So, $\psi_0(x) = A e^{-\frac{\alpha^2 x^2}{2}}$

To calculate A, $\int_{-\infty}^{+\infty} \psi_0^*(x)\, \psi_0(x)\, dx = 1$ (Normalisatio

$$\Rightarrow |A|^2 \int_{-\infty}^{\infty} \exp(-\alpha^2 x^2)\, dx = 1$$

$$2|A|^2 \int_0^{\infty} \exp(-\alpha^2 x^2)\, dx = 1$$

Normalised Wave func^n for nth state of L.H.O.,

$$\boxed{\psi_n(x) = \left(\frac{\alpha}{2^n \cdot n!\, \sqrt{\pi}}\right)^{1/2} e^{-\frac{\alpha^2 x^2}{2}}\, H_n(\alpha x)}$$

$H_n(\alpha x) \rightarrow$ Hermite Polynomial

$$\boxed{H_n(\rho) = (-1)^n e^{\rho^2} \frac{d^n}{d\rho^n} e^{-\rho^2}}$$

for $n = 0$, $H_n(\alpha x) = 1$, $\psi_n(x) \rightarrow$ even func^n

$n = 1$, $H_n(\alpha x) = x$, $\psi_n(x)$ depend on $\underbrace{e^{-\frac{\alpha^2 x^2}{2}}}_{\text{even}}\ \underbrace{x}_{\text{odd}}$

So $\psi_n(x) \rightarrow$ odd func^n.

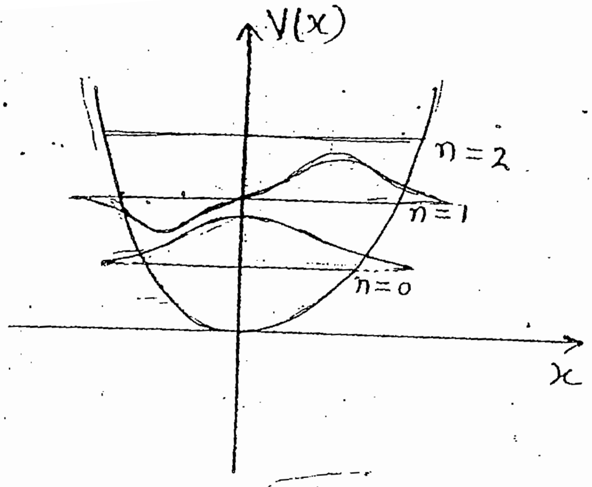
The enegy eigen func^n for Linear harmonic oscillator is even if n is even &

odd if n is odd.

i.e. state is either even or odd so Eigen func^n have definite Parity.

* At $x = 0$, all even func^{n}s for L.H.O. will be Non-zero.

It is valid for all even func^{n}s (particle in box, pot^n well ----)



* At $x=0$, all odd func^n will be zero.

i.e. $\psi = c$, odd value
$\psi \neq c$, even value

Expectation value of ~~Odd operator~~ ($\hat{x} \to$ odd)

$$\langle \hat{x} \rangle = \int \psi_n^* \, \hat{x} \, \psi_n \, dx$$

$$\langle \hat{x} \rangle = \langle n | \hat{x} | n \rangle$$

We can calculate this result by knowing the explicite form of ψ.

for odd operator, expectation value is always zero.
bcoz $|\psi_n|^2 \to$ even & $\hat{x} \to$ odd so Product $\to$ odd & limits are equal & opposite so $\int \psi_n^* \, x \, \psi \, dx = 0$

$$\boxed{\langle \hat{x} \rangle = 0}$$
$$\boxed{\langle \hat{p} \rangle = 0}$$

Also, $\boxed{\langle \hat{x}^m \rangle = 0 = \langle \hat{p}^m \rangle}$ if m is odd

This is valid for all symmetric pot^n.

Expectation value of ~~Even~~ odd operator (by operator method)

$$\langle \hat{x} \rangle = \langle n | \hat{x} | n \rangle \quad \text{———— (A)}$$

We have,
$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}} \, \hat{x} + \frac{i \hat{p}}{\sqrt{2\hbar m\omega}} \quad \text{———— (1)}$$

$$\hat{a}^{+} = \sqrt{\frac{m\omega}{2\hbar}} \, \hat{x} - \frac{i \hat{p}}{\sqrt{2\hbar m\omega}} \quad \text{———— (2)}$$

$$\hat{a}^{+}\hat{a} = \frac{m\omega}{2\hbar} \hat{x}^2 + \frac{1}{2\hbar\omega m} \hat{p}^2 + \frac{i}{2\hbar} [\hat{x}, \hat{p}]$$

$eq^n (1) + (2) \Rightarrow \quad \hat{x} = \sqrt{\frac{\hbar}{2m\omega}} (\hat{a} + \hat{a}^+)$

$eq^n (1) - (2) \Rightarrow \quad \hat{p} = \frac{1}{i} \sqrt{\frac{\hbar m\omega}{2}} (\hat{a} - \hat{a}^+)$

$eq^n (A) \Rightarrow$

$$\langle \hat{x} \rangle = \langle n | \sqrt{\frac{\hbar}{2m\omega}} (\hat{a} + \hat{a}^+) | n \rangle$$

$$= \sqrt{\frac{\hbar}{2m\omega}} \langle n | (\hat{a} + \hat{a}^+) | n \rangle$$

$$= \sqrt{\frac{\hbar}{2m\omega}} \left\{ \langle n | \hat{a} | n \rangle + \langle n | \hat{a}^+ | n \rangle \right\}$$

$$= \sqrt{\frac{\hbar}{2m\omega}} \left\{ \sqrt{n} \underbrace{\langle n | n-1 \rangle}_{0} + \sqrt{n+1} \underbrace{\langle n | n+1 \rangle}_{0} \right\}$$

$[\langle m | n \rangle = \delta_{mn}]$

So, $\boxed{\begin{array}{l} \langle \hat{x} \rangle = \langle n | \hat{x} | n \rangle = 0 \\ \langle \hat{p} \rangle = \langle n | \hat{p} | n \rangle = 0 \end{array}}$

IIly, $\langle \hat{x}^3 \rangle = \langle \hat{p}^3 \rangle = 0$

<u>Expectation value of Even operator</u> :-

$$\langle \hat{x}^2 \rangle = \langle n | \hat{x}^2 | n \rangle = \langle n | \hat{x} \hat{I} \hat{x} | n \rangle$$

$$\langle \hat{p}^2 \rangle = \langle n | \hat{p}^2 | n \rangle$$

<u>Using Closer & completeness condition</u>,

$$\sum_m |m\rangle\langle m| = \hat{I}$$

$$\langle \hat{x}^2 \rangle = \langle n | \hat{x} \hat{I} \hat{x} | n \rangle = \langle n | \hat{x} \sum_m |m\rangle\langle m| \hat{x} | n \rangle$$

$$= \sum_m \langle n | \hat{x} | m \rangle \langle m | \hat{x} | n \rangle = \sum_m | \langle m | \hat{x} | n \rangle |^2$$

Here n is not a single state, there is summission over m, We'll get Non-zero term for $m = n-1$ & $m = n+1$ i.e. $\langle m | n-1 \rangle = 1$ for $m = n-1$ & $\langle m | n+1 \rangle = 1$ for $m = n+1$ for all other terms will be zero.

$$\langle \hat{x}^2 \rangle = \sum_m |\langle m|\hat{x}|n\rangle|^2$$

$$\boxed{\langle \hat{x}^2 \rangle = \frac{\hbar}{m\omega}\left(n+\frac{1}{2}\right)}$$

Illy, for $\boxed{\langle \hat{p}^2 \rangle = \left(n+\frac{1}{2}\right) m\hbar\omega}$

<u>Uncertainity Product</u>, $\Delta x = \sqrt{\langle x^2\rangle - \langle x\rangle^2}$

$$\Delta x = \sqrt{\frac{\hbar}{m\omega}\left(n+\frac{1}{2}\right)} \qquad [\langle x\rangle = 0]$$

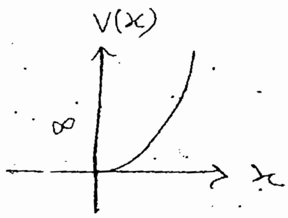
$$\Delta p = \sqrt{\langle p^2\rangle - \langle p\rangle^2} \Rightarrow \Delta p = \sqrt{\left(n+\frac{1}{2}\right) m\hbar\omega}$$

$$\boxed{\Delta x\, \Delta p = \left(n+\frac{1}{2}\right)\hbar}, \quad n = 0, 1, 2 \ldots$$

As $n\uparrow$, Uncertainity $\uparrow$

<u>Problem</u> :- ~~Usin~~ The energy levels of a particle of mass m in a potential of the form

$$V(x) = \begin{cases} \infty, & x \le 0 \\ \frac{1}{2} m\omega^2 x^2, & x > 0 \end{cases}$$



are given by

(a) $\left(n+\frac{1}{2}\right)\hbar\omega$ (b) $\left(2n+\frac{1}{2}\right)\hbar\omega$

(c) $\left(2n+\frac{3}{2}\right)\hbar\omega$ (d) $\left(n+\frac{3}{2}\right)\hbar\omega$ $\Big\}\ n = 0, 1, 2, \ldots \infty$

(e) $\left(n+\frac{1}{2}\right)\hbar\omega$, $n = 1, 3, 5 \ldots$

(f) $\left(n+\frac{3}{2}\right)\hbar\omega$, $n = 0, 2, 4, 6 \ldots$

(g) $\left(n-\frac{1}{2}\right)\hbar\omega$, $n = 0, 2, 4, 6 \ldots$

Wave funcⁿ of L.H.O. for nth state,

$$\psi_n = \left(\frac{\alpha}{2^n n! \sqrt{\pi}}\right)^{1/2} e^{-\frac{\alpha^2 x^2}{2}} H_n(\alpha x)$$

Wave funcⁿ is finite, always

Wave fun^n is continous if $\psi_I = \psi_{II}$ (by in II region $V=\infty$)

$$\text{At } x=0 \Rightarrow \psi = 0$$

for even values of $n = 0, 2, 4, 6 \cdots\cdots$ Wave fun^n is non-zero so these terms will be elliminated. Possible values are odd.

Possible Vaues of $m \Rightarrow m = 1, 3, \cancel{2}, 5, 7 \cdots\cdots$

& $E_m = (m + \frac{1}{2})\hbar\omega$

We have, $m = 0, 1, 2, 3, \cdots\cdots$

Convert these values in odd no.

So Take $n \rightarrow 2n+1 \Rightarrow (2n+1) = 1, 3, 5 \cdots\cdots$

$$E_n = \left(2n+1+\frac{1}{2}\right)\hbar\omega$$

$$E_n = \left(2n+\frac{3}{2}\right)\hbar\omega$$

IIly, for $n = 0, 2, 4, 6$ convert n by $n+1$ to convert even into odd

for $n = 0, 1, 2, 3 \cdots \infty$ $\quad E_n = (2n + \frac{3}{2})\hbar\omega$

$n = 1, 3, 5 \cdots\cdots$ $\quad E_n = (n + \frac{1}{2})\hbar\omega$

$n = 0, 2, 4, 6 \cdots\cdots$ $\quad E_n = (n + \frac{3}{2})\hbar\omega$

Ans.

Problem:- A particle of mass m is confined in the potential

$$V(x) = \begin{cases} \frac{1}{2}m\omega^2 x^2 & x > 0 \\ \infty, & x \le 0 \end{cases}$$

Let the wave fun^n of the particle be given by

$$\psi(x) = \frac{-1}{\sqrt{5}}\psi_0 + \frac{2}{\sqrt{5}}\psi_1$$

where ψ_0 & ψ_1 are the eigen fun^{n}s of ground state & Ist excited state respectivily. The expectation value of energy is.

(a) $\frac{31}{10}\hbar\omega$ (b) $\frac{25}{10}\hbar\omega$ (c) $\frac{13}{10}\hbar\omega$ (d) $\frac{11}{10}\hbar\omega$

If $V = \frac{1}{2}m\omega^2 x^2$ then $E_n = (n+\frac{1}{2})\hbar\omega$, $n = 0, 1, 2, 3 \cdots$

then E_0 $\cancel{E_1} = \frac{1}{2}\hbar\omega$ & $E_1 = \frac{3}{2}\hbar\omega$

$P_0 = \frac{1}{5}$ & $P_1 = \frac{4}{5}$.

$$\langle E \rangle = \sum_n E_n P_n$$
$$= E_0 P_0 + E_1 P_1 = \frac{1}{5}\times\frac{1}{2}\hbar\omega + \frac{4}{5}\times\frac{3}{2}\hbar\omega = \frac{13}{10}\hbar\omega$$

But here, $E_n = (n+\frac{1}{2})\hbar\omega$ ~ $n = 1, 3, 5 \ldots$ (odd values)

Also $E_n = (2n+\frac{3}{2})\hbar\omega$ for $n = 0, 1, 2 \ldots$

$$E_0 = \frac{3}{2}\hbar\omega$$
$$E_1 = \frac{7}{2}\hbar\omega$$

$$\langle E \rangle = \sum_n P_n E_n$$
$$= \frac{1}{5}\times\frac{3}{2}\hbar\omega + \frac{4}{5}\times\frac{7}{2}\hbar\omega$$
$$= \frac{3}{10}\hbar\omega + \frac{28}{10}\hbar\omega = \underline{\underline{\frac{31}{10}\hbar\omega}} \text{ A.}$$

(a)

<u>Problem</u>:- Let $|0\rangle$ & $|1\rangle$ denote the normalized eigen states corresponding to the ground & Ist excited state of a 1 Dim harmonic oscillator. The uncertainity Δp in the state $\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ is

(a) $\Delta p = \sqrt{\hbar m\omega}/2$ (b) $\Delta p = \sqrt{\hbar m\omega/2}$

(c) $\Delta p = \sqrt{\hbar m\omega}$ (d) $\Delta p = \sqrt{2\hbar m\omega}$

We know, for odd o/p $\langle n|\hat{p}|n\rangle = 0$

so $\langle 0|\hat{p}|0\rangle = 0$, & $\langle 1|\hat{p}|1\rangle = 0$

$$\langle 1|\hat{p}|0\rangle = \int_{-\infty}^{+\infty} \psi_1^* \hat{p}\psi_0 \, dx$$

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$$

$$\langle p \rangle = \langle \psi|\hat{p}|\psi\rangle$$
$$= \frac{1}{\sqrt{2}}(\langle 0| + \langle 1|)\,\hat{p}\,\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$$

$$\langle \hat{p} \rangle = \frac{1}{2}\left[\underbrace{\langle 0|\hat{p}|0\rangle}_{0} + \langle 0|\hat{p}|1\rangle + \langle 1|\hat{p}|0\rangle + \underbrace{\langle 1|\hat{p}|1\rangle}_{0}\right]$$

$[\langle n|\hat{p}|n\rangle = 0]$

$$\langle \hat{p}^2 \rangle = \frac{1}{2}\left[\langle 0|\hat{p}^2|0\rangle + \langle 0|\hat{p}^2|1\rangle + \langle 1|\hat{p}^2|0\rangle + \langle 1|\hat{p}^2|1\rangle\right]$$

for $\langle m|\hat{p}^2|n\rangle = 0$ [for different m & n (states)]

$\langle 1|\hat{p}^2|0\rangle \Rightarrow \int_{-\infty}^{+\infty} \psi_1 \hat{p}^2 \psi_0 \, dx \Rightarrow \underset{\text{odd}}{\psi_1} \underset{\text{even}}{\psi_0} \Rightarrow \text{odd}$ & odd × even = odd

$\psi_1 \psi_0 \times p^2 = \text{odd}$

so $\int_{-\infty}^{+\infty} \psi_1 \hat{p}^2 \psi_0 \, dx = 0$

So $\langle 0|\hat{p}^2|1\rangle = \langle 1|\hat{p}^2|0\rangle = 0$

$$\langle 0|\hat{p}^2|0\rangle = (n+\tfrac{1}{2})m\hbar\omega = \tfrac{1}{2}m\hbar\omega = p_0^2$$

$$\langle 1|\hat{p}^2|1\rangle = (1+\tfrac{1}{2})m\hbar\omega = \tfrac{3}{2}m\hbar\omega = p_1^2$$

Now $\langle 1|\hat{p}|0\rangle = ?$ $\langle \phi|\hat{p}|\phi\rangle = ?$

$$\langle 0|\hat{p}|1\rangle = \langle 0|\frac{1}{i}\sqrt{\frac{\hbar m\omega}{2}}(a-a^+)|1\rangle$$

$$= \frac{1}{i}\sqrt{\frac{\hbar m\omega}{2}}\langle 0|(a-a^+)|1\rangle$$

$$= \text{"}\ [\langle 0|a|1\rangle - \langle 0|a^+|1\rangle]$$

$$= \text{"}\ [\underset{1}{\langle 0|0\rangle} - \underset{0}{\langle 0|2\rangle}]$$

$$\langle 0|\hat{p}|1\rangle = \frac{1}{i}\sqrt{\frac{\hbar m\omega}{2}}$$

$\langle 0|\hat{p}|1\rangle$ & $\langle 1|\hat{p}|0\rangle$ are hermitian conjugate of each other so $\underline{\text{||ly}}$, $\langle 1|\hat{p}|0\rangle = -\frac{1}{i}\sqrt{\frac{\hbar m\omega}{2}}$

$$\langle \hat{p}\rangle = \langle 0|\hat{p}|1\rangle + \langle 1|\hat{p}|0\rangle = \frac{1}{i}\sqrt{\frac{\hbar m\omega}{2}} - \frac{1}{i}\sqrt{\frac{\hbar m\omega}{2}} = 0$$

$$\langle \hat{p}^2\rangle = \frac{1}{2}\times p_0^2 + \frac{1}{2}\times p_1^2$$

$$= \frac{1}{2}\times\frac{1}{2}\hbar m\omega + \frac{1}{2}\times\frac{3}{2}\hbar m\omega$$

$$= \hbar m\omega$$

$$\Delta p = \sqrt{\langle p^2\rangle - \langle p\rangle^2} = \sqrt{\cancel{2\hbar m\omega - \hbar m\omega}} = \sqrt{\hbar m\omega - 0}$$

$\boxed{\Delta p = \sqrt{\hbar m\omega}}$ Ans

Problem:- A particle of mass m in 1 Dim moves in a potentia

$$V(x) = \frac{K}{2a}(1-e^{-ax^2})$$

where K & a are +ve constants. If the particles exicutes small oscillations around $x=0$. its Quantum mechanical zero point energy is

(a) $\frac{1}{2}\sqrt{\frac{\hbar^2 K}{m}}$ (b) $\frac{1}{2}\sqrt{\frac{\hbar^2 K}{ma}}$ (c) $\frac{1}{2}\sqrt{\frac{\hbar^2 m}{k}}$ (d) $\frac{1}{2}\sqrt{\frac{\hbar^2 ma}{k}}$

$$V(x) = \frac{K}{2a}(1-e^{-ax^2})$$

$$= \frac{K}{2a}\left[1-\left(1-ax^2+\frac{a^2x^4}{2!}-\frac{a^3x^6}{3!}\cdots\right)\right]$$

neglect higher powers of x.

$$= \frac{K}{2a}\left[\cancel{1}-\cancel{1}+ax^2\right]$$

$$= \frac{K}{2a}ax^2 = \frac{1}{2}Kx^2$$

This is the potn of harmonic oscillator type

for H.O. $E_n = (n+\frac{1}{2})\hbar\omega$, $n = 0, 1, 2 \ldots$

for $n=0$, ground state energy

$$E_0 = \frac{1}{2}\hbar\omega$$

$$\boxed{E_0 = \frac{1}{2}\hbar\sqrt{\frac{K}{m}}} \quad (a) \qquad \left(\sqrt{\frac{K}{m}} = \omega\right)$$

* In all the classical system, ground state energy is always zero.
* When we consider wave motion of particle then Heisenberg uncertainity principal will apply & only then we get non-zero ground state energy.

Problem:- A particle is confined to a 1 Dim harmonic oscillator potential in the region $0<x<\infty$, At $x=0$ there is an infinite barrier. The energy levels of the particle are seperated by

(a) $\frac{1}{2}\hbar\omega$ (b) $\hbar\omega$ (c) $\frac{3}{2}\hbar\omega$ ✓(d) $2\hbar\omega$

for harmonic oscillator $V(x) = \frac{1}{2}m\omega^2 x^2$, $0<x<$
& in this ques, $x=0$ there is barrier.

so $$V(x) = \begin{cases} \frac{1}{2}m\omega^2 x^2, & 0<x<\infty \\ \infty, & x\leq 0 \end{cases} \quad \left[\begin{array}{l} \text{at } x=0 \\ V\to\infty \\ \psi=0 \end{array}\right]$$

At $x=0$, The func's which are zero at $x=0$ are ~~allowed only~~. i.e. $\psi_n(x) \neq 0$, at $x=0$ $n=$ even
$= 0$, at $x=0$ $n=$ odd

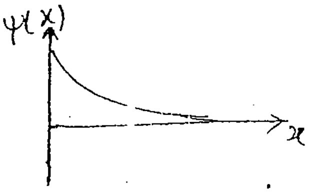
So Energy $E_n = \left(n+\frac{1}{2}\right)\hbar\omega$, $n = 1, 3, 5, 7 \cdots$
allowed for odd value of n.

