AY 2023/2024 final

Q1) (a) (i) If two e^- are in the triplet state, the two e^- can take the following spin states:

$$|\uparrow\uparrow\rangle$$
$$|\downarrow\downarrow\rangle$$
$$\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$$

this state is missing in the description in the question.

(ii) If one e^- is in the spin up state and the other is in the spin down state, $m_s = 0$, but the state can be a superposition of $|s=1, m_s=0\rangle$ and $|s=0, m_s=0\rangle$.

(singlet state: $|s=0, m_s=0\rangle$)

(b) $H = D\left(S_z^2 - \frac{1}{3}S^2\right) + E\left(S_x^2 - S_y^2\right)$

Take $E = 0$, $\hbar = 1$

Basis $\{|s=1, m_s=1\rangle, |s=1, m_s=0\rangle, |s=1, m_s=-1\rangle\}$

In this basis,

$$S_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \qquad (S_z|s,m_s\rangle = \hbar m_s|s,m_s\rangle)$$

$$S_z = \begin{pmatrix} \cdot & \cdot & \cdot \\ 0 & 0 & \cdot \\ 0 & 0 & -1 \end{pmatrix}$$

$$S_z^2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

$$= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$S^2 |s, m_s\rangle = \hbar^2 s(s+1) |s, m_s\rangle$$

Here $s = 1$ $\quad (\hbar = 1)$

So $S^2 |s, m_s\rangle = 2 |s, m_s\rangle$

$$S_z^2 - \frac{1}{3} S^2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} - \frac{2}{3}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$= \begin{pmatrix} \frac{1}{3} & 0 & 0 \\ 0 & -\frac{2}{3} & 0 \\ 0 & 0 & \frac{1}{3} \end{pmatrix}$$

$$\text{So } H = \begin{pmatrix} \frac{D}{3} & 0 & 0 \\ 0 & -\frac{2}{3}D & 0 \\ 0 & 0 & \frac{D}{3} \end{pmatrix}$$

c) $D > 0$, $E = 0$

$|s=1, m_s=1\rangle, \underline{|s=1, m_s=-1\rangle}$ $\quad \frac{D}{3}$

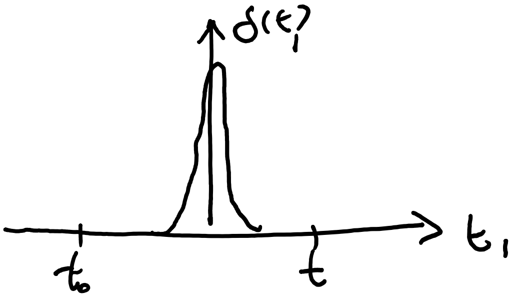
$|s=1, m_s=1\rangle, |s=1, m_s=-1\rangle$ ——— $\frac{D}{3}$

$|s=1, m_s=0\rangle$ ——— $-\frac{2}{3}D$

$\Big\}\ D$

2 a)

$$V(t) = -qE_0 x\,\delta(t)$$



$$P^{(t)}_{e\leftarrow g} = \frac{1}{\hbar^2}\left|\int_{t_0}^{t} \langle e|V(t_1)|g\rangle e^{\frac{i(E_e-E_g)}{\hbar}(t_1-t_0)}\,dt_1\right|^2$$

$$= \frac{E_0^2}{\hbar^2}\left|\int_{t_0}^{t} \underbrace{q\langle e|x|g\rangle}_{d_{eg}}\delta(t_1)\, e^{\frac{i(E_e-E_g)}{\hbar}(t_1-t_0)}\,dt_1\right|^2$$

$$= \frac{E_0^2}{\hbar^2}|d_{eg}|^2\ \underbrace{\left|e^{\frac{-i(E_e-E_g)t_0}{\hbar}}\right|^2}_{1}\ \underbrace{\left|\int_{t_0}^{t}\delta(t_1)\, e^{\frac{i(E_e-E_g)}{\hbar}t_1}\,dt_1\right|^2}_{e^{\frac{i(E_e-E_g)}{\hbar}0}=1}$$

