Quantum Assignment – 2
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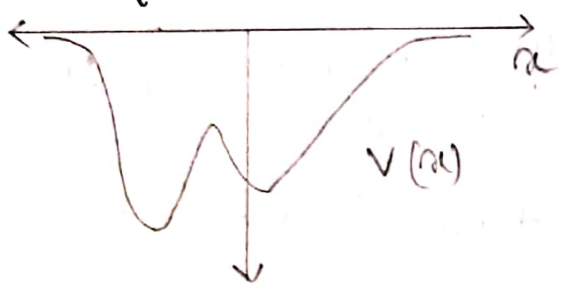
1. To prove that every 1-dimensional attractor potential must have at least one bound state we must consider:

$V(x) \longrightarrow 0$ at $x \to \pm\infty$; $V(x) \leq 0$, $\forall x \in (-\infty, \infty)$

$V(x)$ is piecewise continuous.

The possible (one) graph for $V(x)$ is shown as:



As $V(x) < 0$ everywhere we get $|V(x)| > 0$ & $|V(x)| = -V(x)$.

$$\therefore \; H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - |V(x)|$$

$$\therefore \; \langle H \rangle = \langle T \rangle - \langle |V(x)| \rangle \quad \cdots (1)$$

Clearly $\langle T \rangle$ is always > 0 (as K.E can't be negative)

Now from variational principle we get if for some state $|\psi_\alpha\rangle$ the value of $\langle H \rangle < 0$ then; we must have for the ground state of the actual problem:

$E_0 \leq \langle H \rangle$ i.e $E_0 < 0$ i.e $E_0 < V_{\pm\infty}$

i.e the system has bound state.

For that; we must show; for some ψ_α.

$\langle H\rangle < 0$ i.e $\langle T\rangle - \langle |V|\rangle < 0$

i.e $\dfrac{\langle T\rangle}{\langle |V|\rangle} < 1$ (for some state $|\psi_\alpha\rangle$)

Let's consider $\psi_\alpha = b\, e^{-\frac{\alpha x^2}{2}}$ $(\alpha > 0)$

$\therefore$ by normalization $\int_{-\infty}^{\infty} |\psi_\alpha|^2 dx = b^2 \sqrt{\dfrac{\pi}{\alpha}} = 1$

$\Rightarrow b = \left(\dfrac{\alpha}{\pi}\right)^{1/4}$.

So; $\psi_\alpha = \left(\dfrac{\alpha}{\pi}\right)^{1/4} e^{-\frac{\alpha x^2}{2}}$

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

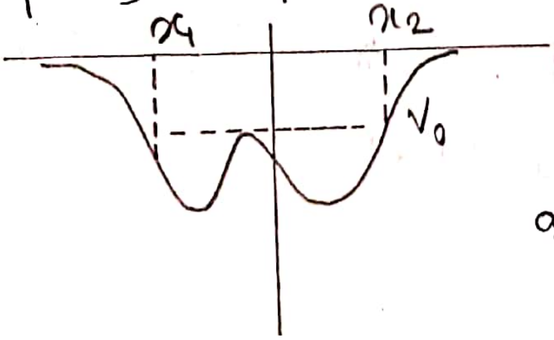
$\downarrow$ using mathematica.

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

$$\langle |V|\rangle = \int_{-\infty}^{\infty} |\psi_\alpha|^2 |V|\, dx = \sqrt{\frac{\alpha}{\pi}} \int_{-\infty}^{\infty} e^{-\frac{2\alpha x^2}{2}} \cdot |V|\, dx$$

$$\therefore \frac{\langle |V|\rangle}{\langle T\rangle} = \frac{4m}{\hbar^2 \sqrt{\pi\alpha}} \int_{-\infty}^{\infty} e^{-\alpha x^2} |V|\, dx \quad \cdots (2).$$

Now, in the V(x) diagram we choose two points x_1 & x_2 as following;



Let in the interval of $[x_1, x_2]$; the maximum of $V(x)$ or minimum of $|V(x)|$ be $|V_0|$ as in fig.

As $|v|$ is always > 0; so:

$$\int_{-\infty}^{\infty} e^{-\alpha x^2} |v| \, dx > \int_{x_1}^{x_2} e^{-\alpha x^2} |v| \, dx$$

And from the last fig; when v_0 is the minimum of $|v|$ in $[x_1, x_2]$:

$$\int_{x_1}^{x_2} |v| e^{-\alpha x^2} dx > \int_{x_1}^{x_2} |v_0| e^{-\alpha x^2} dx$$

but $e^{-\alpha x^2} > e^{-\alpha \cdot \max(x_1^2, x_2^2)}$

($\max(a,b)$ = maximum among a & b)

$$\therefore \int_{x_1}^{x_2} |v_0| e^{-\alpha x^2} dx > \int_{x_1}^{x_2} |v_0| \cdot e^{-\alpha \cdot \max(x_1^2, x_2^2)} dx$$

$$\text{i.e.} > |v_0| (x_2 - x_1) \cdot e^{-\alpha \cdot \max(x_1^2, x_2^2)}$$

Now; if we choose

$$\alpha < \frac{1}{\max(x_1^2, x_2^2)}$$

then $e^{-\alpha \cdot \max(x_1^2, x_2^2)} > e^{-1}$

Combining all of them:

$$\int_{-\infty}^{\infty} |v| e^{-\alpha x^2} dx > |v_0| (x_2 - x_1) \cdot e^{-1}.$$

So from (2) we get:

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$$\frac{\langle |V| \rangle}{\langle T \rangle} > \frac{4m}{\hbar^2 \sqrt{\pi\alpha}} \frac{|V_0| (x_2 - x_1)}{e}$$

$\therefore$ if $\dfrac{4m}{\hbar^2 \sqrt{\pi\alpha}} \cdot \dfrac{|V_0| (x_2 - x_1)}{e} > 1$

i.e $\alpha < \left[\dfrac{4m}{\hbar^2 \sqrt{\pi}} \dfrac{|V_0| (x_2 - x_1)}{e} \right]^2$.

then we get $\dfrac{\langle |V| \rangle}{\langle T \rangle} > 1$

but previously we have taken $\alpha < \dfrac{1}{\max(x_1^2, x_2^2)}$

so by choosing,

$$\alpha < \min \left\{ \frac{1}{\max(x_1^2, x_2^2)}, \left[\frac{4m}{\hbar^2 \sqrt{\pi}} \cdot \frac{|V_0| (x_2 - x_1)}{e} \right]^2 \right\}$$

And as both of the arguments are +ve for $x_1 \neq x_2$ so we get some $\alpha > 0$ (which is trivial) then we must satisfy

$$\frac{\langle |V| \rangle}{\langle T \rangle} > 1 \quad \text{i.e} \left[\langle |V| \rangle - \langle T \rangle \right] \Big|_{\psi_\alpha} > 0$$

i.e $\langle H \rangle_{\psi_\alpha} < 0$

i.e $E_{gs} < 0$. i.e $E_{gs} < V_{\pm\infty}$

i.e there is some bound state.

proved

3. Delta potential attractor:—

$$V = -aV_0\,\delta(x) = -\alpha\,\delta(x) \quad (\alpha = aV_0 > 0 \text{ here.})$$

$$\therefore H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - \alpha\,\delta(x).$$

Now if we use the Gaussian trial f^n:

$$\psi_b = \left(\frac{2b}{\pi}\right)^{1/4} e^{-bx^2}.$$

then $$\langle T\rangle = \sqrt{\frac{2b}{\pi}}\int_{-\infty}^{\infty} e^{-bx^2}\frac{d^2}{dx^2}\left(e^{-bx^2}\right)dx$$

$$= \frac{\hbar^2 b}{2m}$$

(used the ~~result~~ calculation of problem 1)

$$\langle V\rangle = -\alpha\sqrt{\frac{2b}{\pi}}\cdot\int_{-\infty}^{\infty} e^{-2bx^2}\delta(x)\,dx$$

$$= -\alpha\sqrt{\frac{2b}{\pi}}\cdot 1$$

So; $$\langle H\rangle = \frac{\hbar^2 b}{2m} - \alpha\sqrt{\frac{2b}{\pi}}$$

minimizing $\langle H\rangle_{\psi_b}$ by $\frac{\partial\langle H\rangle}{\partial b} = 0$ gives:

$$\frac{\hbar^2}{2m} - \frac{\alpha\sqrt{2}}{2\sqrt{\pi b}} = 0 \Rightarrow \frac{\hbar^2}{2m} = \frac{\alpha}{\sqrt{2\pi b}}$$

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

~~$\Rightarrow \langle H\rangle_{min} = \frac{2m^2\alpha^2}{\pi\hbar^4} \Rightarrow E_{gs} < \frac{2m^2\alpha^2}{\pi\hbar^4}$~~

~~The true ground state is $E^0 =$~~

$$\Rightarrow \langle H \rangle_{min} = \frac{\hbar^2}{\cancel{2}m} \frac{\cancel{2}m^2\alpha^2}{\pi\hbar^4} - \alpha\cdot\sqrt{\frac{2}{\pi}\cdot\frac{2m^2\alpha^2}{\pi\hbar^4}}$$

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

$\therefore E_{gs} < \langle H \rangle_{min}$

i.e $E_{gs} < -\frac{m\alpha^2}{\pi\hbar^2}.$

The true ground state energy is $E_0 = -\frac{m\alpha^2}{2\hbar^2}.$

as $\pi > 2$ so;

$$-\frac{m\alpha^2}{2\hbar^2} < -\frac{m\alpha^2}{\pi\hbar^2}$$

i.e variation gives true result.

2: Spin Orbit interaction energy:-

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

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

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:

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

The magnetic ~~field~~ moment of e^- be given by $\mu_e^S = -\frac{eS}{m}$.