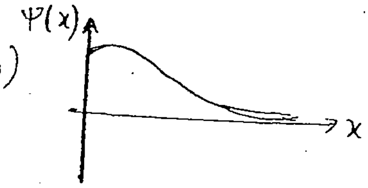
[We can also write the energy as $E_n = (2n+\frac{3}{2})\hbar\omega$, $n=0,1,2,\cdots$ | Here $n \to 2n+1$]

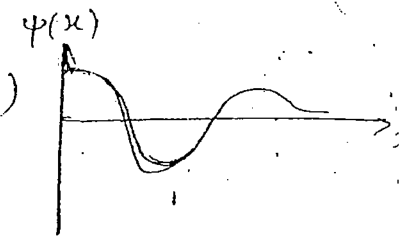
Energy for $n = 1$, $E_1 = \left(1+\frac{1}{2}\right)\hbar\omega = \frac{3}{2}\hbar\omega$
$n = 3$, $E_3 = \left(3+\frac{1}{2}\right)\hbar\omega = \frac{7}{2}\hbar\omega$

Energy level of particle is seperated by
$$\Delta E = E_3 - E_1 = \frac{7}{2}\hbar\omega - \frac{3}{2}\hbar\omega = \frac{4}{2}\hbar\omega$$
$$\boxed{\Delta E = 2\hbar\omega}$$

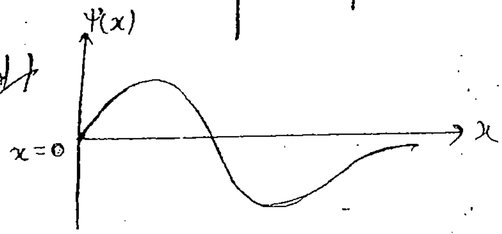
<u>Problem</u> :- Consider a particle in 1 dim pot^n
$$V(x) = \begin{cases} x^2 & \text{for } x>0 \\ \infty & \text{for } x\leq 0 \end{cases}$$
The symmetric form of ground state wave func^n is as follows

(a) 

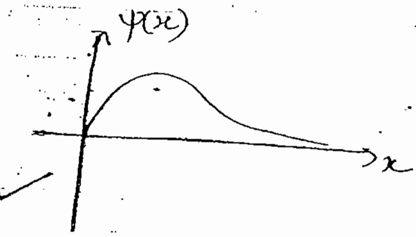
(b) 

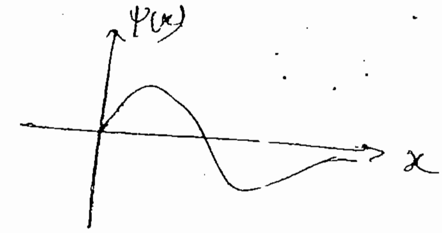
(c) 

At ∞ pot^n, wave func^n is zero. i.e. At $x = \leq 0$, $V(x)=\infty$
so At $x=0$, $\psi(x) = 0$

✓(d) 

If We have





Then this one is appropriate.(bcoz $\psi(x) \to +ve$)

Problem:- For a 1 Dim Harmonic oscillator show that

(1) $\langle K.E. \rangle = \langle P.E. \rangle$

(2) $\langle \hat{x}^4 \rangle$

(3) Calculate the $\langle E_n \rangle$ for the n^{th} state if $\hat{H} = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 - \lambda \hat{x}^4$

for 1 D, H.O., $\quad K.E. = \frac{\hat{p}^2}{2m}$

$$P.E. = \frac{1}{2}m\omega^2\hat{x}^2$$

$$\langle n|\hat{p}^2|n\rangle = \int_{-\infty}^{\infty} \langle n \left| \frac{1}{i^2}\frac{\hbar m\omega}{2}(\hat{a}-\hat{a}^+)\right| n\rangle$$

$$= (n+\tfrac{1}{2})\, m\hbar\omega$$

$$\& \langle n|\hat{x}^2|n\rangle = \langle n \left| \frac{\hbar}{2m\omega}(\hat{a}+\hat{a}^+)\right| n\rangle$$

$$= \cancel{4}\, \frac{\hbar}{m\omega}(n+\tfrac{1}{2})$$

$$\langle K.E.\rangle = (n+\tfrac{1}{2})\frac{\hbar m\omega}{2m} = (n+\tfrac{1}{2})\frac{\hbar\omega}{2}$$

$$\langle P.E.\rangle = \frac{1}{2}m\omega^2\frac{\hbar}{m\omega}(n+\tfrac{1}{2}) = (n+\tfrac{1}{2})\frac{\hbar\omega}{2}$$

$$\boxed{\langle K.E.\rangle = \langle P.E.\rangle}$$

* **Virial theorm**:- if $V \propto x^{n+1}$ then $\overline{T} = \left(\frac{n+1}{2}\right)\overline{U}$

$V \propto x^n$ then $\overline{T} = \left(\frac{n}{2}\right)\overline{U}$

(ii) $\langle \hat{x}^4 \rangle = \langle n | \hat{x}^2 \hat{I} \hat{x}^2 | n \rangle$

$= \langle n | \hat{x}^2 \sum_m |m\rangle\langle m| \hat{x}^2 | n \rangle$

$= \sum_m \langle n | \hat{x}^2 | m \rangle \langle m | \hat{x}^2 | n \rangle$

$\langle \hat{x}^4 \rangle = \sum_m | \langle m | \hat{x}^2 | n \rangle |^2$ ——— (1)

We have $\hat{x} = \sqrt{\frac{\hbar}{2m\omega}} (\hat{a} + \hat{a}^+)$

$\hat{x}^2 = \frac{\hbar}{2m\omega} \left[(\hat{a})^2 + (\hat{a}^+)^2 + 2\hat{a}^+\hat{a} + 1 \right]$.

$\hat{x}^2 |n\rangle = \frac{\hbar}{2m\omega} \left[a^2|n\rangle + (a^+)^2|n\rangle + (2a^+a+1)|n\rangle \right]$

$\because [\hat{a}, \hat{a}^+] = 1 \Rightarrow \hat{a}\hat{a}^+ - \hat{a}^+\hat{a} = 1 \Rightarrow aa^+ = 1 + a^+a$

$= \frac{\hbar}{2m\omega} \left[a\sqrt{n}\,|n-1\rangle + a^+ \sqrt{n+1}\,|n+1\rangle + (2n+1)|n\rangle \right]$

$= \frac{\hbar}{2m\omega} \left[\sqrt{n}\sqrt{n-1}\,|n-2\rangle + \sqrt{n+1}\sqrt{n+2}\,|n+2\rangle + (2n+1)|n\rangle \right]$

Now, $\langle m | x^2 | n \rangle = \frac{\hbar}{2m\omega} \left[\sqrt{n}\sqrt{n-1} \underbrace{\langle m | n-2 \rangle}_{\delta_{m,n-2}} + \sqrt{n+1}\sqrt{n+2} \underbrace{\langle m | n+2 \rangle}_{\delta_{m,n+2}} + (2n+1) \underbrace{\langle m | n \rangle}_{\delta_{m,n}} \right]$.

eqn (1) $\Rightarrow$

$\langle \hat{x}^4 \rangle = \sum_m | \langle m | \hat{x}^2 | n \rangle |^2$

$m = 0, 1, 2, \ldots\ldots, n-2, n-1, n, n+1, n+2, \ldots\ldots$

Except $n-2$, n, $n+2$, all values will be zero.

Take $m = n-2, n, n+2$ respectively.

$\langle \hat{x}^4 \rangle = \left| \frac{\hbar}{2m\omega} (\sqrt{n}\sqrt{n-1}) \right|^2 + \left| \frac{\hbar}{2m\omega} (2n+1) \right|^2 + \left| \frac{\hbar}{2m\omega} \sqrt{n+1}\sqrt{n+2} \right|^2$

$= \frac{\hbar^2}{4m^2\omega^2} n(n-1) + \frac{\hbar^2}{4m^2\omega^2} (4n^2 + 1 + 4n) + \frac{\hbar^2}{4m^2\omega^2} (n^2 + 3n + 2)$

$= \frac{\hbar^2}{4m^2\omega^2} \left[n^2 - n + 4n^2 + 1 + 4n + n^2 + 3n + 2 \right]$

$$\boxed{\langle \hat{x}^4 \rangle = \frac{\hbar^2}{4m^2\omega^2} (6n^2 + 6n + 3)}$$

(iii) $\langle E_n \rangle = ?$

$$H = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2 - \lambda x^4$$

$$\langle E_n \rangle = \left(n+\frac{1}{2}\right)\hbar\omega - \lambda \frac{\hbar^2}{4m^2\omega^2}(6n^2+6n+3)$$ Ans

Problem:- In 1 Dim harmonic oscillator ϕ_1 ϕ_2 ϕ_3 are the ground, Ist, IInd excited state respectively. These three states are normalised & orthogonal to one another. ψ_1 & ψ_2 are 2 states defined by

$$\psi_1 = \phi_0 - 2\phi_1 + 3\phi_2$$

$$\psi_2 = \phi_0 - \phi_1 + \alpha\phi_2 \quad \text{where } \alpha \text{ is constant}$$

(i) The value of α for which ψ_2 is orthogonal to ψ_1, is

(a) 2 (b) 1 (c) -1 (d) -2

(ii) for The value of α determined in (i) part, the expectation value of energy of oscillator in state ψ_2 is.

$$\psi_1 = \phi_0 - 2\phi_1 + 3\phi_2$$

$$\psi_2 = \phi_0 - \phi_1 + \alpha\phi_2$$

(i) If 2 W.fun^n are orthogonal then

$$\sum_n C_n^* C_n' = 0$$

$$\Rightarrow 1 + 2 + 3\alpha = 0$$

$$3\alpha = -3$$

$$\boxed{\alpha = -1}$$

$(\phi_0 - 2\phi_1 + 3\phi_2)(\phi_0 - \phi_1 + \alpha\phi_2)$

$= \langle\phi_0|\phi_0\rangle + 2\langle\phi_1|\phi_1\rangle + 3\alpha\langle\phi_2|\phi_2\rangle$

all other terms $= 0$

$= 1 + 2 + 3\alpha = 0$

$\Rightarrow \alpha = -1$

(ii) $\langle E \rangle = \sum_n E_n P_n$

$\psi_2 = \phi_0 - \phi_1 + \underset{-1}{\alpha}\,\phi_2$ this is not normalised

so Normalised W.fun^n $\psi_2 = \frac{1}{\sqrt{3}}[\phi_0 - \phi_1 - \phi_2]$

$$P_0 = \frac{1}{3} \qquad P_1 = \frac{1}{3} \qquad P_2 = \frac{1}{3}$$

$$\langle E\rangle = \frac{1}{2}\hbar\omega \times \frac{1}{3} + \frac{3}{2}\hbar\omega \times \frac{1}{3} + \frac{5}{2}\hbar\omega \times \frac{1}{3}$$

$$= \frac{1}{3}\hbar\omega\left(\frac{1}{2}+\frac{3}{2}+\frac{5}{2}\right) = \frac{1}{3}\hbar\omega\left(\frac{9}{2}\right)$$

$$\boxed{\langle E\rangle = \frac{3}{2}\hbar\omega}$$

Prob :- A particle is initially in the ground state in 1 dim harmonic oscillator potⁿ $V(x) = \frac{1}{2}kx^2$. If the spring cons. is suddenly doubled. Calculate the probability of finding the particle in ground state of new potⁿ.

$$V(x) = \frac{1}{2}Kx^2$$

ground state wave fucⁿ for this potⁿ is (n = 0)

$$\phi_0 = \left(\frac{\alpha}{\sqrt{\pi}}\right)^{1/2} e^{-\frac{\alpha^2 x^2}{2}}, \quad \alpha^2 = \frac{m\omega}{\hbar}, \quad \omega = \sqrt{\frac{K}{m}}$$

Now K is doubled, i.e. $K \rightarrow 2K = K'$ then new potⁿ

$$V'(x) = \frac{1}{2}K'x^2$$

$$\psi_n(x) = \left(\frac{\alpha'}{2^n n! \sqrt{\pi}}\right)^{1/2} e^{-\frac{\alpha'^2 x^2}{2}} H_n(\alpha' x), \quad \alpha'^2 = \frac{m\omega'}{\hbar}, \quad \omega' = \sqrt{\frac{2K}{m}}$$

$$\phi_0(x) = \sum_n C_n \psi_n$$

$$= C_0\psi_0 + C_1\psi_1 + C_2\psi_2 + \cdots$$

Prob. of finding the particle in ground state

$$P_0 = |C_0|^2$$

$$C_0 = \int_{-\infty}^{+\infty} \psi_0^*(x)\,\phi_0(x)\,dx$$

$$= \int_{-\infty}^{+\infty} \left(\frac{\alpha'}{\sqrt{\pi}}\right)^{1/2} e^{-\frac{\alpha'^2 x^2}{2}} \left(\frac{\alpha}{\sqrt{\pi}}\right)^{1/2} e^{-\frac{\alpha^2 x^2}{2}}\, dx$$

$$= 2\int_0^{\infty} \frac{\sqrt{\alpha\alpha'}}{\sqrt{\pi}}\, e^{-\left(\frac{\alpha^2+\alpha'^2}{2}\right)x^2}$$

$$\left[\int_0^{\infty} e^{-\lambda x^2} x^n\, dx = \frac{\Gamma\left(\frac{n+1}{2}\right)}{2\lambda^{\frac{n+1}{2}}}\right]$$

$$C_0 = \frac{2\sqrt{\alpha\alpha'}}{\sqrt{\pi}}\left[\frac{\sqrt{\frac{1}{2}}}{2\left(\frac{\alpha^2+\alpha'^2}{2}\right)^{1/2}}\right] \qquad (n=0)$$

$$= \frac{\sqrt{\alpha\alpha'}}{\sqrt{\pi}} \frac{\sqrt{\pi}}{\left(\frac{\alpha^2+\alpha'^2}{2}\right)^{1/2}} = \sqrt{\frac{2\alpha\alpha'}{(\alpha'^2+\alpha^2)}}$$

$$P_0 = |C_0|^2 = \left|\frac{\sqrt{2\alpha\alpha'}}{(\alpha'^2+\alpha^2)^{1/2}}\right|^2 = \frac{2\alpha\alpha'}{(\alpha^2+\alpha'^2)}$$

$$P_0 = \frac{2\times\frac{m^2}{\hbar^2}\omega\omega'}{\left[\frac{m^2\omega^2}{\hbar^2}+\frac{m^2\omega'^2}{\hbar^2}\right]} = \frac{2\times\frac{K}{m}\times\sqrt{2}}{\left[\frac{K}{m}+\sqrt{2}\frac{K}{m}\right]}$$

$$\boxed{P_0 = \frac{2^{3/2}}{[1+\sqrt{2}]}}$$

And corresponding Energy,

$$E_n = \left(n+\frac{1}{2}\right)\hbar\omega$$

$$E_n' = \left(n+\frac{1}{2}\right)\hbar\sqrt{2}\,\omega \quad (\text{new energy}) \qquad (\omega'=\sqrt{2}\,\omega)$$

for $n=0$

$$E_0' = \frac{\hbar\omega}{\sqrt{2}}$$

- For 3 Dim Harmonic Oscillator :-

In 3 Dim,

$$H\psi(r) = E\psi(r)$$

$$\Rightarrow \left[-\frac{\hbar^2}{2m}\nabla^2 + \underset{\text{independent of time}}{V(r)}\right]\psi(r) = E\psi(r) \Rightarrow \text{Sch}^r \text{ eq}^n$$

If pot^n $V(x,y,z)$ satisfies the cond^n i.e. pot^n is additive

$$\boxed{V(x,y,z) = V(x)+V(y)+V(z)}$$

then we can reduce 3 dim Sch^r eq^n in three independent 1-dim Sch^r eq^n.

If V is independent of time & only depend on the position then we can write, Energy will be additive & w. fuc^n is multiplicative.

$$E = E_x + E_y + E_z$$

$$\psi(x,y,z) = \psi(x).\psi(y)\,\psi(z)$$

If cross terms occur in pot^n V then we can not seperate 3 dim W. fuc^n in 3 independent w. fuc^{n}s.

Particle in a 3 dim infinite particle in box :-

(1) If length of box in x, y, z dir^n are not equal,

$$L_x \neq L_y \neq L_z$$

$$V(x,y,z) = \begin{cases} 0 , & \text{if } 0<x<L_x ,\ 0<y<L_y ,\ 0<z<L_z \\ \infty , & \text{otherwise} \end{cases}$$

This 3 dim pot^n can be written as sum of 3, 1 dim pot^n

$$V(x,y,z) = V(x) + V(y) + V(z)$$

where,

$$V(x) = \begin{cases} 0 , & \text{if } 0<x<L_x \\ \infty , & \text{otherwise} \end{cases}$$

$$V(y) = \begin{cases} 0 , & \text{if } 0<y<L_y \\ \infty , & \text{otherwise} \end{cases}$$

$$V(z) = \begin{cases} 0 , & \text{if } 0<z<L_z \\ \infty , & \text{otherwise} \end{cases}$$

By Using seperation of variable method,

Sch^r eq^n, $$-\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right]\psi(x,y,z) + \left[V(x)+V(y)+V(z)\right]\psi(x,y,z) = E\,\psi(x,y,z)$$

If pot^n satisfies $V(x)+V(y)+V(z) = V(x,y,z)$ cond^n then wave fuc^n can be sperated as

$$\psi(x,y,z) = \psi(x)\ \psi(y)\,\psi(z)$$

Substitute the value of $\psi(x,y,z) = \psi(x)\psi(y)\psi(z)$ then

$$\Rightarrow \frac{-\hbar^2}{2m}\left[\psi(y)\psi(z)\frac{\partial^2\psi(x)}{\partial x^2} + \psi(x)\psi(z)\frac{\partial^2\psi(y)}{\partial y^2} + \psi(x)\psi(y)\frac{\partial^2\psi(z)}{\partial z^2}\right]$$
$$+ \left[V(x)+V(y)+V(z)\right]\psi(x)\psi(y)\psi(z) = E\,\psi(x)\psi(y)\psi(z)$$

$$\Rightarrow \frac{-\hbar^2}{2m}\left[\frac{1}{\psi(x)}\frac{\partial^2\psi(x)}{\partial x^2} + \frac{1}{\psi(y)}\frac{\partial^2\psi(y)}{\partial y^2} + \frac{1}{\psi(z)}\frac{\partial^2\psi(z)}{\partial z^2}\right] + \left[V(x)+V(y)+V(z)\right] = E$$

— (dividing by $\psi(x)\psi(y)\psi(z)$)

$$\Rightarrow \left[\frac{1}{\psi(x)}\frac{\partial^2\psi(x)}{\partial x^2} + \frac{1}{\psi(y)}\frac{\partial^2\psi(y)}{\partial y^2} + \frac{1}{\psi(z)}\frac{\partial^2\psi(z)}{\partial z^2}\right] = \frac{2m}{\hbar^2}\left[-E + (V(x)+V(y)+V(z))\right]$$

for x part of W. fucⁿ,

$$\frac{1}{\psi(x)}\frac{\partial^2\psi(x)}{\partial x^2} - \frac{2m}{\hbar^2}V(x) = -\frac{2m}{\hbar^2}\left[E - V(y) - V(z)\right]$$
$$= -\frac{2m}{\hbar^2}E_x$$

L.H.S. → x dependent so R.H.S. should be x-dependent.

$$\boxed{\frac{\partial^2\psi(x)}{\partial x^2} + \frac{2m}{\hbar^2}\left[E_x - V(x)\right]\psi(x) = 0}$$

similarly for y & z part,

$$\boxed{\frac{\partial^2\psi(y)}{\partial y^2} + \frac{2m}{\hbar^2}\left[E_y - V(y)\right]\psi(y) = 0}$$

$$\boxed{\frac{\partial^2\psi(z)}{\partial z^2} + \frac{2m}{\hbar^2}\left[E_z - V(z)\right]\psi(z) = 0}$$

Inside the box, potⁿ = 0

$$V(x) = V(y) = V(z) = 0$$

so

$$\frac{\partial^2\psi(x)}{\partial x^2} + \frac{2m}{\hbar^2}E_x\psi(x) = 0, \quad k_x^2 = \frac{2mE_x}{\hbar^2}$$

$$\frac{\partial^2\psi(y)}{\partial y^2} + \frac{2m}{\hbar^2}E_y\psi(y) = 0, \quad k_y^2 = \frac{2mE_y}{\hbar^2}$$

$$\frac{\partial^2\psi(z)}{\partial z^2} + \frac{2m}{\hbar^2}E_z\psi(z) = 0, \quad k_z^2 = \frac{2mE_z}{\hbar^2}$$

Total: $K^2 = K_x^2 + K_y^2 + K_z^2$

$$K^2 = \frac{2m}{\hbar^2}(E_x + E_y + E_z)$$

& Total Energy $E = E_x + E_y + E_z = \frac{\hbar^2 K^2}{2m}$

$$\frac{d^2\psi(x)}{dx^2} + K_x^2\psi(x) = 0$$

$$\frac{d^2\psi(y)}{dy^2} + K_y^2\psi(y) = 0$$

$$\frac{d^2\psi(z)}{dz^2} + K_z^2\psi(z) = 0$$

Most general solution of these eqn will be

$$\psi(x) = A\sin K_x x + B\cos K_x x$$
$$\psi(y) = C\sin K_y y + D\cos K_y y$$
$$\psi(z) = E\sin K_z z + F\cos K_z z$$

On applying B.C. on these wave funcns,

At boundries ψ will be zero [i.e. at $x=0$, $L_x \Rightarrow \psi_x = 0$]

We get $B = D = F = 0$

& $K_x = \frac{n_x \pi x}{L_x}$, $K_y = \frac{n_y \pi y}{L_y}$, $K_z = \frac{n_z \pi z}{L_z}$

$$\psi(x) = A\sin\left(\frac{n_x \pi x}{L_x}\right)$$

$$\psi(y) = C\sin\left(\frac{n_y \pi x}{L_y}\right)$$

$$\psi(z) = E\sin\left(\frac{n_z \pi z}{L_z}\right)$$

Corresponding energies, $E_x = \frac{n_x^2 \pi^2 \hbar^2}{2mL_x^2}$

$E_y = \frac{n_y^2 \pi^2 \hbar^2}{2mL_y^2}$ & $E_z = \frac{n_z^2 \pi^2 \hbar^2}{2mL_z^2}$

Normalization cond^n, $\int \psi^*(x,y,z) \cdot \psi(x,y,z)\, dx\, dy\, dz = 1$

$$\Rightarrow \int_{-\infty}^{+\infty} \psi^*(x)\psi(x)\,dx + \int_{-\infty}^{+\infty} \psi^*(y)\,\psi(y)\,dy + \int_{-\infty}^{+\infty} \psi^*(z)\,\psi(z)\,dz = 1$$

Normalise the wave func^n in each dir^n seperately or normalise combine wave func^n, we'll get same results.

By Normalisation,

$$A = \sqrt{\frac{2}{L_x}}$$

$$CB = \sqrt{\frac{2}{L_y}}$$

$$E = \sqrt{\frac{2}{L_z}}$$

then $\psi(x) = \sqrt{\frac{2}{L_x}} \sin\left(\frac{n_x \pi x}{L_x}\right)$

$$\psi(y) = \sqrt{\frac{2}{L_y}} \sin\left(\frac{n_y \pi y}{L_y}\right)$$

$$\psi(z) = \sqrt{\frac{2}{L_z}} \sin\left(\frac{n_z \pi z}{L_z}\right)$$

Total Wave func^n

$$\psi(x,y,z) = \sqrt{\frac{2}{L_x}}\sqrt{\frac{2}{L_y}}\sqrt{\frac{2}{L_z}} \sin\left(\frac{n_x \pi x}{L_x}\right) \sin\left(\frac{n_y \pi y}{L_y}\right) \sin\left(\frac{n_z \pi z}{L_z}\right)$$

energy, $E_{n_x, n_y, n_z} = \frac{\hbar^2 \pi^2}{2m}\left[\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} + \frac{n_z^2}{L_z^2}\right]$

Pot^n is not symmetric in 1 Dim i.e. No degeneracy. for each eigen value we get only one eigen state. But for heigher dim (symmetric pot^n) we get same eigen value for more than one state i.e. there will be degeneracy.

When $L_x \neq L_y \neq L_z$

Then the eigen value will be ~~dege~~ non-degenerate.

