Lecture 10

Angular momentum & rotational invariance

1. Rotation in 3d:

- on ordinary vectors, e.g. $\vec{r} = (x, y, z)$

$$\vec{r} \xrightarrow{R} \vec{r}\,' = \overleftrightarrow{R}^{(k)} \cdot \vec{r} \iff r_i' = R_{ij}^{(k)} r_j$$

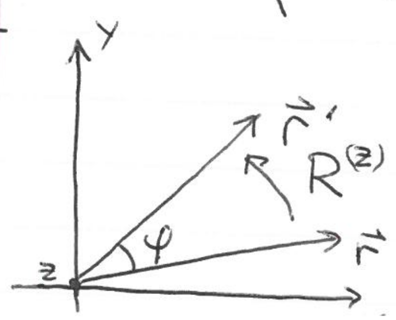
$$R^{(x)} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\varphi & -\sin\varphi \\ 0 & +\sin\varphi & \cos\varphi \end{pmatrix}$$

$$R^{(y)} = \begin{pmatrix} \cos\varphi & 0 & \sin\varphi \\ 0 & 1 & 0 \\ -\sin\varphi & 0 & \cos\varphi \end{pmatrix}$$

preserve scalars: $\vec{E} \cdot \vec{E} = \vec{E}\,' \cdot \vec{E}\,'$

$$R^{(z)} = \begin{pmatrix} \cos\varphi & -\sin\varphi & 0 \\ +\sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

around $\hat{z}$:



$$\overleftrightarrow{R} \cdot \vec{r} = \vec{r}\,' = (x\cos\varphi - y\sin\varphi,\ +x\sin\varphi + y\cos\varphi,\ z)$$

Note: non-Abelian SO(3) group

$R^{(k)} \in SO(3)$ ← orthogonal group of real orthogonal matrices (3×3)

$R^{(x)} R^{(y)} \neq R^{(y)} R^{(x)}$ s.t. $R^T R = \mathbb{1}$

i.e. $R^T = R^{-1}$.

labeled by a "ball" in 3d with radius π

point in a ball $\varphi \hat{n} \equiv \vec{\varphi}$

$0 < \varphi < \pi$ ← angle of rotation

$\hat{n}$ ← axis of rotation.

(also via Euler's angles $\underbrace{\underset{z}{\alpha}, \underset{y}{\beta}, \underset{z}{\gamma}}_{\text{see prob 12.5.7 Shankar}}$)

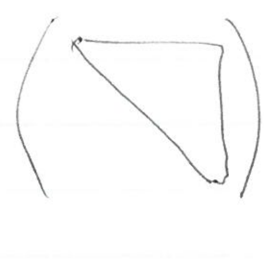
- infinitesimal rots $\varphi = \varepsilon \ll \pi$

e.g. $R_\varepsilon^{(z)} = \begin{pmatrix} 1 & -\varepsilon & 0 \\ +\varepsilon & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$

$\Leftrightarrow \vec{r}\,' = \vec{R}_\varepsilon^{(z)} \cdot \vec{r} = (x - y\varepsilon, +x\varepsilon + y, z)$

$d \times d$ real symm matrix : $\frac{d(d+1)}{2}$
orthogonal

$= 6 \quad (d=3)$



+ d constraint
of orthogonality

$\frac{d(d+1)}{2} - d = \frac{d(d-1)}{2} \underset{d=3}{=} 3.$

$R \simeq \mathbb{1} + \vec{\varepsilon} \cdot \vec{G}$ ← 3 generators ($\frac{d(d-1)}{2}$ planes)

Note: In 2d (only planar rot's), single axis

$\Rightarrow$ abelian, very similar to translations

but compact

$$R_{\varphi\hat{z}} = \begin{pmatrix} \cos\varphi & -\sin\varphi \\ \sin\varphi & \cos\varphi \end{pmatrix}$$

$$R_{\varphi_1} R_{\varphi_2} = R_{\varphi_1 + \varphi_2}$$

$$|R_\varphi \psi\rangle = U_\varphi |\psi\rangle$$

$$U_{\varphi_0}(\psi) = e^{-\varphi_0 \partial_\varphi}$$

c.f. $U_a = e^{-a\partial_x}$

but compact : $0 \leq \varphi_0 < 2\pi$

(important implications)

2. <u>Representation of $R^{(h)}_{\varphi}$ on quantum states & operators</u>

- What <u>unitary</u> operator acts on $|\psi\rangle$ to create a state in which a system is rotated?

i.e.

$$|\psi\rangle \xrightarrow[R_{\vec{\varphi}}]{} |\psi'\rangle \equiv |R_{\vec{\varphi}}\psi\rangle = U_{\vec{\varphi}}|\psi\rangle$$

???

require that

if $\langle\psi|\vec{r}|\psi\rangle = \langle\vec{r}\rangle$ then

$$\langle U_{\vec{\varphi}}\psi|\vec{r}|U_{\vec{\varphi}}\psi\rangle = \overleftrightarrow{R}_{\varphi}\cdot\langle\vec{r}\rangle = \langle\psi|R^{(h)}_{ij}r_j|\psi\rangle$$

what is $U_{\vec{\varphi}}$ representing rotation $R_{\vec{\varphi}}$?

