Orbital Angular Momentum

Higher Dimension

- One dimension:

$$[\hat{X}, \hat{P}] = i\hbar; \hat{P} = -i\hbar\frac{\partial}{\partial x}$$

- Higher dimension extention:

$$[\hat{X}_i, \hat{P}_j] = i\hbar\delta_{ij}; \hat{P}_j = -i\hbar\frac{\partial}{\partial x_j}$$

Angular Momentum

$$\vec{L} = \vec{X} \times \vec{P}$$

$$\hat{L}_x = \hat{y}\hat{P}_z - \hat{z}\hat{P}_y$$

$$\hat{L}_y = \hat{z}\hat{P}_x - \hat{x}\hat{P}_z$$

$$\hat{L}_z = \hat{x}\hat{P}_y - \hat{y}\hat{P}_x$$

$$\hat{L}_i = \sum_{jk} \epsilon_{ijk}\hat{x}_j\hat{P}_k$$

$$\epsilon_{ijk} = -\epsilon_{jik} = -\epsilon_{ikj}$$

Antisymmetric tensor: [xyz]=1, [yxz]= -1, [xxz]=0

Commutation Relation of Angular Momentum

$$[\hat{L}_i, \hat{L}_j] = i\hbar\epsilon_{ijk}\hat{L}_k$$

$$[\hat{x}_i, \hat{L}_j] = i\hbar\epsilon_{ijk}\hat{x}_k$$

$$[\hat{P}_i, \hat{L}_j] = i\hbar\epsilon_{ijk}\hat{P}_k$$

Total Angular momentum:

$$\hat{L}^2 = \hat{L}\cdot\hat{L} = \sum_{i=x,y,z}\hat{L}_i^2$$

$$[\hat{L}^2, \hat{L}_i] = 0$$

More Algebra

- Define

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

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

$$[\hat{L}_+, \hat{L}_-] = 2\hbar\hat{L}_z$$

$$\hat{L}^2 = \hat{L}_+\hat{L}_- + \hat{L}_z^2 - \hbar\hat{L}_z$$

Eigenstates of Angular Momentum

- We can choose $\{\hat{L}^2, \hat{L}_z\}$ to find eigenstates

$$\hat{L}^2|\psi> = L|\psi>; \hat{L}_z|\psi> = M|\psi>$$

- Result:

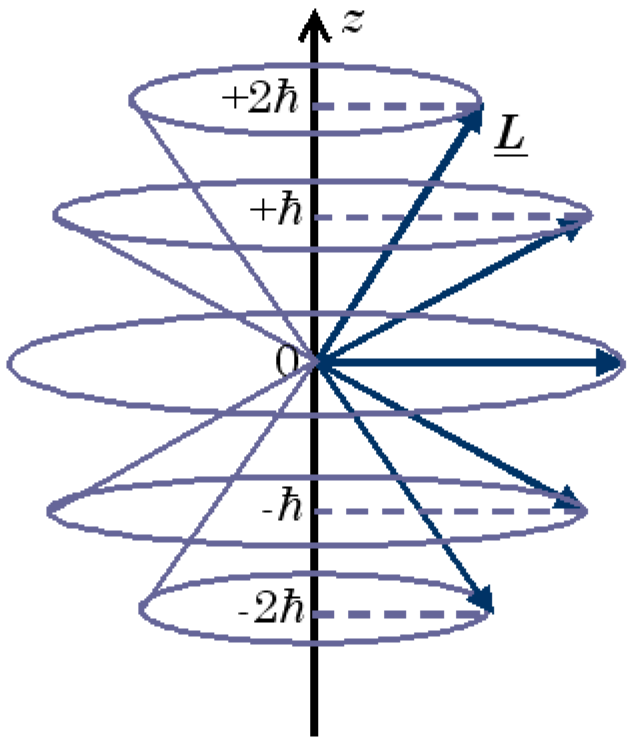
$$|\psi> = |l,m>; l = 1,2..., m = -l, -l+1, ...l$$

$$\hat{L}^2|l,m> = \hbar^2 l(l+1)|l,m>; \hat{L}_z|l,m> = m\hbar|l,m>$$

Eigenstates of Angular Momentum

$$|\psi>=|l,m>; l=1,2...,m=-l,-l+1,...l$$

$$\hat{L}_{\pm}|l,m>=\hbar\sqrt{l(l+1)-m(m\pm 1)}|l,m\pm 1>;$$



Angular Momentum in Spherical Coordinates

$$\vec{r} = r(sin\theta cos\phi, sin\theta sin\phi, cos\theta)$$

$$\vec{e}_\theta = (cos\theta cos\phi, cos\theta sin\phi, -sin\theta)$$

$$\vec{e}_\phi = (-sin\phi, cos\phi, 0)$$

$$\vec{\nabla} = e_r \frac{\partial}{\partial r} + e_\theta \frac{1}{r}\frac{\partial}{\partial \theta} + e_\phi \frac{1}{r sin\theta}\frac{\partial}{\partial \phi}$$

$$\vec{L} = -i\hbar \vec{r} \times \vec{\nabla}$$

$$L_x = -i\hbar(-sin\phi \frac{\partial}{\partial \theta} - cos\phi cot\theta \frac{\partial}{\partial \phi})$$

$$L_y = -i\hbar(cos\phi \frac{\partial}{\partial \theta} - sin\phi cot\theta \frac{\partial}{\partial \phi})$$

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

$$\vec{r} \times \vec{r} = 0; \vec{e}_r \times \vec{e}_\theta = e_\phi; \vec{e}_r \times \vec{e}_\phi = -e_\theta;$$

Angular Momentum in Spherical Coordinates

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

$$Y_l^m(\theta, \phi >=< \vec{r}|lm >$$

$$\hat{L}^2 Y_l^m(\theta, \phi) = l(l+1)\hbar^2 Y_l^m(\theta, \phi)$$

$$\hat{L}_z Y_l^m(\theta, \phi) = m\hbar Y_l^m(\theta, \phi)$$

Y: Spherical hamonics

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

Tables of Spherical Harmoics

L=0:
(S-wave)

$$s = Y_0^0 = \frac{1}{2}\sqrt{\frac{1}{\pi}}$$

L=1:
(P-wave)

$$Y_1^{-1}(\theta,\varphi) = \frac{1}{2}\sqrt{\frac{3}{2\pi}} \cdot e^{-i\varphi} \cdot \sin\theta \quad = \frac{1}{2}\sqrt{\frac{3}{2\pi}} \cdot \frac{(x-iy)}{r}$$

$$Y_1^{0}(\theta,\varphi) = \frac{1}{2}\sqrt{\frac{3}{\pi}} \cdot \cos\theta \quad = \frac{1}{2}\sqrt{\frac{3}{\pi}} \cdot \frac{z}{r}$$

$$Y_1^{1}(\theta,\varphi) = \frac{-1}{2}\sqrt{\frac{3}{2\pi}} \cdot e^{i\varphi} \cdot \sin\theta \quad = \frac{-1}{2}\sqrt{\frac{3}{2\pi}} \cdot \frac{(x+iy)}{r}$$

$$p_x = \sqrt{\frac{1}{2}}\left(Y_1^{-1} - Y_1^{1}\right) = \sqrt{\frac{3}{4\pi}} \cdot \frac{x}{r}$$

$$p_y = i\sqrt{\frac{1}{2}}\left(Y_1^{-1} + Y_1^{1}\right) = \sqrt{\frac{3}{4\pi}} \cdot \frac{y}{r}$$

$$p_z = Y_1^0 = \sqrt{\frac{3}{4\pi}} \cdot \frac{z}{r}$$

L=2:
(d-wave)

$$Y_2^{-2}(\theta,\varphi) = \frac{1}{4}\sqrt{\frac{15}{2\pi}} \cdot e^{-2i\varphi} \cdot \sin^2\theta \quad = \frac{1}{4}\sqrt{\frac{15}{2\pi}} \cdot \frac{(x-iy)^2}{r^2}$$

$$Y_2^{-1}(\theta,\varphi) = \frac{1}{2}\sqrt{\frac{15}{2\pi}} \cdot e^{-i\varphi} \cdot \sin\theta \cdot \cos\theta \quad = \frac{1}{2}\sqrt{\frac{15}{2\pi}} \cdot \frac{(x-iy)z}{r^2}$$

$$Y_2^{0}(\theta,\varphi) = \frac{1}{4}\sqrt{\frac{5}{\pi}} \cdot (3\cos^2\theta - 1) \quad = \frac{1}{4}\sqrt{\frac{5}{\pi}} \cdot \frac{(-x^2-y^2+2z^2)}{r^2}$$

$$Y_2^{1}(\theta,\varphi) = \frac{-1}{2}\sqrt{\frac{15}{2\pi}} \cdot e^{i\varphi} \cdot \sin\theta \cdot \cos\theta \quad = \frac{-1}{2}\sqrt{\frac{15}{2\pi}} \cdot \frac{(x+iy)z}{r^2}$$

$$Y_2^{2}(\theta,\varphi) = \frac{1}{4}\sqrt{\frac{15}{2\pi}} \cdot e^{2i\varphi} \cdot \sin^2\theta \quad = \frac{1}{4}\sqrt{\frac{15}{2\pi}} \cdot \frac{(x+iy)^2}{r^2}$$

$$d_{z^2} = Y_2^0 = \frac{1}{4}\sqrt{\frac{5}{\pi}} \cdot \frac{-x^2-y^2+2z^2}{r^2}$$

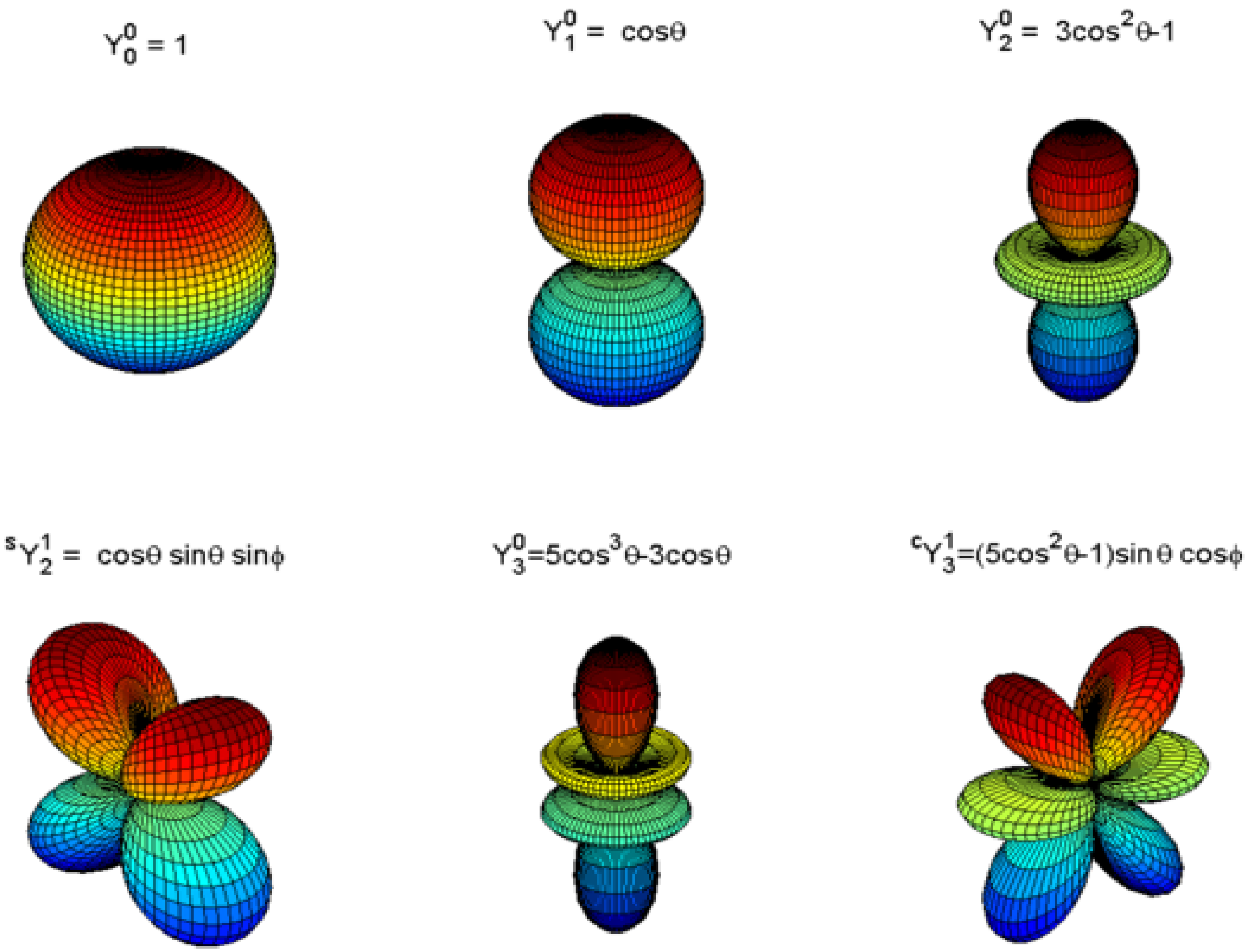
$$d_{yz} = i\sqrt{\frac{1}{2}}\left(Y_2^{-1} + Y_2^{1}\right) = \frac{1}{2}\sqrt{\frac{15}{\pi}} \cdot \frac{yz}{r^2}$$

$$d_{xz} = \sqrt{\frac{1}{2}}\left(Y_2^{-1} - Y_2^{1}\right) = \frac{1}{2}\sqrt{\frac{15}{\pi}} \cdot \frac{zx}{r^2}$$

$$d_{xy} = i\sqrt{\frac{1}{2}}\left(Y_2^{-2} - Y_2^{2}\right) = \frac{1}{2}\sqrt{\frac{15}{\pi}} \cdot \frac{xy}{r^2}$$

$$d_{x^2-y^2} = \sqrt{\frac{1}{2}}\left(Y_2^{-2} + Y_2^{2}\right) = \frac{1}{4}\sqrt{\frac{15}{\pi}} \cdot \frac{x^2-y^2}{r^2}$$

Imagine of orbital



Particle in Central potential

$$\hat{H} = -\frac{\hbar^2}{2m}\vec{\nabla}^2 + V(r)$$

$$\nabla^2 = \frac{1}{2mr^2}\frac{\partial}{\partial r}(r^2\frac{\partial}{\partial r}) - \frac{L^2}{2\hbar^2 r^2}$$

$$\hat{H}\Psi(r,\theta,\phi) == [-\hbar^2\frac{1}{r^2}\frac{\partial}{\partial r}(r^2\frac{\partial}{\partial r}) + \frac{L^2}{2mr^2} + V(r)]\Psi(r,\theta,\phi) = E\Psi(r,\theta,\phi)$$

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

$$\hbar^2[-\frac{1}{r^2}\frac{\partial}{\partial r}(r^2\frac{\partial}{\partial r}) + \frac{l(l+1)^2}{2mr^2} + V(r)]\phi(r) = E\phi(r)$$