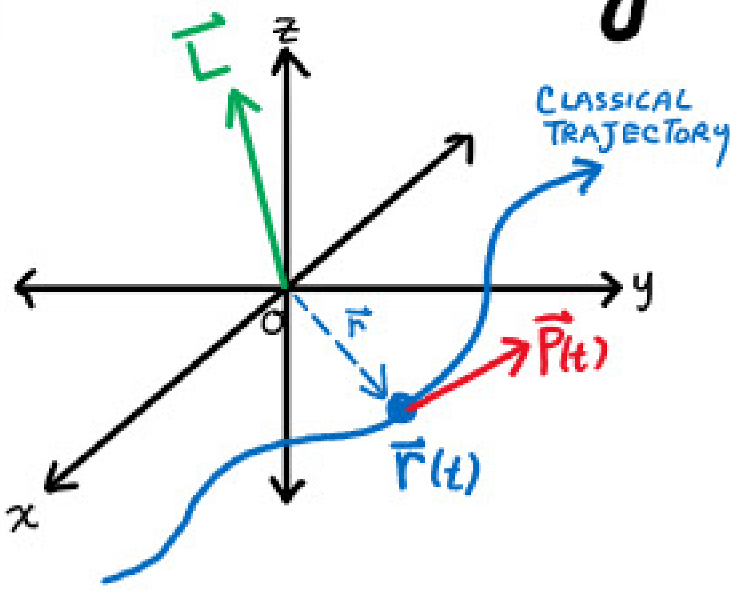
# Orbital Angular Momentum in 3D: Part 1, General Theory




- For a classical particle in 3 spatial dimensions, STATE is determined at time $t$ by 6 numbers:
  - Components of position $\vec{r}$ (relative to some fixed origin $O$)
  - Components of momentum $\vec{P} = m\dot{\vec{r}}$
- All other observables (e.g., kinetic, potential energies) can be computed from $(\vec{r}, \vec{p})$
- "Orbital" angular momentum about origin $O$: $\vec{L} = \vec{r} \times \vec{p}$

## Quantum Mechanics of a (spinless) Particle in 3D

- Classical observables "promoted" to Hermitian operators
  - $x, y, z \Rightarrow \hat{X}, \hat{Y}, \hat{Z} \equiv \{\hat{X}_a\}$, $a \in 1,2,3$
  - $P_x, P_y, P_z \Rightarrow \hat{P}_x, \hat{P}_y, \hat{P}_z \equiv \{\hat{P}_a\}$
  - $L_a = \epsilon_{abc} x_b p_c \Rightarrow \hat{L}_a = \epsilon_{abc} \hat{X}_b \hat{P}_c$

