Applications

Example: Denoting the three terms of ∇^2 in spherical polar by ∇_r^2, ∇_θ^2, ∇_ϕ^2 in an obvious way, evaluate $\nabla_r^2 u$ etc. for the two functions given below and verify that, in each case, although the individual are not necessarily zero their sum $\nabla^2 u$ is zero. Identify the corresponding values of ℓ and m.

(a) $u(r,\theta,\phi) = \left(Ar^2 + \frac{B}{r^3}\right)\frac{3\cos^2\theta - 1}{2}$.

(b) $u(r,\theta,\phi) = \left(Ar + \frac{B}{r^2}\right)\sin\theta \exp i\phi$.

Answer:

In both cases we write $u(r,\theta,\phi)$ as $R(r)\Theta(\theta)\Phi(\phi) \equiv R\Theta\Phi$ with

$$\nabla_r^2 = \frac{1}{r^2}\frac{\partial}{\partial r}(r^2\frac{\partial}{\partial r}), \quad \nabla_\theta^2 = \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right), \quad \nabla_\phi^2 = \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}$$

(a) $u(r,\theta,\phi) = \left(Ar^2 + \frac{B}{r^3}\right)\frac{3\cos^2\theta - 1}{2}$.

$$\nabla_r^2 u = \frac{1}{r^2}\frac{\partial}{\partial r}\left(2Ar^3 - \frac{3B}{r^2}\right)\Theta = \left(6A + \frac{6B}{r^5}\right)\Theta = \frac{6u}{r^2},$$

$$\nabla_\theta^2 u = \frac{R}{r^2}\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}(-3\sin^2\theta\cos\theta) = \frac{R}{r^2}\left(\frac{-6\sin\theta\cos^2\theta + 3\sin^3\theta}{\sin\theta}\right)$$
$$= \frac{R}{r^2}(-9\cos^2\theta + 3) = -\frac{6u}{r^2},$$

$$\nabla_\phi^2 u = 0.$$

Thus, although $\nabla_r^2 u$ and $\nabla_\theta^2 u$ are not individually zero, their sum is. From $\nabla_r^2 u = \ell(\ell+1)u = 6u$, we deduce that $\ell = 2$ and from $\nabla_\phi^2 u = 0$ that $m = 0$.

(b) $u(r,\theta,\phi) = \left(Ar + \frac{B}{r^2}\right)\sin\theta\, e^{i\phi}$.

$$\nabla_r^2 u = \frac{1}{r^2}\frac{\partial}{\partial r}\left(Ar^2 - \frac{2B}{r}\right)\Theta\Phi = \left(\frac{2A}{r} + \frac{2B}{r^4}\right)\Theta\Phi = \frac{2u}{r^2},$$

$$\nabla_\theta^2 u = \frac{R\Phi}{r^2}\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\cos\theta) = \frac{R\Phi}{r^2}\left(\frac{-\sin^2\theta + \cos^2\theta}{\sin\theta}\right)$$
$$= -\frac{u}{r^2} + \frac{\cos^2\theta}{\sin^2\theta}\frac{u}{r^2},$$

$$\nabla_\phi^2 u = \frac{R\Theta}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}(e^{i\phi}) = -\frac{u}{r^2\sin^2\theta}.$$

Hence

$$\nabla^2 u = \frac{2u}{r^2} - \frac{u}{r^2} + \frac{\cos^2\theta}{\sin^2\theta}\frac{u}{r^2} - \frac{u}{r^2\sin^2\theta} = \frac{u}{r^2}\left(1 + \frac{\cos^2\theta - 1}{\sin^2\theta}\right) = 0.$$

Here each individual term is non-zero, but their sum is zero. Further, $\ell(\ell+1) = 2$ and so $\ell = 1$, and from $\nabla_\phi^2 u = -\frac{u}{r^2 \sin\theta}$) it follows that $m^2 = 1$. In fact, from the part $e^{i\phi}$ in u, $m = 1$.

