Orbital Angular Momentum (continued)

Last time, we showed that

$$R_z(d\varphi)|x,y,z\rangle = \mathbb{1} - \frac{i\,d\varphi}{\hbar} L_z |x,y,z\rangle = \mathbb{1} - \frac{i\,d\varphi}{\hbar}(XP_Y - YP_X)|x,y,z\rangle$$

$$= |x - y\,d\varphi,\ y + x\,d\varphi,\ z\rangle$$

$$\begin{pmatrix} 1 & -d\varphi & 0 \\ d\varphi & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = (x - d\varphi\, y,\ y + d\varphi\, x,\ z)^t$$

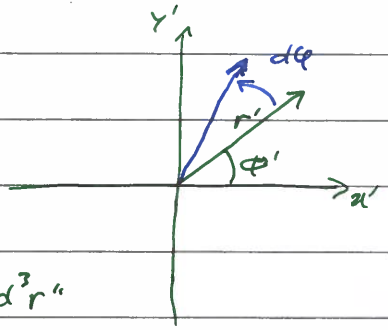
Next consider $R_z(d\varphi)|\psi\rangle$ [$|\psi\rangle$ is a "physical space" ket (with no spin)]

$$= R_z(d\varphi) \int d^3r' |\vec{r}'\rangle\langle\vec{r}'|\psi\rangle$$

$$= \int d^3r' R_z(d\varphi)|\vec{r}'\rangle\langle\vec{r}'|\psi\rangle = \int d^3r' |x' - y'\,d\varphi,\ y' + x'\,d\varphi,\ z'\rangle\langle\vec{r}'|\psi\rangle$$

$$|r', \theta', \phi' + d\varphi\rangle$$

$$= \int d^3r' |r', \theta', \phi' + d\varphi\rangle\langle r', \theta', \phi'|\psi\rangle$$



Change of variable

$$\begin{cases} r'' = r', \ \theta'' = \theta', \ \phi'' = \phi' + d\varphi \\ dr'' = dr', \ d\theta'' = d\theta', \ d\phi'' = d\phi' \Rightarrow d^3r' = d^3r'' \end{cases}$$

$$\int d^3r'' |r'', \theta'', \phi''\rangle\langle r'', \theta'', \phi'' - d\varphi|\psi\rangle$$

$\psi(r'', \theta'', \phi'' - d\varphi)$ → Taylor expand

$$\simeq \int d^3r'' |\vec{r}''\rangle \left(\psi(r'', \theta'', \phi'') - \frac{\partial}{\partial\phi''}\psi(r'', \theta'', \phi'')\,d\varphi + \text{higher orders}\right)$$

$$\simeq \int d^3r'' |\vec{r}''\rangle\langle\vec{r}''|\psi\rangle - d\varphi \int d^3r'' |\vec{r}''\rangle \frac{\partial}{\partial\phi''}\langle\vec{r}''|\psi\rangle + \text{higher orders}$$

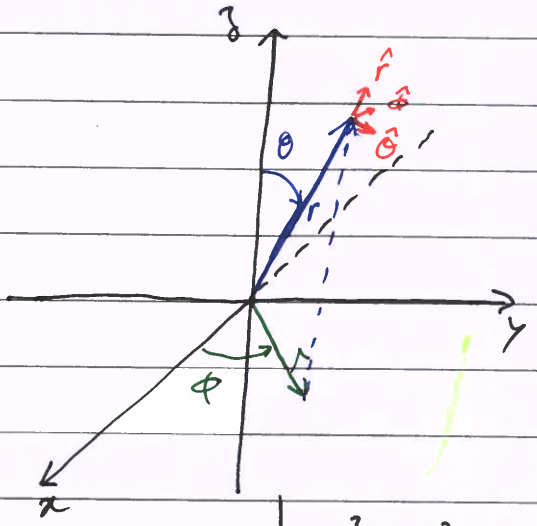
$$\simeq \left[\mathbb{1} - d\varphi\left(\int d^3r'' |\vec{r}''\rangle \frac{\partial}{\partial\phi''}\langle\vec{r}''|\right)\right]|\psi\rangle \Rightarrow \boxed{L_z = -i\hbar \int d^3r\, |\vec{r}\rangle \frac{\partial}{\partial\phi}\langle\vec{r}|}$$

$\mathbb{1}$; $\int d^3r'' |\vec{r}''\rangle \frac{\partial}{\partial\phi''}\langle\vec{r}''| = \frac{i}{\hbar} L_z$

L_z operator in the R-representation

Spherical coordinates reminder

$$x = r\sin\theta\cos\phi$$
$$y = r\sin\theta\sin\phi$$
$$z = r\cos\theta$$
$$r = \sqrt{x^2+y^2+z^2}$$



unit vectors

$\hat{r}\cdot\hat{\theta} = 0,\ \hat{r}\cdot\hat{\phi} = 0,\ \hat{\theta}\cdot\hat{\phi} = 0$