Cubic Potⁿ Box :-

$$V(x,y,z) = \begin{cases} 0 & , \text{ if } 0<x<L,\ 0<y<L,\ 0<z<L \\ \infty & \text{otherwise} \end{cases}$$

i.e. $L_x = L_y = L_z = L$

Energy $E_{n_x, n_y, n_z} = \frac{\hbar^2 \pi^2}{2m}\left[\frac{n_x^2}{L^2} + \frac{n_y^2}{L^2} + \frac{n_z^2}{L^2}\right]$

Wave func $\psi(x,y,z) = \left(\sqrt{\frac{2}{L}}\right)^3 \sin\left(\frac{n_x \pi x}{L_x}\right) \sin\left(\frac{n_y \pi y}{L_y}\right) \sin\left(\frac{n_z \pi z}{L_z}\right)$

generally Energy E. value will be degenerate.

Each eigen value - linearly independent ⇒ more than One state - Degenerate

$\cancel{n_x \neq n_y \neq}$ $n_x, n_y, n_z = 1, 2, 3, \ldots$

$$n^2 = n_x^2 + n_y^2 + n_z^2$$

$$E = \frac{\hbar^2 \pi^2}{2mL^2}(n_x^2 + n_y^2 + n_z^2)$$

Ground state energy $n_x = n_y = n_z = 1$

$$E_{111} = \frac{3\hbar^2 \pi^2}{2mL^2} \qquad g = 1$$

If $\left.\begin{array}{l} n_x = 1 \\ n_y = 1 \\ n_z = 2 \end{array}\right\}$ $\left.\begin{array}{ccc} n_x & n_y & n_z \\ (1 & 1 & 2) \\ (1 & 2 & 1) \\ (2 & 1 & 1) \end{array}\right\}$ there are the possible value of $(n_x n_y n_z)$

$$E_{112} = \frac{6\pi^2 \hbar^2}{2mL^2} \qquad g = 3$$

W.f. $\psi_{112} = \left(\sqrt{\frac{2}{L}}\right)^3 \sin\left(\frac{\pi x}{L}\right) \sin\left(\frac{\pi y}{L}\right) \sin\left(\frac{2\pi z}{L}\right)$

$\psi_{121} = \left(\sqrt{\frac{2}{L}}\right)^3 \sin\left(\frac{\pi x}{L}\right) \sin\left(\frac{2\pi y}{L}\right) \sin\left(\frac{\pi z}{L}\right)$

$\psi_{211} = \left(\frac{2}{L}\right)^3 \sin\left(\frac{2\pi x}{L}\right) \sin\left(\frac{\pi y}{L}\right) \sin\left(\frac{\pi z}{L}\right)$

} for one energy E-value E_{112} there are 3 possible ~~tt~~ states so degeneracy

$$E_{122} = \frac{9\pi^2\hbar^2}{2mL^2}, \quad g = 3$$

n_x	n_y	n_z
1	2	2
2	2	1
2	1	2

$$E_{113} = \frac{11\pi^2\hbar^2}{2mL^2} \quad g = 3$$

$$E_{222} = \frac{12\pi^2\hbar^2}{2mL^2} \quad g = 1$$

for this single value of energy the 3 degenerate state, so there are three eigen value fun.

$E_{113} < E_{222}$

- when all Quantum no's are different i.e.

$n_x \neq n_y \neq n_z$
1 2 3

then $(n_x \; n_y \; n_z) \Rightarrow$ (1 2 3)
(1 3 2)
(2 1 3)
(2 3 1)
(3 1 2)
(3 2 1)

There are 6 possibilities

So degeneracy = 6

Degeneracy / Level :- means the group of states having same energy.

e.g. $E_{112} = \frac{6\pi^2\hbar^2}{2mL^2}$ have degeneracy = 3

$\Downarrow$ This shows the energy level

$\Downarrow$ This shows how many energy states possible in this level.

- Consider the numbering of states in increasing order of energy.

$E_1 \to$ ground state ($n=1$)
$E_2 \to$ Ist excited state ($n=2$)

n is diff. } for particle in box.

CSIR-NET 2012 :

Qu :- A particle of mass m is in a cubic box of size a, the pot^n inside the box $(0<x<a\,;\ 0<y,\ 0<z<a)$ is zero & infinite outside. If the particle is in an eigen state of energy $E = \frac{14\pi^2\hbar^2}{2ma^2}$. Its wave fuc^n is

a) $\psi = \left(\frac{2}{a}\right)^{3/2} \sin\left(\frac{3\pi x}{a}\right) \sin\left(\frac{5\pi y}{a}\right) \sin\left(\frac{6\pi z}{a}\right)$

b) $\psi = \left(\frac{2}{a}\right)^{3/2} \sin\left(\frac{7\pi x}{a}\right) \sin\left(\frac{4\pi y}{a}\right) \sin\left(\frac{3\pi z}{a}\right)$

c) $\psi = \left(\frac{2}{a}\right)^{3/2} \sin\left(\frac{4\pi x}{a}\right) \sin\left(\frac{8\pi y}{a}\right) \sin\left(\frac{2\pi z}{a}\right)$

d) $\psi = \left(\frac{2}{a}\right)^{3/2} \sin\left(\frac{\pi x}{a}\right) \sin\left(\frac{2\pi y}{a}\right) \sin\left(\frac{3\pi z}{a}\right)$ ✓

$$E = \frac{14\pi^2\hbar^2}{2ma^2}$$

for $n_x = 1,\ n_y = 2,\ n_z = 3$ We get

$$n^2 = n_x^2 + n_y^2 + n_z^2 = 1+4+9 = 14$$

i.e. we get $n^2 = 14$ for $(n_x n_y n_z) = (1,2,3)$

so (d) is correct.

Wave fuc^n $\boxed{\psi = \left(\frac{2}{a}\right)^{3/2} \sin\left(\frac{\pi x}{a}\right) \sin\left(\frac{2\pi y}{a}\right) \sin\left(\frac{3\pi z}{a}\right)}$ Ans

Harmonic Oscillator in 3 Dim :-

3 dim pot^n,

$$V(x,y,z) = \frac{1}{2}m\left[\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2\right]$$

Isotropic → property does not change by changing the dir^n.
i.e. property is same in all dir^n. $(\omega_x = \omega_y = \omega_z)$

Anisotropic → " " diff " "

This pot^n is Anisotropic pot^n.

Symmetric → If change $x \to -x$, $y \to -y$, $z \to -z$ then No change in V.

$$V(x,y,z) = V(x) + V(y) + V(z)$$

So Energy & W.func^n can be written as

$$E_{n_x} = \left(n_x + \tfrac{1}{2}\right)\hbar\omega_x$$

$$E_{n_y} = \left(n_y + \tfrac{1}{2}\right)\hbar\omega_y$$

$$E_{n_z} = \left(n_z + \tfrac{1}{2}\right)\hbar\omega_z \qquad n_x, n_y, n_z = 0, 1, 2, 3 \ldots$$

Wave func^n,

$$\psi_{n_x n_y n_z} = \left(\frac{\alpha_x}{2^{n_x} n_x! \sqrt{\pi}}\right)^{1/2} e^{-\frac{\alpha_x^2 x^2}{2}} H_{n_x}(\alpha_x x)$$

$$\times \left(\frac{\alpha_y}{2^{n_y} n_y! \sqrt{\pi}}\right)^{1/2} e^{-\frac{\alpha_y^2 y^2}{2}} H_{n_y}(\alpha_y y)$$

$$\times \left(\frac{\alpha_z}{2^{n_z} n_z! \sqrt{\pi}}\right)^{1/2} e^{-\frac{\alpha_z^2 z^2}{2}} H_{n_z}(\alpha_z z)$$

Total Energy $E = E_{n_x} + E_{n_y} + E_{n_z}$

$$E = \left(n_x + \tfrac{1}{2}\right)\hbar\omega_x + \left(n_y + \tfrac{1}{2}\right)\hbar\omega_y + \left(n_z - \tfrac{1}{2}\right)\hbar\omega_z$$

<u>If pot^n is Isotropic</u> then

$$V(x,y,z) = V(x) + V(y) + V(z) = \tfrac{1}{2} m\omega^2 r^2$$

$$\& \quad \omega_x = \omega_y = \omega_z = \omega$$

then Energy $E_{n_x, n_y, n_z} = \left(n_x + n_y + n_z + \frac{3}{2}\right)\hbar\omega$

$$n_x, n_y, n_z = 0, 1, 2, 3 \ldots$$

Wave func^n,

$$\psi_{n_x n_y n_z} = \left(\frac{\alpha}{2^{n_x} n_x! \sqrt{\pi}}\right)^{1/2} e^{-\frac{\alpha^2 x^2}{2}} H_{n_x}(\alpha x) \times \left(\frac{\alpha}{2^{n_y} n_y! \sqrt{\pi}}\right)^{1/2} e^{-\frac{\alpha^2 y^2}{2}} H_{n_y}(\alpha y)$$

$$\times \left(\frac{\alpha}{2^{n_z} n_z! \sqrt{\pi}}\right)^{1/2} e^{-\frac{\alpha^2 z^2}{2}} H_{n_z}(\alpha z)$$

If $n_x + n_y + n_z = n$ then

$$\boxed{E_n = \left(n + \frac{3}{2}\right)\hbar\omega}$$

$n = n_x + n_y + n_z$

for $n = 1$, 3 possibilities $\Rightarrow$
$$\left.\begin{aligned} 1 &= 0+0+1 \\ &= 1+0+0 \\ &= 0+1+0 \end{aligned}\right\} g = 3$$

~~for n = 2~~, 6 " $\Rightarrow$
$$\left.\begin{aligned} 2 &= 0+1+1 \\ &= 1+0+1 \\ &= 1+1+0 \\ &= 2+0+0 \\ &= 0+2+0 \\ &= 0+0+2 \end{aligned}\right\} g = 6$$

$$\boxed{n = n_x + n_y + n_z}$$ { cond^n shd be s.t. it gives all values of $n = 0, 1, 2, 3 \cdots$

if $n - n_x \to$ fixed $\Rightarrow$ $(n - n_x) = n_y + n_z$

To ~~satisfy~~ satisfy this cond^n, the possibilities

$(n_y, n_z) = (0, n-n_x)$, $(1, n-n_x-1)$; $(2, n-n_x-2)$, $(n-n_x-1, 1)$, $(n-n_x, 0)$

The total no. of possible states $= (n - n_x + 1)$

This is not the total degeneracy bcoz here n_x is fixed.

Total degeneracy $\quad g_n = \sum_{n_x=0}^{n} (n - n_x + 1)$

$$g_n = (n+1) + n + (n-1) + \cdots + 3 + 2 + 1$$

reverse the g_n,

& $g_n = 1 + 2 + 3 + \cdots + (n-1) + n + (n+1)$

add both terms

$$2g_n = (n+2) + (n+2) + \cdots (n+2)$$

Here $(n+2)$ is added $(n+1)$ times so degeneracy will be

$$\boxed{g_n = \frac{(n+1)(n+2)}{2}}$$ $\rightarrow$ degeneracy of Isotropic H.O.

In 1 Dim, Energy seperation $= \hbar\omega$

$$E_n = \left(n+\frac{3}{2}\right)\hbar\omega$$

for $n = 0, 1, 2 \ldots$

$$E_n = \frac{3}{2}\hbar\omega, \frac{5}{2}\hbar\omega, \frac{7}{2}\hbar\omega \ldots$$

i.e. energy seperation is still $\hbar\omega$ while ground state energy is changend.

Problem :- If A Quantum particle of mass m moves in 2 dim in an anisotoopic oscillator potⁿ

$$V(x,y) = \frac{1}{2}m\omega^2x^2 + 2m\omega^2y^2$$

The energy eigen values are (n is +ve integer or zero)
i.e. $n = 0, 1, 2, 3, \ldots$

(a) $\hbar\omega(2n+1)$ (b) $\hbar\omega(n+1)$ (c) $2\hbar\omega(n+1)$ (d) $\hbar\omega\left(n+\frac{3}{2}\right)$

$$\begin{aligned} V(x,y) &= \frac{1}{2}m\omega^2x^2 + 2m\omega^2y^2 \\ &= \underbrace{\frac{1}{2}m\omega^2x^2}_{\text{freq} \to \omega} + \underbrace{\frac{1}{2}m(2\omega)^2y^2}_{\text{freq} \to 2\omega} \end{aligned}$$

If $\omega_y = 2\omega_x$ then Anisotoopic
for Isotoopic $\omega_x = \omega_y$

Energy $E_n = \cancel{\frac{1}{2}m}\left(n_x+\frac{1}{2}\right)\hbar\omega + \left(n_y+\frac{1}{2}\right)\hbar(2\omega)$

$$E_n = \left(n_x + 2n_y + \frac{3}{2}\right)\hbar\omega$$

Suppose $n_x + 2n_y = n$

n_x	n_y	n
0	0	0
1	0	1
1	1	3
0	1	2

i.e. we get all values of n
$n = 0, 1, 2, 3, \ldots$

So $n_x + 2n_y = n$ gives all vales of n so replace (n_x+2n_y) by n

$$\boxed{E_n = \left(n+\frac{3}{2}\right)\hbar\omega}$$

Note :- If Isotropic then $E_n = (n_x+n_y+1)\hbar\omega = (n+1)\hbar\omega$
freq. same

Problem - The degeneracy of the state of energy $E_n = (n+1)\hbar\omega$ where n is an integer (0 or +ve integer) in a 2-Dim isotropic Harmonic Oscillator, with potⁿ

$$V(x,y) = \frac{1}{2}m\omega^2(x^2+y^2) \text{ is}$$

(a) $\frac{n(n-1)}{2}$ (b) $\frac{n(n+1)}{2}$, ✓(c) $n+1$ (d) $n-1$ (e) n

(g) $n(n+1)$ (f) $\frac{(n+1)(n+2)}{2}$

$$V(x,y) = \frac{1}{2}m\omega^2x^2 + \frac{1}{2}m\omega^2y^2$$

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

$$E_n = (n_x+n_y+1)\hbar\omega$$

$$E_n = (n+1)\hbar\omega$$

$$n = n_x + n_y$$

$$(n - n_x) = n_y$$

$$(n_x\ n_y) = (0,n),\ (1,n-1),\ (2,n-2),\ \cdots\cdots (n-1,1),\ (n,0)$$

from 0 to n $\longrightarrow$ $(n+1)$ terms

So degeneracy $\boxed{g = (n+1)}$ Ans

Problem :- Consider a spin less particle of mass m which is moving in a 3 dim potential

$$V(x,y,z) = \begin{cases} \frac{1}{2}m\omega^2z^2, & 0<x<a,\ 0<y<a \\ \infty, & \text{otherwise / elsewhere} \end{cases}$$

(i) Write down the total energy & total Wave fucⁿ for the nth state of the particle,

(ii) Assuming that $\hbar\omega > \frac{5\pi^2\hbar^2}{ma^2}$. Find the energies & corresponding degeneracies for the ground state & Ist excited state

$$V(x,y,z) = 0 + 0 + \frac{1}{2} m\omega^2 z^2$$ { No cond^n on z so for all values of z results will be

$$V(x) = \begin{cases} 0 & 0<x<a \\ \infty & \text{otherwise} \end{cases} \qquad V(y) = \begin{cases} 0 & 0<y<a \\ \infty & \text{otherwise} \end{cases}$$

$$V(z) = \frac{1}{2} m\omega^2 z^2$$

In x-dir^n pot^n is particle in box type
y-dir^n " " "
~~z-dir^n " harmonic Oscillator "~~

So Energy $$E = \frac{n_x^2 \pi^2 \hbar^2}{2ma^2} + \frac{n_y^2 \pi^2 \hbar^2}{2ma^2} + \left(n_z + \frac{1}{2}\right)\hbar\omega$$

$n_x = n_y = 1, 2, 3 \ldots \infty$
$n_z = 0, 1, 2, 3, \ldots$

Wave fun^n,

$$\psi = \sqrt{\frac{2}{a}} \sin\left(\frac{n_x \pi x}{a}\right) \cdot \sqrt{\frac{2}{a}} \sin\left(\frac{n_y \pi y}{a}\right) \cdot \left(\frac{\alpha_z}{2^{n_z} n_z! \sqrt{\pi}}\right)^{1/2} e^{-\frac{\alpha_z^2 z^2}{2}} H_{n_z}(\alpha_z z)$$

for ground state, $n_x = n_y = 1$, $n_z = 0$ $\quad (n_x\, n_y\, n_z) - (1,1,0)$

then energy minimum value, i.e.
Ground state energy $$E = \frac{\pi^2\hbar^2}{2ma^2} + \frac{\pi^2\hbar^2}{2ma^2} + \frac{1}{2}\hbar\omega$$
$$= \pi^2\hbar^2/ma^2 + \frac{1}{2}\hbar\omega$$

for ground state $g = 1$ Non-degenerate

for Ist Excited state, take $n_x = 2$, $n_y = 1$, $n_z = 0$ or $(1,2,0)$

$$E_{120} = \frac{\cancel{4}\pi^2\hbar^2}{2ma^2} + \frac{4\pi^2\hbar^2}{2ma^2} + \frac{1}{2}\hbar\omega$$

$$E_{120} = \frac{5\pi^2\hbar^2}{2ma^2} + \frac{1}{2}\hbar\omega$$

If $\hbar\omega > \frac{5\pi^2\hbar^2}{2ma^2}$

2 fold degenerate
so $g = 2$

$n_x = n_y = n_z = 1$

$E_{111} = \frac{\hbar^2\pi^2}{2ma^2} + \frac{1}{2}\hbar\omega + \hbar\omega$

$E_{111} > E_{210}$

so Ist excited state is E_{210}

$E_{120} = E_{210}$

Problem :- A linear harmonic oscillator is in a state
$$|\psi\rangle = \frac{1}{\sqrt{2}}|\phi_0\rangle + \frac{i}{\sqrt{2}}|\phi_1\rangle$$
$|\phi_0\rangle$ & $|\phi_1\rangle$ are eign states of ground & Ist excited state respectively then expectation value of momentum in this state $|\psi\rangle$ is

(a) 0 (b) $\sqrt{\hbar m\omega}$ ✓(c) $\sqrt{\frac{\hbar m\omega}{2}}$ (d) $\sqrt{\frac{\hbar m\omega}{4}}$

$$|\psi\rangle = \frac{1}{\sqrt{2}}|\phi_0\rangle + \frac{i}{\sqrt{2}}|\phi_1\rangle$$
$$\langle\psi| = \frac{1}{\sqrt{2}}\langle\phi_0| - \frac{i}{\sqrt{2}}\langle\phi_1|$$
$$\langle\hat{p}\rangle = \underbrace{\frac{1}{2}\langle\phi_0|\hat{p}|\phi_0\rangle}_{0} + \frac{i}{2}\langle\phi_0|\hat{p}|\phi_1\rangle - \frac{i}{\cancel{\sqrt{2}}}\langle\phi_1|\hat{p}|\phi_0\rangle + \underbrace{\frac{1}{2}\langle\phi_1|\hat{p}|\phi_1\rangle}_{0}$$
$$= \frac{i}{2}\langle\phi_0|\hat{p}|\phi_1\rangle - \frac{i}{\cancel{\sqrt{2}}}\langle\phi_1|\hat{p}|\phi_0\rangle$$
$$= \frac{i}{2}\langle\phi_0|\frac{1}{i}\sqrt{\frac{\hbar m\omega}{2}}(a-a^+)|\phi_1\rangle - \frac{i}{2}\langle\phi_1|\frac{1}{i}\sqrt{\frac{\hbar m\omega}{2}}(a-a^+)|$$
$$= \frac{1}{2}\sqrt{\frac{\hbar m\omega}{2}}\left[\langle\phi_0|a|\phi_1\rangle - \langle\phi_0|a^+|\phi_1\rangle\right] - \frac{1}{2}\sqrt{\frac{\hbar m\omega}{2}}\left[\langle\phi_1|a|\phi_0\rangle - \langle\phi_1|a^+|\phi_0\rangle\right]$$
$$= \frac{1}{2}\sqrt{\frac{\hbar m\omega}{2}}\left[\langle\phi_0|\phi_0\rangle - \underbrace{\langle\phi_0|\phi_2\rangle}_{0} - \underbrace{\langle\phi_1|\phi_{-1}\rangle}_{0} + \langle\phi_1|\phi_1\rangle\right]$$
$$= \frac{1}{2}\sqrt{\frac{\hbar m\omega}{2}}\left[1+1\right] = \frac{1}{\cancel{2}}\sqrt{\frac{\hbar m\omega}{2}}(\cancel{2})$$
$$\boxed{\langle\hat{p}\rangle = \sqrt{\frac{\hbar m\omega}{2}}}$$
Ans

Problem :- The energy of the first excited quantum state of a particle in the potential $V(x,y) = \frac{1}{2}m\omega^2(x^2+4y^2)$ is

a) $2\hbar\omega$ (b) $3\hbar\omega$ (c) $\frac{3}{2}\hbar\omega$ ✓(d) $\frac{5}{2}\hbar\omega$

$$V(x,y) = \frac{1}{2} m\omega^2 (x^2+4y^2)$$
$$= \frac{1}{2} m\omega^2 x^2 + \frac{1}{2} m (2\omega)^2 y^2$$

$$E_n = \left(n_x + \frac{1}{2}\right)\hbar\omega + \left(n_y + \frac{1}{2}\right)2\hbar\omega$$
$$= \left(\underbrace{n_x + 2n_y} + \frac{3}{2}\right)\hbar\omega$$
$$= \left(n + \frac{3}{2}\right)\hbar\omega \quad , n = 0, 1, 2, \ldots$$

for Ist excited state $n = 1$

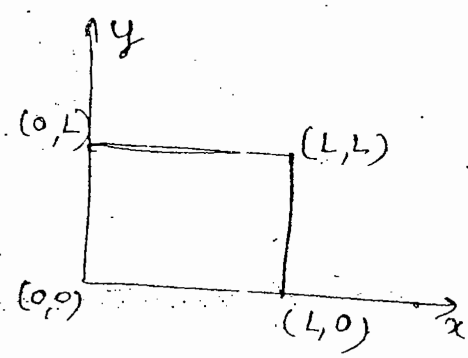
$$E_n = \left(1 + \frac{3}{2}\right)\hbar\omega$$
$$\boxed{E_n = \frac{5}{2}\hbar\omega}$$
✓(d)

Que :- A Quantum particle of mass m is confined to a square region in x-y plane, whose verticies are given by (0,0), (L,0), (L,L) & (0,L). Which of the following rep^n an admissible wave fun^n of the particle (for $l, m, n \to$ +ve integers)

(a) $\frac{2}{L}\sin\left(\frac{n\pi x}{L}\right)\cos\left(\frac{m\pi y}{L}\right)$ (b) $\frac{2}{L}\sin\left(\frac{l\pi x}{L}\right)\cos\left(\frac{n\pi y}{L}\right)$

✓(c) $\frac{2}{L}\sin\left(\frac{m\pi x}{L}\right)\sin\left(\frac{n\pi y}{L}\right)$ (d) $\frac{2}{L}\cos\left(\frac{n\pi y}{L}\right)\sin\left(\frac{l\pi y}{L}\right)$

Sol :- There are 4 boundries i.e. 4 verticies. At these boundaries W. fun^n must be zero.



