Homework 2

Problem 6.11:

$$\langle n'l'm'|\hat{\vec{L}}|nlm\rangle$$

- $\hat{\vec{L}}$ is a pseudovector: $\hat{\vec{L}}' = \hat{\pi}^{\dagger}\hat{\vec{L}}\hat{\pi} = \hat{\vec{L}}$

$$\rightarrow \langle n'l'm'|\hat{\vec{L}}|nlm\rangle = \langle n'l'm'|\hat{\pi}^{\dagger}\hat{\vec{L}}\hat{\pi}|nlm\rangle$$

$$= (-1)^{l'+l}\langle n'l'm'|\hat{\vec{L}}|nlm\rangle$$

- if $l'+l$ is even, then this tells us nothing, but if it's odd, it's saying the matrix element is equal to its negative self, which is only possible when it's zero

$$\Rightarrow \quad \underline{\langle n'l'm'|\hat{\vec{L}}|nlm\rangle = 0 \text{ if } l'+l \text{ is odd}}$$

Problem 6.13

a) $\langle 100|\hat{P}_e|100\rangle$

- we know via the selection rules that

$$\langle n'l'm'|\hat{P}_e|nlm\rangle = 0$$

if $l'+l$ is even

- in this case, $l'+l=0$ which is even, so

$$\langle \hat{P}_e \rangle = 0$$

b) for $n=2$, l can take values $0, 1$, so it's possible to have something like

$$\langle 210|\hat{P}_e|200\rangle$$

where $l'+l=1$ is odd, so it's non-zero

- to construct a single wavefunction, we use a linear combination of two states:

$$|\psi\rangle = \alpha|210\rangle + \beta|200\rangle$$

$$\Rightarrow \langle \vec{r}|200\rangle = R_{20}(r) = \frac{1}{\sqrt{2}} a^{-3/2}\left(1-\frac{1}{2}\frac{r}{a}\right)e^{-r/2a}$$

$$\langle \vec{r}|210\rangle = R_{21}(r) = \frac{1}{2\sqrt{6}} a^{-3/2}\left(\frac{r}{a}\right)e^{-r/2a}$$

- only $l' \neq l$ states survive, so

$$\langle \hat{P}_e\rangle = (\alpha^*\langle 210| + \beta^*\langle 200|)\,\hat{P}_e\,(\alpha|210\rangle + \beta|200\rangle)$$

$$= \alpha^*\beta\langle 210|\hat{P}_e|200\rangle + \beta^*\alpha\langle 200|\hat{P}_e|210\rangle$$

- since $\hat{P}_e = q\hat{\vec{r}}$ and $\hat{\vec{r}}$ is a vector, there are 3 components:

$$\hat{\vec{r}} = (\hat{r}_x, \hat{r}_y, \hat{r}_z)$$

where
$$\hat{r}_x|\psi(r)\rangle = r\sin\theta\cos\phi\,|\psi(r)\rangle$$
$$\hat{r}_y|\psi(r)\rangle = r\sin\theta\sin\phi\,|\psi(r)\rangle$$
$$\hat{r}_z|\psi(r)\rangle = r\cos\theta\,|\psi(r)\rangle$$

- further, $R_{20}(r)$ and $R_{21}(r)$ are entirely real, so

$$\langle \hat{P}_e\rangle = 2(\alpha^*\beta - \beta^*\alpha)\ldots$$
$$= 2q\,\mathrm{Re}\left[\alpha\beta\langle 210|\hat{\vec{r}}|200\rangle\right]$$

$$x \to \hat{i}\left\{q\int d^3r\, R_{21}(r)R_{20}(r)\, r\sin\theta\cos\phi\right\}$$

$=0$ from sole ϕ dependence

$$y \to \hat{j}\left\{q\int d^3r\, R_{21}(r)R_{20}(r)\, r\sin\theta\sin\phi\right\}$$

$=0$ similarly

$$z \to \hat{k}\left\{q\int d^3r \cdot \frac{a^{-3}}{2\sqrt{12}}\left(\frac{r}{a}\right)\left(1-\frac{1}{2}\frac{r}{a}\right)e^{-r/a}\, r\cos\theta\right\}$$

- Just plugged into Mathematica... and let

$$\alpha = \beta = \frac{1}{\sqrt{2}}$$

$$\Rightarrow \boxed{\langle \hat{P}_e\rangle_\psi = -3qa\,\hat{k} \quad \text{for } |\psi\rangle = \frac{|210\rangle + |200\rangle}{\sqrt{2}}}$$

Problem 6.15

$$\text{Eq. (6.34)} \rightarrow [\hat{L}_i, \hat{f}] = 0$$

for some scalar operator $\hat{f}$.

→ Since $\hat{\vec{L}}$ is the generator of rotations, simply by representing (chooring $\hat{n} = \hat{k}$, i.e. z-axis rotation)

$$\hat{R}_z(\phi) = \exp\left[\frac{-i\phi}{\hbar}\hat{L}_z\right]$$

as a power series, then if $\hat{f}$ commutes w/ $\hat{L}_i$, it must commute with $\hat{R}_z(\phi)$. Thus,

$$\hat{f}' = R_z^\dagger(\phi)\,\hat{f}\,R_z(\phi) = R_z^\dagger(\phi)\,R_z(\phi)\,\hat{f} = \hat{f}$$

since $\hat{R}_z(\phi)$ is unitary.

Hence, the above commutation relation implies $\hat{f}$ is unchanged by a rotation.