- $U_{\vec{\varphi}}$ in coordinate representation:

$$|U_{\vec{\varphi}}\psi\rangle = U_{\varphi}|\psi\rangle$$

clearly $U_{\vec{\varphi}}|\vec{r}\rangle = |\overleftrightarrow{R}^{\vec{\varphi}}\cdot\vec{r}\rangle$

guarantees that $\langle\vec{r}\rangle \xrightarrow[R^{\vec{\varphi}}]{} R^{\vec{\varphi}}\cdot\langle\vec{r}\rangle$

since $\hat{\vec{r}}|\vec{r}\rangle = \vec{r}|\vec{r}\rangle$

$$\psi(\vec{r}) \equiv \langle \vec{r} \mid \psi \rangle$$

$$\Rightarrow \psi_{\vec{\varphi}}(\vec{r}) \equiv \langle \vec{r} \mid U_{\vec{\varphi}} \psi \rangle$$

$$= \langle \vec{r} \mid U_{\vec{\varphi}} \mid \psi \rangle$$

$$= \langle \overleftrightarrow{R}^T_{\vec{\varphi}} \cdot \vec{r} \mid \psi \rangle$$

$$\Rightarrow \psi(\vec{r}) \xrightarrow[R_{\vec{\varphi}}]{} \psi_{\vec{\varphi}}(\vec{r}) = \psi(\overleftrightarrow{R}^T_{\vec{\varphi}} \cdot \vec{r})$$

recall $\overleftrightarrow{R}^T_{\varphi\hat{z}} \cdot \vec{r} = (x\cos\varphi + y\sin\varphi,\ y\cos\varphi - x\sin\varphi,\ z)$ — notice reversed signs $\varphi \to -\varphi$

$$\Rightarrow \psi(\vec{r}) \xrightarrow[R_{\varphi\hat{z}}]{} \psi_{\varphi\hat{z}}(\vec{r}) = \psi(x\cos\varphi + y\sin\varphi,\ y\cos\varphi - x\sin\varphi,\ z)$$

$$\underset{\varphi \ll \pi}{\simeq} \psi_{\varepsilon\hat{z}}(\vec{r}) = \psi(x + \varepsilon y,\ y - \varepsilon x,\ z)$$

$$\simeq \psi(x, y, z) + \varepsilon(y\,\partial_x - x\,\partial_y)\psi(x, y, z)$$

$$\Rightarrow \psi(\vec{r}) \to \psi_{\varepsilon\hat{z}}(\vec{r}) = \left(1 - i\varepsilon \frac{1}{\hbar} L_z\right)\psi(\vec{r})$$

where $L_z = (\vec{r} \times \vec{p})_z = x p_y - y p_x$

$$= -i\hbar(x\,\partial_y - y\,\partial_x)$$

$$= -i\hbar\,\partial_\varphi$$

$$(\text{cf. } p = -i\hbar\,\partial_x)$$

z-component of $\vec{L}$ - angular momentum.

Equivalently:

- $\langle \vec{r} | U_{\vec{\varphi}} | \vec{r}\,' \rangle = \langle \vec{r} | \overleftrightarrow{R}_{\vec{\varphi}} \vec{r}\,' \rangle$

$$= \delta^{(3)}(\vec{r} - \overleftrightarrow{R}_{\vec{\varphi}} \cdot \vec{r}\,')$$

infinitesmal

$$\simeq \delta(x - x' + \varepsilon y')\,\delta(y - y' - \varepsilon x')\,\delta(z-z')$$

$$= \delta^{(3)}(\vec{r} - \vec{r}\,') + \varepsilon y' \partial_x \delta(x-x')\delta(y-y')\delta(z-z')$$

$$- \varepsilon x' \partial_y \delta(y-y')\delta(x-x')\delta(z-z')$$

$$\underline{U_{\vec{\varphi}}(\vec{r}, \vec{r}\,') = \left[1 - \varepsilon(x\partial_y - y\partial_x)\right] \delta^{(3)}(\vec{r} - \vec{r}\,')}$$

$$= \left[1 - \frac{i\varepsilon}{\hbar} \hat{L}_z\right]_{r, r'}$$

- "passive" pnt of view via action on operators

$$\langle \psi | \hat{\vec{r}} | \psi \rangle \xrightarrow[R_{\vec{\varphi}}]{} \langle U_{\vec{\varphi}} \psi | \hat{\vec{r}} | U_{\vec{\varphi}} \psi \rangle =$$

$$= \langle \psi | U^{+}_{\vec{\varphi}} \hat{\vec{r}}\, U_{\vec{\varphi}} | \psi \rangle = \overleftrightarrow{R}_{\vec{\varphi}} \cdot \langle \psi | \hat{\vec{r}} | \psi \rangle$$

$$\Rightarrow \quad U^{+}_{\vec{\varphi}} \hat{\vec{r}}\, U_{\vec{\varphi}} = \overleftrightarrow{R}_{\vec{\varphi}} \cdot \hat{\vec{r}}$$

Look at infinitesmal rotation by $\vec{\varphi} = \varepsilon \hat{z}$

$$U_{\vec{\varphi} = \varepsilon \hat{z}} \simeq \mathbb{1} + \underbrace{i \varepsilon G_z}$$