(c) $\frac{2}{L}\sin\left(\frac{m\pi x}{L}\right)\sin\left(\frac{n\pi y}{L}\right)$

At (0,0) $\Rightarrow \frac{2}{L}\sin 0 \sin 0 = 0$
At (0 L) $\Rightarrow$ 0
(L 0) $\Rightarrow$ 0
(L L) $\Rightarrow$ 0

W. fun = 0

Q. Consider a Quantum particle of mass m in a 3-dim Isotropic S.H.O. potential -

$$V(x,y,z) = \frac{1}{2} m\omega^2 (x^2+y^2+z^2)$$

It is known that the particle is in an energy eigen state with eigen value $\frac{7}{2}\hbar\omega$. Which of the following can not be the wavefuncⁿ of the particle [$\alpha = \sqrt{\frac{m\omega}{\hbar}}$ & $H_n(\xi)$ is the hermite polynomial]

(a) $H_2(\alpha x) \exp(-\alpha(y^2+z^2))$ ✓

(b) $H_2(\alpha x) \exp[-\alpha(x^2+y^2+z^2)]$

(c) $H_1(\alpha y) H_1(\alpha z) \exp[-\alpha(x^2+y^2+z^2)]$

(d) $H_1(\alpha x) H_1(\alpha z) \exp[-\alpha(x^2+y^2+z^2)]$

Solⁿ :- For Isotropic S.H.O.,

$$E_n = (n_x + n_y + n_z + \frac{3}{2})\hbar\omega$$

Possible value of n_x, n_y, n_z for obtaining $E = \frac{7}{2}\hbar\omega$ are $n_x = 2$, $n_y = 0$, $n_z = 0$

or $n_x = n_y = 1$, $n_z = 0$

Hermite polynomials should contain all the 3 dirⁿ x, y, z & α is common factor in all the w.funcⁿ, Option (b), (c) & (d) are satisfying the condⁿ of isotropic S.H.O. so option (a) is wrong w.funcⁿ i.e this can not be the w.funcⁿ of particle bcoz it does not contain x-dirⁿ in exponential.

Schrodinger eqn in spherical polar co-ordinate :-

$$H\psi(r,\theta,\phi) = E\psi(r,\theta,\phi)$$

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(r,\theta,\phi)\right]\psi(r,\theta,\phi) = E\psi(r,\theta,\phi)$$

If potn is central potn i.e. V depends on r only then this Schr eqn can be reduced in 3 independent schr eqn one for each r, θ & ϕ.

Central potn $\longrightarrow V(r)$ or $V(|\vec{r}|)$

But $V(\underline{r})$ is not central potn.

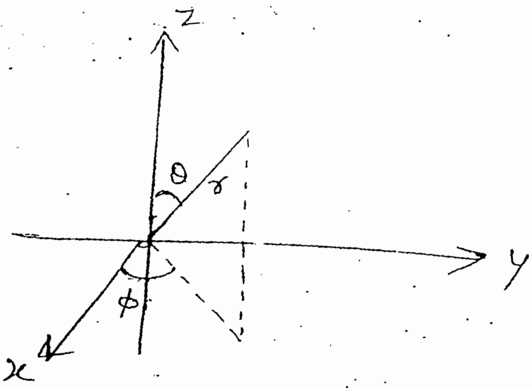
In Cartesian $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$

Convert it in polar form (r,θ,ϕ)

$x = r\sin\theta\cos\phi$

$y = r\sin\theta\sin\phi$

$z = r\cos\theta$



$\Rightarrow r = \sqrt{x^2+y^2+z^2}$

$\tan\phi = \frac{y}{x}$

$\tan\theta = \sqrt{x^2+y^2}/z$

On solving, we get

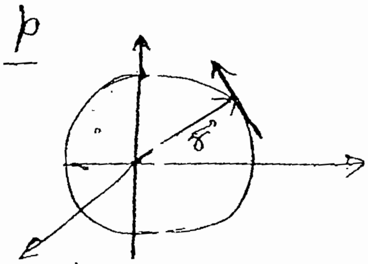
$$\boxed{\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}}$$

~~Ob~~ Orbital Angular Momentum :-

Classically, ang. mom. is $\underline{L} = \underline{r} \times \underline{p}$

$\vec{r} \rightarrow$ position vector

$\vec{p} \rightarrow$ linear mom.



If there is a point like particle then ang. mom. will be $\vec{L} = \vec{r} \times \vec{p}$ in Q.M. as well as C.M.

If we have large no. of particles then there arise a concept of orbital ang. mom.

$$\underline{L} = (xi + yj + zk) \times (p_x i + p_y j + p_z k)$$

$$L_x \hat{i} + L_y \hat{j} + L_z \hat{k} = (x\hat{i} + y\hat{j} + z\hat{k}) \times \left(-i\hbar \frac{\partial}{\partial x}\hat{i} + (-i)\hbar \frac{\partial}{\partial y}\hat{j} + (-i)\hbar\frac{\partial}{\partial z}\hat{k}\right)$$

On ~~seperating~~ the cofficients of $\hat{i}, \hat{j}, \hat{k}$,

$$L_x = -i\hbar\left[y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right] = i\hbar\left[\sin\phi\frac{\partial}{\partial\theta} + \cot\theta\cos\phi\frac{\partial}{\partial\phi}\right]$$

$$L_y = -i\hbar\left[z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right] = i\hbar\left[-\cos\phi\frac{\partial}{\partial\theta} + \cot\theta\sin\phi\frac{\partial}{\partial\phi}\right]$$

$$L_z = -i\hbar\left[x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right] = -i\hbar\frac{\partial}{\partial\phi}$$

<u>Angular Momentum Raising & Lowering operators are</u>

→ $L_+ = L_x + iL_y$ ⟶ Raising o/p

→ $L_- = L_x - iL_y$ ⟶ Lowering "

$$L_+ = i\hbar\left[\sin\phi\frac{\partial}{\partial\theta} + \cot\theta\cos\phi\frac{\partial}{\partial\phi}\right] - \hbar\left[-\cos\phi\frac{\partial}{\partial\theta} + \cot\theta\sin\phi\frac{\partial}{\partial\phi}\right]$$

$$\boxed{L_+ = \hbar e^{i\phi}\left[\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\phi}\right]}$$

& $\boxed{L_- = \hbar e^{-i\phi}\left[\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\phi}\right]}$

$$L^2 = L_x^2 + L_y^2 + L_z^2$$

$$\boxed{L^2 = -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]}$$

- $[L^2, L_x] = [L^2, L_y] = [L^2, L_z] = [L^2, L_\pm] = 0$
- $[L_x, L_y] = i\hbar L_z$, $[L_y, L_x] = -i\hbar L_z$
- $[L_y, L_z] = i\hbar L_x$, $[L_z, L_y] = -i\hbar L_x$
- $[L_z, L_x] = i\hbar L_y$, $[L_x, L_z] = -i\hbar L_y$

$[L_z, L_-] = -\hbar L_-$

- $[\hat{L}_x, \hat{p}_x] = [\hat{L}_x, \hat{x}] = [\hat{L}_x, \hat{L}_x] = 0$

  $[\hat{L}_y, \hat{p}_y] = [\hat{L}_y, \hat{y}] = [\hat{L}_y, \hat{L}_y] = 0$

  $[\hat{L}_z, \hat{p}_z] = [\hat{L}_z, \hat{z}] = [\hat{L}_z, \hat{L}_z] = 0$

- $[L_x, p_y] = i\hbar p_z$

  $[L_y, p_z] = i\hbar p_x$

  $[L_z, p_x] = i\hbar p_y$

- $[L_x, y] = i\hbar z$

  $[L_y, z] = i\hbar x$

  $[L_z, x] = i\hbar y$

- $[L_+, L_-] = L_+L_- - L_-L_+$

$$= (L_x + iL_y)(L_x - iL_y) - (L_x - iL_y)(L_x + iL_y)$$
$$= \cancel{L_x^2} - iL_xL_y + iL_yL_x + \cancel{L_y^2} - \cancel{L_x^2} - iL_xL_y + iL_yL_x - \cancel{L_y^2}$$
$$= 2iL_yL_x - 2iL_xL_y$$
$$= 2i[L_y, L_x] = 2i(-i\hbar L_z)$$

$$\boxed{[L_+, L_-] = 2\hbar L_z}$$

- <u>Spin</u> :- means rotation about centre of mass

In Q.M., a point like particle do 2 type of motion.

(i) spin

(ii) orbital

Spin is an intrinsic property. It is not related with outer space.

All the properties uneffected by outer space are called <u>Intrinsic properties</u>.

We have $L_z = -i\hbar \frac{\partial}{\partial \phi}$ & $J_z = -i\hbar \frac{\partial}{\partial \phi}$

But $S_z \neq -i\hbar \frac{\partial}{\partial \phi}$

Also $\vec{L} = \vec{r} \times \vec{P}$ but $\vec{S} \neq \vec{r} \times \vec{p}$

$$\vec{\mu}_L = \frac{q}{2m}\vec{L} \qquad \vec{\mu}_S = \frac{2q}{2m}\vec{S}$$

If By changing reference frame, value is not changing then it is conserved.
If value change → Not conserved.
Same type of results obtain for S & J

$$[L_x\ L_y] = i\hbar L_z \qquad L^2 = l(l+1)\hbar^2$$
$$\Rightarrow [S_x\ S_y] = i\hbar S_z \qquad S^2 = S(S+1)\hbar^2$$
$$[J_x\ J_y] = i\hbar J_z \qquad J^2 = J(J+1)\hbar^2$$

Eigen values of Angular Momentum operator :-

$$[J^2, J_x] = [J^2, J_y] = [J^2, J_z] = 0$$

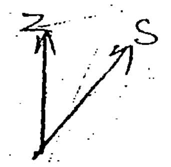
J^2 commute with each component of itself. So J^2 can ha simultanous eigen fuc^n with each fuc^n of itself.

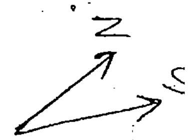
$[J_x\ J_y] = i\hbar J_z \Rightarrow$ J_x & J_y can't have simultanous ei fuc^n with each comp. of itself.

Mostely z-axis is considered the reference axis.
But if we take another reference axis then also the results are same.

$S = \pm \frac{1}{2}$ (quantized)

$S = \pm \frac{1}{2}$





Let $|j, m\rangle$ be the simultaneous eigen fuc^n of J^2 & J_z.

$$J^2 |j, m\rangle = \lambda |j, m\rangle$$
$$J_z |j, m\rangle = m\hbar |j, m\rangle$$

$\lambda \to$ eigen value.

$$J_+ J_- + J_- J_+ = (J_x + iJ_y)(J_x - iJ_y) + (J_x - iJ_y)(J_x + iJ_y)$$
$$= J_x^2 - i\cancel{J_x J_y} + i\cancel{J_y J_x} + J_y^2 + J_x^2 + i\cancel{J_x J_y} - i\cancel{J_y J_x} + J_y^2$$

$$J_+J_- + J_-J_+ = J_x^2 + J_y^2 + J_x^2 + J_y^2 \overset{+2J_z^2 - 2J_z^2}{\wedge} \cancel{+ i[J_zJ_y - J_yJ_z]}$$

$$= 2(J_x^2 + J_y^2 + J_z^2) - 2J_z^2 \cancel{+ i[\,]}$$

$$\boxed{J_+J_- + J_-J_+ = 2(J^2 - J_z^2)}$$

$$2(J^2 - J_z^2)|j, m\rangle = (J_+J_- + J_-J_+)|j,m\rangle$$

$$\Rightarrow \langle j', m'|2(J^2 - J_z^2)|j, m\rangle = \langle j', m'|(J_+J_- + J_-J_+)|j, m\rangle$$

$$\Rightarrow \langle j', m'|2(\lambda^2 - m^2\hbar^2)|j, m\rangle = \underbrace{(\langle j', m'|J_+)(J_-|j, m\rangle)}_{\text{Norm}}$$

$$\underbrace{+ (\langle j', m'|J_-)(J_+|j, m\rangle)}_{\text{Norm}}$$

Hermitian conjugate of each other

$$\Rightarrow 2(\lambda^2 - m^2\hbar^2)\langle j', m'|j, m\rangle = 0$$

$$\because \langle j', m'|j, m\rangle = \delta_{jj'}\delta_{mm'}$$

$$\therefore 2(\lambda^2 - m^2\hbar^2) \geq 0$$

$$\boxed{\lambda \geq m^2\hbar^2}$$

$$\langle j'm'|J_+J_-|j, m\rangle \geq 0$$

$$\langle j'm'|J_-J_+|j, m\rangle \geq 0$$

Eigen value of $\hat{J}$ satisfies this condⁿ.

for $\hbar = 1$, $\boxed{\lambda \geq m^2}$

Effect of Lowering & Raising operator :-

- $$J^2 J_+|j,m\rangle = J_+J^2|j, m\rangle$$
$$= \lambda J_+|j, m\rangle$$

$$[J_z, J_+] = [J_z, J_x + iJ_y]$$

$$= [J_z, J_x] + i[J_z, J_y]$$

$$= i\hbar J_y + i(-i\hbar)J_x$$

$$= \hbar[J_x + iJ_y] = \hbar J_+$$

$$[J_z, J_+] = \hbar J_+$$

$$[J_z, J_-] = \hbar J_-$$

$$[J_z, J_\pm] = \pm i\hbar J_\pm$$

$[J_z, J_+] = \hbar J_+$

$\Rightarrow J_z J_+ - J_+ J_z = \hbar J_+ \Rightarrow J_z J_+ = \hbar J_+ + J_+ J_z$

$\Rightarrow J_z J_+ |j, m\rangle = (\hbar J_+ + J_+ J_z)|j, m\rangle$

$\Rightarrow \qquad = (\hbar J_+ + m\hbar J_+)|j m\rangle$

$\Rightarrow J_z J_+ |j, m\rangle = \hbar(m+1) J_+ |j m\rangle$

$\Rightarrow \boxed{J_z |j, m\rangle = m\hbar |j m\rangle}$

- $\boxed{J_+ |j, m\rangle = C_+ |j, m+1\rangle}$
- $\boxed{J_- |j, m\rangle = C_- |j, m-1\rangle}$

$m = +j, (j-1), (j-2) \cdots\cdots -j$

Maxi. value of $m = j$ so if we operater raising o/p on j then we get 0.

$$\boxed{J_+ |j, +j\rangle = 0}$$

If we operater lowering o/p on min. value of m then we get 0 $\boxed{J_- |j, -j\rangle = 0}$

- $J_- J_+ |j, +j\rangle =$

$(J^2 - J_z^2 - \hbar J_z)|j, +j\rangle = 0$

$(\lambda - j^2\hbar^2 - j\hbar^2)|j, +j\rangle = 0$

$\lambda - j^2\hbar^2 - j\hbar^2 = 0$

$\lambda = j^2\hbar^2 + j\hbar^2$

$\boxed{\lambda = j(j+1)\hbar^2}$

$J_- J_+ = (J_x - iJ_y)(J_x + iJ_y)$

$= J_x^2 + J_y^2 + J_z^2 - J_z^2 - iJ_y J_x + iJ_x J_y$

$= J^2 - J_z^2 + i(i\hbar J_z)$

$= J^2 - J_z^2 - \hbar J_z$

$J_+ J_- |j, -j\rangle = j(j+1)\hbar^2$

$\boxed{J^2 |j, m\rangle = j(j+1)\hbar^2 |j, m\rangle}$ $\qquad \boxed{J_z |j, m\rangle = m\hbar |j, m\rangle}$

$\langle j, m | J_- = \langle j, m+1 | C_+^*$

$\langle j, m | J_- J_+ | j, m \rangle = |C_+|^2 \langle j, m+1 | j, m+1 \rangle$

$\langle j, m | J^2 - J_z^2 - \hbar J_z | j, m \rangle =$

$(j(j+1)\hbar^2 - m^2\hbar^2 - m\hbar^2) \langle j, m | j, m \rangle = |C_+|^2 \delta_{j,j} \delta_{m+1, m+1}$

$C_+ = \sqrt{j(j+1) - m(m+1)}\,\hbar$

$= \sqrt{j^2 + j - m^2 - m}\,\hbar = \sqrt{(j-m)(j+m) + (j-m)}\,\hbar$

$$\boxed{C_+ = \sqrt{(j-m)(j+m+1)}\,\hbar}$$

$\rightarrow \langle j', m' | J^2 | j, m \rangle = j(j+1)\hbar^2 \delta_{jj'} \delta_{mm'}$

$\rightarrow \langle j', m' | J_z | j, m \rangle = m\hbar\, \delta_{jj'} \delta_{mm'}$

$\rightarrow \langle j' m' | J_+ | j, m \rangle = \sqrt{(j-m)(j+m+1)}\,\hbar \langle j' m' | j, m+1 \rangle$
$= \sqrt{(j-m)(j+m+1)}\,\hbar\, \delta_{jj'} \delta_{m', m+1}$

$\rightarrow \langle j' m' | J_- | j, m \rangle = \sqrt{(j+m)(j-m+1)}\,\hbar\, \delta_{jj'} \delta_{m', m-1}$

$S_+ = S_x + iS_y$	$L_+ = L_x + iL_y$
$S_- = S_x - iS_y$	$L_- = L_x - iL_y$

<u>Matrix of J_z</u> :- (i) $J_z = m\hbar$

m' \ m	+1	0	−1
+1	–	0	0
0	0	–	0
−1	0	0	–

digonal elements will be non-zero

(ii) $J^2 = j(j+1)\hbar^2$

→ all digonal elements same → Non digonal zero

(iii) J_+ , $\delta_{jj'} \delta_{m', m+1}$

when $m' = m+1$, elements will be Non-zero. Other elements $= 0$

(iv) J_- ; $\delta_{jj'} \delta_{m', m-1}$

when $m' = m-1$, elements will be non-zero, other elements $= 0$

For $j = 1$, $m = +1, 0, -1$

$j' = 1$, $m = +1, 0, -1$

J^2

j'	m'	j / m	+1 / +1	ϕ / 0	+1 / −1
+1	+1		$2\hbar^2$	0	0
+ϕ	0		0	$2\hbar^2$	0
+1	−1		0	0	$2\hbar^2$

$\langle j'm' | J^2 | jm \rangle = j(j+1)\hbar^2 \delta_{jj'} \delta_{mm'}$

when $m = m'$ then Matrix element → Non zero

J_z

j'	m'	j / m	1 / +1	1 / 0	1 / −1
1	1	~~ħ~~	$\hbar$	0	0
1	0		0	$\hbar$	0
1	−1		0	0	$-\hbar$

$\langle j'm' | J_z | jm \rangle = m\hbar \delta_{jj} \delta_{mm'}$

when $m = m'$ → Non zero

J_+

j'	m'	j / m	1 / +1	1 / 0	1 / −1
1	1		0	$\sqrt{2}\hbar$	0
1	0		0	0	$\sqrt{2}\hbar$
1	−1		0	0	0

$\langle j'm' | J_+ | jm \rangle = \sqrt{(j-m)(j+m+1)}\,\hbar\, \delta_{jj'} \delta_{m', m+1}$

when $m' = m+1$ then Non zero

$\sqrt{(1-0)(1+0+1)}\,\hbar = \sqrt{2}\,\hbar$

$\sqrt{(1+1)(1 \ldots)}$ [illegible]

J_- then $J_+ = J_x + iJ_y$ & $J_- = J_x - iJ_y$

Commutator Relations

$$\psi(r,\theta,\phi) = R(r)\,\Theta(\theta)\,\Phi(\phi)$$

$R(r)$: depand upon Q. No. $n\ell$; $\Theta(\theta)$: ℓm; $\Phi(\phi)$: m

$$= R(r)\, Y_{\ell m}(\theta,\phi)$$

When $Y_{\ell m}(\theta,\phi)$ is called spherical Harmonics & repⁿ by $|\ell, m\rangle$ or $|j,m\rangle$ but $|j,m\rangle$ by symmetry may or may not be spherical harmonic.

If we know ℓ & s then $m_\ell = -\ell \cdots\cdots +\ell$, $m_s = -s \cdots\cdots +s$

$$[J_z, Y_{j,m}] = m\hbar\, Y_{j,m}$$

$$[J_+, Y_{j,m}] = \sqrt{(j-m)(j+m+1)}\,\hbar\, Y_{j,m+1}$$

$$[J_-, Y_{j,m}] = \sqrt{(j+m)(j-m+1)}\,\hbar\, Y_{j,m-1}$$

$$[J^2, Y_{jm}] = j(j+1)\hbar^2\, Y_{j,m}$$

$\{[J_z, Y_{jm}]\psi = J_z(Y\psi) - Y J_z\psi$

Commutator bracket is similar to eigen value.

$J_z|jm\rangle = m\hbar|jm\rangle$

$[J_z, Y_{jm}] = m\hbar\, Y_{jm}$

State $Y_{j,m+1}$ is not the eigen state of J_+ & also $\sqrt{(j-m)(j+m+1)}$ is not the eigen value of J_+ bcoz here state is changend. Illy for J_-.