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

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

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

(I haven't got the proof in usual text books 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 (m, 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 $\langle \vec{S}\cdot\vec{L} \rangle \Big|_{n,l,s,j} = \left\langle \frac{J^2 - L^2 - S^2}{2} \right\rangle_{n,l,s,j}$

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

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

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

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

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):

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

$$= (4.5 \times 10^{-5}) \frac{j(j+1) - l(l+1) - 3/4}{l(l+1/2)\cdot(l+1)} \text{ eV.}$$

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

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

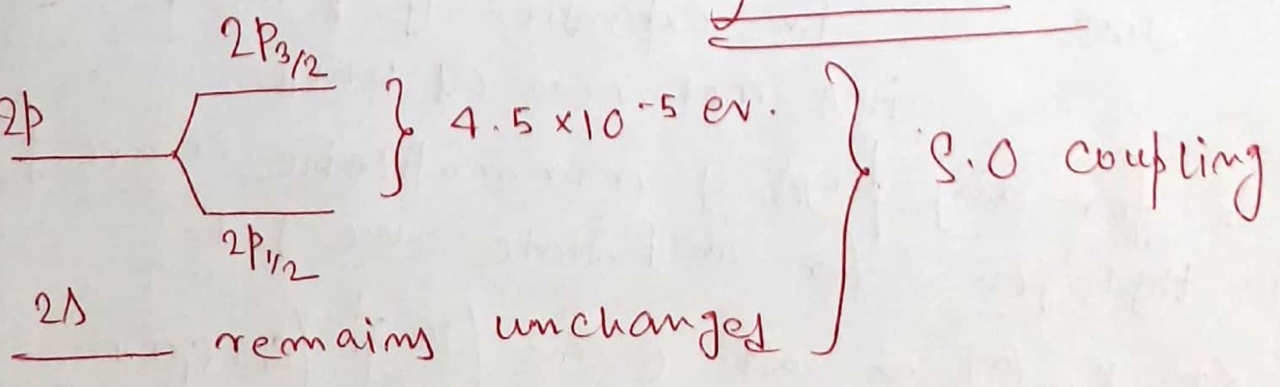
for $l = 0$; the wave fn is spherically symmetric & there will be no splitting. i.e the interaction energy is zero. however for $l = 1$ there is some interaction energy given by: (calculated)

$$E^{So}_{l=1; j=\frac{1}{2}, n=2} = -3 \times 10^{-5} \text{ eV.}$$

$$E^{So}_{l=1, j=\frac{3}{2}, n=2} = 1.5 \times 10^{-5} \text{ eV.}$$

which splits the levels $^2P_{3/2}$ & $^2P_{1/2}$ by an amount $\sim 4.5 \times 10^{-5}$ eV.

Answer



4. $l=1$ Hydrogen State with variational method.

In the true wave fn of H atom; the Radial part varies as:

$$R_{nl}(r) \sim e^{-\frac{r}{na}} \left(\frac{2r}{na}\right)^{l} L_{n-l-1}^{2l+1}\left(\frac{2r}{na}\right)$$

Now the associated ~~Lag~~ Laguerre polys be given by:

$$L_{q-p}^{p}(x) \sim (-1)^{p} \frac{d^{p}}{dx^{p}} L_q(x)$$

when; $L_q(x) = \sum_{j=0}^{q} c_j x^j$ (for some non zero c_j)

as in $L_q(x)$ all powers of x upto $j=q$ is present; hence in it's derivative; there will be at least one term which is constant any non zero. (otherwise the derivative is zero as a whole)

i.e $L_q(x) = \sum_{j=0}^{q} c_j x^j$

$\Rightarrow \frac{d^n}{dx^n} L_q(x) = 0$ if $n > q$ nonzero

& $\frac{d^n}{dx^n} L_q(x)$ has one constant term in expansion if $n \leq q$ i.e it's not zero as whole.

So for any physical normalizable wave fn in Hydrogen for an l state we get

$$\lim_{r\to 0} R_{nl}(r) \sim \lim_{r\to 0} e^{-\frac{r}{na}} \left(\frac{2r}{na}\right)^{l} \left(c_0 + c_1 r + \dots + c_k r^k\right)$$

for some $k \geq 0$ & we get

$C_0, C_1, \cdots, C_k \neq 0$

So; $\lim_{r \to 0} R_{nl}(r) \sim Ae^0 \cdot r^l \cdot (C_0 + 0 + \cdots + 0)$

$\sim r^l.$

Here for the ~~given sta~~ trial state we use that information.

moreover at $r \to \infty$; $e^{-r/na} \cdot r^\alpha \to 0$ for all α. So the good trial fn can be of the form:

$$R_{n1} = Ar^1 e^{-\alpha r} = Are^{-\alpha r}. = \psi_\alpha \text{ (say)}$$

As the Spherical Harmonics are also normalized so we get:

$$1 = \int_0^\infty r^2 R^2 dr = \int_0^\infty A^2 r^2 . r^2 . e^{-2\alpha r} dr$$

$$(2\alpha r = z)$$

$$= A^2 . \int_0^\infty \frac{z^4}{2^4 \alpha^4} \cdot e^{-z} \frac{dz}{2\alpha}.$$

$$= \frac{A^2}{32\alpha^5} \Gamma(5) = \frac{A^2 \times 4 \times 3 \times 2}{32 \alpha^5} = \frac{3A^2}{4\alpha^5}.$$

$$\therefore A = \sqrt{\frac{8\alpha^5}{3 \times 2}}.$$

Now R_{nl} satisfies the eq:

$$-\frac{\hbar^2}{2m} \cdot \frac{1}{r^2} \frac{d}{dr}\left(r^2 \frac{dR}{dr}\right) + \left[\frac{\hbar^2}{2m} \cdot \frac{l(l+1)}{r^2} + V(r)\right]R = ER$$

Here $V(r) = -\frac{e^2}{r}$; $l = 1$ gives:

$$-\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\left(\frac{\hbar^2}{m}\cdot\frac{1}{r^2}-\frac{e^2}{r}\right)R=ER.$$

i.e $$\hat{H}_R=\underbrace{-\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right)}_{\hat{T}_R}+\underbrace{\left(\frac{\hbar^2}{m}\cdot\frac{1}{r^2}-\frac{e^2}{r}\right)}_{\hat{V}_R}$$

At the ~~a~~ trial state ψ_α taken;

$$\langle H_R\rangle=\langle\hat{T}_R\rangle+\langle\hat{V}_R\rangle$$

when $$\langle\hat{A}_R\rangle=\int_0^\infty\left(\psi_\alpha\hat{A}_R\psi_\alpha\right).r^2dr.$$

∴ Here $\langle\hat{T}_R\rangle$

$$=-\int_0^\infty A^2 re^{-\alpha r^2}\left(\frac{\hbar^2}{2m}\right)\cdot\frac{1}{\cancel{r^2}}\frac{d}{dr}\left(r^2\frac{d}{dr}(re^{-\alpha r})\right).\cancel{r^2}\,dr.$$

I've evaluated the integrals in mathematica which gives:

$$\langle\hat{T}_R\rangle_{\psi_\alpha}=\frac{\cancel{3}}{\cancel{8}}\frac{\alpha\hbar^2}{m\alpha^4}\cdot\frac{\cancel{8}\alpha^{\cancel{5}}}{\cancel{3}\times2}\quad\left(\text{using value of } A\right)$$

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

And $$\langle\hat{V}_R\rangle_{\psi_\alpha}=\int_0^\infty\left(\frac{\hbar^2}{mr^2}-\frac{e^2}{r}\right).r^2A^2r^2e^{-2\alpha r}dr$$

$$=-\frac{\cancel{3}}{\cancel{8}}\frac{\cancel{m}e^2}{\cancel{m}\alpha^4}\cdot\frac{\cancel{8}\alpha^{\cancel{5}}}{\cancel{3}\times2}=-\frac{\alpha e^2}{2}.$$

So; $$\langle H\rangle_{\psi_\alpha}=\frac{\alpha^2\hbar^2}{2m}-\frac{\alpha e^2}{2}.$$

varying over α gives:

$$\frac{d\langle H\rangle_{\psi_\alpha}}{d\alpha} = 0 = \frac{2\alpha\hbar^2}{2m} - \frac{e^2}{2}$$

$$\Rightarrow \alpha = \frac{me^2}{2\hbar^2} = \alpha_0$$

$$\therefore \langle H\rangle_{\psi_\alpha}\Big|_{\alpha=\alpha_0} = \left(\frac{\hbar^2\alpha^2}{2m} - \cancel{me}\frac{\alpha e^2}{2}\right)\Bigg|_{\alpha = \frac{me^2}{2\hbar^2}}$$

$$= \frac{\cancel{\hbar^2}}{2\cancel{m}} \cdot \frac{m^{\cancel{2}}e^4}{4\cancel{\hbar^4}\,\hbar^2} - \frac{e^2}{2}\cdot\frac{me^2}{2\hbar^2}$$

$$= -\frac{me^4}{8\hbar^2}.$$

So $E^{gs}\Big|_{l=1} \leq -\dfrac{me^4}{8\hbar^2}$. Ans

The actual energy is given by:

$$E_n = -\frac{me^4}{2n^2\hbar^2} \quad \left(\text{taking } \frac{1}{4\pi\epsilon_0} = 1\right)$$

for $l = 1$ we have $n \geq 2$. (obvious for H)

$$\therefore E_n^{true} = -\frac{me^2}{2n^2\hbar^2} = -\frac{me^2}{8\hbar^2}.$$

$\therefore$ The result is true for $n = 2$.

i.e for all n values ($n = 2, 3, 4, \ldots$) possible for $l=1$; the ground state ($n=2$) exactly matching the energy. This is because of the form of ψ_α. which is equal to the form of $R_{n=2}(r)$ state.

