Lecture $\boxed{26}$, Oct. 30 (Fri.)

Outline for today (& next weeks)

- orbital angular momentum/spherical harmonics from rotations viewpoint (re-deriving "old" results): sec. 3.6 of Sakurai
- Solving Schroedinger's wave equation for spherically symmetric potential: (back to) 3D free particle & (isotropic) SHO (angular momentum viewpoint); Coulomb; ∞ well (sec. 3.7 of Sakurai)
- Addition of angular momenta: sec. 3.8 of Sakurai

What has $\bar{L} = \bar{x} \times \bar{p}$ (operator) to do with rotations?

(i) Commutation relations of $\bar{L}$:

use $[x_i, p_j] = i\hbar\,\delta_{ij}$; $[x_i, x_j] = [p_i, p_j] = 0$

to get : $[L_i, L_j] = i\varepsilon_{ijk} L_k$

i.e., those of angular momentum $(\bar{J})$

$$\left\{ \text{e.g. } [\underset{(\bar{x}\times\bar{p})_x}{L_x}, L_y] = [(y p_z - z p_y), (z p_x - x p_z)] \right.$$

$$= [y p_z, z p_x] + [z p_y, x p_z],$$

do not commute

whereas $[y p_z, x p_z] = 0 = [z p_y, z p_x]$

$$= y p_x \underbrace{[p_z, z]}_{-i\hbar} + p_y x \underbrace{[z, p_z]}_{+i\hbar}$$

$$= i\hbar (x p_y - y p_x) = i\hbar L_z$$

... similarly, $[L_z, L_x]$ & $[L_y, L_z]$

(ii) L ("made of" $x, \vec{p}$) acts on position eigenket, rotating it infinitesimally (using action of p on position eigenkets)

$$\left[1 - i\left(\frac{\delta\phi}{\hbar}\right)L_z\right]|x', y', z'\rangle$$

$$= \left[1 - i\left(\frac{\delta\phi}{\hbar}\right)(x p_y - y p_x)\right]|x', y', z'\rangle$$

switch

$$= \left[1 - i\left(\frac{\delta\phi}{\hbar}\right)(p_y x - p_x y)\right]|x', y', z'\rangle$$

y' x'

$$= \left[1 - i\left(\frac{p_y}{\hbar}\right)(\delta\phi\, x') + i\left(\frac{p_x}{\hbar}\right)(\delta\phi\, y')\right]|x', y', z'\rangle$$

$\left\{\text{Recall : } \left[1 - i\left(\frac{p}{\hbar}\right)(\delta x')\right]|x'\rangle = |x' + \delta x'\rangle \text{ in 1d.}\right\}$

$$= |x' - y'\delta\phi\,, y' + x'\delta\phi\,, z'\rangle$$

$\Rightarrow$ infinitesimal rotation about z-axis [if $\bar{p}$ generates translation, then $\bar{L} = (\bar{x} \times p)$ generates rotations]

— So, $\bar{L}$ is indeed "$\bar{J}$" ("same" footing as $\bar{S}$)

— Use "new" property of $\bar{L}$ ["forget" its origin as $(\bar{x} \times \bar{p})$] to reproduce "old" results:

— $\boxed{\text{How does } \bar{L} \text{ "act" on wavefunctions?}}$

[again, from $\bar{L} = (\bar{x} \times \bar{p})$, we already know L_z "=" $-i\hbar \partial/\partial\phi$ & $|\bar{L}|^2$ is angular part of $\bar{\nabla}'^2$]

— want "analog" of $\langle x'|p|\alpha\rangle = -i\hbar \frac{\partial}{\partial x'} \underbrace{\langle x'|\alpha\rangle}_{\psi_\alpha(x')}$

— infintesimal rotation about z-axis of a ket:

$$\langle x', y', z' | \underbrace{\left[1 - i\left(\frac{\delta\phi}{\hbar}\right) L_z\right] |\alpha\rangle}_{\text{rotated ket}}$$

