

The angular part $Y_{\ell,m} := P_{\ell,m}(\cos\theta)e^{im\phi}$ of the solution (1.12) is a *spherical harmonic function*. It turns out that there is a nonzero $P_{\ell,m}$ whenever ℓ is a nonnegative integer and m is an integer with $|m| \leq \ell$. In Appendix A we will prove this and other facts about spherical harmonic functions. The number ℓ is called the *degree* of the spherical harmonic. From Equation 1.10 we see that each spherical harmonic of degree ℓ satisfies the equation

$$\left(\partial_\theta^2 + \frac{\cos\theta}{\sin\theta}\partial_\theta + \frac{1}{\sin^2\theta}\partial_\phi^2\right) Y_{\ell,m} = -\ell(\ell+1). \tag{1.13}$$

There is one spherical harmonic functions of degree $\ell = 0$:

$$Y_{0,0}(\theta,\phi) := \frac{1}{2\sqrt{\pi}};$$

three of degree $\ell = 1$:

$$\begin{aligned}
Y_{1,1}(\theta,\phi) &:= -\frac{\sqrt{3}}{2\sqrt{2\pi}}\sin\theta e^{i\phi}\\
Y_{1,0}(\theta,\phi) &:= \frac{\sqrt{3}}{2\sqrt{\pi}}\cos\theta\\
Y_{1,-1}(\theta,\phi) &:= \frac{\sqrt{3}}{2\sqrt{2\pi}}\sin\theta e^{-i\phi};
\end{aligned}$$

and five of degree $\ell = 2$:

$$\begin{aligned}
Y_{2,2}(\theta,\phi) &:= \sqrt{\frac{15}{32\pi}}\sin^2\theta e^{2i\phi}\\
Y_{2,1}(\theta,\phi) &:= -\sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta e^{i\phi}\\
Y_{2,0}(\theta,\phi) &:= \sqrt{\frac{5}{16\pi}}(3\cos^2\theta - 1)\\
Y_{2,-1}(\theta,\phi) &:= \sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta e^{-i\phi}\\
Y_{2,-2}(\theta,\phi) &:= \sqrt{\frac{15}{32\pi}}\sin^2\theta e^{-2i\phi}.
\end{aligned}$$

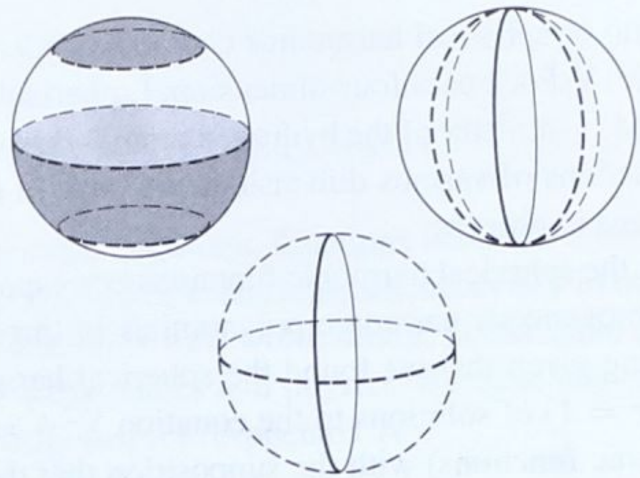

Figure 1.8. The top left sphere shows the positive (shaded) and negative (unshaded) regions for the real-valued function $Y_{2,0}$. The top right sphere shows the pure real (solid) and pure imaginary (dashed) meridian for the function $Y_{2,2}$. The bottom picture shows the zero points (double-dashed) as well as the pure real (solid) and pure imaginary (dashed) meridians of $Y_{2,1}$. There are colored versions of these pictures available on the internet. See, for instance, [Re].

Since spherical harmonics are functions from the sphere to the complex numbers, it is not immediately obvious how to visualize them. One method is to draw the domain, marking the sphere with information about the value of the function at various points. See Figure 1.8. Another way to visualize spherical harmonics is to draw polar graphs of the Legendre functions. See Figure 1.9. Note that for any ℓ, m we have $|Y_{\ell,m}| = |\mathbf{P}_{\ell,m}|$. So the Legendre function carries all the information about the magnitude of the spherical harmonic.

