Lecture 17   137A   Orbital Angular Momentum   1

- Consider particle of mass m, $\vec{p}$, and position $\vec{r}$.

$$\vec{L} = \vec{r} \times \vec{p}$$

$$L_x = y p_z - z p_y$$
$$L_y = z p_x - x p_z$$
$$L_z = x p_y - y p_x$$

In quantum mechanics, in the position rep.,

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

$$\Longrightarrow \quad \hat{L}_x = -i\hbar \left(y \frac{\partial}{\partial z} - z \frac{\partial}{\partial y} \right)$$

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

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

- The commutator is <u>not trivial</u> since we mix up positions and momenta:

$$[\hat{L}_x, \hat{L}_y] = [(\hat{y}\hat{p}_z - \hat{z}\hat{p}_y), \; (\hat{z}\hat{p}_x - \hat{x}\hat{p}_z)]$$

$$= [yP_z, zP_x] + [zP_y, xP_z] - [yP_z, xP_z] - [zP_y - zP_x]$$ ②

$yP_z zP_x - zP_x yP_z$

since y and P_x commute with each other and with z, P_z

$\Downarrow$

$$yP_x\,[P_z, z] = -i\hbar\, yP_x$$

Similarly, $[zP_y, xP_z] = xP_y\,[z, P_z] = i\hbar\, xP_y$

$[zP_y, zP_x]$ vanishes

$$\Longrightarrow \quad [\hat{L}_x, \hat{L}_y] = i\hbar\,(xP_y - yP_x) = i\hbar\,\hat{L}_z \ !$$

Similarly, $[\hat{L}_y, \hat{L}_z] = i\hbar\,\hat{L}_x$

$[\hat{L}_z, \hat{L}_x] = i\hbar\,\hat{L}_y$

$\Longrightarrow$ Cannot measure components of angular momentum separately !!

But....

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

$$[\hat{L}^2, \hat{L}_x] = ?$$

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

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

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

$$= \hat{L}_y [\hat{L}_y, \hat{L}_x] + [\hat{L}_y, \hat{L}_x]\hat{L}_y$$

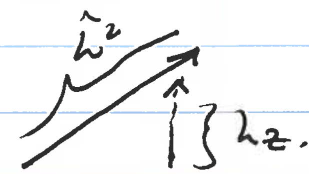
$$+ \hat{L}_z [\hat{L}_z, \hat{L}_x] + [\hat{L}_z, \hat{L}_x]\hat{L}_z$$

$$= -i\hbar (\hat{L}_y \hat{L}_z + \hat{L}_z \hat{L}_y)$$
$$+ i\hbar (\hat{L}_z \hat{L}_y + \hat{L}_y \hat{L}_z) = 0$$

Similarly, $[\hat{L}^2, \hat{L}_y] = [\hat{L}^2, \hat{L}_z] = 0$

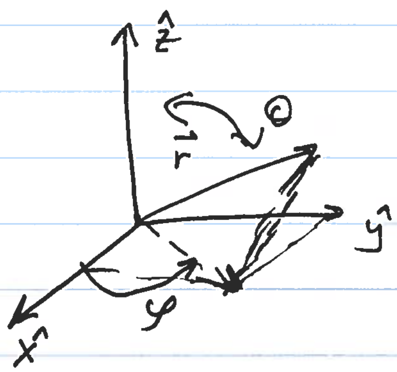
* $\Rightarrow$ Can find simultaneous eigenfunctions of $\hat{L}^2$ and <u>one</u> component of $\hat{L}$, such as $\hat{L}_z$.