Associated Legendre Polynomials

When Helmholtz's equation is separated in spherical polar coordinates, one of the separated ODE's is the associated Legendre equation

Differential equation

$$\left[(1-x^2)\frac{d^2}{dx^2}-2x\frac{d}{dx}+\left\{n(n+1)-\frac{m^2}{(1-x^2)}\right\}\right]P_n^m(x)=0$$

Definition

$$P_n^m(x)=(1-x^2)^{m/2}\frac{d^m}{dx^m}P_n(x); \qquad n=0,1,2,3,\cdots$$

$$m=0,1,2,\cdots,n$$

$$P_n^0(x)=P_n(x)$$

$$P_n^{-m}(x)=(-1)^m\frac{(n-m)!}{(n+m)!}P_n^m(x)$$

$$P_n^m(-x)=(-1)^{n+m}P_n^m(x)$$

$$P_n^m(x)=0 \qquad \text{if } m>n$$

Generating function

$$g(x,h)=(2m-1)!!\frac{(1-x^2)^{m/2}h^m}{\left(1-2xh+h^2\right)^{m+1/2}}=\sum_{n=0}^{\infty}h^nP_n^m(x), \qquad |h|<1, \quad |x|\le +1$$

Recurrence relations

$$(2n+1)xP_n^m(x)=(n+m)P_{n-1}^m(x)+\left(n-m+1\right)P_{n+1}^m(x);$$

$$(2n+1)\sqrt{1-x^2}P_n^m(x)=P_{n-1}^{m+1}(x)-P_{n-1}^{m+1}(x)(x);$$

Orthogonality relation

$$\int_{-1}^{1}P_n^m(x)P_\ell^m(x)dx=\frac{2}{2n+1}\frac{\Gamma(n+m+1)}{\Gamma(n-m+1)}\delta_{n\ell}$$

H.W. Check the following table

m	n	$P_n^m(x)$
1	**1**	$\sqrt{1-x^2}=\sin\theta$
1	**2**	$3x\sqrt{1-x^2}=3\cos\theta\sin\theta$
2	**2**	$3\left(1-x^2\right)=3\sin^2\theta$
1	**3**	$\frac{3}{2}\left(5x^2-1\right)\sqrt{1-x^2}=\frac{3}{2}\left(5\cos^2\theta-1\right)\sin\theta$

Spherical Harmonic Function $Y_{\ell,m}(\theta,\varphi)$

Definition

$$Y_{\ell,m}(\theta,\varphi) = \Theta(\theta)\frac{e^{im\varphi}}{\sqrt{2\pi}}$$

$$= (-1)^m \left[\frac{(2\ell+1)}{4\pi}\frac{(\ell-m)!}{(\ell+m)!}\right]^{1/2} P_\ell^m(\cos\theta)e^{im\varphi}; \qquad m \geq 0$$

$$Y_{\ell,-m}(\theta,\varphi) = (-1)^m Y^*_{\ell,m}(\theta,\varphi);$$

where $\ell = 0,1,2,\cdots;$ $m = -\ell,-\ell+1,\cdots,+\ell$, and

$$\Theta(\theta) = \left[\frac{(2\ell+1)}{2}\frac{(\ell-m)!}{(\ell+m)!}\right]^{1/2} P_\ell^m(\cos\theta)$$

is the normalized angular function. An asterisk * indicates complex conjugation.

l	m	$Y_{lm}(\theta,\varphi)$
0	0	$\frac{1}{\sqrt{4\pi}}$
1	0	$\sqrt{\frac{3}{4\pi}}\cos\theta$
1	±1	$\mp\sqrt{\frac{3}{8\pi}}\sin\theta\ e^{\pm i\varphi}$
2	0	$\sqrt{\frac{5}{16\pi}}\left(3\cos^2\theta-1\right)$
2	±1	$\mp\sqrt{\frac{15}{8\pi}}\cos\theta\sin\theta e^{\pm i\varphi}$
2	±2	$\sqrt{\frac{15}{32\pi}}\sin^2\theta\ e^{\pm 2i\varphi}$

Differential equation

$$\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}+\ell(\ell+1)\right]Y_{\ell,m}(\theta,\varphi)=0$$

Orthogonality relation

$$\langle \ell m | \ell' m\rangle = \int_0^{2\pi} d\varphi \int_0^{\pi}\sin\theta\, d\theta\, Y^*_{\ell,m}(\theta,\varphi)Y_{\ell',m'}(\theta,\varphi) = \int Y^*_{\ell,m}(\theta,\varphi)Y_{\ell',m'}(\theta,\varphi)\,d\Omega = \delta_{\ell\ell'}\delta_{mm'}$$

Also

$$\sum_{m=-\ell}^{\ell}\left|Y_{\ell,m}(\theta,\varphi)\right|^2 = \frac{2\ell+1}{4\pi}$$

