Lecture 3: Spherical Harmonics

Introduction-a

- As we have seen the general differential equation:

$$\left\{\nabla^2 + k^2 - U(r)\right\}\Psi(\mathbf{r}) = 0, \quad k = const \qquad (3.1)$$

- Can be solved with the method of separation of variables, i.e. by considering a solution of the form:

$$\Psi(\mathbf{r}) = R(r)Y(\theta,\varphi) \qquad (3.2)$$

Introduction-b

- The differential equation (3.1) splits in two simpler equations

$$\left\{\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right\}Y\left(\theta,\varphi\right)=-\lambda Y\left(\theta,\varphi\right)\quad(3.3)$$

$$\frac{1}{r^2}\frac{d}{dr}\left(r\frac{dR}{dr}\right)+\left[k^2-U(r)-\frac{\lambda}{r^2}\right]R=0\quad(3.4)$$

Note that the angular dependence is common to all problems with spherical symmetry.

Solution of the angular equation

- Try to consider for Eq. 3.3 a solution of the separating variable form:

$$Y(\theta,\varphi) = \Theta(\theta)\Phi(\varphi) \qquad (3.5)$$

- Then the radial equation is split into two equations:

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)+\left(\lambda-\frac{\mu^2}{\sin^2\theta}\right)\Theta=0 \qquad (3.6)$$

$$\frac{d^2\Phi}{d^2\phi}+\mu^2\Phi=0 \qquad (3.7)$$

The associated Legendre equation

- In physical problems Eq. 3.7 has single valued and periodical solutions only if *m =integer*. In this case

$$\Phi_m \propto \exp(im\phi) \quad (3.8)$$

- With this integer value of *μ,* Eq. (3.6) takes the form:

$$\frac{d}{dx}\left[\left(1-x^2\right)\frac{du}{dx}\right]+\left[\ell(\ell+1)-\frac{m^2}{1-x^2}\right]u=0 \quad (3.9)$$

$$x=\cos\theta, \quad u(x)=\Theta(\theta), \quad \lambda=\ell(\ell+1) \qquad (3.10)$$

The choice $\lambda=l(l+1)$ ensures finite solutions (i.e. physically accepted solutions)

The associated Legendre equation

- This is the so called **associated Legendre equation** and has as its solutions the associated Legendre functions.
- Thus the solutions which correspond to Eq. (3.5) will be a product of associated Legendre functions times the exponentials of the form $e^{\pm im\phi}$. **These are the so called spherical harmonics.**
- The name comes because these function appear when we study the harmonic oscillations of a spherical object like a spherical membrane.

The spherical harmonics

- The **spherical harmonics** are defined as follows:

$$Y_l^m(\theta,\ \phi) = \varepsilon \sqrt{\frac{(2l+1)}{4\pi}\frac{(l-|m|)!}{(l+|m|)!}} P_l^m(\cos\theta)e^{im\phi} \qquad (3.5)$$

$$\varepsilon = \begin{cases} (-1)^m, & m \geq 0 \\ 1 & m < 0 \end{cases}$$

The factor ε is called Condon-Shortley phase and is used to introduce an alternation of sign among the *positive m* spherical harmonics.

$P_l^m(\cos\theta)$ the associated Legendre function

The spherical harmonics

- The **spherical harmonics** are normalized and orthogonal to each other:

$$\int_0^{2\pi}\int_0^{\pi}\left[Y_l^m(\theta,\ \phi)\right]^*\left[Y_{l'}^{m'}(\theta,\ \phi)\right]\sin\theta\, d\theta\, d\phi = \delta_{ll'}\delta_{mm'} \qquad (3.6)$$

- Any function *f*(θ, ϕ), defined on the surface of a sphere and is differentiable and continuous can be expanded in a series of spherical harmonics.

Eq. (3.7) is known as Laplace series

$$f(\theta,\phi) = \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{m=+\ell} A_{\ell m} Y_l^m(\theta,\ \phi) \qquad (3.7)$$

$$A_{\ell m} = \int_0^{2\pi}\int_0^{\pi} f(\theta,\ \phi) Y_\ell^{m*}(\theta,\ \phi)\sin\theta\, d\theta\, d\phi \qquad (3.8)$$