Q. Find the expectation value of $\langle L_+\rangle$ in the state $|\psi\rangle$,

$$|\psi\rangle = \frac{1}{\sqrt3}\left[|1,1\rangle + |1,0\rangle + |1,-1\rangle\right]$$

State for L_+ is in terms of $|\ell, m\rangle$

(so in $|1,0\rangle \Rightarrow \ell=1, m=0$)

Wave funcⁿ is Normalized $\frac13+\frac13+\frac13 = 1$

$$|\psi\rangle = \frac{1}{\sqrt3}\left[|1,1\rangle + |1,0\rangle + |1,-1\rangle\right]$$

$$\langle\psi| = \frac{1}{\sqrt3}\left[\langle 1,1| + \langle 0,0| + \langle -1,1|\right]$$

$$\langle L_+\rangle = \langle\psi|L_+|\psi\rangle$$

$$L_+|1,0\rangle = \sqrt{(\ell-m)(\ell+m+1)}\,\hbar\,\delta_\ell\,\delta_{m+1} = \sqrt{1(1+0+1)}\,\hbar\,|1,1\rangle = \sqrt2\,\hbar\,|1,1\rangle$$

$L_+|1,-1\rangle = \sqrt{(2)(1)}\,\hbar\,|1,0\rangle = \sqrt{2}\hbar|1,0\rangle$

$$L_+|\psi\rangle = \frac{1}{\sqrt{3}}\left[L_+|1,1\rangle + L_+|1,0\rangle + L_+|1,-1\rangle\right]$$

$$= \frac{1}{\sqrt{3}}\left[0 + \sqrt{2}\hbar|1,1\rangle + \sqrt{2}\hbar|1,0\rangle\right]$$

$$\langle\psi|L_+|\psi\rangle = \frac{1}{3}\left[\langle 1,1| + \langle 1,0| + \langle 1,-1|\right]\left[\sqrt{2}\hbar|1,1\rangle + \sqrt{2}\hbar|1,0\rangle\right]$$

$$\cancel{= \frac{1}{3}[\langle N|\sqrt{2}\hbar N}$$

$$= \frac{1}{3}\left[\sqrt{2}\hbar\langle 1,1|1,1\rangle + \sqrt{2}\hbar\langle 1,0|1,0\rangle\right]$$

$$= \frac{1}{3}\,2\sqrt{2}\hbar = \frac{2\sqrt{2}\hbar}{3}\quad \underline{\underline{\text{A}}}$$

Que :- ~~Find the state~~ $|l,m\rangle$, Find the expectation value of operator $\langle\hat{A}\rangle = ?$ if $\hat{A} = \frac{L_xL_y + L_yL_x}{2}$

$$\langle\hat{A}\rangle = \langle l,m|\hat{A}|l,m\rangle$$

$$= \langle l,m|\frac{L_xL_y + L_yL_x}{2}|l,m\rangle$$

$$= \frac{1}{2}\left[\langle l,m|L_xL_y|l,m\rangle + \langle l,m|L_yL_x|l,m\rangle\right]$$

$$\left.\begin{aligned} L_+ &= L_x + iL_y \\ L_- &= L_x - iL_y \end{aligned}\right\}$$

$$\begin{aligned} L_+ &= L_x + iL_y \\ L_- &= L_x - iL_y \\ \hline 2L_x &= L_+ + L_- \end{aligned} \qquad \begin{aligned} L_+ &= L_x + iL_y \\ \underset{-}{L_-} &= \underset{-}{L_x} \underset{+}{-} iL_y \\ \hline 2iL_y &= L_+ - L_- \end{aligned}$$

$$\Rightarrow L_x = \frac{(L_+ + L_-)}{2}, \quad L_y = \frac{(L_+ - L_-)}{2i}$$

$$L_xL_y = \frac{L_+^2}{4i} - \frac{L_-^2}{4i} - \cancel{\frac{1}{4i}L_+L_-} + \cancel{\frac{1}{4i}L_-L_+}$$

$$L_yL_x = \frac{L_+^2}{4i} - \frac{L_-^2}{4i} + \cancel{\frac{1}{4i}L_+L_-} - \cancel{\frac{1}{4i}L_-L_+}$$

Now, $L_xL_y + L_yL_x = \frac{1}{2i}\left[L_+^2 - L_-^2\right]$

If we operate L_+^2 on $|l,m\rangle$ then $m \to m+2$

" " " L_-^2 " $|l,m\rangle$ " $m \to m-2$

But Here ~~It is not given that~~ $m = m+2$, $\delta_{m,m+2} = 1$ & $m = m-2$ $\delta_{m,m-2} = 1$ So here $m \neq m+2$ & $m \neq m-2$

$\delta_{n, m+2} = 0$

$\delta_{n, m-2} = 0$

$\langle \hat{A} \rangle = 0 + 0 = \underline{\underline{0}}$ always.

Q:- A system is known to be in a state described by the wavefunc^n $\psi(\theta, \phi) = \frac{1}{\sqrt{30}}\left[5Y_4^0 + Y_6^0 + 2Y_6^3\right]$

$Y_{l,m}(\theta,\phi)$ are the spherical harmonics. The probability of finding the system in a state with $m = 0$ is

(a) zero (b) $\frac{2}{15}$ (c) $\frac{1}{4}$ (d) $\frac{13}{15}$ ✓

States with $m=0$ are Y_4^0 & Y_6^0

$$P_4 = \left|\frac{5}{\sqrt{30}}\right|^2 = \frac{25}{30}$$

$$P = \left|\frac{1}{\sqrt{30}}\right|^2 = \frac{1}{30}$$

$$\text{Probability} = \frac{25}{30} + \frac{1}{30} = \frac{26}{30} = \underline{\underline{\frac{13}{15}}}$$

{ If what is the prob. for $m=3$ = ?

$$\text{Prob.} = \left|\frac{-2}{\sqrt{30}}\right|^2 = \frac{4}{30} = \frac{2}{15}$$ }

Q:- A measurement of z-comp. of ang. mom. (L_z) is made for a particle moving in the central pot^n with wave func^n

$$\psi_{nlm} = \frac{1}{4}\left[\psi_{100}(r) + 3\psi_{211}(r) - \sqrt{6}\,\psi_{21-1}(r)\right]$$

The expectation value of L_z is - $\underline{nlm}$

$\langle \psi | L_z | \psi \rangle = ?$ $\quad L_z|\psi\rangle = m\hbar|\psi\rangle$

$L_z|l, m\rangle = m\hbar\,|l, m\rangle$

$\psi_{100} \to m = 0$, $\psi_{211} \to m = 1$, $\psi_{21-1} \to m = -1$

$\cancel{\langle\psi|L_z|\psi\rangle} = +\cancel{\frac{3}{4}}\hbar\,|\psi_{211}\rangle + \cancel{\frac{\sqrt{6}}{4}\hbar\,|\psi_{21-1}\rangle}$

$$\therefore \langle\psi|L_z|\psi\rangle = \left(\frac{1}{4}\right)^2 \langle\psi_{100}|L_z|\psi_{100}\rangle + \left|\frac{3}{4}\right|^2 \langle\psi_{211}|L_z|\psi_{211}\rangle + \left|\frac{-\sqrt{6}}{4}\right|^2 \langle\psi_{21-1}|L_z|\psi_{21-1}\rangle$$

$$= 0 + \frac{9}{16}(1)\hbar + \frac{6}{16}(-1)\hbar$$

$$= \left(\frac{9}{16} - \frac{6}{16}\right)\hbar = \frac{3}{16}\hbar \quad \text{Ans}$$

- (Expectation value = Prob. × Eigen value) but when state changes then can't use this.

Prob :- The Normalised wave fucn ψ_1 & ψ_2 corresponding to ground state & Ist excited state of a particle. You are given the information that the operator $\hat{A}$ acts on the wave fucn as $\hat{A}\psi_1 = \psi_2$, $\hat{A}\psi_2 = \psi_1$.

(a) (i) $\langle \hat{A} \rangle = ?$ for $\psi = 3\psi_1 + 4\psi_2$

(a) -0.32 (b) 0.32 (c) 0.75 (d) 0.96

(ii) Which of the following wave functions are eigen fucn of operator $\hat{A}^2$

(a) ψ_1 & ψ_2 (b) ψ_2 & not ψ_1 (c) ψ_1 & not ψ_2

(d) neither ψ_1 nor ψ_2

(ii)
$$\hat{A}\psi_1 = \psi_2 \qquad \hat{A}\psi_2 = \psi_1$$
$$\hat{A}^2\psi_1 = \hat{A}\psi_2 = \psi_1 \qquad \hat{A}^2\psi_2 = \hat{A}\psi_1 = \psi_2$$

So both ψ_1 & ψ_2 will be the eigen fucn of $\hat{A}^2$.

(i) $\psi = 3\psi_1 + 4\psi_2$

ψ_1 & ψ_2 are normalised but their linear combination is not. Normalised wave fucn will be

$$\psi = \frac{3\psi_1 + 4\psi_2}{(|3|^2+|4|^2)} = \frac{3\psi_1 + 4\psi_2}{\sqrt{25}}$$

$$\langle\hat{A}\rangle = \frac{\langle\psi|\hat{A}|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{\langle(3\psi_1+4\psi_2)|\hat{A}|(3\psi_1+4\psi_2)\rangle}{25}$$

$$= \frac{9\langle\psi_1|\hat{A}|\psi_1\rangle + 12\langle\psi_1|\hat{A}|\psi_2\rangle + 12\langle\psi_2|\hat{A}|\psi_1\rangle + 16\langle\psi_2|\hat{A}|}{25}$$

$$= \frac{1}{25}\left[9\underbrace{\langle\psi_1|\psi_2\rangle}_{0} + 12\underbrace{\langle\psi_1|\psi_1\rangle}_{1} + 12\underbrace{\langle\psi_2|\psi_2\rangle}_{1} + 16\underbrace{\langle\psi_2|\psi_1\rangle}_{0}\right]$$

$$= \frac{1}{25}[12+12] = \frac{24}{25}$$

$$\left\{\begin{array}{l}\hat{A}\psi_1 = \psi_2 \\ \hat{A}\psi_2 = \psi_1\end{array}\right.$$

$$\boxed{\langle\hat{A}\rangle = \frac{24}{25} = 0.96}$$

Spin :-

Experimental Need of Spin :-

→ If we include the spin concept then there comes the concept of Fine Specta.

→ If we nclude nuclear spin then there comes the concept of Hyperfine Specta.

→ Anamouly Zeman Effect can't be explain be without concept of spin but Normal zeeman effect can be explained.

→ for $l \neq$, $m_l = +l \cdots\cdots -l$
(mag. q. No.)

In Stein Gerlach exp., as atom is in ground state then a single beam is split by passing inhomogenous $\vec{B}$.

$m_l = +l \cdots\cdots -l$

Interaction with $\vec{B}$ gives $2l+1$ lines

→ Neutral ground state $l=0$

Unpaired e^- also contributes

Hence shifting is not due to l, m & other concept comes it is 'spin'.

Imp $m_j = +j$ to $-j$ $= (2j+1)$

Value of m_j are no. of splitting lines. Total shifting is due to $l+s$. $J = |l+s|$ to $|l-s|$

If $l=0$ then also splitting .....

In Stern-Gerlach Experiment

of Ag atoms:

If a neutral beam is pass through inhomogeneous mag. field then beam split into two parts due to the interaction of mag. moment & mag. field.

Beam split into ~~2s~~ $(2l+1)$ parts.

$$F = \nabla(\mu \cdot B)$$

$$\mu_L = \frac{q}{2m} L$$

Z ↑ B — Mag. field in z-dirⁿ

$$-\mu_L \cdot B = \frac{q}{2m} L_z B$$

where $L_z = m_l \hbar$, $m_l = -l$ to $+l$.

When silver atom in ground state then split into single beam.

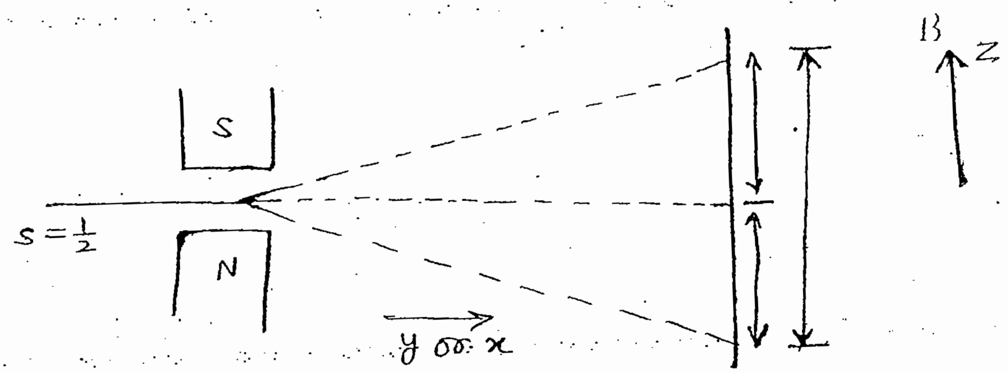
If we consider e^- (of spin ½) then

$$j = |l+s| \text{ to } |l-s| = \underline{1/2}$$

$$m_j = -\frac{1}{2}, +\frac{1}{2}$$

i.e. acc. to Stern Gerlach exp. a single beam split into 2 parts i.e. $\boxed{(2j+1)}$. Beam split in $(2j+1)$ ~~part~~ no. of beams.

Deflection along the z-axis :-



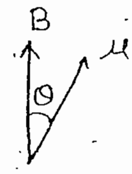
There are 2 comp. of spin for spin ½ particle so there are 2 dirⁿ. of beam splitting.

If $\vec{B}$ is along z-dirⁿ then no velocity along z-dirⁿ then (It is along x or y dirⁿ)
(Force will be in the dirⁿ of $\vec{B}$ i.e. z-dirⁿ)

$$F = q(v \times B)$$

deflection $S = ut + \frac{1}{2} a_z t^2$

$$S = \frac{1}{2} a_z t^2 \quad \text{——(1)} \quad (u = 0, \text{ initially})$$



force, $F = \nabla(\mu \cdot B)$

If μ is const. then $\boxed{\begin{aligned} F &= \mu \cdot \nabla B \\ F &= \mu \nabla B \cos\theta \end{aligned}}$

acceleraion, $\boxed{a = \frac{F}{m} = \frac{\mu \cdot \nabla B}{m} = \frac{\mu \cos\theta}{m} \frac{\partial B}{\partial z}}$

(1) $\Rightarrow$ $s = \frac{1}{2} a_z t^2$

$a_z \rightarrow$ acceleration along z-dis^n

If length of mag. field region is L, particle velocity is v then time $t = \frac{L}{v}$ then ($L \rightarrow$ very small length)

$$S = \frac{1}{2} \frac{\mu \cos\theta}{m} \frac{\partial B}{\partial z} \left(\frac{L}{v}\right)^2$$

$$\boxed{S = \pm \frac{1}{2} \frac{\mu}{m} \frac{\partial B}{\partial z} \frac{L^2}{v^2}} \qquad (\cos\theta = \pm 1)$$

This is the expression for the diflection in stern Garlac exp.

& seperation b/w 2 beams is $= \frac{1}{2} \frac{\mu}{m} \frac{\partial B}{\partial z} \frac{L^2}{v^2} - \left(-\frac{1}{2} \frac{\mu}{m} \frac{\partial B}{\partial z} \frac{L^2}{v^2}\right)$

$$\boxed{\text{Seperation} = \frac{\mu}{m} \frac{\partial B}{\partial z} \frac{L^2}{v^2}}$$

Commuator bracket for spin operator :-

- $[S_x, S_y] = i\hbar S_z$

  $[S_y, S_z] = i\hbar S_x$

  $[S_z, S_x] = i\hbar S_y$

- $S = \frac{1}{2} \hbar \sigma$ $\quad \sigma \rightarrow$ Pauli spin operator

- corresponding components

  $S_x = \hbar/2 \, \sigma_x \qquad [s = \frac{1}{2}]$

  $S_y = \hbar/2 \, \sigma_y$

  $S_z = \hbar/2 \, \sigma_z$

- $\sigma_x^2 = \sigma_y^2 = \sigma_z^2 = 1$

eigen values of each comp of spin is $\pm \frac{\hbar}{2}$
so each σ^2 comp. will be 1.

- $[\sigma_x, \sigma_y] = 2i\sigma_z$
$[\sigma_y, \sigma_z] = 2i\sigma_x$
$[\sigma_z, \sigma_x] = 2i\sigma_y$

Proof $\rightarrow [S_x\, S_y] = i\hbar S_z$

$\Rightarrow \left[\frac{\hbar}{2}\sigma_x, \frac{\hbar}{2}\sigma_y\right] = i\hbar \frac{\hbar}{2}\sigma_z$

$\Rightarrow [\sigma_x, \sigma_y] = 2i\sigma_z$

- Components of Pauli spin operators anticommute.

(i) $\sigma_x\sigma_y + \sigma_y\sigma_x = 0$
$\sigma_y\sigma_z + \sigma_z\sigma_y = 0$
$\sigma_z\sigma_x + \sigma_x\sigma_z = 0$

(i) $\sigma_x\sigma_y + \sigma_y\sigma_x = \frac{1}{2i}[2i\sigma_x\sigma_y + 2i\sigma_y\sigma_x]$

$= \frac{1}{2i}[\sigma_x(2i\sigma_y) + (2i\sigma_y)\sigma_x]$

$= \frac{1}{2i}[\sigma_x[\sigma_z, \sigma_x] + [\sigma_z, \sigma_x]\sigma_x]$

$= \frac{1}{2i}[\sigma_x(\sigma_z\sigma_x - \sigma_x\sigma_z) + (\sigma_z\sigma_x - \sigma_x\sigma_z)\sigma_x]$

$= \frac{1}{2i}[\sigma_x\sigma_z\sigma_x - \sigma_x^2\sigma_z + \sigma_z\sigma_x^2 - \sigma_x\sigma_z\sigma_x]$

$= \frac{1}{2i}[\cancel{\sigma_x\sigma_z\sigma_x} - \cancel{\sigma_z} + \cancel{\sigma_z} - \cancel{\sigma_x\sigma_z\sigma_x}]$

$\boxed{\sigma_x\sigma_y + \sigma_y\sigma_x = 0}$ ✓

or $\boxed{\sigma_x\sigma_y = -\sigma_y\sigma_x}$ ✓

- Also $\sigma_x\sigma_y = i\sigma_z$
$\sigma_y\sigma_z = i\sigma_x$
$\sigma_z\sigma_x = i\sigma_y$

(i) $\sigma_x \sigma_y = i\sigma_z$

We have $\sigma_x\sigma_y + \sigma_y\sigma_x = 0$ —(1)

i.e. $[\sigma_x \sigma_y] = 2i\sigma_z \Rightarrow \sigma_x\sigma_y - \sigma_y\sigma_x = 2i\sigma_z$ —(2)

eqn (1) + (2) $\Rightarrow$ $2\sigma_x\sigma_y = 2i\sigma_z$

$\Rightarrow \boxed{\sigma_x\sigma_y = i\sigma_z}$

- Matrix ~~form of~~ Pauli spin operators,

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

- If we change the reference axis then these matrix will be change. Here ref. axis is z-axis.

- for spin $S = \frac{1}{2}$, $2S+1 \Rightarrow 2$

  So there matrix are of 2 x 2 order

  If spin changes then these matrix forms will be change

  e.g. If $S = 1 \Rightarrow 2S+1 = 3$ then 3 x 3 matrix.

- If Matrix given then Eigen fuc^n = ?

$$\hat{A}\psi = \lambda\psi$$

Any constant multiply with e. fuc^n is the eigen value.

for σ_z, $\sigma_z\psi = \lambda\psi$

$\psi = \begin{bmatrix} a \\ b \end{bmatrix} \Rightarrow$ components = no. of spin comp. $= 2$

so $\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}\begin{bmatrix} a \\ b \end{bmatrix} = \lambda\begin{bmatrix} a \\ b \end{bmatrix}$

Eigen Value of $\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$ are ± 1

for +1, $\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}\begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} a \\ b \end{bmatrix}$

$\Rightarrow$ $1\cdot a + 0\cdot b = a$

$0\, a + -1 \times b = b$

$\Rightarrow b = -b$ Not possible, Only for $b=0$, it is pos

$\Rightarrow -2b = 0$

$\Rightarrow \boxed{b=0}$ always

a is unknown.

So for $+1$ E. value the Eigen func^n is $\begin{bmatrix} a \\ 0 \end{bmatrix}$.

Normalisation, $\langle \psi | \psi \rangle = 1$

$$\Rightarrow A^* \begin{bmatrix} a^* & 0 \end{bmatrix} A \begin{bmatrix} a \\ 0 \end{bmatrix} = 1$$

$$\Rightarrow |A|^2 |a|^2 = 1$$

$$A = \frac{1}{a}$$

So Normalised eigen state is $|\psi(z)\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$

& any eigen state obtained by multiplying this state with a const. is also the eigen state i.e. of same eigen value.

$$i \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} i \\ 0 \end{bmatrix}$$

$$-1 \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} -1 \\ 0 \end{bmatrix}$$

These eigen states are linearly dependent on each other.

for -1 E. value, z-comp. of E. state $= \begin{bmatrix} 0 \\ 1 \end{bmatrix}$.

i.e. $|\psi(z)\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} (+)$, $\begin{bmatrix} 0 \\ 1 \end{bmatrix} (-)$

$|\psi(y)\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ i \end{bmatrix} (+)$, $\frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -i \end{bmatrix} (-)$

$|\psi(x)\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix} (+)$, $\frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix} (-)$

$\downarrow$ for +ve E. value $\qquad$ $\downarrow$ for -ve E. value

- If this $|\psi(x)\rangle$ is the E. state of S_x then E. value will be $\hbar/2$.

The Eigen state for spin comp. will be same as σ but Eigen value will be different.

for +ve eigen value $\Rightarrow +\frac{\hbar}{2}$, -ve eigen value $\Rightarrow -\frac{\hbar}{2}$.

$\therefore$ Expectation Value of any operator,

In Sch. notation $\Rightarrow$ $\langle \hat{A} \rangle = \dfrac{\int \psi^* \hat{A} \psi \, d\tau}{\int \psi^* \psi \, d\tau}$

dirac " $\Rightarrow$ $\langle \hat{A} \rangle = \langle \psi | \hat{A} | \psi \rangle$

$\Downarrow$

multiply 3 matrix.

Problem.1:- If a spin 1 particle is in the state $|m=0\rangle$ w.r.to a quantisation axis $\hat{n}$. Which of the following is correct

✓(A) $\langle \underline{S} \rangle = 0$

(B) $\langle \underline{S} \rangle = \hat{n}$

(C) $\langle \underline{S} \rangle = \sqrt{9}\, \hat{n}$

(D) $\langle \underline{S} \rangle = -\hat{n}$

$S = \sqrt{s(s+1)}\,\hbar$

$\underline{S} = S_x \hat{i} + S_y \hat{j} + S_z \hat{k}$

Suppose quantisation axis is z-axis.

So $\langle S_x \rangle = 0$

$\langle S_y \rangle = 0$

$\langle S_z \rangle = \langle m=0 | S_z | m=0 \rangle$

$= m\hbar = 0$ $(\because m=0)$

So $\langle \underline{S} \rangle = \langle S_x \rangle \hat{i} + \langle S_y \rangle \hat{j} + \langle S_z \rangle \hat{k}$

$\boxed{\langle \underline{S} \rangle = 0}$ ✓

$|s, m_s\rangle$

$\Rightarrow |1,+1\rangle$ $|+1\rangle$

$\Rightarrow |1,0\rangle$ $|0\rangle$

$\Rightarrow |1,-1\rangle$ $|-1\rangle$

for a particular value of m_s, rotating about a particular angle so Expectation value of S will be zero in remaining two dirn

If $|m=1\rangle$ then if Quantisation Δ is Z-axis $\langle S_x\rangle = 0$

$\langle S_y\rangle = 0$

$$\langle S_z\rangle = \langle m=1|S_z|m=1\rangle$$
$$= m\hbar = \hbar \quad (\because m=1)$$

If we consider all angles together then always $m=0$.