Often use $\hat{L}^2$ and $\hat{L}_z$



④

Can convert these expressions in spherical polar coordinates (r, θ, φ)



$$x = r \sin\theta \cos\varphi$$
$$y = r \sin\theta \sin\varphi$$
$$z = r \cos\theta$$

$$r \in [0, \infty]$$
$$\theta \in [0, \pi]$$
$$\varphi \in [0, 2\pi]$$

$$\hat{L}_x = -i\hbar \left(-\sin\varphi \frac{\partial}{\partial\theta} - \cot\theta \cos\varphi \frac{\partial}{\partial\varphi} \right)$$

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

$$\hat{L}_z = -i\hbar \frac{\partial}{\partial\varphi}$$

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

<u>Note:</u> $\hat{L}_x, \hat{L}_y, \hat{L}_z$ are purely angular and do not depend on the coordinate r.

$$\left.\begin{array}{l} [L_x, f(r)] \\ [L_y, f(r)] \\ [L_z, f(r)] \\ [L^2, f(r)] \end{array}\right\} = 0$$

Generator of rotations: (5)

To generate a rotation of $\delta\alpha$ along the $\hat{z}$ axis, can use

$$\hat{\mathcal{U}}_z(\delta\alpha) = \hat{I} - \frac{i}{\hbar} \cancel{\text{sim}}\ \underbrace{\delta\alpha}_{\text{Small \#}} L_z$$

For a finite rotation about $\hat{n}$:

$$\hat{\mathcal{U}}_{n}(\alpha) = \exp\left(-\frac{i}{\hbar}\alpha\hat{n}\cdot\hat{L}\right)$$

• Note, for an isolated system, $[\hat{L}, \hat{H}] = 0$ and total angular momentum is conserved.

Eigenvalues and Eigenvectors of $\hat{L}^2, \hat{L}_z$:

L_z: let $\Phi_m(\varphi)$ be an eigenfunction with eigenvalue $m\hbar$

$$\hat{L}_z \Phi_m(\varphi) = m\hbar\,\Phi_m(\varphi)$$

$$-i\frac{\partial}{\partial\varphi}\Phi_m(\varphi) = m\,\Phi_m(\varphi)$$

$$\longrightarrow \quad \Phi_m(\varphi) = \frac{1}{\sqrt{2\pi}} e^{im\varphi}$$

Require $\Phi_m(2\pi) = \Phi_m(0)$ or $e^{2\pi i m} = 1 \rightarrow m = 0, \pm 1, \pm 2, \ldots$

**

→ The measurement of the angular momentum along any axis is quantized! ⑥

Φ_m is part of a complete orthonormal set:

$$\int_0^{2\pi} \Phi_{m'}^*(\varphi)\,\Phi_m(\varphi)\,d\varphi = \delta_{mm'}$$

$$f(\varphi) = \sum_{m=-\infty}^{m=\infty} a_m \Phi_m(\varphi) \quad ; \quad a_m = \int_0^{2\pi} \Phi_m^*(\varphi) f(\varphi)\,d\varphi$$

Now, let's try to find simultaneous eigenfunctions of L^2 and L_z:

Let's call these functions $Y_{lm}(\theta,\varphi)$
Let the eigenvalues be $l(l+1)\hbar^2$

$$L^2 Y_{lm}(\theta,\varphi) = l(l+1)\hbar^2 Y_{lm}(\theta,\varphi)$$
$$L_z Y_{lm}(\theta,\varphi) = m\hbar\, Y_{lm}(\theta,\varphi)$$

Look for separable solutions

$$Y_{lm}(\theta,\varphi) = \Theta_{lm}(\theta)\,\Phi_m(\varphi)$$

Convert $\hat{L}^2$ into (r, θ, φ) coordinates (7)

$$\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right] Y_{lm}(\theta,\varphi)$$

$$= -l(l+1)\, Y_{lm}(\theta,\varphi)$$

Substitute form $Y = \Theta\,\Phi$

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

Let $w = \cos\theta$ and $F_{lm}(w) = \Theta_{lm}(\theta)$

$w \in [-1, 1]$

$$\left[(1-w^2)\frac{d^2}{dw^2} - 2w\frac{d}{dw} + l(l+1) - \frac{m^2}{1-w^2}\right] F_{lm}(w) = 0$$

