Today

I. Last Time

II. Derivation of the Angular Momentum Eigenfunctions… Continued

III. Radial Equation

I. Last time

* Two compatible angular momentum observables L^2, L_z.
* We started studying the ang. mom. eigenfunctions using a separation ansatz: $f_\ell^m(\theta, \phi) = \Theta(\theta)\Phi(\phi)$.
* Found L_z and L^2 in spherical coordinates. We also found each component and the ladder operators in these coord.s

I. Derivation of angular momentum eigenfunctions.

Classically, $\overrightarrow{L} = \vec{r} \times \overrightarrow{p}$. We want to convert this into operators

$$\hat{\overrightarrow{L}} = \frac{\hbar}{i} \vec{r} \times \overrightarrow{\nabla}.$$

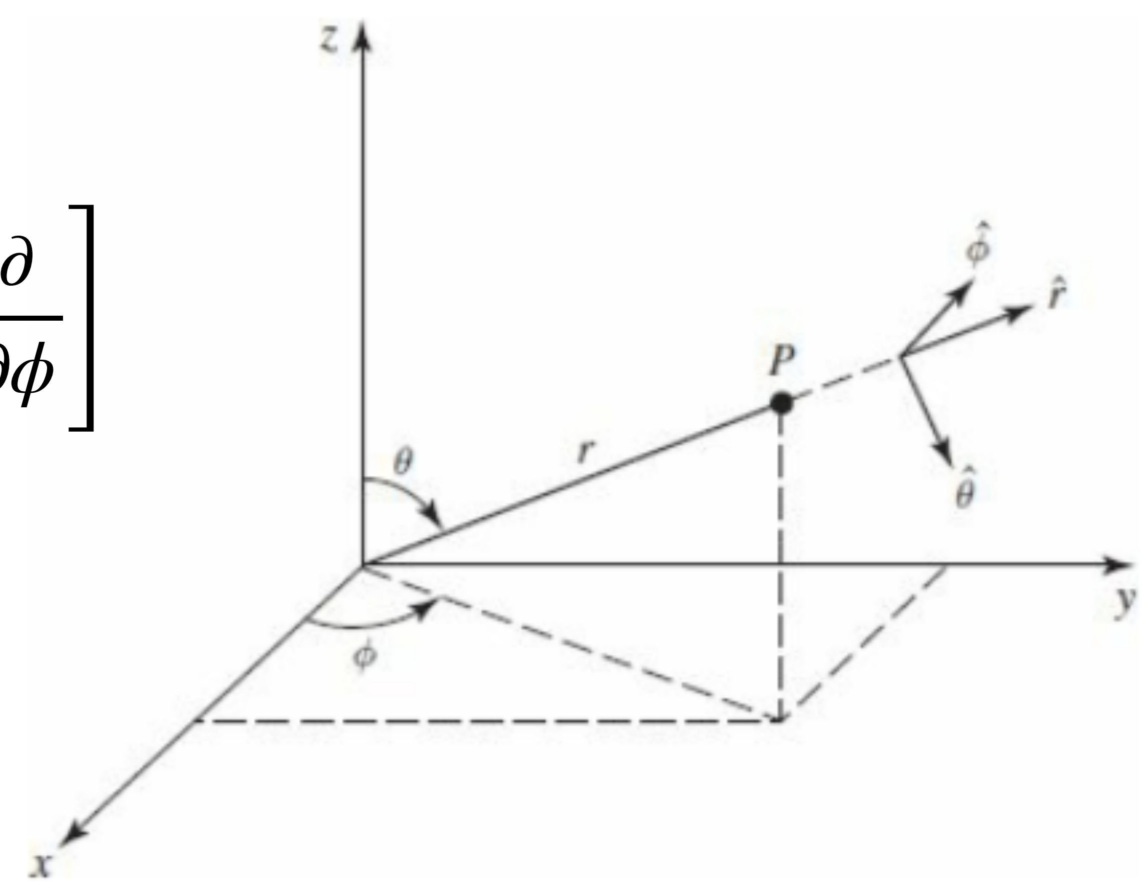
In spherical coords. (natural for ang. momentum and rotations)

$$\overrightarrow{\nabla} = \hat{r}\frac{\partial}{\partial r} + \hat{\theta}\frac{1}{r}\frac{\partial}{\partial \theta} + \hat{\phi}\frac{1}{r\sin\theta}\frac{\partial}{\partial \phi}.$$