The spherical harmonics

- The spherical harmonics are eigenfunctions of the square angular momentum operator and of the angular momentum operator along the *z*-direction

$$\mathbf{l}^2 Y_l^m = \hbar^2 l(l+1) Y_l^m, \quad l_z Y_l^m = \hbar m Y_l^m \tag{3.9}$$

the first few spherical harmonics

$$Y_0^0 = \left(\frac{1}{4\pi}\right)^{1/2}$$

$$Y_1^0 = \left(\frac{3}{4\pi}\right)^{1/2} \cos\theta$$

$$Y_1^{\pm1} = \mp\left(\frac{3}{8\pi}\right)^{1/2} \sin\theta e^{\pm i\phi}$$

$$Y_2^0 = 3\left(\frac{5}{16\pi}\right)^{1/2} \left(3\cos^2\theta - 1\right)$$

$$Y_2^{\pm1} = \mp3\left(\frac{15}{8\pi}\right)^{1/2} \sin\theta\cos\theta e^{\pm i\phi}$$

$$Y_2^{\pm2} = \left(\frac{15}{32\pi}\right)^{1/2} \sin^2\theta e^{\pm2i\phi}$$

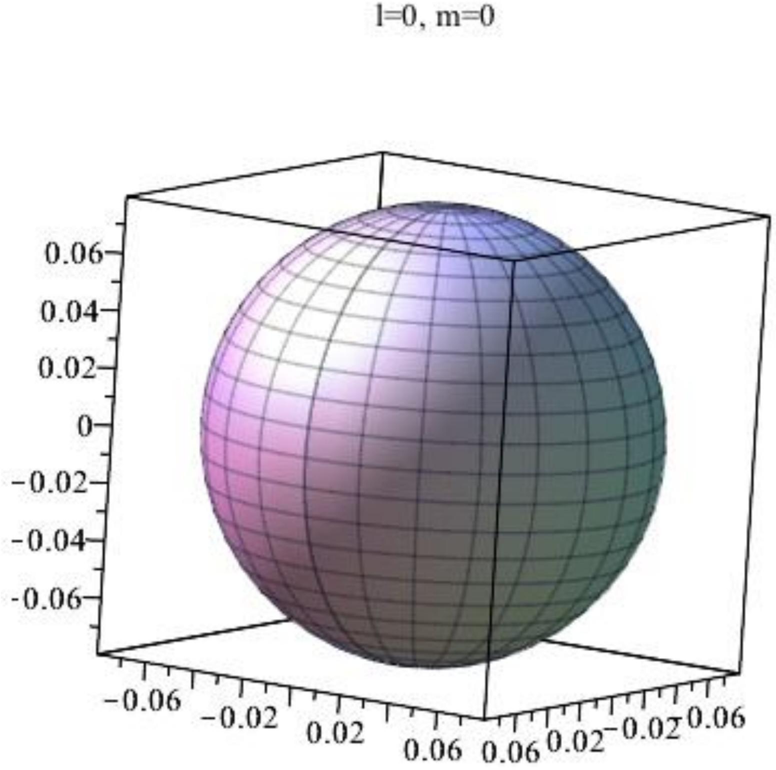
$$Y_3^0 = \left(\frac{7}{16\pi}\right)^{1/2} \left(5\cos^3\theta - 3\cos\theta\right)$$

$$Y_3^{\pm1} = \mp\left(\frac{21}{16\pi}\right)^{1/2} \sin\theta\left(5\cos^2\theta - 1\right)e^{\pm i\phi}$$

$$Y_3^{\pm2} = \left(\frac{105}{32\pi}\right)^{1/2} \sin^2\theta\cos\theta e^{\pm2i\phi}$$

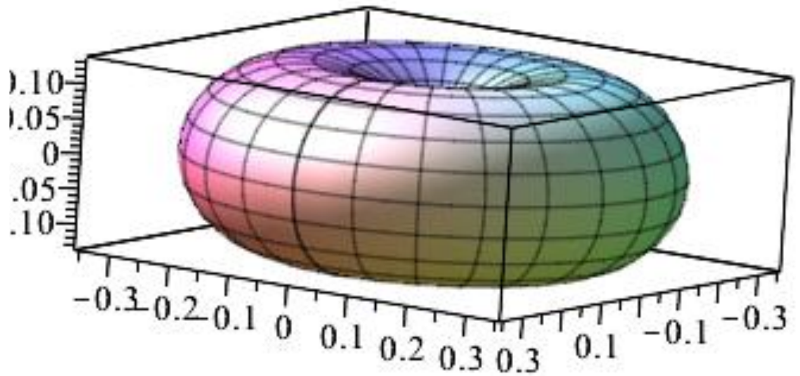
$$Y_3^{\pm3} = \mp\left(\frac{35}{64\pi}\right)^{1/2} \sin^3\theta e^{\pm3i\phi}$$

