Angular Momentum Wavefunctions

In the position basis,

$$\hat{L}_x = \hat{Y}\hat{P}_z - \hat{Z}\hat{P}_y = \frac{\hbar}{i}\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)$$

$$\hat{L}_y = \hat{Z}\hat{P}_x - \hat{X}\hat{P}_z = \frac{\hbar}{i}\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)$$

$$\hat{L}_z = \hat{X}\hat{P}_y - \hat{Y}\hat{P}_x = \frac{\hbar}{i}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)$$

Transform to spherical

From Mathworld being careful to exchange $\phi \longleftrightarrow \theta$

$$x = r\cos\phi\sin\theta$$

$$y = r\sin\phi\sin\theta$$

$$z = r\cos\theta$$

$$\frac{\partial}{\partial x} = \cos\phi\sin\theta\frac{\partial}{\partial r} - \frac{\sin\phi}{r\sin\theta}\frac{\partial}{\partial\phi} + \frac{\cos\phi\cos\theta}{r}\frac{\partial}{\partial\theta}$$

$$\frac{\partial}{\partial y} = \sin\phi\sin\theta\frac{\partial}{\partial r} + \frac{\cos\phi}{r\sin\theta}\frac{\partial}{\partial\phi} + \frac{\sin\phi\cos\theta}{r}\frac{\partial}{\partial\theta}$$

$$\frac{\partial}{\partial z} = \cos\theta\frac{\partial}{\partial r} - \frac{\sin\theta}{r}\frac{\partial}{\partial\theta}$$

<u>So</u>

$$L_z = \frac{\hbar}{i}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)$$

$$= \frac{\hbar}{i}\Bigg(r\cos\phi\sin\theta\cdot\left[\sin\phi\sin\theta\frac{\partial}{\partial r} + \frac{\cos\phi}{r\sin\theta}\frac{\partial}{\partial\phi} + \frac{\sin\phi\cos\theta}{r}\frac{\partial}{\partial\theta}\right]$$

$$- r\sin\phi\sin\theta\left[\cos\phi\sin\theta\frac{\partial}{\partial r} - \frac{\sin\phi}{r\sin\theta}\frac{\partial}{\partial\phi} + \frac{\cos\phi\cos\theta}{r}\frac{\partial}{\partial\theta}\right]$$

$$\hat{L}_z = \frac{\hbar}{i}\left[\cos^2\phi \frac{\partial}{\partial\phi} + \sin^2\phi \frac{\partial}{\partial\phi}\right]$$

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

By a similar and equally horrible calculation,

$$\hat{L}_x = i\hbar\left(\sin\phi \frac{\partial}{\partial\theta} + \frac{\cos\phi}{\tan\theta}\frac{\partial}{\partial\phi}\right)$$

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

<u>and</u>

$$\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$$

$$= -\hbar^2\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right)$$

$$\hat{L}_+ = \hat{L}_x + i\hat{L}_y$$

$$= i\hbar\left[\sin\phi\frac{\partial}{\partial\theta} + \frac{\cos\phi}{\tan\theta}\frac{\partial}{\partial\phi}\right.$$

$$\left. - i\cos\phi\frac{\partial}{\partial\theta} + \frac{i\sin\phi}{\tan\theta}\frac{\partial}{\partial\phi}\right]$$

$$= \hbar\left[(\cos\phi + i\sin\phi)\frac{\partial}{\partial\theta} + i(\cos\phi + i\sin\phi)\cot\theta\frac{\partial}{\partial\phi}\right]$$

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

Likewise, $\hat{L}_- = \hat{L}_x - i\hat{L}_y$

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

We know we can find a function $f_\ell^m(\theta,\phi)$ that is simultaneously an eigenfunction of $\hat{L}^2$ and $\hat{L}_z$.

$$\hat{L}^2 f_\ell^m = \ell(\ell+1)\hbar^2 f_\ell^m$$

$$\hat{L}_z f_\ell^m = m\hbar f_\ell^m$$

Propose a separated solution

$$f_\ell^m = T_\ell^m(\theta)\,\Phi_\ell^m(\phi)$$

<u>Solve L_z eqn</u>

$$L_z f_\ell^m = m\hbar f_\ell^m$$

$$\frac{\hbar}{i}\frac{\partial f_\ell^m}{\partial\phi} = m\hbar \frac{\partial f_\ell^m}{\partial\phi}$$

$$\frac{\hbar}{i} T_\ell^m \frac{\partial \Phi_\ell^m}{\partial\phi} = m\hbar\, T_\ell^m \Phi_\ell^m$$