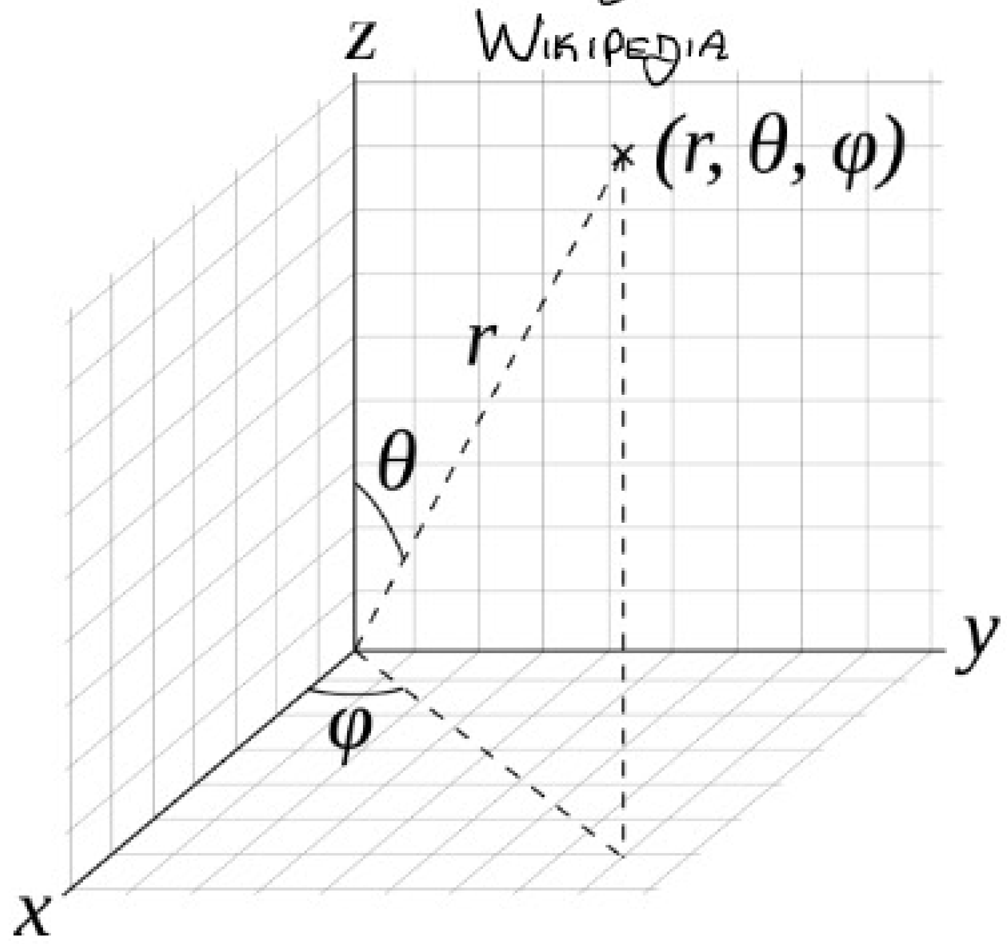
Explicitly,

① $\hat{L}_x = \hat{Y}\hat{P}_z - \hat{Z}\hat{P}_y \xrightarrow{\text{Position Basis}} -i\hbar(y\partial_z - z\partial_y)$

② $\hat{L}_y = \hat{Z}\hat{P}_x - \hat{X}\hat{P}_z \longrightarrow -i\hbar(z\partial_x - x\partial_z)$

③ $\hat{L}_z = \hat{X}\hat{P}_y - \hat{Y}\hat{P}_x \longrightarrow -i\hbar(x\partial_y - y\partial_x) = -i\hbar \dfrac{\partial}{\partial\phi}$ Lec. 15, p. 4:

Image Credit: Wikipedia




Spherical Polar Coords

$x = r\cos\phi \sin\theta$

$y = r\sin\phi \sin\theta$

$z = r\cos\theta$

The angular momentum operators satisfy the same SO(3) Lie algebra as spin generators of rotation:

$$\boxed{[\hat{L}_a, \hat{L}_b] = i\hbar \epsilon_{abc} \hat{L}_c}$$

$\therefore$ Expect $\hat{L}$ generates rotations of functions on $\mathbb{R}^3$

$$\therefore \langle \vec{r} | e^{-i\frac{\hat{L}\cdot\vec{\Theta}}{\hbar}} | \psi \rangle = \psi(\hat{R}^{-1}_{(\vec{\Theta})}\vec{r})$$

Ordinary 3x3 Rot. Matrix acting on components of $\vec{r}$

e.g., XY-plane rotation: (Lec. 15)

$$\langle \vec{r} | e^{-i\frac{\hat{L}_z \phi_0}{\hbar}} | \psi \rangle = \psi(r, \theta, \phi - \phi_0)$$

**SQUARED-NORM:** $\hat{\vec{L}}^2 = \hat{\vec{L}}\cdot\hat{\vec{L}} = (\hat{L}_x)^2 + (\hat{L}_y)^2 + (\hat{L}_z)^2 = \hat{L}_a \hat{L}_a$ EINSTEIN SUM $a \in 1,2,3$

SINCE IT IS INVARIANT UNDER ROTATIONS, EXPECT $[\hat{\vec{L}}^2, \hat{L}_a] = 0$

CHECK: $[\hat{L}_b \hat{L}_b, \hat{L}_a] = \hat{L}_b[\hat{L}_b, \hat{L}_a] + [\hat{L}_b, \hat{L}_a]\hat{L}_b$

$$= \underset{\substack{\text{ANTISYM. UNDER} \\ \text{EXCHANGE} \\ b \leftrightarrow c}}{\epsilon_{bac}} \underbrace{(\hat{L}_b \hat{L}_c + \hat{L}_c \hat{L}_b)}_{\substack{\text{SYM. UNDER} \\ \text{EXCHANGE} \\ b \leftrightarrow c}} = 0 \checkmark$$