$\Rightarrow$

Taylor expansion in ε

(actually know that by unitarity of $U_{\vec{\varphi}}$ $\quad U_{\vec{\varphi}} = e^{i \vec{\varphi} \cdot \vec{G}} \quad G^{+} = G$)

$$\hat{U}^{\dagger}_{\varepsilon\hat{z}}\,\hat{\vec{r}}\,\hat{U}_{\varepsilon\hat{z}} = (\mathbb{1} - i\varepsilon\hat{G}_z)\,\hat{\vec{r}}\,(\mathbb{1} + i\varepsilon\hat{G}_z)$$

$$\approx \hat{\vec{r}} + i\varepsilon[\hat{\vec{r}}, \hat{G}_z] = \overleftrightarrow{R}_{\varepsilon\hat{z}} \cdot \hat{\vec{r}}$$

$$\hat{r}_i + i\varepsilon[\hat{r}_i, \hat{G}_z] = \hat{r}_i - \varepsilon\epsilon_{ijz}\hat{r}_j$$

$$\Rightarrow [\hat{r}_i, \hat{G}_z] = +i\epsilon_{ijz}\hat{r}_j$$

repeat for rotations about other 2 axes, $\hat{x}, \hat{y}$:

$$[\hat{r}_i, \hat{G}_k] = +i\epsilon_{ijk}\hat{r}_j$$

$$\Rightarrow \hat{\vec{G}} = -\frac{1}{\hbar}\hat{\vec{r}} \times \hat{\vec{p}} = -\frac{1}{\hbar}\hat{\vec{L}}$$

check by using $[\hat{r}_i, \hat{p}_j] = i\hbar\delta_{ij}$

$$\frac{1}{\hbar}[r_i, (\vec{r}\times\vec{p})_k] = \frac{1}{\hbar}[r_i, \epsilon_{jnk} r_j p_n]$$

$$= \frac{\epsilon_{jnk}}{\hbar} r_j \underbrace{[r_i, p_n]}_{i\hbar\delta_{in}} = i\epsilon_{jik} r_j$$

$$\Rightarrow \boxed{[\hat{r}_i, \hat{L}_k] = -i\hbar\epsilon_{ijk} r_j}$$

extends to any <u>vector</u> operator $\hat{\vec{E}}$

$$[\hat{E}_i, \hat{L}_k] = -i\hbar\epsilon_{ijk}\hat{E}_j \quad \leftarrow \text{defn of vector operator.}$$

$$\boxed{\hat{U}_{\vec{\varepsilon}} = \mathbb{1} - i\frac{\vec{\varepsilon}}{\hbar}\cdot\hat{\vec{L}}}$$ ← unitary op for rotation by $|\vec{\varepsilon}|$ about $\vec{\varepsilon}$ axis.

- Finite (large) rotation:

$$\hat{U}_{\vec{\varphi}} = \left(\hat{U}_{\frac{\varphi}{N}\hat{n}}\right)^N = \left(\mathbb{1} - \frac{i}{\hbar}\frac{\varphi}{N}\hat{n}\cdot\vec{L}\right)^N$$

$$\boxed{\hat{U}_{\vec{\varphi}} \underset{N\to\infty}{=} e^{-\frac{i}{\hbar}\vec{\varphi}\cdot\hat{\vec{L}}}}$$

$$= e^{-i/\hbar\,\varphi_0(-i\hbar\partial_\varphi)} = e^{-\varphi_0\partial_\varphi} \quad (\text{cf. } T_a = e^{a\partial_x})$$

equivalently:

Note: $\vec{E} \xrightarrow[R_\varphi]{} \vec{E}' = \vec{E} + \delta\vec{E}$

where,

$$\delta\hat{\vec{E}} = -i\frac{\varepsilon}{\hbar}[\hat{\vec{E}}, \hat{L}_z]$$

$$\frac{\partial\hat{\vec{E}}}{\partial\varphi} = -\frac{i}{\hbar}[\hat{\vec{E}}, \hat{L}_z]$$

differential eqn for "evolution" in φ via generator $\hat{L}_z/\hbar$ (cf evolution in t via $\frac{\hat{H}}{\hbar}$]

solved by $\hat{\vec{E}}_\varphi = e^{+\frac{i}{\hbar}\varphi\hat{L}_z}\hat{\vec{E}}\,e^{-\frac{i}{\hbar}\varphi\hat{L}_z}$

(cf $\hat{O}_t = e^{\frac{i}{\hbar}t\hat{H}}\hat{O}\,e^{-\frac{i}{\hbar}t\hat{H}}$)

$$\Rightarrow \boxed{U_{\vec{\varphi}} = e^{-\frac{i}{\hbar}\varphi\hat{n}\cdot\hat{\vec{L}}}} \quad \text{cf } U_{\vec{a}} = e^{-\frac{i}{\hbar}\vec{a}\cdot\vec{p}}$$

3. Symmetry (rotational):

Any scalar operator (by defn) must not transform under rotation, i.e.

$$\hat{U}^{+}_{\vec{\varphi}} \hat{O} \hat{U}_{\vec{\varphi}} = \hat{O} \iff [\hat{O}, \hat{\vec{L}}] = 0$$

System is symmetric under rotation when $\hat{H}$ is a scalar operator

i.e. $[\hat{H}, \hat{\vec{L}}] = 0$

Ex. $\hat{H} = \frac{\hat{p}^2}{2m} + V(|\vec{r}|)$ ✓

scalar ($\hat{p}^2$)

scaler, potential only depends on distance $|\vec{r}|$ not x, y, z separately.

(show this for hw 6)

$$[\hat{H}, \hat{\vec{L}}] = 0$$

can diagonalize $\hat{H}$ & $\hat{L}_x, \hat{L}_y, \hat{L}_z$ simultaneously?

No! since $[L_i, L_j] = i\hbar \epsilon_{ijk} L_k$

$\Rightarrow L_i, L_j$ do not commute for $i \neq j$.

what to do?

pick any one, or even any one linear combination, i.e. pick quantization axis, e.g. $\hat{z}$

but also note that $[\hat{L}^2, \vec{\hat{L}}] = 0$, since $\hat{L}^2$ scalar, & $[H, \hat{L}^2] = 0$, since $[H, \vec{L}] = 0$

$\Rightarrow$ "complete" set of commuting ops, whose eigenvalues can be used to label $|E\rangle$ are:

$$\underline{\hat{H}, \hat{L}^2, \hat{L}_z}$$; also $\underline{L^2 \text{ \& } L_z \text{ are conserved}}$
$\Leftrightarrow$ const. of motion!

