Quantum final Exam :
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Problem: 12

Given: $E(t) = E_0 \hat{x}$ for $0 < t \leq \tau$
$= 0$ o/w

So from $\vec{E} = -\vec{\nabla} V$ we get the potential is:

$$V = V(x) = -eE_0 x \; ; \; 0 < t \leq \tau$$
$$= 0 \; ; \; \text{o/w}$$

(e is charge of e^- with sign)

As the electric field changes suddenly so the $\frac{\partial \vec{E}}{\partial t}$ term is zero for all other time & we can approximate the induced $\vec{B}$ field only lasts for a infinitely small interval & doesn't need to be considered in the given problem.

Now if the initial state & final state be $|i\rangle$ & $|f\rangle$ then the transition probability amp from $|i\rangle \to |f\rangle$ at a time $t \geq \tau$ be given by (from the formula of time dependent perturbation):

$$c_{i \to f} = -\frac{i}{\hbar} \int_0^t H'_{if} \, e^{i\omega_0 t} \, dt \, .$$

$$= -\frac{i}{\hbar} \int_0^\tau \langle i | -eE_0 x | f \rangle \, e^{i\omega_0 t} \, dt \, .$$

Here $|i\rangle = |100\rangle$; $|f\rangle = |210\rangle, |21,\pm 1\rangle$

$$\therefore \omega_0 = \frac{E_2 - E_1}{\hbar} \, .$$

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So; $C_{i\to f} = \frac{ieE_0}{\hbar}\langle i|x|f\rangle \int_0^{\tau} e^{i\omega_0 t}\,dt$.

$$= \frac{ieE_0}{\hbar}\langle i|x|f\rangle \left(\frac{e^{i\omega_0\tau}-1}{i\omega_0}\right)$$

$$= \frac{ieE_0}{\omega_0\hbar}\langle i|x|f\rangle \exp\left(\frac{i\omega_0\tau}{2}\right) \sin\left(\frac{\omega_0\tau}{2}\right) \quad \cdots (1)$$

Now for $|f\rangle = |210\rangle, |200\rangle$ & $|i\rangle = |100\rangle$
the ϕ integral in $\langle i|x|f\rangle$ gives:

$$I_\phi \sim \int_0^{2\pi} \cos\phi \, d\phi = 0.$$

So; $\langle 100|x|210\rangle = 0 = \langle 100|x|200\rangle$.

for $|f\rangle = |211\rangle$; $\langle 100|x|211\rangle$ gives:

$$I = \int_0^{\infty} r \cdot R_{21}(r) \cdot R_{10}(r) \cdot r^2\,dr \cdot \int_0^{\pi} \frac{\sin\theta}{\sqrt{4\pi}} \cdot \left(-\sqrt{\frac{3}{8\pi}}\right) \sin^2\theta\,d\theta$$

$$\int_0^{2\pi} \cos\phi\,(\cos\phi + i\sin\phi)\,d\phi.$$

$$(\because e^{i\phi} = \cos\phi + i\sin\phi)$$

Now $\int_0^{2\pi} \sin\phi\cos\phi\,d\phi = 0$ & hence Using Mathematica the other integral gives:

$$I = -\sqrt{\frac{3}{32\pi^2}} \int_0^{\infty} r^3 \cdot 2a^{-3/2} e^{-r/a} \cdot \frac{1}{\sqrt{24}} a^{-3/2} \cdot \frac{r}{a} e^{-\frac{r}{2a}}\,dr$$

$$\int_0^{\pi} \sin^3\theta\,d\theta \cdot \int_0^{2\pi} \cos^2\phi\,d\phi.$$

$$= -\sqrt{\frac{3}{32\pi^2}} \cdot \frac{128}{81} \cdot \sqrt{\frac{2}{3}}\ a \cdot \pi \cdot \frac{4}{3}.$$

$$= -\frac{128\,a}{243}.$$

for $|f\rangle = |21\,{-1}\rangle$; the difference is in $Y_l^m(\theta,\phi)$;

$-\sqrt{\frac{3}{8\pi}} \longrightarrow +\sqrt{\frac{3}{8\pi}}$ & $e^{i\phi} \rightarrow e^{-i\phi}$; but the

$\sin\phi\cos\phi$ integral again vanishes. Hence.

$$\langle 100|x|21\,{-1}\rangle = +\frac{128a}{243}.$$

$\therefore$ The transition amplitude & probabilities are:

$$C_{|100\rangle\to|210\rangle} = 0 \ ; \quad P_{|100\rangle\to|210\rangle} = 0$$

$$C_{|100\rangle\to|200\rangle} = 0 \ ; \quad P_{|100\rangle\to|210\rangle} = 0.$$

$$C_{|100\rangle\to|211\rangle} = -\frac{128a}{\cancel{81}\ 243} \cdot \frac{ieE_0}{\hbar\omega_0}\, e^{\frac{i\omega_0\tau}{2}} \sin\left(\frac{\omega_0\tau}{2}\right)$$

$$\text{i.e } P_{|100\rangle\to|211\rangle} = |c|^2 = \left(\frac{128a}{243}\right)^2 \cdot \frac{e^2E_0^2}{\hbar^2\omega_0^2} \sin^2\left(\frac{\omega_0\tau}{2}\right)$$

$$C_{|100\rangle\to|21\,{-1}\rangle} = \frac{128\,a}{243} \cdot \frac{ieE_0}{\hbar\omega_0}\, e^{\frac{i\omega_0\tau}{2}} \sin\left(\frac{\omega_0\tau}{2}\right)$$

$$\therefore P_{|100\rangle\to|21\,{-1}\rangle} = \left(\frac{128a}{243}\right)^2 \cdot \frac{e^2E_0^2}{\hbar^2\omega_0^2}\ \cancel{\&}\ \sin^2\left(\frac{\omega_0\tau}{2}\right)$$

Ans

$\left(\omega_0 = \frac{E_2 - E_1}{\hbar}\right.$; for H atom $\left.\begin{array}{l} E_2 = -3.4\ \text{ev} \\ E_1 = -13.6\ \text{ev} \end{array}\right\}\Big)$

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VII Problem: 6

a) Given: $H = H_0 + V$

$$= \underbrace{\frac{p_x^2 + p_y^2}{2m} + \frac{m\omega^2(x^2+y^2)}{2}}_{H_0} + \underbrace{\alpha m\omega^2 xy}_{V}. \quad (\alpha \ll 1)$$

Clearly; for the unperturbed condition $(\alpha = 0)$; the oscillator is just a 2-dimensional L.H.O with no coupling term between x & y. The eigenstate should be obviously the product of $\psi_{LHO}^{n_x}(x)$ & $\psi_{LHO}^{n_y}(y)$ that will satisfy T.I.S.E with eigenvalue

$$E_n = E_{n_x} + E_{n_y}.$$

This can also be shown by taking the ~~trial~~ wave fn

$$\psi(x,y) = \psi_x(x)\cdot\psi_y(y).$$

$\therefore \quad H_0\psi(x,y) = E_0\psi(x,y)$ gives:

$$\left(\frac{p_x^2}{2m} + \frac{m\omega^2 x^2}{2}\right)\psi_x(x)\psi_y(y) + \left(\frac{p_y^2}{2m} + \frac{m\omega^2 y^2}{2}\right)\psi_x(x)\psi_y(y)$$

$$= E_0\psi_x(x)\cdot\psi_y(y).$$

Breaking $E_0 = E_x + E_y$ & using the property that $p_{x/y}$ will only act on $\psi_{x/y}$; we get

$$\psi_y(y)\left\{\left(\frac{p_x^2}{2m} + \frac{m\omega^2 x^2}{2}\right)\psi_x(x) - E_x\psi_x(x)\right\} +$$
$$\psi_x(x)\left\{\left(\frac{p_y^2}{2m} + \frac{m\omega^2 y^2}{2}\right)\psi_y(y) - E_y\psi_y(y)\right\} = 0$$

Clearly the eq will be solved (& the eig fn s will form complete set) if

$$\left.\begin{aligned}\left(\frac{p_x^2}{2m}+\frac{m\omega^2x^2}{2}\right)\psi_x &= E_x\psi_x\\ \&\ \left(\frac{p_y^2}{2m}+\frac{m\omega^2y^2}{2}\right)\psi_y &= E_y\psi_y\end{aligned}\right\}$$

i.e $\psi_{x'}(x') = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\frac{1}{\sqrt{2^n n!}}H_n(\xi)\,e^{-\xi^2/2}$

$\left(\xi = \sqrt{\frac{m\omega}{\hbar}}\,x' \ ;\ x' = (x, y)\right)$

with eigenvalue: $\left.\begin{aligned}E_x &= \left(n_x+\frac{1}{2}\right)\hbar\omega\\ E_y &= \left(n_y+\frac{1}{2}\right)\hbar\omega\end{aligned}\right]$

i.e the actual eig-val of the whole H_0 is:

$E_0 = (E_x + E_y) = (n_x + n_y + 1)\hbar\omega.$

$(n_x, n_y = 0, 1, 2, \ldots)$

i.e $E_0 = (n+1)\hbar\omega \quad (n = n_x + n_y).$

1) ground state: $n = 0$; $E = \hbar\omega$

only possible: $(n_x, n_y) = (0, 0)$

$\longrightarrow$ no degeneracy.

ii) 1st excited state: $n = 1$; $E = 2\hbar\omega.$

$(n_x, n_y) = (1, 0), (0, 1)$

$\longrightarrow$ two fold degeneracy.

iii) 2nd excited state : $n = 2$; $E = 3\hbar\omega$
$(n_x, n_y) = (1,1), (2,0), (0,2)$
$\longrightarrow$ 3 fold degeneracy.

Ans

6.b

For ground state $|00\rangle$; the first order theory gives (as no degeneracy)

$$E' = \langle 00 | \underbrace{xy\alpha m\omega^2}_{H'} | 00 \rangle$$

$$= \alpha m\omega^2 \underbrace{\langle 0|x|0\rangle_x}_{0} \cdot \underbrace{\langle 0|y|0\rangle_y}_{0} = 0.$$

So there is no first order energy shift . Ans

For 1st excited state , there is 2 fold degeneracy

$\therefore$ The elements of W matrix be

$$W_{ij} = \alpha m\omega^2 \langle i | xy | j \rangle .$$

Now, $\langle 01 | xy | 01 \rangle = \underbrace{\langle 0|x|0\rangle_x}_{0} \underbrace{\langle 1|y|1\rangle_y}_{0} = 0$

Similarly $\langle 10 | xy | 10 \rangle = 0.$

$\langle 01 | xy | 10 \rangle = \langle 0|x|1\rangle_x \langle 1|y|0\rangle_y$

$$= \frac{\hbar}{2m\omega} \left\{ \langle 0 | (a_+^x + a_-^x) | 1 \rangle \langle 1 | (a_+^y + a_-^y) | 0 \rangle \right\}$$

$$= \frac{\hbar}{2m\omega}\left\{ \underbrace{\langle 0 | a_-^x | 1\rangle}_{1} \cdot \underbrace{\langle 1 | a_+^y | 0\rangle}_{1} \right\}$$

$$= \frac{\hbar}{2m\omega}. \qquad \text{i.e } W_{12} = \frac{\hbar}{2m\omega}\cdot \alpha m\omega^2 = \frac{\alpha\hbar\omega}{2}.$$

As $W_{ij} = W_{ji}^*$ so $W = \frac{\alpha\hbar\omega}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & \beta \\ \beta & 0 \end{pmatrix}$

$\left(\beta = \frac{\alpha\hbar\omega}{2}\right)$

$\therefore$ The eig-val eq: $\lambda^2 - \beta^2 = 0$

$\Rightarrow \lambda = \pm\beta.$

$\therefore$ The energy shift be $\pm \frac{\alpha\hbar\omega}{2}.$

Ans the eig state:

$\lambda = \pm\beta$, $\begin{pmatrix} 0 & \beta \\ \beta & 0 \end{pmatrix}\begin{pmatrix} x \\ y \end{pmatrix} = \pm\beta\begin{pmatrix} x \\ y \end{pmatrix}$

$\Rightarrow \begin{pmatrix} \beta y \\ \beta x \end{pmatrix} = \pm\begin{pmatrix} \beta x \\ \beta y \end{pmatrix} \Rightarrow x = \pm y$

i.e eig states are: $\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$; $\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$

So the good ~~unpe~~ unperturbed states are

$$\frac{1}{\sqrt{2}}\left(|10\rangle \pm |01\rangle\right);$$

$|10\rangle ; |01\rangle$

$E = E_0 = 2\hbar\omega$

$\frac{|10\rangle + |01\rangle}{\sqrt{2}}$; $E_0 + \frac{\alpha\hbar\omega}{2}$

$\frac{|10\rangle - |01\rangle}{\sqrt{2}}$; $E_0 - \frac{\alpha\hbar\omega}{2}$

Ans

For 2nd excited state:

By similar way $W_{11}, W_{22}; W_{33} = 0$.

& $\langle 11|xy|20\rangle \quad (\sim W_{12})$

$$= \frac{\hbar}{2m\omega}\left\{\langle 1|\cancel{x+2}\, a_+^x + a_-^x|2\rangle \cdot \langle 1|\cancel{y}\, a_+^y + a_-^y|0\rangle\right\}$$

$$= \frac{\hbar}{2m\omega}\left\{\sqrt{2}\cdot 1\right\} = \frac{\hbar}{\sqrt{2}m\omega}.$$

$$\therefore W_{12} = \frac{\hbar}{\sqrt{2}m\omega}\cdot \alpha m\omega^2 = \frac{\alpha\hbar\omega}{\sqrt{2}}.$$

$\langle 11|xy|02\rangle \quad (\sim W_{13})$

$$= \frac{\hbar}{2m\omega}\left\{\langle 1|a_+^x + a_-^x|0\rangle \cdot \langle 1|a_+^y + a_-^y|2\rangle\right\}$$

$$= \frac{\hbar}{2m\omega}\left\{1\cdot\sqrt{2}\right\} = \frac{\hbar}{\sqrt{2}m\omega}$$

$$\therefore W_{13} = \frac{\alpha\hbar\omega}{\sqrt{2}}$$

~~$\langle 02|xy|20\rangle$~~ $\langle 20|xy|02\rangle \quad (\sim W_{23})$

$$= \frac{\hbar}{2m\omega}\left\{\underbrace{\langle 2|a_+^x + a_-^x|0\rangle}_{0} \cdot \underbrace{\langle 0|a_+^y + a_-^y|2\rangle}_{0}\right\}$$

$= 0$ i.e. $W_{23} = 0$.

$\therefore$ W matrix be given by (using $W^\dagger = W$)

$$W = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}\cdot\frac{\alpha\hbar\omega}{\sqrt{2}} = \beta\begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}$$

Using Wolfram online the eig vals & eig vectors:

$$\left.\begin{aligned}
\lambda_1 &= -\beta\sqrt{2} = -\alpha\hbar\omega \longrightarrow |x_1\rangle = \frac{1}{2}\begin{pmatrix} -\sqrt{2} \\ 1 \\ 1 \end{pmatrix} \\
\lambda_2 &= \beta\sqrt{2} = \alpha\hbar\omega \longrightarrow |x_2\rangle = \frac{1}{2}\begin{pmatrix} \sqrt{2} \\ 1 \\ 1 \end{pmatrix} \\
\lambda_3 &= 0 \longrightarrow |x_3\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ -1 \\ 1 \end{pmatrix}
\end{aligned}\right\}$$

$$\frac{|11\rangle, |20\rangle, |02\rangle}{E_0 = E_0 = 3\hbar\omega} \left\{\begin{aligned}
&\frac{1}{2}\left(\sqrt{2}|11\rangle + |02\rangle + |20\rangle\right); (\alpha+3)\hbar\omega \\
&\frac{1}{\sqrt{2}}\left(|02\rangle - |20\rangle\right); 3\hbar\omega \\
&\frac{1}{2}\left(-\sqrt{2}|11\rangle + |02\rangle + |20\rangle\right); (3-\alpha)\hbar\omega
\end{aligned}\right\}$$

<u>Ans</u>

<u>6.c</u>. If we take the variable change as:

$$z = \frac{x+y}{\sqrt{2}}; \quad \eta = \frac{x-y}{\sqrt{2}}.$$

then
$$\frac{\partial}{\partial x} = \frac{\partial}{\partial z}\frac{\partial z}{\partial x} + \frac{\partial}{\partial \eta}\frac{\partial \eta}{\partial x} = \frac{1}{\sqrt{2}}\left(\partial_z + \partial_\eta\right)$$

$$\frac{\partial}{\partial y} = \frac{\partial}{\partial z}\frac{\partial z}{\partial y} + \frac{\partial}{\partial \eta}\frac{\partial \eta}{\partial y} = \frac{1}{\sqrt{2}}\left(\partial_z - \partial_\eta\right)$$

$$\therefore \partial_x^2 = \frac{1}{2}\left(\partial_z + \partial_\eta\right)^2 = \frac{1}{2}\left(\partial_z^2 + \partial_\eta^2 + 2\partial_z\partial_\eta\right)$$

$$\partial_y^2 = \frac{1}{2}\left(\partial_z - \partial_\eta\right)^2 = \frac{1}{2}\left(\partial_z^2 + \partial_\eta^2 - 2\partial_z\partial_\eta\right)$$

$$\therefore \frac{p_x^2}{2m} = -\frac{\hbar^2}{2m}\partial_x^2 = -\frac{\hbar^2}{4m}\left(\partial_z^2 + \partial_\eta^2 + 2\partial_z\partial_\eta\right)$$

$$\frac{p_y^2}{2m} = -\frac{\hbar^2}{2m}\partial_y^2 = -\frac{\hbar^2}{4m}\left(\partial_z^2 + \partial_\eta^2 - 2\partial_z\partial_\eta\right)$$

$$\therefore \frac{p_x^2 + p_y^2}{2m} = -\frac{\hbar^2}{2m}\left(\partial_z^2 + \partial_\eta^2\right)$$

i.e the T.I.S.E for H gives: $(H\psi = E\psi)$

$$\Rightarrow -\frac{\hbar^2}{2m}\left(\partial_z^2 + \partial_\eta^2\right)\psi(z,\eta) + \frac{1}{2}m\omega^2\left(z^2+\eta^2\right)\psi(z,\eta)$$

$$+ \alpha m\omega^2\frac{\left(z^2-\eta^2\right)}{2}\psi(z,\eta) = E\psi(z,\eta)$$

$$\left(\because x^2+y^2 = z^2+\eta^2 \;;\; x^2-y^2 = \frac{z^2-\eta^2}{2}\right)$$

Taking $\psi(z,\eta) = \psi_z(z)\cdot\psi_\eta(\eta)$ & $E = (E_z + E_\eta)$

the T.I.S.E gives:

$$\psi_\eta(\eta)\left(-\frac{\hbar^2}{2m}\partial_z^2 + \frac{m\omega^2}{2}(1+\alpha)z^2 - E_z\right)\psi_z(z)$$

$$+ \psi_z(z)\left(-\frac{\hbar^2}{2m}\partial_\eta^2 + \frac{m\omega^2}{2}(1-\alpha)\eta^2 - E_\eta\right)\psi_\eta(\eta) = 0$$

This is a two dimensional L.H.O eq for two coordinates (z,η) with $\omega_z^2 = \omega^2(1+\alpha)$

& $\omega_\eta^2 = \omega^2(1-\alpha)$. i.e the solutions are:

$$\psi(z,\eta) = \psi_{LHO}^{\omega_z}(z)\cdot\psi_{L.HO}^{\omega_\eta}(\eta)$$

with energy $E = (E_z + E_\eta) = \left(n_z + \frac{1}{2}\right)\hbar\omega_z + \left(n_\eta + \frac{1}{2}\right)\hbar\omega_\eta$

$\therefore$ ground state : $n_z = 0$; $n_y = 0$: (E_{00} in xy)

$$E_0 = \frac{\hbar}{2}(\omega_z + \omega_y)$$

$$= \frac{\hbar\omega}{2}\left(\sqrt{1+\frac{2\alpha}{2}} + \sqrt{1-\frac{2\alpha}{2}}\right)$$

(upto 1st order) $\simeq \frac{\hbar\omega}{2}\left(1+\frac{4\alpha}{4}+1-\frac{4\alpha}{4}\right) = \hbar\omega$. Ans

1st excited state: $n_z = 0$; $n_y = 1$ ($\because \omega_z > \omega_y$)

$$\therefore E_1 = \frac{\hbar\omega_z}{2} + \frac{3}{2}\hbar\omega_y$$

$$= \frac{\hbar\omega}{2}\sqrt{1+\frac{2\alpha}{2}} + \frac{3}{2}\hbar\omega\sqrt{1-2\alpha/2}$$

$$\simeq \frac{\hbar\omega}{2}\left(1+\frac{4\alpha}{4}\right) + \frac{3}{2}\hbar\omega\left(1-\frac{4\alpha}{4}\right)$$

$$= 2\hbar\omega - \frac{\alpha\hbar\omega}{2}$$ Ans

2nd excited state: $n_z = 1$; $n_y = 0$

$$\therefore E_2 = \frac{3}{2}\hbar\omega_z + \frac{1}{2}\hbar\omega_y$$

$$= \frac{3}{2}\hbar\omega\sqrt{1+\alpha} + \frac{\hbar\omega}{2}\sqrt{1-\alpha}.$$

$$\simeq \frac{3\hbar\omega}{2}\left(1+\frac{\alpha}{2}\right) + \frac{\hbar\omega}{2}\left(1-\frac{\alpha}{2}\right)$$

$$= 2\hbar\omega + \frac{\alpha\hbar\omega}{2}$$ Ans

The results are completely equal to the perturbative results in part b.

