The Spherical Harmonics

1. Solution to Laplace's equation in spherical coordinates

In spherical coordinates, the Laplacian is given by

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

We shall solve Laplace's equation,

$$\vec{\boldsymbol{\nabla}}^{\mathbf{2}} T(r,\theta,\phi) = 0\,, \tag{2}$$

using the method of separation of variables, by writing

$$T(r,\theta,\phi) = R(r)\Theta(\theta)\Phi(\phi)\,.$$

Inserting this decomposition into the Laplace equation and multiplying through by $r^2/R\Theta\Phi$ yields

$$\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \frac{1}{\Theta}\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) + \frac{1}{\Phi}\frac{1}{\sin^2\theta}\frac{d^2\Phi}{d\phi^2} = 0\,.$$

Hence,

$$\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2} = -\frac{\sin^2\theta}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) - \frac{\sin\theta}{\Theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) = -m^2\,, \tag{3}$$

where $-m^2$ is the separation constant, which is chosen negative so that the solutions for $\Phi(\phi)$ are periodic in ϕ,

$$\Phi(\phi) = \begin{cases} e^{im\phi} \\ e^{-im\phi} \end{cases} \qquad \text{for } m = 0, 1, 2, 3, \ldots .$$

Note that m must be an integer since ϕ is a periodic variable and $\Phi(\phi+2\pi) = \Phi(\phi)$. In the case of $m=0$, the general solution is $\Phi(\phi) = a\phi + b$, but we must choose $a=0$ to be consistent with $\Phi(\phi+2\pi) = \Phi(\phi)$. Hence in the case of $m=0$, only one solution is allowed.

One can now recast eq. (3) in the following form,

$$\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) = -\frac{1}{\Theta}\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\,\frac{d\Theta}{d\theta}\right) + \frac{m^2}{\sin^2\theta} = \ell(\ell+1)\,, \tag{4}$$

where the separation variable at this step is denoted by $\ell(\ell+1)$ for reasons that will shortly become clear. The resulting radial equation,

$$r^2\frac{d^2R}{dr^2} + 2r\frac{dR}{dr} - \ell(\ell+1)R = 0\,, \tag{5}$$

is recognized to be an Euler equation. This means that the solution is of the form $R = r^s$. To determine the exponent s, we insert this solution back into eq. (5). The end result is

$$s(s+1) = \ell(\ell+1) \qquad \Longrightarrow \qquad s = \ell \;\text{ or }\; s = -\ell - 1\,.$$

That is,

$$R(r) = \begin{cases} r^{\ell} \\ r^{-\ell-1} \end{cases}$$

Eq. (4) also yields

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

Changing variables to $x = \cos\theta$ and $y = \Theta(\theta)$, the above differential equation reduces to

$$(1-x^2)\frac{d^2y}{dx^2} - 2x\frac{dy}{dx} + \left[\ell(\ell+1) - \frac{m^2}{\sin^2\theta}\right]y = 0\,. \tag{6}$$

This is the differential equation for associated Legendre polynomials,

$$y(x) = P_\ell^m(x)\,, \qquad \text{for } \ell = 0, 1, 2, 3, \ldots \text{ and } m = -\ell, -\ell+1, \ldots, \ell-1, \ell\,.$$

The restrictions of ℓ and $|m|$ to non-negative integers with $|m| \leq \ell$ is a consequence of the requirement that $P_\ell^m(x)$ should be non-singular at $\cos\theta = \pm 1$. On p. 583, Boas gives the following result in eq. (10.6),

$$P_\ell^m(x) = \frac{1}{2^\ell\,\ell!}\,(1-x^2)^{m/2}\frac{d^{\,\ell+m}}{dx^{\,\ell+m}}\left(x^2-1\right)^\ell\,, \qquad \text{for } m = -\ell, -\ell+1, \ldots, \ell-1, \ell\,. \tag{7}$$

The differential equation for the associated Legendre polynomials, given in eq. (6), depends on m^2 and is therefore not sensitive to the sign of m. Consequently, $P_\ell^m(x)$ and $P_\ell^{-m}(x)$ must be equivalent solutions and hence proportional to each other. Using eq. (7), it is straightforward to prove that

$$P_\ell^{-m}(\cos\theta) = (-1)^m\frac{(\ell-m)!}{(\ell+m)!}\,P_\ell^m(\cos\theta)\,. \tag{8}$$

Combining all the results obtained above, we have found that the general solution to Laplace's equation is of the form

$$T(r,\theta,\phi) = \begin{Bmatrix} r^\ell \\ r^{-\ell-1} \end{Bmatrix} P_\ell^m(\cos\theta) \begin{Bmatrix} e^{im\phi} \\ e^{-im\phi} \end{Bmatrix}\,.$$

where $\ell = 0, 1, 2, 3, \ldots$ and $m = -\ell, -\ell+1, \ldots, \ell-1, \ell$.