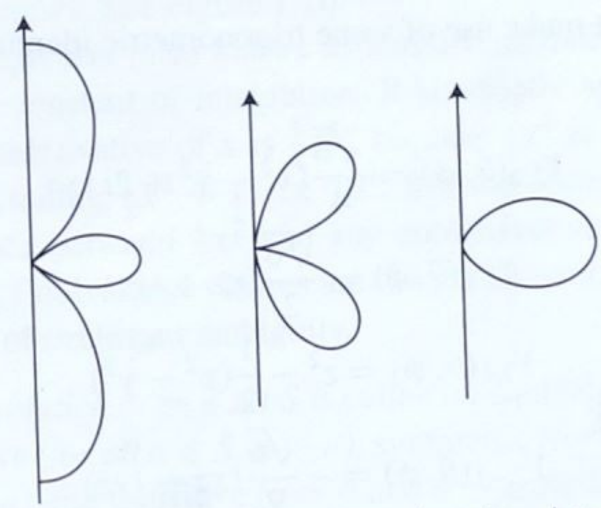

Figure 1.9. Polar graphs of, left to right, $|\mathbf{P}_{2,2}|$, $|\mathbf{P}_{2,1}|$ and $|\mathbf{P}_{2,0}|$. Rotate each graph around the vertical axis to obtain the spherical graph of the absolute value of the spherical harmonics. Three-dimensional versions of these pictures, with color added to indicate the phase $e^{im\phi}$, are available on the internet. See for instance [Sw].

The construction of spherical harmonics can be extended to other dimensions. For example, V. Fock uses four-dimensional spherical harmonics in his article on the $SO(4)$ symmetry of the hydrogen atom — see Chapter 9. Spherical harmonic functions of various dimensions are used in many spherically symmetric problems in physics.

It turns out that the spherical harmonic functions correspond exactly to the restrictions of homogeneous harmonic polynomials in three variables. This is not too surprising given that we found the spherical harmonics by taking the angular part ($r = 1$) of solutions to the equation $\nabla^2\psi = 0$ (the defining property of harmonic functions) with the supposition that the radial part has the form r^ℓ. A proof of the exact correspondence is in Appendix A. For the moment, we will simply verify that the spherical harmonics above are indeed restrictions of harmonic polynomials. Recall that on the unit sphere we have $(x, y, z) = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$. For $\ell = 0$ we have a constant function, which is a polynomial of degree 0. For $\ell = 1$ it is easy to compute from the definitions that

$$Y_{1,1}(\theta,\phi) = -\frac{\sqrt{3}}{2\sqrt{2\pi}}(x+iy)$$

$$Y_{1,0}(\theta,\phi) = \frac{\sqrt{3}}{2\sqrt{\pi}}z$$

$$Y_{1,-1}(\theta,\phi) = \frac{\sqrt{3}}{2\sqrt{2\pi}}(x-iy).$$

For $\ell = 2$ we must make use of some trigonometric identities to see that

$$Y_{2,2}(\theta,\phi) = \frac{\sqrt{6}}{4}(x^2 - y^2 + 2ixy)$$

$$Y_{2,1}(\theta,\phi) = \frac{\sqrt{6}}{2}(xz + iyz)$$

$$Y_{2,0}(\theta,\phi) = z^2 - \frac{1}{2}(x^2 - y^2)$$

$$Y_{2,-1}(\theta,\phi) = -\frac{\sqrt{6}}{2}(xz - iyz)$$

$$Y_{2,-2}(\theta,\phi) = \frac{\sqrt{6}}{4}(x^2 - 2ixy - y^2).$$

The right-hand side of each equation is a homogeneous polynomial of degree two in x, y and z. Each is harmonic, as the reader may check by direct calculation. For example,

$$\left(\partial_x^2 + \partial_y^2 + \partial_z^2\right) \frac{\sqrt{6}}{4}(x^2 - 2ixy - y^2) = \frac{\sqrt{6}}{4}(2 + 0 - 2) = 0.$$

Relating the spherical harmonic functions introduced here to the homogeneous harmonic polynomials is not logically necessary in this book. Morally, however, the calculation is well worth doing, in the name of better communication between mathematics and physics. Because this calculation is a bit tricky, we have postponed it to Appendix A.

1.7 Equivalence Classes

We will encounter *equivalence relations* and *equivalence classes* several times in our story. Equivalence is ubiquitous in mathematics. Because mathematicians insist on defining every object rigorously, and rigor often requires technical details, we need a mechanism to suppress any details that are irrelevant to our main point. The reader may have encountered this technique before in studying vectors and indefinite integration. In many courses, vectors are introduced as *directed line segments*, or arrows from one point to another point. See, for example, Marsden, Tromba and Weinstein [MTW]. This geometric image is very useful for developing intuition about vectors. For instance, one can interpret vector addition as a picture of a parallelogram made up of these arrows. See Figure 1.10.

In indefinite integration (also knows as antidifferentiation), there is extra information in the constant of integration. It is, strictly speaking, incorrect to say that "*the* antiderivative of x is $\frac{1}{2}x^2$" because $\frac{1}{2}x^2$ is only one of many antiderivatives, including $\frac{1}{2}x^2 + 1.7 \times 10^3$. But the statement is correct in spirit: the difference between $\frac{1}{2}x^2$ and any antiderivative of x is irrelevant for most purposes. Equivalence classes are the mathematician's way to make precise the notion of irrelevant ambiguity.

