Lecture 27: Orbital Angular Momentum

Phy851 Fall 2009

The General Theory of Angular Momentum

- Starting point:
  - Assume you have three operators that satisfy the commutation relations:

$$[J_x, J_y] = i\hbar J_z$$

$$[J_y, J_z] = i\hbar J_x$$

$$[J_z, J_x] = i\hbar J_y$$

  - Let: $J^2 = J_x^2 + J_y^2 + J_z^2$

$$J_\pm = J_x \pm iJ_y$$

- Conclusions:
  - Simultaneous eigenstates of J^2 and J_z exist
  - They must satisfy:

$$J^2 |j,m\rangle = \hbar^2 j(j+1) |j,m\rangle$$

$$J_z |j,m\rangle = \hbar m |j,m\rangle$$

$$J_\pm |j,m\rangle = \hbar\sqrt{j(j+1) - m(m\pm 1)}\, |j,m\pm 1\rangle$$

  - Where the quantum numbers take on the values:

$$j = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \frac{5}{2}, 3, \ldots$$

$$m = -j, -j+1, -j+2, \ldots, j-1, j$$

Orbital Angular Momentum

- For orbital angular momentum we have:

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

- So that: $L_z = XP_y - YP_x$

- In coordinate representation we have:

$$\vec{L} \rightarrow -i\hbar\left(\vec{r} \times \vec{\nabla}\right)$$

$$\vec{r} \times \vec{\nabla} = \det\begin{vmatrix} \vec{e}_r & \vec{e}_\theta & \vec{e}_\phi \\ r & 0 & 0 \\ \frac{\partial}{\partial r} & \frac{1}{r}\frac{\partial}{\partial \theta} & \frac{1}{r\sin\theta}\frac{\partial}{\partial \phi} \end{vmatrix}$$

$$= -\vec{e}_\theta \frac{1}{\sin\theta}\frac{\partial}{\partial \phi} + \vec{e}_\phi \frac{\partial}{\partial \theta}$$

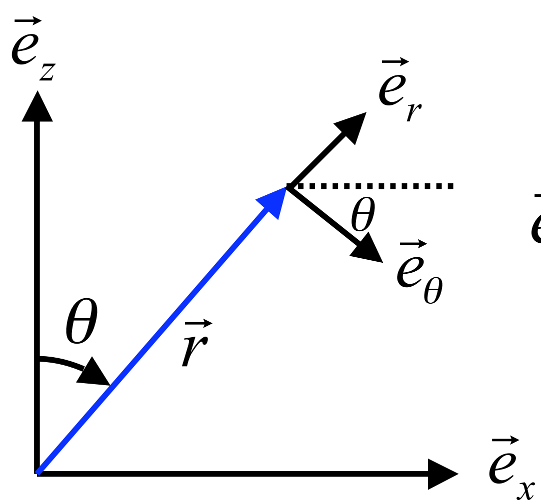
$$\vec{L} = -i\hbar\left(-\vec{e}_\theta \frac{1}{\sin\theta}\frac{\partial}{\partial \phi} + \vec{e}_\phi \frac{\partial}{\partial \theta}\right)$$

The z-component of L

$$\vec{L} \rightarrow -i\hbar\left(-\vec{e}_\theta \frac{1}{\sin\theta}\frac{\partial}{\partial\phi} + \vec{e}_\phi \frac{\partial}{\partial\theta} \right)$$

- L_z is defined by:

$$L_z = \vec{e}_z \cdot \vec{L}$$



$$\vec{e}_z = \cos\theta\, \vec{e}_r - \sin\theta\, \vec{e}_\theta$$

$$\vec{e}_z \cdot \vec{L} = \cos\theta\, \vec{e}_r \cdot \vec{L} - \sin\theta\, \vec{e}_\theta \cdot \vec{L}$$

$$\vec{e}_r \cdot \vec{L} = 0 \qquad \vec{e}_\theta \cdot \vec{L} = -\frac{1}{\sin\theta}\frac{\partial}{\partial\phi}$$

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

Laplacian

- In spherical coordinates, the Laplacian is given by:

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}$$

- In QM, the Kinetic Energy obeys:

$$\langle\vec{r}|\frac{P^2}{2M}|\psi\rangle = -\frac{\hbar^2}{2M}\nabla^2\psi(\vec{r})$$

$$= \frac{\hbar^2}{2Mr^2}\left[\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]\psi(\vec{r})$$