SIMILARLY,

- $[\hat{L}_a, \hat{X}_b] = i\hbar\epsilon_{abc}\hat{X}_c$ ; $[\hat{L}_a, \hat{X}_b\hat{X}_b] = 0$ ;
- $[\hat{L}_a, \hat{P}_b] = i\hbar\epsilon_{abc}\hat{P}_c$ ; $[\hat{L}_a, \hat{P}_b\hat{P}_b] = 0$

FOR A ROTATIONALLY INVARIANT HAMILTONIAN, e.g.

$$\hat{H} = \frac{\hat{\vec{P}}^2}{2\mu} + \hat{V}\left(\sqrt{\hat{\vec{X}}\cdot\hat{\vec{X}}}\right) \Rightarrow -\frac{\hbar^2}{2\mu}\vec{\nabla}^2 + v(r)$$

[PARTICLE SUBJECT TO A CENTRAL POTENTIAL (E.G., COULOMB $V(r) = \frac{q_1 q_2}{r}$), IN 3 SPATIAL DIMENSIONS]

USE $\mu$ FOR MASS TO AVOID CONFUSION WITH $\hat{L}_z$ E'VALUE $\hbar m_z$

WE CAN SIMULTANEOUSLY DIAGONALIZE $\hat{H}$, $\hat{\vec{L}}^2$, AND $\hat{L}_z$.

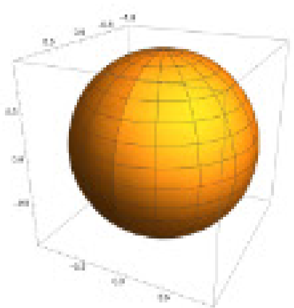
**RESULT:** "FAMILIES" OF EIGENFUNCTIONS THAT TRANSFORM ONLY AMONGST "FAMILY MEMBERS" UNDER ROTATIONS

$\equiv$ IRREDUCIBLE REPRESENTATIONS OF ANGULAR MOMENTUM

$\ell = 0$

1 s-ORBITAL

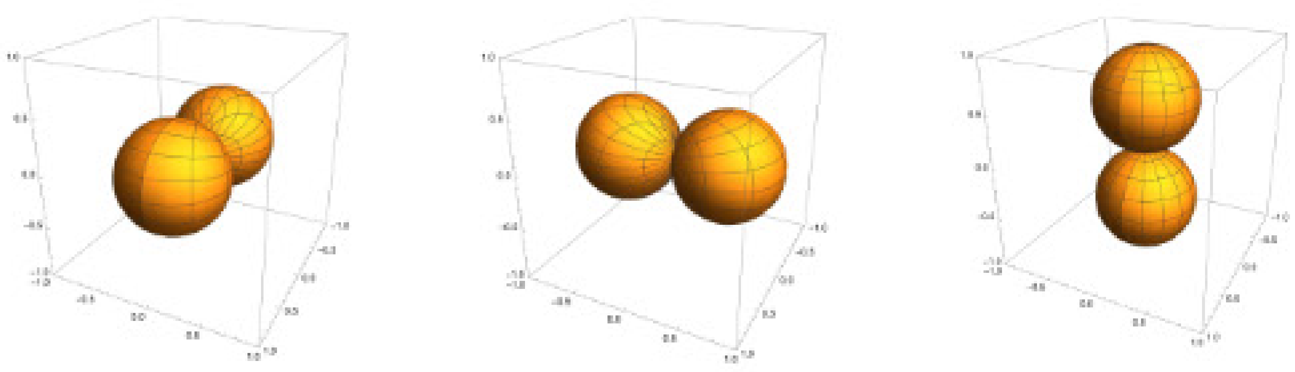
$\sim$ SPIN-0!