6.d From perturbative method the results were

$|00\rangle \longrightarrow$ unchanged $E_0 = \hbar\omega$.

$|10\rangle, |01\rangle \longrightarrow$ splits $\frac{|10\rangle - |01\rangle}{\sqrt{2}}$; $E_1 = 2\hbar\omega - \frac{\alpha\hbar\omega}{2}$

$\frac{|10\rangle + |01\rangle}{\sqrt{2}}$; $E_2 = 2\hbar\omega + \frac{\alpha\hbar\omega}{2}$

So degeneracy was splitted in xy L.H.O by perturbation & the energy levels were

$$\underbrace{\hbar\omega, \quad 2\hbar\omega - \frac{\alpha\hbar\omega}{2}, \quad 2\hbar\omega + \frac{\alpha\hbar\omega}{2}} \quad (\alpha \gtrsim 0)$$

which is same to the result given by exact sol^n of T.I.S.E with variable change. i.e same results are recovered.

Proved

6.e As given the e^-'s are subjected to the same H; it means to keep H unchanged; we need to assume that there is no coloumb / spin-spin interactions between the electrons.

As the energy depends only on the spatial part of ϕ (total wave f^n); the ground state is when both of the e^-'s are in ground state (symmetric configuration)

i.e $\phi(r_1, r_2) = |0\rangle_1 |0\rangle_2$ $(|0\rangle = \text{ground state})$

explicitly $|0\rangle \equiv |n_z = 0; n_\eta = 0\rangle$

i.e $\psi_{|0\rangle} = \left(\frac{m\omega_z}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^0 \cdot 0!}} H_0(z') e^{-\frac{z'^2}{2}} \cdot \left(\frac{m\omega_\eta}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^0 \cdot 0!}} H_0(\eta') e^{-\frac{\eta'^2}{2}}$

$\left(z' = z\sqrt{\frac{m\omega_z}{\hbar}} ; \eta' = \sqrt{\frac{m\omega_\eta}{\hbar}} \cdot \eta\right)$

Now there ~~are~~ are 4 spin states: $|+\rangle_1|+\rangle_2$; $|-\rangle_1|-\rangle_2$; $|+\rangle_1|-\rangle_2$; $|-\rangle_1|+\rangle_2$.

As the spacial wave fn is symmetric so the spin part must be antisymmetric. But the only antisymmetric configuration made out of these states is singlet one $|00\rangle = \dfrac{|+\rangle_1|-\rangle_2 - |-\rangle_1|+\rangle_2}{\sqrt{2}} = |\chi_1\rangle$

$\therefore$ The total ground state wave fn be given by:

$$|\psi_1\rangle = |\phi_1\rangle \cdot |\chi_1\rangle = |0\rangle_1 |0\rangle_2 \cdot \frac{(|+\rangle_1|-\rangle_2 - |-\rangle_1|+\rangle_2)}{\sqrt{2}}$$ Ans

And there is $\boxed{\text{no degeneracy.}}$

For the 1st excited state we need: $|\phi\rangle = |1\rangle_1|0\rangle_2$ or $|0\rangle_1|1\rangle_2$

$$\left(|1\rangle = |n_z = 0; n_m = 1\rangle = \left(\frac{m\omega_z}{\pi\hbar}\right)^{1/4} \cdot e^{-z'^2/2} \cdot \left(\frac{m\omega_m}{\pi\hbar}\right)^{1/4} \cdot e^{-\frac{\eta'^2}{2}} \frac{H_1(\eta')}{\sqrt{2}}\right)$$

For the symmetric space configuration there is the singlet state; i.e Antisymmetric spin configuration.

$$|\psi_2\rangle^{(1)} = \frac{|1\rangle_1|0\rangle_2 + |0\rangle_1|1\rangle_2}{\sqrt{2}} \times \frac{|+\rangle_1|-\rangle_2 - |-\rangle_1|+\rangle_2}{\sqrt{2}} = |\phi_2\rangle^{(1)} \cdot |00\rangle$$

For the Antisymm space configuration there is the triplet state (symmetric spin configuration)

$$|\psi_2\rangle^{(2)} = \frac{|1\rangle_1|0\rangle_2 - |0\rangle_1|1\rangle_2}{\sqrt{2}} \times |++\rangle \equiv |\phi_2\rangle^{(2)} \cdot |11\rangle$$

$$|\psi_2\rangle^{(3)} = \frac{|1\rangle_1|0\rangle_2 - |0\rangle_1|1\rangle_2}{\sqrt{2}} \times |--\rangle \equiv |\phi_2\rangle^{(3)} \cdot |1-1\rangle$$

$$|\psi_2\rangle^{(4)} = \frac{|1\rangle_1|0\rangle_2 - |0\rangle_1|1\rangle_2}{\sqrt{2}} \times \frac{|+-\rangle + |-+\rangle}{\sqrt{2}} \equiv |\phi_2\rangle^{(4)} |10\rangle$$

Ans

Clearly there is $\boxed{\text{4 fold degeneracy}}$ Ans

☑ Problem: 2 →

2a $$H = -\frac{\hbar^2}{2m}\left(\nabla_1^2+\nabla_2^2\right) + \frac{m\omega^2}{2}\left(r_1^2+r_2^2\right) - \frac{\lambda m\omega^2}{4}\left|\vec{r}_1-\vec{r}_2\right|^2$$

for $\lambda=0$; the Hamiltonian is simply the spherical oscillator for two particles:

$$H_0 = \left(-\frac{\hbar^2}{2m}\nabla_1^2 + \frac{m\omega^2 r_1^2}{2}\right) + \left(-\frac{\hbar^2\nabla_2^2}{2m} + \frac{m\omega^2 r_2^2}{2}\right)$$

Clearly these ~~at~~ are sum of two spherical oscillator ~~oo~~ Hamiltonians. For any one of the ~~spherical~~ spherical oscillators the T.I.S.E in cartesian coordinate be given by:

$$\left\{-\frac{\hbar^2}{2m}\left(\partial_x^2+\partial_y^2+\partial_z^2\right) + \frac{m\omega^2}{2}\left(x^2+y^2+z^2\right)\right\}\psi(x,y,z) = E\psi(x,y,z).$$

by taking $\psi(x,y,z) = \psi_x(x)\cdot\psi_y(y)\cdot\psi_z(z)$ & $E = E_x + E_y + E_z$ we get T.I.S.E splits into 3 parts:

$$\psi_y\psi_z\left\{\left(-\frac{\hbar^2}{2m}\partial_x^2 + \frac{m\omega^2x^2}{2} - E_x\right)\psi_x\right\} + \psi_z\psi_x\left\{\left(-\frac{\hbar^2}{2m}\partial_y^2 + \frac{m\omega^2y^2}{2} - E_y\right)\psi_y\right\} + \psi_x\psi_y\left\{\left(-\frac{\hbar^2\partial_z^2}{2m} + \frac{m\omega^2z^2}{2} - E_z\right)\psi_z\right\} = 0.$$

The eq is satisfied if $\psi_x(x)$, $\psi_y(y)$, $\psi_z(z)$ are soln s of linear L.H.O with freq ω

i.e $\psi_i(x_i) \sim |n_{x_i}\rangle$ with energy $E_{x_i} = \left(n_{x_i} + \frac{1}{2}\right)\hbar\omega$.

$\therefore \psi(x,y,z) = |n_x n_y n_z\rangle$; $E = \left(n_x + n_y + n_z + \frac{3}{2}\right)\hbar\omega$.

So for two particle system the ground state is:

$$\psi_0(r_1, r_2) = |0\,0\,0\rangle_1 |0\,0\,0\rangle_2$$

$$= \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{\tilde{x}_1^2}{2}} \cdot \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{\tilde{y}_1^2}{2}} \cdot \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{\tilde{z}_1^2/2}$$

$$\times \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{\tilde{x}_2^2}{2}} \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{\tilde{y}_2^2}{2}} \cdot \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{\tilde{z}_2^2}{2}}.$$

$$= \left(\frac{m\omega}{\pi\hbar}\right)^{3/2} e^{-\frac{\tilde{r}_1^2 + \tilde{r}_2^2}{2}} = \left(\frac{\alpha}{\pi}\right)^{3/2} e^{-\frac{\tilde{r}_1^2 + \tilde{r}_2^2}{2}}.$$

$$\left(\text{as } \tilde{r} = r\sqrt{\frac{m\omega}{\hbar}} = r\sqrt{\alpha}\right) \left(\tilde{x}_i = x_i\sqrt{\alpha}\right)$$

i.e $\psi_0(r_1, r_2) = \left(\frac{\alpha}{\pi}\right)^{3/2} e^{-\frac{\sqrt{\alpha}^2 (r_1^2 + r_2^2)}{2}}$.

combining with the spin part (which must be antisymmetric singlet state due to the symmetric spacial part) we get the total ground state is given by: (normalized)

$$\psi_0^{tot} = \underbrace{\left(\frac{\alpha}{\pi}\right)^{3/2} e^{-\frac{\alpha(r_1^2 + r_2^2)}{2}}}_{\psi_0(r_1, r_2)} \times \underbrace{\left(\frac{|+\rangle_1 |-\rangle_2 - |-\rangle_1 |+\rangle_2}{\sqrt{2}}\right)}_{|0\,0\rangle}$$

with energy:

$$E_0 = 2 \times \frac{3}{2}\hbar\omega = 3\hbar\omega \quad \underline{\text{Ans}}$$

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2.b Now for $\lambda \neq 0$; we use perturbative method to estimate the perturbed energy of the system

Here $H' = -\frac{\lambda m \omega^2}{4} |(\vec{r}_1 - \vec{r}_2)|^2$.

$\therefore$ The ground state shift be given by:

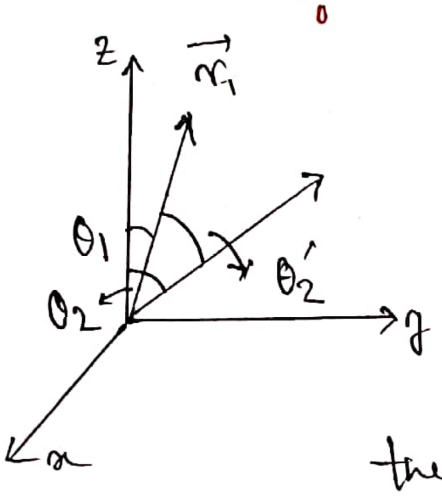
$$\Delta E_0 = \langle 000 | H' | 000 \rangle = -\frac{\lambda m \omega^2}{4} \langle 000 | |\vec{r}_1 - \vec{r}_2|^2 | 000 \rangle$$

but $|000\rangle = \left(\frac{\alpha}{\pi}\right)^{3/2} e^{-\frac{\sqrt{\alpha^2}(r_1^2 + r_2^2)}{2}}$; And hence:

$$\Delta E_0 = \left(\left(\frac{\alpha}{\pi}\right)^{3/2}\right)^2 \left(-\frac{\lambda m \omega^2}{4}\right) \int e^{-\sqrt{\alpha^2}(r_1^2 + r_2^2)} |\vec{r}_1 - \vec{r}_2|^2 d^3\vec{r}_1 \, d^3\vec{r}_2$$

$$= -\frac{\lambda m \omega^2}{4} \cdot \left(\frac{\alpha}{\pi}\right)^3 \int e^{-\sqrt{\alpha^2} r_1^2} d^3\vec{r}_1 \times$$

$$\int_0^\infty e^{-\sqrt{\alpha^2} r_2^2} \cdot r_2^2 \, dr_2 \int_0^\pi (r_1^2 + r_2^2 - 2 r_1 r_2 \cos\theta_2') \sin\theta_2' d\theta_2' \int_0^{2\pi} d\phi'$$



Here I have changed the integral by first integrating over r_2 as the polar axis along $\vec{r}_1$ (fixed) & the polar angle be θ_2' (not θ_2); then the integral on $\vec{r}_1$

And used $|\vec{r}_1 - \vec{r}_2| = (r_1^2 + r_2^2 - 2 r_1 r_2 \cos\theta_2')^{1/2}$.

Now, $\int_0^{2\pi} d\phi' = 2\pi$.

And $\int_0^\pi (r_1^2 + r_2^2 - 2 r_1 r_2 \cos\theta_2') \sin\theta_2' d\theta_2'$

$$= \int_{\theta_2'=0}^{\pi} \frac{x \, dx}{2 r_1 r_2}$$

$$\left(\begin{array}{l} r_1^2 + r_2^2 - 2 r_1 r_2 \cos\theta_2' = x \\ \sin\theta_2' \, d\theta_2' = \frac{dx}{2 r_1 r_2} \end{array} \right)$$

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$$= \left. \frac{(r_1^2 + r_2^2 - 2r_1r_2\cos\theta_2')^2}{2r_1r_2 \times 2} \right|_{\theta_2'=0}^{\pi}$$

$$= \frac{(r_1+r_2)^4 - (r_1-r_2)^4}{4r_1r_2} = \frac{8r_1r_2(r_1^2+r_2^2)}{4r_1r_2} = 2(r_1^2+r_2^2)$$

$\therefore$ The r_2 integral gives:

$$I_2 = 2\pi \int_0^\infty r_2^2 e^{-\sqrt{\alpha^2} r_2^2}\, 2(r_1^2+r_2^2)\, dr_2 .$$

$\Big\downarrow$ using Mathematica.

$$= \frac{\pi^{3/2}(3 + 2r_1^2\alpha^2)}{2\alpha^{5/2}}$$

So finally the quantity:

$$\Delta E_0 = -\frac{\lambda m \omega^2}{4}\left(\frac{\alpha}{\pi}\right)^3 \cdot \int_0^\infty r_1^2 e^{-\alpha^2 r_1^2} \cdot \frac{\pi^{3/2}(3+2r_1^2\alpha^2)}{2\alpha^{5/2}}\, dr_1 .$$

$$\times \int_0^\pi \sin\theta_1\, d\theta_1 \int_0^{2\pi} d\phi_1 .$$

$$= -\frac{\lambda m \omega^2}{4} \cdot \left(\frac{\alpha}{\pi}\right)^3 \times 4\pi \times \frac{3\pi^2}{4\alpha^4}$$

(Using Mathematica)

$$\boxed{= -\frac{3m\lambda\omega^2}{4\alpha}}$$

So the corrected G.S energy is:

$$E = E_0 + \Delta E_0 = 3\hbar\omega - \frac{3m\lambda\omega^2}{4\alpha}$$

Ans

2.c I've taken first order perturbation. Now we know that the 2nd order perturbation is always negative. any higher orders give smaller & smaller contributions.

i.e contribution from (2nd order + higher orders) < 0.

As infinite order perturbation gives exact result; hence the sign of error is +ve here.

i.e $\begin{pmatrix}\text{calculated result using} \\ \text{1st order perturbation}\end{pmatrix} >$ exact result.
in part 2.b

2.d Let's introduce $\vec{z} = \dfrac{\vec{r}_1 + \vec{r}_2}{\sqrt{2}}$; $\vec{\eta} = \dfrac{\vec{r}_1 - \vec{r}_2}{\sqrt{2}}$.

$$\therefore \nabla_z = \frac{\nabla_1 + \nabla_2}{\sqrt{2}} \; ; \; \nabla_\eta = \frac{\nabla_1 - \nabla_2}{\sqrt{2}}.$$

$$\therefore \nabla_z^2 + \nabla_\eta^2 = \left(\frac{\nabla_1 + \nabla_2}{\sqrt{2}}\right)^2 + \left(\frac{\nabla_1 - \nabla_2}{\sqrt{2}}\right)^2 = \nabla_1^2 + \nabla_2^2.$$

And $z^2 + \eta^2 = \frac{1}{2}\left\{(\vec{r}_1 + \vec{r}_2)^2 + (\vec{r}_1 - \vec{r}_2)^2\right\} = r_1^2 + r_2^2$

And $|(\vec{r}_1 - \vec{r}_2)|^2 = r_1^2 + r_2^2 - 2\vec{r}_1 \cdot \vec{r}_2 = (\vec{r}_1 - \vec{r}_2)^2 = 2\eta^2$.