Clearly the ~~value~~ value is indp of m.
m only takes part for determinging "Angular" part. $(Y_l^m(\theta,\phi))$

<u>Ans</u>

Problem: 5

Using diagonalization:-

<u>5.a</u> For the two charge system; the 4 orthogonal spin states are:

$|++\rangle; |+-\rangle; |-+\rangle; |--\rangle$

we represents, these states as (4×1) column matrix as:

$$|++\rangle = \begin{pmatrix}1\\0\\0\\0\end{pmatrix}; \quad |+-\rangle = \begin{pmatrix}0\\1\\0\\0\end{pmatrix}; \quad |-+\rangle = \begin{pmatrix}0\\0\\1\\0\end{pmatrix}; \quad |--\rangle = \begin{pmatrix}0\\0\\0\\1\end{pmatrix}$$

Now Given Hamiltonian:

$$\hat{H} = A\,\vec{S_1}\cdot\vec{S_2} + \frac{eB}{m_e c}(S_{1z} - S_{2z})$$

$$\text{Now}\quad \vec{S_1}\cdot\vec{S_2} = S_1^x \otimes S_2^x + S_1^y \otimes S_2^y + S_1^z \otimes S_2^z.$$

$$= \frac{\hbar^2}{2^2}\left[\begin{pmatrix}0&1\\1&0\end{pmatrix}\otimes\begin{pmatrix}0&1\\1&0\end{pmatrix} + \begin{pmatrix}0&-i\\i&0\end{pmatrix}\otimes\begin{pmatrix}0&-i\\i&0\end{pmatrix} + \begin{pmatrix}1&0\\0&-1\end{pmatrix}\otimes\begin{pmatrix}1&0\\0&-1\end{pmatrix}\right]$$

$$= \frac{\hbar^2}{2^2}\left[\begin{pmatrix}0&0&0&1\\0&0&1&0\\0&1&0&0\\1&0&0&0\end{pmatrix} + \begin{pmatrix}0&0&0&-1\\0&0&1&0\\0&1&0&0\\-1&0&0&0\end{pmatrix} + \begin{pmatrix}1&0&0&0\\0&-1&0&0\\0&0&-1&0\\0&0&0&1\end{pmatrix}\right]$$

$$= \frac{\hbar^2}{4}\begin{pmatrix}1&0&0&0\\0&-1&2&0\\0&2&-1&0\\0&0&0&1\end{pmatrix}$$

$$S_1^z - S_2^z = S_1^z \otimes \mathbb{I}_{S_2} - \mathbb{I}_{S_1} \otimes S_2^z$$

$$= \frac{\hbar}{2}\left[\begin{pmatrix}1&0\\0&-1\end{pmatrix}\otimes\begin{pmatrix}1&0\\0&1\end{pmatrix} - \begin{pmatrix}1&0\\0&1\end{pmatrix}\otimes\begin{pmatrix}1&0\\0&-1\end{pmatrix}\right]$$

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$$= \frac{\hbar}{2}\left[\begin{pmatrix}1&&&0\\&1&&\\&&-1&\\0&&&-1\end{pmatrix} - \begin{pmatrix}1&&&0\\&-1&&\\&&1&\\0&&&-1\end{pmatrix}\right] = \hbar\begin{pmatrix}0&&&0\\&1&&\\&&-1&\\0&&&0\end{pmatrix}$$

$$\hat{H} = \underbrace{A\,\vec{S_1}\cdot\vec{S_2}}_{\hat{H}_1} + \underbrace{\frac{eB}{m_e c}\left(S_1^z - S_2^z\right)}_{\hat{H}_2}$$

$\therefore$ The W matrix $\left(W_{ij} = \langle i|\hat{H}|j\rangle\right)$ be given by:

$$W_{ij} = W^1_{ij} + W^2_{ij} \quad ; \quad \left.\begin{array}{l} W^1_{ij} = \langle i|\hat{H}_1|j\rangle \\ W^2_{ij} = \langle i|\hat{H}_2|j\rangle \end{array}\right\}$$

$$W^1_{11} = \frac{\hbar^2 A}{4}\begin{pmatrix}1&0&0&0\end{pmatrix}\begin{pmatrix}1&0&0&0\\0&-1&2&0\\0&2&-1&0\\0&0&0&1\end{pmatrix}\begin{pmatrix}1\\0\\0\\0\end{pmatrix} = \frac{\hbar^2 A}{4}\begin{pmatrix}1&0&0&0\end{pmatrix}\begin{pmatrix}1\\0\\0\\0\end{pmatrix} = \frac{\hbar^2 A}{4}.$$

$$W^1_{22} = \frac{\hbar^2 A}{4}\begin{pmatrix}0&1&0&0\end{pmatrix}\begin{pmatrix}1&0&0&0\\0&-1&2&0\\0&2&-1&0\\0&0&0&1\end{pmatrix}\begin{pmatrix}0\\1\\0\\0\end{pmatrix} = \frac{\hbar^2 A}{4}\begin{pmatrix}0&1&0&0\end{pmatrix}\begin{pmatrix}0\\-1\\2\\0\end{pmatrix} = -\frac{\hbar^2 A}{4}.$$

$$W^1_{33} = \frac{\hbar^2 A}{4}\begin{pmatrix}0&0&1&0\end{pmatrix}\begin{pmatrix}1&0&0&0\\0&-1&2&0\\0&2&-1&0\\0&0&0&1\end{pmatrix}\begin{pmatrix}0\\0\\1\\0\end{pmatrix} = \frac{\hbar^2 A}{4}\begin{pmatrix}0&0&1&0\end{pmatrix}\begin{pmatrix}0\\2\\-1\\0\end{pmatrix} = -\frac{\hbar^2 A}{4}.$$

$$W^1_{44} = \frac{\hbar^2 A}{4}\begin{pmatrix}0&0&0&1\end{pmatrix}\begin{pmatrix}1&0&0&0\\0&-1&2&0\\0&2&-1&0\\0&0&0&1\end{pmatrix}\begin{pmatrix}0\\0\\0\\1\end{pmatrix} = \frac{\hbar^2 A}{4}\begin{pmatrix}0&0&0&1\end{pmatrix}\begin{pmatrix}0\\0\\0\\1\end{pmatrix} = \frac{\hbar^2 A}{4}.$$

$$W^1_{12} = \frac{\hbar^2 A}{4}\begin{pmatrix}1&0&0&0\end{pmatrix}\begin{pmatrix}1&0&0&0\\0&-1&2&0\\0&2&-1&0\\0&0&0&1\end{pmatrix}\begin{pmatrix}0\\1\\0\\0\end{pmatrix} = \frac{\hbar^2 A}{4}\begin{pmatrix}1&0&0&0\end{pmatrix}\begin{pmatrix}0\\-1\\2\\0\end{pmatrix} = 0.$$

$$W^1_{23} = \frac{\hbar^2 A}{4}\begin{pmatrix}0&1&0&0\end{pmatrix}\begin{pmatrix}\ast\end{pmatrix}\begin{pmatrix}0\\0\\1\\0\end{pmatrix} = \frac{\hbar^2 A}{4}\begin{pmatrix}0&1&0&0\end{pmatrix}\begin{pmatrix}0\\2\\-1\\0\end{pmatrix} = \frac{\hbar^2 A}{2}$$

$$W^1_{34} = \frac{\hbar^2 A}{4}\begin{pmatrix}0&0&1&0\end{pmatrix}\begin{pmatrix}0\\0\\0\\1\end{pmatrix} = 0.$$

$$W^1_{13} = \frac{\hbar^2 A}{4}\begin{pmatrix}1&0&0&0\end{pmatrix}\begin{pmatrix}0\\2\\-1\\0\end{pmatrix} = 0$$

$$W^1_{24} = \frac{\hbar^2 A}{4}\begin{pmatrix}0&1&0&0\end{pmatrix}\begin{pmatrix}0\\0\\0\\1\end{pmatrix} = 0.$$

$$W^1_{14} = \frac{\hbar^2 A}{4}(1\,0\,0\,0)\begin{pmatrix}0\\0\\0\\1\end{pmatrix} = 0.$$

Now; for W^2 matrix we get: $\left(\text{let } x = \frac{eB\hbar}{m_e c}\right)$

$$W^2_{11} = x\,(1\,0\,0\,0)\begin{pmatrix}0&0&0&0\\0&1&0&0\\0&0&-1&0\\0&0&0&0\end{pmatrix}\begin{pmatrix}1\\0\\0\\0\end{pmatrix} = x \times 0 = 0$$

$$W^2_{22} = x\,(0\,1\,0\,0)\begin{pmatrix}0&0&0&0\\0&1&0&0\\0&0&-1&0\\0&0&0&0\end{pmatrix}\begin{pmatrix}0\\1\\0\\0\end{pmatrix} = x\,(0\,1\,0\,0)\begin{pmatrix}0\\1\\0\\0\end{pmatrix} = x$$

$$W^2_{33} = x\,(0\,0\,1\,0)\begin{pmatrix}0&0&0&0\\0&1&0&0\\0&0&-1&0\\0&0&0&0\end{pmatrix}\begin{pmatrix}0\\0\\1\\0\end{pmatrix} = x\,(0\,1\,0\,0)\begin{pmatrix}0\\0\\-1\\0\end{pmatrix} = -x.$$

$$W^2_{44} = x\,(0\,0\,0\,1)\begin{pmatrix}0&0&0&0\\0&1&0&0\\0&0&-1&0\\0&0&0&0\end{pmatrix}\begin{pmatrix}0\\0\\0\\1\end{pmatrix} = x \times 0 = 0.$$

$$W^2_{12} = x\,(1\,0\,0\,0)\begin{pmatrix}0\\1\\0\\0\end{pmatrix} = 0.$$

However we don't have to evaluate W^2_{ij} for $i \neq j$.
As ~~W^2 is diagonal~~ $\hat{H}_2$ is diagonal so W_2 is also.

$\hat{W}$ matrix be given by: $W = W^1 + W^2$

$$\Rightarrow W_{ij} = W^1_{ij} + W^2_{ij}$$

$$\therefore W = \alpha\begin{pmatrix}1&0&0&0\\0&-1&2&0\\0&2&-1&0\\0&0&0&1\end{pmatrix} + x\begin{pmatrix}0&0&0&0\\0&1&0&0\\0&0&-1&0\\0&0&0&0\end{pmatrix} \qquad \left(\alpha = \frac{\hbar^2 A}{4},\quad x = \frac{eB\hbar}{m_e c}\right)$$

$$= \begin{pmatrix}\alpha&0&0&0\\0&x-\alpha&2\alpha&0\\0&2\alpha&-x-\alpha&0\\0&0&0&\alpha\end{pmatrix}$$

Clearly two eigenvalues of W are α & α.
for other two eig-vals; we have to solve the eq:

$$\{\lambda - (x-\alpha)\}\{\lambda + (x+\alpha)\} - 4\alpha^2 = 0$$

$\Rightarrow \lambda^2 - \lambda(x-\alpha) + \lambda(x+\alpha) + (-x^2 + \alpha^2 - 4\alpha^2) = 0$

$\cancel{\Rightarrow \lambda^2 - 2\lambda x + (x^2 - 5\alpha^2) = 0.}$

$\cancel{\Rightarrow \lambda = \dfrac{2x \pm \sqrt{4x^2 - 4(x^2 - 5\alpha^2)}}{2}}$

$\cancel{= \dfrac{2x \pm 2\sqrt{x^2 - x^2 + 5\alpha^2}}{2} = x \pm \alpha\sqrt{5}}$