2. The spherical harmonics

In obtaining the solutions to Laplace's equation in spherical coordinates, it is traditional to introduce the spherical harmonics, $Y_\ell^m(\theta,\phi)$,

$$Y_\ell^m(\theta,\phi) = (-1)^m \sqrt{\frac{(2\ell+1)}{4\pi}\,\frac{(\ell-m)!}{(\ell+m)!}}\; P_\ell^m(\cos\theta)\, e^{im\phi}\,, \qquad \text{for } \begin{cases} \ell = 0,1,2,3,\ldots\,, \\ m = -\ell, -\ell+1, \ldots, \ell-1, \ell\,. \end{cases} \tag{9}$$

The phase factor $(-1)^m$, introduced originally by Condon and Shortley, is convenient for applications in quantum mechanics. Note that eq. (8) implies that

$$Y_\ell^{-m}(\theta,\phi) = (-1)^m Y_\ell^m(\theta,\phi)^*\,, \tag{10}$$

where the star means complex conjugation. The normalization factor in eq. (9) has been chosen such that the spherical harmonics are normalized to one. In particular, these functions are orthonormal and complete. The orthonormality relation is given by:

$$\int Y_\ell^m(\theta,\phi)\, Y_{\ell'}^{m'}(\theta,\phi)\, d\Omega = \delta_{\ell\ell'}\,\delta_{mm'}\,, \tag{11}$$

where $d\Omega = \sin\theta\, d\theta\, d\phi$ is the differential solid angle in spherical coordinates. The completeness of the spherical harmonics means that these functions are linearly independent and there does not exist any function of θ and ϕ that is orthogonal to all the $Y_\ell^m(\theta,\phi)$ where ℓ and m range over all possible values as indicated above. The completeness property of the spherical harmonics implies that any well-behaved function of θ and ϕ can be written as

$$f(\theta,\phi) = \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell} a_{\ell m} Y_\ell^m(\theta,\phi)\,. \tag{12}$$

for some choice of coefficients $a_{\ell m}$. For convenience, we list the spherical harmonics for $\ell = 0,1,2$ and non-negative values of m.

$$\ell = 0\,, \qquad Y_0^0(\theta,\phi) = \frac{1}{\sqrt{4\pi}}$$

$$\ell = 1\,, \qquad \begin{cases} Y_1^1(\theta,\phi) = -\sqrt{\dfrac{3}{8\pi}}\sin\theta e^{i\phi} \\[2ex] Y_1^0(\theta,\phi) = \sqrt{\dfrac{3}{4\pi}}\cos\theta \end{cases}$$

$$\ell = 2\,, \qquad \begin{cases} Y_2^2(\theta,\phi) = \dfrac{1}{4}\sqrt{\dfrac{15}{2\pi}}\sin^2\theta e^{2i\phi} \\[2ex] Y_2^1(\theta,\phi) = -\sqrt{\dfrac{15}{8\pi}}\sin\theta\cos\theta e^{i\phi} \\[2ex] Y_2^0(\theta,\phi) = \dfrac{1}{2}\sqrt{\dfrac{5}{4\pi}}(3\cos^2\theta - 1) \end{cases}$$

The corresponding spherical harmonics for negative values of m are obtained using eq. (10).

In addition, eq. (9) yields the following useful relation,

$$Y_\ell^0(\theta,\phi) = \sqrt{\frac{2\ell+1}{4\pi}}\, P_\ell(\cos\theta)\,, \qquad \text{for } \ell = 0,1,2,3,\ldots, \tag{13}$$

which relates the Legendre polynomials to the spherical harmonics with $m = 0$.

In terms of the spherical harmonics, the general solution to Laplace's equation can be written as:

$$T(r,\theta,\phi) = \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell} (a_{\ell m} r^\ell + b_{\ell m} r^{-\ell-1}) Y_\ell^m(\theta,\phi)\,.$$

In particular,

$$\vec{\boldsymbol{\nabla}}^{\mathbf{2}}\left[(a_{\ell m} r^\ell + b_{\ell m} r^{-\ell-1}) Y_\ell^m(\theta,\phi)\right] = 0\,.$$

Making use of eq. (1) for the Laplacian and using

$$\left[\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)\right] f(r) = \ell(\ell+1) f(r)\,, \qquad \text{for } f(r) = ar^\ell + br^{-\ell-1}\,,$$

it follows from eq. (2) that[1]

$$-r^2\vec{\boldsymbol{\nabla}}^{\mathbf{2}} Y_\ell^m(\theta,\phi) = \ell(\ell+1) Y_\ell^m(\theta,\phi)\,. \tag{15}$$

3. The Laplace series

As noted in the previous section, the completeness property of the spherical harmonics implies that any well-behaved function of θ and ϕ can be written as

$$f(\theta,\phi) = \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell} a_{\ell m} Y_\ell^m(\theta,\phi)\,. \tag{16}$$

[1]Indeed, eq. (1) can be written as

$$\vec{\boldsymbol{\nabla}}^{\mathbf{2}} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{\vec{\boldsymbol{L}}^{\mathbf{2}}}{r^2}\,, \tag{14}$$

where $\vec{\boldsymbol{L}}^{\mathbf{2}}$ is the differential operator,

$$\vec{\boldsymbol{L}}^{\mathbf{2}} \equiv -\frac{1}{\sin^2\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) - \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\,,$$

which depends only on the angular variables θ and ϕ. Then, eqs. (14) and (15) imply that:

$$\vec{\boldsymbol{L}}^{\mathbf{2}} Y_\ell^m(\theta,\phi) = \ell(\ell+1) Y_\ell^m(\theta,\phi)\,.$$

That is, the spherical harmonics are eigenfunctions of the differential operator $\vec{\boldsymbol{L}}^{\mathbf{2}}$, with corresponding eigenvalues $\ell(\ell+1)$, for $\ell = 0,1,2,3,\ldots$.