Definition 1.3 *A relation $\sim$ on a set S is called an* equivalence relation *if and only if $\sim$ is* reflexive *(for all $a \in S$, $a \sim a$),* symmetric *(for all $a, b \in S$, $a \sim b$ if and only if $b \sim a$) and* transitive *($a \sim b$ and $b \sim c$ implies $a \sim c$). Given a set S, an equivalence relation $\sim$ and an element $a \in S$, the* equivalence class *of a is the set*

$$[a] := \{b \in S : b \sim a\}$$

and the set of all equivalence classes of elements of S is denoted $S/\sim$.

Exercise 11.6 (Used in Proposition 11.1) *Suppose V and W are finite-dimensional vector spaces and let $T: V \otimes W \to Hom(V^*, W)$ denote the isomorphism from the proof of Proposition 5.14. Suppose $\Pi: W \to W$ is an orthogonal projection and consider $x \in V \otimes W$. Set $X := T(x)$. Show that*

$$T(\tilde{\Pi}x) = \Pi X \in \operatorname{Hom}(V^*, W),$$

where $\tilde{\Pi}$ is defined in Formula 11.2.

Next suppose $Q: V^* \to V^*$ is a orthogonal projection. Define P as in Exercise 11.5. Show that

$$T(\tilde{P}x) = XQ \in \operatorname{Hom}(V^*, W).$$

Exercise 11.7 *For each nonnegative integer ℓ, decompose the representation of $SU(2)$ on $\mathcal{P}^\ell \otimes \mathbb{C}^2$ into a Cartesian sum of its irreducible components. Conclude that this representation is reducible. Is there a meaningful physical consequence or interpretation of this reducibility?*

Exercise 11.8 *Show that if H is any operator on $L^2(\mathbb{R}^3)$ and p is any direction in $\mathbb{R}^3$, then measurement of H and measurement of the spin in the p-direction commute on the state space of a mobile particle with spin 1/2.*

Exercise 11.9 *Show that the complex scalar product on the tensor product $L^2(\mathbb{R}^3) \otimes \mathbb{C}^2$, defined in terms of the complex scalar products on $L^2(\mathbb{R}^3)$ and $\mathbb{C}^2$ from Equation 5.2, agrees with the complex scalar product given in Equation 11.6.*

Appendix A
Spherical Harmonics

The goal of this appendix is to prove that the restrictions of harmonic polynomials of degree ℓ to the sphere do in fact correspond to the spherical harmonics of degree ℓ. Recall that in Section 1.6 we used solutions to the Legendre equation (Equation 1.11) to define the spherical harmonics. In this appendix we construct bona fide solutions $\mathbf{P}_{\ell,m}$ to the Legendre equation; then we show that each of the span of the spherical harmonics of degree ℓ is precisely the set of restrictions of harmonic polynomials of degree ℓ to the sphere.

Physicists and chemists know the Legendre functions well. One very useful explicit expression for these functions is given in terms of derivatives of a polynomials.

Definition A.1 *Let ℓ be a nonnegative integer and let m be an integer satisfying $0 \leq m \leq \ell$. Define the ℓ, m* Legendre function *by*

$$\mathbf{P}_{\ell,m}(t) := \frac{(-1)^m}{\ell! 2^\ell}(1-t^2)^{m/2}\partial_t^{\ell+m}(t^2-1)^\ell.$$

For each ℓ, the function $\mathbf{P}_{\ell,0}$ is called the Legendre polynomial *of degree ℓ.*

Note that the so-called Legendre polynomial is in fact a polynomial of degree ℓ, as it is the ℓth derivative of a polynomial of degree 2ℓ. Legendre functions with $m \neq 0$ are often called *associated Legendre functions*.

Recall the Legendre equation (Equation 1.11):

$$(1-t^2)P''(t) - 2tP'(t) + \left(\ell(\ell+1) - \frac{m^2}{(1-t^2)}\right)P(t) = 0. \tag{A.1}$$

Proposition A.1 *The Legendre functions of Definition A.1 satisfy the Legendre equation.*

There are many ways to prove this proposition. Our proof is straightforward, elementary and rather ugly. For a more elegant proof via the "Rodrigues formula," see [WW, Chapter XV] or [DyM, Section 4.12].

Proof. First we will show that the Legendre polynomial of degree ℓ satisfies the Legendre equation with $m = 0$. Then we will deduce that for any $m = 1, \ldots, \ell$, the Legendre function $\mathbf{P}_{\ell,m}$ satisfies the Legendre equation.