Let's start with $m = 0$

$$\left[(1-w^2)\frac{d^2}{dw^2} - 2w\frac{d}{dw} + l(l+1)\right] F_{l0}(w) = 0$$

Legendre Equation

Legendre

- Power series solution

$l = 0, 1, 2, \ldots$ for non-divergent solution

- Solution is a set of Legendre polynomials

$$P_l(w) = 2^{-l} (l!)^{-1} \frac{d^l}{dw^l} (w^2-1)^l$$

$$P_0(w) = 1$$
$$P_1(w) = w$$
$$P_2(w) = \tfrac{1}{2}(3w^2-1)$$
$$\ldots$$

For the general case of m: ← original eqn on fcn of m^2

Define Associated Legendre Functions $P_l^{|m|}(w)$

$$P_l^{|m|}(w) = (1-w^2)^{|m|/2} \frac{d^{|m|}}{dw^{|m|}} P_l(w)$$

degree $l = 0, 1, 2, 3 \ldots$

order m

$|m| = 0, 1, 2, \ldots$

We get the restriction that

$$m = -l, -l+1, \ldots l$$

which reflects

$$\langle L^2 \rangle \geq \langle L_z^2 \rangle$$

$$P_1^1(w) = (1-w^2)^{1/2}$$
$$P_2^1(w) = 3(1-w^2)^{1/2} w$$

$$P_2^2(w) = 3(1-w^2)$$

$$\Theta_{\ell m}(\theta) = (-1)^m \left[\frac{(2\ell+1)(\ell-m)!}{2(\ell+m)!}\right]^{1/2} P_\ell^m(\cos\theta)$$ 9

$m \geq 0$

$$= (-1)^m \,\Theta_{\ell|m|}(\theta) \text{ for } m < 0$$

Spherical Harmonics

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

$m \geq 0$

$$= (-1)^m \, Y^*_{\ell,-m}(\theta,\varphi) \quad \text{for } m < 0$$

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

$m = -\ell, -\ell+1, \ldots \ell$

Orthonormal:

$$\int Y^*_{\ell' m'}(\theta,\varphi)\, Y_{\ell m}(\theta,\varphi)\, \underbrace{d\Omega}_{\sin\theta\, d\theta\, d\varphi} = \delta_{\ell\ell'}\delta_{mm'}$$

Complete set:

$$f(\theta,\varphi) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} a_{\ell m} Y_{\ell m}(\theta,\varphi)$$

$$a_{\ell m} = \int Y^*_{\ell m}(\theta,\varphi)\, f(\theta,\varphi)\, d\Omega$$

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

$\updownarrow \; \updownarrow \; \updownarrow \; \downarrow$

s p d f   Spectroscopic notation

Low-order spherical harmonics

ℓ	m	$Y_{\ell m}$
0	0	$Y_{00} = \frac{1}{\sqrt{4\pi}}$
1	0	$Y_{10} = \sqrt{\frac{3}{4\pi}} \cos\theta$
	± 1	$Y_{1,\pm 1} = \mp \left(\frac{3}{8\pi}\right)^{1/2} \sin\theta \, e^{\pm i\varphi}$
2	0	$Y_{2,0} = \left(\frac{5}{16\pi}\right)^{1/2} (3\cos^2\theta - 1)$
	± 1	$Y_{2,\pm 1} = \mp \left(\frac{15}{8\pi}\right)^{1/2} \sin\theta\cos\theta \, e^{\pm i\varphi}$
	± 2	$Y_{2,\pm 2} = \left(\frac{15}{32\pi}\right)^{1/2} \sin^2\theta \, e^{\pm 2i\varphi}$

Lecture 18 Angular Momentum Ladder Operators

$$\hat{L}_+ = \hat{L}_x + i\hat{L}_y \qquad ; \qquad \hat{L}_+^{\dagger} = \hat{L}_-$$
$$\hat{L}_- = \hat{L}_x - i\hat{L}_y \qquad \qquad \hat{L}_-^{\dagger} = \hat{L}_+$$