So the Hamiltonian separates, (in terms of z, η)

$$H = -\frac{\hbar^2 \nabla_z^2}{2m} - \frac{\hbar^2 \nabla_\eta^2}{2m} + \frac{1}{2} m\omega^2 (z^2 + \eta^2) - \frac{m\omega^2 \lambda \eta^2}{2}.$$

$$= \left(-\frac{\hbar^2 \nabla_z^2}{2m} + \frac{m\omega^2 z^2}{2}\right) + \left(-\frac{\hbar^2 \nabla_\eta^2}{2m} + \frac{m\omega^2}{2}(1-\lambda)\eta^2\right)$$

This is the sum of two L.H.O Hamiltonians (indp) with freq $\omega_z^2 = \omega^2$; $\omega_\eta^2 = \omega^2 (1-\lambda)$

The solutions are $|\psi_{n_z n_\eta}\rangle = |n_z, n_\eta\rangle$

with energy $E_{n_z n_\eta} = \left(n_z + \frac{3}{2}\right)\hbar\omega_z + \left(n_\eta + \frac{3}{2}\right)\hbar\omega_\eta$

($\frac{3}{2}$ due to 3 spacial dimension)

∴ The ground state is:

$$|\psi_{00}\rangle = |0\;0\rangle = \left(\frac{m\omega_z}{\pi\hbar}\right)^{1/4} \cdot \left(\frac{m\omega_\eta}{\pi\hbar}\right)^{1/4} e^{-\frac{m^2\omega_z^2 z^2}{\hbar^2}} \cdot e^{-\frac{m^2\omega_\eta^2 \eta^2}{\hbar^2}}$$

With energy $E_{00} = \frac{3}{2}\hbar\left(\omega_z + \omega_\eta\right)$

$$= \frac{3}{2}\hbar\left(\omega + \omega\sqrt{1-\lambda}\right)$$

$$\simeq \frac{3}{2}\hbar\left(\omega + \omega\left(1 - \frac{\lambda}{2} - \frac{3\lambda^2}{8} - \cdots\right)\right)$$

$$= 3\hbar\omega - \frac{3}{4}\hbar\lambda\omega - O(\lambda^2).$$

Ans

~~Here first order correction is~~ $\cancel{-\frac{3}{4}\left(\frac{m\omega}{\hbar}\right)\cdot\left(\frac{\lambda\hbar^2}{m}\right) = -\frac{3\lambda\hbar^2\alpha}{4}}$.

~~To satisfy part (c) we need~~

$\cancel{-\frac{3m\lambda\omega^2}{4\alpha} > -\frac{3\hbar\lambda\omega}{4}}$ ~~i.e~~ $\cancel{\frac{m\omega}{\alpha^5\hbar} < 1}$

~~i.e~~ $\cancel{\frac{1}{\alpha^6} < 1}$ ~~i.e~~ $\cancel{\alpha^6 > 1}$ ~~i.e~~ $\cancel{\alpha > 1}$.

~~i.e~~ $\cancel{\frac{\alpha}{\alpha^5} < 1}$ ~~i.e~~ $\cancel{\alpha > 1}$

~~Ans~~

Here the 1st order correction is:

$$-\frac{3}{4}\hbar\lambda\omega = -\frac{3}{4}\frac{\hbar m}{m\omega}\lambda\omega^2 = -\frac{3}{4}\frac{\lambda m\omega^2}{\alpha}$$

proved

Which matches with the perturbative result.

Now the 2nd order correction $= -\frac{3}{8}\lambda^2\hbar\omega \times \frac{3}{2} < 0$

i.e exact result < perturbative result.

i.e it satisfies the argument in part (c)

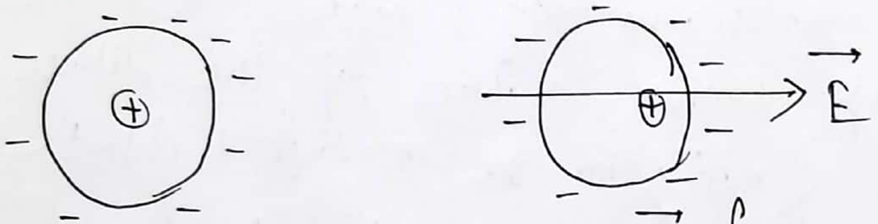
And part (b) too

proved

Problem : 10

a) As the atomic system (given) is a constantly/uniformly distributed charged sphere; the dipole moment; without any external field is obviously zero due to symmetry.

Now in presence of external $\vec{E}$ field; the ~~cet~~ central positive charge shifts a little bit (or the charged sphere in the opposite of $\vec{E}$) in the direction of $\vec{E}$ field..

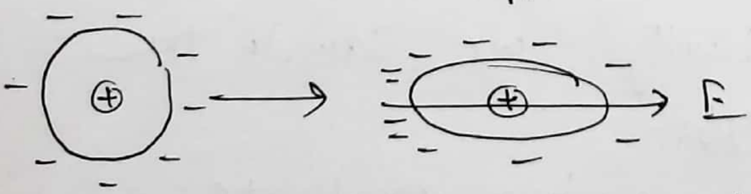


No field

in $\vec{E}$ field

The shifting goes on until the internal ~~fit~~ field due to the distance between +ve & −ve charge ~~centres~~ centres cancells out the external field.

(Here however; a change of spherical shape also occures and the '-ve' charge concentration increases in the opposite end and the shape becomes



But this brings a lot of complexity & we neglect that here.)

Now if the distance in equilibrium becomes d; then the electric field due to sphere at the position of '+ve' charge:

$$E = \frac{1}{4\pi\epsilon_0} \times \frac{ed}{a^3}$$ (This is a standard result $\vec{E} = \int d\vec{E} = \frac{1}{4\pi\epsilon_0}\int_0^d \frac{(4\pi r^2)\rho(r)}{d^2}\,dr = \frac{1}{4\pi\epsilon_0}\frac{q\vec{d}}{a^3}$)

$$\therefore d = \frac{4\pi\epsilon_0 a^3 E}{e}$$

i.e the induced dipole moment: $\mu = ed = 4\pi\epsilon_0 a^3 E$ } Ans

& polarizibility: $\alpha = \frac{\mu}{E} = 4\pi\epsilon_0 a^3$ Ans

~~10.b Quantum mechanically; here we have to find the expectation value of the dipole moment $\langle\mu\rangle = \langle e\vec{r}\rangle$ in the modifies state due to perturbation for external field.~~

~~Now the perturbing Hamiltonian is given by:~~

~~$H' = -eV'$; but $\vec{E} = E\hat{x} \Rightarrow V' = -\hat{x}E$~~

~~$\therefore H' = \hat{x}eE$~~

~~As the e^- was initially~~

10.b Quantum mechanically; we can do the problem in two ways,

i) find the modifies state & then evaluate $\langle\mu\rangle = \langle e\vec{r}\rangle$

ii) Find the energy shift & equate it with $\frac{1}{2}\alpha E^2$

i.e $|\Delta E_{100}| = \frac{1}{2}\alpha E^2$

I'm however going to do with the 2nd way.

Now given $\vec{E} = E\hat{x}$; i.e $\hat{V}' = -\hat{x}E$

$\therefore H' = -eV' = eEx$

Now the energy shift be given by:

$$\Delta E_1^{(1)} = \langle H' \rangle = +eE \underbrace{\langle \psi_{100} | x | \psi_{100} \rangle}_{0}$$

correction

$\therefore$ 1st order term is zero.

We go for 2nd order correction.

$$\Delta E_1^{(2)} = \sum_{n=2} - \frac{|\langle nlm | H' | 100 \rangle|^2}{E_2^0 - E_1^0}$$

(As it's told to take only $n=2$ (2s, 2p) states)

$$= \frac{e^2E^2}{E_2^0 - E_1^0} \sum_{n=2} |\langle nlm | x | 100 \rangle|^2.$$

now if $|nlm\rangle = |200\rangle$ then we get $\langle 200 | x | 100 \rangle$; the ϕ integral is: $\int_0^{2\pi} \cos\phi \, d\phi = 0$.

$\therefore \langle 200 | x | 100 \rangle = 0$.

for $\langle nlm | = \langle 211 |$:

$\langle 211 | x | 100 \rangle$

$$= \int_0^\infty r R_{21}(r) \cdot R_{10}(r) \cdot r^2 dr \int_0^\pi \left(-\frac{1}{\sqrt{4\pi}} \cdot \sqrt{\frac{3}{8\pi}} \right) \sin^3\theta \, d\theta$$

$$\int_0^{2\pi} \cos\phi \, (\cos\phi - i\sin\phi) \, d\phi.$$

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The integral was previously evaluated in problem (12) & is given by:

$$\langle 211 | x | 100 \rangle = -\frac{2^7 a_0}{3^5}.$$

for $|nlm\rangle = |21\,{-1}\rangle$ similarly from previous problem we get:

$$\langle 21\,{-1} | x | 100 \rangle = \frac{2^7 a_0}{3^5}.$$

$$\therefore \Delta E_1^{(2)} = -\frac{e^2 E^2}{E_2^0 - E_1^0} \left[\left(\frac{2^7 a_0}{3^5}\right)^2 + \left(-\frac{2^7 a_0}{3^5}\right)^2 \right]$$

$$= \frac{-e^2 E^2}{E_2^0 - E_1^0} \times \frac{2^{15} a_0^2}{3^{10}}.$$

$\therefore$ from the relation $|\Delta E^{(2)}| = \frac{\alpha E^2}{2}$ we get:

$$\frac{\alpha \cancel{E^2}}{2} = \frac{e^2 \cancel{E^2}}{E_2^0 - E_1^0} \cdot \frac{2^{15} a_0^2}{3^{10}}.$$

$$\therefore \alpha = \text{polarizibity} = \frac{2^{16} e^2 a_0^2}{3^{10}(E_2^0 - E_1^0)}$$ Ans

The dipole moment is $\vec{\mu} = -\alpha \vec{E}$

$$\therefore \vec{\mu} = -\frac{2^{16} e^2 a_0^2 \vec{E}}{3^{10}(E_2^0 - E_1^0)}$$ Ans

(Here for H: $E_2^0 = -3.4$ eV
$E_1^0 = -13.6$ eV)

10.c experimentally we can't directly find $\vec{\mu}$. But we can find the modified energy states & their gaps. So if we calculate the energy shift of $n=2$ states in similar way (there we've to use degenerate perturbation theory) & then from the spectra of that H atom from experimental data; we can compare the two results to check the validity of the mathematical procedure.

On the other hand; we can measure the permittivity (ϵ) of polarized H atom experimentally (easy). By putting some H in between two plates of a parallel capacitor this can be done. Then we use two relations

$$\text{i)}\quad \alpha = \frac{n^2-1}{n^2+2} \cdot \frac{3}{4\pi N} \longrightarrow \text{Lorentz eq}$$

$$\text{ii)}\quad n \propto \sqrt{\epsilon} \longrightarrow \text{clasius Mossoti eq}$$

(n = electrical refractive index)

Calculating α from here experimentally we check if it matches or not with the previous result. Ans

Problem: 5 →

a As both of neutron & proton are spin $\frac{1}{2}$ particles so total ~~spin spin~~ of spin of deuteron is 0 or 1. Ans

b. for $S(=S_p+S_n)=1$: we get $m_s=\pm 1, 0$.
if the coupled state is given by curvy bracket $|\,)$ & uncoupled state by $|\,\rangle$ then obviously:

$$|1\,1) = |\uparrow_p\rangle|\uparrow_n\rangle = |\tfrac{1}{2}\rangle_p|\tfrac{1}{2}\rangle_n \quad \text{Ans}$$

$$\therefore J^-|1\,1) = J_p^-|\tfrac{1}{2}\rangle_p|\tfrac{1}{2}\rangle_n + J_n^-|\tfrac{1}{2}\rangle_p|\tfrac{1}{2}\rangle_n$$

J_p & J_n acts only on $|\tfrac{1}{2}\rangle_p$ & $|\,\rangle_n$. So we get:

$$\sqrt{(1+1)(1-1+1)}\,|1\,0) = \sqrt{(\tfrac{1}{2}+\tfrac{1}{2})(\tfrac{1}{2}-\tfrac{1}{2}+1)}\left\{|-\tfrac{1}{2}\rangle_p|\tfrac{1}{2}\rangle_n + |\tfrac{1}{2}\rangle_p|-\tfrac{1}{2}\rangle_n\right\}$$

$$\Rightarrow |1\,0) = \frac{1}{\sqrt{2}}\left(|\tfrac{1}{2}\rangle_p|-\tfrac{1}{2}\rangle_n + |-\tfrac{1}{2}\rangle_p|\tfrac{1}{2}\rangle_n\right)$$

And obviously; $|1\,{-1}) = |-\tfrac{1}{2}\rangle_p|-\tfrac{1}{2}\rangle_n = |\downarrow\rangle_p|\downarrow\rangle_n$ Ans

for $S=0$; $m_s=0$:

Now let $|0\,0) = a|\tfrac{1}{2}\rangle_p|-\tfrac{1}{2}\rangle_n + b|-\tfrac{1}{2}\rangle_p|\tfrac{1}{2}\rangle_n$

(other C-G coefficients will be zero as $m_1+m_2=m$ is to be satisfied.)

$$J_-|0\,0) = 0 = a\left\{J_p^-|\tfrac{1}{2}\rangle_p|-\tfrac{1}{2}\rangle_n + \cancel{J_n^-|\tfrac{1}{2}\rangle_p|-\tfrac{1}{2}\rangle_n}^{\,0}\right\}$$
$$+\, b\left\{J_p^-|-\tfrac{1}{2}\rangle_p|\tfrac{1}{2}\rangle_n + J_n^-|-\tfrac{1}{2}\rangle_p|\tfrac{1}{2}\rangle_n\right\}$$

i.e $(a+b)\,|-\tfrac{1}{2}\rangle_p|-\tfrac{1}{2}\rangle_n = 0$ i.e $a=-b$.

Now $a^2+b^2 = 1$ So; $a = \sqrt{\tfrac{1}{2}}$; $b = -\tfrac{1}{\sqrt{2}}$.

$\therefore |0\,0) = \frac{1}{\sqrt{2}}\left(|\tfrac{1}{2}\rangle_p|-\tfrac{1}{2}\rangle_n - |-\tfrac{1}{2}\rangle_p|\tfrac{1}{2}\rangle_n\right)$ Ans

This are total spin eigenstates of Deuteron with.

$$\left.\begin{aligned} S^2|1;\pm1,0) &= \hbar^2\sqrt{2}\,|1;\pm1,0) \\ \& \; S^2|0,0) &= 0 \end{aligned}\right\}$$

5.c We get: $\hat{S}_p\cdot\hat{S}_n = \dfrac{S^2 - S_p^2 - S_n^2}{2}$.

Now for Deuteron spin state $S = \left(\tfrac{1}{2}+\tfrac{1}{2}\right) = 1$; we get:

$$\langle\sigma_n\cdot\sigma_p\rangle = \frac{1}{2}\langle\sigma^2 - \sigma_n^2 - \sigma_p^2\rangle \times 4$$

(4 because $S = \frac{\hbar}{2}\sigma$ i.e $S^2 = \frac{\hbar^2\sigma^2}{4}$)

$$= \frac{1}{2}\left(S(S+1) - \tfrac{1}{2}\times\left(\tfrac{1}{2}+1\right)\times 2\right)\times 4$$

$$= \frac{4}{2}\left(2 - \frac{3}{2}\right) = \frac{4}{4} = 1$$

~~i.e $V_{S=1}(r) = \frac{V_c(r)}{2}\left(1+\frac{1}{4}\right) = \frac{5V_c(r)}{8}$; $(r<a)$~~

for $S=0$;

$$\langle\sigma_n\cdot\sigma_p\rangle = \frac{4}{2}\left(0(0+1) - \tfrac{1}{2}\left(\tfrac{1}{2}+1\right)\times 2\right)$$

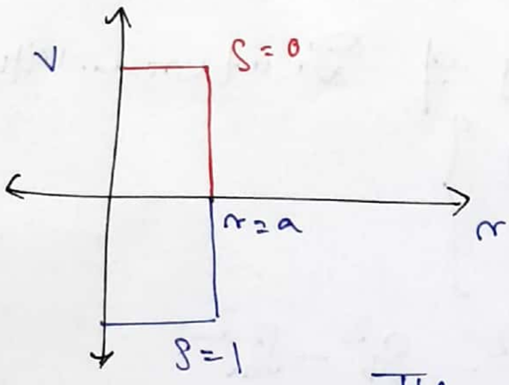
$$= -\frac{3}{4}\times 4 = -3$$

~~$\therefore V_{S=0}(r) = \frac{V_c(r)}{2}\left(1-\frac{3}{4}\right) = \frac{V_c(r)}{8}$, $(r<a)$~~

$$\therefore V_{S=1}(r) = \frac{V_c(r)}{2}(1+1) = V_c(r) = -V_0 \quad (r \leq a)$$

$$\& \; V_{S=0}(r) = \frac{V_c(r)}{2}(1-3) = -V_c(r) = V_0 \quad (r \leq a).$$

So; The potential looks like:



As $V_{S=0,1}(r) = 0$ for $r > a$

So the bound state is formed for which ~~then~~ there is a well; i.e $S=1$ (triplet) state.

The singlet $(S=0)$ state gives unbounded wavefn.

5. d As the potential minima is smaller for the triplet state; it forms the true ground state. Now here told that $l=0$; i.e T.I.S.E says:

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} + V(r)\Big|_{S=1} \cdot u = E(u).$$

for bound state $-V_0 < E < 0$.

So for $r \leq a$; T.I.S.E gives:

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} \cancel{+} - V_0 u = Eu$$

$$\Rightarrow \frac{d^2u}{dr^2} = -\frac{2m}{\hbar^2}(V_0+E)u = -k^2u \qquad \left(\begin{array}{c}\because |V_0| > |E| \\ \& \; E<0 \\ V_0 > 0\end{array}\right)$$

i.e $u = A\sin(kr) + B\cos(kr)$.

For $r > a$:

$$\frac{d^2u}{dr^2} = -\frac{2mE}{\hbar^2}u = \eta^2 u$$

$$\Rightarrow u = Ce^{\eta r} + De^{-\eta r}.$$

As $\underset{r\to 0}{\text{Lt}}\ u(r) = 0$ so we must have $B=0$.

$\underset{r\to\infty}{\text{Lt}}\ u(r) = 0$ " " " " $C=0$

$$\therefore \left.\begin{aligned} u_{in}(r) &= A\sin(kr) \\ u_{out}(r) &= D e^{-\eta r}. \end{aligned}\right\}$$ Unnormalized W.F

Ans

Continuity of u & u' at $r=a$ gives:

$$A\sin ka = De^{-\eta a}$$

$$kA\cos ka = -\eta D e^{-\eta a}$$

Which gives: $\frac{\tan(ka)}{k} = -\frac{1}{\eta}$ ... (1)

This eq helps to find the allowed value of energy.

So the total G.S is (for $l=0$)

$$|\psi\rangle_{G.S} = A\frac{\sin(kr)}{r}Y_0^0(\theta,\phi)\cdot|r,\theta,\phi\rangle\cdot|\text{triplet}\rangle \quad r\leq a$$

$$= D\frac{e^{-\eta r}}{r}Y_0^0(\theta,\phi)|r,\theta,\phi\rangle|\text{triplet}\rangle \quad r>a$$

with possible values of E given by eq (1).