- Now from Classical Mechanics, we know that:

$$K.E. = \frac{p_r^2}{2M} + \frac{L^2}{2Mr^2}$$

- By comparison, we see that we must have:

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

Changing coordinate system and/or basis

- Coordinate representation in spherical coordinates: $\left\{ \left| r\theta\phi \right\rangle \right\}$

$$R \rightarrow r \qquad P_r \rightarrow -i\hbar \frac{\partial}{\partial r}$$

$$\Theta, \Phi \rightarrow \theta, \phi \qquad \vec{L} \rightarrow -\vec{e}_\theta \frac{1}{\sin\theta} \frac{\partial}{\partial\phi} + \vec{e}_\phi \frac{\partial}{\partial\theta}$$

- Note that the angular momentum operator didn't depend on r or $\partial/\partial r$:

$$[\vec{L}, R] = 0 \qquad [\vec{L}, P_r] = 0$$

- Decompose as tensor product:

$$\left| r\theta\phi \right\rangle = \left| r \right\rangle^{(R)} \otimes \left| \theta\phi \right\rangle^{(\Omega)}$$

- Alternate basis sets:

$$\left| r \right\rangle^{(R)} \leftrightarrow \left| p_r \right\rangle^{(R)} \qquad \left| \theta\phi \right\rangle^{(\Omega)} \leftrightarrow \left| \ell m \right\rangle^{(\Omega)}$$

- Can be combined to give four basis choices:

$$\left\{ \left| r,\theta,\phi \right\rangle \right\} \; \left\{ \left| p_r,\theta,\phi \right\rangle \right\} \; \left\{ \left| r,\ell,m \right\rangle \right\} \; \left\{ \left| p_r,\ell,m \right\rangle \right\}$$

Allowed quantum numbers for orbital angular momentum

- In coordinate representation, the eigenvalue equation for L_z becomes:

$$L_z\left|\ell,m\right\rangle = \hbar m\left|\ell,m\right\rangle$$

$$-i\hbar\frac{\partial}{\partial\phi}\left\langle\theta,\phi\middle|\ell,m\right\rangle = \hbar m\left\langle\theta,\phi\middle|\ell,m\right\rangle$$

- Which has the solution:

$$\left\langle\theta,\phi\middle|\ell,m\right\rangle = \left\langle\theta,0\middle|\ell,m\right\rangle e^{im\phi}$$

- The wave-function must be single-valued, so that:

$$e^{im2\pi} = 1$$

$$m = 0,\pm1,\pm2,\pm3,\ldots$$

- Integer *m* values occur only for integer ℓ values
- Therefore half-integer ℓ values are forbidden for the case of orbital angular momentum

$$\ell = 0,1,2,3,\ldots$$

Spherical Harmonics

- The transformation coefficients from angular to angular momentum representation are called `Spherical Harmonics'
  - Denoted as:

$$\langle \theta,\phi | \ell, m \rangle = Y_\ell^m(\theta,\phi)$$

  - In Mathematica:

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SphericalHarmonicY[l,m,_,_]
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- Some properties:

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

$$\int_0^\pi \sin\theta d\theta \int_0^{2\pi} d\phi \left(Y_\ell^m(\theta,\phi)\right)^* Y_{\ell'}^{m'}(\theta,\phi) = \delta_{\ell,\ell'}\delta_{m,m'}$$

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

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

- Any function of θ and ϕ can be expanded onto Spherical Harmonics:

$$f\left(\theta,\phi\right) = \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell} c_{\ell,m} Y_\ell^m(\theta,\phi)$$

$$c_{\ell,m} = \int_0^\pi \sin\theta d\theta \int_0^{2\pi} d\phi \left(Y_\ell^m(\theta,\phi)\right)^* f(\theta,\phi)$$

Orbitals

- We call the different ℓ states 'orbitals'

$\ell=0$ 'S' orbitals $$Y_0^0(\theta,\phi) = \frac{1}{\sqrt{4\pi}}$$

m=0

$\ell=1$ 'P' orbitals

m=-1,0,1

$\ell=2$ 'D' orbitals

m=-2,-1,0,1,2

$\ell=3$ 'F' orbitals

m=-3,-2,-1,0,1,2,3

etc…

- The number of sub-orbitals (*m*-states) is given by:

$$N_\ell = 2\ell + 1$$