$\hat{r}\times\hat{\theta} = \hat{\phi},\ \hat{\theta}\times\hat{\phi} = \hat{r},\ \hat{\phi}\times\hat{r} = \hat{\theta}$

$$\hat{r} = \sin\theta\cos\phi\,\hat{x} + \sin\theta\sin\phi\,\hat{y} + \cos\theta\,\hat{z}$$
$$\hat{\theta} = \cos\theta\cos\phi\,\hat{x} + \cos\theta\sin\phi\,\hat{y} - \sin\theta\,\hat{z}$$
$$\hat{\phi} = -\sin\phi\,\hat{x} + \cos\phi\,\hat{y}$$

$$d^3r = r^2\sin\theta\,dr\,d\theta\,d\phi = dx\,dy\,dz$$

Derivative:
$$\vec{\nabla} = \frac{\partial}{\partial r}\hat{r} + \frac{1}{r}\frac{\partial}{\partial\theta}\hat{\theta} + \frac{1}{r\sin\theta}\frac{\partial}{\partial\phi}\hat{\phi}$$

$$\nabla^2 = \underbrace{\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)}_{\frac{1}{r}\frac{\partial^2}{\partial r^2}(r\psi)} + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}$$

In the R-representation:

$$L_z = XP_y - YP_x \longrightarrow \langle\vec{r}\,|\,L_z\,|\psi\rangle = -i\hbar\left[x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right]\psi(\vec{r})$$

$$\Leftrightarrow \boxed{\langle\vec{r}\,|\,L_z\,|\psi\rangle = -i\hbar\frac{\partial}{\partial\phi}\psi(r,\theta,\phi)}$$

$$L_x = yP_z - zP_y \rightarrow \langle \vec{r}|L_x|\psi\rangle = -i\hbar\left[y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right]\psi(\vec{r})$$

$$\Longleftrightarrow \boxed{\langle \vec{r}|L_x|\psi\rangle = -i\hbar\left[-\sin\phi\frac{\partial}{\partial\theta} - \cot\theta\cos\phi\frac{\partial}{\partial\phi}\right]\psi(r,\theta,\phi)}$$

$$L_y = zP_x - xP_z \rightarrow \langle \vec{r}|L_y|\psi\rangle = -i\hbar\left[z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right]\psi(\vec{r})$$

$$\Longleftrightarrow \boxed{\langle \vec{r}|L_y|\psi\rangle = -i\hbar\left[\cos\phi\frac{\partial}{\partial\theta} - \cot\theta\sin\phi\frac{\partial}{\partial\phi}\right]\psi(r,\theta,\phi)}$$

Since $L_\pm = L_x \pm iL_y$, then

$$\boxed{\langle \vec{r}|L_\pm|\psi\rangle = -i\hbar\, e^{\pm i\phi}\left[\pm i\frac{\partial}{\partial\theta} - \cot\theta\frac{\partial}{\partial\phi}\right]\psi(r,\theta,\phi)}$$

After some algebra, we have

$$\boxed{\langle \vec{r}|\vec{L}^2|\psi\rangle = -\hbar^2\left[\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)\right]\psi(r,\theta,\phi)}$$

Spherical Harmonics

The spherical harmonics are the eigenstates of $\vec{L}^2$ and L_z: $|l,m\rangle$

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

$$L_z|l,m\rangle = \hbar m|l,m\rangle$$

$$\langle \vec{r}|l,m\rangle = Y_l^m(\theta,\phi)$$

$$\langle \vec{r} | L_z | l,m \rangle = \hbar m \langle \vec{r} | l,m \rangle$$

$$\Leftrightarrow -i\hbar \frac{\partial}{\partial \phi} Y_l^m(\theta,\phi) = \hbar m Y_l^m(\theta,\phi)$$

$$\Leftrightarrow \frac{\partial}{\partial \phi} Y_l^m(\theta,\phi) = i m Y_l^m(\theta,\phi)$$

$$\Rightarrow \boxed{Y_l^m(\theta,\phi) = e^{im\phi} f_{lm}(\theta)}$$

$\Rightarrow$ m must be an integer (not a half-integer) for the function to be single-valued since $0 \leq \phi < 2\pi$

$\Rightarrow$ orbital angular momentum requires l = integer.