The coefficients $a_{\ell m}$ can be determined from eq. (11). Namely, multiply both sides of eq. (16) by $Y_{\ell'}^{m'}(\theta,\phi)^*$ and then integrate over all solid angles. Using eq. (11), the right hand side of eq. (16) becomes

$$\sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell} a_{\ell m}\delta_{\ell\ell'}\delta_{mm'} = a_{\ell'm'}\,.$$

Dropping the primes, we conclude that

$$a_{\ell m} = \int f(\theta,\phi)Y_\ell^m(\theta,\phi)^* d\Omega\,. \tag{17}$$

Two special cases are notable. First, suppose that the function $f(\theta,\phi)$ is independent of ϕ. In this case, we write $f(\theta,\phi)=f(\theta)$ and eq. (17) yields

$$a_{\ell m} = N_{\ell m}\int_0^{2\pi} e^{-im\phi}d\phi \int_{-1}^{1} f(\theta)P_\ell^m(\cos\theta)d\cos\theta\,,$$

where we have written $Y_\ell^m(\theta,\phi) = N_{\ell m}P_\ell^m(\cos\theta)e^{im\phi}$, where $N_{\ell m}$ is the normalization constant exhibited in eq. (9). However, the integral over ϕ is straightforward,

$$\int_0^{2\pi} e^{-im\phi}d\phi = 2\pi\delta_{m0}\,,$$

where the Kronecker delta indicates that the above integral is nonzero only when $m=0$. Using eq. (13), we end up with

$$a_{\ell 0} = \sqrt{\pi(2\ell+1)}\int_{-1}^{1} f(\theta)P_\ell(\cos\theta)d\cos\theta\,.$$

This means that the Laplace series reduces to a sum over Legendre polynomials,

$$f(\theta) = \sum_{\ell=0}^{\infty} c_\ell P_\ell(\cos\theta)\,, \qquad \text{where } c_\ell = \frac{2\ell+1}{2}\int_{-1}^{1} f(\theta)P_\ell(\cos\theta)d\cos\theta\,.$$

The coefficients c_ℓ are related to the $a_{\ell 0}$ by

$$c_\ell = a_{\ell 0}\sqrt{\frac{2\ell+1}{4\pi}}\,.$$

That is, for problems with azimuthal symmetry, the Laplace series reduces to a sum over Legendre polynomials.

The second special case of interest is one in which $f(\theta,\phi)$ satisfies

$$-r^2\vec{\boldsymbol{\nabla}}^{\mathbf{2}} f(\theta,\phi) = \ell(\ell+1)f(\theta,\phi)\,. \tag{18}$$

In this case, we can conclude that

$$f(\theta,\phi) = \sum_{m=-\ell}^{\ell} b_m Y_\ell^m(\theta,\phi)\,. \tag{19}$$

The proof is simple. First, we expand $f(\theta,\phi)$ in a Laplace series,

$$f(\theta,\phi)=\sum_{\ell'=0}^{\infty}\sum_{m'=-\ell'}^{\ell'} a_{\ell' m'} Y_{\ell'}^{m'}(\theta,\phi)\,. \tag{20}$$

If we operate on both sides of the above equation with the Laplacian and use eqs. (14) and (18), then it follows that:

$$\sum_{\ell'=0}^{\infty}\sum_{m'=-\ell'}^{\ell'}\left[\ell(\ell+1)-\ell'(\ell'+1)\right] a_{\ell' m'} Y_{\ell'}^{m'}(\theta,\phi)=0\,.$$

Since the spherical harmonics are linearly independent (and complete), the overall coefficient of $Y_{\ell'}^{m'}(\theta,\phi)$ in the above equation must vanish for any choice of ℓ' and m'. Thus, for $\ell'\neq\ell$ we conclude that

$$a_{\ell' m'}=0\,,\qquad \text{for } \ell'\neq\ell \;\text{ and }\; m'=-\ell',-\ell'+1,\ldots,\ell'-1,\ell'\,.$$

Inserting this result into eq. (20), only the term $\ell'=\ell$ survives in the sum over ℓ', and we end up with

$$f(\theta,\phi)=\sum_{m'=-\ell}^{\ell} a_{\ell m'} Y_{\ell}^{m'}(\theta,\phi)\,.$$

Dropping the primes on m and identifying $a_{\ell m}\equiv b_m$, we end up with eq. (19), as was to be proven.