$\Rightarrow$ common eigenstates $|E, L^2, L_z\rangle = ?$

4. Eigenstates of $\hat{L}^2$ & $\hat{L}_z$:

$$\hat{L}^2 |l, m\rangle = \hbar^2 \underbrace{l(l+1)}_{} |l, m\rangle$$

must have: $l \geq 0$ dimensions convenient way to write eigenvalue of $\hat{L}^2$.

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

$|l, m\rangle$, l, $m = ?$

Could do everything in coordinate representation, $|\theta, \varphi\rangle$

i.e. in terms of wavefncs

$$\psi_{lm}(\theta, \varphi) = \langle \theta, \varphi | l m\rangle \quad (\text{cf } \psi_n(x) = \langle x|n\rangle)$$

by solving differential eqn:
$$\begin{cases} L^2 \psi_{lm}(\theta, \varphi) = \hbar^2 l(l+1) \psi_{lm} \\ L_z \psi_{lm} = \hbar m \psi_{lm} \end{cases}$$
diff'l. op's

... but most of the information can be obtained from operator formalism.
(cf harmonic oscillator via solving Sch. Eqn vs using creation/annihil. ops)

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

consider (non Hermitian) "ladder" operators.

$$\hat{L}_\pm \equiv \hat{L}_x \pm i \hat{L}_y \;; \quad \hat{L}_+^+ = \hat{L}_-$$

(like a^+, a)

<u>with properties</u>:

- $[\hat{L}_z, \hat{L}_\pm] = \pm \hbar L_\pm$

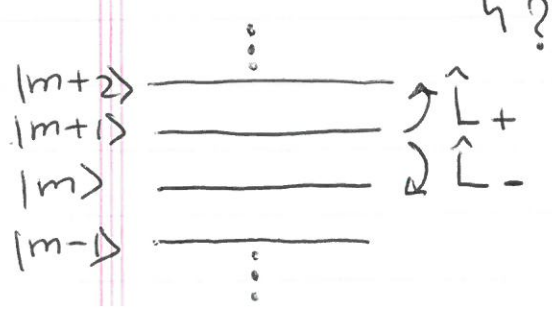
- $[L_+, L_-] = 2\hbar L_z$

→ look at state: $(L_\pm |\ell m\rangle)$

$$L_z (L_\pm |\ell m\rangle) = (L_\pm L_z \pm \hbar L_\pm) |\ell m\rangle$$
$$= \hbar(m \pm 1)(L_\pm |\ell m\rangle)$$

$$\Rightarrow L_\pm |\ell m\rangle = \underbrace{C_m^{(\pm)}}_{???} |\ell\ m \pm 1\rangle$$

hence L_x, L_y have no matrix elements between ℓ & ℓ' for $\ell \neq \ell'$
block-diagonal in ℓ, ℓ'



Harmonic oscillator analogues:

- $[\hat{n}, \hat{a}^+] = a^+$
  $[\hat{n}, \hat{a}] = -a$

- $[a, a^+] = 1$

→ look at state: $(a^+ |n\rangle)$

$$a^+ |n\rangle = C_n^{(+)} |n+1\rangle$$
$$a |n\rangle = C_n^{(-)} |n-1\rangle$$
$$C_n^{(\pm)} = ???$$
$$\langle n | a a^+ | n\rangle = |C_n^{(+)}|^2 = n+1$$
$$\Rightarrow C_n^{(+)} = \sqrt{n+1}$$
$$\underline{C_n^{(-)} = \sqrt{n}}$$

SU(2) special unitary group

2×2 complex matrices with $\det U = 1$

$$U = \begin{pmatrix} a & b \\ -b^* & a^* \end{pmatrix} \Rightarrow U^+ U = 1$$

$$\begin{pmatrix} a^* & -b \\ b^* & a \end{pmatrix}\begin{pmatrix} a & b \\ -b^* & a^* \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$\downarrow$

with constraint (unimodular)

$$|a|^2 + |b|^2 = 1 \rightarrow 3 \text{ parameters for } SU(2)$$

SU(2) subgroup of U(2) which does not have unimodular constraint.

$$e^{i\gamma}\begin{pmatrix} a & b \\ -b^* & a^* \end{pmatrix} \in U(2)$$

SU(2) locally isomorphic to SO(3) but globally different.

e.g. $U_{2\pi\hat{z}} = e^{-\frac{i}{\hbar}\vec{S}\cdot 2\pi\hat{z}} = e^{-i\pi} \neq \mathbb{1}$

but rot. by 2π is $= \mathbb{1}$.