$\Rightarrow \lambda^2 + 2\alpha\lambda - (3\alpha^2 + x^2) = 0.$

$$\therefore \lambda = \frac{-2\alpha \pm \sqrt{4\alpha^2 + 4(3\alpha^2 + x^2)}}{2}$$

$$= \frac{-2\alpha \pm \sqrt{16\alpha^2 + 4x^2}}{2} = \frac{-2\alpha \pm 2\sqrt{x^2 + 4\alpha^2}}{2}$$

$$= -\alpha \pm \sqrt{x^2 + 4\alpha^2}$$

$\therefore$ The energy values are:

$\epsilon_1 = \alpha$; $\epsilon_2 = \alpha$

$\epsilon_3 = -\alpha + \sqrt{x^2 + 4\alpha^2}$; $\epsilon_4 = -\alpha - \sqrt{x^2 + 4\alpha^2}$. **Ans**

Clearly $-\alpha \pm \sqrt{x^2 + 4\alpha^2} = -\alpha \pm x\sqrt{1 + \dfrac{4\alpha^2}{x^2}}$

letting $\alpha \ll x$: $\simeq -\alpha \pm x\left(1 + \dfrac{1}{2}\cdot\dfrac{4\alpha^2}{x^2}\right)$

$$\simeq \pm x\left(1 \mp \frac{\alpha}{x} + \frac{2\alpha^2}{x^2}\right)$$

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$\therefore$ upto 2nd order approximation of α/x:

$$\epsilon_1 = \alpha \,;\; \epsilon_2 = \alpha \,;\; \epsilon_3, \epsilon_4 = \pm x\left(1 \mp \frac{\alpha}{x} + \frac{2\alpha^2}{x^2}\right)$$

$$\left(\alpha = \frac{\hbar^2 A}{4} \,;\; x = \frac{eB\hbar}{m_e c}\right)$$

Ans

Using perturbation :—

$$\hat{H} = \underbrace{\frac{eB}{m_e c}\left(S_1^z - S_2^z\right)}_{H_0} + \underbrace{A\left(\vec{S_1}\cdot\vec{S_2}\right)}_{H' = \text{perturbation}}$$

The eigenstate of H_0 are $|++\rangle; |+-\rangle; |-+\rangle, |--\rangle$.

& $$H_0|++\rangle = \frac{eB}{m_e c}\left(\frac{\hbar}{2} - \frac{\hbar}{2}\right) = 0$$

$$H_0|+-\rangle = \frac{eB}{m_e c}\left(\frac{\hbar}{2} + \frac{\hbar}{2}\right) = \frac{eB\hbar}{m_e c} = x$$

$$H_0|-+\rangle = \frac{eB}{m_e c}\left(-\frac{\hbar}{2} - \frac{\hbar}{2}\right) = -\frac{eB\hbar}{m_e c} = -x.$$

$$H_0|--\rangle = \frac{eB}{m_e c}\left(-\frac{\hbar}{2} + \frac{\hbar}{2}\right) = 0.$$

Now, $H' = A\vec{S_1}\cdot\vec{S_2}$.

~~Here $\vec{S} = \vec{S_1} + \vec{S_2}$ is conserved, as there is~~
~~any external torque~~

Now, $\vec{S_1} + \vec{S_2} = \vec{S}$ (let)

$$\rightarrow S^2 = S_1^2 + S_2^2 + 2\vec{S_1}\cdot\vec{S_2}$$

$$\rightarrow \vec{S_1}\cdot\vec{S_2} = \frac{S^2 - S_1^2 - S_2^2}{2}.$$

$\therefore$ The eig-states of $\vec{S_1}\cdot\vec{S_2}$ are simultaneously eig-states of S^2, S_1^2, S_2^2.

i.e $$|10\rangle = \frac{|+-\rangle + |-+\rangle}{\sqrt{2}} \; ; \; |11\rangle = |++\rangle$$
$$|00\rangle = \frac{|+-\rangle - |-+\rangle}{\sqrt{2}} \; ; \; |1-1\rangle = |--\rangle \quad \cdots (1)$$

~~for; $|\psi\rangle = |11\rangle$~~

$$\cancel{\langle\psi|H'|\psi\rangle = \frac{1^2 - \left(\frac{1}{2}\right)^2 - \left(\frac{1}{2}\right)^2}{2} \times A\hbar^2 = \frac{\left(1-\frac{1}{2}\right)A\hbar^2}{2} = \frac{A\hbar^2}{4} = \alpha}$$

$$\cancel{\left(\langle\vec{S_1}\cdot\vec{S_2}\rangle = \frac{\langle S^2 - S_1^2 - S_2^2\rangle}{2}\right.}$$

Now, the amount of perturbed energy in state $|\psi\rangle$ given by (1) be:

$$\langle H'\rangle\Big|_{|\psi\rangle} = \langle\psi|H'|\psi\rangle = A\langle\vec{S_1}\cdot\vec{S_2}\rangle_{|\psi\rangle}$$
$$= \frac{A}{2}\langle S^2 - S_1^2 - S_2^2\rangle = \frac{A}{2}\left(s(s+1) - \frac{3}{4} - \frac{3}{4}\right)\hbar^2$$
$$= \frac{A}{2}\left(s(s+1) - \frac{3}{2}\right)\hbar^2$$

for $|\psi\rangle = |11\rangle; |10\rangle; |1-1\rangle$:

$$\langle H'\rangle = \frac{A\hbar^2}{2}\left(2 - \frac{3}{2}\right) = \frac{A\hbar^2}{4} = \alpha$$

$|\psi\rangle = |00\rangle$:

$$\langle H'\rangle = \frac{A\hbar^2}{2}\left(0 - \frac{3}{2}\right) = -\frac{3A\hbar^2}{4}.$$

The eig-states of H' are simultaneous eig-states of S^2, S_1^2, S_2^2. The states are:

$$\left.\begin{array}{l} |11\rangle = |++\rangle \; ; \; |10\rangle = \dfrac{|+-\rangle + |-+\rangle}{\sqrt{2}} \\ |00\rangle = \dfrac{|+-\rangle - |-+\rangle}{\sqrt{2}} \; ; \; |1\,-1\rangle = |--\rangle \end{array}\right\}$$

So; $|+-\rangle = \dfrac{|10\rangle + |00\rangle}{\sqrt{2}}$; $|-+\rangle = \dfrac{|10\rangle - |00\rangle}{\sqrt{2}}$.

Now; $\langle ++|H'|++\rangle = \langle 11|H'|11\rangle$

$$= \frac{A}{2}\langle 11|\left(S^2 - S_1^2 - S_2^2\right)|11\rangle$$

$$= \frac{A\hbar^2}{2}\langle 11|\,2 - \tfrac{3}{2}\,|11\rangle = \frac{A\hbar^2}{4} = \alpha$$

Similarly:

$$\langle --|H'|--\rangle = \langle 1\,-1|H'|1\,-1\rangle = \alpha.$$

And, $\langle +-|H'|+-\rangle = \dfrac{\langle 10| + \langle 00|}{\sqrt{2}}\left(H'\right)\left(\dfrac{|10\rangle + |00\rangle}{\sqrt{2}}\right)$

$$= \frac{A}{4}\left(\langle 10| + \langle 00|\right)\left(S^2 - \frac{3\hbar^2}{2}\right)\left(|10\rangle + |00\rangle\right)$$

$$= \frac{A\hbar^2}{4}\left(\langle 10| + \langle 00|\right)\left(\left(2 - \frac{3}{2}\right)|10\rangle + \left(0 - \frac{3}{2}\right)|00\rangle\right)$$

$$= \frac{A\hbar^2}{4}\left(\langle 10| + \langle 00|\right)\left(\frac{1}{2}|10\rangle - \frac{3}{2}|00\rangle\right)$$

$$= \frac{A\hbar^2}{4}\left(\frac{1}{2} - \frac{3}{2}\right) = -\frac{A\hbar^2}{4} = -\alpha.$$

Similarly: $\langle -+| H' | -+\rangle$

$$= \frac{A\hbar^2}{4}\left(\langle 10| - \langle 00|\right)\left(\frac{1}{2}|10\rangle + \frac{3}{2}|00\rangle\right)$$

$$= \frac{A\hbar^2}{4}\left(\frac{1}{2} - \frac{3}{2}\right) = -\frac{A\hbar^2}{4} = -\alpha.$$

So upto first order perturbation the energy of the states are: (the left states are although not modifies eig-states.)

$$|++\rangle \longrightarrow 0 + \alpha = \alpha$$

$$|--\rangle \longrightarrow 0 + \alpha = \alpha$$

$$|+-\rangle \longrightarrow x - \alpha = x\left(1 - \frac{\alpha}{x}\right)$$

$$|-+\rangle \longrightarrow -x - \alpha = -x\left(1 + \frac{\alpha}{x}\right)$$

Ans

i.e $\epsilon_1 = \epsilon_2 = \alpha$; $\epsilon_3, \epsilon_4 = \pm x\left(1 \mp \frac{\alpha}{x}\right)$

The result is completely same (upto first order correction) with the exact value of ϵ given by diagonalization evaluated before

Proved

5. b. For the given atomic Hydrogen:

$$H = \underbrace{A\,\vec{S_1}\cdot\vec{S_2}}_{H_1} + \underbrace{\frac{eB}{m_e c}\left(\vec{S_1}\cdot\vec{B}\right)}_{H_2}$$

Here $A\vec{S}_1\cdot\vec{S}_2 = \frac{A\hbar^2}{4}\begin{pmatrix}1&0&0&0\\0&-1&2&0\\0&2&-1&0\\0&0&0&1\end{pmatrix}$ (evaluated before).