(use action of L on position eigenkets)

[use $(\langle\alpha| X) \Longleftrightarrow X^{\dagger}|\alpha\rangle$]

$$= \langle x' + y'\delta\phi, \; y' - x'\delta\phi, \; \underset{\text{unchanged}}{z'} |\alpha\rangle$$

— Switch to spherical: $\langle x', y', z'| \rightarrow \langle r, \theta, \phi|$

$$\langle r, \theta, \phi| \left[1 - i\left(\frac{\delta\phi}{\hbar}\right) L_z\right] |\alpha\rangle = \langle r, \theta, \phi - \delta\phi | \alpha\rangle$$

$$\simeq \langle r, \theta, \phi | \alpha\rangle - \delta\phi \frac{\partial}{\partial\phi} \langle r, \theta, \phi | \alpha\rangle$$

$$\Rightarrow \langle \bar{x}' | L_z | \alpha\rangle = -i\hbar \frac{\partial}{\partial\phi} \langle x' | \alpha\rangle$$

[L_z "=" $-i\hbar\, \partial/\partial\phi$]

"acting on" wavefunctions

– Similarly, $\delta\phi_x$ rotation about x-axis:

$$\langle x', y', z' | \left[1 - i\left(\frac{\delta\phi}{\hbar}\right)L_x\right] |\alpha\rangle = \langle x', y' + z'\delta\phi, z' - y'\delta\phi | \alpha\rangle;$$

express x', y', z' in terms of r, θ, ϕ (including derivatives) to give

$$\langle \bar{x}' | L_x |\alpha\rangle = -i\hbar\left(-\sin\phi\frac{\partial}{\partial\theta} - \cot\theta\cos\phi\frac{\partial}{\partial\phi}\right)\langle x'|\alpha\rangle$$

and $$\langle \bar{x}' | L_y |\alpha\rangle = -i\hbar\left(\cos\phi\,\partial/\partial\theta - \cot\theta\sin\phi\frac{\partial}{\partial\phi}\right)\langle \bar{x}'|\alpha\rangle$$

– As usual, raising/lowering operators: $L_\pm = L_x \pm iL_y$ so that

$$\langle \bar{x}' | L_\pm |\alpha\rangle = -i\hbar e^{\pm i\phi}\left(\pm i\frac{\partial}{\partial\theta} - \cot\theta\frac{\partial}{\partial\phi}\right)\langle \bar{x}'|\alpha\rangle$$

– Finally $|\bar{L}|^2 = L_z^2 + \frac{1}{2}(L_+L_- + L_-L_+)$:

$$\langle \bar{x}' | |\bar{L}|^2 |\alpha\rangle = -\hbar^2\left[\frac{1}{\sin^2\theta}\partial^2/\partial\phi^2 + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\,\partial/\partial\theta)\right]\langle \bar{x}'|\alpha\rangle$$

$|\bar{L}|^2$ ("upto" $-\hbar^2 r^2$) "=" angular part of $\bar{\nabla}'^2$

— Note: above only used $\bar{L}$ generates rotation [and not $\bar{L} = \bar{x} \times \bar{p}$ per say]

... can get $\bar{L}$, $|\bar{L}|^2$ action on wavefunction also from $\bar{L} = (\bar{x} \times \bar{p})$, with $\bar{p}$ "=" $-i\hbar\bar{\nabla}'$

— Actually, more "physically/elegantly", $|\bar{L}|^2$ action on wavefunction via "old" picture:

$$|\bar{L}|^2 = |\bar{x}|^2 |\bar{p}|^2 - (\bar{x} \cdot \bar{p})^2 + i\hbar\, \bar{x} \cdot \bar{p}$$

[using $\bar{L} = (\bar{x} \times \bar{p})$] ...