$$\frac{\partial \Phi_\ell^m}{\partial\phi} = im\Phi_\ell^m \implies \Phi^m = e^{im\phi}$$

$$f_\ell^m = T_\ell^m(\theta)\, e^{im\phi}$$

Solve L^2 eqn

$$L^2 f_\ell^m = \ell(\ell+1)\hbar^2 f_\ell^m$$

$$-\hbar^2\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}f_\ell^m + \frac{1}{\sin^2\theta}\frac{\partial^2 f_\ell^m}{\partial\phi^2}\right)$$

$$= \ell(\ell+1)\hbar^2 f_\ell^m$$

Use $f_\ell^m = T(\theta)\, e^{im\phi}$

$$\frac{\partial^2 f_\ell^m}{\partial\phi^2} = -T(\theta)\, m^2 e^{im\phi}$$

$$-\hbar^2 e^{im\phi}\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial T}{\partial\theta} - \frac{m^2 T}{\sin^2\theta}\right)$$

$$= \ell(\ell+1)\hbar^2 T e^{im\phi}$$

Divide by $-\hbar^2 e^{im\phi}$

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\sin\theta\frac{dT}{d\theta} - \frac{m^2}{\sin^2\theta}T = -l(l+1)T$$

or

$$\sin\theta\frac{d}{d\theta}\sin\theta\frac{dT}{d\theta} + \left[l(l+1)\sin^2\theta - m^2\right]T = 0$$

This is the same equation we got separating the spherical harmonics.

$$T(\theta) = P_l^m(\cos\theta)$$

$$f_l^m = A P_l^m(\cos\theta)\, e^{im\phi}$$

$$= Y_l^m(\theta, \phi)$$

$\Longrightarrow$ The eigenfunctions of L^2, L_z are the spherical harmonics.

$$L^2 Y_l^m = l(l+1)\hbar^2 Y_l^m$$

$$L_z Y_l^m = m\hbar Y_l^m$$

This means we can build the spherical harmonics with the ladder operators.

$$\hat{L}_+ Y_l^l = 0$$

$$\hbar e^{i\phi}\left(\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\phi}\right) Y_l^l = 0$$

$$Y_l^l = T(\theta)e^{il\phi}$$

$$\frac{\partial Y_l^l}{\partial\phi} = ilTe^{il\phi}$$

$$\frac{\partial}{\partial\theta}Te^{il\phi} + i\cot(\theta)\left(ilTe^{il\phi}\right) = 0$$

$$\frac{\partial}{\partial\theta}T - l\cot(\theta)T = 0$$

$$T = A(\sin\theta)^{\ell}$$

$$Y_{\ell}^{\ell} = A \sin^{\ell}\theta \, e^{i\ell\phi}$$

$\Rightarrow$ We can lower this to build the rest.

Ex The infinite spherical well contains a particle in state

$$\psi = A(r^2 - a^2) \sin\theta \, e^{-i\phi}$$

What values of the angular momentum L^2 and the can be observed.

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

$\Longrightarrow \quad \ell = 1 \qquad m = -1$

$$L^2 = \ell(\ell+1)\hbar^2$$

$$= 1(1+1)\hbar^2 = 2\hbar^2$$

$$L = \sqrt{2}\,\hbar$$

$L_z = -\hbar$

100% prob.

There were elements of the proceeding that were somewhat unnatural. For a radial potential $V(r)$ it would have been natural to write.

$$H = \frac{P_r^2}{2m} + \frac{1}{2} I \omega^2 + V(r)$$

P_r - radial component of momentum

I - moment of inertia

ω - angular frequency

Since the angular momentum is conserved, $L = I\omega$ is a constant.

$$H = \frac{P_r^2}{2m} + \frac{1}{2}\frac{L^2}{I} + V(r)$$

For a point particle orbiting the origin in the x-y plane, $I = mr^2$

$$H = \frac{P_r^2}{2m} + \frac{1}{2}\frac{L^2}{mr^2} + V(r)$$

Quantize

Classically $\quad P_r = \vec{P} \cdot \hat{r}$

QM $\quad \hat{P}_r = \frac{1}{2}\left(\hat{\vec{P}} \cdot \frac{\hat{\vec{R}}}{r} + \frac{\hat{\vec{R}}}{r} \cdot \vec{P} \right)$

$$= \frac{\hbar}{2i}\left(\nabla \cdot \hat{r} + \hat{r} \cdot \nabla \right)$$ dangerous.