$$H_2^0 = \frac{eB}{m_e c}\,\vec{S}_1\cdot\vec{B} = \frac{eB^2}{m_e c}\,S_1^z$$

$$S_1^z = S_1^z \otimes \mathbb{I}_{S_2} = \frac{\hbar}{2}\begin{pmatrix}1&0\\0&-1\end{pmatrix}\otimes\begin{pmatrix}1&0\\0&1\end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix}1&&&0\\&1&&\\&&-1&\\0&&&-1\end{pmatrix}$$

$$\therefore\ H_2^0 = \frac{eB^2\hbar}{2m_e c}\begin{pmatrix}1&&&0\\&1&&\\&&-1&\\0&&&-1\end{pmatrix}$$

$$\text{So; } \hat{H} = \underbrace{\frac{A\hbar^2}{4}}_{\alpha}\begin{pmatrix}1&0&0&0\\0&-1&2&0\\0&2&-1&0\\0&0&0&1\end{pmatrix} + \underbrace{\frac{eB^2\hbar}{2m_e c}}_{\eta}\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&-1&0\\0&0&0&-1\end{pmatrix}$$

$$= \alpha\begin{pmatrix}1&0&0&0\\0&-1&2&0\\0&2&-1&0\\0&0&0&1\end{pmatrix} + \eta\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&-1&0\\0&0&0&-1\end{pmatrix}$$

$$= \begin{array}{c c}\begin{pmatrix}\alpha+\eta&0&0&0\\0&\eta-\alpha&2\alpha&0\\0&2\alpha&-\eta-\alpha&0\\0&0&0&\alpha-\eta\end{pmatrix} & \begin{matrix}|++\rangle\\|+-\rangle\\|-+\rangle\\|--\rangle\end{matrix}\\ \begin{matrix}\langle ++| & \langle +-| & \langle -+| & \langle --|\end{matrix} & \end{array}$$

clearly two eigenvalues of H are: $\alpha\pm\eta$

for other two values we have to solve the eq:

$$\{\lambda-(\eta-\alpha)\}\{\lambda+(\eta+\alpha)\} - 4\alpha^2 = 0.$$

$$\Rightarrow \lambda^2 - \lambda(\eta-\alpha) + \lambda(\eta+\alpha) - \eta^2 + \alpha^2 - 4\alpha^2 = 0.$$

$$\Rightarrow \lambda^2 + 2\alpha\lambda - \eta^2 - 3\alpha^2 = 0.$$

$$\therefore\ \lambda = \frac{-2\alpha \pm \sqrt{4\alpha^2 + 4(3\alpha^2+\eta^2)}}{2} = \frac{-2\alpha \pm 2\sqrt{\eta^2+4\alpha^2}}{2}$$

$$= -\alpha \pm \sqrt{\eta^2 + 4\alpha^2}.$$

So; the energy eigenvalues of $\hat{H}$ are:

$$\left.\begin{aligned} \epsilon_1 &= \alpha + \eta \\ \epsilon_2 &= \alpha - \eta \\ \epsilon_3 &= -\alpha + \sqrt{\eta^2 + 4\alpha^2} \\ \epsilon_4 &= -\alpha - \sqrt{\eta^2 + 4\alpha^2} \end{aligned}\right\} \quad \underline{\underline{\text{Ans}}} \;\cdots\cdots\; (A)$$

These are although the exact answer.

Using perturbation:-

$$\hat{H} = \underbrace{\eta \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}}_{H^0} + \underbrace{\alpha \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 2 & 0 \\ 0 & 2 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}}_{H'}$$

Clearly the eigenstates of H^0 are $|+\pm\rangle, |-\pm\rangle$.
with energy eig-val $\eta;\ \eta;\ -\eta;\ -\eta$.

Now the 1st order correction term due to H' for the state $|i\rangle$ be: $\langle i|H'|i\rangle$.

$\therefore$ for $|i\rangle = |++\rangle$:

$$\epsilon' = \alpha\,(1\,0\,0\,0) \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 2 & 0 \\ 0 & 2 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} = \alpha\,(1\,0\,0\,0) \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} = \alpha$$

for $|--\rangle$:

$$\epsilon' = \alpha\,(0\,0\,0\,1) \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 2 & 0 \\ 0 & 2 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} = \alpha\,(0\,0\,0\,1) \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} = \alpha.$$

for $|i\rangle = |+-\rangle$:

$$\varepsilon' = \alpha\,(0\,1\,0\,0)\begin{pmatrix}1&0&0&0\\0&-1&2&0\\0&2&-1&0\\0&0&0&1\end{pmatrix}\begin{pmatrix}0\\1\\0\\0\end{pmatrix} = \alpha\,(0\,1\,0\,0)\begin{pmatrix}0\\-1\\2\\0\end{pmatrix} = -\alpha$$

for $|-+\rangle$:

$$\varepsilon' = \alpha\,(0\,0\,1\,0)\begin{pmatrix}1&0&0&0\\0&-1&2&0\\0&2&-1&0\\0&0&0&1\end{pmatrix}\begin{pmatrix}0\\0\\1\\0\end{pmatrix} = \alpha\,(0\,0\,1\,0)\begin{pmatrix}0\\2\\-1\\0\end{pmatrix} = -\alpha$$

So first order correction gives the correction:

$$\left.\begin{array}{lll}|++\rangle \longrightarrow & \varepsilon_1 = \eta + \alpha \\ |--\rangle \longrightarrow & \varepsilon_2 = -\eta + \alpha \\ |+-\rangle \longrightarrow & \varepsilon_3 = \eta - \alpha \\ |-+\rangle \longrightarrow & \varepsilon_4 = -\eta - \alpha\end{array}\right\}$$

Ans

(with modified eig-states undetermined)

The answer is true (upto first order $\frac{\alpha}{\eta}$ correction) and matches with values given by eigenvalue of full Hamiltonian $\hat{H} = H^0 + H'$

$$\left(\because -\alpha \pm \sqrt{\eta^2 + 4\alpha^2} = -\alpha \pm \eta\left(1 + 4\frac{\alpha^2}{\eta^2}\right)^{1/2}\right.$$

$$\simeq -\alpha \pm \eta\left(1 - \frac{2\alpha^2}{\eta^2} + \cdots\right)$$

$$\left.\simeq \pm\eta\left(1 \mp \frac{\alpha}{\eta} - \frac{2\alpha^2}{\eta^2}\right)\right)$$

Proved

8. Time dependent perturbation for two state system :-

$$H'(t) = V(t) = \lambda \cos(\omega t)$$

If $|\psi(t)\rangle = C_a(t)|1\rangle + C_b(t)|2\rangle$ then; at time t; $C_b(t)$ be as given $C_a(0) = 1$; then at time t; $C_b(t)$ be given by the formula: (first order)

$$C_b'(t) = -\frac{i}{\hbar}\int_0^t \langle 2|H'|1\rangle e^{i\omega_0 t}\, dt.$$

$$= -\frac{i}{\hbar}\int_0^t \lambda \cos(\omega t)\, e^{i\omega_0 t}\, dt.$$

$$\left(\omega_0 = (E_2^0 - E_1^0)/\hbar\right)$$

$$= -\frac{i\lambda}{2\hbar}\int_0^t \left\{e^{i(\omega+\omega_0)t} + e^{i(\omega_0-\omega)t}\right\} dt.$$

$$= -\frac{\lambda}{2\hbar}\left\{\frac{e^{i(\omega_0+\omega)t}-1}{\omega_0+\omega} + \frac{e^{i(\omega_0-\omega)t}-1}{\omega_0-\omega}\right\}$$

As $E_2^0 - E_1^0$ is not close to $\hbar\omega$
i.e $|\omega - \omega_0| \gg 0$ so we cant neglect any term.

However simplyfying $C_b'(t)$ in mathematica and evaluating the absolute value we get the probability (first order) to get the system in state $|2\rangle$ at time t i.e $\left|C_b^1(t)\right|^2 = P_{1\to 2}(t)$

$$= \frac{\chi^2}{2\hbar^2(\omega_0^2-\omega^2)}\Big[3\omega_0^2 - \omega^2 - 2\omega\omega_0\cos\{(\omega_0-\omega)t\}$$

$$-4\omega_0^2\cos(\omega_0 t)\cos(\omega t) + \cos(2\omega t)(\omega_0^2-\omega^2)$$

$$+2\omega_0\omega\cos\{(\omega_0+\omega)t\}\Big]$$

Ans

And the transcition ~~probabi~~ rate be given by:

$$R(t) = \frac{\partial P_{1\to 2}}{\partial t}$$

$$= \frac{\chi^2}{2\hbar^2(\omega_0^2-\omega^2)}\Big[4\omega_0^3\cos(\omega_0 t)\sin(\omega_0 t) +$$

$$2\omega_0(\omega_0-\omega)\omega\sin\{(\omega_0-\omega)t\} + 4\omega_0^2\omega\cos(\omega_0 t).$$

$$\sin(\omega t) - 2\omega_0^2\omega\sin(2\omega t) +$$

$$2\omega^3\sin(2\omega t) - 2\omega_0\omega(\omega+\omega_0)\sin\{(\omega+\omega_0)t\}\Big]$$

Ans

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Problem: 10

The particle was confined in infinite square well before introducing the perturbation.

Now (as not mentioned) I assume the particle start from ground state at time $t=0$.

The goal is to find transition probability and rate at time t; from ground state to 1st excited state.

Applying the formula for time dependent perturbation we get the probability amplitude be given by:

$$C_1(t) = -\frac{i}{\hbar}\int_0^t \langle \psi_1 | H' | \psi_0 \rangle e^{i t \Omega_1} dt.$$

(upto first order correction)

Here $H'(t) = \lambda(1+x)e^{-i\omega_0 t}$

$$\Omega_1 = \frac{E_1 - E_0}{\hbar} = \frac{(2^2-1^2)\pi^2\hbar}{2mL^2} = \frac{3\pi^2\hbar}{2mL^2}$$

$$\psi_0 = \sqrt{\frac{2}{L}}\sin\left(\frac{\pi x}{L}\right); \quad \psi_1 = \sqrt{\frac{2}{L}}\sin\left(\frac{2\pi x}{L}\right)$$

$$\therefore \langle \psi_1 | H' | \psi_0 \rangle = \langle \psi_1 | \lambda(1+x)e^{-i\omega_0 t} | \psi_0 \rangle$$

$$= \lambda e^{-i\omega_0 t}\left\{ \underbrace{\cancel{\langle \psi_1 | \psi_0 \rangle}}_{0} + \langle \psi_1 | x | \psi_0 \rangle \right\}$$

Now, $\langle \psi_1 | x | \psi_0 \rangle = \int_0^L \frac{2}{L} x \sin\left(\frac{\pi x}{L}\right) \sin\left(\frac{2\pi x}{L}\right) dx$

$$= -\frac{16L}{9\pi^2} \quad \text{(from Mathematica)}$$

So; $C_{1\to 2}(t) = +\frac{i}{\hbar} \times \frac{16L}{9\pi^2} \int_0^t \lambda e^{i(\Omega - \omega_0)t} dt$.

$$= \frac{16\lambda L i}{9\pi^2 \hbar} \left\{ \int_0^t \left(\cos(\Omega - \omega_0)t + i \sin(\Omega - \omega_0)t \right) dt \right\} \quad \cdots (1)$$

The ~~transmission~~ transcition probability be given by: $P_{1\to 2} = |C_{1\to 2}(t)|^2$

from expression (1) using mathematica I found out the integral to be given by:

$$\boxed{\cancel{P_{1\to 2} = \left(\frac{16L\lambda}{9\pi^2 (\Omega - \omega_0)\hbar}\right)^2 \times \left(\cos^2(\Omega - \omega_0)t + \sin^2(\Omega - \omega_0)t\right)}}$$

$$P_{1\to 2}(t) = \frac{512 L^2 \lambda^2}{81 \pi^4 \hbar^2 (\Omega - \omega_0)^2} \left\{ -\cos((\Omega - \omega_0)t) + 1 \right\}$$

And the transcition rate:

$$R_{1\to 2}(t) = \frac{\partial P}{\partial t} = \frac{512 L^2 \lambda^2 \sin((\Omega - \omega_0)t)}{81 \pi^4 \hbar^2 (\Omega - \omega_0)}$$

Ans

(L = length of infinite sq well
$\Omega = \frac{3\hbar\pi^2}{2ma^2}$)

VI Problem: 11

Quantum H.O in time dependent field :-

Here let the freq of the original H.O be ω_0.