5.e. for $|E|\ll V_0$ we get: $\tan ka = -\frac{k}{\eta}$

$$\Rightarrow \tan\left\{a\sqrt{\frac{2m(V_0-|E|)}{\hbar^2}}\right\} = -\sqrt{\frac{V_0-|E|}{|E|}} = -\sqrt{\frac{V_0}{|E|}-1}$$

but for $|E|\ll V_0$; $\frac{V_0}{|E|}\gg 1$; i.e R.H.S $\to -\infty$.

$$\therefore \tan a\frac{\sqrt{2m(V_0-|E|)}}{\hbar^2} \approx -\infty \text{ i.e } \approx \tan\left(-\frac{\pi}{2}\right)$$

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$$\therefore \quad \frac{a\sqrt{2m(V_0-|E|)}}{\hbar} \approx -\frac{\pi}{2}.$$

$$\Rightarrow \quad 2m(V_0-|E|) \approx \frac{\pi^2\hbar^2}{4a^2} \quad \Rightarrow \quad V_0 - |E| \approx \frac{\pi^2\hbar^2}{8ma^2}.$$

$$\therefore \quad V_0 \approx |E| + \frac{\pi^2\hbar^2}{8ma^2}.$$

or by further using the approximation:

$$V_0 \approx \frac{\pi^2\hbar^2}{8ma^2}. \quad \underline{\underline{\text{Ans}}}$$

Using values (given $a = 1.5$ fm) ($\because m^{(\text{effective})}_{\text{deuteron}} \approx \frac{m_p}{2}$)

$$V_0 \approx \frac{\pi^2\hbar^2}{8\times\left(\frac{m_p}{2}\right)\times a^2} \approx 7.28\times10^{-12} \text{ J} \quad \underline{\underline{\text{Ans}}}$$

Problem: 8 :→

a) Given $V(r) = \alpha\,\delta(r-r_0)$

∴ T.I.S.E. for $E>0$ gives the radial eq:

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} + \left(V + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}\right)u = Eu.$$

Now for S wave ($l=0$) & $r \gtrless r_0$ gives:

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} = Eu$$

$$\Rightarrow \quad u''(r) = -\frac{2mE}{\hbar^2}u = -k^2u.$$

$$\therefore \quad u = A\sin(kr) + B\cos(kr).$$

$$\therefore \quad R = \frac{u}{r} = A\frac{\sin(kr)}{r} + B\frac{\cos(kr)}{r}.$$

For $r<r_0$; $B=0$; o/w the wave fn blows up at origine.

$$\therefore \quad R_{in}(r) = A\frac{\sin(kr)}{r}. \quad \underline{\text{Ans}}$$

For outside region both of sin & cos terms are permitted.

$$\therefore \quad R_{out}(r) = C\frac{\sin(kr)}{r} + D\frac{\cos(kr)}{r}. \quad \underline{\text{Ans}}$$

continuity of R at $r=r_0$ gives:

$$A\frac{\sin(kr_0)}{r_0} = C\frac{\sin(kr_0)}{r_0} + D\frac{\cos(kr_0)}{r_0}.$$

$$\text{or} \quad A\sin(kr_0) = C\sin(kr_0) + D\cos(kr_0) \quad \cdots (1)$$

$$= P\sin(kr_0+\delta) \quad \cdots (2)$$

Now T.I.S.E gives: due to discontinuity of u' at $r = r_0$:

$r_0 + \epsilon$

$$-\frac{\hbar^2}{2m}\int_{r_0-\epsilon}^{r_0+\epsilon}\frac{d^2u}{dr^2}\,dr + \int_{r_0-\epsilon}^{r_0+\epsilon}\alpha\,\delta(r-r_0)\,u(r)\,dr = \int_{r_0-\epsilon}^{r_0+\epsilon}E\,u(r)\,dr$$

at $\epsilon \to 0$ limit this gives:

$$-\frac{\hbar^2}{2m}\Delta u'(r_0) + \alpha u(r_0) = 0$$

$$\therefore \Delta u(r_0) = \frac{2m\alpha}{\hbar^2}u(r_0).$$

Using values we get:

$$pk\cos(kr_0+\delta) - Ak\cos(kr_0) = \frac{2m\alpha}{\hbar^2}A\sin(kr_0).$$

$$\Rightarrow A\left(\frac{2m\alpha}{\hbar^2}\sin kr_0 + k\cos kr_0\right) = pk\cos(kr_0+\delta) \quad \cdots (3)$$

from (2) & (3) we get:

$$\frac{2m\alpha}{\hbar^2} + k\cot(kr_0) = k\cot(kr_0+\delta) \quad \cdots (4)$$

i.e the phase shift be given by:

$$\left.\begin{aligned} \cot(kr_0+\delta) &= \cot(kr_0) + \frac{2m\alpha}{k\hbar^2} \\ \text{i.e } \delta &= -kr_0 + \cot^{-1}\left[\cot(kr_0) + \frac{2m\alpha}{\hbar^2 k}\right] \end{aligned}\right\}\ \text{Ans}$$

As the scattering state is not normalizable; we get when by using values of δ & p the inside radial wave fn is given by:

$$R_{in}(r) \sim A\,\frac{\sin(kr)}{r}$$

the outside wave fn be like:

$$R_{out}(r) \sim A\,\frac{\sin(kr_0)}{\sin(kr_0+\delta)}\cdot \sin(kr+\delta)$$

Ans

[where δ = phase shift (previously evaluated)]

Q.b at long wave length i.e when $k \to 0$; $\lambda \to \infty$

we get $\cot(kr_0) = \dfrac{1}{\tan(kr_0)} \approx \dfrac{1}{kr_0}$.

∴ from eq (4) we get:

$$\cot(kr_0+\delta) = \cot(kr_0) + \frac{2m\alpha}{\hbar^2 k}$$

$$\Rightarrow \frac{\cot(kr_0)\cot\delta - 1}{\cot(kr_0)+\cot\delta} = \cot(kr_0) + \frac{2m\alpha}{\hbar^2 k}$$

$$\Rightarrow \frac{\frac{1}{kr_0}\cot\delta - 1}{\cot\delta + \frac{1}{kr_0}} \simeq \frac{1}{kr_0} + \frac{2m\alpha}{\hbar^2 k}$$

$$\Rightarrow \frac{\cot\delta - kr_0}{kr_0\cot\delta + 1} = \frac{1}{kr_0} + \frac{2m\alpha}{\hbar^2 k}$$

$$\Rightarrow \cancel{\cot\delta} - kr_0 = \cancel{\cot\delta} + \frac{2m\alpha r_0}{\hbar^2}\cot\delta + \frac{1}{kr_0} + \frac{2m\alpha}{\hbar^2 k}$$

$$\Rightarrow \cot\delta = -\left(kr_0 + \frac{1}{kr_0} + \frac{2m\alpha}{\hbar^2 k}\right)\times\frac{\hbar^2}{2m\alpha r_0}$$

~~Now~~ Now $\cot\delta \simeq \frac{1}{\delta}$ here so

$$\frac{1}{\delta} \simeq -\left(kr_0 + \frac{1}{kr_0} + \frac{2m\alpha}{\hbar^2 k}\right) \times \frac{\hbar^2}{2m\alpha r_0}$$

$$\therefore \delta \simeq -\left(kr_0 + \frac{1}{r_0 k} + \frac{2m\alpha}{\hbar^2 k}\right)^{-1} \times \frac{2m\alpha r_0}{\hbar^2} \Bigg\} \underline{\text{Ans}}$$

~~We also get an tangent alternative expansion from~~

However as $O\left(\frac{1}{k}\right) \gg O(k)$ so we get:

$$\frac{1}{\delta} \simeq -\left(\frac{1}{kr_0} + \frac{2m\alpha}{\hbar^2 k}\right) \cdot \frac{\hbar^2}{2m\alpha r_0}.$$

$$= -\left(\frac{1}{r_0 k} + \frac{\hbar^2}{2m\alpha r_0^2 k}\right)$$

$$= -\left(\frac{\hbar^2 + 2m\alpha r_0}{2m\alpha r_0^2 k}\right)$$

$$\text{i.e. } \delta \simeq -\frac{2m\alpha r_0^2 k}{\hbar^2 + 2m\alpha r_0} = -\frac{r_0 k}{1 + \frac{\hbar^2}{2m\alpha r_0}} \Bigg\} \underline{\text{Ans}}$$

The scattering length a is defined by:

$$\lim_{k\to 0} k\cot\delta = -\frac{1}{a}$$

$$\text{i.e. } -\frac{1}{a} = -k \cdot \frac{\left(1 + \frac{\hbar^2}{2m\alpha r_0}\right)}{kr_0} = -\frac{\left(1 + \frac{\hbar^2}{2m\alpha r_0}\right)}{r_0}.$$

$$\therefore a = \text{Scattering length} = \frac{r_0}{1 + \frac{\hbar^2}{2m\alpha r_0}} \Bigg\} \underline{\text{Ans}}$$

8-c For bound state we have $E<0$ (& $\alpha<0$ i.e delta well spherical)

$\therefore$ TISE gives for $r \neq r_0$: (for $l=0$)

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} = Eu \Rightarrow u''(r) = -\frac{2mE}{\hbar^2}u = \eta^2 u$$

$$\left(\eta^2 = -\frac{2mE}{\hbar^2}\right)$$

i.e $u = Ae^{\eta r} + Be^{-\eta r}$.

Now for $r < r_0$ to keep $u(0) = 0$ (o/w $R(0)$ blows up) $B = -A$ & hence

$$u_{in}(r) = A \sinh(\eta r)$$

for $r > r_0$ to keep $\lim_{r \to \infty} u(r) = 0$; $A = 0$

$$\therefore u_{out}(r) = Be^{-\eta r}.$$

Continuity of u gives: $A \sinh \eta r_0 = Be^{-\eta r_0}$ ... (1).

discontinuity of $u'(r)$ at $r = r_0$ gives,

$$-\frac{\hbar^2}{2m}\int_{r_0-\epsilon}^{r_0+\epsilon}\frac{d^2u}{dr^2}dr + \int_{r_0-\epsilon}^{r_0+\epsilon}\alpha\,\delta(r-r_0)\,u(r)\,dr = \int_{r_0-\epsilon}^{r_0+\epsilon}E\,u(r)\,dr$$

at $\epsilon \to 0$ limit we get:

$$-\frac{\hbar^2}{2m}\Delta u'(r_0) + \alpha u(r_0) = 0$$

$$\Rightarrow \Delta u'(r_0) = +\frac{2m\alpha}{\hbar^2}u(r_0) \quad \text{... (2)}$$

$$\Rightarrow -B\eta e^{-\eta r_0} - A\eta\cosh(\eta r_0) = \frac{2m\alpha}{\hbar^2}Be^{-\eta r_0}$$

$$\Rightarrow Be^{-\eta r_0}\left(\eta + \frac{2m\alpha}{\hbar^2}\right) = -A\eta\cosh(\eta r_0) \quad \text{... (3)}$$

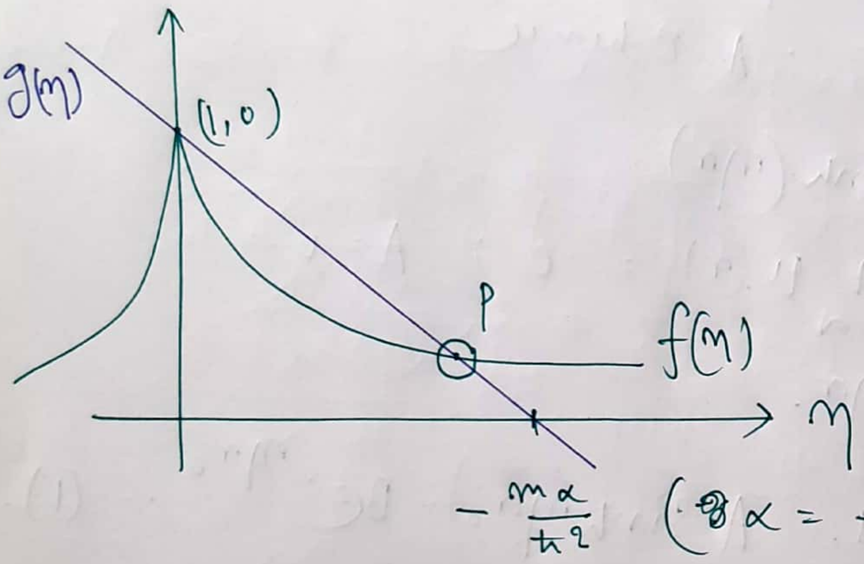
from (1) & (3) we get:

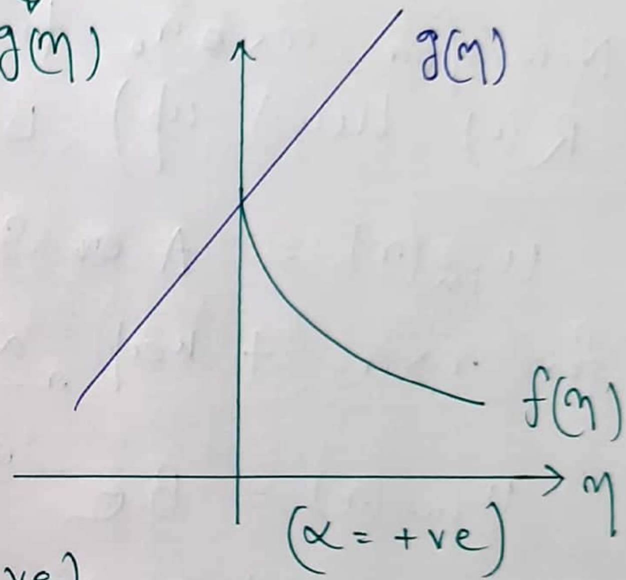
$$-\frac{\eta\cosh(\eta r_0)}{\sinh(\eta r_0)} = \left(\eta + \frac{2m\alpha}{\hbar^2}\right)$$

$$\Rightarrow \frac{e^{\eta r_0} + e^{-\eta r_0}}{e^{\eta r_0} - e^{-\eta r_0}} = -\left(1 + \frac{2m\alpha}{\eta \hbar^2}\right)$$

$$\Rightarrow \frac{e^{\eta r_0}}{e^{-\eta r_0}} = \frac{-1 - \frac{2m\alpha}{\eta\hbar^2} + 1}{-1 - \frac{2m\alpha}{\eta\hbar^2} - 1} = \frac{\frac{\cancel{2}m\alpha}{\eta\hbar^2}}{\cancel{2} + \frac{\cancel{2}m\alpha}{\eta\hbar^2}} = \frac{1}{1 + \frac{\eta\hbar^2}{m\alpha}}$$

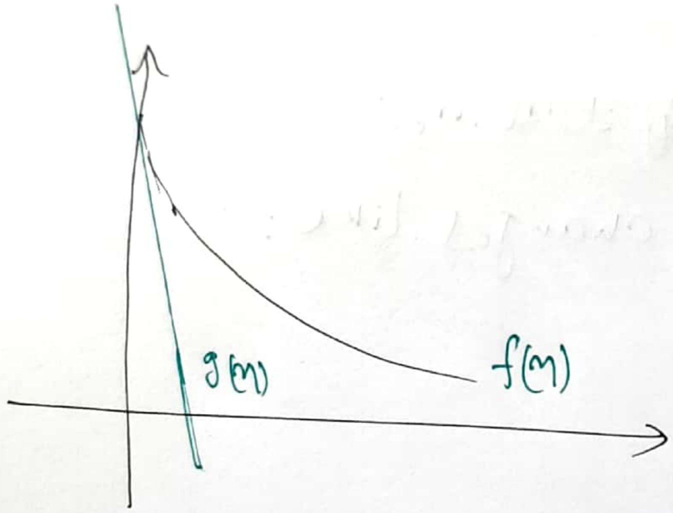
$$\Rightarrow \frac{e^{-\eta r_0}}{e^{\eta r_0}} = \underbrace{e^{-2\eta r_0}}_{f(\eta)} = \underbrace{1 + \frac{\eta\hbar^2}{m\alpha}}_{g(\eta)}$$





Clearly there is at most $\boxed{\text{one solution}}$ i.e one bound state exist iff $\alpha < 0$ i.e we ~~get~~ take ~~det~~ delta well & not barrier. <u>Ans</u>

Now if the slope of $f(\eta)$ at $\eta = 0$ is so small that it doesn't cut ~~f~~ $g(\eta)$ then we don't get a bound state. i.e the situation be like:



So as both slopes are $-ve$ at $\eta = 0$ the condition for getting solution be :

$$|f'(\eta=0)| > |g'(\eta=0)|$$

i.e $2r_0 > \frac{\hbar^2}{m|\alpha|}$

i.e $|\alpha| > \frac{\hbar^2}{2mr_0}$

but as $\alpha < 0$ so we must have $\alpha < -\frac{\hbar^2}{2mr_0}$.

So the condition on α to get bound state be

$$\boxed{\alpha < -\frac{\hbar^2}{2mr_0}}$$ Ans

8.d previously I got Scattering length:

$$a = \frac{r_0}{1 + \frac{\hbar^2}{2m\alpha r_0}}$$

In part c it was shown first bound state occures when $\alpha \lesssim -\frac{\hbar^2}{2mr_0}$ at $E \simeq 0$ (obvious)

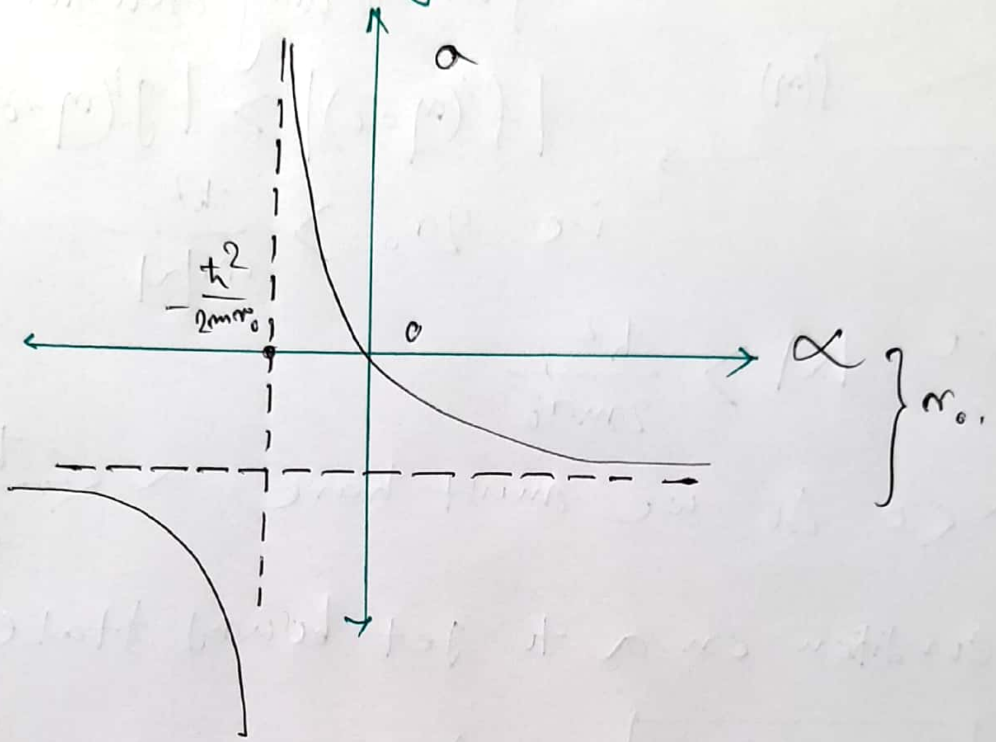
i.e $\frac{\hbar^2}{2m\alpha r_0} \approx -1$

i.e $a \to \infty$

Ans for $\alpha = 0$ we get $a = 0$. $\left(a = \frac{1}{1+\infty} = 0\right)$

And $\alpha = \pm\infty$, $a \longrightarrow r_0$.

