Last Time

Thinking about $\hat{\Pi}$ in $D=3$. We saw that

$\hat{\Pi}|n\ell m\rangle = (-1)^\ell |n\ell m\rangle$

so $|n\ell m\rangle$ is an e-state of both $\hat{H}$ & $\hat{\Pi}$.

What is: $[\hat{\Pi},\hat{H}] = ?$

$[\hat{\Pi},\hat{H}] = \frac{1}{2m}[\hat{\Pi},\hat{\vec{p}}^2] + [\hat{\Pi},U]$

w/ $\bar{\hat{p}}^2 = (-\hat{\vec{p}})\cdot(-\hat{\vec{p}}) \overset{!}{=} \hat{\vec{p}}^2 = \hat{\Pi}^+\hat{\vec{p}}^2\hat{\Pi}$

so $[\hat{\Pi},\hat{\vec{p}}^2] = 0$

& sim.,

$\bar{U} = U(-r) = U(r)$

& $\bar{U} = U = \hat{\Pi}^+ U \hat{\Pi}$ gives

$[\hat{\Pi}, U] = 0$.

then: $[\hat{\Pi},\hat{H}] = 0$.

Laporte's Rule

Suppose we have a vector operator, w/ parity, so that:

$$\bar{\hat{\vec{V}}} = -\hat{\vec{V}} = \hat{\Pi}^+\hat{\vec{V}}\hat{\Pi}$$

Take 2 Hydrogen states: $|n\ell m\rangle$ & $|n'\ell'm'\rangle$, then the matrix elt. of $\hat{\vec{V}}$, $\langle n'\ell'm'|\hat{\vec{V}}|n\ell m\rangle$ has:

$$\langle n'\ell'm'|\hat{\vec{V}}|n\ell m\rangle = -\langle n'\ell'm'|\hat{\Pi}^+\hat{\vec{V}}\hat{\Pi}|n\ell m\rangle$$

& $\hat{\Pi}|n\ell m\rangle = (-1)^\ell |n\ell m\rangle$,

$(\hat{\Pi}|n'\ell'm'\rangle)^+ = \langle n'\ell'm'|\hat{\Pi}^+(-1)^{\ell'}$, so

$$\langle n'\ell'm'|\hat{\vec{V}}|n\ell m\rangle = -(-1)^\ell(-1)^{\ell'}\langle n'\ell'm'|\hat{\vec{V}}|n\ell m\rangle$$

which tells us that

$$\langle n'\ell'm'|\hat{\vec{V}}|n\ell m\rangle = 0 \text{ if } (\ell+\ell') \text{ is } \underline{\text{even}}.$$

a "selection rule" – good for computing!

example: the dipole operator: $\hat{\vec{p}}_e = q\hat{\vec{r}}$ ← vector has:

$$\langle 100|\hat{\vec{p}}_e|100\rangle = 0$$

(makes sense for the spherically symmetric ground state).

but we know more than this: $\langle n'\ell m'|\hat{\vec{p}}_e|n\ell m\rangle = 0$, for for any n', m', n & m, (w/ $\ell' = \ell$) – true for any vector operator.

If we run the same argument w/ a pseudovector: $\bar{\hat{\vec{W}}} = \hat{\vec{W}} = \hat{\Pi}^+\hat{\vec{W}}\hat{\Pi}$,

then

$$\langle n'\ell'm'|\hat{\vec{W}}|n\ell m\rangle = \langle n'\ell'm'|\hat{\Pi}^+\hat{\vec{W}}\hat{\Pi}|n\ell m\rangle$$
$$\overset{!}{=} \langle n'\ell'm'|(-1)^{\ell'}\hat{\vec{W}}(-1)^\ell|n\ell m\rangle$$
$$\overset{!}{=} (-1)^{\ell+\ell'}\langle n'\ell'm'|\hat{\vec{W}}|n\ell m\rangle$$

so $\langle n'\ell'm'|\hat{\vec{W}}|n\ell m\rangle = 0$ if $\ell+\ell'$ odd.

example of $\hat{\vec{W}}$?