"=" $-\hbar^2 \bar{\nabla}'^2$

$$\langle \bar{x}' | |\bar{L}|^2 | \alpha \rangle = r^2 \langle \bar{x}' | |\bar{p}|^2 | \alpha \rangle + \hbar^2 \left(r^2 \frac{\partial^2}{\partial r^2} \langle x' | \alpha \rangle + 2r \frac{\partial}{\partial r} \langle x' | \alpha \rangle \right)$$

radial part of $\bar{\nabla}'^2$ (upto r^2)

$\Rightarrow \langle \bar{x}' | |\bar{L}|^2 | \alpha \rangle =$ angular part of $\bar{\nabla}'^2$, "upto" $-\hbar^2 r^2$

... as before

Similarly, new viewpoint on $\boxed{\text{spherical harmonics}}$: $Y_\ell^m(\theta,\phi)$

- "Old" way: Y_ℓ^m appear when solving wave equation (e.g. Schroedinger's) or Laplace's equation (e.g., electrostatic potential in charge free region), with (ℓ, m) as separation constants (no rotations/angular momentum connection per say)...

... whereas now see (angular) functions parametrized by (ℓ, m) as angular momentum eigenvalues must be present due to rotational invariance

$\Rightarrow$ "define" $Y_\ell^m(\theta,\phi)$ in terms of $|\ell, m\rangle$ (angular momentum eigenkets), "recovering" usual/known properties of Y_ℓ^m based on those of $|\ell, m\rangle$

— Also, rotation matrices, $\mathcal{D}^{(\ell)}_{m'm}(\alpha, \beta, \gamma)$ "related to" $Y_\ell^m(\theta, \phi)$ ...

Earlier exposure to $Y_\ell^m(\theta, \phi)$; e.g., solving Schroedinger's wave equation for potential which is spherically symmetric by $\boxed{\text{separation of variables}}$ in coordinates: energy eigenstates look like

$$\underbrace{\langle \bar{x}' |}_{r,\theta,\phi} \underbrace{n}_{\text{"radial/principal" quantum number}}, \ell, m\rangle = R_{n\ell}(r) \times \boxed{Y_\ell^m(\theta, \phi)}$$

(e.g. one electron atom)

$\boxed{\ell, m}$: separation constants ...

... but also angular momentum eigenvalues as per new viewpoint

... what's connection?

Rotational $\boxed{\text{invariance}}$: $H = V(r \text{ only}) + |\bar{p}|^2/(2m)$

$$\text{"="} \; V(r) - \frac{\hbar^2}{2m}\left(\text{radial part of } \bar{\nabla}'^2\right) \qquad -\hbar^2 \bar{\nabla}'^2$$

crucial

$$+ \left(\text{angular part of } \bar{\nabla}'^2\right)\left(\frac{-\hbar^2}{2m}\right) \Big\} \; |\bar{L}|^2/(2mr^2)$$

$$\Rightarrow [H, |\bar{L}|^2] = 0 = [H, L_z]$$

$\Rightarrow$ energy eigenstates are also eigenkets of $|\bar{L}|^2$, L_z (but not $L_{x,y}$)

& L_K's commute "like" J_K's

$\Rightarrow$ eigenvalues of $|\bar{L}|^2$, L_z are $(\ell+1)\ell\hbar^2$ & $m\hbar$ ($m = -\ell \ldots +\ell$) : ℓ, m "label" energy eigenstates ...