So the Scattering angle changes like:



Problem: 4

<u>a</u> The interaction is due to the Hyperfine part of hydrogen - Hamiltonian. i.e the proton's magnetic moment (dipole moment) makes a field $\vec{B} \sim \alpha\{3(\vec{\mu}_p\cdot\hat{r})\hat{r} - \vec{\mu}_p\} + \beta\,\delta^3(\vec{r})$ $(\vec{\mu}_p \sim \hat{S}_p)$

And due to the e^-'s dipole moment $\sim \hat{S}_e$; it sets up the Hamiltonian of the form:

$$H' \sim \frac{\alpha'}{r^3}\left(3(\hat{S}_p\cdot\hat{r})(\hat{S}_e\cdot\hat{r}) - \hat{S}_p\cdot\hat{S}_e\right) + \beta'\,\hat{S}_p\cdot\hat{S}_e\,\delta^3(\vec{r})$$

$\left(\alpha, \beta = \text{constants depend on } g_p, g_e\right)$

for the 1s state (or $L=0$ state), the expectation of 1st term is zero & the 2nd term remains.

Ans

$$\therefore \langle H'_{l=0}\rangle \sim \langle S_p\cdot S_e\rangle \cdot |\psi_{l=0}(0)|^2.$$

<u>b</u>. $$H_1 = \frac{8\pi}{3}\frac{g_p g_e}{4m_p m_e c^2}\,\vec{S}_p\cdot\vec{S}_e\,\delta^3(\vec{r}).$$

$\therefore$ The energy shift $\Delta E = \langle H\rangle = \frac{8\pi}{3}\frac{g_p g_e}{4m_p m_e c^2}\langle \hat{S}_p\cdot\hat{S}_e\rangle |\psi(0)|^2$

Now for the given state (1s) ψ_{100} we know

$$|\psi(0)|^2 = \frac{1}{\pi a_0^3} \qquad \left(\psi_{100} = \frac{e^{-r/a_0}}{\sqrt{\pi a_0^3}}\right)$$

Now in absence of external $\vec{B}$ field $(\vec{S}_p + \vec{S}_e) = \vec{F}$ is conserved.

$$\therefore \vec{F} = (\vec{S}_p + \vec{S}_e) \quad \text{i.e } F^2 = S_p^2 + S_e^2 + 2\vec{S}_p\cdot\vec{S}_e$$

$$\text{i.e } \hat{S}_p\cdot\hat{S}_e = \frac{F^2 - S_p^2 - S_e^2}{2}$$

$$\therefore \langle \hat{S}_p \cdot \hat{S}_e \rangle = \frac{1}{2} \langle -\hat{S}_p^2 - \hat{S}_e^2 + \hat{F}^2 \rangle$$

Now in eigenstate of $\hat{S}_e, \hat{S}_p, \hat{F}$ we get the quantity to be:

$$\langle \hat{S}_p \cdot \hat{S}_e \rangle = \frac{1}{2}\left(F(F+1) - \frac{1}{2}\left(\frac{1}{2}+1\right) \times 2 \right) \hbar^2$$

$$= \frac{\hbar^2}{2}\left(F(F+1) - 3/2 \right)$$

$\therefore$ The energy shift: $\Delta E = \frac{8\pi}{3} \cdot \frac{g_p g_e \hbar^2 \left(F(F+1) - 3/2\right)}{4 m_p m_e c^2 \cdot 2 \times \pi a_0^3}$

$$\therefore \Delta E = \frac{g_p g_e \hbar^2}{3 m_p m_e c^2 a_0^3} \times \begin{cases} 1/2 \rightarrow F=1 \text{ triplet} \\ -3/2 \rightarrow F=0 \text{ singlet} \end{cases}$$

~~Using values it gives~~; So the energy splitting is:

$$\delta(\Delta E) = \Delta E_{F=1} - \Delta E_{F=0} = \underbrace{\frac{2 g_p g_e \hbar^2}{3 m_p m_e c^2 a_0^3}}_{\text{Ans}}$$

4.C In presence of the $\vec{B}_{ext}$ field (assuming $\vec{B}_{ext}$ along z direction); the perturbing Hamiltonian be

$$H'' = -(\mu_e + \mu_p) \cdot B = -\frac{g_p e B}{2m_p} S_{pz} + \frac{g_e e B}{2m_e} S_{ez}.$$

$$= \mu_B B \left(g_e S_{ez} - g_p S_{pz} \right)$$

Clearly the lowest energy state of the system is

$$|\psi_{low}\rangle = |F=0\rangle \cdot |G.S \text{ of } H\rangle \quad \text{(as done previously)}$$

$\therefore$ The first order correction of H'' gives:

$$\langle H'' \rangle = -\frac{g_p e B}{2m_p} \langle \psi_{low} | S_{pz} | \psi_{low} \rangle + \frac{g_e e B}{2m_e} \langle \psi_{low} | S_{ez} | \psi_{low} \rangle$$

Now $\langle F=0 | S_{pz} | F=0 \rangle = \left\langle \frac{\uparrow_p \downarrow_e - \downarrow_p \uparrow_e}{\sqrt{2}} \middle| S_{pz} \middle| \frac{\uparrow_p \downarrow_e - \downarrow_p \uparrow_e}{\sqrt{2}} \right\rangle$

$$= \frac{\hbar}{2}\Big[\langle \uparrow_p \downarrow_e | \tfrac{1}{2} | \uparrow_p \downarrow_e \rangle - \cancel{\langle \uparrow_p \downarrow_e | -\tfrac{1}{2} | \downarrow_p \uparrow_e \rangle}^{\,0}$$

$$- \cancel{\langle \downarrow_p \uparrow_e | \tfrac{1}{2} | \uparrow_p \downarrow_e \rangle}^{\,0} + \langle \downarrow_p \uparrow_e | -\tfrac{1}{2} | \downarrow_p \uparrow_e \rangle \Big]$$

$$= \frac{\hbar}{2}\left[\frac{1}{2} \times 1 - \frac{1}{2} \times 1 \right] = 0$$

$(\because \langle \uparrow_p \downarrow_e | \uparrow_p \downarrow_e \rangle = 1 ; \langle \uparrow_p \downarrow_e | \downarrow_p \uparrow_e \rangle = 0$ etc$)$

Similarly $\langle F=0 | S_{ez} | F=0 \rangle = 0$.

as $|\psi_{low}\rangle = |F=0\rangle |G.S\rangle$ Hence we finally get,

$\langle H'' \rangle = 0$ i.e 1st order correction is zero.

We go for 2nd order:

$$\delta E^{(2)}(B) = \sum_{F=1} \frac{|\langle \psi_{low} | H' | F=1 \rangle | G.S \rangle|^2}{E^0_{F=0} - E^0_{F=1}}$$

$$= \frac{\mu_B^2 B^2}{E^0_{F=0} - E^0_{F=1}} \sum_{F_m=-1}^{1} |\langle G.S | F=0 | g_e S_{ez} - g_p S_{pz} | F=1, F_m | G.S \rangle|^2$$

The H atom G.S does not interact with spin operators & hence we get $\langle G.S | G.S \rangle = 1$

$$\therefore \delta E^{(2)}(B) = \frac{\mu_B B}{E^0_{F=0} - E^0_{F=1}} \sum_{F_m=-1}^{1} |\langle F=0 | g_e S_{ez} - g_p S_{pz} | F=1; F_m \rangle|^2$$

For $F_m = 0$; $F = 1$:

$\langle F=0 | -g_p S_{pz} + g_e S_{ez} | F=1 ; F_m = 0 \rangle$ gives:

$$\left\langle \frac{\uparrow_p \downarrow_e - \downarrow_p \uparrow_e}{\sqrt{2}} \right| g_e S_{ez} - g_p S_{pz} \left| \frac{\uparrow_p \downarrow_e + \downarrow_p \uparrow_e}{\sqrt{2}} \right\rangle$$

$$= \frac{g_e \hbar}{2} \Big[\langle \uparrow_p \downarrow_e | -\tfrac{1}{2} | \uparrow_p \downarrow_e \rangle + \cancel{\langle \uparrow_p \downarrow_e | \tfrac{1}{2} | \downarrow_p \uparrow_e \rangle}^{\,0}$$
$$- \cancel{\langle \downarrow_p \uparrow_e | -\tfrac{1}{2} | \uparrow_p \downarrow_e \rangle}^{\,0} - \langle \downarrow_p \uparrow_e | \tfrac{1}{2} | \downarrow_p \uparrow_e \rangle \Big]$$

$+$ Similar for S_{pz}. with $(+\frac{1}{2})$ terms.

$$= \frac{g_e \hbar}{2} \left[-\frac{1}{2} - \frac{1}{2} \right] - \frac{g_p \hbar}{2} \left[\frac{1}{2} + \frac{1}{2} \right]$$
$$= -\frac{\hbar}{2} (g_e + g_p)$$

$F_m = 1$; $F = 1$:

$\langle F=0 | g_e S_{ez} - g_p S_{pz} | F=1 ; F_m = 1 \rangle$

$$= \left\langle \frac{\uparrow_p \downarrow_e - \downarrow_p \uparrow_e}{\sqrt{2}} \right| g_e S_{ez} - g_p S_{pz} \left| \uparrow_p \uparrow_e \right\rangle$$

$= 0$ (obviously) $\left(\text{as } \langle \uparrow_p \downarrow_e | \uparrow_p \uparrow_e \rangle = 0 = \langle \downarrow_p \uparrow_e | \uparrow_p \uparrow_e \rangle \right)$

Similarly for $F_m = -1$; $F = 1$:

$\langle F=0 | g_e S_{ez} - g_p S_{pz} | F_m = -1 ; F = 1 \rangle = 0$.

So finally we get,

$$\delta E^{(2)}(B) = \frac{\mu_B^2 B^2}{E^0_{F=0} - E^0_{F=1}} \times \frac{\hbar^2}{4}(g_e + g_p)^2.$$

$$= -\frac{\mu_B^2 B^2 \cancel{\hbar^2}}{4} \cdot \frac{3 m_p m_e c^2 a_0^3}{2 g_p g_e \cancel{\hbar^2}} (g_e + g_p)^2.$$

So for the lowest Hyperfine state we got (by 2nd order perturbation):

$$\delta E(B) = -\frac{3\mu_B^2 B^2 m_p m_e c^2 a_0^3}{8 g_p g_e}(g_p + g_e)^2.$$

Ans

4.d And the magnetic polarizibility is given by:

$$\alpha_B = -\frac{\partial^2(\delta E(B))}{\partial B^2}$$

$$= +\frac{3\mu_B^2 m_p m_e c^2 a_0^3}{4(g_p g_e)}(g_p + g_e)^2$$

Ans

power of a_0 in $\alpha_B = 3$; i.e a_0^3.

Ans

Problem – 11

Given: $\vec{E} = E_0 \vec{u}_x \cos(\omega t - kz)$

$$\therefore \vec{\nabla} \times \vec{E} = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ E_0 \cos(\omega t - kz) & 0 & 0 \end{vmatrix} = -\hat{j} \cdot \left\{ 0 - \frac{\partial}{\partial z} E_0 \cos(\omega t - kz) \right\}$$

$$= kE_0 \sin(\omega t - kz)\,\hat{j}$$

But $\vec{\nabla} \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}$; So; $\frac{\partial \vec{B}}{\partial t} = -kE_0 \sin(\omega t - kz)\,\hat{j}$

$\therefore B_x = 0 = B_z$

$$B_y = -kE_0 \int \sin(\omega t - kz)\,dt = \frac{kE_0 \cos(\omega t - kz)}{\omega}$$

And the vector potential is given by:

$$\vec{E} = -\vec{\nabla}\phi - \frac{\partial \vec{A}}{\partial t}.$$

$$\text{i.e. } \vec{A} = -\int \vec{E}\,dt = -\int E_0 \vec{u}_x \cos(\omega t - kz)\,dt$$

$$= -\frac{E_0}{\omega} \vec{u}_x \sin(\omega t - kz)$$

$$\therefore \vec{\nabla} \cdot \vec{A} = -\frac{E_0}{\omega} \vec{\nabla} \cdot \left(\sin(\omega t - kz) \cdot \hat{x} \right)$$

$$= -\frac{E_0}{\omega} \cdot \frac{\partial}{\partial x} \left\{ \sin(\omega t - kz) \right\} = 0$$

(~~Lorentz~~ coloumb Gauge condition)

Now the Hamiltonian in presence of ~~magn~~ field be given by,

$$H = \frac{(\vec{p} + e\vec{A})^2}{2m} + V_0(\vec{r}) - e\phi$$

Here Scalar pot $\phi = 0$; V_0 = unperturbed pot.
($-e$ is charge of e^-)

i.e $H = \frac{1}{2m}\left(p^2 + e^2A^2 + e\vec{p}\cdot\vec{A} + e\vec{A}\cdot\vec{p}\right) + V_0(\vec{r})$

$$= \frac{1}{2m}\left(p^2 + e^2A^2 + 2e\vec{A}\cdot\vec{p}\right) + V_0(\vec{r})$$

$(\because [p, A] = -i\hbar\, \vec{\nabla}\cdot\vec{A} = 0$ in coloumb Gauge$)$

$$= \frac{p^2}{2m} + \frac{e}{m}\vec{A}\cdot\vec{p} + \frac{e^2A^2}{2m} + V_0\vec{r}$$

If we neglect A^2 as a 2nd order perturbing term; then it gives,

$$H' = H - H^{(0)} = \frac{e}{m}\vec{A}\cdot\vec{p}$$

$$= \frac{e}{m}\cdot\frac{E_0}{\omega}\hat{}\overset{(\hat{x}\cdot\vec{p})}{}\sin(kz - \omega t)$$

$$= \frac{eE_0}{m\omega}(\hat{x}\cdot\vec{p})\cdot\frac{e^{i(kz-\omega t)} - e^{-i(kz-\omega t)}}{2i}$$

$$= \frac{eE_0}{m\omega} \times \left\{(\,)\times e^{i\omega t} + (\,)\times e^{-i\omega t}\right\}$$

Here $e^{i\omega t}$ term represents stimulated emission & $e^{-i\omega t}$ for absorption. As there is no chance for emission of the H atom was in ground state we get finally:

$$H'(t) = \frac{eE_0}{m\omega}\times\frac{1}{2i}\cdot(\hat{x}\cdot\vec{p})\, e^{ikz}\cdot e^{-i\omega t}$$

$$= \frac{eE_0}{m\omega}\cdot\frac{1}{2i}\, p_x\, e^{ikz}\cdot e^{-i\omega t}.$$

$$= \frac{eE_0}{m\omega}\cdot\frac{1}{2i}\, e^{ikz}\cdot p_x\, e^{i\omega t} \qquad (\because [p_x, z] = 0)$$

Now using dipole appx we get by taking first power of the expansion of e^{ikz};

$$e^{ikz} = 1 + \underbrace{ikz + \frac{(ikz)^2}{2!} + \cdots}_{\text{neglect.}}$$

$$\therefore \langle \psi_f | e^{ik_z z} \hat{x}\cdot p | \psi_i \rangle \simeq \langle \psi_f | (1+\cdots) p_x | \psi_i \rangle$$

$$= \langle \psi_f | \hat{p}_x | \psi_i \rangle$$

Now, $[\hat{x}, \hat{H}_0] = [\hat{x}, \frac{p^2}{2m} + V(\vec{r}_0)] = [\hat{x}, \frac{p^2}{2m}]$

$$= [\hat{x}, \frac{p_x^2}{2m}] = \frac{i\hbar}{m} \hat{p}_x$$

$$\therefore \langle \psi_f | e^{ikz} \hat{x}\cdot p | \psi_i \rangle = \frac{m}{i\hbar} \langle \psi_f | [\hat{x}, H_0] | \psi_i \rangle$$

but for $f \neq i$; $\langle \psi_f | H_0 | \psi_i \rangle = 0$

($\because \psi_i, \psi_f$ are eigenstates of H_0)

$$\therefore \langle \psi_f | e^{ikz} \hat{x}\cdot p | \psi_i \rangle \simeq \frac{m}{i\hbar} (E_i - E_f) \langle \psi_f | \hat{x} | \psi_i \rangle$$

$\therefore$ The transition amplitude be given by:

$$C_{i\to f}(t) = -\frac{i}{\hbar} \int e^{i\omega_0 t} H'_{fi}(t)\, dt$$

when $H'_{fi} = \frac{E_0 e}{m\omega} \cdot \frac{1}{2i} e^{-i\omega t} \langle \psi_f | e^{ikz} p_x | \psi_i \rangle$

$$= \frac{eE_0}{m\omega} \cdot \frac{1}{2i} \cdot \frac{m}{i\hbar} (E_i - E_f) \langle \psi_f | \hat{x} | \psi_i \rangle$$

$$= \frac{eE_0 \omega_0}{2\omega} \langle \psi_f | \hat{x} | \psi_i \rangle$$

$\left(\omega_0 = \dfrac{E_f - E_i}{\hbar}\right)$

So the dipole selection rule depends on $\langle \psi_f | \hat{x} | \psi_i \rangle$

as $m_i = 1$; $m_f = 2$ (mentioned in question)

& $\hat{x} = r \sin\theta \cos\phi$ so for states $|210\rangle$ &

$|200\rangle$ the ϕ integral gives:

$\int_0^{2\pi} \cos\phi \, d\phi = 0.$; i.e $\left\langle \begin{matrix} 210 \\ 200 \end{matrix} \text{ or} \middle| \hat{x} \middle| 100 \right\rangle = 0.$

$\therefore$ ~~Ut~~ Under dipole approx there is no transition from $|100\rangle \to |210\rangle, |200\rangle$.