Recurrence relations

$$\cos\theta Y_{\ell,m}(\theta,\varphi)=\left[\frac{(\ell+1+m)(\ell+1-m)}{(2\ell+1)(2\ell+3)}\right]^{1/2}Y_{\ell+1,m}(\theta,\varphi)$$
$$+\left[\frac{(\ell+m)(\ell-m)}{(2\ell+1)(2\ell-1)}\right]^{1/2}Y_{\ell-1,m}(\theta,\varphi);$$

$$\sin\theta Y_{\ell,m}(\theta,\varphi)=\left[\frac{(\ell+1-m)(\ell+2-m)}{(2\ell+1)(2\ell+3)}\right]^{1/2}Y_{\ell+1,m-1}(\theta,\varphi)$$
$$+\left\{\left[\frac{(\ell+m)(\ell+m-1)}{(2\ell+1)(2\ell-1)}\right]^{1/2}Y_{\ell-1,m-1}(\theta,\varphi)\right\}e^{i\varphi}$$

The statement of completeness is that any function $f\ (\theta,\varphi)$ can be represented as a sum over spherical harmonics:

$$f(\theta,\phi)=\sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell}f_{\ell m}Y_{\ell m}(\theta,\phi) \tag{2.5.8}$$

for some coefficients $f_{\ell m}$. By virtue of Eq. (2.5.7), these can in fact be calculated as

$$f_{\ell m}=\int f(\theta,\phi)Y^*_{\ell m}(\theta,\phi)\,d\Omega. \tag{2.5.9}$$

Equation (2.5.8) means that the spherical harmonics form a complete set of *basis functions* on the sphere.

It is interesting to see what happens when Eq. (2.5.9) is substituted into Eq. (2.5.8). To avoid confusion we change the variables of integration to θ' and ϕ':

$$\begin{aligned} f(\theta,\phi) &= \sum_\ell\sum_m Y_{\ell m}(\theta,\phi)\int f(\theta',\phi')Y^*_{\ell m}(\theta',\phi')\,d\Omega' \\ &= \int f(\theta',\phi')\left[\sum_\ell\sum_m Y^*_{\ell m}(\theta',\phi')Y_{\ell m}(\theta,\phi)\right]d\Omega'. \end{aligned}$$

The quantity within the large square brackets is such that when it is multiplied by $f(\theta',\phi')$ and integrated over the primed angles, it returns $f(\theta,\phi)$. This must therefore be a product of two δ-functions, one for θ and the other for ϕ. More precisely stated,

$$\sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell}Y^*_{\ell m}(\theta',\phi')Y_{\ell m}(\theta,\phi)=\frac{\delta(\theta-\theta')\delta(\phi-\phi')}{\sin\theta}, \tag{2.5.10}$$

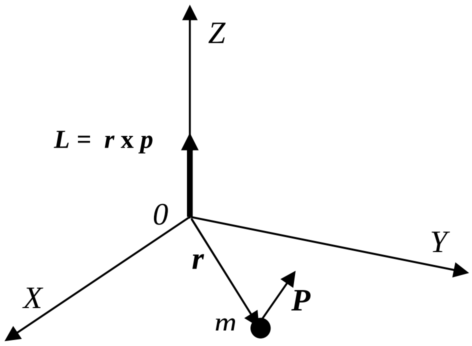
where the factor of $1/\sin\theta$ was inserted to compensate for the factor of $\sin\theta'$ in $d\Omega'$ (the δ-function is enforcing the condition $\theta' = \theta$). Equation (2.5.10) is known as the *completeness relation* for the spherical harmonics. This is analogous to a well-known identity,

$$\int \left(\frac{1}{\sqrt{2\pi}} e^{ikx'}\right)^* \left(\frac{1}{\sqrt{2\pi}} e^{ikx}\right) dk = \delta(x - x'),$$

in which the integral over dk replaces the discrete summation over ℓ and m; the basis functions $(2\pi)^{-1/2} e^{ikx}$ are then analogous to the spherical harmonics.

Angular Momentum Operators

$$\boldsymbol{L} = \boldsymbol{r} \times \boldsymbol{p} = \begin{vmatrix} \boldsymbol{e}_X & \boldsymbol{e}_Y & \boldsymbol{e}_Z \\ x & y & z \\ p_x & p_y & p_z \end{vmatrix}$$