$\Rightarrow$ 2 elements of SU(2) $\rightarrow$ 1 of SO(3)

$\Uparrow$

has $s = \frac{1}{2}$ represent.

$$C_m^{\pm} = ??? \xrightarrow{} \text{positive definite} \Rightarrow l(l+1) \geq m(m\pm 1)$$

$$\underbrace{\langle l\, m | L_- L_+ | l\, m\rangle}_{?} = |C_m^{(+)}|^2 \underbrace{\langle l\ m+1 | l\ m+1\rangle}_{1}$$

Note: $L^2 = L_- L_+ + L_z^2 + \hbar L_z$

$$= L_+ L_- + L_z^2 - \hbar L_z$$

$$\Rightarrow \langle l m | L_- L_+ | l m\rangle = \hbar^2 [l(l+1) - m(m+1)]$$

$$\langle l m | L_+ L_- | l m\rangle = \hbar^2 [l(l+1) - m(m-1)]$$

$$\Rightarrow \boxed{C_m^{(\pm)} = \hbar \sqrt{\underbrace{l(l+1) - m(m\pm 1)}_{\text{must be positive}}}}$$

To keep $C_m^{(\pm)}$ real need to have max & min values of m_*, s.t. $C_{m_*}^{(\pm)} = 0$

also because require $L_z^2 < L^2$

$$\Rightarrow -l \leq m \leq l$$

$$m = l,\ l-1,\ l-2,\ \ldots,\ l-n = -l$$

$n \in \mathbb{Z}$; in order to vanish $C_{m=-l}^{(-)} = 0$

$$\Rightarrow l - n = -l$$

$$2l = n \Rightarrow \boxed{l = \frac{1}{2} n}$$

i.e. SU(2)/SO(3) rotational group (non Abelian) structure

requires $l = \frac{1}{2} n$, i.e. integer or half integer

that's it!

orbital $\vec{L}$ spin $\vec{S}$

<u>scalar operator</u>: $[\hat{h}, \vec{L}] = 0 \Rightarrow$

$$\Rightarrow [\hat{h}, \hat{L}_+] = 0$$

$$\langle nlm | (\hat{h} \hat{L}_+ - \hat{L}_+ \hat{h}) | n'l'm' \rangle$$

$$\langle n l m | \underset{\substack{\uparrow \\ \text{diagonal} \\ \text{in } l, m}}{\hat{h}} \underset{\substack{\uparrow \\ \text{diagonal in } ll \\ \text{connects } m \,\&\, m' = m-1}}{\hat{L}_+} | n'l'm' \rangle - \langle n l m | \hat{L}_+ \hat{h} | n'l'm' \rangle$$

$$\sum_{\substack{m'' \\ l'' \\ n''}} \Big(\langle n l m | \hat{h} | n'' l'' m'' \rangle \langle n'' l'' m'' | \hat{L}_+ | n' l' m' \rangle - \langle n l m | \hat{L}_+ | n'' l'' m'' \rangle \langle n'' l'' m'' | \hat{h} | n' l' m' \rangle \Big)$$

$$= \langle n l m | \hat{h} | n' l m \rangle \langle n' l m | \hat{L}_+ | n' l \, m-1 \rangle$$

$$- \langle n l m | \hat{L}_+ | n l \, m-1 \rangle \langle n l \, m-1 | \hat{h} | n' l \, m-1 \rangle = 0$$

$$\Rightarrow \langle n l m | \hat{h} | n' l m \rangle = \langle n l \, m-1 | \hat{h} | n' l \, m-1 \rangle$$

independent of m!

$\Rightarrow$ <u>$2l+1$ degeneracy</u>.

More generally, expect degeneracy when:

- $[J_1, J_2] \neq 0$ but $[H, J_{1,2}] = 0$

on

- H invariant under nonAbelian group with irreducible representations of $d > 1$ dimensions.

Focus on orbital L with $\ell \in \mathbb{Z}$. (spin ½ later)

Each ℓ has $2\ell+1$ m states.

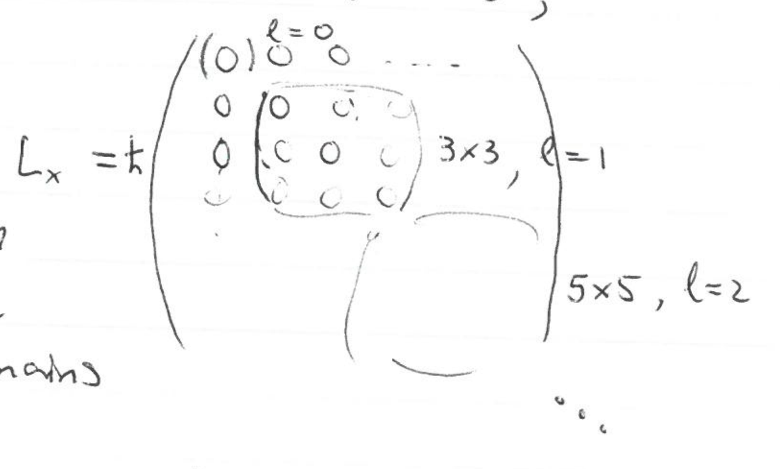
- Degeneracy:

H is a scalar $\Rightarrow$ cannot depend on L_z alone, only through L^2

$\Rightarrow H[L^2, \cancel{L_z}] \Rightarrow$ independent of L_z eigenvalue m $\Rightarrow$ each $|E, \ell, m\rangle$ is (at least) $\boxed{(2\ell+1)\text{-fold degenerate}}$

Note: operator $\vec{L}$, represented by a matrix valued vector $\vec{L}_{\ell m; \ell' m'}$ is block-diagonal with ℓ^{th} block a matrix $\vec{L}^{(\ell)}_{m,m'}$ $(2\ell+1)\times(2\ell+1)$;

each block is independent called $2\ell+1$ dimensional representation of $\vec{L}$. Each subspace has fixed L^2, that remains unchanged by $\vec{L}$



$\Rightarrow$ guaranteed degeneracy iff non Abelian group with representation >1, and $[H, L_\pm]=0$, where $L_\pm$ is a ladder op moving between