$\therefore \quad E_n^{\text{original}} = \left(n + \frac{1}{2}\right)\hbar\omega_0.$

Assuming the system starts ~~at~~ from state $|0\rangle$; the prob amplitude to find it in state $|1\rangle$ at time t be given by: (upto first order):

$$C_1(t) = -\frac{i}{\hbar}\int_0^t \langle 1|H'|0\rangle e^{i\Omega_1 t}\, dt$$

$$\Omega_1 = \frac{(E_1 - E_0)}{\hbar} = \frac{\hbar\omega_0}{\hbar} = \omega_0$$

$$H' = \frac{eE_0}{2}\left[\frac{p}{m\omega}\sin\omega t - x\cos\omega t\right]$$

$$\therefore \langle 1|H'|0\rangle = \frac{eE_0}{2}\left[\frac{p}{m\omega}\sin\omega t\cdot \underbrace{\cancel{\langle 1|0\rangle}}_{0} - \cos(\omega t)\cdot\langle 1|x|0\rangle\right]$$

$$= -\frac{eE_0}{2}\cos(\omega t)\cdot\langle 1|x|0\rangle.$$

Now; $$\langle 1|x|0\rangle = \sqrt{\frac{\hbar}{2m\omega_0}}\langle 1|(a_+ + a_-)|0\rangle$$

$$= \sqrt{\frac{\hbar}{2m\omega_0}}\left(\langle 1|1\rangle + \langle 1|\times 0\right) = \sqrt{\frac{\hbar}{2m\omega_0}}$$

$$\therefore \langle 1|H'|0\rangle = -\frac{eE_0}{2}\cdot\sqrt{\frac{\hbar}{2m\omega_0}}\cdot\cos(\omega t)$$

So; $$C_{0\to 1}(t) = \frac{ieE_0}{2\hbar}\sqrt{\frac{\hbar}{2m\omega_0}}\int_0^t \cos(\omega t)\cdot e^{i\omega_0 t}\, dt.$$

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$$= \frac{i e E_0}{2\sqrt{2m\omega_0\hbar}} \times \cancel{\frac{1}{2}} \int_0^t \left\{ \cos(\omega t)\cdot\cos(\omega_0 t) + i\,\cos(\omega t)\cdot\sin(\omega_0 t) \right\} dt.$$

The probability to find the system in state $|1\rangle$ is $P_{0\to1}(t) = |C_{1\to2}(t)|^2$; And the rate is given by:

$$R_{0\to1}(t) = \frac{\partial P}{\partial t}$$

Using mathematica I've calculated the value $R_{0\to1}$ to be

$$R_{0\to1}(t) = \frac{\partial |C_{0\to1}|^2}{\partial t}$$

(The intermediate expressions are very long & I've not written down here. They are in Mathematica file. I've sent the file too.)

$$= \frac{e^2 E_0^2}{16\, m\,\omega_0 \hbar\,(\omega^2-\omega_0^2)^2}\Big[4\omega_0^3\cos(\omega t)\sin(\omega_0 t) + 2\omega_0(\omega_0-\omega)\,\omega\sin((\omega_0-\omega)t) + 4\omega\omega_0^2\cos(\omega_0 t)\sin(\omega t) - 2\omega\omega_0^2\sin(2\omega t) + 2\omega^3\sin(2\omega t) - 2\omega\omega_0(\omega+\omega_0)\sin((\omega+\omega_0)t)\Big]$$

Ans

Problem: 7: Charged particle in magnetic field.

In presence of magnetic field $\vec{B} = \vec{B}(x,y,z)$; the Hamiltonian is given by: (in Gaussian unit):

$$H = \frac{(\vec{p} - e\vec{A}/c)^2}{2m} = \frac{\vec{\pi}^2}{2m} \quad ; \quad \vec{\pi} = \vec{p} - \frac{e\vec{A}}{c} = m\vec{v} \quad (\vec{B} = \vec{\nabla}\times\vec{A})$$

Now, $$\frac{d\vec{\pi}}{dt} = \frac{i}{\hbar}[H, \vec{\pi}] \quad \text{i.e} \quad \frac{d\pi_i}{dt} = \frac{i}{\hbar}[H, \pi_i]$$

$\left(\because \vec{\pi} = \vec{\pi}(x,y,z) \Rightarrow \frac{\partial \vec{\pi}}{\partial t} = 0 \text{ i.e the magnetic field is only space varying; not time varying.}\right)$

Now, $$[H, \pi_i] = \left[\frac{\pi^2}{2m}, \pi_i\right] = \sum_j \frac{1}{2m}[\pi_j^2, \pi_i]$$

$$= \frac{1}{2m}\sum_j \left\{\pi_j[\pi_j, \pi_i] + [\pi_j, \pi_i]\pi_j\right\}$$

Now, $$[\pi_i, \pi_j] = \left[p_i - \frac{eA_i}{c}, p_j - \frac{eA_j}{c}\right]$$

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

$(\because A_i = A_i(x,y,z) \ \& \ [r_i, r_j] = 0)$

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

$$\therefore [H, \pi_x] = \frac{1}{2mc}\Big(\pi_y[\pi_y, \pi_x] + [\pi_y, \pi_x]\pi_y + \pi_z[\pi_z, \pi_x] + [\pi_z, \pi_x]\pi_z\Big)$$

$$= \frac{1}{2mc}\times i\hbar e\left(-B_z\pi_y - \pi_y B_z + \pi_z B_y + B_y\pi_z\right)$$

$$= \frac{i\hbar e}{2mc}\Big((p_z - eA_z)B_y + B_y(p_z - eA_z) - B_z(p_y - eA_y) - (p_y - eA_y)B_z\Big)$$

$$= \frac{i\hbar e}{2mc}\Big[p_zB_y + B_yp_z - 2eA_zB_y - B_zp_y - p_yB_z + 2eA_yB_z\Big]$$

$(\because [B_i, A_j] = 0)$

$$= \frac{i\hbar e}{2mc}\left(2\pi_z B_y - 2\pi_y B_z + [B_y, \pi_z] - [B_z, \pi_y]\right)$$

But $[B_i, \pi_j] = [B_i, p_j - \frac{eA_j}{c}] = [B_i, p_j] = i\hbar \frac{\partial B_i}{\partial x_j}$

~~So; $[H, \pi_x] = \frac{i\hbar}{2m}\left(2p_z B_y - 2eA_z B_y - 2\right.$~~

So; $$[H, \pi_x] = \frac{i\hbar e}{2mc}\left[2(\pi_z B_y - \pi_y B_z) + i\hbar\left(\frac{\partial B_y}{\partial x_z} - \frac{\partial B_z}{\partial x_y}\right)\right]$$

$$= \frac{-2i\hbar e}{2mc}(\vec{\pi} \times \vec{B})_x + \frac{i^2\hbar^2 e}{2mc}(-\vec{\nabla} \times \vec{B})_x$$

$$= -\frac{\cancel{2}i\hbar e}{\cancel{2}mc}(\vec{\pi} \times \vec{B})_x - \frac{e\hbar^2}{2mc}(\vec{\nabla} \times \vec{B})_x$$

So $$[H, \vec{\pi}] = -\frac{\cancel{2}i\hbar e}{\cancel{2}mc}(\vec{\pi} \times \vec{B}) - \frac{e\hbar^2}{2mc}(\vec{\nabla} \times \vec{B})$$

i.e $$\frac{d\vec{\pi}}{dt} = \frac{i}{\hbar}[H, \vec{\pi}] = \frac{e}{mc}(\vec{\pi} \times \vec{B}) + \frac{ie\hbar}{2mc}(\vec{\nabla} \times \vec{B})$$

Using $\vec{\pi} = m\vec{v}$ we get:

$$\boxed{\frac{d\vec{v}}{dt} = \frac{i}{\hbar}[H, \vec{v}] = \frac{e}{c}(\vec{v} \times \vec{B}) + \frac{ie\hbar}{2m^2c}(\vec{\nabla} \times \vec{B})}$$

Proved

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

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

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

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

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

$= \sum_i [p_i, A_i]$

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:

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

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

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

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

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

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

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

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

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

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

$\therefore\ [a^+, a] = 1.$ or $[a, a^+] = 1.$

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

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

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

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

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

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

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

VIII Eigenstates:-

The Schrodinger eq be given by

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

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)

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

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

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

This is TISE of the form:

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

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 energy levels are infinitely degenerate. These are the so called Landau Levels.

14. Hypothetical He Atom :-

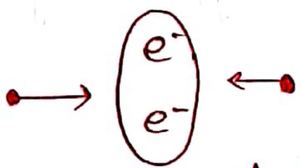
As they are spin 1 particles, so they will follow B-E statistics and will form symmetric ground state.

Now symmetric ground state can be formed in two ways

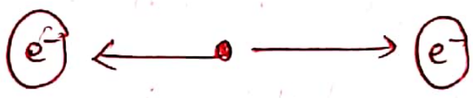
i) Symmetric spacial configuration and symmetric spin configuration.

ii) Antisymmetric spacial and Antisymmetric spin configuration.

As Antisymmetrisation gives separation so that's not energitically favourable & do not form less energy ground state. Symmetrisation needs less energy ground state. Symmetrisation is the true ground state of He & hence ① is the true ground state of He



Symmetrisation
= Closeness



Antisymmetrization
= Separation.