$\therefore$ for $\psi_f = |211\rangle$; $\langle \psi_f | \hat{x} | \psi_i \rangle = \langle 211 | \hat{x} | 100 \rangle$

$$= \int_0^\infty r \cdot R_{21}(r) \cdot R_{10}(r) \cdot r^2 dr \int_0^\pi -\frac{1}{\sqrt{4\pi}} \cdot \sqrt{\frac{3}{4\pi}} \sin^3\theta \, d\theta$$
$$\int_0^{2\pi} \cos\phi \cdot (\cos\phi - i\sin\phi) \, d\phi.$$

Using Mathematica (The result was already calculated ~~for~~ for problem 12)

$$= -\frac{128 a_0}{243} = -\frac{2^7 a_0}{3^5}.$$

Similarly for $|\psi_f\rangle = |21-1\rangle$; $\langle \psi_f | \hat{x} | \psi_i \rangle = \langle 21-1 | \hat{x} | 100 \rangle$

$$= \frac{2^7 a_0}{3^5}.$$ (again previously evaluated)

So the transition amplitude for $|100\rangle \to |211\rangle$

$$C_{|211\rangle} = -\frac{i}{\hbar} \frac{e E_0 \omega_0}{2\omega} \int_0^t \left(-\frac{2^7 a_0}{3^5}\right) \cdot e^{i\omega_0 t'} dt'$$

$$= \frac{i}{\hbar} \frac{eE_0 \cancel{\omega_0}}{\omega} \left(\frac{2^6 a_0}{3^5}\right) \frac{\left(e^{i\omega_0 t} - 1\right)}{i\cancel{\omega_0}}$$

$$= \frac{i}{\hbar} \frac{eE_0}{\omega} \frac{2^7 a_0}{3^5} \cdot e^{\frac{i\omega_0 t}{2}} \left(\frac{e^{\frac{i\omega_0 t}{2}} - e^{-\frac{i\omega_0 t}{2}}}{2i}\right)$$

$$= \frac{i}{\hbar} \frac{eE_0}{\omega} \frac{2^7 a_0}{3^5} \cdot e^{\frac{i\omega_0 t}{2}} \sin\left(\frac{\omega_0 t}{2}\right)$$

The transcition amp for $|100\rangle \to |21-1\rangle$ could just differ by a '-ve' sign due to $\langle 21-1|x|100\rangle$ & is,

$$C_{|21-1\rangle} = -\frac{i}{\hbar} \frac{eE_0}{\omega} \frac{2^7 a_0}{3^5} \cdot e^{\frac{i\omega_0 t}{2}} \sin\left(\frac{\omega_0 t}{2}\right).$$

As the transcition prob $P = |c|^2$ So;

$$P_{|100\rangle \to |21\pm1\rangle} = \left(\frac{eE_0 a_0}{\hbar\omega}\right)^2 \cdot \frac{2^{14}}{3^{10}} \sin^2\left(\frac{\omega_0 t}{2}\right)$$

Ans

The over all probability for any of the n=2 transcition

$$P_{|100\rangle \to n=2} = P_{|21+1\rangle} + P_{|21-1\rangle}$$

$$= \frac{2^{15}}{3^{10}} \cdot \frac{e^2 E_0^2 a_0^2}{\hbar^2\omega^2} \sin^2\left(\frac{\omega_0 t}{2}\right)$$

Ans

(When $\omega_0 = \frac{E_2 - E_1}{\hbar}$ & for H atom: $E_2 = 3.4$ ev
$E_1 = 13.6$ ev)

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Problem: 7

Charged particle in e-m field:-

The classical Hamiltonian of a charged particle in E-M field be given by:

$$H = \frac{(\vec{p} - e\vec{A})^2}{2m} + q\phi$$

when $\vec{A}$ & ϕ are related by the gauge transformations:

$$\left.\begin{aligned} \vec{A} &\longrightarrow \vec{A} + \vec{\nabla}\chi(\vec{r},t) \\ \phi &\longrightarrow \phi - \frac{\partial\chi(\vec{r},t)}{\partial t} \end{aligned}\right\}$$

Now our physical quantities ~~remain~~ remaining unchanged under gauge transformation.

As $\vec{p}$ is canonical momentum & $\vec{p} = m\dot{\vec{r}} - e\vec{A}$.

So $\vec{p} \longrightarrow \vec{p} + e\vec{\nabla}\chi$

but $(\vec{p} - e\vec{A}) = m\dot{\vec{r}}$ ~~change~~ do not change under gauge transformation

$\therefore$ $H = \frac{(\vec{p} - e\vec{A})^2}{2m} + q\phi$ only change under gauge transformation iff $\phi \neq 0$.

And the change is like $H \longrightarrow H - q\frac{\partial\chi(\dot{\vec{r}},t)}{\partial t}$

Clearly H is not a physical quantity if $\phi \neq 0$.

But $\phi = 0$ means we are in a constant magnetic field and there is no electric field. (i.e when $\vec{A} \neq 0$)

~~[illegible]~~ Only then; the quantity H is related to something physical.

Now in Q.M if we use TISE

$H\psi = E\psi$

then H must be a physical quantity & when we try to measure H we get the physical value to be E.

So if H is not ~~const~~ unchanged under gauge transformations we cant use TISE.

** This can be shown in another way.

$$H = \frac{(\vec{p} - e\vec{A})^2}{2m} + q\phi$$

And $\phi \longrightarrow \phi - \underbrace{\frac{\partial \chi(\vec{r},t)}{\partial t}}$

due to this term

H is explicitly dependent on t.

And we cant use TISE.

▨ For constant magnetic field under gauge transformation $H \rightarrow H$ & we can use TISE and get a particular value of energy.

▨ $\vec{p} = -i\hbar\vec{\nabla}$ is canonical momentum operator in QM.

$$H = \frac{(-i\hbar\vec{\nabla} - e\vec{A})^2}{2m} = \left\{\frac{(\hat{p} - e\vec{A})^2}{2m}\right\}$$

Velocity operator of the particle is:

$$\dot{\vec{x}} = \frac{\vec{P}_{mec}}{m} = \frac{\hat{p} - e\vec{A}}{m} = \hat{v} \quad (\hat{p} = P_{canonical})$$ Ans

b) Now proceed to solve the problem of a charged particle in const magnetic field

Let $\vec{B} = B_0 \hat{z}$

$\therefore \vec{\nabla} \times \vec{A} = \vec{B}$ gives: $\begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ A_x & A_y & A_z \end{vmatrix} = B_0 \hat{z}$

$$\Rightarrow \left.\begin{aligned} \frac{\partial A_z}{\partial y} - \frac{\partial A_y}{\partial z} &= 0 \\ \frac{\partial A_z}{\partial x} - \frac{\partial A_x}{\partial z} &= 0 \\ -\frac{\partial A_x}{\partial y} + \frac{\partial A_y}{\partial x} &= B_0 \end{aligned}\right\}$$

But from symmetry A should not depend on z coordinate.

$\Rightarrow \frac{\partial}{\partial z}(A_x, A_y) = 0$

Moreover from $\frac{\partial A_z}{\partial y} = 0$ we get $A_z = A_z(x)$

& $\frac{\partial A_z}{\partial x} = 0$ " " $A_z = A_z(y)$

Both of this can be satisfied iff $A_z =$ const.

we can take $A_z = 0$.

$$\therefore -\frac{\partial A_x}{\partial y} + \frac{\partial A_y}{\partial x} = B_0 \quad \cdots (1)$$

For coulomb gauge $\vec{\nabla} \cdot \vec{A} = 0 \Rightarrow \frac{\partial A_x}{\partial x} + \frac{\partial A_y}{\partial y} + \cancelto{0}{\frac{\partial A_z}{\partial z}} = 0$

So one choice is:

$A_x = A_x(y)$; $A_y = A_y(x)$

such that (1) is valid.

This can be made by taking $A_x = -B_0 y$; $A_y = 0$

or, $A_x = 0$; $A_y = +B_0 x$

or $A_x = -\frac{B_0 y}{2}$; $A_y = +\frac{B_0 x}{2}$

.... etc.

Let's start with $A_x = -B_0 y$; $A_y = 0$.

$\therefore \vec{A} = (-B_0 y, 0, 0)$; And $\vec{\nabla} \cdot \vec{A} = 0$ (also)

Now, $H = \frac{(\vec{p} - e\vec{A})^2}{2m}$

$$= \frac{1}{2m}\left\{(\vec{p} - e\vec{A})\cdot(\vec{p} - e\vec{A})\right\}$$

$$= \frac{1}{2m}\left\{p^2 + e^2A^2 - e\vec{p}\cdot\vec{A} - e\vec{A}\cdot\vec{p}\right\}$$

Here we get $[p_x, A_x] = -i\hbar\frac{\partial A_x}{\partial x}$

$$\therefore [\vec{p}, \vec{A}] = \vec{p}\cdot\vec{A} - \vec{A}\cdot\vec{p}$$

$$= \sum_i [p_i, A_i] = -i\hbar\,\vec{\nabla}\cdot\vec{A}$$

For the current choice of gauge: $\vec{\nabla}\cdot\vec{A} = 0$

So: $H = \frac{1}{2m}\left\{p^2 + e^2A^2 - 2e\vec{p}\cdot\vec{A}\right\}$

The velocity of the particle be given by:

$$m\dot{\vec{x}} = \vec{p} - e\vec{A} = \vec{\pi}$$

$$\therefore [\pi_i, \pi_j] = [p_i - eA_i, p_j - eA_j]$$

$$= \underbrace{\cancel{[p_i, p_j]}}_{0} - e[A_i, p_j] - e[p_i, A_j] + e^2\underbrace{\cancel{[A_i, A_j]}}_{0}$$

$$= -i\hbar e\frac{\partial A_i}{\partial x_j} + i\hbar e\frac{\partial A_j}{\partial x_i}$$

$$= -i\hbar e\left(\frac{\partial A_i}{\partial x_j} - \frac{\partial A_j}{\partial x_i}\right)$$

$$= +i\hbar e\,\epsilon_{ijk}B_k$$

i.e $\cancel{m^2[\hat{x}_i, A}$ $m^2[\hat{v}_i, \hat{v}_j] = i\hbar e \epsilon_{ijk} B_k$

$$\therefore \left.[\hat{v}_i, \hat{v}_j] = \frac{i\hbar e \epsilon_{ijk} B_k}{m^2}\right\}$$ Ans

And, $[\hat{\pi}_i, \hat{x}_j] = m[\hat{v}_i, \hat{x}_j] = [\hat{p}_i - e\vec{A}_i, x_j]$

$$= [\hat{p}_i, \hat{x}_j] - e\underbrace{[\vec{A}_i(\vec{x}), \hat{x}_j]}_{0}$$

$$= -i\hbar \cdot \delta_{ij}$$

$$\therefore \left.[\hat{v}_i, \hat{x}_j] = -\frac{i\hbar \delta_{ij}}{m}\right\}$$ Ans

- As canonical and mechanical momenta are different in presence of magnetic field; (by the relation $p_m \longrightarrow p_c - eA$) hence the $[\hat{v}_i, \hat{x}_j]$ relation (or $\frac{1}{m}[\hat{p}_{m_i}, x_j]$) remaining unchanged.

But $[\hat{v}_i, \hat{v}_j]$ changes & it is only non zero when the 3rd component (k-th) of $\vec{B}$ field is nonzero. So for $\vec{B} = 0$; the relation matches with usual result. $[\hat{p}_{m_i}, \hat{p}_{m_j}] = 0 = [\hat{p}_{c_i}, \hat{p}_{c_j}]$

Here for $\vec{B} \neq 0$; $[\hat{p}_{c_i}, \hat{p}_{c_j}] = 0$ but $p_m \neq p_c$ & hence $[\hat{p}_{m_i}, \hat{p}_{m_j}] \neq 0$ or $[\hat{v}_i, \hat{v}_j] \neq 0$

Moreover the commutation is indep of Gauge choice. (As $\vec{B} = (\vec{\nabla} \times \vec{A})$; is a physical unchanged quantity)

Ans

7.c) i) Let $a = \frac{\pi_x + i\pi_y}{\sqrt{2\hbar e B_0}} \Rightarrow a^\dagger = \frac{\pi_x - i\pi_y}{\sqrt{2\hbar e B_0}}$

Now, $[a^\dagger, a] = \frac{1}{2\hbar e B_0}\left[(\pi_x - i\pi_y)(\pi_x + i\pi_y) - (\pi_x + i\pi_y)(\pi_x - i\pi_y)\right]$

$$= \frac{1}{2\hbar eB}\left\{ \cancel{\pi_x^2} + i\pi_x\pi_y - i\pi_y\pi_x + \cancel{\pi_y^2} - \cancel{\pi_x^2} + i\pi_x\pi_y - i\pi_y\pi_x - \cancel{\pi_y^2} \right\}$$

$$= \frac{2i[\pi_x, \pi_y]}{2\hbar eB_0} = \frac{2i \times (+i\hbar eB_0)}{2\hbar eB_0} = -1.$$

$$\therefore [a^+, a] = -1. \quad \text{or,} \quad [a, a^+] = 1.$$

$$H = \frac{(p_x - eA_x)^2}{2m} + \frac{(p_y - eA_y)^2}{2m} + \frac{p_z^2}{2m} \quad (\because A_z = 0)$$

$$= \frac{\pi_x^2 + \pi_y^2}{2m} + \frac{p_z^2}{2m}$$

$$a^+a = \frac{1}{2\hbar eB_0}\left(\pi_x^2 + \pi_y^2 - i\{[\pi_x, \pi_y]\}\right)$$

$$= \frac{\pi_x^2 + \pi_y^2}{2\hbar eB_0} - \frac{1}{2}$$

But $\pi_x^2 + \pi_y^2 = 2mH - p_z^2$

So, $$a^+a = \frac{2mH - p_z^2}{2\hbar eB_0} - \frac{1}{2}$$

$$\Rightarrow 2mH - p_z^2 = \left(a^+a + \frac{1}{2}\right)$$

i.e $$H = \frac{\left(a^+a + \frac{1}{2}\right)2\hbar eB}{2m} + \frac{p_z^2}{2m}$$

$$= \frac{\hbar eB}{m}\left(a^+a + \frac{1}{2}\right) + \frac{p_z^2}{2m}$$

as $[a^+, a] = -1$ so a & a^+ are equivalent to a_+ and a_- in Harmonic oscillator solution.

i.e $H = \frac{\hbar e B_0}{m}\left(a_{\mp} a_{\pm} \mp \frac{1}{2}\right) + \frac{p_z^2}{2m}$

$$= \hbar\omega_D \left(a_{\mp} a_{\pm} \mp \frac{1}{2}\right) + \frac{p_z^2}{2m}$$

$$= H_1 + H_2$$

When H_1 is the Hamiltonian of a Harmonic oscillator & H_2 is of a free particle along z direction.

As here $[H_1, H_2] = 0$ (clearly) so clearly the eigenvalue of the hamiltonian would be = eig val of H_1 + eig val of H_2

$$= \left(n + \frac{1}{2}\right)\hbar\omega_D + \frac{\hbar^2 k_z^2}{2m}$$

$$\boxed{\begin{array}{l} \text{Let } H|\psi\rangle = E|\psi\rangle \\ \Rightarrow (H_1 + H_2)|\psi\rangle = H_1|\psi\rangle + H_2|\psi\rangle = E_1|\psi\rangle + E_2|\psi\rangle \\ \qquad\qquad = (E_1 + E_2)|\psi\rangle \\ \Rightarrow E = E_1 + E_2 \\ \text{when } [H_1, H_2] = 0 \text{; i.e } |\psi\rangle \text{ is simultaneous eigenfn of } H_1 \,\&\, H_2 \end{array}}$$

(iii) This part was by operator approach. Here is the soln of T.I.S.E as asked in question.

VIII Eigenstates:-

The Schrodinger eq be given by

$$\underbrace{\left\{\frac{(p_x + eB_0 y)^2}{2m} + \frac{p_y^2}{2m} + \frac{p_z^2}{2m}\right\}}_{H} \psi = E\psi$$

Here $[p_x, H] = 0$; $[p_z, H] = 0$

as there is no x or z dependence.

$\therefore$ The eigenfn will be simultaneous eigenfn of p_x & p_z.

if $\psi(x,y,z) = \phi_1(x)\phi_2(y)\phi_3(z)$ (Separating vars)

then $p_x\psi = -i\hbar\,\phi_2(y)\phi_3(z)\dfrac{\partial\phi_1(x)}{\partial x}$

$= \alpha\psi = \alpha\phi_1(x)\phi_2(y)\phi_3(z)$

$$\therefore \frac{\partial\phi_1(x)}{\partial x} = \frac{i\alpha}{\hbar}\phi_1(x)$$

$$\Rightarrow \frac{d\phi_1}{\phi_1} = \frac{\alpha i\,dx}{\hbar} \Rightarrow \phi_1(x) = e^{\frac{i\alpha x}{\hbar}}$$

$$= e^{ik_x \cdot x}$$

Similarly $\phi_3(z) = e^{ik_z \cdot z}$

$\therefore$ TISE gives:

$$\left\{\frac{(\hbar k_x + eB_0 y)^2}{2m} + \frac{p_y^2}{2m} + \frac{\hbar^2 k_z^2}{2m}\right\}\psi = E\psi.$$

$$\Rightarrow -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial y^2} + \frac{e^2B_0^2}{2m}\left(y + \frac{\hbar k_x}{eB}\right)^2\psi = \underbrace{\left(E - \frac{\hbar^2 k_z^2}{2m}\right)}_{= E'}\psi.$$

Let; $\eta = y + \dfrac{\hbar k_x}{eB_0} \Rightarrow \dfrac{\partial^2\psi}{\partial y^2} = \dfrac{\partial^2\psi}{\partial\eta^2}$;

$$\Rightarrow -\frac{\hbar^2}{2m}\frac{\partial^2\phi_2}{\partial\eta^2} + \frac{e^2B^2}{2m}\eta^2\phi_2 = E'\phi_2$$

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This is TISE of the form:

$$-\frac{\hbar^2}{2m}\frac{d^2\varphi}{dx^2} + \frac{1}{2}m\omega^2 x^2 \varphi = E\varphi.$$

with $\frac{1}{2}m\omega^2 = \frac{e^2B_0^2}{2m}$, $\omega = \frac{eB_0}{m}$.

i.e Harmonic oscillator potential.

So: $\phi_2(\eta) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n \cdot n!}} H_n(\xi) \cdot e^{-\xi^2/2}$.

where $\xi = \sqrt{\frac{m\omega}{\hbar}}\,\eta = \sqrt{\frac{m\omega}{\hbar}}\left(y + \frac{\hbar k_x}{eB_0}\right)$

with energy eigenvalue $= \left(n+\frac{1}{2}\right)\hbar\omega$.

$\therefore$ $E - \frac{\hbar^2 k_z^2}{2m} = \left(n+\frac{1}{2}\right)\hbar\omega$.

$\Rightarrow$ $E = \frac{\hbar^2 k_z^2}{2m} + \left(n+\frac{1}{2}\right)\hbar\omega$.

Due to infinite possible values of k_x; these ~~these~~ energy levels are infinitely degenerate.
These are the so called Landau Levels.

