Homework III

Problem 1

2p states

$$V = \lambda (x^2 - y^2)$$

2s and 2p are degenerate but $\underset{+\ \ +\ \ -}{\langle 2s | V | 2p\, l_z \rangle} = 0$ by parity

We can ignore the 2s states.

$$\langle 2p\, l_z' | V | 2p\, l_z \rangle$$

$$x^2 - y^2 \Rightarrow \begin{cases} 1 \otimes 1 = 0 \oplus 1 \oplus 2 \\ l_z = \pm 1 \pm 1 = -2, 0, 2 \\ \pi = + \end{cases} \rightarrow \underbrace{l_z' = l_z}_{\text{diagonal}} \text{ or } \underbrace{l_z' = l_z \pm 2}_{\substack{-1 \to 1 \\ 1 \to -1}}$$

We can compute the diagonal $l_z' = l_z$ case or be more precise and look at

$$x^2 - y^2 = r^2 s^2\theta (c^2\varphi - s^2\varphi) = r^2 s^2\theta\, c\, 2\varphi = \frac{r^2 s^2\theta}{2} (e^{2i\varphi} + e^{-2i\varphi})$$

$e^{2i\varphi} \rightarrow q = +2 \qquad e^{-2i\varphi} \rightarrow q = -2$ so, actually, there is no $q = 0$

$\Rightarrow$ diagonal $= 0$

Either by direct computation or by previous argument $\langle l_z | V | l_z \rangle = 0$

We still need

$$\langle 2p\, l_z = -1 | V | 2p\, l_z = +1 \rangle$$

$$\langle \vec{x} \,|\, 2p\; l_z=+1\rangle = R_{21}(r)\, Y_{11}(\theta,\varphi)$$

$$R_{21}(r) = \frac{1}{(2a_0)^{3/2}}\,\frac{1}{\sqrt{3}}\,\frac{r}{a_0}\; e^{-r/2a_0}$$

$$Y_{11}(\theta,\varphi) = -\sqrt{\frac{3}{8\pi}}\, s\theta\; e^{i\varphi} \qquad Y_{1-1} = \sqrt{\frac{3}{8\pi}}\; s\theta\, e^{-i\varphi}$$

$$\langle 2p\; l_z=-1 \,|\, x^2-y^2 \,|\, 2p\; l_z=+1\rangle = \int r^2 dr\, s\theta\, d\theta\, d\varphi\; \underbrace{\sqrt{\frac{3}{8\pi}}\, s\theta\, e^{i\varphi}\, R_{21}}_{\psi^*_{21-1}}\; \underbrace{\frac{r^2 s^2\theta}{2}\,(e^{2i\varphi}+e^{-2i\varphi})}_{x^2-y^2}\,\cdot$$

$$R_{21}\,(-)\sqrt{\frac{3}{8\pi}}\; s\theta\, e^{i\varphi}$$

$$= -\frac{\cancel{8}}{2\times 8\pi}\,\frac{1}{(2a_0)^3}\,\frac{1}{\cancel{3}}\,\frac{\cancel{3}}{a_0^2}\int r^2 dr\, s\theta\, d\theta\, d\varphi\;\; s^4\theta\;\; \underset{R_{21}^2}{r^2}\,\underset{x^2-y^2}{r^2}\,(e^{4i\varphi}+1)\; e^{-r/a_0}$$

$$= -\frac{1}{128\pi a_0^5}\int_0^\infty r^6 e^{-r/a_0}\,dr \int_{-1}^{1} d\mu\,(1-\mu^2)^2 \int_0^{2\pi} d\varphi\,(\underset{2\pi}{1}+\underset{0}{e^{4i\varphi}})$$

$$\mu=\cos\theta \qquad (1-2\mu^2+\mu^4)$$

$$1\cdot\cancel{2}\cdot 3\cdot\cancel{4}\cdot 5\cdot\cancel{6}$$

$$= -\frac{a_0^7}{\underset{\cancel{16}\;\cancel{8}\;4}{128\cancel{\pi}\, a_0^5}}\; 6!\times 2\cancel{\pi}\times\left(\mu - 2\frac{\mu^3}{3}+\frac{\mu^5}{5}\right)\Big|_{-1}^{1} = -a_0^2\,\frac{\overset{3}{\cancel{45}}}{\underset{2}{\cancel{4}}}\times 2\left(1-\frac{2}{3}+\frac{1}{5}\right)$$

$$\frac{15-10+3}{\cancel{18}}$$

$$= \frac{3}{\cancel{2}}\,a_0^2\times\overset{4}{\cancel{8}} = 12 a_0^2$$

$$\langle 2p\; l_z=-1 \,|V|\, 2p\; l_z=+1\rangle = -12\lambda a_0^2$$

$$\langle V\rangle = \begin{array}{c|ccc} & -1 & 0 & 1 \\ \hline -1 & 0 & 0 & -12\lambda a_0^2 \\ 0 & 0 & 0 & 0 \\ 1 & -12\lambda a_0^2 & 0 & 0 \end{array}$$