Problem 6.16

Eq. (6.38) $\rightarrow$ $[\hat{L}_i, \hat{V}_j] = i\hbar \varepsilon_{ijk} \hat{V}_k$

$$\rightarrow \hat{\vec{V}}' = \hat{R}_y^T(\delta)\, \hat{\vec{V}}\, \hat{R}_y(\delta)$$

$$= \left(1 + \frac{i\delta}{\hbar}\hat{L}_y\right)\begin{pmatrix}\hat{V}_x \\ \hat{V}_y \\ \hat{V}_z\end{pmatrix}\left(1 - \frac{i\delta}{\hbar}\hat{L}_y\right)$$

$$= \begin{pmatrix}\hat{V}_x \\ \hat{V}_y \\ \hat{V}_z\end{pmatrix} + \frac{i\delta}{\hbar}\begin{pmatrix}[\hat{L}_y, \hat{V}_x] \\ [\hat{L}_y, \hat{V}_y] \\ [\hat{L}_y, \hat{V}_z]\end{pmatrix} + \mathcal{O}(\delta^2)$$

$$= \begin{pmatrix}\hat{V}_x \\ \hat{V}_y \\ \hat{V}_z\end{pmatrix} + \frac{i\delta}{\hbar}\begin{pmatrix}-i\hbar \hat{V}_z \\ 0 \\ i\hbar \hat{V}_x\end{pmatrix}$$

$$\begin{pmatrix}\hat{V}_x' \\ \hat{V}_y' \\ \hat{V}_z'\end{pmatrix} = \begin{pmatrix}\hat{V}_x + \delta\hat{V}_z \\ \hat{V}_y \\ \hat{V}_z - \delta\hat{V}_x\end{pmatrix}$$

- by inspection,

$$\begin{pmatrix}\hat{V}_x' \\ \hat{V}_y \\ \hat{V}_z\end{pmatrix} = \underbrace{\begin{pmatrix}1 & 0 & \delta \\ 0 & 1 & 0 \\ -\delta & 0 & 1\end{pmatrix}}\begin{pmatrix}\hat{V}_x \\ \hat{V}_y \\ \hat{V}_z\end{pmatrix}$$

Problem 6.17

$$\langle \vec{r} | \hat{R}_{\hat{n}} | nlm \rangle = \sum_{m'} D_{m'm} \psi_{nlm}$$

$$\hat{R}_{\hat{n}}(\delta)\psi_{nlm} = \sum_{m'} D_{m'm} \psi_{nlm}$$

- infinitesimal form:

$$\left(1 - \frac{i\delta}{\hbar}\hat{n}\cdot\hat{\vec{L}}\right)\psi_{nlm} = \sim$$

$$\rightarrow \hat{n}\cdot\hat{\vec{L}} = n_x\hat{L}_x + n_y\hat{L}_y + n_z\hat{L}_z$$

- cannot know these simultaneously, but we know: $\hat{L}_\pm = \hat{L}_x \pm i\hat{L}_y$

$$\rightarrow \hat{L}_+ = \hat{L}_x + i\hat{L}_y$$
$$\hat{L}_- = \hat{L}_x - i\hat{L}_y$$

$$\Rightarrow A\hat{L}_+ + B\hat{L}_- = n_x\hat{L}_x + n_y\hat{L}_y$$

$$A(\hat{L}_x + i\hat{L}_y) + B(\hat{L}_x - i\hat{L}_y) = \sim$$

$$(A+B)\hat{L}_x + i(A-B)\hat{L}_y = n_x\hat{L}_x + n_y\hat{L}_y$$

$$\rightarrow \begin{cases} A+B = n_x \\ i(A-B) = n_y \end{cases} \rightarrow \begin{matrix} A+B = n_x \\ A-B = -in_y \end{matrix}$$

$$\rightarrow A = \frac{n_x - in_y}{2}$$

$$\frac{n_x - in_y}{2} + B = n_x \rightarrow B = \frac{n_x + in_y}{2}$$

- Back to original eq:

$$\psi_{nlm} - \frac{i\delta}{\hbar}\left(\frac{n_x - in_y}{2}\hat{L}_+ + \frac{n_y + in_y}{2}\hat{L}_- + n_z\hat{L}_z\right)\psi_{nlm}$$

- we know

$$\hat{L}_+\psi_{nlm} = \hbar\sqrt{l(l+1) - m(m+1)}\,\psi_{nlm+1}$$
$$\hat{L}_-\psi_{nlm} = \hbar\sqrt{l(l+1) - m(m-1)}\,\psi_{nlm-1}$$

$$\rightarrow \psi_{nlm} - \frac{i\delta}{\hbar}\Big[\left(\frac{n_x - in_y}{2}\right)\hbar\sqrt{l(l+1) - m(m+1)}\,\psi_{nlm+1}$$
$$+ \left(\frac{n_x + in_y}{2}\right)\hbar\sqrt{l(l+1) - m(m-1)}\,\psi_{nlm-1}$$
$$+ n_z\hbar m\,\psi_{nlm}\Big]$$

(grouping like eigenfuncs)

$$= (1 - in_z\delta m)\psi_{nlm}$$
$$- \frac{i\delta}{2}(n_x + in_y)\sqrt{l(l+1) - m(m-1)}\,\psi_{nlm-1}$$
$$- \frac{i\delta}{2}(n_x - in_y)\sqrt{l(l+1) - m(m+1)}\,\psi_{nlm+1} = \sum_{m'} D_{m'm}\psi_{nlm'}$$

- we can define the coefficient/function D to be:

$$D_{m'm} = \begin{cases} 1 - in_z\delta m & \text{if } m' = m \\ -\frac{i\delta}{2}(n_x + in_y)\sqrt{l(l+1) - m(m-1)} & \text{if } m' = m-1 \\ -\frac{i\delta}{2}(n_x - in_y)\sqrt{l(l+1) - m(m+1)} & \text{if } m' = m+1 \\ 0 & \text{otherwise} \end{cases}$$