Plots of the modulus squared of some spherical harmonics

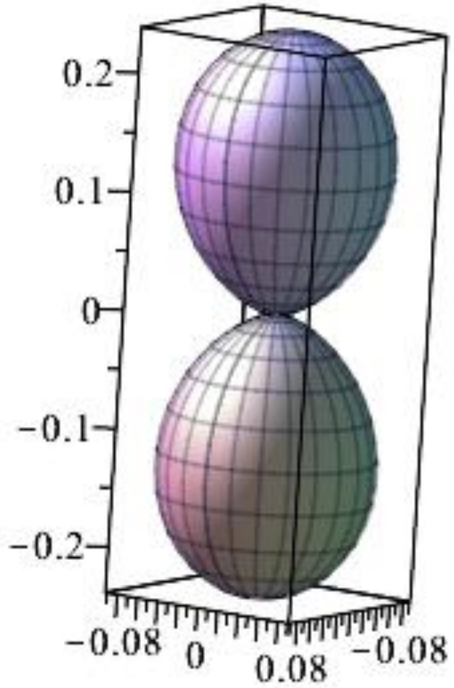


Plots of the modulus squared of some spherical harmonics

l=1, m=1 or m=-1

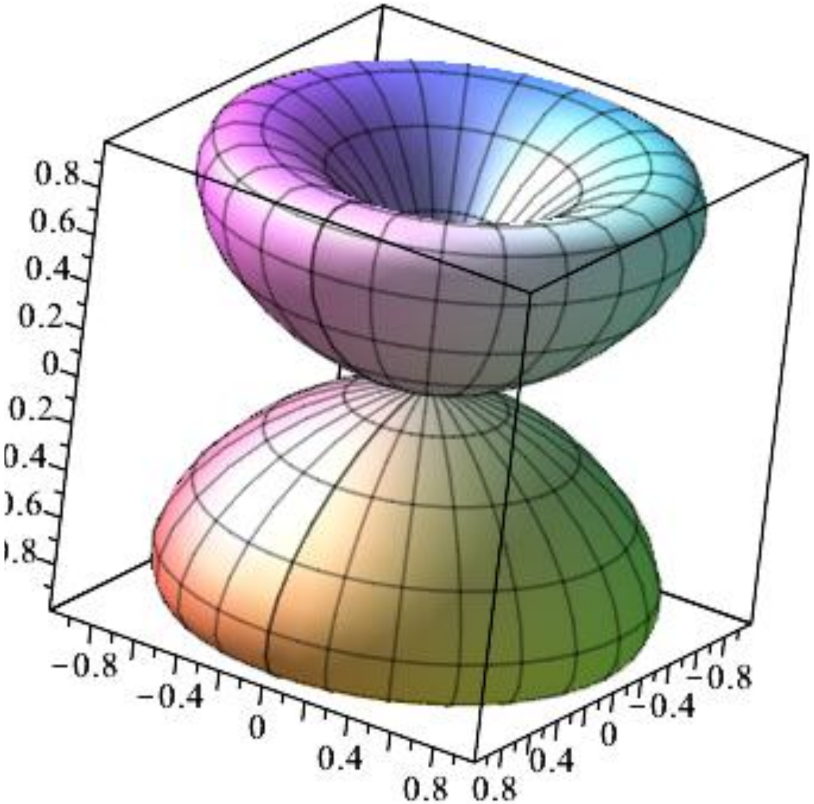


l=1, m=0

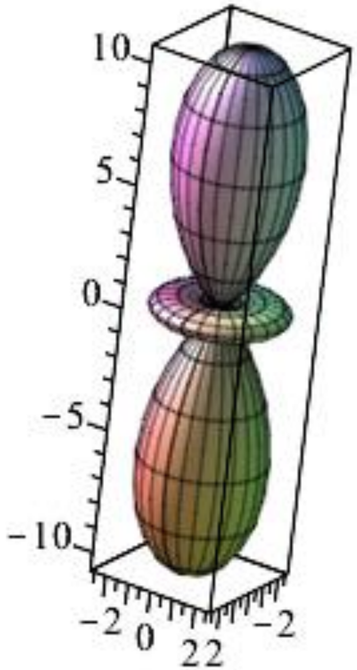


Plots of the modulus squared of some spherical harmonics

l=2, m=+1 or -1



l=2, m=0



The addition theorem

- The addition theorem for the spherical harmonics states that:

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