Rotations

A rotation is defined by ($\hat{z}$-axis, e.g.)

$$\begin{pmatrix}\bar{x}\\ \bar{y}\\ \bar{z}\end{pmatrix} = \begin{pmatrix}\cos\Theta & -\sin\Theta & 0\\ \sin\Theta & \cos\Theta & 0\\ 0 & 0 & 1\end{pmatrix}\begin{pmatrix}x\\ y\\ z\end{pmatrix} \quad (*)$$

anything that responds to this transformation in the same way as the coordinates (meaning, as in (*)), is a "vector" under rotations.

example: $\vec{E}(\vec{r}) = \frac{q}{4\pi\epsilon_0 r^3}(x\hat{x} + y\hat{y} + z\hat{z})$

has

$$\bar{\vec{E}} = \frac{q}{4\pi\epsilon_0 \underbrace{\bar{r}^3}_{= r^3}}\left[(x\cos\theta - y\sin\theta)\hat{x} + (x\sin\theta + y\cos\theta)\hat{y} + z\hat{z}\right]$$

so

$$\begin{pmatrix}\bar{E}^x \\ \bar{E}^y \\ \bar{E}^z\end{pmatrix} = \begin{pmatrix}\cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1\end{pmatrix}\begin{pmatrix}E^x \\ E^y \\ E^z\end{pmatrix}$$

✓ $\vec{E}$ is a vector under rotations.

How about $\vec{B}(\vec{r})$?

$I \uparrow$ $\vec{B} = \frac{\mu_0 I}{2\pi s^2}(-y\hat{x} + x\hat{y})$ has

$B^x = \frac{\mu_0 I}{2\pi s^2}(-y)$, $B^y = \frac{\mu_0 I}{2\pi s^2}(x)$, $B^z = 0$

and

$$\bar{\vec{B}} = \frac{\mu_0 I}{2\pi \underbrace{\bar{s}^2}_{= s^2}}\left[-(x\sin\theta + y\cos\theta)\hat{x} + (x\cos\theta - y\sin\theta)\hat{y}\right]$$

so $\bar{\vec{B}} = (-B^y\sin\theta + B^x\cos\theta)\hat{x} + (B^y\cos\theta + B^x\sin\theta)\hat{y}$

or

$$\begin{pmatrix}\bar{B}^x \\ \bar{B}^y \\ \bar{B}^z\end{pmatrix} = \begin{pmatrix}\cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1\end{pmatrix}\begin{pmatrix}B^x \\ B^y \\ B^z\end{pmatrix}$$

✓ $\vec{B}$ is a vector under rotations.

Rotation Operator

We know the infinitesimal form of the rotation matrices:

$$\underbrace{\begin{pmatrix}\cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1\end{pmatrix}}_{O_z} \doteq \begin{pmatrix}1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1\end{pmatrix} + \theta\underbrace{\begin{pmatrix}0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0\end{pmatrix}}_{L_z}$$

and

$$O_z = e^{\theta L_z}$$

similarly for L_x, L_y, & we had the "classical" commutator:

$$[L_i, L_j] = \epsilon_{ijk} L_k$$

since $\hat{L}_i = \sum_{j,k=1}^{3} \epsilon_{ijk}\hat{r}_j\hat{p}_k$

w/ $[\hat{r}_j, \hat{p}_k] = i\hbar\delta_{jk}$, we expect

$[\hat{L}_i, \hat{L}_j] = i\hbar\epsilon_{ijk}\hat{L}_k$. (serves to define momentum operators)

∴ $\hat{R}_z(\theta) = e^{-i/\hbar\,\theta\hat{L}_z}$ (like $\hat{T}(a) = e^{-i/\hbar\,a\hat{p}}$)

How about the classical generator – does our CM → QM story hold up?