7.c.ii) For the ground state of y, the wave f^n is:

$$\left|\psi_{n_y=0}(x,y,z)\right\rangle = e^{ik_x \cdot x}\, e^{ik_z \cdot z} \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\xi^2/2}$$

$$= e^{ik_x x}\, e^{ik_z \cdot z}\, |n_y = 0\rangle \cdot |x\rangle |z\rangle$$

$$\left(\omega = \frac{eB_0}{m};\ \xi = \sqrt{\frac{m\omega}{\hbar}}\left(y + \frac{\hbar k_x}{eB_0}\right)\right)$$

the energy is $E = \dfrac{\hbar^2 k_z^2}{2m} + \dfrac{\hbar\omega}{2}$ $(n_y = 0)$

So for the lowest energy level we need $k_z = 0$.

the wave f^n is:

$$\left.\psi_{G.S}(x,y,z) = e^{ik_x \cdot x} \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\xi^2/2}.\right\}\ \underline{\text{Ans}}$$

i.e. $\left|\psi_{G.S}(x,y,z)\right\rangle = e^{ik_x \cdot x} \left(\dfrac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\xi^2/2}\, |x\rangle |y\rangle |z\rangle$

7.c.iii) If we pick ~~bea~~ a recangle of size $L_x \times L_y$ then no of states that can fit inside comes from the B.C: ~~$\psi(x, y+L_y$~~

$$\psi(x+L_x, y, z) = \psi(x,y,z) \quad \text{i.e. } e^{ik_x L_x} = 1$$

$\therefore k_x$ is quantized in units of $\dfrac{2\pi}{L_x}$.

due to the term exp$\left\{\left(\sqrt{\frac{m\omega}{\hbar}}\right)^2 \left(y + \frac{\hbar k_x}{eB_0}\right)^2\right\}$ in ψ we get; the wave f^n is ~~down~~ exponentially falling outside $y^2 = \dfrac{\hbar^2 k_x^2}{(eB_0)^2} \Rightarrow |y| > l^2 k_x$ $\left(l = \sqrt{\dfrac{\hbar}{eB_0}}\right)$

i.e we expect that allowed k_x values goes between $0 \le k_x \le L_y/l^2$

i.e The degeneracy is given by:

$$\mathcal{D}_N = \frac{L_x}{2\pi}\int_0^{L_y/l^2} dk = \frac{L_x L_y}{2\pi l^2} = \frac{eB L_x L_y}{2\pi\hbar} = \frac{eBA}{2\pi\hbar}$$ Ans

<u>7.d</u> $L_z = (\vec{r}\times\vec{p})_z = xp_y - yp_x$

$$V_z = \frac{p_z - eA_z}{m}$$

$$\therefore [L_z, V_z] = \frac{1}{m}[xp_y - yp_x,\ p_z - eA_z]$$

$$= \frac{1}{m}\left\{ \cancel{[xp_y, p_z]}^{\,0} - e[xp_y, A_z] - \cancel{[yp_x, p_z]}^{\,0} + e[yp_x, A_z] \right\}$$

$$= \frac{e}{m}\left\{ y[p_x, A_z] - x[p_y, A_z] \right\} \quad (\because [x_i, A] = 0)$$

$$= \frac{e}{m}\left\{ i\hbar x\frac{\partial A_z}{\partial y} - i\hbar y\frac{\partial A_z}{\partial x} \right\}$$

$$= \frac{e}{m}\left\{ yp_x A_z - xp_y A_z \right\}$$

$$= \frac{e}{m} L_z A_z$$

Ans

Here for the Given case for all Gauge $A_z = 0$

So for this problem $[L_z, V_z] = 0$.

(iii) explain:- The commutation depends on the choice of Gauge for a general case. Now Gauge is not a physical quantity. Hence the particular commutation is not physical ~~fo~~ operator.

In Q.M; we just borrow names from C.M. Now here Angular momenta operator $\vec{L}$ is just a canonical quantity of the angular ~~of~~ coordinate ϕ. Like the canonical momenta $\left(p_i = -i\hbar \frac{\partial}{\partial x_i}\right)$ it has no mechanical sense. The canonical momenta also doesn't have any physical sence unless $p_{canonical} = p_{mechanical}$.

Here similarly $\vec{L} = \vec{r} \times \vec{p}_{canonical}$ does not have a mechanical (physical). Hence like the classical quantity: $\vec{L}_{cl} = m\vec{r} \times \left(\frac{d\vec{v}}{dt}\right)$ (as $\vec{v}$ is physical)

hence the commutator operator depends on Gauge.

Here for $\vec{B} = B\hat{z}$; $p_z^{(canonical)} = -i\hbar \frac{\partial}{\partial z} = p_z^{(mechanical)}$

as $p_i^{(cano)} = p_i^{(mecha)} + qA_i$ & for z component $A_i = A_z = 0$ here.

Hence the canonical ~~mo~~ z component of momenta as well as the operator L_z both are indp of Gauge.

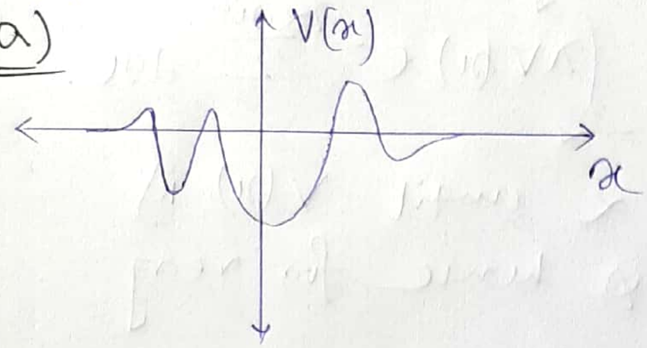
Hence here for all Gauge choice,

$$[L_z, V_z] = [L_z^{(mecha)}, V_z] = \text{physical quantity} = 0$$

Ans

Problem: 3

a)



The potential is mostly attractive i.e

$$\int_{-\infty}^{\infty} V(x)\, dx < 0.$$

And we have another constrain: $\left. \begin{array}{l} V(x) \simeq 0 \\ x \to \pm\infty. \end{array} \right\}$

Now let the trial wave fn be $\psi(x) = A e^{-\frac{\alpha x^2}{2}}$

Normalization gives $\int_{-\infty}^{\infty} A^2 e^{-\alpha x^2} dx = 1 \quad (\alpha > 0)$

i.e $A^2 \cdot \sqrt{\frac{\pi}{\alpha}} = 1 \Rightarrow A = \left(\frac{\alpha}{\pi}\right)^{1/4}.$

$\therefore \psi_\alpha(x) = \left(\frac{\alpha}{\pi}\right)^{1/4} \cdot e^{-\frac{\alpha x^2}{2}}. \quad \left(\alpha = \text{variational parameter}\right)$

For existance of bound state, we must get

$\langle H \rangle_\alpha = \langle T + \lambda V \rangle_\alpha < 0 \quad \left(\langle \cdot \rangle_\alpha \equiv \text{expectation at state } \psi_\alpha \right)$

then by variational principle we say $E_{gs} < \langle H \rangle_\alpha$

Now, $\langle T \rangle = -\frac{\hbar^2}{2m} \sqrt{\frac{\alpha}{\pi}} \int_{-\infty}^{\infty} e^{-\frac{\alpha x^2}{2}} \cdot \frac{d^2}{dx^2}\left(e^{-\frac{\alpha x^2}{2}}\right) dx$

Using mathematica.

$$= \frac{\hbar^2 \alpha}{4m}.$$

Let $\langle H \rangle_\alpha = f(\alpha)$ (a fn of α)

$\therefore \langle H \rangle_\alpha = f(\alpha) = \dfrac{\hbar^2\alpha}{4m} + \sqrt{\dfrac{\alpha}{\pi}} \displaystyle\int_{-\infty}^{\infty} \lambda V(x) \cdot e^{-\frac{2\alpha x^2}{2}} dx$

$\Rightarrow \dfrac{f(\alpha)}{\sqrt{\alpha}} = \dfrac{\hbar^2\sqrt{\alpha}}{4m} + \dfrac{1}{\sqrt{\pi}} \displaystyle\int_{-\infty}^{\infty} \lambda V(x) e^{-\frac{2\alpha x^2}{2}} dx.$

This is a continuous fn of α until $V(x)$ is well behaved. Now $\alpha > 0$ & hence for very small α $(\alpha \to 0_+)$

$$\lim_{\alpha \to 0+} f(\alpha) = \lim_{\alpha \to 0+} \left\{ \frac{\hbar^2\sqrt{\alpha}}{4m} + \frac{\lambda}{\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-\frac{2\alpha x^2}{2}} V(x) dx \right\}$$

$$= 0 + \frac{\lambda}{\sqrt{\pi}} \int_{-\infty}^{\infty} V(x) dx < 0 \quad \left(\text{if } \lambda > 0\right)$$

$$\left(\because \int_{-\infty}^{\infty} V(x) dx < 0 \right)$$

$\therefore$ There exists some small α for which $\dfrac{f(\alpha)}{\sqrt{\alpha}}$ is just below (tightest bound) 0. i.e

$\dfrac{f(\alpha)}{\sqrt{\alpha}} < 0$ i.e $\dfrac{\langle H \rangle_\alpha}{\sqrt{\alpha}} < 0$ i.e $\langle H \rangle_\alpha < 0$.

This ensures that a bound state exists if $\lambda > 0$ and $\int V(x) dx < 0$.

proved

3.c By scaling argument we can ~~by~~ say if or if not there will be a bound state in higher spacial dimensions.

Suppose in D dimensions: a negative potential with range r_0 has a bound state described by a wave fn that extends over a range R_0. In the limit $R_0 \gg r_0$

The K.E scales as $\frac{\hbar^2}{mR_0^2}$ and can be made arbitrarily small.

This would suggest; there indeed any slightly negative potential would give a total energy $(E+V)$ negative and form a bound state. However as the wave fn extends far beyond the range of the potential, the P.E V scales as $\left(\frac{r_0}{R_0}\right)^D$. For $D<2$ & R_0 sufficiently large the '-ve' potential energy $(\sim R_0^{-D})$ can always beat the '+ve' K.E ~~but~~ $(\sim R_0^{-2})$; but for $D>2$, that's not the case.

So for the given 3d case there is not surely a bound state. It may exist or may not. There is no surity. Ans

3.b $\langle H\rangle_\alpha = f(\alpha) = \frac{\hbar^2\alpha}{2m} + \lambda\sqrt{\frac{\alpha}{\pi}}\int_{-\infty}^{\infty} e^{-\alpha x^2}V(x)\,dx$

For $\lambda \ll 1$; we must have $\alpha \ll 1$; o/w the 1st term will dominate for effectively zero potential.

$$\therefore \frac{\partial f}{\partial \alpha} = 0 = \frac{\hbar^2}{2m} + \frac{\lambda}{2\sqrt{\alpha\pi}}\int_{-\infty}^{\infty} e^{-\alpha x^2}V(x)\,dx - \lambda\sqrt{\frac{\alpha}{\pi}}\int_{-\infty}^{\infty} x^2 e^{-\alpha x^2}V(x)\,dx$$

for $\alpha \ll 1$ we neglect last term w.r.t 2nd & 1st terms & get:

$$\frac{\hbar^2}{4m} = \frac{\lambda}{2\sqrt{\alpha\pi}} \int_{-\infty}^{\infty} e^{-\alpha x^2} V(x)\, dx$$

but approximating $\int_{-\infty}^{\infty} \cancel{\alpha x}\, e^{-\alpha x^2} V(x)\, dx \approx \int_{-\infty}^{\infty} V(x)\, dx$

for $(\alpha \approx 0)$ we get:

$$\frac{\hbar^2}{4m} \approx \frac{\lambda}{2\sqrt{\alpha\pi}} \left(\int_{-\infty}^{\infty} V(x)\, dx \right)$$

$$\therefore \sqrt{\alpha} \approx \frac{2m\lambda}{\hbar^2\sqrt{\pi}} \left(\int_{-\infty}^{\infty} V(x)\, dx \right)$$

$$\therefore \alpha \Big|_{\frac{\partial f}{\partial \alpha} = 0} = \tilde{\alpha} = \frac{4m^2\lambda^2}{\hbar^4 \pi} \left(\int_{-\infty}^{\infty} V(x)\, dx \right)^2.$$

$$\therefore \langle H \rangle_{\tilde{\alpha}} = f(\tilde{\alpha}) = \frac{\cancel{\hbar^2}}{\cancel{4m}} \frac{\cancel{4}m^{\cancel{2}}\lambda^2}{\pi \cancel{\hbar^4}\,\hbar^2} I^2 - \frac{\lambda}{\sqrt{\pi}} \times \frac{2m\lambda I}{\hbar^2 \sqrt{\pi}} \times I$$

$$\left(I = \int_{-\infty}^{\infty} V(x)\, dx \right)$$

$$\therefore f(\tilde{\alpha}) = \frac{m\lambda^2 I^2}{\pi \hbar^2} - \frac{2m\lambda^2 I^2}{\pi \hbar^2} = -\frac{m\lambda^2 I^2}{\pi \hbar^2} < 0.$$

So $E_{gs} \leq -\dfrac{m\lambda^2 I^2}{\pi \hbar^2}$

i.e. $E_{g.s} \leq -\dfrac{m\lambda^2}{\pi \hbar^2} \left(\displaystyle\int_{-\infty}^{\infty} V(x)\, dx \right)^2.$

Ans

Problem: 1

a) i) Given $\pi^- + d \longrightarrow n + n$

Now π^- has spin 0 & deuteron has spin 1.

initial $L = 0$.

$\therefore$ $S = 1$; $L = 0$ i.e $J = 1$.

$\therefore$ final state also have $J = 1$. There are two possibility

I) $S = 0$ i.e antisymmetric spin configuration.

So we must have $L = 1$.

but $L = 1$ is again antisymmetric configuration. So it makes total wave fn symmetric.

So this is not possible as neutron is a fermion.

II) $S = 1$; i.e to make $J = 1$ we need $L = 0, 1, 2$.

Here spin is symmetric & hence we need spacial symmetry i.e $L = 1$.

So the final state is $J = 1$; $L = 1$; $S = 1$.

Ans

a. ii) $d = n + p$

$\therefore$ d has parity $+1$.

final state $L = 1 \longrightarrow -1$ (under parity transform $L \rightarrow (-1)^l \cdot L$)

$n, n \longrightarrow +1$.

$$\therefore \eta_{\pi^-} = \eta_n \times \eta_n \times \eta_{L=1} = (-1)^L; \text{ but } L = 1$$

$$\text{so } \eta_{\pi^-} = -1.$$

Ans

1.1.6 Spin Orbit interaction energy:-

In the H atom; from e^- frame there is a rotating proton; creating a magnetic field due to current.

$$\vec{B} = \frac{\mu_0 I}{2r} \cdot \hat{n}.$$

when $I = \frac{e}{T}$ & $L = mvr = \frac{2\pi m r^2}{T}$

So; $$\vec{B} = \frac{\mu_0}{2r} \cdot \frac{eL}{2\pi m r^2} \cdot \hat{n}.$$

as $\vec{L}$ & $\vec{B}$ points similar direction:

$$\vec{B} = \frac{e}{4\pi\epsilon_0 m c^2 r^3} \cdot \vec{L}$$ (using $c^2 = \frac{1}{\mu_0 \epsilon_0}$)

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The magnetic ~~field~~ moment of e^- be given by $\mu^S_{e,z} = -\frac{eS}{m}$

(i.e the spin of e^- is being coupled through the $\vec{B}$ arising due to $\vec{L}$. So the name.)

$$\therefore H' = -\vec{\mu}\cdot\vec{B} = \frac{e^2}{4\pi\epsilon_0 m^2c^2r^3}\,\vec{S}\cdot\vec{L}$$

However due to Thomson precession there is an extra term of $\frac{1}{2}$.

(I haven't got the proof in usual text book but I know the result.)

$$\therefore H' = \frac{e^2}{8\pi\epsilon_0 m^2c^2r^3}\,\vec{S}\cdot\vec{L}$$

As in spin orbit coupling spin tries to rotate $\vec{L}$ & $\vec{L}$ tries to rotate $\vec{S}$ so none of them are conserved. Rather as on the whole system, there is no external field; so $\vec{L}+\vec{S} = \vec{J}$ is conserved.

This can be verified through fact that

$$[\vec{L}\cdot\vec{S}, \vec{L}],\ [\vec{L}\cdot\vec{S}, \vec{S}] \neq 0$$

$$[\vec{L}\cdot\vec{S}, \vec{J}] = 0 = [\vec{L}\cdot\vec{S}, L^2] = [\vec{L}\cdot\vec{S}, S^2]$$

$$\therefore J^2 = (\vec{L}+\vec{S})^2 = L^2 + S^2 + 2\vec{L}\cdot\vec{S}$$

$$\Rightarrow \vec{L}\cdot\vec{S} = \frac{1}{2}(J^2 - L^2 - S^2)$$

Here however (n, L, S) forms complete set of basis.

So; in the state labeled by n, l, s, j

$$\langle H' \rangle = \frac{e^2}{8\pi\epsilon_0 m^2 c^2} \left\langle \frac{1}{r^3} \right\rangle \cdot \langle \vec{S}\cdot\vec{L} \rangle$$

but $$\langle \vec{S}\cdot\vec{L} \rangle \Big|_{n,l,s,j} = \left\langle \frac{J^2 - L^2 - S^2}{2} \right\rangle_{n,l,s,j}$$

$$= \frac{j(j+1) - l(l+1) - s(s+1)}{2} \hbar^2$$

here $S = \frac{1}{2}$ for e^- $\Rightarrow s(s+1) = 3/4$

Now $\left\langle \frac{1}{r^3} \right\rangle$ depends only on n & l (which is quite obvious for central potential)

Here I've used the standard result from online

$$\left\langle \frac{1}{r^3} \right\rangle = \frac{1}{l(l+\frac{1}{2})(l+1) n^3 a^3} \quad \begin{pmatrix} a = \text{Bohr} \\ \text{radius} \end{pmatrix}$$

(The proof is too long algebric mess. I think that's not needed here and not also the part of actual problem.)

$$\text{So: } \langle H' \rangle = \frac{e^2}{8\pi\epsilon_0 m^2 c^2} \frac{\hbar^2}{2} \frac{j(j+1) - l(l+1) - 3/4}{l(l+\frac{1}{2})(l+1) n^3 a^3}$$

Now for $n=2$ the interaction energy at state labeled by $n=2, l, j$ is given by: (using values of e, ϵ_0, m, c, a):

$$\langle H'_{so} \rangle_{n=2} = E^{so}_{l,j,n=2}$$

$$= (4.5\times10^{-5}) \, \frac{j(j+1) - l(l+1) - 3/4}{l(l+1/2)\cdot(l+1)} \text{ eV.}$$

Here possible values of l are: $l = 0, 1$.