$\ell = 1$

3 p-ORBITALS

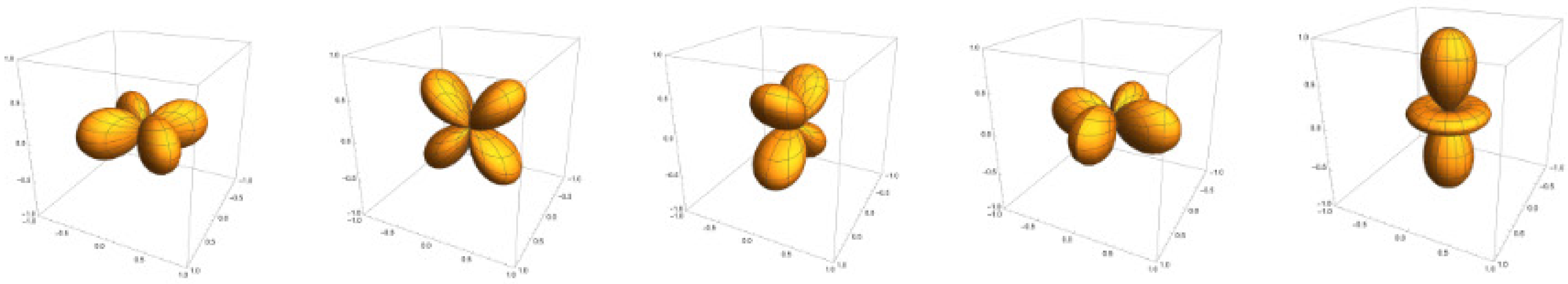
$\sim$ SPIN-1!



$\ell = 2$

5 d-ORBITALS

$\sim$ SPIN-2!



# General Representation Theory of Angular Momentum

$$\hat{J}_\pm \equiv \hat{J}_x \pm i\hat{J}_y \;;\; [\hat{J}_z, \hat{J}_\pm] = \pm\hbar\hat{J}_\pm \;;\; [\hat{J}_+, \hat{J}_-] = 2\hbar\hat{J}_z$$

**Squared-Norm: ("Casimir Op.")** $\hat{\vec{J}}^2 = (\hat{J}_x)^2 + (\hat{J}_y)^2 + (\hat{J}_z)^2$

$$= \underbrace{\tfrac{1}{2}[\hat{J}_+\hat{J}_- + \hat{J}_-\hat{J}_+]}_{\text{Hermitian}} + (\hat{J}_z)^2$$

Hermitian — $i\hat{J}_x\hat{J}_y$, etc. terms cancel.

Let
1. $\hat{\vec{J}}^2|\alpha,\beta\rangle = \alpha|\alpha,\beta\rangle$
2. $\hat{J}_z|\alpha,\beta\rangle = \beta|\alpha,\beta\rangle$

No restrictions for now on $\alpha, \beta$, except: $\alpha = \alpha^*$, $\beta = \beta^*$ Real.

Consider:

- $\hat{J}_z\hat{J}_+|\alpha,\beta\rangle = (\hat{J}_+\hat{J}_z + \hbar\hat{J}_+)|\alpha,\beta\rangle = (\beta+\hbar)\hat{J}_+|\alpha,\beta\rangle$
- $\hat{J}_z\hat{J}_-|\alpha,\beta\rangle = (\hat{J}_-\hat{J}_z - \hbar\hat{J}_-)|\alpha,\beta\rangle = (\beta-\hbar)\hat{J}_-|\alpha,\beta\rangle$

$\therefore$ Eigenstates of $\hat{J}_z$ have E'values separated by units of $\hbar$,

$\ldots, \beta+2\hbar, \beta+\hbar, \beta, \beta-\hbar, \beta-2\hbar, \ldots$

**Expect:** "$\hat{\vec{J}}^2 \geq (\hat{J}_z)^2$", i.e. $\langle\alpha,\beta|\hat{\vec{J}}^2|\alpha,\beta\rangle \geq \langle\alpha,\beta|(\hat{J}_z)^2|\alpha,\beta\rangle$

$\therefore$ $\alpha \geq \beta^2$. $\Rightarrow$ There must exist $\beta_{MAX}$, $\beta_{MIN}$, such that

$$\hat{J}_+|\alpha,\beta_{MAX}\rangle = \hat{J}_-|\alpha,\beta_{MIN}\rangle = 0$$