Q.2:- for a spin $\frac{1}{2}$ particle, the expectation value of $S_x S_y S_z$ where (S_x, S_y, S_z are spin operators) is

(A) $\frac{i\hbar^3}{8}$ (B) $-\frac{i\hbar^3}{8}$ (C) $\frac{i\hbar^3}{16}$ (D) $-\frac{i\hbar^3}{16}$

$$S_x S_y S_z = \frac{\hbar}{2}\sigma_x \frac{\hbar}{2}\sigma_y \frac{\hbar}{2}\sigma_z$$
$$= \frac{\hbar^3}{8}\sigma_x \sigma_y \sigma_z$$
$$= \frac{\hbar^3}{8}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$
$$= \frac{\hbar^3}{8}\begin{bmatrix} i & 0 \\ 0 & -i \end{bmatrix}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} = \frac{\hbar^3}{8}\begin{bmatrix} i & 0 \\ 0 & i \end{bmatrix} = \frac{i\hbar^3}{8}\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$|\psi\rangle = \begin{bmatrix} a \\ b \end{bmatrix}$$

then $[a^* \; b^*]\frac{\hbar^3 i}{8}\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}\begin{bmatrix} a \\ b \end{bmatrix}$

$$\Rightarrow \frac{\hbar^3 i}{8}[a^* \; b^*]\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}\begin{bmatrix} a \\ b \end{bmatrix} = \frac{i\hbar^3}{8}[a^* \; b^*]\begin{bmatrix} a \\ b \end{bmatrix}.$$
$$= \frac{i\hbar^3}{8}[a^*a + b^*b]$$
$$= \frac{i\hbar^3}{8}$$

$\langle\psi|\psi\rangle = 1$

$\Rightarrow [a^* \; b^*]\begin{bmatrix} a \\ b \end{bmatrix} = 1$

$\Rightarrow a^*a + b^*b = 1$

OR

Another method,
$$S_x S_y S_z = \frac{\hbar^3}{8}\sigma_x \sigma_y \sigma_z$$
$$= \frac{\hbar^3}{8} i\,\sigma_z^2 \qquad (\sigma_x\sigma_y = i\sigma_z)$$
$$= \frac{\hbar^3}{8} i \qquad (\sigma_z^2 = 1)$$

$$\langle S_x S_y S_z\rangle = \langle\psi|S_x S_y S_z|\psi\rangle$$
$$= \langle\psi|\, i\frac{\hbar^3}{8}|\psi\rangle = \frac{i\hbar^3}{8}\langle\psi|\psi\rangle$$

$\langle \psi | \psi \rangle = 1$ then

$$\langle S_x S_y S_z \rangle = \frac{i\hbar^3}{8} \;//$$

Q.3:- A spin $\frac{1}{2}$ particle is in the state $S_z = \frac{\hbar}{2}$. The expectation value of S_x, S_x^2, S_y & S_y^2 are given by

(A) $0, 0, \frac{\hbar^2}{4}, \frac{\hbar^2}{4}$

(B) $0, \frac{\hbar^2}{4}, \frac{\hbar^2}{4}, 0$

(C) ✓ $0, \frac{\hbar^2}{4}, 0, \frac{\hbar^2}{4}$

(D) $\frac{\hbar^2}{4}, \frac{\hbar^2}{4}, 0, 0$

$S_z = \frac{\hbar}{2}$ corresponding E. state $= \begin{bmatrix} 1 \\ 0 \end{bmatrix}$

then $\langle S_x \rangle = 0$

$\langle S_y \rangle = 0$

but $\langle S_x^2 \rangle$ and $\langle S_y^2 \rangle \neq 0$

So (c) ✓

$\left\{ S_x = \frac{\hbar}{2}\sigma_x = \frac{\hbar}{2}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \right.$

By method, $\langle S_x \rangle = [1, 0]\, \frac{\hbar}{2} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = 0$

$\left.\langle S_x^2 \rangle = \frac{\hbar^2}{4}\right\} \langle S_x \rangle = 0 \qquad = \frac{\hbar}{2}[1, 0]\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}\begin{bmatrix} 1 \\ 0 \end{bmatrix} = \frac{\hbar}{2}(1, 0)\begin{bmatrix} 0 \\ 1 \end{bmatrix} = \frac{\hbar}{2}(($

$\left\{ \begin{array}{l} \text{If } S_x = \frac{\hbar}{2} \text{ is given then E. state} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 1 \end{bmatrix} \text{ then} \\ \langle S_x \rangle = \hbar/2, \quad \langle S_x^2 \rangle = \frac{\hbar^2}{4} \\ \text{then } \frac{\hbar^2}{2}, \frac{\hbar^2}{4}, 0, \frac{\hbar^2}{4} \end{array} \right\}$

Ans:- Now $\langle S_x^2 \rangle = [1, 0]\, \frac{\hbar^2}{4} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}^2 \begin{bmatrix} 1 \\ 0 \end{bmatrix}$

$\langle S_x^2 \rangle = \frac{\hbar^2}{4}[1, 0]\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}\begin{bmatrix} 1 \\ 0 \end{bmatrix}$

$= [1, 0]\, \frac{\hbar^2}{4}\begin{bmatrix} 1 \\ 0 \end{bmatrix} = \frac{\hbar^2}{4}[1, 0]\begin{bmatrix} 1 \\ 0 \end{bmatrix} = \frac{\hbar^2}{4}$

So $0, \frac{\hbar^2}{4}, 0, \frac{\hbar^2}{4}$ Option (c) is correct.

Q.4 :- An e^- is in the state with spin wave fuc^n

$$\phi_s = \begin{bmatrix} \frac{\sqrt{3}}{2} \\ \frac{1}{2} \end{bmatrix}$$

is in the S_z representation. What is the probability of finding the z-component of its spin along the $-\hat{z}$ dir^n.

Expand ϕ_s in z-comp of Eigen fuc^n of S.

$$\phi_s = \begin{bmatrix} \sqrt{3}/2 \\ 1/2 \end{bmatrix} = C_1 \underset{(\text{along } +z)}{\begin{bmatrix} 1 \\ 0 \end{bmatrix}} + C_2 \underset{(\text{along } -z \text{ dir}^n)}{\begin{bmatrix} 0 \\ 1 \end{bmatrix}}$$

$$\Rightarrow \quad C_1 \cdot 1 + C_2 \cdot 0 = \sqrt{3}/2 \quad \Rightarrow \quad \sqrt{3}/2 = C_1$$

$$C_1 \cdot 0 + C_2 \cdot 1 = 1/2 \quad \Rightarrow \quad 1/2 = C_2.$$

i.e. $$\begin{bmatrix} \sqrt{3}/2 \\ 1/2 \end{bmatrix} = \frac{\sqrt{3}}{2}\begin{bmatrix} 1 \\ 0 \end{bmatrix} + \frac{1}{2}\begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

Prob. of finding the particle $= \left|\frac{\sqrt{3}}{2}\right|^2 + \left|\frac{1}{2}\right|^2$

Total prob. $= \frac{3}{4} + \frac{1}{4} = 1$

Prob. of finding the z-comp. of spin along $(-z)$ dir^n $= \frac{1}{4}$ Ans

Q.5 :- Suppose a spin $\frac{1}{2}$ particle is in the state

$$|\phi\rangle = \frac{1}{\sqrt{6}}\begin{bmatrix} 1+i \\ 2 \end{bmatrix}$$

What are the probabilities of getting $+\frac{\hbar}{2}$ & $-\frac{\hbar}{2}$. If

(i) z-comp. of spin is measured

(ii) x-comp. of spin is measured

(iii) Calculate the expectation value of S_x i.e. $\langle S_x \rangle$

(i) z-comp. of S.

$$|\phi\rangle = \frac{1}{\sqrt{6}}\begin{bmatrix} 1+i \\ 2 \end{bmatrix} = C_1\begin{bmatrix} 1 \\ 0 \end{bmatrix} + C_2\begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

$$\Rightarrow \frac{1}{\sqrt6}(1+i) = C_1$$

$$\frac{1}{\sqrt6}\,2 = C_2$$

So $\frac{1}{\sqrt5}\begin{bmatrix}1+i\\2\end{bmatrix} = \frac{1}{\sqrt6}(1+i)\begin{bmatrix}1\\0\end{bmatrix} + \frac{1}{\sqrt6}2\begin{bmatrix}0\\1\end{bmatrix}$

Prob. of getting $+\frac{\hbar}{2} = |C_1|^2 = \left|\frac{1}{\sqrt6}(1+i)\right|^2 = \frac{1}{6}(1+i)(1-i)$
$= \frac{1}{6}(1+1)$

$$= \frac{1}{3} \text{ Ans}$$

Prob. of getting $-\frac{\hbar}{2} = |C_2|^2 = \left|\frac{2}{\sqrt6}\right|^2 = \frac{4}{6} = \frac{2}{3}$ Ans

(ii) x-comp.

$$|\phi\rangle = \frac{1}{\sqrt6}\begin{bmatrix}1+i\\2\end{bmatrix} = C_1\frac{1}{\sqrt2}\begin{bmatrix}1\\1\end{bmatrix} + C_2\frac{1}{\sqrt2}\begin{bmatrix}1\\-1\end{bmatrix}$$

$$\Rightarrow \frac{C_1}{\sqrt2} + \frac{C_2}{\sqrt2} = \frac{1}{\sqrt6}(1+i)$$

$$\frac{C_1}{\sqrt2} - \frac{C_2}{\sqrt2} = \frac{1}{\sqrt6}(2)$$

add, $2\frac{C_1}{\sqrt2} = \frac{1}{\sqrt6}[1+i+2]$

$$\sqrt2\,C_1 = \frac{1}{\sqrt6}[i+3] \Rightarrow C_1 = \frac{1}{\sqrt2}\left[\frac{(i+3)}{\sqrt6}\right]$$

Subs. $\Rightarrow 2\frac{C_2}{\sqrt2} = \frac{1}{\sqrt6}(1+i-2)$

$$\sqrt2\,C_2 = \frac{1}{\sqrt6}(i-1) \Rightarrow C_2 = \frac{1}{\sqrt2}\left[\frac{-1+i}{\sqrt6}\right]$$

Prob. of getting $+\frac{\hbar}{2} = |C_1|^2 = \left|\frac{1}{\sqrt2}\left(\frac{i+3}{\sqrt6}\right)\right|^2$

$$= \frac{1}{2}\frac{(3+i)(3-i)}{6} = \frac{1}{2}\frac{(9+1)}{6} = 5/6 \text{ Ans}$$

Prob. of getting $-\frac{\hbar}{2} = |C_2|^2 = \left|\frac{1}{\sqrt2}\frac{(-1+i)}{\sqrt6}\right|^2$

$$= \frac{1}{6} \text{ Ans}$$

(iii) $\langle S_x \rangle = ?$

$$\langle S_x \rangle = \text{Prob} \times \text{Ei. value} + \text{Prob} \times \text{Eigen value}$$
$$= P_1 \times \frac{\hbar}{2} + P_2 \times \left(\frac{\hbar}{2}\right) = \frac{5}{6} \times \frac{\hbar}{2} - \frac{1}{6} \times \frac{\hbar}{2}$$
$$= \frac{\hbar}{2 \times 6}[5-1] = \frac{4\hbar}{2 \times 6} = \frac{\hbar}{3} \text{ Ans}$$

OR If Prob. is not given then

$$\langle S_x \rangle = \frac{1}{\sqrt{6}}(1-i,\ 2)\frac{\hbar}{2}\underbrace{\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}}_{(\sigma_x)}\frac{1}{\sqrt{6}}\begin{bmatrix} 1+i \\ 2 \end{bmatrix}$$
$$= \frac{\hbar}{12}[1-i,\ 2]\begin{bmatrix} 2 \\ 1+i \end{bmatrix} = \frac{\hbar}{12}\left[2(1-i)+2(1+i)\right] = \frac{\hbar}{3} \text{ Ans}$$

Q.6 :- The wave func^n of an e^- at a given time is given by $\psi = f(r,\theta)\, e^{2i\phi}\, \chi_{1/2}$. Calculate the ~~ex~~ average value of z-comp. of its magnetic moments.

$$\psi = \underbrace{f(r,\theta)}_{\text{depends on } r \,\&\, \theta}\ \underbrace{e^{2i\phi}}_{\text{on } \phi}\ \underbrace{\chi_{1/2}}_{\text{spin wave func}^n}$$

for H_2 atom, $\psi_{nlm} \propto e^{im_l\phi}$

$$\chi_{1/2} = \begin{bmatrix} 1 \\ 0 \end{bmatrix} = |1/2, +1/2\rangle$$
$$\chi_{-1/2} = \begin{bmatrix} 0 \\ 1 \end{bmatrix} = |1/2, -1/2\rangle$$

$$\begin{cases} L_z|\psi\rangle = m_l\hbar|\psi\rangle \\ S_z|\psi\rangle = m_s\hbar|\psi\rangle \end{cases}$$

expectation value of mag. moment,

$$\mu = \underbrace{\mu_L}_{\text{depends on } L_z} + \underbrace{\mu_S}_{\text{depends on } S_z} = \frac{-e}{2m}L + \left(\frac{-2e}{2m}\right)S$$

z-comp.

$$\langle \mu_z \rangle = \mu_{Lz} + \mu_{Sz} = \frac{-e}{2m}L_z + \left(\frac{-2e}{2m}\right)S_z$$
$$= \frac{-e}{2m}\hbar m_l + \frac{-2e}{2m}\hbar m_s$$

Bohr magneton $\mu_B = \frac{e\hbar}{2m}$

$$\langle \mu_z \rangle = \langle \psi|\mu_z|\psi\rangle = \langle \psi|-\mu_B m_l|\psi\rangle - \langle \psi|2\mu_B \tfrac{1}{2}|\psi\rangle$$
$$= -\mu_B m_l\langle\psi|\psi\rangle - 2\mu_B\tfrac{1}{2}\langle\psi|\psi\rangle$$
$$= -2\mu_B - \mu_B = -3\mu_B$$

$\langle \mu_z \rangle = \langle \psi | \mu_{Lz} | \psi \rangle + \langle \psi | \mu_{Sz} | \psi \rangle$

$= \langle \psi | -\frac{e}{2m} m_l | \psi \rangle + \langle \psi | \left(\frac{-2e}{2m}\right) S_z | \psi \rangle$

$\psi = f(r,\theta)\, e^{2i\phi} \chi_{1/2}$

L_z will operate on ψ then L_z operate only on $e^{2i\phi}$

S_z " " " S_z " " " $\chi_{1/2}$

$m_l = 2, \; L_z = m_l\hbar \Rightarrow 2\hbar$

$S_z = m_s\hbar = \frac{\hbar}{2}$

$\therefore \langle \mu_z \rangle = \langle \psi | \frac{-e}{2m} 2\hbar | \psi \rangle + \langle \psi | \left(-\frac{2e}{2m}\right) \frac{1}{2}\hbar | \psi \rangle$

$= -2\mu_B \langle \psi | \psi \rangle - \mu_B \langle \psi | \psi \rangle$

$\underline{\langle \mu_z \rangle = -3\mu_B}$ A

Qu. 7 :- The wave func^n of an e^- at a given time is
$|\psi\rangle = f(r)\left[-2\chi_{1/2} + 3\chi_{-1/2}\right]$ or $f(r)\left[-2|\uparrow\rangle + 3|\downarrow\rangle\right]$
calculate the expectation value of z-comp. of magnetic moment (5/13)

$|\psi\rangle = \underbrace{f(r)}_{\text{depend on } r}\left[-2\chi_{1/2} + 3\chi_{-1/2}\right]$

independent on θ & ϕ i.e. l & m_l , ~~$l \neq 0$~~

A func^n will be independent on θ & ϕ only if $\rightarrow$ $\boxed{l=0}$ & $\boxed{m_l = 0}$

If $f(r,\theta,\phi) \Rightarrow$ then $n, l, m_l \neq 0$

$|\psi\rangle$ is not normalised so

$|\psi\rangle = \frac{f(r)\left[-2\chi_{1/2} + 3\chi_{-1/2}\right]}{\sqrt{4+9}} = \frac{f(r)\left[-2\chi_{1/2} + 3\chi_{-1/2}\right]}{\sqrt{13}}$

$\langle \psi | = \frac{f(r)\left[-2\chi_{1/2} + 3\chi_{-1/2}\right]}{\sqrt{13}}$

$\langle \mu_z \rangle = \langle \psi | \mu_{Lz} | \psi \rangle + \langle \psi | \mu_{Sz} | \psi \rangle$

$$\langle \mu_z \rangle = \frac{\langle \psi | \mu_{sz} | \psi \rangle}{\langle \psi | \psi \rangle} \qquad L = \sqrt{l(l+1)}$$

$$\langle \mu_z \rangle = \langle \psi | \mu_{sz} | \psi \rangle$$

$$= \langle \psi | \left(\frac{-2e}{2m}\right) S_z | \psi \rangle$$

$$= \left\langle \left(\frac{-2\chi_{1/2} + 3\chi_{-1/2}}{\sqrt{13}}\right) \middle| \left(\frac{-2e}{2m}\right) S_z \middle| \left(\frac{-2\chi_{1/2} + 3\chi_{-1/2}}{\sqrt{13}}\right) \right\rangle$$

$$= \frac{1}{13} \left[4 \langle \chi_{1/2} | \frac{-2e}{2m} S_z | \chi_{1/2} \rangle + 9 \langle \chi_{-1/2} | \frac{-2e}{2m} S_z | \chi_{-1/2} \rangle \right]$$

$$= \frac{1}{13} \left[4 \frac{-2e}{2m} \frac{\hbar}{2} \langle \chi_{1/2} | \chi_{1/2} \rangle + 9 \left(\frac{-2e}{2m}\right)\left(\frac{-\hbar}{2}\right) \langle \chi_{-1/2} | \chi_{-1/2} \rangle \right]$$

$$= \frac{1}{13} \left[-4\mu_B + 9\mu_B \right]$$

$$= \frac{1}{13} 5 \mu_B$$

$$\boxed{\langle \mu_z \rangle = \frac{5}{13} \mu_B}$$

Que:- For Pauli spin operator, Prove that

(i) $e^{i\theta \sigma \cdot \hat{n}} = \cos\theta + i \sigma \cdot \hat{n} \sin\theta$

where θ is any arbitrary angle.

(ii) $e^{i\alpha\sigma_x} \sigma_z e^{-i\alpha\sigma_x} = \sigma_z \cos 2\alpha + \sigma_y \sin 2\alpha$

where α is any arbitrary angle.

(i) $$e^{i\theta\sigma\cdot\hat{n}} = 1 + i\theta\sigma\cdot\hat{n} + \frac{(i\theta\sigma\cdot\hat{n})^2}{2!} + \frac{(i\theta\sigma\cdot\hat{n})^3}{3!} + \frac{(i\theta\sigma\cdot n)^4}{4!} + \cdots$$

$$= 1 + \frac{(i\theta\sigma\cdot\hat{n})^2}{2!} + \frac{(i\theta\sigma\cdot\hat{n})^4}{4!} + \cdots (i\theta\sigma\cdot\hat{n}) + \frac{(i\theta\sigma\cdot\hat{n})^3}{3!} + \cdots \quad (1)$$

$$(\sigma\cdot\hat{n})^2 = \left[(\sigma_x i + \sigma_y j + \sigma_z k)\cdot\frac{(\hat{i}+\hat{j}+\hat{k})}{\sqrt{3}}\right]^2 = \frac{\sigma_x^2 + \sigma_y^2 + \sigma_z^2}{3}$$

$$= \frac{3}{3} = 1$$

$(\sigma\cdot\hat{n})^4 = 1$

(i) $\Rightarrow e^{i\theta\sigma\cdot\hat{n}} = 1 - \frac{\theta^2}{2!} + \frac{\theta^4}{4!} \cdots\cdots + i\sigma\cdot\hat{n}\left[\theta - \frac{\theta^3}{3!} + \frac{\theta^5}{5!} \cdots\right]$

$$\boxed{e^{i\theta\sigma\cdot\hat{n}} = \cos\theta + i\sigma\cdot\hat{n}\sin\theta}$$ Proofed

(ii) $e^{i\alpha\sigma_x}\sigma_z e^{-i\alpha\sigma_x}$

Using $e^{i\theta\sigma\cdot\hat{n}} = \cos\theta + i\sigma\cdot\hat{n}\sin\theta$

$$e^{i\alpha\sigma_x}\sigma_z e^{-i\alpha\sigma_x} = (\cos\alpha + i\sigma_x\sin\alpha)\sigma_z(\cos\alpha - i\sigma_x\sin\alpha)$$

$$= \cos\alpha\,\sigma_z\cos\alpha - i\cos\alpha\,\sigma_z\sigma_x\sin\alpha + i\sigma_x\sin\alpha\,\sigma_z\cos\alpha + \sigma_x\sin\alpha\,\sigma_z\sigma_x\sin\alpha$$

$$= \sigma_z\cos^2\alpha + \sigma_x\sigma_z\sigma_x\sin^2\alpha + i\cos\alpha\sin\alpha\,[\sigma_x\sigma_z - \sigma_z\sigma_x]$$

$$= \sigma_z\cos^2\alpha - \sigma_z\sigma_x\sigma_x\sin^2\alpha + i\cos\alpha\sin\alpha\,[\sigma_x,\sigma_z]$$

$$= \sigma_z\cos^2\alpha - \sigma_z\sigma_x^2\sin^2\alpha + i\cos\alpha\sin\alpha\,(-i2\sigma_y)$$

$$= \sigma_z(\cos^2\alpha - \sin^2\alpha) + 2\cos\alpha\sin\alpha\,\sigma_y \qquad \{[\sigma_z,\sigma_x] = 2i\sigma_y$$

$$= \sigma_z\cos 2\alpha + \sin 2\alpha\,\sigma_y$$

$$= \sigma_z\cos 2\alpha + \sigma_y\sin 2\alpha$$

Que :- The Hamiltonian of an e^- in a constant mag. field B is given by $H = \mu\sigma\cdot B$ where μ is the const. & $\sigma = (\sigma_1, \sigma_2, \sigma_3)$ denotes the Pauli matrices. Let $\omega = \frac{\mu B}{\hbar}$ & I be 2×2 unit matrix then the operator $e^{\frac{iHt}{\hbar}}$ simplifies to

a) $I\cos\frac{\omega t}{2} + \frac{i\sigma\cdot B}{B}\sin\frac{\omega t}{2}$

b) $I\cos\omega t + \frac{i\sigma\cdot B}{B}\sin\omega t$

c) $I\sin\omega t + \frac{i\sigma\cdot B}{B}\cos\omega t$

d) $I\sin 2\omega t + \frac{i\sigma\cdot B}{B}\cos 2\omega t$

e) $I\cos 2\omega t + \frac{i\sigma\cdot B}{B}\sin 2\omega t$

$$H = \mu\sigma \cdot B \Rightarrow H = \mu\sigma \cdot B\hat{n} = \mu B\sigma\cdot\hat{n}$$

$$e^{\frac{iHt}{\hbar}} = e^{\frac{i\mu\sigma\cdot Bt}{\hbar}} = e^{\frac{i\mu\sigma\cdot B\hat{n}t}{\hbar}} = e^{i\left(\frac{\mu B t}{\hbar}\right)\sigma\cdot\hat{n}}$$

On comparing with $e^{i\theta\sigma\cdot\hat{n}}$ we get

$$\theta = \frac{\mu Bt}{\hbar} \Rightarrow \omega \cancel{t} = \frac{\mu B\cancel{t}}{\hbar} \Rightarrow \omega = \frac{\mu B}{\hbar}$$

So
$$e^{\frac{iHt}{\hbar}} = \cos\left(\frac{\mu Bt}{\hbar}\right) + i\sigma\cdot\hat{n}\,\sin\left(\frac{\mu Bt}{\hbar}\right)$$
$$= \cos\omega t + i\sigma\cdot\hat{n}\,\sin\omega t$$
$$e^{\frac{iHt}{\hbar}} = \cos\omega t + i\frac{\sigma\cdot B}{B}\sin\omega t \quad \text{Ans}$$
$$\left\{\hat{n} = \frac{\vec{B}}{B}\right.$$

* $$H\psi = E\psi$$

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V\right]\psi(r,\theta,\phi) = E\psi(r,\theta,\phi)$$

$$-\frac{\hbar^2}{2m}\left\{\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right\} + V(r)\,\psi(r,\theta,\phi)$$
$$= E\psi(r,\theta,\phi) \quad \text{——— (1)}$$

If potⁿ is fucⁿ of r only then potⁿ is central potⁿ i.e. dependent on position part.

$$V = V(r) \rightarrow \text{central}$$

Ex → rigid rotator, hydrogen atom

$V(\vec{r}) \rightarrow$ Non central

for any central potⁿ, 3 dim Schʳ eqⁿ can be seperated in 3 independent Eqⁿs.

$$\psi(r,\theta,\phi) = R(r)\,\Theta(\theta)\,\Phi(\phi)$$

(1) Rigid Rotator :- (for fixed plane)

for rigid rotator, $\theta = 90°$ (angle is fixed)

So θ part will be elliminated from wave func^n & also ~~from~~ for rigid rotator $r = R$

Only ϕ is variable now.