Use the spherical coordinates to prove the following expressions:

$$\hat{L}_x = -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right) = i\hbar\left(\sin\varphi\frac{\partial}{\partial\theta} + \cot\theta\cos\phi\frac{\partial}{\partial\varphi}\right)$$

$$\hat{L}_y = -i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right) = i\hbar\left(-\cos\varphi\frac{\partial}{\partial\theta} + \cot\theta\sin\phi\frac{\partial}{\partial\varphi}\right)$$

$$\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2 = -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right], \qquad \hat{L}_z = -i\hbar\frac{\partial}{\partial\phi}$$

$$\boxed{\begin{aligned} &\hat{L}^2 Y_{\ell,m}(\theta,\varphi) = \hat{L}^2\left|\ell,m\right\rangle = \ell(\ell+1)\left|\ell,m\right\rangle; \\ &\hat{L}_z Y_{\ell,m}(\theta,\varphi) = m\left|\ell,m\right\rangle = m\left|\ell,m\right\rangle \\ &\hat{L}_\pm\left|\ell,m\right\rangle = C_\pm\left|\ell,m\right\rangle = \sqrt{\ell(\ell+1) - m(m\pm1)}\left|\ell,m\pm1\right\rangle \\ &\hat{L}_\pm \equiv \hat{L}_x \pm i\hat{L}_y = \pm e^{\pm i\varphi}\left[\frac{\partial}{\partial\theta} \pm i\frac{\cos\theta}{\sin\theta}\frac{\partial}{\partial\phi}\right] \end{aligned}}$$

Example:

$$Y_{l,0} = \sqrt{\frac{2l+1}{4\pi}}P_l(\cos\theta)$$

Example:

$$Y_{3,0} = \sqrt{\frac{7}{4\pi}}P_3(\cos\theta) = \sqrt{\frac{7}{4\pi}}\frac{1}{2}(5\cos^2\theta - 3\cos\theta) = \frac{1}{4}\sqrt{\frac{7}{\pi}}\cos\theta(5\cos\theta - 3)$$

$$= \frac{1}{4}\sqrt{\frac{7}{\pi}}\frac{z}{r}\left(5\frac{z^2}{r} - 3\right) = \frac{1}{4}\sqrt{\frac{7}{\pi}}\frac{z}{r^3}\left(5z^2 - 3r^2\right)$$

Example:

$$\psi = x + iy = r\sin\theta\,(\cos\varphi + i\,\sin\varphi) = r\sin\theta\, e^{i\varphi}$$

$$= -\sqrt{\frac{8\pi}{3}}\, r\, Y_{1,1}$$

Example:

$$\sin\theta\left(\sin\varphi + \cos\theta\cos\varphi\right) = -\frac{1}{2i}\sqrt{\frac{8\pi}{3}}Y_{1,1} - \frac{1}{2i}\sqrt{\frac{8\pi}{3}}Y_{1,-1} - \frac{1}{2}\sqrt{\frac{8\pi}{15}}Y_{2,1} + \frac{1}{2}\sqrt{\frac{8\pi}{15}}Y_{2,-1}$$

Example: $\sin\theta(1-\cos\theta)e^{i\varphi} = -\sqrt{\frac{8\pi}{3}}Y_{1,1} - \sqrt{\frac{8\pi}{15}}Y_{2,1}$

Example: $\sqrt{\pi} - \sqrt{3\pi}\cos^2\theta = -\pi\sqrt{\frac{16}{5}}Y_{2,0}$

Example: $\sin\theta\cos\varphi = -\sqrt{\frac{2\pi}{3}}Y_{1,1} + \sqrt{\frac{2\pi}{3}}Y_{1,-1}$

Homework: Establish the following equations

$(i)\quad \frac{x}{r} = \sin\theta\cos\varphi = \sqrt{\frac{2\pi}{3}}\left[-Y_{1,1}+Y_{1,-1}\right] \qquad (ii)\quad \frac{y}{r} = i\sqrt{\frac{2\pi}{3}}\left[Y_{2,2}-Y_{2,-2}\right]$

$(iii)\quad xz = r^2\sqrt{\frac{2\pi}{15}}\left[-Y_{2,1}+Y_{2,-1}\right] \qquad (iv)\quad x^2-y^2 = r^2\sqrt{\frac{8\pi}{15}}\left[Y_{2,2}+Y_{2,-2}\right]$

$(v)\quad x\,y = \frac{r^2}{i}\sqrt{\frac{2\pi}{15}}\left[-Y_{2,2}-Y_{2,-2}\right] \qquad (vi)\quad \sin^2\theta\cos 2\varphi = \sqrt{\frac{8\pi}{15}}\left[Y_{2,2}+Y_{2,-2}\right]$