"Highest Weight State" "Lowest Weight State"

NOTE: • $\hat{\vec{J}}^2 = \frac{1}{2}[\hat{J}_+\hat{J}_- + \hat{J}_-\hat{J}_+] + \hat{J}_z^2 = \frac{1}{2}[2\hat{J}_-\hat{J}_+ + 2\hbar\hat{J}_z] + (\hat{J}_z)^2$

$$= \hat{J}_-\hat{J}_+ + \hbar\hat{J}_z + (\hat{J}_z)^2$$

• $\hat{\vec{J}}^2 = \frac{1}{2}[\hat{J}_+\hat{J}_- + \hat{J}_-\hat{J}_+] + \hat{J}_z^2 = \frac{1}{2}[2\hat{J}_+\hat{J}_- - 2\hbar\hat{J}_z] + (\hat{J}_z)^2$

$$= \hat{J}_+\hat{J}_- - \hbar\hat{J}_z + (\hat{J}_z)^2$$

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THEN: ① $\hat{J}_-\hat{J}_+|\alpha,\beta_{MAX}\rangle = (\hat{\vec{J}}^2 - \hbar\hat{J}_z - \hat{J}_z^2)|\alpha,\beta_{MAX}\rangle$

$$= (\alpha - \hbar\beta_{MAX} - \beta_{MAX}^2)|\alpha,\beta_{MAX}\rangle = 0$$

$$\therefore \alpha = \beta_{MAX}(\beta_{MAX} + \hbar)$$

② $\hat{J}_+\hat{J}_-|\alpha,\beta_{MIN}\rangle = (\hat{\vec{J}}^2 + \hbar\hat{J}_z - \hat{J}_z^2)|\alpha,\beta_{MIN}\rangle$

$$= (\alpha + \hbar\beta_{MIN} - \beta_{MIN}^2)|\alpha,\beta_{MIN}\rangle = 0$$

$$\therefore \alpha = \beta_{MIN}(\beta_{MIN} - \hbar)$$

$\Rightarrow \beta_{MIN} = -\beta_{MAX}$; $\beta_{MAX} - \beta_{MIN} = 2\beta_{MAX} = \hbar \cdot n$, $n \in \{0, 1, 2, 3, \ldots\}$

HERE $n$ IS THE "DEPTH OF THE WEIGHT STRING"

$$\beta \in \{\underbrace{\beta_{MAX}, \beta_{MAX} - \hbar, \beta_{MAX} - 2\hbar, \ldots, -\beta_{MAX} + \hbar, -\beta_{MAX}}_{n+1 \text{ EIGENSTATES}}\}$$

$$\therefore \beta_{MAX} = j \cdot \hbar, \quad j \in \{0, \tfrac{1}{2}, 1, \tfrac{3}{2}, \ldots\}$$

$j$ IS CALLED THE ANGULAR MOMENTUM OF THE STATE $|\alpha,\beta\rangle$

$$\alpha = \beta_{MAX}(\beta_{MAX} + 1) = \hbar^2 \cdot j(j+1)$$

SWITCHING TO CONVENTIONAL NOTATION:

1. $\hat{J}_z |j, m_z\rangle = \hbar m_z |j, m_z\rangle \quad ; \quad -j \le m_z \le j$ $\Rightarrow n+1 = 2j+1$ STATES IN THE "IRREDUCIBLE" REPRESENTATION WITH ANGULAR MOMENTUM $j$,
2. $\hat{\vec{J}}^2 |j, m_z\rangle = \hbar^2 j(j+1) |j, m_z\rangle$