(ℓ not yet restricted to be integer)

$\Rightarrow$ angular dependence of energy eigenstates (for any spherically symmetric potential) characterized by l, m : define $Y_l^m(\theta, \phi)$ using angular momentum eigenkets (cf. originally from separating variables)

$$\underbrace{\langle \hat{n} |}_{\text{"direction" eigenbra}} l, m\rangle \equiv Y_l^m \underbrace{(\theta, \phi)}_{\text{polar, azimuthal angles of } \hat{n} \text{ (unit vector)}}$$

[$Y_l^m(\theta, \phi)$: amplitude for $|l, m\rangle$ "to be found" in $\hat{n}$]

$\boxed{\text{Check}}$ Properties of above "version" of $Y_l^m(\theta, \phi)$

(differential equations satisfied,

actual functional form)

"inherited" from $|\ell, m\rangle$ ...

same as before (separation of variables, not quite related to rotations/angular momentum), e.g.,

$\boxed{\text{action of } \bar{L}}$ on $\boxed{|\ell, m\rangle}$ → DE's for Y_ℓ^m:

$$\langle \hat{n} | L_z | \ell, m\rangle = m\hbar \langle \hat{n} | \ell, m\rangle$$

Use $\langle \bar{x}' | L_z | \alpha\rangle = -i\hbar \frac{\partial}{\partial\phi} \langle \bar{x}' | \alpha\rangle \left(\begin{array}{l} \bar{x}' \to \hat{n} \\ \alpha \to \ell, m \end{array} \right)$

(again, "based on" rotations) ⇒

$$-i\hbar \frac{\partial}{\partial\phi} \langle \hat{n} | \ell, m\rangle = m\hbar \langle \hat{n} | \ell, m\rangle$$

$$\partial/\partial\phi \; Y_\ell^m(\theta, \phi) = i m \, Y_\ell^m(\theta, \phi)$$

$$\Rightarrow Y_\ell^m(\theta, \phi) \propto e^{im\phi}$$

Similarly $|\bar{L}|^2 |\ell, m\rangle = \ell(\ell+1)\hbar^2 |\ell, m\rangle \Rightarrow$

$$\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}+(\ell+1)\ell\right]Y_\ell^m = 0$$

"using rotations"

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

$$= \int d\Omega_{\hat{n}} \langle \ell', m' | \hat{n}\rangle \langle \hat{n} | \ell, m\rangle$$

$$\Rightarrow \int_0^{2\pi} d\phi \int_{-1}^{+1} d(\cos\theta)\, Y_{\ell'}^{m'*}(\theta,\phi)\, Y_\ell^m(\theta,\phi) = \delta_{\ell'\ell}\delta_{m'm}$$

... same as known from separation of variables

What do $Y_\ell^m(\theta,\phi)$ look like (know already $e^{im\phi}$ part)?

Again, use "new" insight (from $|\ell, m\rangle$):

start with $Y_\ell^{\boxed{\ell\,(=m)}} = e^{i\ell\phi} f_\ell(\theta) = \langle \hat{n} | \ell, \ell\rangle$

$f_\ell(\theta) \hookrightarrow$ to be determined

Use $L_+ |\ell, \ell\rangle = 0$

and $\langle \bar{x}' | L_+ | \alpha \rangle = -i\hbar e^{+i\phi} \left(i \partial / \partial\theta - \cot\theta \frac{\partial}{\partial\phi} \right) \langle \bar{x}' | \alpha \rangle$

with $x' \to \hat{n}$
$\alpha \to l, m$

to get

1^{st} order DE vs. 2^{nd} above

$$-i\hbar e^{i\phi} \left[i \frac{\partial}{\partial\theta} - \cot\theta \frac{\partial}{\partial\phi} \right] \underbrace{\langle \hat{n} | l, l \rangle}_{Y_l^l(\theta,\phi) = e^{il\phi} f_l(\theta)} = 0$$

$\Rightarrow$

$$\frac{d f_l(\theta)}{d\theta} = (\cot\theta)\, l\, f_l(\theta)$$

$$\Rightarrow \frac{d f_l(\theta)}{f_l(\theta)} = \left(\frac{d(\sin\theta)}{\sin\theta} \right) l \; ; \; d(\ln f_l) = l\, d(\ln \sin\theta);$$

$$\ln f_l = (\ln \sin\theta + \text{constant}) \Rightarrow \boxed{f_l(\theta) \propto (\sin\theta)^l} \ldots$$

$$Y_l^l(\theta,\phi) = c_l\, e^{il\phi} (\sin\theta)^l, \text{ with}$$

c_l (normalization)

$$= \left[(-1)^l / (2^l\, l!) \right] \sqrt{\frac{(2l+1)(2l)!}{4\pi}}$$

How to get $Y_\ell^{m<\ell}(\theta,\phi)$?