but that notation is ambiguous, an operator must operate on something, let it be arbitrary function f.

$$\hat{P}_f f = \frac{\hbar}{2i}\left(\nabla \cdot (\hat{r} f) + \hat{r} \cdot \nabla f \right)$$

Griffiths Cover

$$\nabla \cdot (f\vec{A}) = f\,\nabla \cdot \vec{A} + \vec{A} \cdot \nabla f$$

$$\hat{P}_r f = \frac{\hbar}{2i}\left(f\,\nabla\cdot\hat{r} + \hat{r}\cdot\nabla f + \hat{r}\cdot\nabla f \right)$$

$$\nabla\cdot\hat{r} = \frac{2}{r}$$

$$\hat{P}_r f = \frac{\hbar}{2i}\left(\frac{2f}{r} + 2\,\hat{r}\cdot\nabla f \right)$$

$$= \frac{\hbar}{i}\left(\frac{1}{r} + \hat{r}\cdot\nabla \right) f$$

$$\hat{r}\cdot\nabla = \frac{\partial}{\partial r}$$

$$\hat{P}_r f = \frac{\hbar}{i}\left(\frac{1}{r} + \frac{\partial}{\partial r} \right) f$$

$$= \frac{\hbar}{i}\left(\frac{1}{r}\frac{\partial}{\partial r} r \right) f$$

$$\hat{P}_r = \frac{\hbar}{i}\,\frac{1}{r}\,\frac{\partial}{\partial r}$$

Radial TISE

$$\left[\frac{\hat{p}_r^{\,2}}{2m} + \frac{L^2}{2mr^2} + V(r)\right]\psi = E\psi$$

$$\frac{-\hbar^2}{2m}\frac{1}{r}\frac{\partial}{\partial r} r \frac{1}{r}\frac{\partial}{\partial r} r\psi + \frac{L^2\psi}{2mr^2} + V\psi = E\psi$$

$$\frac{-\hbar^2}{2m}\frac{1}{r}\frac{\partial^2}{\partial r^2} r\psi + \frac{L^2\psi}{2mr^2} + V\psi = E\psi$$

or $$\frac{-\hbar^2}{2mr^2}\frac{\partial}{\partial r} r^2 \frac{\partial\psi}{\partial r} + \frac{\hat{L}^2\psi}{2mr^2} + V\psi = E\psi$$

Rigid Rotor

Consider a moleculer with rotational and translational degrees of freedom. The molecules has moment of inertia I.

$$H = \frac{\vec{P}^2}{2m} + \frac{L^2}{2I} + V$$

If $V=0$, we can separate the rotational and translational energies.

$$E = E_t + E_r$$

$$H_t = \frac{-\hbar^2}{2m} \nabla^2 \quad \text{(operator on center of mass)}$$

$$H_r = \frac{L^2}{2I}$$

Rotational Energies

$$H_r |\psi_n\rangle = E_{rn} |\psi_n\rangle$$

$$\frac{L^2}{2I} |\psi_n\rangle = E_{rn} |\psi_n\rangle$$

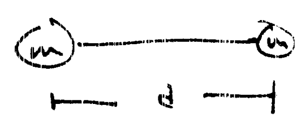
but the eigenvectors of L^2 are $|l\, m\rangle$

$$|\psi_n\rangle = |l\, m\rangle$$

$$\frac{L^2}{2I} |l\, m\rangle = \frac{l(l+1)\hbar^2}{2I} |l\, m\rangle$$

$$E_r = \frac{l(l+1)\hbar^2}{2I}$$

If the object is two masses on a stick



$$I = 2\left(\frac{d}{2}\right)^2 m$$

$$= \frac{1}{2} m d^2$$

The smollest principle moment for woter is

$$I = 1.2\times10^{-40}\ \mathrm{gm\,cm^2}$$

$$= 1.2\times10^{-47}\ \mathrm{Kg\,m^2}$$

The lowest rotational energy is $l=0 \rightarrow E=0$

The second lowest state is $l=1$

$$E_1 = \frac{\hbar^2}{I} = \frac{(1.05\times10^{-34}\ \mathrm{J\cdot s})^2}{1.2\times10^{-47}\ \mathrm{Kg\,m^2}}$$

$$= 9.2\times10^{-22}\ \mathrm{J}$$

$$= hf$$

$$f = 1.4\times10^{12}\ \mathrm{s^{-1}}$$

$$\lambda = \frac{c}{f} = 2.2\times10^{-4}\ \mathrm{m} = 0.2\ \mathrm{mm}$$