Now, $\vec{r} = r\hat{r}$, so

$$\overrightarrow{L} = \frac{\hbar}{i}\left[r(\hat{r}\times\hat{r})\frac{\partial}{\partial r} + (\hat{r}\times\hat{\theta})\frac{\partial}{\partial\theta} + \frac{\hat{r}\times\hat{\phi}}{\sin\theta}\frac{\partial}{\partial\phi}\right]$$

$$= \frac{\hbar}{i}\left[\hat{\phi}\frac{\partial}{\partial\theta} - \frac{\hat{\theta}}{\sin\theta}\frac{\partial}{\partial\phi}\right]$$



I. Derivation of angular momentum eigenfunctions.

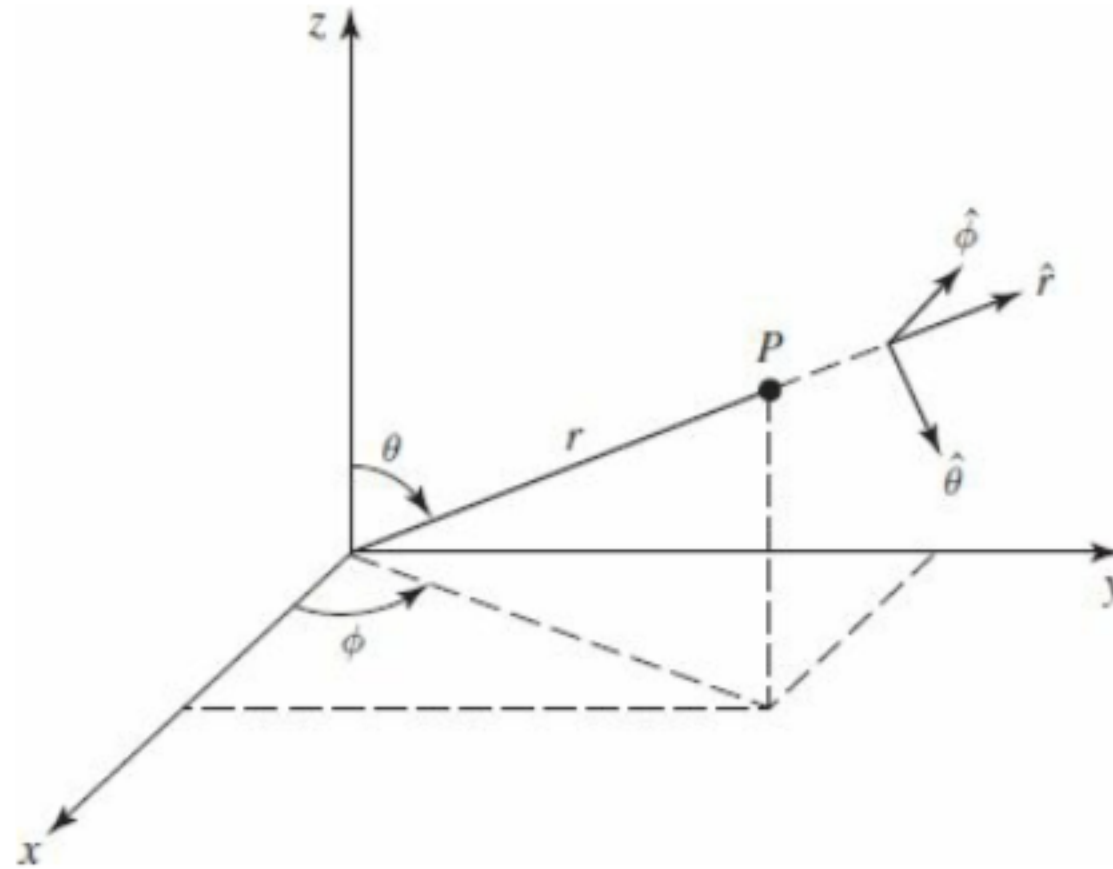
Then,

$$L_z = \frac{\hbar}{i}\frac{\partial}{\partial\phi}$$

while

$$L_x = \frac{\hbar}{i}\left(-s\phi\frac{\partial}{\partial\theta} - \cot\theta c\phi\frac{\partial}{\partial\phi}\right)$$

$$L_y = \frac{\hbar}{i}\left(c\phi\frac{\partial}{\partial\theta} - \cot\theta s\phi\frac{\partial}{\partial\phi}\right)$$