$$= \frac{|d_{eg}|^2}{\hbar^2}E_0^2 \qquad \left(\int \delta(t_1) f(t_1)\,dt_1 = f(0)\right)$$

b) $|g\rangle = |1\ 0\ 0\rangle$

$n_g = 1, \quad l_g = 0, \quad m_g = 0$

The selection rules for $\langle e|x|g\rangle$ are that $\langle e|x|g\rangle$ is non-zero only if $\Delta l = \pm 1$ and $\Delta m = 0, \pm 1$

$l_g = 0, \quad \Delta l = \pm 1 \Rightarrow l_e = 1$
(since $l \geq 0$)

$m_g = 0, \quad \Delta m = 0, \pm 1 \Rightarrow m_e = 0, \pm 1$

since $l \leq (n-1)$,
$n_e \geq l_e + 1 = 2$

So if $|e\rangle \equiv |n\,l\,m\rangle$, for $P_{e \leftarrow g} \neq 0$,

we need $l = 1, \quad m = 0, \pm 1,$

n is an integer ≥ 2.

3) $$H_0 = \frac{p_x^2 + p_y^2}{2m} + \frac{m\omega^2}{2}(x^2 + y^2)$$

Eigenstates $|n_x, n_y\rangle$

$$E_{n_x, n_y} = \hbar\omega\left(n_x + \frac{1}{2}\right) + \hbar\omega\left(n_y + \frac{1}{2}\right).$$

Refer to W10L1 Eg. on 2D harmonic oscillator,

$$\varphi_{n_x, n_y}(x, y) = \varphi_{n_x}(x)\, \varphi_{n_y}(y)$$

(a) $\qquad \vec{B} = B\vec{e}_z$

$$U = -\vec{\mu}_L \cdot \vec{B} \quad , \quad \vec{\mu}_L = -\frac{\mu_B}{\hbar}\vec{L}$$

$$U = -\vec{\mu}_L \cdot \vec{B}$$

$$= \frac{\mu_B}{\hbar} B\, \vec{L} \cdot \vec{e}_z$$

$$= \frac{\mu_B B}{\hbar} (\vec{r} \times \vec{p})_z \qquad \vec{r} = \begin{pmatrix} x \\ y \\ z \end{pmatrix} \quad \vec{p} = \begin{pmatrix} p_x \\ p_y \\ p_z \end{pmatrix}$$

$$= \frac{\mu_B B}{\hbar} (x p_y - y p_x)$$

(b) Ground state: $n_x = 0, n_y = 0$

$$\varphi_{00}(x, y) = \varphi_0(x)\, \varphi_0(y)$$

Not degenerate.

So $E_0^{(1)} = \langle \underset{\substack{\uparrow \\ n_x}}{0}, \underset{\substack{\uparrow \\ n_y}}{0} | \hat{U} | \underset{\substack{\uparrow \\ n_x}}{0}, \underset{\substack{\uparrow \\ n_y}}{0} \rangle$

$$= \frac{\mu_B B}{\hbar} \left(\langle 0, 0 | x p_y - y p_x | 0, 0 \rangle \right)$$

$$= \frac{\mu_B B}{\hbar} \left(\langle \underset{\underset{n_x}{\uparrow}}{0}, \underset{\underset{n_y}{\uparrow}}{0} | x p_y - y p_x | \underset{\underset{n_x}{\uparrow}}{0}, \underset{\underset{n_y}{\uparrow}}{0} \rangle \right)$$

$$= \frac{\mu_B B}{\hbar} \left(\langle \underset{\underset{n_x}{\uparrow}}{0}, \underset{\underset{n_y}{\uparrow}}{0} | x \otimes p_y - p_x \otimes y | \underset{\underset{n_x}{\uparrow}}{0}, \underset{\underset{n_y}{\uparrow}}{0} \rangle \right)$$