Example: for l = 1; find the matrix form of $<\hat{L}^2>$, and $<\hat{L}_z>$

Answer:

$$\left(\hat{L}^2\right) = <l'|\hat{L}^2|l> = l(l+1)\hbar^2 \underbrace{<l'|l>}_{\delta_{l'l}} = 2\hbar^2 \begin{array}{cc} \begin{array}{ccc} <11| & <10| & <1-1| \end{array} & \\ \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} & \begin{array}{l} |11> \\ |10> \\ |1-1> \end{array} \end{array}$$

$$<\hat{L}^2> = \begin{pmatrix} <11|\hat{L}^2|11> & <11|\hat{L}^2|10> & <11|\hat{L}^2|1-1> \\ <10|\hat{L}^2|11> & <10|\hat{L}^2|10> & <10|\hat{L}^2|1-1> \\ <1-1|\hat{L}^2|11> & <1-1|\hat{L}^2|10> & <1-1|\hat{L}^2|1-1> \end{pmatrix} = 2\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix};$$

$$<\hat{L}_z> = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

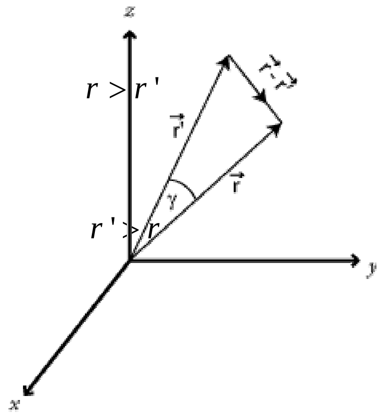
Example: Is the following function the eigenfunction of $\hat{L}^2$? of $\hat{L}_z$?

$$x^2 - y^2 = r^2\sqrt{\frac{8\pi}{15}}\left[Y_{2,2}+Y_{2,-2}\right]$$

It is an eigen function of $\hat{L}^2$, not $\hat{L}_z$

Prove that: $\hat{L}_z\left(\cos^2\varphi - \sin^2\varphi + 2i\cos\varphi\sin\varphi\right) = 2\hbar e^{2i\varphi}$

H. W. Multipole expansion: It easy to extend this expansion to the general one as:



$$\frac{1}{|\vec{r}-\vec{r}'|}=\frac{1}{r\sqrt{1+\left(\frac{r'}{r}\right)^2-2\left(\frac{r'}{r}\right)\cos\theta}}=\frac{1}{r}\sum_{\ell=0}^{\infty}\left(\frac{r'}{r}\right)^{\ell}P_\ell(x=\cos\theta),$$

$$=\frac{1}{r'\sqrt{1+\left(\frac{r}{r'}\right)^2-2\left(\frac{r}{r'}\right)\cos\theta}}=\frac{1}{r'}\sum_{\ell=0}^{\infty}\left(\frac{r}{r'}\right)^{\ell}P_\ell(x=\cos\theta),$$

Answer:

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

Where γ is the angle between the two vectors $\vec{r}$ and $\vec{\mathbf{r}}'$.

Case I: $r > r'$

$$\frac{1}{|\vec{r}-\vec{r}'|}=\frac{1}{r}\left\{1-\frac{2r'}{r}\mu+\left(\frac{r'}{r}\right)^2\right\}^{-\frac{1}{2}}=\frac{1}{r}\left\{1-\frac{r'}{r}\left(2\mu-\frac{r'}{r}\right)\right\}^{-\frac{1}{2}}$$

$$=\frac{1}{r}\left\{1+\frac{1}{2}\frac{r'}{r}\left(2\mu-\frac{r'}{r}\right)+\frac{3}{8}\left(\frac{r'}{r}\right)^2\left(2\mu-\frac{r'}{r}\right)^2+\cdots\right\}$$

$$=\frac{1}{r}+\frac{r'}{r^2}\mu+\frac{r'^2}{r^3}\left(\frac{3\mu^2-1}{2}\right)+\cdots$$

$$=\frac{1}{r}P_0(\mu)+\frac{r'}{r^2}P_1(\mu)+\frac{r'^2}{r^3}P_2(\mu)+\cdots$$

$$\boxed{\frac{1}{|\vec{r}-\vec{r}'|}=\frac{1}{r}\sum_{\ell=0}^{\infty}\left(\frac{r'}{r}\right)^{\ell}P_\ell(\mu)}$$

Case I: $r < r'$

$$\frac{1}{|\vec{r}-\vec{r}'|}=\frac{1}{r'}\sum_{\ell=0}^{\infty}\left(\frac{r}{r'}\right)^{\ell}P_\ell(\mu)$$

In general, we can write (see Jackson 3.38):

$$\frac{1}{|\vec{r}-\vec{r}'|}=\sum_{\ell=0}^{\infty}\frac{r_<^{\ell}}{r_<^{\ell+1}}P_\ell(\mu),:$$

In spherical coordinates, we can define the two vectors $\vec{r}$ and $\vec{\mathbf{r}}'$ such as: