Lecture 7 : Orbital angular momentum

A particle which moves through physical space can posess angular momentum associated with its "orbit".

$$\hat{\vec{L}} = \hat{\vec{x}} \times \hat{\vec{p}}$$

Using the canonical commutator $[\hat{x}_i, \hat{p}_j] = i\hbar\, \delta_{ij}$, we have shown in homework that

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

$\Rightarrow$ $\hat{\vec{L}}$ is the generator of rotations in physical space.

$\Rightarrow$ $\hat{D}(\phi) = e^{-i \hat{L}_z \phi/\hbar}$ = rotation operator about z-axis

$$\hat{D}^\dagger(\phi)\, \hat{x}_i\, \hat{D}(\phi) = R_{ij}(\phi)\, \hat{x}_j$$

where $\mathbb{R}(\phi) = \begin{bmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$

The eigenvectors of $\mathbb{R}(\phi)$ $\Rightarrow$ "Spherical basis"

$$\vec{e}_\pm = \mp \left(\frac{\vec{e}_x \pm i \vec{e}_y}{\sqrt{2}} \right) \qquad \vec{e}_0 = \vec{e}_z$$

phase convention

$q = 0, \pm 1 \qquad \mathbb{R}(\phi)\, \vec{e}_q = e^{-iq\phi}\, \vec{e}_q$

Position representation $\quad \hat{\vec{p}} \doteq -i\hbar \vec{\nabla}$

$$\hat{\vec{x}} \doteq \vec{x}$$

Cartesian coords:

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

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

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

$$\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2 = \hat{L}_\mp \hat{L}_\pm \pm \hat{L}_z(\hat{L}_z \pm 1)$$

$$\hat{L}_\pm = \hat{L}_x \pm i\hat{L}_y = \hbar\left[(-x-iy)\frac{\partial}{\partial z} + z\left(\frac{\partial}{\partial x} + i\frac{\partial}{\partial y}\right)\right]$$

Spherical basis $\quad \left(x_\pm \equiv \mp\left(\frac{x \pm iy}{\sqrt{2}}\right),\ z\right)$

$$\Rightarrow \frac{\partial}{\partial x} = \frac{1}{\sqrt{2}}\left(-\frac{\partial}{\partial x_+} + \frac{\partial}{\partial x_-}\right), \quad \frac{\partial}{\partial y} = \frac{-i}{\sqrt{2}}\left(\frac{\partial}{\partial x_+} + \frac{\partial}{\partial x_-}\right)$$

Dimensionless operators: $\hat{\vec{\ell}} \equiv \hat{\vec{L}}/\hbar$

$$\Rightarrow \boxed{\begin{aligned} \hat{\ell}_z &\doteq x_+\frac{\partial}{\partial x_+} - x_-\frac{\partial}{\partial x_-} \\ \hat{\ell}_+ &\doteq \sqrt{2}\left(x_+\frac{\partial}{\partial z} + z\frac{\partial}{\partial x_-}\right) \\ \hat{\ell}_- &\doteq -\sqrt{2}\left(x_-\frac{\partial}{\partial z} + z\frac{\partial}{\partial x_+}\right) \\ \hat{\ell}^2 &= \hat{\ell}_\mp \hat{\ell}_\pm + \hat{\ell}_z(\hat{\ell}_z \pm 1) \end{aligned}}$$

Solid Harmonics

Abstract eigenkets $|l,m\rangle$: $\hat{l}^2|l,m\rangle = l(l+1)|l,m\rangle$

$\hat{l}_z|l,m\rangle = m|l,m\rangle$

We seek position representation:

$$\langle\vec{x}|l,m\rangle \equiv \mathcal{Y}_l^m(\vec{x}) \; : \; \text{"solid harmonics"}$$

"spherical tensors"

___: $x_\pm$ and z are eigenfunctions with $l=1$ and $m=\pm 1$ and 0

$$\hat{l}_z x_\pm = \left(x_+ \frac{\partial}{\partial x_+} - x_- \frac{\partial}{\partial x_-}\right) = (\pm 1)\, x_\pm$$

$$\hat{l}_z z = 0$$

$$\hat{l}_+ x_+ = 0 \, , \quad \hat{l}_- x_- = 0 \, , \quad \begin{cases} \hat{l}_\pm x_\mp = \sqrt{2}\, z \\ \hat{l}_\pm z = \sqrt{2}\, x_\pm \end{cases}$$

$$\Rightarrow \hat{l}^2 x_\pm = \left(\hat{l}_\mp \hat{l}_\pm + \hat{l}_z(\hat{l}_z \pm 1)\right) x_\pm = 1(1+1)\, x_+$$

$$= 2\, x_\pm = l(l+1)\, x_\pm \quad \text{with } l = 1$$

$$\hat{l}^2 z = \hat{l}_- \hat{l}_+ z = \sqrt{2}\, \hat{l}_- x_+ = 2z = l(l+1)\, z$$

$$\Rightarrow \mathcal{Y}_1^{\pm 1} = N_1\, x_\pm = \pm \frac{N_1}{\sqrt{2}}(x \pm iy)$$

$$\mathcal{Y}_1^0 = N_1\, z = N_1\, z$$

where N_1 is a normalization constant

Lemma: $(x_+)^\ell$ is the eigenfunction $\langle\vec{x}|\,\ell,\underset{\substack{\uparrow\\ \text{max } m}}{\ell}\,\rangle$

Proof: $\hat{\ell}_z (x_+)^\ell = \left(x_-\frac{\partial}{\partial x_-} + x_+\frac{\partial}{\partial x_+}\right)(x_+)^\ell$

$$= x_+ \frac{d}{dx_+}(x_+)^\ell = x_+\left(\ell\, x_+^{\ell-1}\right) = \underset{\substack{\uparrow\\ m}}{\ell}(x_+)^\ell$$

$$\hat{\ell}^2 (x_+)^\ell = \left[\hat{\ell}_-\hat{\ell}_+ + \hat{\ell}_z(\hat{\ell}_z+1)\right](x_+)^\ell = \ell(\ell+1)\,(x_+)^\ell$$

$\Rightarrow$ q.e.d.

c_ℓ in text

Thus $$y_\ell^\ell(\vec{x}) = \underset{\substack{\Uparrow\\ \text{Normalization}}}{N_\ell}\,(x_+)^\ell = (\mp 1)^\ell \frac{N_\ell}{2^{\ell/2}}(x \pm iy)^\ell$$

Find other m-values with ladder operators

$$\hat{\ell}_-\, y_\ell^m(\vec{x}) = \sqrt{\ell(\ell+1) - m(m-1)}\; y_\ell^{m-1}(\vec{x})$$

$$= \sqrt{2}\left(x_-\frac{\partial}{\partial z} + z\frac{\partial}{\partial x_+}\right) y_\ell^m$$

$$\Rightarrow \boxed{y_\ell^{m-1}(\vec{x}) = \sqrt{\frac{2}{\ell(\ell+1)-m(m-1)}}\left(x_-\frac{\partial}{\partial z} + z\frac{\partial}{\partial x_+}\right) y_\ell^m}$$

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<u>Examples:</u>

- $\underline{l=0}$ $\quad Y_0^0 = N_0 (x_+)^0 = N_0$ $\quad$ <u>constant</u>

- $\underline{l=1}$ $\quad \boxed{Y_1^1 = N_1 (x_+) = -\frac{N_1}{\sqrt{2}}(x+iy)}$ $\qquad m=1$

$$\hat{l}_- Y_1^1 = \sqrt{1(1+1)-1(1-1)}\; Y_1^0 = \sqrt{2}\, Y_1^0$$

$$= \sqrt{2}\left(x_- \frac{\partial}{\partial z} + z\frac{\partial}{\partial x_+}\right) N_1 x_+ = \sqrt{2}\, N_1\, z$$

$$\Rightarrow \boxed{Y_1^0 = N_1 z} \qquad m=0$$

$$\hat{l}_- Y_1^0 = \sqrt{1(1+1)-0(1-0)}\; Y_1^{-1} = \sqrt{2}\, Y_1^{-1}$$

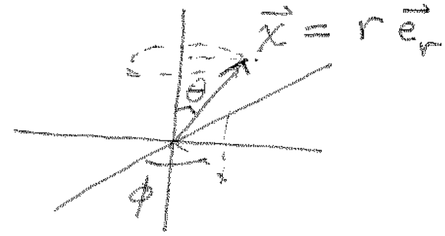
$$= \sqrt{2}\left(x_- \frac{\partial}{\partial z} + z\frac{\partial}{\partial x_+}\right) N_1 z = \sqrt{2}\, N_1\, x_-$$

$$\Rightarrow \boxed{Y_1^{-1} = N_1 x_- = \frac{N_1}{\sqrt{2}}(x-iy)}$$

- <u>Similarly</u> $l=2$

$$\boxed{\begin{aligned} Y_2^{\pm 2} &= N_2 (x_\pm)^2 = \frac{N_2}{2}(x \pm iy)^2 \\ Y_2^{\pm 1} &= \mp N_2\, x_\pm z = \mp N_2 (x \pm iy) z \\ Y_2^0 &= \frac{N_2}{\sqrt{6}}(x_+ x_- + 2z^2) = \frac{N_2}{\sqrt{\;}}(3z^2 - r^2) \end{aligned}}$$

Spherical Harmonics



Spherical coordinates:
(r, θ, ϕ)

$\vec{e}_r \equiv \frac{\vec{x}}{r}$ direction in space

$$\left.\begin{aligned} x &= r\sin\theta\cos\phi \\ y &= r\sin\theta\sin\phi \end{aligned}\right\} \Rightarrow x_\pm = \mp r\, e^{\pm i\phi}$$

$$z = r\cos\theta$$

Rotation about the z-axis by ϕ_0: $\hat{D} = e^{-i\phi_0 \hat{\ell}_z}$

Start with state $|\psi\rangle$ $\quad\begin{pmatrix} r \to r,\ \theta \to \theta \\ \phi \to \phi + \phi_0 \end{pmatrix}$

Rotated state $|\psi'\rangle = \hat{D}|\psi\rangle$

$$\psi'(\vec{x}) = \psi'(r,\theta,\phi) = \langle \vec{x}|\psi'\rangle = \psi(r,\theta,\phi-\phi_0)$$

shifted by ϕ_0

Suppose infinitesimal $\phi_0 = \delta\phi$

$$\Rightarrow \psi'(\vec{x}) = \psi(r,\theta,\phi) - \delta\phi \frac{\partial \psi}{\partial \phi}(r,\theta,\phi) \quad \text{to first order}$$

But $\psi'(\vec{x}) = (1 - i\delta\phi\, \hat{\ell}_z)\,\psi(\vec{x})$

$$\Rightarrow \boxed{\hat{\ell}_z \doteq -i\frac{\partial}{\partial\phi}} \quad \text{Generator of rotation } \phi \to \phi + \phi_0$$

Eigenfunctions $\hat{\ell}_z \Phi_m(\phi) = m\,\Phi_m(\phi)$

$$\Rightarrow \boxed{\Phi_m(\phi) = A_m e^{+im\phi}}$$

Single valued $\Rightarrow e^{i2\pi m} = 1$
$\Rightarrow m$ integer

Can show: $\begin{cases} \hat{\ell}_x = i\left(\sin\phi \frac{\partial}{\partial\theta} + \frac{\cos\phi}{\tan\theta} \frac{\partial}{\partial\phi}\right) \\ \hat{\ell}_y = i\left(-\cos\phi \frac{\partial}{\partial\theta} + \frac{\sin\phi}{\tan\theta} \frac{\partial}{\partial\phi}\right) \end{cases}$

$\Rightarrow$ Eigenfunctions of $\hat{\ell}_i$ depend only on <u>direction in space</u>, $\vec{e}_r$ and not $|\vec{x}| = r$

Define: $\boxed{\text{Spherical Harmonics}: \; Y_\ell^m(\theta,\phi) \equiv \mathcal{Y}_\ell^m\left(\frac{\vec{x}}{r}\right)}$

Note $\mathcal{Y}_\ell^m\left(\frac{\vec{x}}{r}\right) = \frac{1}{r^\ell} \mathcal{Y}_\ell^m$

$\therefore \; Y_0^0 = N_0$

$$\begin{cases} Y_1^{\pm 1} = \mp \frac{N_1}{\sqrt{2}} \left(\frac{x \pm iy}{r}\right) = \mp \frac{N_1}{\sqrt{2}} \sin\theta \, e^{\pm i\phi} \\ Y_1^0 = N_1\left(\frac{z}{r}\right) = N_1 \cos\theta \end{cases}$$

$$\begin{cases} Y_2^{\pm 2} = \frac{N_2}{2} \left(\frac{x \pm iy}{r}\right)^2 = \frac{N_2}{2} \sin^2\theta \, e^{\pm 2i\phi} \\ Y_2^{\pm 1} = \mp N_2 \left(\frac{x \pm iy}{r}\right)\left(\frac{z}{r}\right) = \mp N_2 \sin\theta\cos\theta \, e^{i\phi} \\ Y_2^0 = \frac{N_2}{\sqrt{6}} \left(\frac{3z^2 - r^2}{r^2}\right) = \frac{N_2}{\sqrt{6}} \left(3\cos^2\theta - 1\right) \end{cases}$$

Note: $\boxed{Y_\ell^m(\theta,\phi) = \underbrace{P_\ell^m}_{\text{Associate Legendre polynomial}}(\cos\theta) \, e^{im\phi}}$

Properties of Spherical Harmonics

Can think of $Y_\ell^m(\theta,\phi) = \langle \vec{e}_r | \ell, m\rangle$

where $|\vec{e}_r\rangle$ is the "direction eigenket" $|\frac{\vec{x}}{r}\rangle$

$$\langle \vec{e}_r | \vec{e}_r{}'\rangle = \delta(\phi-\phi')\,\delta(\cos\theta - \cos\theta')$$

Integration over sphere: solid angle $d\Omega_{\vec{e}_r}$

$$da = r^2 d\Omega_{\vec{e}_r} = r^2\, d(\cos\theta)\, d\phi$$

$$-1 < \cos\theta < 1$$

Inner product over sphere:

$$\langle f|g\rangle = \int d\Omega_{e_r}\, f^*(\theta,\phi)\, g(\theta,\phi)$$

Orthogonality

$$\langle \ell m | \ell' m'\rangle = \delta_{\ell,\ell'}\,\delta_{mm'}$$

$$\Rightarrow \boxed{\int d\Omega_{\vec{e}_r}\, Y_\ell^{m*}(\theta,\phi)\, Y_{\ell'}^{m'}(\theta,\phi) = \delta_{\ell,\ell'}\,\delta_{mm'}}$$

Completeness: $\sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} |\ell m\rangle\langle \ell m| = \hat{\mathbb{1}}$

$$\Rightarrow \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell} Y_\ell^m(\theta,\phi)\, Y_\ell^{m*}(\theta',\phi') = \delta(\phi-\phi')\,\delta(\cos\theta-\cos\theta')$$

$$|\Psi\rangle = \sum_{\ell,m} \psi_{\ell,m}|\ell,m\rangle \Rightarrow \psi(\theta,\phi) = \sum_{\ell,m} \psi_{\ell,m}\, Y_\ell^m(\theta,\phi)$$

$$\psi_{\ell,m} = \langle \ell m|\psi\rangle$$

Normalization constant: $Y_\ell^\ell = N_\ell \frac{(-1)^\ell}{2^{\ell/2}} \sin^\ell\theta \, e^{i\ell\phi}$

$$\langle \ell\ell | \ell\ell \rangle = 1 = \int d\Omega \, |Y_\ell^\ell|^2 = \frac{|N_\ell|^2}{2^\ell} \underbrace{\int d\Omega \sin^{2\ell}\theta}_{\frac{4\pi}{(2\ell+1)!} 2^{2\ell}(\ell!)^2}$$

$$\Rightarrow N_\ell = \frac{1}{\ell!} \frac{1}{2^{\ell/2}} \sqrt{\frac{(2\ell+1)!}{4\pi}} \quad \text{(phase convention)}$$

$$\Rightarrow \boxed{Y_\ell^\ell = \frac{(-1)^\ell}{\ell! \, 2^\ell} \left(\frac{(2\ell+1)!}{4\pi}\right)^{1/2} \sin^\ell\theta \, e^{i\ell\phi}}$$

Other properties:

- $$Y_\ell^m(\theta,\phi)^* = (-1)^m \, Y_\ell^{-m}(\theta,\phi)$$

- Parity: $\vec{x} \Rightarrow -\vec{x} \Rightarrow \begin{matrix} \phi \Rightarrow \phi \\ \cos\theta \Rightarrow -\cos\theta \end{matrix}$

$$\mathcal{Y}_\ell^m\left(\frac{\vec{x}}{r}\right) \Rightarrow \boxed{\mathcal{Y}_\ell^m\left(-\frac{\vec{x}}{r}\right) = (-1)^\ell \, \mathcal{Y}_\ell^m\left(\frac{\vec{x}}{r}\right)}$$

Spherical harmonics are eigenfunctions of parity with eigenvalue $(-1)^\ell$