When $m = 0$ the Legendre equation reduces to

$$(1-t^2)P''(t) - 2tP'(t) + \ell(\ell+1)P(t) = 0. \tag{A.2}$$

We use the binomial expansion to find the coefficients of the Legendre polynomial of degree ℓ. For convenience, we multiply through by $2^\ell \ell!$:

$$\begin{aligned}(2^\ell \ell!)\mathbf{P}_{\ell,0}(t) &= \partial_t^\ell (t^2-1)^\ell \\ &= \partial_t^\ell \sum_{k=0}^{\ell} \binom{\ell}{k} (-1)^{\ell-k} t^{2k} \\ &= \sum_{k=(\ell+\epsilon)/2}^{\ell} \binom{\ell}{k} (-1)^{\ell-k} \frac{(2k)!}{(2k-\ell)!} t^{2k-\ell}.\end{aligned}$$

Differentiating once we find

$$(2^\ell \ell!)\mathbf{P}'_{\ell,0}(t) = \sum_{k=1+(\ell-\epsilon)/2}^{\ell} \binom{\ell}{k} (-1)^{\ell-k} \frac{(2k)!}{(2k-\ell-1)!} t^{2k-\ell-1}$$

and, differentiating again,

$$(2^\ell \ell!)\mathbf{P}''_{\ell,0}(t) = \sum_{k=1+(\ell+\epsilon)/2}^{\ell} \binom{\ell}{k} (-1)^{\ell-k} \frac{(2k)!}{(2k-\ell-2)!} t^{2k-\ell-2},$$

where $\epsilon = 0$ if ℓ is even and $\epsilon = 1$ if ℓ is odd. Hence to show that

$$(1-t^2)\mathbf{P}''_{\ell,0}(t) - 2t\mathbf{P}'_{\ell,0}(t) + \ell(\ell+1)\mathbf{P}_{\ell,0}(t) = 0,$$

it suffices to show the vanishing of the following expression:

$$\sum_{k=1+(\ell+\epsilon)/2}^{\ell} \binom{\ell}{k} \frac{(-1)^{\ell-k}(2k)!}{(2k-\ell-2)!} t^{2k-\ell-2}$$
$$- \sum_{k=1+(\ell+\epsilon)/2}^{\ell} \binom{\ell}{k} \frac{(-1)^{\ell-k}(2k)!}{(2k-\ell-2)!} t^{2k-\ell}$$
$$-2 \sum_{k=1+(\ell-\epsilon)/2}^{\ell} \binom{\ell}{k} \frac{(-1)^{\ell-k}(2k)!}{(2k-\ell-1)!} t^{2k-\ell}$$
$$+\ell(\ell+1) \sum_{k=(\ell+\epsilon)/2}^{\ell} \binom{\ell}{k} \frac{(-1)^{\ell-k}(2k)!}{(2k-\ell)!} t^{2k-\ell}.$$

We will show that the coefficient of each power of t is zero. The coefficient of t^ℓ is

$$-\frac{(2\ell)!}{(\ell-2)!} - 2\frac{(2\ell)!}{(\ell-1)!} + \ell(\ell+1)\frac{(2\ell)!}{\ell!}$$
$$= \frac{2\ell}{(\ell-1)!}\left(-(\ell-1) - 2 + (\ell+1)\right) = 0.$$

The coefficients of $t^{\ell-1}$ through t^2 take the form (with an appropriate choice of k, and ignoring an overall factor of $(-1)^{\ell-k}$):

$$-\binom{\ell}{k}\frac{(2k+2)!}{(2k-\ell)!} - \binom{\ell}{k}\frac{(2k)!}{(2k-\ell-2)!} - 2\binom{\ell}{k}\frac{(2k)!}{(2k-\ell-1)!}$$
$$+\ell(\ell+1)\binom{\ell}{k}\frac{(2k)!}{(2k-\ell)!}$$
$$= \binom{\ell}{k}\frac{(2k)!}{(2k-\ell)!}\Big(-2(\ell-k)(2k+1) - (2k-\ell-1)(2k-\ell)$$
$$- 2(2k-\ell) + \ell(\ell+1)\Big) = 0.$$

There is one more term: t^1 if ℓ is odd and t^0 if ℓ is even. We will leave the even case to the reader. If ℓ is odd, then the coefficient of t^1 is

$$\binom{\ell}{(\ell+3)/2}(-1)^{\frac{\ell+1}{2}}(\ell+3)! - 2\binom{\ell}{(\ell+1)/2}(-1)^{(\ell-1)/2}(\ell+1)!$$
$$+\ell(\ell+1)\binom{\ell}{(\ell+1)/2}(-1)^{(\ell-1)/2}(\ell+1)!$$
$$= \binom{\ell}{(\ell+1)/2}(\ell+1)!\,((\ell+2)(\ell+1) + 2 - \ell(\ell+1)) = 0.$$

The calculation for the case of even ℓ is similar. So we have shown that the Legendre polynomial $\mathbf{P}_{\ell,0}$ of degree ℓ satisfies the Legendre equation with $m = 0$.