$\boxed{J_x}$

$\langle j'm' | J_x | jm \rangle$

$$
\begin{array}{c|cccccc}
{}_{j'm'} \backslash {}^{jm} & (0,0) & (\frac{1}{2},\frac{1}{2}) & (\frac{1}{2},-\frac{1}{2}) & (1,1) & (1,0) & (1,-1) \ldots \\
\hline
 & 0 & 0 & 0 & 0 & 0 & 0 \\
 & 0 & 0 & \hbar/2 & 0 & 0 & 0 \\
 & 0 & \hbar/2 & 0 & 0 & 0 & 0 \\
 & 0 & 0 & 0 & 0 & \hbar/\sqrt{2} & 0 \\
 & 0 & 0 & 0 & \frac{\hbar}{\sqrt{2}} & 0 & \frac{\hbar}{\sqrt{2}} \\
 & 0 & 0 & 0 & 0 & \frac{\hbar}{\sqrt{2}} & 0
\end{array}
$$

5. Coordinate representation: $\vec{L} = \vec{r} \times \vec{p}$

- $L^2 = -\frac{\hbar^2}{\sin\theta}\partial_\theta \sin\theta\, \partial_\theta - \frac{\hbar^2}{\sin^2\theta}\partial_\varphi^2$

$L_z = -i\hbar\,\partial_\varphi$; $L_\pm = \hbar e^{\pm i\varphi}(\pm\partial_\theta + i\cot\theta\,\partial_\varphi)$

$\Psi_{lm}(\theta,\varphi) \equiv \langle \theta,\varphi | l\, m\rangle \equiv Y_{lm}(\theta,\varphi)$

the (so-called) spherical harmonics

$$\begin{cases} L^2\Psi_{lm}(\theta,\varphi) = \hbar^2 l(l+1)\Psi_{lm}(\theta,\varphi) \\ -i\hbar\,\partial_\varphi\Psi_{lm} = \hbar m\Psi_{lm} \end{cases}$$

→ these two diff. eqns can be solved directly via series solns method. $\Rightarrow Y_{lm}(\theta,\varphi)$.

→ easy via separation of vars $\Psi_{lm}(\theta,\varphi) = \Theta_{lm}(\theta)\Phi_m(\varphi)$

$\Rightarrow \partial_\varphi \Phi_m(\varphi) = im\,\Phi_m(\varphi)$

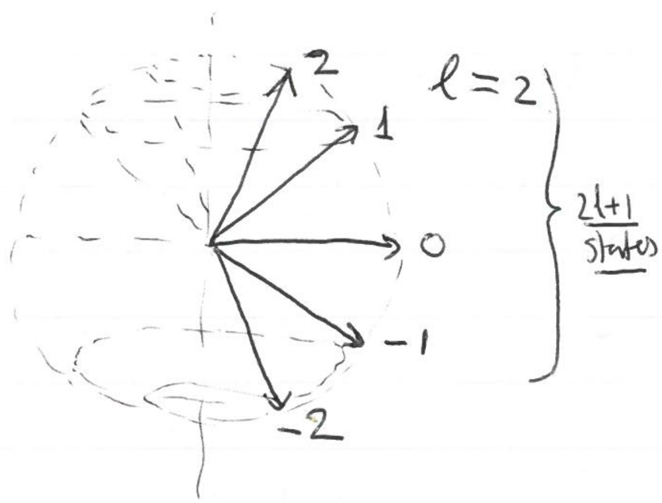
$\Rightarrow \Phi_m(\varphi) = \frac{1}{\sqrt{2\pi}} e^{im\varphi}$ (Normalization: $\int_0^{2\pi} d\varphi\, |\Phi_m|^2 = 1$)

Note: $\varphi \to \varphi + 2\pi$: $\Phi_m(\varphi) \to \Phi_m(\varphi+2\pi) = e^{i2\pi m}\Phi_m(\varphi)$

cannot require $e^{i2\pi m} = 1$ since $\Phi(\varphi)$ can be multivalued, i.e. this is not the argument for $m \in \mathbb{Z}$ quantization. Related to why in 2d ok to have fractional m. $m \in \mathbb{Z}$ (or $\frac{1}{2}\mathbb{Z}$) due to 3D rots & its non Abelian nature.

- <u>Note</u> orthonormality

$$\langle lm | lm' \rangle = \delta_{mm'} = \frac{1}{2\pi}\int_0^{2\pi} d\varphi \, e^{-i(m-m')\varphi}$$



<u>Note:</u> only L_z has a definite value of m
L_x, L_y are not defined
i.e. can be measured to be any value
cartoon: precession about $\hat{z}$ axis.

<u>Note:</u> $L^2 = \hbar^2 l(l+1) > L_z^2 = m^2\hbar^2 = l^2\hbar^2$

$\sqrt{l(l+1)} > l \Rightarrow$ even in $m=l$ state

$\vec{L}$ vector is <u>not</u> straight up! Why?

uncertainty in L_x & L_y

$$L^2 = L_x^2 + L_y^2 + L_z^2$$

$$\langle lm | L^2 | lm \rangle = \hbar^2 l(l+1) = \langle L_\perp^2 \rangle + m^2\hbar^2$$

$\Rightarrow$ <u>for $m=l$</u> $\hbar^2(l(l+1) - l^2) = \hbar^2 l = \langle L_\perp^2 \rangle$

$$\Rightarrow \underline{L_\perp^{rms} = \hbar\sqrt{l}}$$

$\Rightarrow$ large l, uncertainty in $L_\perp << L^2$

$\Rightarrow$ <u>classical limit</u> for large l.

$$\langle lm | L_x^2 | lm \rangle = \langle lm | L_y^2 | lm \rangle = \frac{1}{2}\hbar^2 (l(l+1) - m^2)$$