HIGHEST WEIGHT STATE $|j, j\rangle$

# REPRESENTATIONS OF SO(3) OR SU(2)

| ANGULAR MOMENTUM | STATES | PHYSICAL REALIZATION |
|---|---|---|
| 1. $j = 0$ | $\|0,0\rangle$ | e.g. SPIN SINGLET $\frac{1}{\sqrt{2}}(\|\uparrow\downarrow\rangle - \|\downarrow\uparrow\rangle)$; S-ORBITAL |
| 2. $j = \frac{1}{2}$ | $\|\frac{1}{2},\frac{1}{2}\rangle, \|\frac{1}{2},-\frac{1}{2}\rangle$ | SPIN-$\frac{1}{2}$ |
| 3. $j = 1$ | $\|1,1\rangle, \|1,0\rangle, \|1,-1\rangle$ | SPIN-1; P-ORBITALS |
| 4. $j = \frac{3}{2}$ | $\|\frac{3}{2},\frac{3}{2}\rangle, \|\frac{3}{2},\frac{1}{2}\rangle, \|\frac{3}{2},-\frac{1}{2}\rangle, \|\frac{3}{2},-\frac{3}{2}\rangle$ | SPIN-$\frac{3}{2}$ |
| $\vdots$ | $\vdots$ | $\vdots$ |

WE KNOW FROM STUDYING E'STATES OF $\hat{L}_z$ FOR A PARTICLE IN THE PLANE, THAT $m_z \in \mathbb{Z}$

LEC. 15, p. 4: $\hat{L}_z |m_z\rangle = m_z \hbar |m_z\rangle \Rightarrow -i \frac{\partial}{\partial \phi} \psi_m(r,\phi) = m \psi_m(r,\phi)$

$$\Rightarrow \psi_m(r,\phi) = \psi_m(r) e^{im\phi} \; ; \; \psi_m(r, \phi + 2\pi) = \psi_m(r,\phi) \Rightarrow m \in \text{INTEGER}$$

∴ ONLY INTEGER-$j$ REPRESENTATIONS CAN DESCRIBE SPINLESS WAVEFUNCTIONS.

We are not quite done. Need matrix elements (including coefficients) of $\hat{J}_\pm$.

Let $\quad \hat{J}_\pm |j, m_z\rangle \equiv C^{(\pm)}_{jm_z} |j, m_z \pm 1\rangle$

Consider

① $$\langle j, m_z | \hat{J}_- \hat{J}_+ | j, m_z\rangle = |C^{(+)}_{jm_z}|^2 \underbrace{\langle j, m_z+1 | j, m_z+1\rangle}_{=1}$$

$$= \langle j, m_z | \hat{\vec{J}}^2 - \hbar \hat{J}_z - (\hat{J}_z)^2 | j, m_z\rangle$$

$$= \hbar^2 j(j+1) - \hbar^2 m_z(m_z+1)$$

$$\therefore \quad C^{(+)}_{jm_z} = \hbar\sqrt{j(j+1) - m_z(m_z+1)} \, ; \quad C^{(+)}_{jj} = 0 \checkmark$$

② $$\langle j, m_z | \hat{J}_+ \hat{J}_- | j, m_z\rangle = |C^{(-)}_{jm_z}|^2 \underbrace{\langle j, m_z-1 | j, m_z-1\rangle}_{=1}$$

$$= \langle j, m_z | \hat{\vec{J}}^2 + \hbar \hat{J}_z - (\hat{J}_z)^2 | j, m_z\rangle$$

$$= \hbar^2 j(j+1) - \hbar^2 m_z(m_z-1)$$

$$\therefore \quad C^{(-)}_{jm_z} = \hbar\sqrt{j(j+1) - m_z(m_z-1)} \, ; \quad C^{(-)}_{j\,-j} = 0 \checkmark$$

Some examples:

① $j = \frac{1}{2}$ ; $j(j+1) = 3/4$

$$\hat{J}_+ |\tfrac{1}{2}, -\tfrac{1}{2}\rangle = \hbar\sqrt{3/4 - (-\tfrac{1}{2})(-\tfrac{1}{2}+1)} \, |\tfrac{1}{2}, \tfrac{1}{2}\rangle = \hbar\sqrt{3/4 + 1/4} \, |\tfrac{1}{2}, \tfrac{1}{2}\rangle = \hbar |\tfrac{1}{2}, \tfrac{1}{2}\rangle \checkmark$$

Lec. 13, p.2

② $j = 1$ ; $j(j+1) = 2$

$$\hat{J}_+ |1, 0\rangle = \hbar\sqrt{2 - 0} \, |1,1\rangle = \sqrt{2}\hbar |1,1\rangle \checkmark$$

e.g., Lec. 11 p.6