- $[\hat{L}^2, \hat{L}_\pm] = 0$

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

Effect of $\hat{L}_\pm$!

$$\hat{L}_z |lm\rangle = m\hbar |lm\rangle$$

Act on left by $\hat{L}_\pm$

$$\underbrace{\hat{L}_\pm \hat{L}_z}_{\text{switch order}} |lm\rangle = m\hbar \hat{L}_\pm |lm\rangle$$

$$(\hat{L}_z \hat{L}_\pm \mp \hbar \hat{L}_\pm)|lm\rangle = m\hbar \hat{L}_\pm |lm\rangle$$

$$\hat{L}_z \underbrace{\hat{L}_\pm |lm\rangle}_{} = (m\pm 1)\hbar \hat{L}_\pm |lm\rangle$$

eigenfunction of $\hat{L}_z$ with one more (less) $\hbar$!

②

- $\hat{L}^2|lm\rangle = l(l+1)\hbar^2|lm\rangle$

(act on left w. $\hat{L}_\pm$) $\quad \underbrace{\hat{L}_\pm L^2}_{\text{commute}}|lm\rangle = l(l+1)\hbar^2\hat{L}_\pm|lm\rangle$

$$\hat{L}^2\left[\hat{L}_\pm|lm\rangle\right] = l(l+1)\left[\hat{L}_\pm|lm\rangle\right]$$

$\longrightarrow$ The effect of $\hat{L}_\pm$ on $|lm\rangle$ is to raise (lower) m but leave $\underline{l}$ unchanged

Can normalize kets to find coefficients:

$$\hat{L}_\pm|lm\rangle = \hbar\left[l(l+1) - m(m\pm1)\right]^{1/2}|l, m+1\rangle$$

- $\hat{L}_x = \frac{1}{2}(\hat{L}_+ + \hat{L}_-)$

  $\hat{L}_y = \frac{1}{2i}(\hat{L}_+ - \hat{L}_-)$

- Note $\langle L_x\rangle$ for a state $|lm\rangle$

$$= \langle lm|\hat{L}_x|lm\rangle = \frac{1}{2}\langle lm|\hat{L}_+ + \hat{L}_-|lm\rangle$$

$$= 0$$

$\longrightarrow \langle L_y\rangle = \langle L_z\rangle = 0$

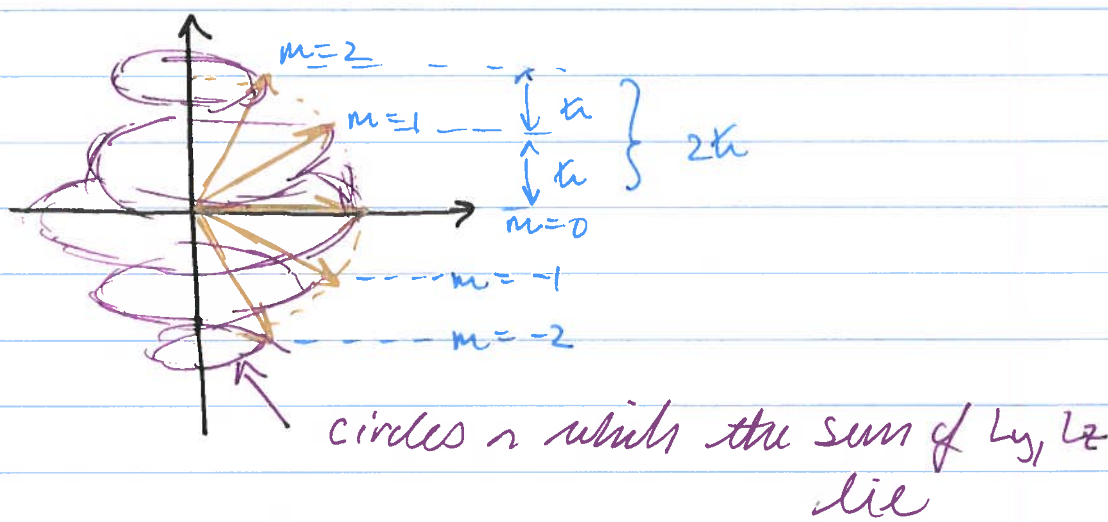
But....