$\langle \hat{n} | \ell m \rangle = \langle \theta, \varphi | \ell m \rangle \equiv Y_{\ell m}(\theta,\varphi)$ (c.f. $\langle x | p \rangle = \psi_p(x)$)

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

consider infinitesimal rots. or use r & p in coord. repres.

$$\Rightarrow \quad L^x = -i\hbar \left(-\sin\varphi \frac{\partial}{\partial\theta} - \cot\theta \cos\varphi \, \partial_\varphi \right)$$

$$L^y = -i\hbar \left(\cos\varphi \frac{\partial}{\partial\theta} - \cot\theta \sin\varphi \, \partial_\varphi \right)$$

$$L^2 = \vec{r}^{\,2} \vec{p}^{\,2} - (\vec{r} \cdot \vec{p})^2 + i\hbar \, \vec{r} \cdot \vec{p}$$

- Wavefncs $Y_{\ell m}(\theta,\varphi)$ via ladder operators.

Recall treatment of harmonic oscillator:

$$a|0\rangle = 0 \Rightarrow \int_{x'} \underbrace{\langle x|a|x'\rangle}_{a_{xx'}} \underbrace{\langle x'|0\rangle}_{\psi_0(x)}$$

$$a_{xx'} = \frac{1}{\sqrt{2}}(x+\partial_x)\delta(x-x')$$

$$\Rightarrow (x+\partial_x)\psi_0(x) = 0$$

$$\Rightarrow \psi_0(x) = N e^{-x^2/2}$$

$$\psi_1(x) = \langle x|1\rangle = a^+|0\rangle = \frac{1}{\sqrt{2}}(x-\partial_x)\psi_0(x)$$

$$\psi_1(x) = \langle x|1\rangle = \frac{1}{\sqrt{2}}(x-\partial_x)e^{-x^2/2}N$$

$$\vdots \qquad \vdots$$

$$\psi_n(x) = \langle x|n\rangle = \left(\frac{1}{\sqrt{2}}\right)^n \frac{1}{\sqrt{n!}}(x-\partial_x)^n e^{-x^2/2} N$$

similarly with $|\ell m\rangle$, L_+, L_-:

$$L_+|\ell\ell\rangle = 0,$$ annihilation of "top most" (highest weight) state.

$$L_\pm = \pm\hbar e^{\pm i\varphi}(\partial_\theta \pm i\cot\theta\,\partial_\varphi)$$

$$\Rightarrow (\partial_\theta + i\cot\theta\,\partial_\varphi)\psi_{\ell\ell}(\theta,\varphi) = 0$$

$$\psi_{\ell\ell}(\theta,\varphi) = \Theta_{\ell\ell}(\theta)\,e^{i\ell\phi}$$

$$\Rightarrow (\partial_\theta - \ell\cot\theta)\Theta_{\ell\ell}(\theta) = 0 \Rightarrow \Theta_{\ell\ell}(\theta) = (\sin\theta)^\ell \propto Y_{\ell\ell}$$

$$P_\ell(x) = P_\ell^{m=0}(x) = N \frac{d^\ell}{dx^\ell}\left[(1-x^2)^\ell\right]$$

$$P_\ell^m(x) = (1-x^2)^{m/2} \frac{d^m}{dx^m} P_\ell(x)$$

with proper normalization

$$Y_{\ell\ell}(\theta,\varphi) = (-1)^\ell \left[\frac{(2\ell+1)!}{4\pi}\right]^{1/2} \frac{1}{2^\ell \ell!} \underbrace{(\sin\theta)^\ell}_{\text{strongly confined to xy plane}} e^{i\ell\varphi}$$

$$L_-|\ell\ell\rangle = \hbar\,[\underbrace{\ell(\ell+1)-\ell(\ell-1)}_{2\ell}]^{1/2}\,|\ell\,\ell-1\rangle$$

$$\Rightarrow Y_{\ell\,\ell-1}(\theta,\varphi) = \frac{1}{\hbar\sqrt{2\ell}}\left[-\hbar e^{-i\varphi}(\partial_\theta - i\cot\theta\,\partial_\varphi)\right] Y_{\ell\ell}(\theta,\varphi)$$

$$= \frac{1}{\sqrt{2\ell}\,\hbar}\left[(-\hbar)e^{i(\ell-1)\varphi}(\partial_\theta + \ell\cot\theta)(\sin\theta)^\ell\right]$$

Note: $(\partial_\theta + \ell\cot\theta) f(\theta) = \frac{1}{(\sin\theta)^\ell}\partial_\theta\left((\sin\theta)^\ell f(\theta)\right)$

$$\Rightarrow Y_{\ell\,\ell-1} = C_\ell \frac{e^{i(\ell-1)\varphi}}{(\sin\theta)^\ell}(-\partial_\theta)\left[(\sin\theta)^{2\ell}\right]$$

$\vdots$

$$\boxed{Y_{\ell m}(\theta,\varphi) = C_{\ell m}\frac{e^{im\varphi}}{(\sin\theta)^m}\left(\frac{\partial}{\partial u}\right)^{\ell-m}\left[(1-u^2)^\ell\right]}$$

where, $u = \cos\theta$

Normalization $\langle Y_{\ell m}|Y_{\ell m}\rangle = 1 = \int_0^{2\pi} d\varphi \int_{-1}^{1} du\, |C|^2 \left[\frac{1}{(1-u^2)^{m/2}}\partial_u^{\ell-m}(1-u^2)^\ell\right]^2$

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

$$Y_{\ell,-m} = (-1)^m Y_{\ell m}^*\,;\quad P_\ell^m(u) = (-1)^{\ell+m}\frac{(\ell+m)!}{(\ell-m)!}\,\frac{(1-u^2)^{-m/2}}{2^\ell \ell!}\,\partial_u^{\ell-m}(1-u^2)^\ell$$

Associated Legendre polynomials $P_\ell^m(u)$

other props:

- $$\int_{-1}^{1} P_\ell(\cos\theta)\, P_{\ell'}(\cos\theta)\, d(\cos\theta) = \frac{2}{2\ell+1}\,\delta_{\ell,\ell'}$$

- $$P_\ell(x) = \frac{1}{2^\ell \ell!}\frac{d^\ell}{dx^\ell}(x^2-1)^\ell$$ Legendre Polyn.