$= \langle \hat{n} \,|\, \ell, m < \ell \rangle$..

use action of L_- on wavefunction

$$\langle \hat{n} \,|\, \ell, m-1 \rangle = \frac{\langle \hat{n} | L_- | \ell, m \rangle}{\sqrt{(\ell+m)(\ell-m+1)}\,\hbar}$$

$$= \frac{e^{-i\phi}\left(-\partial/\partial\theta + i\cot\theta\, \partial/\partial\phi\right)\langle \hat{n} \,|\, \ell, m \rangle}{\sqrt{(\ell+m)(\ell-m+1)}\,\hbar}$$

used repeatedly ... to give

$Y_\ell^{m=\ell-1\ldots 0}$ (fixed ℓ, $\ell > m \geq 0$)

$$= \frac{(-1)^\ell}{2^\ell \ell!}\sqrt{\frac{(2\ell+1)(\ell+m)!}{4\pi(\ell-m)!}}\; \boxed{e^{im\phi}}\; \frac{1}{\sin^m\theta} \times \frac{d^{(\ell-m)}}{d(\cos\theta)^{\ell-m}} (\sin\theta)^{2\ell}$$

with $Y_\ell^{-m} = (-1)^m \underbrace{\left[Y_\ell^m(\theta,\phi)\right]^*}_{e^{-im\phi} f_\ell(\theta)}$

- Note/recall: $f_\ell(\theta)$ is $(\sin\theta)^{|m|}\times$ polynomial in $\cos\theta$ of degree $(\ell-|m|)$: associated Legendre functions $\left[P_\ell^m(\cos\theta)\right]$

- For $\boxed{m=0}$, $Y_\ell^0(\theta,\phi)=\sqrt{\dfrac{2\ell+1}{4\pi}}\,P_\ell(\cos\theta)$

- Another way to get Legendre polynomials

- Remarkably simpler way to obtain $Y_\ell^m(\theta,\phi)$ using rotations/ket "language", cf. solving 2nd order PDE postulating series solution, requiring termination... in old approach (separation of variables)

- Can ℓ, m be half-integers (allowed so far)? No

- wavefunction $\propto Y_\ell^m(\theta,\phi)$
$\propto e^{im\phi}$

$\Rightarrow$ If m = half-integer, then 2π rotation ($\phi \to \phi + 2\pi$) flips sign of wavefunction... ... but that's same physical point! $\Rightarrow$ $\boxed{m \text{ (hence } \ell) \text{ is integer}}$

[More formally, L generates rotation of $|\bar{x}'\rangle$, with "2π-rotated" $|\bar{x}'\rangle = |\bar{x}'\rangle$ $\Rightarrow$

wavefunction of 2π rotated $\begin{pmatrix}\text{about} \\ z\text{-axis}\end{pmatrix}$ state =

$$\langle \bar{x}' | \exp\left(\frac{-iL_z 2\pi}{\hbar}\right) |\alpha\rangle$$

$\boxed{\mathcal{D}(\phi \text{ about } z\text{-axis}) = \exp\left(\frac{-iL_z\phi}{\hbar}\right)}$

rotated state

act on eigenbra

$= \langle (-2\pi)\text{-rotated } x' | \alpha \rangle$ $\quad (\langle \beta | X \leftrightarrow X^{+} | \beta \rangle)$

$= \langle x' | \alpha \rangle$, i.e., wavefunction is unchanged ...

more "mathematical" arguments in Sakurai]