Next we fix an integer m with $1 \le m \le \ell$ and show that $\mathbf{P}_{\ell,m}$ satisfies the Legendre equation (Equation A.1). Since the function $\mathbf{P}_{\ell,0}$ satisfies Equation A.2, we have

$$(1-t^2)\mathbf{P}''_{\ell,0}(t) - 2t\mathbf{P}'_{\ell,0}(t) + \ell(\ell+1)\mathbf{P}_{\ell,0}(t) = 0.$$

Differentiating m times with respect to t, we find that

$$\Big((1-t^2)\partial_t^{m+2} - 2(m+1)t\partial_t^{m+1} + \big(\ell(\ell+1) - m(m+1)\big)\partial_t^m\Big)\mathbf{P}_{\ell,0}(t) = 0. \quad (A.3)$$

Define $c := (-1)^m/(\ell!2^\ell)$. From Definition A.1 we know that $c\,\partial_t^m\mathbf{P}_{\ell,0}(t) = (1-t^2)^{(-\frac{m}{2})}\mathbf{P}_{\ell,m}(t)$. Differentiating this expression twice in a row we obtain

$$\begin{aligned} c\,\partial_t^{m+1}\mathbf{P}_{\ell,0}(t) &= (1-t^2)^{(-\frac{m}{2})}\Big(\frac{mt}{1-t^2}\mathbf{P}_{\ell,m}(t) + \mathbf{P}'_{\ell,m}(t)\Big)\\ c\,\partial_t^{m+2}\mathbf{P}_{\ell,0}(t) &= (1-t^2)^{(-\frac{m}{2})}\Big(\frac{m}{1-t^2} + \frac{(m+2)t^2}{(1-t^2)^2}\Big)\mathbf{P}_{\ell,m}(t)\\ &\quad + (1-t^2)^{(-\frac{m}{2})}\Big(\frac{2mt}{1-t^2}\mathbf{P}'_{\ell,m}(t) + \mathbf{P}''_{\ell,m}(t)\Big). \end{aligned}$$

Here we have used the fact (easily verified by induction) that for any sufficiently differentiable function $f(t)$ we have

$$\partial_t^m(1-t^2)f(t) = (1-t^2)\partial_t^m f + 2mt\partial_t^{m-1}f(t) + m(m-1)\partial_t^{m-2}f(t).$$

Plugging these expressions into Equation A.3, multiplying by $c(1-t^2)^{(m/2)}$ and simplifying we find that

$$0 = (1-t^2)\mathbf{P}''_{\ell,m}(t) - 2t\mathbf{P}'_{\ell,m}(t) + \left(\ell(\ell+1) - \frac{m}{1-t^2}\right)\mathbf{P}_{\ell,m}(t).$$

In other words, the function $\mathbf{P}_{\ell,m}$ satisfies the Legendre equation (Equation A.1).

□

It is natural to wonder whether there are any other solutions to Legendre's equation. Since the equation is linear (in P, P' and P''), there should be two solutions for each value of m^2. For $m^2 \neq 0$ there are indeed two solutions: $\mathbf{P}_{\ell,\pm m}$. The case $m^2 = 0$ is discussed in detail in Simmons' undergraduate text on ordinary differential equations [Sim, Sections 28, 29 and 44]. The point is that a solution corresponds to a continuous function on the sphere only if it is bounded near $t = \pm 1$ and only one of the solutions to the Legendre equation is bounded near $t = \pm 1$.

Now we are ready to define the spherical harmonic functions. In Section 1.6 we gave examples for $\ell = 0, 1, 2$; here is the general definition.

Definition A.2 *Let ℓ be a nonnegative integer and let m be an integer satisfying $-\ell \leq m \leq \ell$. Define the ℓ, m* spherical harmonic function $Y_{\ell,m} : [0, \pi] \oplus (-\pi, \pi] \to \mathbb{C}$ *by*

$$Y_{\ell,m}(\theta, \phi) := c_{\ell,m} \mathbf{P}_{\ell,|m|}(\cos\theta) e^{im\phi},$$

where the the constant $c_{\ell,m}$ takes the value

$$\sqrt{\frac{(\ell - m)!(2\ell + 1)}{(\ell + m)! 4\pi}}.$$

For each ℓ, linear combinations of the vectors

$$\left\{Y_{\ell,m} : m = -\ell, \ldots, \ell\right\}$$

are spherical harmonics of degree ℓ.

In fact, every spherical harmonic function is the restriction to the sphere of a harmonic polynomial on $\mathbb{R}^3$. Recall the vector space $\mathcal{Y}^\ell$ of S^2 in $\mathbb{R}^3$ of a harmonic polynomial on $\mathbb{R}^3$. Recall the vector space $\mathcal{Y}^\ell$ of restrictions of harmonic polynomials of degree ℓ in three variables to the sphere S^2 (Definition 2.6).

Proposition A.2 *Suppose ℓ is a nonnegative integer. Then the span of the set $\{Y_{\ell,-\ell}, \ldots, Y_{\ell,\ell}\}$ is $\mathcal{Y}^\ell$.*

Proof. First we will show that the set $\left\{Y_{\ell,m} : m = -\ell, \ldots, \ell\right\}$ is linearly independent. Next we will show it is a subset of $\mathcal{Y}^\ell$. The proof ends with a dimension count.