$$\langle L_x^2 \rangle = \langle L_y^2 \rangle = \frac{1}{2} \langle L^2 - L_z^2 \rangle$$
$$= \frac{1}{2} [\ell(\ell+1) - m^2]\hbar^2$$

Thus, you always have some L_x, L_y components even when $L_z = \pm \ell \hbar$

Consider a vector model:

$\ell = 2, \quad m = +2, +1, 0, -1, -2$



Example of the Rigid Rotor:

Consider a particle of mass μ:

Kinetic Energy $\hat{T} = \frac{\hat{p}^2}{2\mu} = \frac{-\hbar^2}{2\mu}\nabla^2$

In spherical coordinates:

$$\hat{T} = \frac{-\hbar^2}{2\mu}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2}\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right]$$

$$= \frac{-\hbar^2}{2\mu}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{\hat{L}^2}{\hbar^2 r^2}\right]$$

If the particle is constrained to move on the surface of a sphere of radius a.

Then $r = a$ and the first term is 0.

$$\hat{T} = \frac{\hat{L}^2}{2\mu a^2} = \frac{\hat{L}^2}{2I}$$ ← moment of inertia

- Add a potential $\hat{H} = \frac{\hat{L}^2}{2I} + \hat{V}(\theta, \varphi)$

Time independent Schrödinger now reads:

$$\left[\frac{\hat{L}^2}{2I} + \hat{V}(\theta,\varphi)\right]\psi(\theta,\varphi) = E\,\psi(\theta,\varphi)$$

If we set $\hat{V}=0 \rightarrow$ Rigid Rotor

$\hat{H} = \frac{\hat{L}^2}{2I} \longrightarrow$ Eigenfunctions are $Y_{lm}(\theta,\varphi)$!

$E_l = \frac{\hbar^2}{2I}\,l(l+1) \qquad l = 0, 1, 2, \ldots$

$(2l+1)$ - fold degenerate

Can apply this model to a diatomic molecule $\rightarrow$ rotations at far-IR or μ-wave.

Lecture 19 Generalized Angular Momentum & Matrix representation

(1)

- Can have intrinsic properties that behave as an angular momentum.

Call a general angular momentum $\vec{J}$

Most important properties, one by one
Note: Must work for $\hat{L}$.

- $[\hat{J}_x, \hat{J}_y] = i\hbar \hat{J}_z$ and other permutations.

- $\hat{J}^2 = \hat{J}_x^2 + \hat{J}_y^2 + \hat{J}_z^2$
$[\hat{J}^2, \hat{J}_x] = 0$

- Eigenfunctions of $\hat{J}^2, \hat{J}_z$ $|j\,m\rangle$

$\hat{J}^2 |jm\rangle = j(j+1)\hbar^2 |jm\rangle$
$\hat{J}_z |j\,m\rangle = m\hbar |jm\rangle$ $j(j+1) \geq m^2$

Since $\langle J^2 \rangle \geq \langle J_z^2 \rangle$

- $\hat{J}_+ = \hat{J}_x + i\hat{J}_y$
$\hat{J}_- = J_x - i\hat{J}_y$

- $\hat{J}_+^{\dagger} = \hat{J}_- \qquad \hat{J}_-^{\dagger} = \hat{J}_+$

- $[\hat{J}^2, \hat{J}_\pm] = 0$

- $\hat{J}_\pm \hat{J}_\mp = \hat{J}^2 - \hat{J}_z^2 \pm \hbar \hat{J}_z$
- $[\hat{J}_+, \hat{J}_-] = 2\hbar \hat{J}_z$
- $[\hat{J}_z, \hat{J}_\mp] = \mp \hbar \hat{J}_\mp$

$$\hat{J}_+ |jm\rangle = [j(j+1) - m(m+1)]^{1/2} \hbar |j, m+1\rangle$$
$$J_- |jm\rangle = [j(j+1) - m(m-1)]^{1/2} \hbar |j, m-1\rangle$$