Ignoring the hyperfine structure without any calculation we can tell that for spin 1 particles; we get symmetrization of 2 spin 1 particles (i.e more than one possibility.)

$s = s_1 + s_2 = 0, 1, 2$

So clearly there will be degeneracy.

From clebsch Gordon table we get :

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

Symmetric (+ve in interchange)

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$$|2\ 2\rangle = |1\,1\rangle|1\,1\rangle$$

$$|2\ 0\rangle = \frac{1}{\sqrt{6}}\left(|1\,1\rangle|1\,\bar{1}\rangle + |1\,\bar{1}\rangle|1\,1\rangle\right) - \sqrt{\frac{2}{3}}\,|1\,0\rangle|1\,0\rangle$$

$$|2\ 1\rangle = \frac{1}{\sqrt{2}}\left(|1\,0\rangle|1\,1\rangle + |1\,1\rangle|1\,0\rangle\right)$$

$$|2\ \bar{1}\rangle = \frac{1}{\sqrt{2}}\left(|1\,0\rangle|1\,\bar{1}\rangle + |1\,\bar{1}\rangle|1\,0\rangle\right)$$

$$|2\,{-2}\rangle = |1\,\bar{1}\rangle|1\,\bar{1}\rangle$$

Symmetric

$$|1\ 1\rangle = \frac{1}{\sqrt{2}}\left(|1\,1\rangle|1\,0\rangle - |1\,0\rangle|1\,1\rangle\right)$$

$$|1\ \bar{1}\rangle = \frac{1}{\sqrt{2}}\left(|1\,{-1}\rangle|1\,0\rangle - |1\,0\rangle|1\,\bar{1}\rangle\right)$$

$$|1\ 0\rangle = \frac{1}{\sqrt{2}}\left(|1\,\bar{1}\rangle|1\,1\rangle - |1\,1\rangle|1\,\bar{1}\rangle\right)$$

Anti Symmetric (due to −ve sign in interchange)

So the ground state of that He is 6 fold degenerate; for which the spacial wave fn be given by:

$$\psi^{sp}_{He} = \psi_g(r_1)\,\psi_g(r_2).$$

Ans

And spin part: $\chi_{He} = |0\,0\rangle, |2, (0, \pm 1, \pm 2)\rangle$

For normal He it's not degenerate as for spin $\frac{1}{2}$ particle the only antisymmetric (needed for spin $\frac{1}{2}$ Fermion) state is $|0\,0\rangle$. Which has only one l_z value.

$2\times 0 + 1 = 1 \rightarrow$ no degeneracy.

Problem: 6

i) For the 1d box of length L, with 3 non interacting spin $\frac{1}{2}$ distinguishable particles the first 3 lowest possible states will be:

$$E_1 = 3 \times \left(\frac{\pi^2 n^2 \hbar^2}{2mL^2}\right)_{n=1} = \frac{3\pi^2\hbar^2}{2mL^2}$$ no degeneracy

A B C
o o o $n = 1$ i.e. $\Psi_g = \psi_0(r_1) \cdot \psi_0(r_2)\, \psi_0(r_3)$

(As the particles are distinguishable so there's no quantum indistinguishability & hence no antisymmetrization needed. So any no of particle can stay in one single state.)

$$E_2 = \frac{2^2\pi^2\hbar^2}{2mL^2} \times 1 + \frac{1^2\pi^2\hbar^2}{2mL^2} \times 2 = \frac{6\pi^2\hbar^2}{2mL^2}$$

$n=2$: A ; $n=1$: B C   or $n=2$: B ; $n=1$: A C   or $n=2$: C ; $n=1$: A B

$$\left.\begin{array}{l} \Psi_{1st\ ex} = \psi_0(r_1)\, \psi_0(r_2)\, \psi_1(r_3) \\ \text{or} \\ \psi_1(r_1)\, \psi_0(r_2)\, \psi_0(r_3) \\ \text{or} \\ \psi_0(r_1)\, \psi_1(r_2)\, \psi_0(r_3) \end{array}\right\} \text{degeneracy} = 3.$$

$$E_3 = 2 \times \frac{2^2\pi^2\hbar^2}{2mL^2} + \frac{\pi^2\hbar^2}{2mL^2} = \frac{9\pi^2\hbar^2}{2mL^2}$$

$n=2$: A B ; $n=1$: C | $n=2$: B C ; $n=1$: A | $n=2$: C A ; $n=1$: B $\longrightarrow$ degeneracy $= 3$.

$$\psi_{2nd\ excited} = \psi_0(r_1)\,\psi_1(r_2)\,\psi_1(r_3)$$
or
$$\psi_1(r_1)\,\psi_0(r_2)\,\psi_1(r_3)$$
or
$$\psi_1(r_1)\,\psi_1(r_2)\,\psi_0(r_3)$$
$\Rightarrow$ 3 states.

ii) In case of 4 distinguishable non interacting particle:

$$E_1 = \frac{4\pi^2\hbar^2}{2mL^2} = \frac{2\pi^2\hbar^2}{mL^2} \longrightarrow \underline{\ A\ B\ C\ D\ }\ \ n=1.$$

$$\psi_g = \psi_0(r_1)\,\psi_0(r_2)\,\psi_0(r_3)\,\psi_0(r_4) \longrightarrow \text{no degeneracy.}$$

$$E_2 = \frac{3\pi^2\hbar^2}{2mL^2} + \frac{4\pi^2\hbar^2}{2mL^2} = \frac{7\pi^2\hbar^2}{2mL^2}$$

D	A	B	C
A B C	B C D	C D A	A D B

$$\psi_{first\ excited} = \psi_0(r_1)\,\psi_0(r_2)\,\psi_0(r_3)\,\psi_1(r_4)$$
$\vdots$
4 permutations

degeneracy = 4 fold.

$$E_3 = 2\times\frac{4\pi^2\hbar^2}{2mL^2} + 2\frac{\pi^2\hbar^2}{2mL^2} = \frac{10\pi^2\hbar^2}{2mL^2} = \frac{5\pi^2\hbar^2}{mL^2}.$$

A B	B C	A C	A D	B D	C D
C D	A D	B D	B C	A C	A B

$$\psi_{2nd\ excited} = \psi_0(r_1)\,\psi_0(r_2)\,\psi_1(r_3)\,\psi_1(r_4)$$
$\vdots$
total 6 permutations

6 fold degeneracy.

12. H atom in external $\vec{E}$ field :-

given $\left.\begin{aligned} \vec{E} &= E_0 e^{-\Gamma t}\hat{k} & t \geq 0 \\ &= 0 & t < 0 \end{aligned}\right\}$

So for $t \geq 0$; applying $\vec{E} = -\vec{\nabla} V$; we get

$$V(t) = -zE_0 e^{-\Gamma t}$$

For the e^- of the H atom; the perturbing field is given by: $V' = eV = -zeE_0 e^{-\Gamma t}$.

Taking E_0 to be small & as the perturbation decreases exponentially with time; we can ~~use~~ use first order perturbation for even large t.

Now, $\langle nlm|V|n'l'm'\rangle \sim \langle nlm|z|n'l'm'\rangle$

$$\sim \int_0^\infty r^3 R_{nl}(r) R_{n'l'}(r)\, dr \cdot \int Y_l^{m*}(\theta,\phi) Y_{l'}^{m'}(\theta\,\phi) \cos\theta \sin\theta\, d\theta\, d\phi$$

The ϕ integral gives: $\sim \int_0^{2\pi} e^{i(m-m')\phi}\, d\phi$

$\neq 0$ iff $m = m'$

So for all 2p states; only $|21\,0\rangle$ is involved in perturbation. Other matrix elements are 0.

$$\therefore \langle \underbrace{100}_{\text{state } i}|z|\underbrace{210}_{\text{state } f}\rangle = \int_0^\infty r^3 R_{10} R_{21}\, dr \int Y_0^{0*} Y_1^0 \sin\theta\cos\theta\, d\theta\, d\phi$$

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

$$\times \int_0^\pi \frac{1}{\sqrt{4\pi}} \cdot \sqrt{\frac{3}{4\pi}} \sin\theta \cos^2\theta\, d\theta \int_0^{2\pi} d\phi$$

$$= \frac{2a^{-3}}{a\sqrt{24}} \cdot \frac{256a^5}{81} \times 2\pi \cdot \frac{1}{2\sqrt{3}\pi} = \frac{2^7\sqrt{2}\,a}{3^5}$$

$\therefore$ The transcition amplitude is $(C_{1s\to 2p})$:

$$= -\frac{i}{\hbar}\int_0^t \langle 100|z|210\rangle \cdot \left(-eE_0 e^{-\Gamma t}\right) \cdot e^{i\omega_0 t}\, dt$$

$$= +\frac{i}{\hbar} \cdot eE_0 \times \frac{2^7\sqrt{2}\,a}{3^5} \int_0^t e^{-t(-i\omega_0 + \Gamma)}\, dt. \quad \left(\omega_0 = \frac{E_2 - E_1}{\hbar}\right)$$

$$= \frac{2^7\sqrt{2}\,a e E_0 i}{3^5 \hbar} \int_0^t e^{-\Gamma t}\left(\cos(\omega_0 t) + i\sin(\omega_0 t)\right) dt.$$

Using mathematica the result is given to be:

$$C(t) = \frac{2^7\sqrt{2}\,a e E_0 i}{3^5\hbar}\left[\frac{e^{-\Gamma t}}{\Gamma^2+\omega_0^2}\left(e^{t\Gamma}\cdot\Gamma + \omega_0 \sin(\omega_0 t) - \Gamma\cos(\omega_0 t)\right) + \frac{ie^{-\Gamma t}}{\Gamma^2+\omega_0^2}\cdot\left(\omega_0 e^{\Gamma t} - \Gamma\sin(\omega_0 t) - \omega_0\cos(\omega_0 t)\right)\right]$$

$\therefore$ The transcition probability from $|100\rangle \to |210\rangle$ is:

$$P(t) = |C(t)|^2 \xrightarrow[\text{mathematica}]{\text{using}} \frac{2^{15}a^2}{3^{10}} \cdot \frac{1 + e^{-2\Gamma t} - 2e^{-\Gamma t}\cos(\omega_0 t)}{\Gamma^2 + \omega_0^2}.$$

So transcition rate:

$$R(t) = \frac{\partial P}{\partial t} = \frac{2^{15}a^2}{3^{10}} \times \frac{-2e^{-2\Gamma t}\cdot\Gamma + 2e^{-\Gamma t}\left(\cos(\omega_0 t)\cdot\Gamma + \omega_0\sin(\omega_0 t)\right)}{\Gamma^2+\omega_0^2}.$$

Clearly at $t \to \infty$ limit $\boxed{R(t) \to 0.}$ Ans

This is also clear from the nature of perturbing field. At $t \to \infty$; $V'(t) \to 0$. i.e the perturbation goes off. So there is no new trans~~ition~~cition at very large t. All transcition effectively happens between $t \in [0, T]$ when T is a sufficiently large number.