To show linear independence, consider an arbitrary linear combination equalling zero:

$$0 = \sum_{m=-\ell}^{\ell} C_m \mathbf{P}_{\ell,|m|}(\cos\theta) e^{im\phi}.$$

We must show that each $C_m = 0$. By Exercise 2.2, the set

$$\left\{e^{im(\cdot)} : m = -\ell, \ldots, \ell\right\},$$

where $e^{im(\cdot)}: [0,\pi] \to \mathbb{C}, x \to e^{imx}$, is linearly independent, so we can conclude that for each m we have $C_m \mathbf{P}_{\ell,m} = 0$. Hence we will be done with the proof of linear independence if we can show that for each m, the function $\mathbf{P}_{\ell,m}(\cos\theta)$ is not the zero function. Now $(-1)^m/\ell!2^\ell$ is a nonzero constant, and $(1-\cos^2(\pi/2))^{m/2} \neq 0$, so it suffices to show that $\partial_t^{\ell+m}(t^2-1)^\ell$ is not the zero polynomial. But $(t^2-1)^\ell$ is a polynomial of degree 2ℓ in t, so its first 2ℓ derivatives are nonzero. Since $m \le \ell$, it follows that $\mathbf{P}_{\ell,m}$ is not the zero function. We have shown the required linear independence.

A longer argument is required to show that $\{Y_{\ell,m}: m = -\ell, \ldots, \ell\} \subset \mathcal{Y}^\ell$. We begin by showing that for any nonnegative integer k the expression $\partial_t^k(t^2-1)^\ell$ is a polynomial in the variables $\alpha := 1-t^2$ and $\beta := t$. According to the chain rule for partial derivatives we have $\partial_t = 2\beta\partial_\alpha + \partial_\beta$, so applying ∂_t to any polynomial in α and β yields a polynomial in α and β. Consider $(t^2-1)^\ell = \alpha^\ell$, which is a polynomial in α and β. Hence, by induction on k, we can conclude that $\partial_t^k(t^2-1)^\ell$ is a polynomial in α and β.

Another induction on k shows that for any nonnegative integer k the expression $\partial_t^k(t^2-1)^\ell$ is a homogeneous polynomial of degree $2\ell - k$ in the variables $\sqrt{\alpha}$ and β. The key to the inductive step is that $(t^2-1)^\ell = \sqrt{\alpha}^{2\ell}$, a polynomial of degree 2ℓ, while applying $\partial_t = 2\beta\partial_\alpha + \partial_\beta$ lowers the degree (in $\sqrt{\alpha}$ and β) by one.

The point is that if $t = \cos\theta$, then we have

$$r^2\alpha = r^2(1-t^2) = r^2\sin^2\theta = x^2 + y^2$$
$$r\beta = r\cos\theta = z.$$

So a polynomial of degree d in $\sqrt{\alpha}$ and β that is also a polynomial in α will be homogeneous of degree d in x, y and z. Setting $k = \ell + m$ and applying the results of our inductions above, we find that

$$r^{\ell-m}\partial_t^{\ell+m}(t^2-1)^\ell$$

is a polynomial of degree $\ell - m$ in x, y, and z. Also,

$$r^m(1-t^2)^{m/2}e^{\pm im\phi} = r^m\sin^m\theta(\cos\phi \pm i\sin\phi)^m = (x \pm iy)^m,$$

which is a homogeneous polynomial in x and y of degree m when $m \ge 0$. Note that $\theta \in [0,\pi]$, so $\sin\theta \ge 0$. Hence the function

$$r^\ell(1-t^2)^{m/2}\partial_t^{\ell+m}(t^2-1)^\ell e^{im\phi}$$

is a polynomial of degree ℓ in x, y and z; by inspection, it is homogeneous. We know from Equation 1.12 and Proposition A.1 that if we evaluate this function at $t = \cos\theta$ we obtain a harmonic function. Restricting this homogeneous polynomial to the sphere we obtain $\mathbf{P}_{\ell,m}$. Hence $\mathbf{P}_{\ell,m} \in \mathcal{Y}^\ell$ for $m = 0, 1, \ldots, \ell$.

Next we show that the harmonic function from Equation 1.12 is a polynomial in x, y and z of degree ℓ even when $m < 0$. To see this, note that (by yet another induction, this time on $-m$ and left to the reader), for any nonnegative integer ℓ and any integer m with $-\ell \le m < 0$ there is a polynomial q of two variables such that $q(\alpha, \beta)$ has degree $\ell + m$ in $\sqrt{\alpha}$ and β and

$$\partial_t^{\ell+m}(t^2 - 1)^\ell = \alpha^{-m} q(\alpha, \beta).$$

Note that $r^{\ell+m} q(\alpha, \beta)$ is a polynomial of degree $\ell + m$ in x, y and z. Hence, for $m < 0$ we have