$$\det\begin{pmatrix} -\varepsilon^{(1)} & 0 & -12\lambda a_0^2 \\ 0 & 0 & 0 \\ -12\lambda a_0^2 & 0 & -\varepsilon^{(1)} \end{pmatrix} = 0 \qquad \varepsilon^{(1)} = -12\lambda a_0^2\ ,\ 0,\ 12\lambda a_0^2$$

$$\varepsilon^{(1)} = -12\lambda a_0^2 \rightarrow \frac{1}{\sqrt{2}}\Big(|\,l_z = 1\rangle - |\,l_z = -1\rangle\Big)$$

$$\varepsilon^{(1)} = 0 \longrightarrow |\,l_z = 0\rangle$$

$$\varepsilon^{(1)} = 12\lambda a_0^2 \rightarrow \frac{1}{\sqrt{2}}\Big(|\,l_z = 1\rangle + |\,l_z = -1\rangle\Big)$$

$\uparrow$ first order correction to the energy

$\uparrow$ 0^{th} order eigenstates

Time-reversal:

$$\Theta\,|\,l_z\rangle = (-)^{l_z}\,|-l_z\rangle$$

$[\Theta, H_0 + V] = 0 \Rightarrow \Theta\,|E\rangle$ is a state with the same energy.

$$\Theta\,|\,\varepsilon^{(1)} = -12\lambda a_0^2\rangle = \frac{1}{\sqrt{2}}\Big(-|\,l_z = 1\rangle + |\,l_z = -1\rangle\Big) = -\,|\,\varepsilon^{(1)} = -12\lambda a_0^2\rangle$$

$$\Theta\,|\,\varepsilon^{(1)} = 12\lambda a_0^2\rangle = -\,|\,\varepsilon^{(1)} = 12\lambda a_0^2\rangle$$

$$\Theta\,|\,\varepsilon^{(1)} = 0\rangle = |\,\varepsilon^{(1)} = 0\rangle$$

They are all time-reversal eigenstates as they should.

Also eigenstates of Π but not l_z.

Problem 2

$$H = AL^2 + BL_z + CL_y$$

a) $B \gg C$

$$H_0 = AL^2 + BL_z$$

we use $|l\, l_z\rangle$ basis.

$$\mathcal{E} = A\hbar^2\, l(l+1) + B\hbar\, l_z$$

non-degenerate eigenstates.

$\langle l l_z | L_y | l l_z \rangle = 0$ by l_z selection rule.

$l_z = \pm 1$ $\quad L_\pm = L_x \pm i L_y \quad L_+ - L_- = 2i L_y$

$L_y = \frac{1}{2i}(L_+ - L_-)$

$\Rightarrow$ second order.

$$\mathcal{E}^{(2)} = -\sum_{l_z' \neq l_z} \frac{|\langle l_z' | C L_y | l_z \rangle|^2}{\mathcal{E}_{l_z'} - \mathcal{E}_{l_z}}$$

$$= -\frac{1}{4}|C|^2 \sum_{l_z' \neq l_z} \frac{|\langle l_z' | L_+ - L_- | l_z \rangle|^2}{\hbar B\,(l_z' - l_z)}$$

only $l_z' = l_z \pm 1$ contribute.

$$\mathcal{E}^{(2)} = -\frac{|C|^2}{4}\frac{1}{\hbar B}\left(|\langle l_z+1|L_+|l_z\rangle|^2 - |\langle l_z-1|L_-|l_z\rangle|^2\right)$$

$$\left(\sqrt{l(l+1)-l_z(l_z+1)}\right)^2 - \left(\sqrt{l(l+1)-l_z(l_z-1)}\right)^2$$

$$\cancel{l(l+1)}\cancel{-l_z^2}-l_z - \cancel{l(l+1)}\cancel{+l_z^2}-l_z$$

$$-2l_z\hbar^2$$

$$\mathcal{E}^{(2)} = \frac{|C|^2}{4\cancel{\hbar}B}2l_z\hbar^{\cancel{2}}$$

$$E \simeq A\hbar^2 l(l+1) + B\hbar l_z + \frac{1}{2}\frac{C^2}{B}\hbar l_z.$$

$$\boxed{E \simeq A\hbar^2 l(l+1) + \left(B+\frac{1}{2}\frac{C^2}{B}\right)\hbar l_z} \quad (1)$$

2nd order pert. theory in C.

where $l_z : -l \ldots l$

c) Exact solution: ~~the ex~~ Define vector $\hat{n} = \frac{1}{\sqrt{B^2+C^2}}(0, C, B)$

then

$$H = AL^2 + \sqrt{B^2+C^2}\,(\vec{L}\cdot\hat{n})$$

the eigenvalues of $(\vec{L}\cdot\hat{n})$ are $-\hbar l \ldots \hbar l$ for any unit vector $\hat{n}$ (since all directions are equivalent).

$$\mathcal{E}^{(exact)} = A\hbar^2 l(l+1) + \sqrt{B^2+C^2}\,\hbar\tilde{l}_z \quad ; \tilde{l}_z = -l \ldots l.$$

$$\simeq A\hbar^2 l(l+1) + \left(B+\frac{1}{2}\frac{C^2}{B}\right)\hbar\tilde{l}_z$$ agrees w/ (1) ✓