13. The spectroscopic notation for all states of H $n=1$, $n=2$ be given by:

$n=1 \longrightarrow {}^2S_{1/2}$ (1s)

$n=2 \longrightarrow {}^2S_{1/2}$ (2s)

${}^2P_{3/2}$ (2p ; $j=3/2$)

${}^2P_{1/2}$ (2p ; $j=1/2$)

Ans

14. The given corrections are:

i) fine structure $\longrightarrow$ comes from spin-orbit coupling or L-S coupling (good name) & relativistic effect of the e^- from nucleus frame.

ii) Hyperfine structure $\longrightarrow$ comes from the ~~mag~~ magnetic interaction between e^- & the proton's spin. (if they are parallel ($\uparrow\uparrow / \downarrow\downarrow$) or if they are antiparallel ($\uparrow\downarrow / \downarrow\uparrow$)

(no symmetrization / antisymmetrization as they are distinguishable mutually; i.e. e^- & p)

iii) relativistic effect: comes due to relativistic effect of e^- (included in fine structure)

iv) Lamb shift $\longrightarrow$ comes from vaccume energy fluctuation in different orbitals. It's totally a phenomenon of QED.

Now $E_r = -\frac{\alpha^2 z^4}{4n^4}\left(\frac{4n}{l+\frac{1}{2}} - 3\right) \times 13.6 \text{ eV} \sim \alpha^2$

$$E_{so} = \cancel{\frac{\alpha^2 z^4}{n^3}} \frac{(13.6)^2}{mc^2} \times \frac{n\left[j(j+1) - l(l+1) - \frac{3}{4}\right]}{l(l+1)(l+1/2)} \quad (\text{in eV})$$

$$\sim \alpha^2 \times E_1 \text{ ie } \sim \alpha^4$$

$$E_{hyp} = \frac{4 g_p \hbar^4}{3 m_e m_p a^4 c^2}$$

$$E_{Lamb} = \alpha^5 mc^2 \times \frac{1}{6\pi} \ln\left(\frac{1}{\alpha\pi}\right)$$

i) for $n = 1$ state $(1s)$; E_r is present ; $E_{so} = 0$.
So fine structure is present. (~~at~~ only due to E_r)
$s_e = \pm\frac{1}{2} \Rightarrow$ hyperfine (E_{hyp}) is present.

ii) for $n = 2$: E_r & E_{so} both are non zero. for $l = 1$
$E_r \neq 0$; $E_{so} = 0$ for $l = 0$

so as E_r is always so ~~E_A~~ $E_{fs} = E_r + E_{so} \neq 0$.
$\therefore$ fine structure is present.
Hyperfine structure is present.

iii) by order of magnitude strength we get

Answer

$$\underbrace{E_r \sim E_{so} \sim E_{fs}\overset{ie}{(E_r + E_{so})}}_{\sim \alpha^4 m_e c^2} \gg \underset{\sim \alpha^5 mc^2}{E_{Lamb}} > \underset{\sim \frac{m_e}{m_p}\alpha^4 m_e c^2}{E_{hyp}}$$

Problem: 16

From Fermi's rule decay const is given by:

$$\lambda = \frac{2\pi}{\hbar}|M|^2 \rho(E_f) \; ; \quad M = \int \psi_f^* V \psi_i \, d^3x.$$

In the reaction eq: parent nucleus $\rightarrow$ product nucleus $+ e^- + \bar{\nu}$

Let the ~~initial~~ final K.E $= Q$

K.E of product nucleus $= T$

$\therefore$ K.E of $(e^- + \bar{\nu}) = (Q - T)$

Now the no of states of e^- & $\bar{\nu}$ with magnitude of ~~KE~~ momentum between $(p_e$ & $p_e + dp_e)$ and $(p_\nu$ & $p_\nu + dp_\nu)$ are proportional to $4\pi p_e^2 \, dp_e$ & $4\pi p_\nu^2 \, dp_\nu$.

$\therefore$ Total no of momentum states,

$$= A \times 16\pi^2 p_e^2 p_\nu^2 \, dp_e \, dp_\nu \times \delta\left(p_\nu c + p_e c - (Q-T)\right)$$

$(\because E_{tot} = p_{tot} c = p_\nu c + p_e c + T = Q)$

$=$ conserved quantity.

$\therefore$ Total no of momentum states for all possible momentum value

$$= A \int p_e^2 p_\nu^2 \, \delta\left(p_\nu c + p_e c - (Q-T)\right) dp_\nu \, dp_e$$

$$= A \int p_e^2 \times \left(\frac{Q-T}{c} - p_e\right)^2 dp_e \quad = \Gamma \text{ (let)}$$

but value of p_e changes from 0 to $\frac{Q-T}{c}$

(when the e^- gets zero momentum & when the neutrino gets zero momentum.)

$$\therefore \Gamma = A \int_0^{\frac{Q-T}{c}} p_e^2 \left(\frac{Q-T}{c} - p_e\right)^2 dp_e .$$

let $x = \frac{c p_e}{Q-T} \Rightarrow dx = \frac{c\, dp_e}{Q-T}$;

p_e	0	$\frac{Q-T}{c}$
x	0	1

$$\therefore \Gamma = A \cdot \left(\frac{Q-T}{c}\right)^2 \int_0^1 x^2 \times \left(\frac{p_e}{x} - p_e\right)^2 \times \frac{Q-T}{c} \cancel{dp_e}\, dx$$

$$= A \cdot \left(\frac{Q-T}{c}\right)^2 \int_0^1 \cancel{x^2}\, p_e^2 \frac{(1-x^2)}{\cancel{x^2}} \cdot \frac{Q-T}{c}\, dx$$

$$= A \left(\frac{Q-T}{c}\right)^3 \int_0^1 \left(\frac{Q-T}{c}\right)^2 x^2 (1-x^2)\, dx$$

$$= A \frac{(Q-T)^5}{c^5} \int_0^1 x^2 (1-x^2)\, dx$$

So; $\Gamma \propto (Q-T)^5$.

$P(E_f^e) \sim p_e^f c$

i.e $P(E_f^e) \sim (Q-T)^5$.

i.e $\Lambda \sim (Q-T)^5$.

So at leading order; half life is proportional to 5th power of the K.E of isotope.

proved

Problem: 9

Sp coupling:– The given potential:

$$\therefore V = \lambda\left[\delta^3(x)\cdot\vec{S}\cdot\vec{p} + \vec{S}\cdot\vec{p}\cdot\delta^3(x)\right]$$

And the states in presence of the potential:

$$|n\,l\,m\,j\rangle \longrightarrow |n\,l\,m\,j\rangle + \Sigma_1\, C_{n'l'j'm'}\,|n'\,l'\,j'\,m'\rangle$$

Clearly from 1st order perturbation; we get:

$$C_{n'l'j'm'} = \frac{\langle n'\,l'\,j'\,m'|V|n\,l\,m\,j\rangle}{E_{nlj} - E_{n'l'j'}}$$

As $\pi^\dagger p\pi = -p$ & $\pi^\dagger\vec{S}\pi = \vec{S}$; so $\pi^\dagger(\vec{S}\cdot\vec{p})\pi = -\vec{S}\cdot\vec{p}$

i.e $\vec{S}\cdot\vec{p}$ is a pseudo-scalar.

So; $\langle n'\,l'\,j'\,m'|\vec{S}\cdot\vec{p}|n\,l\,j\,m\rangle = \langle n'\,l'\,j'\,m'|\pi^\dagger\pi\,\vec{S}\cdot\vec{p}\,\pi^\dagger\pi|n\,l\,j\,m\rangle$

$$= (-1)^{l'}\cdot(-1)^{l}\cdot(-1)\,\langle n'\,l'\,j'\,m'|\vec{S}\cdot\vec{p}|n\,l\,j\,m\rangle$$

$$= (-1)^{1+l+l'}\langle n'\,l'\,j'\,m'|\vec{S}\cdot\vec{p}|n\,l\,j\,m\rangle.$$

So for non vanishing matrix element:

$$(-1)^{1+l+l'} = 1 = (-1)^{2} \Rightarrow l+l' = 1.\ \boxed{\Rightarrow l' = 1-l.}$$

Again as $\vec{S}\cdot\vec{p}$ is a pseudoscalar: $\vec{S}\cdot\vec{p} = T^0_0$.

$$\therefore \langle n'\,l'\,j'\,m'|\vec{S}\cdot\vec{p}|n\,l\,j\,m\rangle \cong \langle n'\,l'\,j'\,m'|T^0_0|n\,l\,j\,m\rangle$$

$$= \langle j\,0;\,m\,0|j\,0;\,j'\,m'\rangle \times \frac{\langle n'\,l'\,j'\|T^0\|n\,l\,j\rangle}{\sqrt{2j+1}}$$

$$= \delta_{jj'}\,\delta_{mm'}\cdot\frac{\langle n'\,l'\,j'\|T^0\|n\,l\,j\rangle}{\sqrt{2j+1}}$$

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So for non vanishing matrix element $\boxed{j = j' ; \ m = m'}$

R_{nl} (for Hydrogen) go like r^l.

So ~~Rad~~ $\langle n'l'j'm' | V | nljm \rangle_{Radial} \sim \int r^l \delta^3(r) . r^{l'} \times f(r) \, dr$

(with some $f(r)$ for which $f(0) \neq 0$)

i.e $\langle nljm | V | nljm \rangle \sim \int r^{2l} \delta^3(r) . f(r) \, dr$

$\neq 0$

iff $r^{2l} = 1 \Rightarrow 2l = 0$

i.e $l = 0$.

$\therefore \ l' = 1 - l = 1 - 0 = 1$.

$\therefore$ the only interacting states are $S_{1/2}$ and $P_{1/2}$.

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