(see Sakurai & Napolitano p193-194)

Next, we consider the largest value of $m = l$

$\rightarrow$ we know that $\langle \vec{r} | L_+ | l,m \rangle = 0$

$$\Leftrightarrow -i\hbar e^{\pm i\phi} \left[\frac{i\partial}{\partial\theta} - \cot\theta \frac{\partial}{\partial\phi} \right] \underbrace{Y_l^m(\theta,\phi)}_{e^{il\phi} f_{ll}(\theta)} = 0$$

$$\Rightarrow \frac{\partial}{\partial\theta} f_{ll}(\theta) e^{il\phi} - \underbrace{\cot\theta}_{\frac{\cos\theta}{\sin\theta}} (il) e^{il\phi} f_{ll}(\theta) = 0$$

$$\Leftrightarrow \sin\theta \frac{\partial}{\partial\theta} f_{ll}(\theta) = l \cos\theta f_{ll}(\theta)$$

$$\Rightarrow f_{ll}(\theta) = \sin^l(\theta)$$

normalization

$$\Rightarrow \boxed{Y_l^l(\theta,\phi) = N_{ll} e^{il\phi} \sin^l\theta}$$

Normalization: we require $\langle l, m=l \mid l, m=l \rangle = 1$

$$\Leftrightarrow \int Y_l^{*l}(\theta,\phi)\, Y_l^{l}(\theta,\phi)\, d\Omega = 1$$

$d\Omega = r^2 \sin\theta\, dr\, d\theta\, d\phi$

$$\Leftrightarrow |N_{ll}|^2 \int_0^{2\pi}\int_0^{\pi} \left(e^{-il\phi}\sin^l(\theta)\right)\left(e^{il\phi}\sin^l(\theta)\right)\sin\theta\, d\theta\, d\phi = 1$$

$$\Leftrightarrow |N_{ll}|^2 2\pi \int_0^{\pi} \underbrace{\sin^{2l+1}(\theta)\, d\theta}_{\sin\theta\,(\sin^2\theta)^l \,=\, \sin\theta\,(1-\cos^2\theta)^l} = 1$$

change of variable

$z = \cos\theta$

$dz = -\sin\theta\, d\theta$

$$\Rightarrow |N_{ll}|^2 2\pi (-1)\int_1^{-1} (1-z^2)^l\, dz = 1 \Leftrightarrow |N_{ll}|^2 2\pi \underbrace{\int_{-1}^{1} (1-z^2)^l\, dz}_{\frac{2\cdot 2^{2l}(l!)^2}{(2l)!(2l+1)}} = 1$$

$$\Rightarrow N_{ll} = \frac{(-1)^l}{2^l l!}\sqrt{\frac{(2l+1)(2l)!}{4\pi}}$$

$(-1)^l$ is a phase convention

$$\Rightarrow Y_{ll}(\theta,\phi) = N_{ll}\, e^{il\phi}\sin^l(\theta) = \frac{(-1)^l}{2^l l!}\sqrt{\frac{(2l+1)(2l)!}{4\pi}}\, e^{il\phi}\sin^l\theta$$

Next, $L_-|l, m\rangle = \sqrt{l(l+1)-m(m-1)}\,|l, m-1\rangle$

$$\Rightarrow -i\hbar\, e^{-i\phi}\left(-i\frac{\partial}{\partial\theta} - \cot\theta\, i\frac{\partial}{\partial\phi}\right) Y_l^m(\theta,\phi) = \hbar\sqrt{l(l+1)-m(m-1)}\, Y_l^{m-1}(\theta,\phi)$$

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

$$\Rightarrow Y_\ell^{m-1}(\theta,\phi) = \frac{1}{\sqrt{\ell(\ell+1)-m(m-1)}}\left(-\frac{\partial}{\partial\theta} - m\cot\theta\right) Y_\ell^m(\theta,\phi)$$

Examples:

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

$\underline{\ell=1} \Rightarrow \begin{cases} Y_1^0(\theta,\phi) = \sqrt{\frac{3}{4\pi}}\cos\theta = \sqrt{\frac{3}{4\pi}}\frac{z}{r} \\ Y_1^{\pm1}(\theta,\phi) = \mp\sqrt{\frac{3}{8\pi}}\sin\theta\cdot e^{\pm i\phi} \\ \quad = \mp\sqrt{\frac{3}{8\pi}}\frac{x\pm iy}{r} \end{cases}$

"spherical components of a cartesian vector"

$\underline{\ell=2} \Rightarrow \begin{cases} Y_2^0(\theta,\phi) = \sqrt{\frac{5}{16\pi}}\left(3\cos^2\theta - 1\right) \\ Y_2^{\pm1}(\theta,\phi) = \mp\sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta\cdot e^{\pm i\phi} \\ Y_2^{\pm2}(\theta,\phi) = \sqrt{\frac{15}{32\pi}}\sin^2\theta\cdot e^{\pm i2\phi} \end{cases}$