$$\begin{aligned} r^\ell (1 - t^2)^{m/2} \partial_t^{\ell+m}(t^2 - 1)^\ell e^{im\phi} &= r^\ell \alpha^{-m/2} (e^{-i\phi})^{-m} q(\alpha, \beta) \\ &= (x - iy)^{-m} r^{\ell+m} q(\alpha, \beta), \end{aligned}$$

which is a polynomial of degree $-m + \ell + m = \ell$ in x, y and z. This polynomial is clearly homogeneous, and by Equation 1.12 it is harmonic. Restricting this homogeneous polynomial to the sphere we obtain $\mathbf{P}_{\ell,m}$. Hence $\mathbf{P}_{\ell,m} \in \mathcal{Y}^\ell$ for $m = -\ell, \ldots, -1$. Thus we have shown that each function $\mathbf{P}_{\ell,m}$ is the restriction to the sphere S^2 of a harmonic polynomial of degree ℓ on $\mathbb{R}^3$. In other words, $\{Y_{\ell,m} : m = -\ell, \ldots, \ell\} \subset \mathcal{Y}^\ell$.

Finally, since the $Y_{\ell,m}$'s are linearly independent, they span a $(2\ell + 1)$-dimensional subset of $\mathcal{Y}^\ell$. But we know by Proposition 7.1 that $\mathcal{Y}^\ell$ has dimension at most $(2\ell + 1)$. Hence $\mathcal{Y}^\ell$ is equal to the span of the $Y_{\ell,m}$'s. □

The following proposition justifies the reliance on spherical harmonics in spherically symmetric problems involving the Laplacian. To state it succinctly, we introduce the vector space $C_2 \subset L^2(\mathbb{R}^3)$ of continuous functions whose first and second partial derivatives are all continuous.

Proposition A.3 *Suppose D is a differential operator of the form*

$$D = \nabla^2 + u(r),$$

where u is a real-valued function of r. Then the vector space

$$K := \left\{ f \in L^2(\mathbb{R}^3) : f \in C_2 \text{ and } Df = 0 \right\}$$

of solutions to the differential equation $Df = 0$ is spanned by solutions of the form $\alpha \otimes Y_{\ell,m}$, where $\alpha \in \mathcal{I}$, ℓ is a nonnegative integer and m is an integer such that $|m| \le \ell$.

The technical conditions on f are quite reasonable: if a physical situation has a discontinuity, we might look for solutions with discontinuities in the function f and its derivatives. In this case, we might have to consider, e.g., piecewise-defined combinations of smooth solutions to the differential equation. These solutions might not be linear combinations of spherical harmonics.

Proof. Let V denote the set of solutions in $L^2(\mathbb{R}^3)$ obtained by multiplying a spherical harmonic by a spherically symmetric function:

$$V := \left\{\alpha \otimes Y_{\ell,m} \in \mathcal{I} \otimes \mathcal{Y} \colon \alpha \in C_2 \text{ and } D(\alpha \otimes Y_{\ell,m}) = 0\right\}.$$

It suffices to show that $K \cap \left(V^{\perp}\right) = 0$. So suppose that $f \in K \cap \left(V^{\perp}\right)$, i.e., suppose that f and its first and second partial derivatives are continuous, that $Df = 0$ and that f is orthogonal to every solution obtained by separation of variables. We will show that $f = 0$.

By Fubini's Theorem (Theorem 3.1), the function $\|f\|_{S^2}$ defined by

$$\|f\|_{S^2} : r \mapsto \sqrt{\int_{S^2} |f(r,\theta,\phi)|^2 \, \sin\theta \, d\theta d\phi}$$

lies in $\mathcal{I}$ because $f \in L^2(\mathbb{R}^3)$. Now for any nonnegative integer ℓ and any integer m with $|m| \le \ell$, the function $Y_{\ell,m} f$ is measurable and

$$\int_{\mathbb{R}^3} \left|Y_{\ell,m}(\theta,\phi) f(r,\theta,\phi)\right|^2 r^2 \, dr \, \sin\theta \, d\theta d\phi < \infty$$

because $Y_{\ell,m}$ is bounded and $f \in L^2(\mathbb{R}^3)$. Again by Fubini's Theorem,

$$\alpha_{\ell,m}(r) := \int_{S^2} Y_{\ell,m}(\theta,\phi) f(r,\theta,\phi) \, \sin\theta \, d\theta d\phi = \left\langle Y_{\ell,m}, f(r,\cdot,\cdot)\right\rangle_{S^2}$$

defines a measurable function $\alpha_{\ell,m}$ on $\mathbb{R}^{\ge 0}$. Note that by the Schwarz Inequality (Proposition 3.6) on $L^2(S^2)$ we have

$$\left|\alpha_{\ell,m}\right|^2 = \left|\int_{S^2} Y_{\ell,m}(\theta,\phi) f(\cdot,\theta,\phi) \sin\theta \, d\theta d\phi\right|^2 \le \left\|Y_{\ell,m}\right\|_{S^2}^2 \|f\|_{S^2}^2.$$

Since $\left\|Y_{\ell,m}\right\|^2$ does not depend on r and $\|f\|_{S^2} \in \mathcal{I}$, it follows that $\alpha_{\ell,m} \in \mathcal{I}$.