The ladder operator are slightly simpler

$$L_\pm = L_x \pm iL_y = \frac{\hbar}{i}\left[(-s\phi \pm ic\phi)\frac{\partial}{\partial\theta} - (c\phi \pm is\phi)\cot\theta\frac{\partial}{\partial\phi}\right]$$

$$= \pm\hbar e^{\pm i\phi}\left[\frac{\partial}{\partial\theta} \pm i\cot\theta\frac{\partial}{\partial\phi}\right]$$

I. Derivation of angular momentum eigenfunctions.

From which

$$L_+L_- = -\hbar^2\left[\frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta} + \cot^2\theta\frac{\partial^2}{\partial\phi^2} + i\frac{\partial}{\partial\phi}\right]$$

$$L^2 = -\hbar^2\left[\frac{1}{s\theta}\frac{\partial}{\partial\theta}\left(s\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{s^2\theta}\frac{\partial^2}{\partial\phi^2}\right]$$

Now, recall

$L^2 f_\ell^m = \hbar^2\ell(\ell+1)f_\ell^m$, where $f_\ell^m = f_\ell^m(\theta,\phi)$. Let's suppose

$f_\ell^m(\theta,\phi) = \Theta(\theta)\Phi(\phi)$ (separation ansatz) to find

$$\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2} = -m^2 \quad (1)$$

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

II. Derivation of angular momentum eigenfunctions.

Let's focus on (1) at first

$$\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2} = -m^2 \quad (1)$$

It has solutions

$$\Phi(\phi) = e^{im\phi}.$$

Boundary conditions tell us the allowed values for m, in the present case they are

$$\Phi(\phi + 2\pi) = \Phi(\phi).$$

Let's impose this

$$e^{im(\phi+2\pi)} = e^{im\phi} \quad \Longrightarrow \quad e^{im2\pi} = 1,$$

The last condition is satisfied when

$$m = 0, \pm 1, \pm 2, \dots .$$

II. Derivation of angular momentum eigenfunctions.

Let's focus on (2) at first

$$\left\{ \frac{1}{\Theta} \left[s\theta \frac{d}{d\theta} \left(s\theta \frac{d\Theta}{d\theta} \right) \right] + \ell(\ell+1)s^2\theta \right\} = m^2 \quad (2)$$

It has solutions

$$\Theta(\theta) = AP_\ell^m(\cos\theta),$$

where P_ℓ^m is the associated Legendre polynomial (or function),

$$P_\ell^m(x) = (1-x^2)^{|m|/2} \left(\frac{d}{dx} \right)^{|m|} P_\ell(x),$$

which in turn is defined in terms of the Legendre polynomial

$$P_\ell(x) = \frac{1}{2^\ell \ell!} \left(\frac{d}{dx} \right)^\ell (x^2-1)^\ell.$$

This last formula is called the Rodrigues formula.

II. Derivation of angular momentum eigenfunctions.

This all amounts to having found the "spherical harmonics"

$$Y_\ell^m(\theta,\phi) = \Phi(\phi)\Theta(\theta) = \sqrt{\frac{(2\ell+1)(\ell-|m|)!}{4\pi(\ell+|m|)!}}e^{im\phi}P_\ell^m(\cos\theta).$$

These are also orthogonal (why?). So,

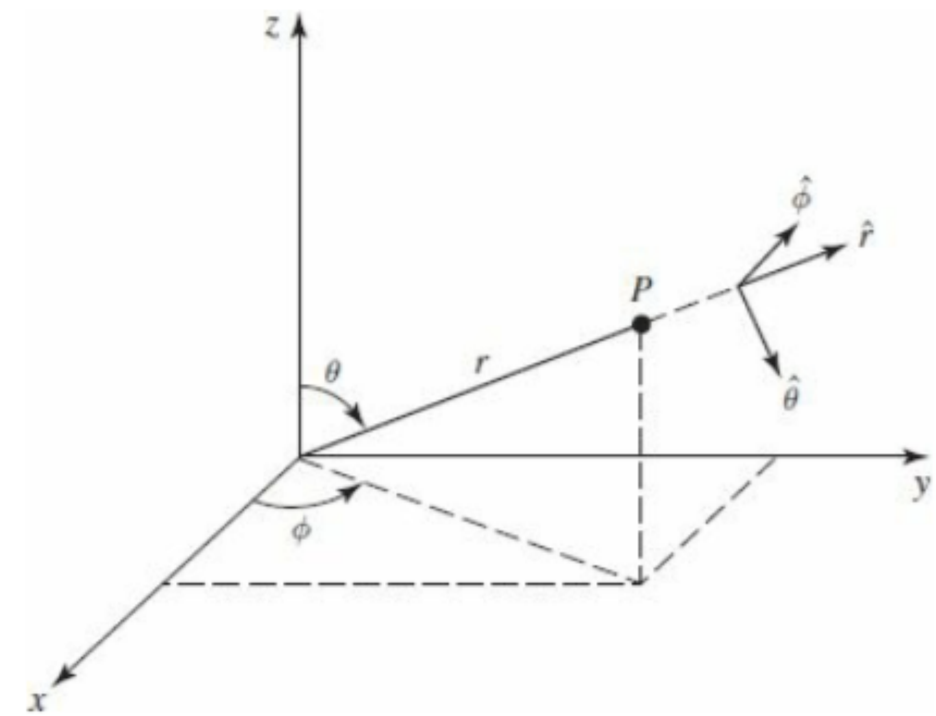
$\int_0^{2\pi}\int_{\theta=0}^{\pi}\left[Y_\ell^m(\theta,\phi)\right]^*\left[Y_{\ell'}^{m'}(\theta,\phi)\right]\sin\theta d\theta d\phi = \delta_{\ell\ell'}\delta_{mm'}$. (Beware the Condon-Shortley phase. Also the Geodesy convention, which is a real basis for spherical harmonics.)