4. The addition formula for the spherical harmonics

Suppose we have two vectors

$$\vec{\boldsymbol{r}}=(r,\theta,\phi)\,,\qquad \vec{\boldsymbol{r}}\,'=(r',\theta',\phi')\,,$$

which are designated by their spherical coordinates, as shown in Figure 1 below.
The angle between these two vectors, denoted by γ, is easily computed. Noting that the unit vectors are given by

$$\hat{\boldsymbol{r}}=\hat{\boldsymbol{\imath}}\sin\theta\cos\phi+\hat{\boldsymbol{\jmath}}\sin\theta\sin\phi+\hat{\boldsymbol{k}}\cos\theta\,,$$

and similarly for $\hat{\boldsymbol{r}}\,'$, it follows that

$$\cos\gamma=\hat{\boldsymbol{r}}\cdot\hat{\boldsymbol{r}}\,'=\cos\theta\cos\theta'+\sin\theta\sin\theta'\cos(\phi-\phi')\,. \tag{21}$$

The addition theorem for the spherical harmonics is

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

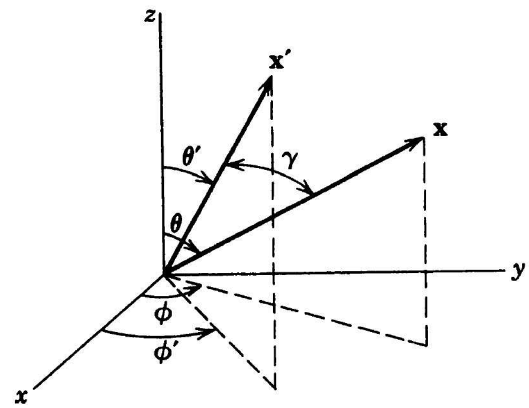

Figure 1: The two vectors $\vec{\boldsymbol{r}}$ and $\vec{\boldsymbol{r}}'$ are denoted in this figure by $\mathbf{x}$ and $\mathbf{x}'$, respectively. The angle between the two vectors is denoted by γ.

Note that if one sets $\ell = 1$ in the addition theorem and employs $P_1(\cos\gamma) = \cos\gamma$, then the result coincides with eq. (21) (check this!). That is, the addition theorem generalizes the geometric relation exhibited by eq. (21).

To prove the addition theorem, we first note that

$$-r^2\vec{\boldsymbol{\nabla}}^{\mathbf{2}} P_\ell(\cos\gamma) = \ell(\ell+1)P_\ell(\cos\gamma)\,. \tag{22}$$

This result is justified by considering a coordinate system in which the z-axis is aligned along $\vec{\boldsymbol{r}}'$. In this coordinate system, γ is the polar angle of the vector $\vec{\boldsymbol{r}}$. Noting that

$$P_\ell(\cos\gamma) = \sqrt{\frac{4\pi}{2\ell+1}}\,Y_\ell^0(\gamma,\beta)\,,$$

where β is the corresponding azimuthal angle in the new coordinate system, it then follows that eq. (22) is a consequence of eq. (15). However, $\vec{\boldsymbol{\nabla}}^{\mathbf{2}}$ is a scalar operator which is invariant with respect to rigid rotations of the coordinate system. The length r is also invariant with respect to rotations. Thus, eq. (22) must be true in the original coordinate system as well!

By virtue of eq. (21), $P_\ell(\cos\gamma)$ can be viewed as a function of θ and ϕ (where θ' and ϕ' are held fixed). Thus, we can expand this function in a Laplace series,

$$P_\ell(\cos\gamma) = \sum_{m=-\ell}^{\ell} b_m(\theta',\phi')Y_\ell^m(\theta,\phi)\,, \tag{23}$$

where the coefficients b_m depend on the fixed parameters θ' and ϕ'. Note that this Laplace series is of the form given by eq. (19) as a result of eq. (22). We solve for the coefficients b_m in the usual way,

$$b_m(\theta',\phi') = \int P_\ell(\cos\gamma)Y_\ell^m(\theta,\phi)^* d\Omega\,. \tag{24}$$

Using eq. (21), we must evaluate

$$b_m(\theta',\phi') = \int P_\ell(\cos\theta\cos\theta' + \sin\theta\sin\theta'\cos(\phi-\phi'))Y_\ell^m(\theta,\phi)^* d\Omega\,,$$

which is difficult to compute directly. Instead, we will deduce the value of $b_m(\theta', \phi')$ with a clever indirect approach that avoids a messy calculation of a difficult integral.

In the coordinate system in which the z-axis lies along $\vec{\boldsymbol{r}}'$, the vector $\vec{\boldsymbol{r}}$ has polar angle γ and azimuthal angle β. The angles θ and ϕ are functions of the angles γ and β so we can write the following Laplace series,

$$Y_{\ell m}(\theta, \phi)^* = \sum_{m'=-\ell}^{\ell} B_{mm'} Y_{\ell m'}(\gamma, \beta)\,, \tag{25}$$

where we have been careful to choose a new dummy index m' to avoid confusion with the fixed index m. The coefficients $B_{mm'}$ can be determined as usual,

$$B_{mm'} = \int Y_{\ell m}(\theta, \phi)^* Y_{\ell m'}(\gamma, \beta)^* d\Omega_\gamma\,,$$

where $d\Omega_\gamma$ indicates the differential solid angle in the new coordinate system. In particular, setting $m' = 0$ and using eq. (13) yields

$$B_{m0} = \int Y_{\ell m}(\theta, \phi)^* Y_{\ell 0}(\gamma, \beta)^* d\Omega_\gamma = \sqrt{\frac{2\ell+1}{4\pi}} \int Y_{\ell m}(\theta, \phi)^* P_\ell(\cos\gamma) d\Omega_\gamma\,.$$