Next we introduce some convenient notation. By Exercise 1.12 we know that $\nabla^2 = \nabla_r^2 + \nabla_{\theta,\phi}^2$, where we set

$$\nabla_r^2 := \partial_r^2 + \frac{2}{r}\partial_r$$
$$\nabla_{\theta,\phi}^2 := \frac{1}{r^2}\partial_\theta^2 + \frac{\cos\theta}{r^2\sin\theta}\partial_\theta + \frac{1}{r^2\sin^2\theta}\partial_\phi^2.$$

Note that $\nabla^2_{\theta,\phi}$ is Hermitian-symmetric on $L^2(S^2)$ by Exercise 3.26. Since $Df = 0$ we have $(\nabla_r^2 + u)f = -\nabla^2_{\theta,\phi} f$. Hence for $r \in (0, \infty)$ we have

$$\begin{aligned}(\nabla_r^2 + u)\alpha_{\ell,m}(r) &= \left\langle Y_{\ell,m}, (\nabla_r^2 + u) f(r, \cdot, \cdot)\right\rangle_{S^2} \\ &= -\left\langle Y_{\ell,m}, \nabla^2_{\theta,\phi} f(r, \cdot, \cdot)\right\rangle_{S^2} \\ &= -\left\langle \nabla^2_{\theta,\phi} Y_{\ell,m}, f(r, \cdot, \cdot)\right\rangle \\ &= \ell(\ell+1)\left\langle Y_{\ell,m}, f(r, \cdot, \cdot)\right\rangle \\ &= \ell(\ell+1)\alpha_{\ell,m}(r).\end{aligned}$$

Here the first equality follows from the fact that $f \in C_2$. The technical continuity condition on f and its first and second partial derivatives allows us to exchange the derivative and the integral sign (disguised as a complex scalar product). See, for example, [Bart, Theorem 31.7]. The third equality follows from the Hermitian symmetry of $\nabla^2_{\theta,\phi}$. It follows that $\alpha_{\ell,m} Y_{\ell,m}$ is an element of the kernel of $D = \nabla^2 + u$, as we can verify:

$$\begin{aligned}(\nabla^2 + u)\alpha_{\ell,m}(r) Y_{\ell,m}(\theta, \phi) &= \left((\nabla_r^2 + u)\alpha_{\ell,m}(r)\right) Y_{\ell,m}(\theta, \phi) \\ &\qquad + \alpha_{\ell,m}(r)\nabla^2_{\theta,\phi} Y_{\ell,m}(\theta, \phi) \\ &= \ell(\ell+1)\alpha_{\ell,m}(r) Y_{\ell,m}(\theta, \phi) \\ &\qquad - \alpha_{\ell,m}(r)\ell(\ell+1) Y_{\ell,m}(\theta, \phi) \\ &= 0.\end{aligned}$$

Hence $\alpha_{\ell,m} \otimes Y_{\ell,m} \in V$. Next we examine the norm of $\alpha_{\ell,m} = 0$ and recall that $f \in V^{\perp}$ by hypothesis:

$$\begin{aligned}\left\|\alpha_{\ell,m}\right\|^2_{\mathcal{I}} = \left\langle \alpha_{\ell,m}, \langle Y_{\ell,m}, f\rangle_{S^2}\right\rangle &= \int_0^\infty \int_{S^2} \alpha^*_{\ell,m} Y^*_{\ell,m} f \\ &= \left\langle \alpha_{\ell,m} Y_{\ell,m}, f\right\rangle_{\mathbb{R}^3} \\ &= 0.\end{aligned}$$

Hence $\alpha_{\ell,m} = 0$. But this implies that for any $h \otimes Y \in (\mathcal{I} \otimes \mathcal{Y})$ we have

$$\langle h \otimes Y, f\rangle_{\mathbb{R}^3} = \int_0^\infty \langle Y, f(r, \cdot, \cdot)\rangle_{S^2}\, r^2\, dr = \left\langle h, \alpha_{\ell,m}\right\rangle_{\mathbb{R}^{\geq 0}} = 0.$$

But, by Proposition 7.5, $\mathcal{I} \otimes \mathcal{Y}$ spans $L^2(\mathbb{R}^3)$. Hence $f = 0$. □

Note that the application of Fubini's Theorem here mirrors the argument in Proposition 7.7. Also note that this proposition could easily be generalized to differential operators of the form

$$\nabla^2 + \mathcal{O},$$

where $\mathcal{O}$ is a differential operator depending only on r. One would need appropriate technical hypotheses on f. Specifically, if we let n denote the minimum of 2 and the order of the differential operator $\mathcal{O}$, then f and all its partial derivatives up to the nth order would have to be continuous.