Our first example of a basis for functions were sin and cos in the context of Fourier analysis. The intuition for spherical harmonics is exactly the same—they provide a basis of functions for the sphere.

III. The Radial Equation

In 3D we realized that we could do many of the same things that we had done in 1D:

$$i\hbar\frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi + V(r,\theta,\phi,t)\Psi.$$



Just as in 1D if $V = V(\vec{r})$, then

$$\Psi_n(\vec{r},t) = \psi_n(\vec{r})e^{-iE_n t/\hbar}.$$

As in 1D we interpret

$$|\Psi(\vec{r},t)|^2 d^3\vec{r}$$

as the probability of finding the particle in a volume $d^3\vec{r}$. We also again have

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi$$

Let's study a very special case, one where

$$V(\vec{r}) = V(r)$$

only depends on the radial distance $r = |\vec{r}|$.

III. The Radial Equation

In these spherical coordinates

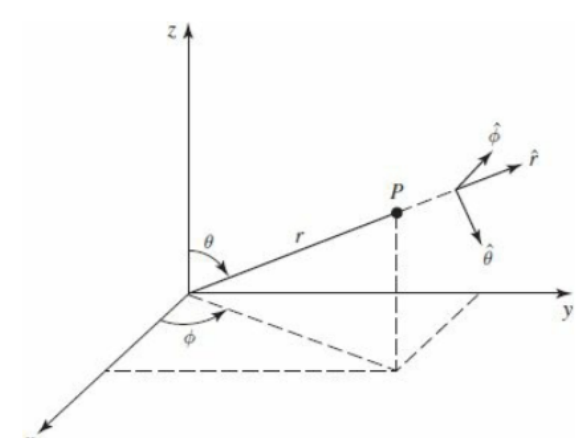
$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2 s\theta}\frac{\partial}{\partial\theta}\left(s\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2 s^2\theta}\frac{\partial^2}{\partial\phi^2}$$

Notice that part of this (the last two terms) is exactly

$$-\frac{1}{\hbar^2 r^2}L^2.$$

Once again we're tempted to try and use separation of variables

$\psi(r,\theta,\phi) = R(r)Y(\theta,\phi)$.



Then

$$-\frac{\hbar^2}{2m}\nabla^2(RY) + V(RY) = E(RY)$$

$$\implies -\frac{\hbar^2}{2mr^2}Y\frac{\partial}{\partial r}\left(r^2\frac{dR}{dr}\right) + \frac{\hbar^2}{\hbar^2 2mr^2}RL^2Y + VRY = ERY$$

III. The Radial Equation

$$-\frac{\hbar^2}{2mr^2}Y\frac{\partial}{\partial r}\left(r^2\frac{dR}{dr}\right)+\frac{\hbar^2}{\hbar^2 2mr^2}RL^2Y+VRY=ERY$$

Dividing by RY and multiplying by $-2mr^2/\hbar^2$:

$$\left\{\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)-\frac{2mr^2}{\hbar^2}\left[V(r)-E\right]\right\}+\frac{1}{Y}\left\{\frac{1}{s\theta}\frac{\partial}{\partial\theta}\left(s\theta\frac{\partial Y}{\partial\theta}\right)+\frac{1}{s^2\theta}\frac{\partial^2 Y}{\partial\phi^2}\right\}=0$$