However,

$$d\Omega_\gamma = d\Omega\,, \tag{26}$$

since a rigid rotation of the coordinate system leaves the infinitesimal solid angle element invariant.[2] Hence,

$$B_{m0} = \sqrt{\frac{2\ell+1}{4\pi}} \int P_\ell(\cos\gamma) Y_{\ell m}(\theta, \phi)^* d\Omega = \sqrt{\frac{2\ell+1}{4\pi}} b_m(\theta', \phi')\,, \tag{27}$$

where the last identification is a consequence of eq. (24). However, we can also determine B_{m0} directly from eq. (25) by taking the $\gamma \to 0$ limit. Note that[3]

$$Y_{\ell m}(0, \beta) = N_{\ell m} P_\ell^m(1) e^{im\phi} = \delta_{m0} N_{\ell 0} = \delta_{m0}\sqrt{\frac{2\ell+1}{4\pi}}\,,$$

where $N_{\ell m}$ is the normalization factor in eq. (9). Hence, in the $\gamma \to 0$ limit, only the $m' = 0$ term of the sum in eq. (25) survives, and we are left with

$$\lim_{\gamma\to 0} Y_{\ell m}(\theta, \phi)^* = B_{m0}\sqrt{\frac{2\ell+1}{4\pi}}\,.$$

However, in the limit where $\gamma \to 0$, the vectors $\vec{\boldsymbol{r}}$ and $\vec{\boldsymbol{r}}'$ coincide, in which case $\theta \to \theta'$ and $\phi \to \phi'$. Thus, we conclude that

$$Y_{\ell m}(\theta', \phi')^* = \sqrt{\frac{2\ell+1}{4\pi}} B_{m0}\,.$$

[2]Note that $r^2 d\Omega$ is the infinitesimal surface area on a sphere of radius r subtended by the infinitesimal solid angle $d\Omega$. Clearly, the area of this infinitesimal surface is unchanged by a rigid rotation.

[3]One can quickly check that $P_\ell^m(1) = 0$ unless $m = 0$, in which case we can write $P_\ell^m(1) = \delta_{m0}$.

Finally, substituting for B_{m0} using eq. (27), we arrive at

$$b_m(\theta',\phi') = \frac{4\pi}{2\ell+1} Y_{\ell m}(\theta',\phi')^* \,.$$

Inserting this result back into eq. (23) yields the addition theorem,

$$P_\ell(\cos\gamma) = \frac{4\pi}{2\ell+1}\sum_{m=-\ell}^{\ell} Y_\ell^m(\theta,\phi) Y_\ell^m(\theta',\phi')^* \,. \tag{28}$$

5. An application of the addition formula for the spherical harmonics

The inverse distance between two vectors arises often in physics,

$$\frac{1}{|\vec{\boldsymbol{r}} - \vec{\boldsymbol{r}}'|} = \frac{1}{\sqrt{r^2 + r'^2 - 2rr'\cos\gamma}}\,, \tag{29}$$

where $r \equiv |\vec{\boldsymbol{r}}|$ and $r' \equiv \vec{\boldsymbol{r}}'$. In the case of $r' < r$,

$$\frac{1}{|\vec{\boldsymbol{r}} - \vec{\boldsymbol{r}}'|} = \frac{1}{r}\left(1 + \frac{r'^2}{r^2} - \frac{2r'}{r}\cos\gamma\right)^{-1/2} = \frac{1}{r}\sum_{\ell=0}^{\infty}\left(\frac{r'}{r}\right)^{\ell} P_\ell(\cos\gamma)\,, \tag{30}$$

where we made use of the generating function of the Legendre polynomials at the last step. In the case of $r' > r$, it is sufficient to interchange r and r' in eq. (30) to obtain the correct result. It is convenient to introduce the notation where $r_<$ is lesser of the two quantities r and r', and $r_>$ is the greater of the two quantities r and r'. In equations,

$$r_< = \min\{r\,,\,r'\}\,, \qquad r_> = \max\{r\,,\,r'\}\,.$$

Using this notation,

$$\frac{1}{|\vec{\boldsymbol{r}} - \vec{\boldsymbol{r}}'|} = \frac{1}{r_>}\sum_{\ell=0}^{\infty}\left(\frac{r_<}{r_>}\right)^{\ell} P_\ell(\cos\gamma)\,, \tag{31}$$

which is convergent for all $r \neq r'$.[4]

We now invoke the addition theorem of the spherical harmonics by inserting eq. (28) for $P_\ell(\cos\gamma)$ into eq. (31). The end result is the following expansion for the inverse distance between two vectors,

$$\boxed{\frac{1}{|\vec{\boldsymbol{r}} - \vec{\boldsymbol{r}}'|} = 4\pi\sum_{\ell=0}^{\infty}\frac{1}{2\ell+1}\frac{r_<^{\ell}}{r_>^{\ell+1}}\sum_{m=-\ell}^{\ell} Y_\ell^m(\theta,\phi) Y_\ell^m(\theta',\phi')^*} \tag{32}$$

[4]In the case of $r = r'$, we have $\vec{\boldsymbol{r}} = r\hat{\boldsymbol{r}}$ and $\vec{\boldsymbol{r}}' = r\hat{\boldsymbol{r}}'$. In this case, eq. (31) naively yields

$$\frac{1}{|\hat{\boldsymbol{r}} - \hat{\boldsymbol{r}}'|} = \frac{1}{2|\sin\left(\frac{1}{2}\gamma\right)|} = \sum_{\ell=0}^{\infty} P_\ell(\cos\gamma)\,,$$

after using $1 - \cos\gamma = 2\sin^2\left(\frac{1}{2}\gamma\right)$. Unfortunately, the infinite sum over Legendre polynomials is not convergent in the usual sense. Nevertheless, it is common practice to *define* the sum by taking the limit of eq. (31) as $r' \to r$, in which case $\sum_{\ell=0}^{\infty} P_\ell(\cos\gamma)$ is assigned the value $\{2|\sin(\frac{1}{2}\gamma)|\}^{-1}$.