We have, $L^2 = -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]$

Substituting these values in (1) then Sch^r eq^n for spherical polar coordinates changes to

$$\left[-\frac{\hbar^2}{2m}\left\{\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{L^2}{\hbar^2 r^2}\right\} + V(r)\right]\psi(r,\theta,\phi) = E\psi(r,\theta,\phi)$$

In x-y plane, $\theta = 90°$

If particle is moving in x-y fixed plane then angular momentum will be in z-dir^n so $L \to L_z$

$$\frac{L_z^2}{2mR^2}\psi = E\psi \quad \text{———— (i)} \qquad \{\text{Position part} = 0\}$$

$L_z = m_l\hbar \Rightarrow \boxed{E = \frac{m_l^2\hbar^2}{2mR^2}}$

This is the energy for a rigid rotator with fixed plane

$$L_z = -i\hbar\frac{\partial}{\partial\phi}$$

$$\Rightarrow L_z^2 = -\hbar^2\frac{\partial^2}{\partial\phi^2}$$

(i) $\Rightarrow \quad -\frac{\hbar^2}{2mR^2}\frac{\partial^2}{\partial\phi^2}\psi = E\psi \quad \Rightarrow \quad \frac{-\hbar^2}{2I}\frac{\partial^2\psi}{\partial\phi^2} = E\psi$

$$\Rightarrow \frac{\partial^2\psi}{\partial\phi^2} = -\frac{2EI}{\hbar^2}\psi$$

$$\Rightarrow \frac{\partial^2\psi}{\partial\phi^2} + \frac{2EI}{\hbar^2}\psi = 0$$

Let $K^2 = \frac{2EI}{\hbar^2}$ then $\frac{\partial^2 \psi}{\partial \phi^2} + K^2\psi = 0$.

solution of this eqn, $\psi = A e^{ik\phi} + B e^{-ik\phi}$ ——— (ii)

Condition, $\psi(2\pi + \phi) = \psi(\phi)$

i.e. wave funcn will repeat after 2π.

This condn is satisfied in eqn (ii)

~~(ii) ⇒ $\psi(\phi) = A e^{ik(2\pi+\phi)}$~~ $+ B e^{-ik(2\pi+\phi)}$

$= A e^{ik\phi} + B e^{-ik\phi}$

$\psi = A e^{im\phi}$

$K = 0, \pm 1, \pm 2$

$m = 0, \pm 1, \pm 2$

Normalisation Condn :-

$$\int_0^{2\pi} \psi^* \psi \, d\phi = 1$$

(ψ only depends on ϕ)

$$\Rightarrow \int_0^{2\pi} A^* e^{-im\phi} A e^{im\phi} d\phi = 1$$

$$\Rightarrow |A|^2 \int_0^{2\pi} e^{im\phi} e^{-im\phi} d\phi = 1$$

$$\Rightarrow A = \frac{1}{\sqrt{2\pi}}$$

so $\psi = \frac{1}{\sqrt{2\pi}} e^{im\phi}$

If potn is 0, $V = 0$ then

$$\boxed{E = \frac{m^2\hbar^2}{2I}}, \quad m = 0, \pm 1, \pm 2 \ldots$$

If potn $= V_0$ then

$$E - V_0 = \frac{m^2\hbar^2}{2I}$$

$$\boxed{E = \frac{m^2\hbar^2}{2I} + V_0}$$

Wave func will be same

For Variable Plane (Rigid Rotator)

for rigid rotator r is fixed so r part elliminated. Only 2 variables → θ & ϕ

$$-\frac{\hbar^2}{2m}\left[\frac{-L^2}{\hbar^2 R^2}\right]\psi = E\psi$$

$$\frac{L^2}{2mR^2}\psi = E\psi$$

$$\boxed{\frac{L^2}{2I}\psi = E\psi}$$

We know $L^2\psi = l(l+1)\hbar^2$

so $$\boxed{\frac{l(l+1)\hbar^2}{2I}\psi = E\psi}$$

$$\Rightarrow \boxed{E = \frac{l(l+1)\hbar^2}{2I}}$$

- Possible values of l, $l = 0, 1, 2, 3, \ldots\ldots$ (zero or +ve intiger)

$$L^2 = -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]$$

In this case, wave fun^n will depand on θ & ϕ both.

$$\psi = \Theta(\theta)\,\Phi(\phi)$$

$$\psi = \Theta(\theta)\frac{1}{\sqrt{2\pi}}e^{im\phi}$$

$$\boxed{Y_{lm}(\theta,\phi) = \Theta(\theta)\frac{1}{\sqrt{2\pi}}e^{im\phi} = |l, m\rangle}$$

→ θ part depand on l & m both

→ ϕ " " " m only.

$Y_{l,m}(\theta,\phi)$ is known as Spherical Harmonics.

- for Each central pot^n, ϕ dependent part be remain same always. $\left(\frac{1}{\sqrt{2\pi}}e^{im\phi}\right)$

θ dependent part,

$$\boxed{\Theta_{l,m}(\theta) = \sqrt{\frac{(2l+1)}{2}\cdot\frac{(l-|m|)!}{(l+|m|)!}}\; P_l^{|m|}(\cos\theta)}$$

Hydrogen Atom :-

Pot^n depands only on r,

$$V = -\frac{1}{4\pi\epsilon_0}\frac{e^2}{r}$$

~~In~~ Wave fuc^n, r, θ, ϕ all three are variable $\rightarrow \psi(r,\theta,\phi)$.

To Solve Sch^r eq^n for hydrogen atom, we have to introduce Legurre Polinomial. It is complicated.

position dependent part,

$$R_{nl}(r) = \sqrt{\left(\frac{2Z}{na_0}\right)^3 \frac{(n-l-1)!}{2n\{(n+l)!\}^3}}\; e^{-\frac{Zr}{na_0}} \times \left(\frac{2Zr}{na_0}\right)^l \times L_{n+l}^{2l+1}\left(\frac{2Zr}{na_0}\right)$$

$$\Theta_{l,m}(\theta) = \sqrt{\frac{(2l+1)}{2}\frac{(l-|m|)!}{(l+|m|)!}}\; P_l^{|m|}(\cos\theta) \quad (\theta \text{ dependent Part})$$

$$\Phi(\phi) = \frac{1}{\sqrt{2\pi}} e^{im\phi} \quad (\phi \text{ dependent part})$$

If $\Theta_{l,m}(\theta) \times \Phi(\phi) \propto e^{\underline{\underline{im}}\phi}$ by ~~them~~ this m is obtained.

$R_{nl}(r) \propto e^{-\frac{2r}{na_0}}$ by this we get n {for m, only cheak $e^{im\phi}$ part}

for l, cheak θ dependent part $(\cos\theta)$

If $l = 0$, no θ depandancy

$l \neq 0$, θ dependancy is there.

$l = 1 \longrightarrow \cos\theta$

$l = 2 \longrightarrow (\cos\theta)^2$

Energy $$\boxed{E_n = \frac{-mz^2e^4}{2(4\pi\varepsilon_0)^2 n^2\hbar^2}} = \frac{-13.6}{n^2}\,eV \quad (M.K.S.)$$

$$\boxed{E_n = \frac{-mz^2e^4}{2\hbar^2 n^2}} \quad (C.G.S.)$$

In C.G.S., $V = -\frac{ze^2}{r}$

If nucleus is at rest then mass it of mass of e^- but ~~If nucleus is not at rest~~, ~~it is~~ in motion then mass m will be change by reduced mass in energy expression

$$\mu = \frac{m_1 m_2}{m_1 + m_2}$$

$$E = \frac{-\mu z^2 e^4}{2(4\pi\varepsilon_0)^2 n^2 \hbar^2}$$

i.e. $E \propto$ mass , $E \propto z^2$, $E \propto e^4$

for Deutron,

(Mass is comparable ($m_p \approx m_e$) Not heavy)

$$\mu = \frac{m.m}{m+m} = \frac{m}{2}$$

If ~~nu~~ mass of nucleus is heavy then

$m_p >> m_e$

$\mu \approx m_e$

<u>First Bohr Radius :-</u>

$$a_0 = \frac{4\pi\varepsilon_0\hbar^2}{Z\mu e^2}$$

a_0 depand on z & μ both.

Potn $V = -\frac{Z}{4\pi\varepsilon_0}\frac{e^2}{r} = (\ )\frac{1}{n^2}$

As orbit changes, radius ↑.

Angular mom. concept

$$\boxed{mvr = n\hbar} \quad ; \quad n = 1, 2, \ldots$$

~~for different~~ orbits for $n = 1, 2 \ldots$, we can calcula
the velocity v.

Probability, $|\psi(x,t)|^2 = \psi^* \psi$
in region $x, x+dx$

In Central pot^n, there comes the concept of Radial Probability density. (Radial Prob. density means change in radius, but no change in θ & ϕ)

Prob. of finding the particle in region r to $r+dr$

$$|\psi|^2 d\tau = |\psi|^2 r^2 dr \sin\theta \, d\theta \, d\phi$$

$r \to r+dr$
$\begin{Bmatrix} \theta \to \theta + d\theta \\ \phi \to \phi + d\phi \end{Bmatrix}$

This is the total probability.

Now Radial prob. density,

$$\int_0^{\pi}\int_0^{2\pi} |\psi|^2 d\tau = \int_0^{\pi}\int_0^{2\pi} |\psi|^2 r^2 dr \sin\theta \, d\theta \, d\phi / r^2$$

$$= 4\pi |\psi|^2 r^2 dr / r^2$$

$|\psi|^2 r^2 \Rightarrow$ Radial probability density.

ψ At $r = 0$, $|\psi|^2 \neq 0$ but if at $r = 0$, $|\psi|^2 = 0$ i.e. (e$^-$ will not exist at the cen.x of nucleus Not possible)

$$\psi_{100} = \psi_{1s} = \left(\frac{Z^3}{\pi a_0^3}\right)^{1/2} e^{-\frac{Zr}{a_0}}$$

$$\psi_{200} = \psi_{2s} = \left(\frac{Z^3}{32\pi a_0^3}\right)^{1/2} e^{-\frac{Zr}{2a_0}} \left(2 - \frac{Zr}{a_0}\right)$$

$\psi_{210} \Rightarrow \psi_{2p}$ if distribution in z dir^n then ψ_{2pz}
" y " ψ_{2py}
" x " ψ_{2px}

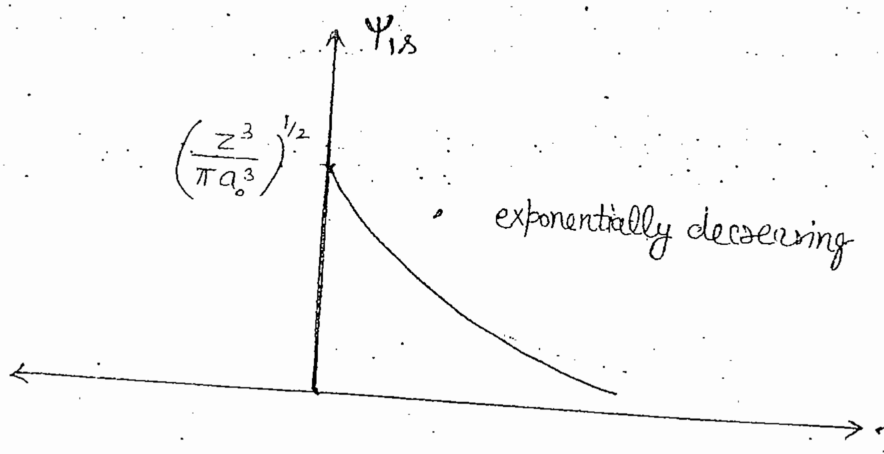
$\Psi_{210} \Rightarrow \Psi_{2p_z}$

& linear combination of Ψ_{211} & $\Psi_{21\bar{1}}$ will give info. about x & y
i.e. P_x , P_y

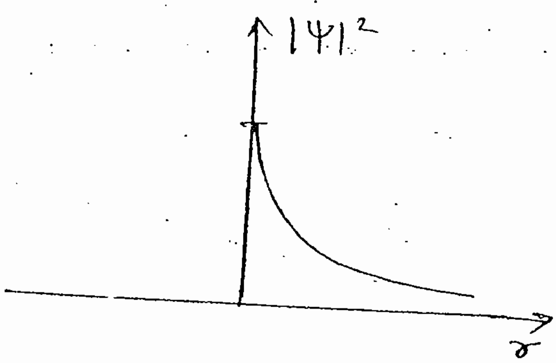
$$\Psi_{210} = \left(\frac{Z^3}{32\pi a_0^3}\right)^{1/2} \left(\frac{Zr}{2a_0}\right) e^{-\frac{Zr}{2a_0}} \cos\theta$$

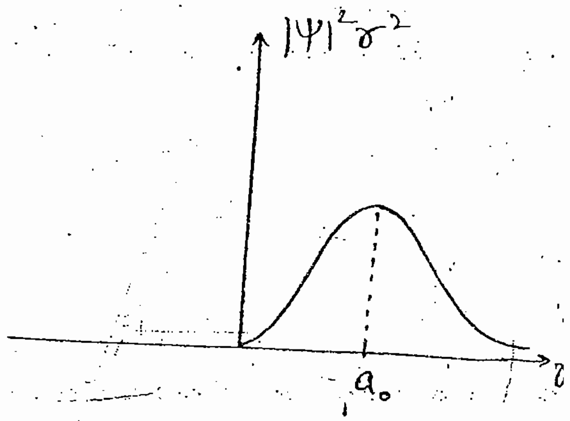
$$\Psi_{211} = \left(\frac{Z^3}{32\pi a_0^3}\right)^{1/2} \left(\frac{Zr}{2a_0}\right) e^{-\frac{Zr}{2a_0}} \sin\theta \, e^{i\phi}$$

$$\Psi_{21\bar{1}} = \left(\frac{Z^3}{32\pi a_0^3}\right)^{1/2} \left(\frac{Zr}{2a_0}\right) e^{-\frac{Zr}{2a_0}} \sin\theta \, e^{-i\phi}$$



(for H_2 atom origin at nucleus i.e at proton





$|\Psi|^2 r^2 \Rightarrow r \updownarrow$, $|\Psi|^2 \downarrow \uparrow$

The value at which $|\Psi|^2 r^2$ is maximum $\Rightarrow$ Most probable distance $\rightarrow a_0$
(radial prob.)

$$\frac{d}{dr}\left\{ |\Psi|^2 r^2 \right\} = 0 \Rightarrow r = ? \quad \text{(Most probable distance)}$$

for each state , at $r = 0$, Radial prob. $= 0$ always.
So e^- can not be inside the nucleus.

1) The most probable distance for the nth state for hydrogen atom $= n^2 a_0$ [with maximum value of $l \Rightarrow l = n-1$]

$1S$ $n=1$ $l=0$ $2S, 2p$ $n=2$ $l=0, 1$ for 2S, we get 2 maxima. for 2S $n^2 a_0$ is not valid.

(2) The no. of radial nodes in the wave fuc^n for hydrogen atom $= n-l-1$ (Excluding the node at $r=0$)

3) Expactation value of r for nth state,

- $\langle r \rangle = \langle nl | r | nl \rangle = \frac{1}{2}\left[3n^2 - l(l+1)\right] a_0$
- $\langle r^2 \rangle = \frac{1}{2} n^2 \left[5n^2 + 1 - 3l(l+1)\right] a_0^2$
- $\langle \frac{1}{r} \rangle = \frac{1}{n^2 a_0}$
- $\langle \frac{1}{r^2} \rangle = \frac{2}{n^3 (2l+1) a_0^2}$

Prob. 1 :- The radial wave fuc^n of the e^- in the state with $n=1$ & $l=0$ in hydrogen atom is

$$R_{10} = \frac{2}{a_0^{3/2}} \exp\left[\frac{-r}{a_0}\right],$$ where a_0 is Ist Bohr radius. The most probable value of r for an e^- is.

(a) a_0 (b) $2a_0$ (c) $4a_0$ (d) $8a_0$

Most prob. value of $r = n^2 a_0$

$$r = (1)^2 a_0$$
$$r = a_0$$

Q.2 :- Let $|\psi_0\rangle$ denothe the ground state of H_2 atom, Choose the correct statement from given below,

(a) $[L_x, L_y] |\psi_0\rangle = 0$

(b) $J^2|\psi_0\rangle = 0$

(c) $\underline{L}\cdot\underline{S}\,|\psi_0\rangle = 0$

(d) $[S_x, S_y]|\psi_0\rangle = 0$

for ground state of H_2 atom, $l=0, s=\frac{1}{2}$

$J=\frac{1}{2}$

$$J^2|\psi_0\rangle = j(j+1)|\psi_0\rangle = \cancel{\tfrac{1}{2}(\tfrac{1}{2}+1) \neq 0}$$

$$L\cdot S\,|\psi_0\rangle = \frac{J^2 - L^2 - S^2}{2}$$

$$\neq 0$$

$$[S_x, S_y]|\psi_0\rangle = i\hbar S_z|\psi_0\rangle = i\hbar m_s\hbar|\psi_0\rangle \neq 0$$

$$[L_x, L_y]|\psi_0\rangle = i\hbar L_z|\psi_0\rangle = i\hbar m_l\hbar|\psi_0\rangle = 0$$

for $l=0$ $(m_l = 0)$

(a) is correct.

Q.3:- The ground state wave func^n of H_2 atom is given b

$$\psi(r) = \left(\frac{1}{\pi a^3}\right)^{1/2} e^{-r/a} \quad \text{where a is constant.}$$

If $P(r)\,dr$ is the probability of finding the e^- b/w r & $r+dr$ then

(a) $P(r) = 0$ at $r=0$

(b) $P(r)$ is maximum at $r=0$

(c) $P(r)$ is maximum at $r=a$

(d) $\int_0^\infty P(r)\,dr = 1$

Prob. is maxi. at Ist Bohr radius a_0 but here a is not Ist bohr radius, it is a const.

$$|\psi(r)|^2 r^2 = P(r) = 0 \quad \text{at } r=0$$

Degeneracy :-

Wave fucⁿ of hydrogen atom depends on n, l, m without considering spin.

for a given n,

$$l = 0, 1, 2, \cdots n-1$$

$$\& \quad m = -l, \cdots\cdots, +l$$

Eigen energy $E_n = \frac{-13.6}{n^2}$ eV. depends only on n.

~~e.g. $n=2$~~

$l = 0, 1$

$m = 0 \;, \; -1, 0, +1$

ψ depends on n, l, m but E_n depends on n only.

Degeneracy of nth ~~atom~~ level of H_2 atom, i.e. no of different wave fucⁿ for a given n $\Rightarrow$ $g_n = \sum_{l=0}^{n-1} 2l+1$

This is the degeneracy without considering the spin.

(ii) By considering spin, ψ depends on n, l, m_l, n_s then

$$g_n = 2 \sum_{l=0}^{n-1} 2l+1$$

$$= 2\left[1+3+5+ \cdots\right]$$

$$= \cancel{2} \times \frac{n}{\cancel{2}}\left[2(1) + (n-1)2\right] = n\left[\cancel{2} + 2n - \cancel{2}\right] = 2n^2$$

$$\boxed{\begin{array}{ll} g_n = 2n^2 & \text{(including spin)} \\ g_n = n^2 & \text{(Excluding spin)} \end{array}}$$

Note :- If there is no idea of spin then we consider $g_n = 2n^2$ i.e. maximum degeneracy.