" " of j " : $j = 1/2$ for $l = 0$
$= \frac{1}{2}, \frac{3}{2}$ for $l = 1$

for $l = 0$; the wave fn is spherically symmetric & there will be no splitting.
i.e the interaction energy is zero.
however for $l = 1$ there is some interaction energy given by: (calculated)

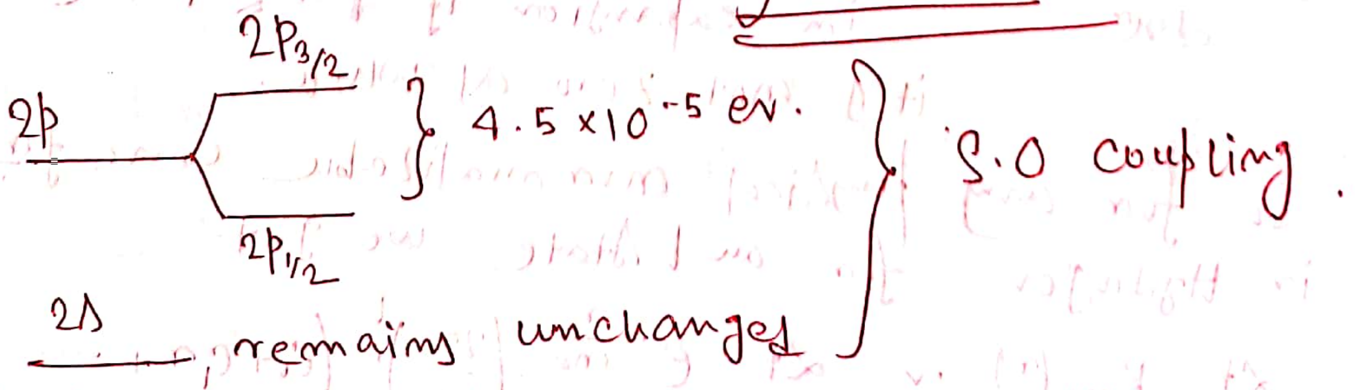
$$E^{so}_{l=1; j=\frac{1}{2}, n=2} = -3\times10^{-5} \text{ eV.}$$

$$E^{so}_{l=1, j=\frac{3}{2}, n=2} = 1.5\times10^{-5} \text{ eV.}$$

which splits the levels $^2P_{3/2}$ & $^2P_{1/2}$

by an amount $\sim 4.5\times10^{-5}$ eV.

Answer



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1.c i) $H = AK^2\hat{I} + B(\vec{K}\cdot\vec{J})^2$

Let's take the $\hat{z}$ axis along $\vec{K}$; i.e $\vec{K} = K\hat{z}$

$\therefore H = AK^2\hat{I} + BK^2J_z^2$

Clearly J_z commutes with H & hence they have simultaneous eigenvectors. Now clearly from the expressions of H we get: eig val of H

$\lambda = K^2(A + Bm^2\hbar^2)$ ($m\hbar$ is eig val of J_z)

Now as given $J = \frac{3}{2}$; $m = \pm\frac{3}{2}, \pm\frac{1}{2}$.

for $m = \pm\frac{3}{2} \rightarrow \lambda = K^2(A^2 + \frac{9B\hbar^2}{4}) \rightarrow$ two fold degeneracy

$m = \pm\frac{1}{2} \rightarrow \lambda = K^2(A^2 + \frac{B\hbar^2}{4}) \rightarrow$ "

ii) The Hamiltonian is not cubic symmetric: i.e it changes by exchange of x, y, z.

To make it cubic symmetric we have to add ~~$BK^2(x^2+y^2)$~~ $BK^2(J_x^2 + J_y^2)$ with H.

i.e The new Hamiltonian would be: $AK^2\hat{I} + BK^2J^2$.

1.d i) $V = \sum_q (-1)^q S_K^q T_K^{-q}$ (S, T = vector op)

$R S_K^q R^+ = \sum_{q'} R_K^{qq'} S_K^{q'}$

$R T_K^q R^+ = \sum_{q'} R_K^{qq'} T_K^{q'}$

$\therefore RVR^+ = \sum_q (-1)^q (RS_K^q R^+)(RT_K^{-q} R^+)$

$= \sum_q (-1)^q \sum_{q'} R_K^{qq'} S_K^{q'} \sum_{q''} R_K^{-qq''} T_K^{-q''}$

$= \sum_{qq'q''} (-1)^q R_K^{qq'} R_K^{-qq''} T_K^{-q''} S_K^{q'} \neq V$

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So V is not a scalar.

And V does not change sign like a vector

$(R v^i \neq \Sigma_i R^{ij}_B v_j)$ So v is not vector

So $V = \Sigma_i (-1)^q S^q_k T^{-q}_k$ is Tensor.

Ans

ii) $\Theta x \Theta^{-1} = x$; $\Theta p \Theta^{-1} = -p$

$\therefore \Theta L_z \Theta^{-1} = \Theta (x p_y - y p_x) \Theta^{-1}$

$= - x p_y + y p_x = -L_z.$

$\therefore \Theta \vec{L} \Theta^{-1} = -\vec{L}$;

For $\vec{S}$ we use the same analogy as that's another version of angular momenta.

$\therefore \Theta \vec{S} \Theta^{-1} = -\vec{S}$

And generally $\Theta \vec{J} \Theta^{-1} = -\vec{J}$

(iii) $\Theta (\vec{S}\cdot\vec{B}) \Theta^{-1} = (\Theta \vec{S} \Theta^{-1}) \cdot \vec{B} = -\vec{S}\cdot\vec{B}$

$\therefore (\vec{S}\cdot\vec{B})$ changes sign under time reversal. Ans

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1.2.(iii) $\langle 2 1 \tfrac{3}{2} \tfrac{3}{2} | \hat{P}_z | 2 1 \tfrac{3}{2} \tfrac{1}{2} \rangle$

Now the $|n l j m_j\rangle$ states can be decoupled in $|n l m_l\rangle |s m_s\rangle$ form using C.G coefficient as:

$$|2 1 \tfrac{3}{2} \tfrac{3}{2}\rangle = |2 1 1\rangle |\tfrac{1}{2} \tfrac{1}{2}\rangle$$

$$|2 1 \tfrac{3}{2} \tfrac{1}{2}\rangle = \frac{1}{\sqrt{3}} |2 1 1\rangle |\tfrac{1}{2} -\tfrac{1}{2}\rangle + \sqrt{\tfrac{2}{3}} |2 1 0\rangle |\tfrac{1}{2} \tfrac{1}{2}\rangle$$

So the given quantity

$$= \langle 2 1 1 | \langle \tfrac{1}{2} \tfrac{1}{2} | \hat{P}_z | \left\{ \frac{1}{\sqrt{3}} |2 1 1\rangle |\tfrac{1}{2} -\tfrac{1}{2}\rangle + \sqrt{\tfrac{2}{3}} |2 1 0\rangle |\tfrac{1}{2} \tfrac{1}{2}\rangle \right\}$$

As $\hat{P}_z$ never acts on spin; they directly gives inner products. i.e the quantity becomes:

$$\langle 2 1 \tfrac{3}{2} \tfrac{3}{2} | \hat{P}_z | 2 1 \tfrac{3}{2} \tfrac{1}{2} \rangle$$

$$= \frac{1}{\sqrt{3}} \langle 2 1 1 | \hat{P}_z | 2 1 1 \rangle \cdot \cancel{\langle \tfrac{1}{2} \tfrac{1}{2} | \tfrac{1}{2} -\tfrac{1}{2} \rangle} \to 0 \; +$$

$$\sqrt{\tfrac{2}{3}} \langle 2 1 1 | \hat{P}_z | 2 1 0 \rangle \underbrace{\langle \tfrac{1}{2} \tfrac{1}{2} | \tfrac{1}{2} \tfrac{1}{2} \rangle}_{1}$$

$$= \sqrt{\tfrac{2}{3}} \langle 2 1 1 | \hat{P}_z | 2 1 0 \rangle$$

Now $P_z = -i\hbar \frac{\partial}{\partial z} = -i\hbar \left\{ \cos\theta \frac{\partial}{\partial r} - \frac{\sin\theta}{r} \frac{\partial}{\partial \theta} \right\}$

(by variable transform)

(not proved; collected from online. The proof is long)

Clearly $\hat{p}_z$ does not act ~~any~~ any way on the ϕ coordinate & hence the ϕ integral gives:

$$\int_0^{2\pi} \underbrace{e^{-i\phi}}_{\text{coming from } |211\rangle^{+}} \cdot \underbrace{1}_{\text{coming from } |210\rangle} \, d\phi$$

$$= \left.\frac{e^{-i\phi}}{-i}\right|_0^{2\pi} = 0. \quad ; \text{ i.e } \langle 211|\hat{p}_z|210\rangle = 0.$$

So: $\langle 2\,1\,\tfrac{3}{2}\,\tfrac{3}{2}|\hat{p}_z|2\,1\,\tfrac{3}{2}\,\tfrac{1}{2}\rangle = 0.$

Ans

Here I've to find $\langle 1\,0\,\tfrac{1}{2}\,\tfrac{1}{2}|p_i p_j|1\,0\,\tfrac{1}{2}\,\tfrac{1}{2}\rangle$

Using CG coefficient & breaking $|n\,l\,j\,m_j\rangle$ into $|n\,l\,m_l\rangle|s\,m_s\rangle$ we get,

$$|1\,0\,\tfrac{1}{2}\,\tfrac{1}{2}\rangle = |1\,0\,0\rangle|\tfrac{1}{2}\,\tfrac{1}{2}\rangle$$

So $\langle 1\,0\,\tfrac{1}{2}\,\tfrac{1}{2}|p_i p_j|1\,0\,\tfrac{1}{2}\,\tfrac{1}{2}\rangle$

$$= \langle 100|\langle\tfrac{1}{2}\,\tfrac{1}{2}|p_i p_j|100\rangle|\tfrac{1}{2}\,\tfrac{1}{2}\rangle$$

(but p_i does not act on $|s\,m_s\rangle$ & hence)

$$= \langle 100|p_i p_j|100\rangle \underbrace{\langle\tfrac{1}{2}\,\tfrac{1}{2}|\tfrac{1}{2}\,\tfrac{1}{2}\rangle}_{1}$$

$= \langle 100 | p_i p_j | 100 \rangle$

Now, $p_{x_i} = -i\hbar \frac{\partial}{\partial x_i}$, & the transformations be:

$$\frac{\partial}{\partial x} \equiv \sin\theta \cos\phi \frac{\partial}{\partial r} + \frac{\cos\theta \cos\phi}{r} \frac{\partial}{\partial \theta} - \frac{\sin\phi}{r \sin\theta} \frac{\partial}{\partial \phi}$$

$$\frac{\partial}{\partial y} = \sin\theta \sin\phi \frac{\partial}{\partial r} + \frac{\cos\theta \sin\phi}{r} \frac{\partial}{\partial \theta} + \frac{\cos\phi}{r \sin\theta} \frac{\partial}{\partial \phi}.$$

$$\frac{\partial}{\partial z} \equiv \cos\theta \frac{\partial}{\partial r} - \frac{\sin\theta}{r} \frac{\partial}{\partial \theta}.$$

So in $p_x p_y$ (or $p_y p_x$) the present terms would be

$$\sim \frac{\partial^2}{\partial r^2}, \frac{\partial^2}{\partial \theta^2}, \frac{\partial^2}{\partial \phi^2}, \frac{\partial^2}{\partial r \partial \theta}, \frac{\partial^2}{\partial r \partial \phi}, \frac{\partial^2}{\partial \theta \partial \phi}$$

As $|100\rangle$ is spherically symmetric so except $\frac{\partial^2}{\partial r^2}$ all will be zero. i.e $Y_0^0(\theta, \phi) = \text{const}$.

So $\frac{\partial^2}{\partial \theta^2} \psi_{100} = 0$; $\frac{\partial^2}{\partial \theta \partial \phi} \psi_{100} = 0$; ... etc.

but the coefficient of $\frac{\partial^2}{\partial r^2}$ is $\sim \sin^2\theta \sin\phi \cos\phi$

So the ϕ integral gives:

$$\int_0^{2\pi} \sin\phi \cos\phi \, d\phi = 0.$$

i.e $\langle 100 | p_x p_y | 100 \rangle = \langle 1 0 \tfrac{1}{2} \tfrac{1}{2} | p_x p_y | 1 0 \tfrac{1}{2} \tfrac{1}{2} \rangle$

$= \langle 1 0 \tfrac{1}{2} \tfrac{1}{2} | p_y p_x | 1 0 \tfrac{1}{2} \tfrac{1}{2} \rangle = 0.$

Now $p_x p_z$ (or $p_z p_x$ as they commute) has all terms except $\frac{\partial^2}{\partial\phi^2}$; And by similar reasoning only $\frac{\partial^2}{\partial r^2}$ term survives. But that has coefficient as $\sin\theta\cos\theta\cos\phi\frac{\partial^2}{\partial r^2}$.

$\therefore$ the ϕ integral gives: $\int_0^{2\pi}\cos\phi\, d\phi = 0$.

$$\therefore \langle 100|p_x p_z|100\rangle = \langle 1 0 \tfrac{1}{2}\tfrac{1}{2}|p_x p_z|100\rangle$$
$$= \langle 1 0 \tfrac{1}{2}\tfrac{1}{2}|p_z p_x|100\rangle = 0,$$

Similarly we get $\langle 1 0 \tfrac{1}{2}\tfrac{1}{2}|p_y p_z|1 0 \tfrac{1}{2}\tfrac{1}{2}\rangle = 0$.

Now, for $i=j$ in $p_i p_j$ it gives p_i^2; Here as $|100\rangle$ state is spherically symmetric so we should get:

$$\langle p_x^2\rangle = \langle p_y^2\rangle = \langle p_z^2\rangle \quad \ldots (1)$$

$$\& \sum_{i=1}^{3}\langle 100|p_i^2|100\rangle = 2m \times \langle 100|\frac{p^2}{2m}|100\rangle$$
$$= 3\times\underbrace{\langle 100|p_i^2|100\rangle}_{i=1/2/3} = 2m\langle K.E\rangle = 2m\times\left\{-\frac{\langle E\rangle_{100}}{2}\right\}$$

(Using Virial th: $\langle K.E\rangle = -\frac{\langle P.E\rangle}{2}$)

$$\therefore \langle 1 0 \tfrac{1}{2}\tfrac{1}{2}|p_i^2|1 0 \tfrac{1}{2}\tfrac{1}{2}\rangle = -\frac{m}{3}\langle E_{100}\rangle \to (\text{due to (1)})$$

So in general:

$$\langle 1 0 \tfrac{1}{2}\tfrac{1}{2}|p_i p_j|1 0 \tfrac{1}{2}\tfrac{1}{2}\rangle = -\frac{m}{3}\langle E_{100}\rangle\,\delta_{ij}$$

(Where $\langle E_{100}\rangle = -13.6$ eV)

Ans

Problem: 9 →

b. ☒ In scattering process; as energy of incident particle becomes lower & lower; the particles are effectively shows a cross section of an impenetrable sphere in that limiting case. The radius of this sphere is called scattering length. (a)

☒ The formula for scattering length be

$$a = \lim_{K \to 0} \frac{\tan \delta_0}{K} \quad \left(\delta_0 \text{ is phase shift for } S \text{ wave} \right)$$

If $a > 0$: implies either the existance of repulsive potential / scattering instead of existance of attractive potential.

$a < 0$: implies bound state forms due to attractive potential only.

☒ Neutron-proton ~~Act~~ scattering length ~ 5.4 fm.

Now Radius of nucleus ~ 1 fm. n & p forms a bound state as nucleus. So the potential must be attractive. i.e a is '$-$ve'. Now if it is repulsive then the bound state can only be formed iff $a_0 \sim 1$ fm i.e short range force.

c. The radial eq gives: $\left(-\frac{\hbar^2}{2m}\partial_r^2 + V_r\right)u = Eu \quad (l=0)$

For $E<0$ i.e $E = -E_0$; $E_0 > 0$ we get the solution for u be:

$$u_{out}(r) = u(r>a) = Ae^{kr} + Be^{-kr}$$

$$k^2 = \frac{2mE_0}{\hbar^2}.$$

Ans; $u(r \leq a) = u_{in}(r) = C \sin(\eta r) + D \cos(\eta r)$

$$\eta = \frac{\sqrt{2m(V_0 - E_0)}}{\hbar^2} \quad (\because V_0 > 0)$$

Clearly as $u(r \to 0) = 0$; $u(r \to \infty) = 0$ so we get : $D = 0$; $A = 0$.

$$\therefore u(r) = \left.\begin{array}{ll} C \sin(\eta r) & r \leq a \\ = B e^{-kr} & r > a \end{array}\right\}$$

Continuity of u & u' gives:

$$\left.\begin{array}{l} C \sin \eta a = B e^{-ka} \quad \cdots (1) \\ \eta C \cos \eta a = -kB e^{-ka} \quad \cdots (2) \end{array}\right\}$$

which gives : $$\frac{\tan \eta a}{\eta} = -\frac{1}{k} \quad \cdots (3)$$

Now for $E > 0$ both solutions are of sinusoidal form.

let for $E > 0$;

$u(r > a) = A \sin(\tilde{k}r + \delta_0)$ (~~k will not change as V is still zero outside~~)

$$\left(\tilde{k} = \frac{\sqrt{2mE}}{\hbar}\right)$$

Ans; $u(r < a) = C \sin(\tilde{\eta} r)$ $\left(\tilde{\eta} = \frac{\sqrt{2m(E+V_0)}}{\hbar}\right)$

(once again the cosine will vanish for $r < a$)

Again by continuity of u & u' at $r = a$ gives:

$$\left.\begin{array}{l} A \sin(\tilde{k}a + \delta_0) = C \sin(\tilde{\eta} a) \\ \tilde{k} A \cos(\tilde{k}a + \delta_0) = \tilde{\eta} C \cos(\tilde{\eta} a) \end{array}\right\}$$

i.e $$\frac{\tan(\tilde{k}a + \delta_0)}{\tilde{k}} = \frac{\tan(\tilde{\eta} a)}{\tilde{\eta}} \quad \cdots (4)$$

Now the S wave scattering amplitude gives:

$$f_0 = \frac{e^{i\delta_0}\sin\delta_0}{\tilde{k}} = \frac{1}{\tilde{k}\,\mathrm{cosec}\,\delta_0\,(\cos\delta_0 - i\sin\delta_0)}$$

$$= \frac{1}{\tilde{k}\cot\delta_0 - i\tilde{k}} = \frac{1}{\tilde{k}(\cot\delta_0 - i)}$$

Clearly f_0 has a simple pole at $\cot\delta_0 = i$. Ans

(complex phase shift).

Now for $E<0$ we got $\tilde{\eta} = \eta$. So; from (4) we get:

~~$\eta\cot(\eta a) = \tilde{k}\cot\tilde{k}a+$~~

$$\frac{\tan(\tilde{k}a+\delta_0)}{\tilde{k}} = \frac{\tan(\tilde{\eta}a)}{\tilde{\eta}} = \frac{\tan(\eta a)}{\eta}$$

$\therefore$ ~~cot k~~ but $\tilde{k} = ik$; so;

$$\frac{\tan(ika+\delta_0)}{ik} = \frac{\tan(\eta a)}{\eta}$$

$$\therefore \cot(ika+\delta_0) = -i\frac{\eta}{k}\cot(\eta a)$$

~~So to get the pole we need cot i~~

$$\therefore ika+\delta_0 = -\cot^{-1}\left(\frac{i\eta}{k}\cot\eta a\right)$$

$$\therefore \cot\delta_0 = \cot\left[-ika - \cot^{-1}\left(\frac{i\eta}{k}\cot\eta a\right)\right]$$

$\therefore$ To get the pole we need: $\cot\delta_0 = i$

i.e. $$\cot\left[-ika - \cot^{-1}\left(\frac{i\eta}{k}\cot\eta a\right)\right] = i$$

proved