Although eq. (32) looks quite complicated, it can be very useful in evaluating certain integrals. As a simple example, consider

$$\int \frac{d\Omega}{|\vec{\boldsymbol{r}} - \vec{\boldsymbol{r}}\,'|}\,. \tag{33}$$

One could try to integrate this directly by using eqs. (21) and (29),

$$\int_0^{2\pi} d\phi \int_{-1}^{1} d\cos\theta \frac{1}{\sqrt{r^2 + r'^2 - 2rr'\left[\cos\theta\cos\theta' + \sin\theta\sin\theta'\cos(\phi-\phi')\right]}}\,.$$

Actually, it is easier to first fix the coordinate system such that $\vec{\boldsymbol{r}}\,'$ lies along the z-axis. Then it is permissible to set $\theta' = \phi' = 0$ without loss of generality and evaluate:

$$\int_0^{2\pi} d\phi \int_{-1}^{1} \frac{d\cos\theta}{\sqrt{r^2 + r'^2 - 2rr'\cos\theta}}\,.$$

Changing variables to $x = r^2 + r'^2 - 2rr'\cos\theta$, the resulting integrals are elementary,

$$\int \frac{d\Omega}{|\vec{\boldsymbol{r}} - \vec{\boldsymbol{r}}\,'|} = \frac{\pi}{rr'}\int_{(r-r')^2}^{(r+r')^2} \frac{dx}{\sqrt{x}} = \frac{2\pi}{rr'}\left(r + r' - |r - r'|\right) = \begin{cases} \dfrac{4\pi}{r}\,, & \text{if } r > r'\,, \\[2ex] \dfrac{4\pi}{r'}\,, & \text{if } r < r'\,. \end{cases} \tag{34}$$

Employing eq. (32) provides an even simpler technique for evaluating eq. (33),

$$\int \frac{d\Omega}{|\vec{\boldsymbol{r}} - \vec{\boldsymbol{r}}\,'|} = 4\pi \sum_{\ell=0}^{\infty} \frac{1}{2\ell+1}\frac{r_<^\ell}{r_>^{\ell+1}} \sum_{m=-\ell}^{\ell} Y_\ell^m(\theta',\phi')^* \int Y_\ell^m(\theta,\phi)d\Omega\,. \tag{35}$$

The integration over the solid angles can be done by inspection by noting that

$$\sqrt{4\pi}\, Y_0^0(\theta,\phi)^* = 1\,.$$

Consequently, the integral over solid angles in eq. (35) can be written as:

$$\int Y_\ell^m(\theta,\phi)d\Omega = \sqrt{4\pi}\int Y_\ell^m(\theta,\phi)Y_0^0(\theta,\phi)^* d\Omega = \sqrt{4\pi}\,\delta_{\ell 0}\delta_{m0}\,,$$

after employing the orthonormality relations given in eq. (11). Inserting this result back into eq. (35), we see that only the $\ell = m = 0$ term of the sum survives. Hence, the end result is

$$\int \frac{d\Omega}{|\vec{\boldsymbol{r}} - \vec{\boldsymbol{r}}\,'|} = \frac{4\pi}{r_>}\sqrt{4\pi}\,Y_0^0(\theta',\phi')^* = \frac{4\pi}{r_>} = \begin{cases} \dfrac{4\pi}{r}\,, & \text{if } r > r'\,, \\[2ex] \dfrac{4\pi}{r'}\,, & \text{if } r < r'\,, \end{cases}$$

which reproduces in a very simple way the result of eq. (34).

APPENDICES

A. Alternate proof of the addition theorem

In this Appendix, I shall provide an alternative proof of the addition theorem, which differs somewhat from the one presented in Section 4 of these notes.[5] Our starting point is eq. (23), reproduced below,

$$P_\ell(\cos\gamma) = \sum_{m=-\ell}^{\ell} b_m(\theta',\phi') Y_\ell^m(\theta,\phi)\,, \tag{36}$$

where the coefficients b_m depend on the fixed parameters θ' and ϕ'. In obtaining eq. (36) $P_\ell(\cos\gamma)$ is viewed as a function of θ and ϕ (where θ' and ϕ' are held fixed). However, one can also view $P_\ell(\cos\gamma)$ as a function of θ' and ϕ' (where θ and ϕ are held fixed). Thus, it must be possible to write:

$$P_\ell(\cos\gamma) = \sum_{m=-\ell}^{\ell}\sum_{m'=-\ell}^{\ell} b_{mm'} Y_\ell^m(\theta,\phi) Y_\ell^{m'}(\theta',\phi')\,,$$