$$\Big(\text{c.f. } \langle \underset{\underset{n_x}{\uparrow}}{0} | x | \underset{\underset{n_x}{\uparrow}}{0} \rangle = \int dx \, \varphi^*_{n_x=0}(x) \, x \, \varphi_{n_x=0}(x)$$

$$\langle \underset{\underset{n_x}{\uparrow}}{0} | p_x | \underset{\underset{n_x}{\uparrow}}{0} \rangle = \int dx \, \varphi^*_{n_x=0}(x) \, p_x \, \varphi_{n_x=0}(x)$$

$$\langle \underset{\underset{n_y}{\uparrow}}{0} | y | \underset{\underset{n_y}{\uparrow}}{0} \rangle = \int dy \, \varphi^*_{n_y=0}(y) \, y \, \varphi_{n_y=0}(y)$$

$$\langle \underset{\underset{n_y}{\uparrow}}{0} | p_y | \underset{\underset{n_y}{\uparrow}}{0} \rangle = \int dy \, \varphi^*_{n_y=0}(y) \, p_y \, \varphi_{n_y=0}(y) \Big)$$

$$E_0^{(1)} = \frac{\mu_B B}{\hbar} \left(\langle 0|x|0\rangle \langle 0|p_y|0\rangle - \langle 0|p_x|0\rangle \langle 0|y|0\rangle \right)$$

Because $\hat{x}$, $\hat{y}$, $\hat{p}_x$, $\hat{p}_y$ are all odd operators and $|0\rangle$ has definite parity, the expectation values of these operators in state $|0\rangle$ are zero.

So $E_0^{(1)} = 0$

(c) $E_{n_x, n_y} = \hbar\omega(n_x + \frac{1}{2}) + \hbar\omega(n_y + \frac{1}{2})$

$n_x = 0, 1, 2, \ldots$

$n_y = 0, 1, 2, \ldots$

So the 1st excited state has:

$n_x = 0$ ~~and~~ $n_y = 1$;

$n_x = 1$ and $n_y = 0$

$E_{n_x, n_y} = \hbar\omega\left(1 + \frac{1}{2} + \frac{1}{2}\right) = 2\hbar\omega$

(d) First excited state is degenerate.

So we need to find the matrix for U in the degenerate subspace $\{|n_x = 1, n_y = 0\rangle, |n_x = 0, n_y = 1\rangle\}$.

These states have definite parity so the diagonal elements are zero (similar to (b)).

$$U = \frac{\mu_B B}{\hbar}\left(x \otimes p_y - p_x \otimes y\right)$$

$$\langle n_x = 1, n_y = 0 \,|\, x \otimes p_y \,|\, n_x = 0, n_y = 1 \rangle$$

$$= i\sqrt{\frac{\hbar}{2m\omega}} \cdot \sqrt{\frac{\hbar m\omega}{2}} \langle n_x = 1, n_y = 0 | \underbrace{(\hat{a}^\dagger + \hat{a})}_{\text{for } x} \underbrace{(\hat{b}^\dagger - \hat{b})}_{\text{for } p_y} | n_x = 0, n_y = 1 \rangle$$

$$= -\frac{i\hbar}{2} \langle n_x = 1, n_y = 0 | \hat{a}^\dagger \hat{b} \,|\, n_x = 0, n_y = 1 \rangle$$

$$= -\frac{i\hbar}{2}$$

$$\langle n_x = 0, n_y = 1 \,|\, \hat{x} \otimes \hat{p}_y \,|\, n_x = 1, n_y = 0 \rangle$$

$$= \langle n_x = 1, n_y = 0 \,|\, \hat{x} \otimes \hat{p}_y \,|\, n_x = 0, n_y = 1 \rangle^*$$

$$= \frac{i\hbar}{2}$$

$$\langle n_x = 1, n_y = 0 \,|\, \hat{p}_x \otimes \hat{y} \,|\, n_x = 0, n_y = 1 \rangle$$