Let's now let m_T be the max value of J_z
m_B min

- $J_+ |j\, m_T\rangle = 0$

Act with $\hat{J}_-$ from the left

$$\hat{J}_- (J_+ |j m_T\rangle) = (\hat{J}^2 - \hat{J}_z^2 - \hbar \hat{J}_z) |j\, m_T\rangle$$
$$= [(j(j+1)) - m_T^2 - m_T] \hbar^2 |j\, m_T\rangle$$
$$= 0$$
$$\longrightarrow j(j+1) = m_T^2 + m_T$$

Similarly, $J_- |j\, m_B\rangle = 0$
$J_+ J_- |j\, m_B\rangle = (J^2 - J_z^2 + \hbar J_z) |j\, m_B\rangle$

$$0 = \left(j(j+1) - m_B^2 + m_B\right)\hbar^2 |j\, m_B\rangle \qquad (3)$$

$$\longrightarrow \quad j(j+1) = m_B^2 - m_B$$

Combine the two expressions,

$$m_T^2 + m_T = m_B^2 - m_B$$

$$\Longrightarrow \quad m_T = -m_B \quad \text{or} \quad \cancel{m_T^2 + m_T = m_B^2 - m_B}$$

$$\cancel{m_T = m_B - 1}$$

we know $m_T - m_B$ = integer

since

$$\hat{J}_z\left[\hat{J}_\pm |j\, m\rangle\right] = (m \pm 1)\hbar\, |j\, m\rangle$$

Thus $m_T = j$

$m_T = -j$

$\underset{\substack{\| \\ 2j}}{m_T - m_B}$ is a positive integer or zero.

$$\longrightarrow \quad j = 0,\ \tfrac{1}{2},\ 1,\ \tfrac{3}{2},\ 2,\ \tfrac{5}{2},\ \ldots$$

Angular momentum can in general have half-integers

Matrix representation

(4)

$$\langle j'm' | jm \rangle = \delta_{jj'}\delta_{mm'}$$

- $[J^2]_{j'm'jm} = \langle j'm' | \hat{J}^2 | jm \rangle$

  $= j(j+1)\hbar^2 \delta_{jj'}\delta_{mm'}$

  diagonal.

- $[\hat{J}_z]_{j'm'jm} = \langle j'm' | \hat{J}_z | jm \rangle$

  $= m\hbar\, \delta_{jj'}\delta_{mm'}$

  diagonal

- $[\hat{J}_+]_{j'm',jm} = [j(j+1) - m(m+1)]^{1/2}\hbar\, \delta_{jj'}\underbrace{\delta_{m',m+1}}_{\text{one off diagonal}}$

  $[\hat{J}_-]_{j'm'jm} = [j(j+1) - m(m-1)]^{1/2}\hbar\, \delta_{jj'}\delta_{m',m-1}$ diagonal

- $\hat{J}_x = \frac{1}{2}(\hat{J}_+ + \hat{J}_-) \qquad \hat{J}_y = \frac{1}{2i}(\hat{J}_+ - \hat{J}_-)$

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$j = 0$

$J_x = 0 \qquad J_y = 0 \qquad J_z = 0 \qquad J^2 = 0$

$j = 1/2$

$$J_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad J_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

$$J_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \qquad J^2 = \frac{3}{4}\hbar^2\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$j = 1$

$$J_x = \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \qquad J_y = \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}$$

$$J_z = \hbar\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \qquad J^2 = 2\hbar^2\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Can also express all of them in block diagonal format

$$\begin{pmatrix} (j=0) & & & \\ & (j=1/2) & & \\ & & (j=1) & \\ & & & \ddots \end{pmatrix}$$