where the coefficients $b_{mm'}$ are independent of θ and ϕ. Since $P_\ell(\cos\gamma)$ depends on the azimuthal angles only via the combination $\phi-\phi'$ [cf. eq. (21)], it follows that the only possible terms that can survive in eq. (37) are $m'=-m$.[6] After using eq. (10), one finds that

$$P_\ell(\cos\gamma) = \sum_{m=-\ell}^{\ell} c_m Y_\ell^m(\theta,\phi) Y_\ell^m(\theta',\phi')^*\,, \tag{38}$$

where $c_m \equiv (-1)^m b_{m,-m}$. Moreover, since $P_\ell(\cos\gamma)$ is real and invariant under the interchange of the unprimed and primed coordinates, it follows that the $c_m = c_{-m}$ are real coefficients. This is easily proved by writing $Y_\ell^m(\theta,\phi) = N_{\ell m}P_\ell^m(\cos\theta)e^{im\phi}$ and using eq. (8) to show that

$$[N_{\ell m}]^2 P_\ell^m(\cos\theta)P_\ell^m(\cos\theta') = [N_{\ell,-m}]^2 P_\ell^{-m}(\cos\theta)P_\ell^{-m}(\cos\theta')\,.$$

To determine the c_m, we perform two operations on eq. (38). First, we set $\vec{\boldsymbol{r}} = \vec{\boldsymbol{r}}\boldsymbol{'}$. Then, we have $\theta'=\theta$, $\phi'=\phi$ and $\cos\gamma = 1$. The latter implies that $P_\ell(1)=1$ so that

$$\sum_{m=-\ell}^{\ell} c_m |Y_\ell^m(\theta,\phi)|^2 = 1\,.$$

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[5] This proof is inspired by a similar proof presented in Appendix B of a book by Francis E. Low, *Classical Field Theory: Electromagnetism and Gravitation* (John Wiley & Sons, Inc., New York, 1997).

[6] To see this explicitly, we write $Y_\ell^m(\theta,\phi) = N_{\ell m}P_\ell^m(\cos\theta)e^{im\phi}$. Then the relevant double sum over m and m' is

$$\sum_{m=-\ell}^{\ell}\sum_{m'=-\ell}^{\ell} b_{mm'}P_\ell^m(\cos\theta)P_\ell^{m'}(\cos\theta')e^{i(m\phi+m'\phi')}\,. \tag{37}$$

In order for this sum to a function of θ, θ' and $\phi-\phi'$, the only possible terms that can survive in eq. (37) are $m'=-m$.

Integrating over all solid angles and using the orthonormality of the spherical harmonics, it follows that

$$\sum_{m=-\ell}^{\ell} c_m = 4\pi \,. \tag{39}$$

Second, take the absolute square of eq. (38) to obtain

$$[P_\ell(\cos\gamma)]^2 = \sum_{m=-\ell}^{\ell} c_m Y_\ell^m(\theta,\phi) Y_\ell^m(\theta',\phi')^* \sum_{m'=-\ell}^{\ell} c_{m'} Y_\ell^{m'}(\theta,\phi)^* Y_\ell^{m'}(\theta',\phi') \,, \tag{40}$$

where we have used the fact that the constants c_m are real. Integrate both sides over $d\Omega$. Integrating the left hand side of eq. (40) yields

$$\int [P_\ell(\cos\gamma)]^2 d\Omega = [P_\ell(\cos\gamma)]^2 d\Omega_\gamma = 2\pi \int_{-1}^{1} [P_\ell(\cos\gamma)]^2 d\cos\gamma = \frac{4\pi}{2\ell+1} \,,$$

after using eq. (26) and the normalization integral for the Legendre polynomials. Integrating the right hand side of eq. (40) and using the orthonormality of the spherical harmonics, we end up with

$$\frac{4\pi}{2\ell+1} = \sum_{m=-\ell}^{\ell} c_m^2 |Y_\ell^m(\theta',\phi')|^2 \,. \tag{41}$$

Integrating both sides of eq. (41) over $d\Omega' = d\cos\theta' d\phi'$ and using $\int d\Omega' = 4\pi$ on the left and the orthonormality of the spherical harmonics on the right, it follows that

$$\sum_{m=-\ell}^{\ell} c_m^2 = \frac{(4\pi)^2}{2\ell+1} \,. \tag{42}$$

Remarkably, eqs. (39) and (42) are sufficient to determine all the c_m uniquely! This follows from the observation that:

$$\left(\sum_{m=-\ell}^{\ell} c_m\right)^2 = (2\ell+1)\left(\sum_{m=-\ell}^{\ell} c_m^2\right) = (4\pi)^2 \,. \tag{43}$$

However, according to Cauchy's inequality, which is proved in Appendix B,

$$\left(\sum_{k=1}^{n} a_k\right)^2 \leq n \left(\sum_{k=1}^{n} a_k^2\right) \,, \tag{44}$$

with the equality achieved if and only if all the a_k are equal. Applying this to eq. (43) with $n = 2\ell+1$,[7] we conclude that the c_m must be equal for all m. Using this result along with eq. (39) then yields

$$c_m = \frac{4\pi}{2\ell+1} \,. \tag{45}$$

[7]Since $m = -\ell, -\ell+1, \ldots, \ell-1, \ell$ it follows that there are $2\ell+1$ terms in each of the sums in eq. (43).