- $$\int_0^1 (1-x^2)^m\, dx = \frac{2m!!}{(2m+1)!!}$$

- isotropy of closed ℓ shell: $$\sum_m |Y_{\ell m}(\theta,\varphi)|^2 = \frac{2\ell+1}{4\pi}$$

- generating fnc.: $$\frac{1}{\sqrt{1+s^2-2sx}} = \sum_{\ell=0}^{\infty} P_\ell(x)\, s^\ell$$ ← multipole expansion

$$\int \frac{\rho(\vec r\,')}{|\vec r - \vec r\,'|}\, d^3\vec r\,'$$

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

- $$P_\ell(\hat n\cdot\hat n') = \frac{4\pi}{2\ell+1}\sum_{m=-\ell}^{\ell} Y^*_{\ell m}(\hat n')\, Y_{\ell m}(\hat n)$$

$\hat n'$ ← quantization axis

$$Y^{\hat n'}_{\ell 0}(\hat n) = \sum_m C_{\ell m}(\hat n')\, Y^{\hat z}_{\ell m}(\hat n)$$

$\|$ rotation of $\hat z \to \hat n'$ complete set. $\|$

$$= Y^{\hat n}_{\ell 0}(\hat n') = \sum_m C_{\ell m}(\hat n)\, Y^{\hat z}_{\ell m}(\hat n')$$

$$\Rightarrow C_{\ell m}(\hat n) = Y^{\hat z}_{\ell m}(\hat n)\,!$$

- Closure relation ($\Rightarrow$): $$\int P_\ell(\hat n\cdot\hat n')\, P_{\ell'}(\hat n\cdot\hat n'')\, d\Omega_{\hat n} = \frac{4\pi}{2\ell+1}\,\delta_{\ell\ell'}\, P_\ell(\hat n'\cdot\hat n'')$$

- Parity: $r\to r$, $\theta\to\pi-\theta$, $\phi\to\phi+\pi$: $Y_{\ell m}(\theta,\varphi)\to(-1)^\ell\, Y_{\ell m}(\theta,\varphi)$
  $\Leftrightarrow (\vec r \to -\vec r)$

$$[P, L_\pm] = 0$$

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

spherical harmonics: $\propto (\sin\theta)^{|m|}\big(\underbrace{P_{\ell-|m|}}_{\text{highest monomial}}(\cos\theta)\big)$

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

complete orthonormal basis.

$$\psi(r,\theta,\varphi) = \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell} C_{\ell m}(r)\, Y_{\ell m}(\theta,\varphi)$$

Explicit list: Hydrogen orbitals.

$$Y_{0,0} = \frac{1}{\sqrt{4\pi}}$$

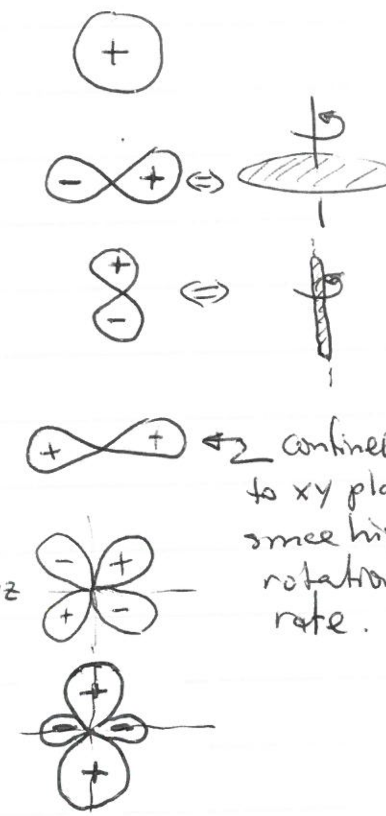
$$Y_{1,\pm1} = \mp\left(\frac{3}{8\pi}\right)^{1/2}\sin\theta\, e^{\pm i\varphi} \propto x \pm iy$$

$$Y_{1,0} = \left(\frac{3}{4\pi}\right)^{1/2}\cos\theta \propto z$$

$$Y_{2,\pm2} = \left(\frac{15}{32\pi}\right)^{1/2}\sin^2\theta\, e^{\pm i2\varphi} \propto x^2 - y^2 \pm i2xy$$

$$Y_{2,\pm1} = \mp\left(\frac{15}{8\pi}\right)^{1/2}\sin\theta\cos\theta\, e^{\pm i\varphi} \propto xz \pm iyz$$

$$Y_{2,0} = \left(\frac{5}{16\pi}\right)^{1/2}(3\cos^2\theta - 1) \propto 3z^2 - 1$$



confined to xy plane since high rotation rate.

cartesian tensors $x_i x_j x_k = T_{ijk}$; $Q_{ij} = x_i x_j$

traceless $\frac{3\cdot 4}{2} - 1$