For $J(\vec{r}, \vec{p})$, we have

$\bar{x}^j = x^j + \epsilon\frac{\partial J}{\partial p_j}$ $\quad \bar{p}_j = p_j - \epsilon\frac{\partial J}{\partial x^j}$

An infinitesimal rotation about the z-axis has:

$$\bar{x} = x - \epsilon y \qquad \bar{y} = y + \epsilon x \qquad \bar{z} = z$$

$$\frac{\partial J}{\partial p_x} \qquad \frac{\partial J}{\partial p_y}$$

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

& sim. for $L_x = y p_z - z p_y$ & $L_y = z p_x - x p_z$.

We can compute Poisson Brackets:

$$\{L_x, L_z\}_{P.B.} = \frac{\partial L_x}{\partial x}\frac{\partial L_z}{\partial p_x} + \frac{\partial L_x}{\partial y}\frac{\partial L_z}{\partial p_y} + \cancel{\frac{\partial L_x}{\partial z}\frac{\partial L_z}{\partial p_z}}$$

$$- \cancel{\frac{\partial L_x}{\partial p_x}\frac{\partial L_z}{\partial x}} - \frac{\partial L_x}{\partial p_y}\frac{\partial L_z}{\partial y} - \cancel{\frac{\partial L_x}{\partial p_z}\frac{\partial L_z}{\partial z}}$$

$$= x p_z - z p_x = -L_y$$

& we have $\{L_i, L_j\}_{P.B.} = \epsilon_{ijk} L_k$

This becomes the QM

$$[\hat{L}_i, \hat{L}_j] = i\hbar \epsilon_{ijk} \hat{L}_k$$

Since any vector responds in the same way to rotations, we know that

$$[\hat{L}_i, \hat{V}_j] = i\hbar \epsilon_{ijk} \hat{V}_k$$

for all vector operators $\hat{\vec{V}}$.

Spherically Symmetric Hamiltonians

For $\hat{H} = \hat{p}^2/2m + U(r)$
a function only of radial coord. r.

we have: $\hat{p}^2 = \hat{\vec{p}} \cdot \hat{\vec{p}}$

&

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

$$[\hat{L}_z, \hat{p}_x] = +i\hbar \hat{p}_y \quad [\hat{L}_z, \hat{p}_y] = -i\hbar \hat{p}_x \quad [\hat{L}_z, \hat{p}_z] = 0$$

& for $[A, B] = C$, $[A^2, B] = AC + CA$, so

$$[\hat{L}_z, \hat{p}_x^2] = -i\hbar(\hat{p}_x \hat{p}_y + \hat{p}_y \hat{p}_x)$$

$$[\hat{L}_z, \hat{p}_y^2] = +i\hbar(\hat{p}_y \hat{p}_x + \hat{p}_x \hat{p}_y)$$

& $[\hat{L}_z, \hat{p}^2] = 0$ & sim. for $\hat{L}_x$ & $\hat{L}_y$, so

$$[\hat{L}_i, \hat{p}^2] = 0$$

rot. about $\hat{z}$ axis

We also have: $\bar{U} = \underbrace{\hat{R}_z^\dagger U(r) \hat{R}_z = U(r)}$

& $\hat{R}^{-1} = \hat{R}^\dagger$, so

$$[\hat{R}_z, U] = 0$$

& since $\hat{R}_z(\epsilon) = e^{-i/\hbar \, \epsilon \hat{L}_z} \approx (1 - i/\hbar \, \epsilon \hat{L}_z)$

$$[1 - i/\hbar \, \epsilon \hat{L}_z, U] = 0 \Rightarrow [\hat{L}_z, U] = 0$$

& similarly for $\hat{R}_x(\phi)$, $\hat{R}_y(\phi)$

so $[\hat{H}, \hat{L}_i] = 0$ & then $[\hat{H}, \hat{L}^2] = 0$.