Inserting this result for the c_m back into eq. (38), we obtain

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

which is the addition theorem for the spherical harmonics.

For completeness, I briefly mention another technique for deriving eq. (45). The method requires an examination of the behavior of $Y_\ell^m(\theta,\phi)$ under a rigid rotation of the coordinate system. One can show[8] that under any rigid rotation of the coordinate system, the quantity

$$\sum_{m=-\ell}^{\ell} Y_\ell^m(\theta,\phi)Y_\ell^m(\theta',\phi')^*$$

is unchanged. Likewise, $P_\ell(\cos\gamma)$ is unchanged since the angle γ between the two vectors $\vec{\boldsymbol{r}}$ and $\vec{\boldsymbol{r}}'$ does not depend on the choice of the coordinate system. It then follows from eq. (38) that the c_m must be independent of m. With this result in hand, it is sufficient to compute c_0 by setting $\theta' = \phi' = 0$ (which is equivalent to choosing the positive z-axis of the coordinate system to lie along $\vec{\boldsymbol{r}}'$). Noting that

$$Y_\ell^m(0,0) = \sqrt{\frac{2\ell+1}{4\pi}}\,\delta_{m0}\,,$$

and using eq. (13), it follows from eq. (38) that

$$\sqrt{\frac{4\pi}{2\ell+1}}\,Y_\ell^0(\theta,\phi) = c_0\sqrt{\frac{2\ell+1}{4\pi}}\,Y_\ell^0(\theta,\phi)\,.$$

Solving for c_0 yields

$$c_0 = \frac{4\pi}{2\ell+1}\,.$$

Since we have argued that the c_m are independent of m, we have recovered the result of eq. (45). Inserting this result into eq. (38) yields the addition theorem as before.

B. The Cauchy Inequality

The Cauchy inequality states that for real numbers a_k and b_k (for $k = 1, 2, 3, \ldots, n$),

$$\left(\sum_{k=1}^{n} a_k b_k\right)^2 \leq \left(\sum_{k=1}^{n} a_k^2\right)\left(\sum_{k=1}^{n} b_k^2\right)\,,$$

and the equality holds only if the sequences $\{a_k\}$ and $\{b_k\}$ are proportional. In Appendix A, we need only a special case of this inequality in which $b_k = 1$ for all k,

$$\left(\sum_{k=1}^{n} a_k\right)^2 \leq n\left(\sum_{k=1}^{n} a_k^2\right)\,, \tag{46}$$

with the equality achieved if and only if all the a_k are equal.

[8]For details, see e.g. Section 6.3.3 of M. Chaichian and R. Hagedorn, *Symmetries in Quantum Mechanics: From Angular Momentum to Supersymmetry* (Institute of Physics Publishing, Bristol, UK, 1998).

To prove the inequality given in eq. (46),[9] consider the function

$$F(x) = (a_1x-1)^2 + (a_2x-1)^2 + \cdots + (a_nx-1)^2 = x^2\sum_{k=1}^n a_k^2 - 2x\sum_{k=1}^n a_k + n\,. \qquad (47)$$

Note that $F(x)$ is a quadratic polynomial in x and $F(x)\geq 0$ since it is the sum of squares. Thus, the polynomial equation $F(x)=0$ either as a double real root or a complex root, which means that its discriminant is non-positive.[10] That is,

$$\left(\sum_{k=1}^n a_k^2\right)^2 - n\sum_{k=1}^n a_k^2 \leq 0\,,$$

which yields the desired inequality [cf. eq. (46)]. Equality is achieved if and only if $F(x)=0$, which occurs if the quadratic polynomial $F(x)$ has a double root at x. From eq. (47), this means that $a_kx=1$ for all k, which implies that all the $a_k=1/x$ must be equal. The proof of eq. (46) is now complete.

References for further study:

An excellent pedagogical introduction to the spherical harmonics, along with a derivation of the addition theorem as presented in Section 4 can be found in

1. George B. Arfken, Hans J. Weber and Frank E. Harris, *Mathematical Methods for Physicists*, 7th edition (Academic Press, Elsevier, Inc., Waltham, MA, 2013).

2. Susan M. Lea, *Mathematics for Physicists* (Brooks/Cole—Thomson Learning, Belmont, CA, 2004).

A more profound understanding of the spherical harmonics can be found in the study of group theory and the properties of the rotation group. The addition theorem follows almost immediately from the transformation properties of the spherical harmonics under rotations. Two excellent introductions for physicists are:

3. Wu-Ki Tung, *Group Theory in Physics* (World Scientific Publishing Co., Singapore, 1985).

4. M. Chaichian and R. Hagedorn, *Symmetries in Quantum Mechanics: From Angular Momentum to Supersymmetry* (Institute of Physics Publishing, Bristol, UK, 1998).

[9]The more general Cauchy inequality can be proved by a simple generalization of the proof given here. I leave this generalization to the reader. A good reference for inequalities is D.S. Mitrinović, *Analytic Inequalities* (Springer-Verlag, Berlin, 1970).

[10]Given a quadratic polynomial $F(x)=Ax^2+Bx+C$, its discriminant is defined as B^2-4AC. Then $F(x)\geq 0$ if and only if $B^2-4AC\leq 0$.