$$= \frac{i\hbar}{2} \langle n_x = 1, n_y = 0 | (\hat{a}^\dagger - \hat{a}) \otimes (\hat{b}^\dagger + \hat{b}) | n_x = 0, n_y = 1 \rangle$$

$$= \frac{i\hbar}{2} \langle n_x = 1, n_y = 0 \,|\, \hat{a}^\dagger \hat{b} \,|\, n_x = 0, n_y = 1 \rangle$$

$$= \frac{i\hbar}{2}$$

$$\langle n_x = 0, n_y = 1 \,|\, \hat{p}_x \otimes \hat{y} \,|\, n_x = 1, n_y = 0 \rangle$$

$$= \langle n_x = 1, n_y = 0 \mid \hat{p}_x \otimes \hat{y} \mid n_x = 0, n_y = 1 \rangle^*$$

$$= -\frac{i\hbar}{2}$$

In the basis $\{ |1,0\rangle, |0,1\rangle \}$,

$$U = \frac{\mu_B B}{\hbar} \cdot \frac{i\hbar}{2} \left(\begin{array}{cc} |1,0\rangle & |0,1\rangle \\ \left(\begin{matrix} 0 \\ 1 \end{matrix} \right. & \left. \begin{matrix} -1 \\ 0 \end{matrix} \right) \end{array} - \begin{array}{ccc} |1,0\rangle & |0,1\rangle & \\ \left(\begin{matrix} 0 \\ -1 \end{matrix} \right. & \left. \begin{matrix} 1 \\ 0 \end{matrix} \right) & \begin{matrix} |1,0\rangle \\ |0,1\rangle \end{matrix} \end{array} \right)$$

$$= \frac{\mu_B B}{\hbar} \cdot \frac{i\hbar}{2} \begin{pmatrix} 0 & -2 \\ 2 & 0 \end{pmatrix}$$

$$= i \mu_B B \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$

Let $\tilde{U} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$.

$$\det (\tilde{U} - \tilde{\lambda} \mathbb{1}) = 0$$

$$\begin{vmatrix} -\tilde{\lambda} & -1 \\ 1 & -\tilde{\lambda} \end{vmatrix} = 0$$

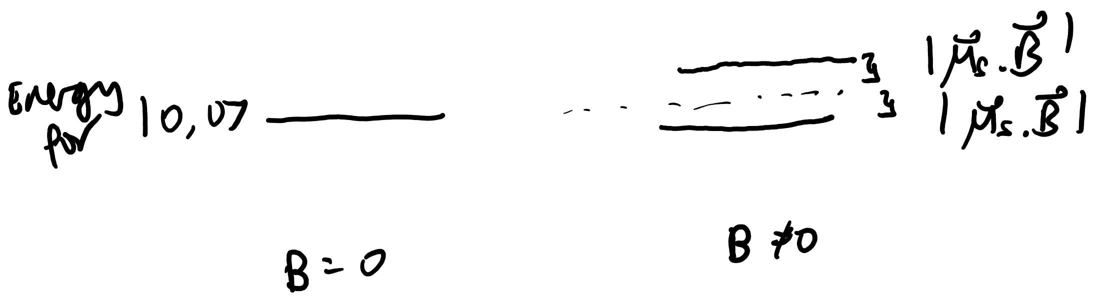
$$\Rightarrow \quad \tilde{\lambda}^2 + 1 = 0 \quad \Rightarrow \tilde{\lambda} = \pm i$$

So the eigenvalues of U in the degenerate subspace are $\lambda = \pm i (i \mu_B B)$

$$= \mp \mu_B B$$

By degenerate perturbation theory, the 1st order corrections to the 1st excited state energy are $\pm \mu_B B$.

(e) An electron has spin $s = \frac{1}{2}$ and the spin magnetic moment $\vec{\mu}_s$ also interacts with $\vec{B}$.



(Here, when spin is taken into account, the ground state becomes two-fold degenerate (spin ↑ and spin ↓ have the same energy), when $B=0$.

The B field breaks this two-fold degeneracy.)