Problem :- Calculate the expectation value of $\langle \frac{1}{r} \rangle$ for a single charged Helium ion in ground state.

ground state wave fucⁿ for He atom;

$$\psi_{100} = \left(\frac{z^3}{\pi a_0^3}\right)^{1/2} e^{-\frac{zr}{a_0}}$$

for He ion, $z=2$. $\quad \psi_{100} = \left(\frac{8}{\pi . a_0^3}\right)^{1/2} e^{-\frac{2r}{a_0}}$

$$\left\langle \frac{1}{r} \right\rangle = \int \psi^* \frac{1}{r} \psi \, d\tau = \int_0^\infty \int_0^\pi \int_0^{2\pi} \frac{8}{\pi a_0^3} e^{-\frac{2r}{a_0}} \frac{1}{r} e^{-\frac{2r}{a_0}} r^2 dr \ldots d\theta \ldots$$

$$= \frac{8}{\pi a_0^3} \int_0^\infty \frac{1}{r} e^{-\frac{4r}{a_0}} 4\pi r^2 dr = \frac{8}{\pi a_0^3} 4\pi \int_0^\infty e^{-\frac{4r}{a_0}} r \, dr$$

$$= \frac{8\times 4}{a_0^3} \left[\frac{e^{-\frac{4r}{a_0}}}{-\frac{4}{a_0}} r - \frac{e^{-\frac{4r}{a_0}}}{\left(-\frac{4}{a_0}\right)^2} \right]_0^\infty = \frac{8\times 4}{a_0^3} \left[-\frac{a_0 r}{4} e^{-\frac{4r}{a_0}} + \frac{a_0^2}{16} e^{-\frac{4r}{a_0}} \ldots \right]$$

$$= \frac{8\times 4}{a_0^3} \left[\frac{a_0^2}{16} \right] = \frac{2}{a_0}$$

$$= \underline{\frac{2}{a_0}} \text{ Ans}$$

<u>Problem</u>:- The e^- in a H_2 atom has wave funcⁿ

$$\psi(r) = \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0} \quad , \quad a_0 = 0.53\,\text{Å} \text{ ; first Bohr r…}$$

And the origin is taken at proton. Find the probability that the e^- will be found outside the Ist Bohr radius.

$$\psi(r) = \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0}$$

for outside the a_0 then take limit for $a_0 \to \infty$

{ we can also find P_{in} … by limit 0 to a_0 & … for outside $(1 - P_{in})$ }

$$P = \int |\psi(r)|^2 d\tau$$

$$= \int_{a_0}^\infty \frac{1}{\pi a_0^3} e^{-\frac{2r}{a_0}} 4\pi r^2 dr$$

$$= \frac{4}{a_0^3} \int_{a_0}^\infty r^2 e^{-\frac{2r}{a_0}} dr$$

$$= \frac{4}{a_0^3} \left[r^2 \frac{e^{-\frac{2r}{a_0}}}{-\frac{2}{a_0}} - \int_{a_0} 2r \frac{e^{-\frac{2r}{a_0}}}{-\frac{2}{a_0}} dr \right]$$

$$= \frac{4}{a_0^3} \left[-\frac{r^2 a_0}{2} e^{-\frac{2r}{a_0}} + a_0 \int_{a_0}^\infty r e^{-\frac{2r}{a_0}} dr \right]$$

$$= \frac{4}{a_0^3} \left[-\frac{r^2 a_0}{2} e^{-\frac{2r}{a_0}} + a_0 r \frac{e^{-\frac{2r}{a_0}}}{-\frac{2}{a_0}} - a_0 \frac{e^{-\frac{2r}{a_0}}}{\left(-\frac{2}{a_0}\right)^2} \right]_{a_0}^\infty$$

$$= \frac{4}{a_0^3} \left[0 + 0 - 0 + \frac{a_0^3}{2} e^{-2} + \frac{a_0^3}{2} e^{-2} + \frac{a_0^3}{4} e^{-2} \right]$$

$$= \frac{4}{a_0^3} \left[\frac{a_0^3}{e^2} + \frac{a_0^3}{4e^2} \right] = 4 \left[\frac{1}{e^2} + \frac{1}{4e^2} \right] = 4 \left[\frac{5}{4e^2} \right]$$

$$= \frac{5}{e^2} = \underline{0.68} \text{ Ans}$$

Prob. that e^- is found outside $= \underline{0.68}$ Ans

Inside the Ist Bohr radius,

$$\text{Probability} = 1 - 0.68 \doteq 1 - \frac{5}{e^2} = \underline{0.32} \quad \text{Ans}$$

Que:– The energy levels of the non-relativistic e^- in a H_2 atom i.e. in a coulomb potⁿ $V(r) \propto -\frac{1}{r}$ are given by $E_{nlm} \propto -\frac{1}{n^2}$ where n is the principle Q. No. and the corresponding wave functions are given by ψ_{nlm} where l is the orbital angular mom. Q. No. and m is the magnetic Q. No. The spin of the e^- is not considered. Which of the following is a correct statement,

(i) There are exactly $(2l+1)$ different wave functions ψ_{nlm} for each E_{nlm}

ii) There are $l(l+1)$ different wave fuc's ψ_{nlm} for each E_{nlm}

iii) E_{nlm} does not depend on l & m for the coulomb potⁿ.

iv) There is a unique wave fucⁿ for each E_{nlm}.

for coulomb potⁿ energy depends on n, no – on l & m

(i) is not correct bcoz $(2l+1)$ is for a given l but for a given l there are $\sum_{l=0}^{n-1}(2l+1)$ different w. fucⁿs.

Que:– Let ψ_{nlm} denotes the eigen fucⁿs of a hamiltonian for a
2012 spherically symmetric potⁿ $V(r)$,

$$\psi = \frac{1}{4}\left[\psi_{210} + \sqrt{5}\,\psi_{21-1} + \sqrt{10}\,\psi_{211}\right]$$

is an eigen fucⁿ only of

1) H, L^2 & L_z

2) H & L_z

3) H & L^2

4) L^2 & L_z

for L_z, $L_z = m\hbar$

$$L_z\psi = \frac{\hbar}{4}\left[0 - \sqrt{5}\,\psi_{21-1} + \sqrt{10}\,\psi_{211}\right]$$

ψ_{nlm}

$\therefore \quad L^2 \psi = l(l+1)\hbar \, \psi$

So $L^2\psi =$ l is same for all 3, ψ so wave fuc^n is not charg

So This is not the E. fuc^n of L_z but E. fuc^n of L^2.

$$\lambda = E = -\frac{13.6}{n^2}$$

(3) option is correct,

Que:- The normalised w. fuc^n of a H_2 atom are denoted by ψ_{nl} where n, ~~l & m are principal, azimuthal & magnetic Q. No.~~ respectively. Now consider an e^- is in the state

$$\psi(\vec{r}) = \frac{1}{3}\psi_{100}(\vec{r}) + \frac{2}{3}\psi_{210}(\vec{r}) + \frac{2}{3}\psi_{322}(\vec{r})$$

The expectation value of energy of the e^- in eV will be approx -te

a) -1.5 ✓b) -3.7 c) -13.6 d) -80.1

$$\langle E \rangle = \sum P_r E_r$$

$$\langle E_n \rangle = \frac{1}{9}\left[\frac{-13.6}{1}\right] + \frac{4}{9}\left[\frac{-13.6}{4}\right] + \frac{4}{9}\left[\frac{-13.6}{9}\right] \qquad \left\{E_n = \frac{-13.6}{n^2}\right.$$

$$\cancel{= 4.533 + 2.266 + 1.0074}$$

$$= -1.511 \mp 1.544 \mp 0.671$$

$$= -3.7266$$

$$\simeq \underline{-3.7} \; \underline{\underline{Ans}}$$

Que:- An H_2 atom is in $2p$ state. All possible values of z-comp. of orbital angular mom. are equally probab. Write the wave fuc^n of H_2 atom.

H_2 in $2p$ state, $n=2$, for p, $l=1$, $m = 0, 1, 0,$

for $2p$ state, $\Rightarrow m = -1, 0, +1$

ψ_{210}, ψ_{211}, $\psi_{21\bar{1}}$ $\Rightarrow$ these 3 w. fuc^n are possible

So by their linear combination, we get

$$\psi = C_1\psi_{210} + C_2\psi_{211} + C_3\psi_{21\bar{1}}$$

$$|C_1|^2 + |C_2|^2 + |C_3|^2 = 1$$

$$|C_1|^2 = \frac{1}{3}$$

$$l_z = m_l \hbar$$
$$= \hbar\ , 0\ ; -\hbar$$

So $\boxed{\psi = \frac{1}{\sqrt{3}}\left[\psi_{210} + \psi_{211} + \psi_{21\bar{1}}\right]}$

Que :- Positronium is an atom formed by an e^- and positron The mass of the positron is same as that of an e^- and its charge is ~~equal in~~ magnitude but opposite in sign to that ~~of an e^-. The positronium atom is thus similar to the H_2~~ atom with the positron replacing the proton.

(i) The Binding energy of a positronium atom is

(a) 13.6 eV ✓(b) 6.8 eV (c) 27.2 eV (d) 3.4 eV

(ii) If a positronium atom makes a transition from the state with $n=3$ to a state with $n=2$, The energy of the photon that is ~~im~~ emitted in the transition is closest to

(a) 1.88 eV ✓(b) 0.94 eV (c) 27.2 eV (d) 2.27 eV

In H_2 atom, 1p & 1e^-, p is heavier than e^-, so we consider p at rest

But here in positronium, e^- & e^+ have same mass. So we can't take e^+ at rest so

$$\text{reduced mass } \mu = \frac{m_1 m_2}{m_1+m_2} = \frac{m\cdot m}{m+m}$$
$$\mu = \frac{m}{2}$$

So $E_n \propto$ mass $\Rightarrow E_n \propto \frac{m}{2}$ So $E = \frac{13.6}{2}$

$$E_n = 6.8\text{ eV}$$

(ii) $n = 3 \longrightarrow n = 2$

$$E = \frac{hc}{\lambda}$$

$E_3 = \frac{-13.6}{9}$

$E_2 = \frac{-13.6}{4}$

$$E_3 - E_2 = \frac{1}{2}\left(-\frac{13.6}{9} + \frac{13.6}{4}\right)$$
$$= \frac{1}{2}[13.6]\left[\frac{-1}{9} + \frac{1}{4}\right] = 6.8\left[\frac{-4+9}{36}\right] = 6.8 \times \frac{5}{36}$$
$$= 0.9444$$

Ionisation for $-13.6\left(\frac{1}{\infty}-\frac{1}{n^2}\right) = 0 + \frac{13.6}{n^2}$

for $n=1$, first ionisation

$n=2$, second "

Que :- If σ_x and σ_y are defined as

$$\sigma_x = (f^+ + f) \text{ and } \sigma_y = -i(f^+ - f)$$

where σ's are Pauli spin matrices. And f^+, f obey anticommutation relations, $\{f,f\}=0$, $\{f,f^+\}=1$ then σ_z is given by

(a) $ff^+ - 1$ ✓(b) $2f^+f - 1$ (c) $2f^+f+1$ (d) f^+f

Using, $\sigma_x \sigma_y = i\sigma_z$

$$(f^+ + f)(-i)(f^+ - f) = i\sigma_z$$

$$-i\left[f^+f^+ - f^+f + ff^+ - ff\right] = i\sigma_z$$

$$\sigma_z = -\left[f^+f^+ - f^+f + ff^+ - ff\right]$$

$$\sigma_z = -(-f^+f + ff^+)$$

$\{f,f\}=0$

$ff + ff = 0$

$2ff = 0 \Rightarrow ff =$

by Hermitian conjug

$(ff)^+ = 0$

$f^+f^+ = 0$

Now $\{f, f^+\} = 1$

$$ff^+ + f^+f = 1 \Rightarrow ff^+ = 1 - f^+f$$

$$\sigma_z = -(-f^+f + 1 - f^+f) = -(1 - 2f^+f)$$

$$\sigma_z = 2f^+f - 1$$

✓(b)

Identical Particles :- The particles having same intrinsic properties ~~are~~ (charge, mass, spin) are known as identical. These particles can not be distinguish by intrinsic properties

These are of 2 types,

(i) Classical Identical Particles

(ii) Quantum " ".

Classical identical particles are those that can be (in gen ~~distinguish from each other.~~

Quantum I.P. are in general indistinguishable,

Quantum Identical Particles

↓ Bosons

↓ Fermions

Bosons → Identical particles with 0 or integral spin

$S = 0, 1, 2, 3 \cdots$

fermions → Identical particles having half integral spin.

$\text{spin} = \frac{1}{2} \times (\text{odd})$

For Bosons :- Total system wave fun^n will be symmetric

$$\psi_{Total} = \psi_{space} \times \psi_{spin} \times \psi_{isospin}$$

For fermions :- Total system wave fun^n will be antisymmetric.

Total w. fun^n should be antisymmetric (may be ψ_{space} will be symmetric or other two not)

System of Distinguishable Non-Interacting particle

OR

System of classical non-interacting identical particle :-

Suppose we consider a system of N non-interacting distinguishable particles. Hamiltonian of the system

$$H = \sum_{i=1}^{N} \left[\frac{p_i^2}{2m_i} + V_i(r_i) \right]$$

{ there is no cross terms s.t. r_{12}

for N non-interacting distinguishable Identicle partic mass will be.

$$H = \sum_{i=1}^{N} \left[\frac{p_i^2}{2m} + V_i(r_i) \right]$$

when fctⁿ is additive for each particles (non-interactings)

so $\psi(\underline{r}_1, \underline{r}_2, \underline{r}_3 \dots \underline{r}_N) = \psi(\underline{r}_1)\, \psi_2(\underline{r}_2) \dots \psi_N(\underline{r}_N)$

For classical identical particles, there is no definate symmetry (parity) $\{ e^x \neq \pm e^x \}$ i.e. Unsymmetric & Energy $E = \sum_{i=1}^{N} \varepsilon_i$

for Quantum Identicle particle

For N, non-interacting Indistinguishable Identicle par

$$H = \sum_{i=1}^{N} \left[\frac{p_i^2}{2m} + V_i(\underline{r}_i) \right]$$

Quantum Identicle particles have definate symmetry.

Construction of Symmetric & antisymmetric wave fucⁿ from Unsymmetric wave fucⁿ :-

Consider a 2 particle system then wave fucⁿ $\psi(1,2)$ & Interchange in pair $\psi(2,1)$

$$\psi(1,2) = \psi_1(\underline{r}_1)\, \psi_2(\underline{r}_2)$$

$$\psi(2,1) = \psi_2(\underline{r}_1)\, \psi_1(\underline{r}_2)$$

Total W. fucⁿ will be the superposition of these 2 w. fu

for Bosons, $\psi_{Boson} = \frac{1}{\sqrt{2}}\left[\psi(1,2) + \psi(2,1)\right]$ symmetric

All W. fucⁿs are equally probable for bosons.

for fermions, $\psi_{fermion} = \frac{1}{\sqrt{2}}\left[\psi(1,2) - \psi(2,1)\right]$ Antisym

change in even no. of co-ordinate will be add (+)

" odd " " " (+)

for 3 particle system, $\psi(1\,2\,3)$. On interchanging, possi[ble] wave fuc^{n}s are

✓ $\psi(1\,2\,3)$

✓ $\psi(1\,3\,2)$

✓ $\psi(2\,1\,3)$

$\psi(2\,3\,1)$

✓ $\psi(3\,2\,1)$

$\psi(3\,1\,2)$

There are 6 diff. w. fuc^n for 3 identical particles.

$$\cancel{\psi_{Boson}} = \psi_S = \frac{1}{\sqrt{6}}\left[\psi(1,2,3) + \psi(1,3,2) + \psi(2,1,3) + \psi(2,3,1) + \psi(3,2,1) + \psi(3,1,2)\right]$$

$$\psi_S = \frac{1}{\sqrt{3!}}\left[\psi(1,2,3) + \psi(1,3,2) + \psi(2,1,3) + \psi(2,3) + \psi(3,2,1) + \psi(3,1,2)\right]$$

$$\psi_A = \frac{1}{\sqrt{3!}}\left[\psi(1,2,3) + \psi(2,3,1) + \psi(3,1,2) - \psi(1,3,2) - \psi(2,1,3) - \psi(3,2,1)\right]$$

for N no. of particles, there will be

$N!$ = different wave fuc^{n}s (Energy will be same)

Wave-fuc^n $\rightarrow$ diff, Energy $\rightarrow$ same so Energy Eigen value will be degenerate by $N!$ fold.

$N!$ = degenerate Energy Eigen value

= Exchange degeneracy (bcoz particles change in pairs)

- Quantum identicle particles are indistinguishable but they can be distinguishable in some cases. for Ex - i - we consider the concept of spin.

  But in general Q.I.P. are indistinguishable.

- If at $t=0$, ψ is symmetric then at time $t+dt$ what is the symmetry of w. fuc^n,

$$\psi_s(t) \longrightarrow \psi(t+dt)$$

$$H\psi_s = i\hbar \frac{\partial \psi_s}{\partial t}$$

If W. fuc^n is symmetric then its time derivative will be sy

$\psi_s \rightarrow$ sym. then $\frac{d\psi_s}{dt} \rightarrow$ sym.

→ H is always symmetric for identical particle.

then $\psi(t+dt) = \underset{\text{sym}}{\psi(t)} + \underset{\text{sym.}}{\left(\frac{\partial \psi}{\partial t}\right)} dt$ then total W. fuc^n → S

If $\psi \rightarrow$ antisym. $H\psi_A = i\hbar \frac{\partial \psi_A}{\partial t}$

$$\underset{\text{antisym.}}{\psi(t+dt)} = \underset{\text{antisym.}}{\psi(t)} + \underset{\text{antisym.}}{\left(\frac{\partial \psi}{\partial t}\right)} dt$$

- Symmetry character does not change w.r. to time.

<u>Particle Exchange operator</u> :- The operator that exchange the particles in pair is called Particle <u>Exchange operator</u>.

Suppose P_{12} is particle exchange o/p.

$$P_{12}\psi(1,2) = \psi(2,1)$$

$$\boxed{P_{12}\psi(\underline{r}_1, s_1; \underline{r}_2, s_2) = \psi(\underline{r}_2, s_2; \underline{r}_1, s_1)}$$

This is the eq^n of action of Particle exchange o/p.

<u>Eigen Value</u>:-

$$P_{12}\psi(\underline{r}_1, s_1, \underline{r}_2; s_2) = \lambda\psi(\underline{r}_1, s_1, \underline{r}_2; s_2)$$

$$P_{12}^2\psi(\underline{r}_1, s_1, \underline{r}_2, s_2) = \lambda^2\psi(\underline{r}_1 s_1, \underline{r}_2 s_2) \Rightarrow P_{12}^2\psi(1,2) = \psi($$

$$\lambda^2 = 1$$

$$\boxed{\lambda = \pm 1}$$

- Particle exchange o/p is Hermitian o/p.
- Particle exchange o/p commutes with Hamiltonian if potentially symmetric under the exchange of particles.

$$[H, P_{12}] = 0$$

Q. Particle exchange o/p for a system of non-interacting identical partic commutes with hamiltonian

1) always
2) Never
3) depends on the form of pot^n

for Non-interacting, identical particles, P_{12} always commute with hamiltonian. (i.e. pot^n is symmetric)

If particle not identical then (3) ✓

• for 2 e^- system,

$$S' = \left|\tfrac{1}{2}+\tfrac{1}{2}\right| \cdots\cdots \left|\tfrac{1}{2}-\tfrac{1}{2}\right| = 1\ ;\ 0$$

• for 3 e^- system,

$$S = \left|\underbrace{\tfrac{1}{2}+\tfrac{1}{2}}_{S'}+\tfrac{1}{2}\right| \cdots\cdots \left|\tfrac{1}{2}+\tfrac{1}{2}-\tfrac{1}{2}\right|$$

$$= |S'+S_3| \cdots\cdots |S'-S_3| = \tfrac{3}{2},\ \tfrac{1}{2},\ \tfrac{1}{2}$$

If no. of constraints is even (Bosons) → then Boson
" " " " odd → " Fermions

for Nucleus, If n_1+p_1 = even then boson
n_1+p_1 = odd then fermons

for atom; If $n_1+p_1+e_1$ = even → boson
= odd → fermion

Pauli Exclusion Principle :- "No two identical fermions can exist in the same Quantum state."

for 2 particle system,

spin wave fuc^{n}s ⇒ $|\uparrow\uparrow\rangle,\ |\downarrow\downarrow\rangle,\ \underbrace{|\uparrow\downarrow\rangle,\ |\downarrow\uparrow\rangle}_{\frac{1}{\sqrt{2}}\left[|\uparrow\downarrow\rangle \pm |\downarrow\uparrow\rangle\right]}$

$s = |s_1 + s_2| \text{ ---- } |s_1 - s_2|$

$s = 1, 0$

$m_s = +1, 0, -1, 0$

$|s, m_s\rangle = |0,0\rangle, |1,+1\rangle, |1,0\rangle, |1,-1\rangle$

There are 4 different W.fue^ns.

for $|\uparrow\uparrow\rangle \Rightarrow |s=1, m_s=+1\rangle$

$|\downarrow\downarrow\rangle \Rightarrow |s=1, m_s=-1\rangle$

$\frac{1}{\sqrt{2}}[|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle] = |s=1, m_s=0\rangle$ for symmetric $s =$

$\frac{1}{\sqrt{2}}[|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle] = |s=0, m_s=0\rangle$ for Antisymmetric $s=0$

- If $\Psi_{spin} \rightarrow$ Sym. then Ψ_{space} will be Antisym. bcoz total product $\rightarrow$ Ant

& If $\Psi_{spin} \rightarrow$ Antisym. then Ψ_{space} will be symmetric.

- All four states are equally probable.
- Total states $= (2)^3 = 8$ (Possible Microstates)
- for 1 particle, $(2S+1)$ microstates so
  for N " $(2S+1)^N$ "

For 3 particle System,

$S = \frac{3}{2}, \frac{1}{2}, \frac{1}{2}$

$(2S+1) = 4, 2, 2$

Total microstates $= 8$

i.e. 8 possibilities $\Rightarrow |\uparrow\uparrow\uparrow\rangle, |\downarrow\downarrow\downarrow\rangle$, -----

Prob :- Which of the following may rep^n a valid quantum state for 2 e^-'s in a He-atom.

(a) $[1s(1)\ 2s(2)]\ \chi_{1/2}(1)\ \chi_{1/2}(2)$

(b) $[1s(1)\ 2s(2) + 1s(2)\ 2s(1)]\ \chi_{1/2}(1)\ \chi_{1/2}(2)$

(c) $[1s(1)\ 2s(2) - 1s(2)\ 2s(1)]\ \chi_{1/2}(1)\ \chi_{1/2}(2)$

(d) $[1s(1)\ 2s(2) - 1s(2)\ 2s(1)]\ \chi_{1/2}(1)\ \chi_{-1/2}(2)$

(e) $[1s(1)\ 2s(2) - 1s(2)\ 2s(1)]\ [\chi_{1/2}(1)\ \chi_{-1/2}(2) + \chi_{1/2}(2)\ \chi_{-1/2}(1)]$

constraints are fermions (2 e^-) so, W. fu^n will be antisymmetric

$$\psi_{as} = \psi_{as} \times \psi_{s}$$
Total
$$= \psi_s \times \psi_{as}$$

- For a system of identical Bosons, the total wave function of the system will be symmetric under the exchange of particles in pairs.

- for a system of identical Fermions...... $\psi \rightarrow$ antisymmetric

e.g. $_2He^3$ $\rightarrow$ constraints are fermion
$= 5$ odd $\rightarrow$ fermion

$_7N^{14}$ $\rightarrow$ $7 + 14 = 21$ constraints in atom $\rightarrow$ fermions
(odd)
$= 14$ constraints in nucleus $\rightarrow$ Even $\rightarrow$ Bosons

Problem :- A system of 2 identical Boson's each of mass m is placed in a 1-dim box of length L. Both particles are in same spin state. The energy of the system is $\frac{5\pi^2\hbar^2}{2mL^2}$ What is the space part of the ~~syste~~ wave fu^n ?

$$E = \frac{5\pi^2\hbar^2}{2mL^2}$$

$$\left\{ E_n = \frac{n^2\pi^2\hbar^2}{2mL^2} \right.$$

$$n^2 = 5$$

$$\Rightarrow n_x^2 + n_y^2 = 5 \quad \Rightarrow \quad \begin{array}{c|c} n_x = 1 & n_x = 2 \\ n_y = 2 & n_y = 1 \end{array}$$

for single particle, Energy of system (particle in box)

$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}.$$

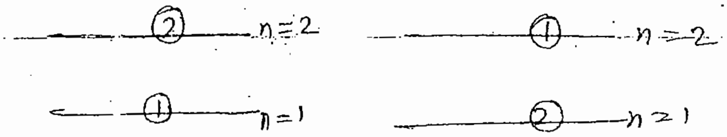
& $\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$

for a system of 2 identical boson,

$$E = \frac{n_1^2 \pi^2 \hbar^2}{2mL^2} + \frac{n_2^2 \pi^2 \hbar^2}{2mL^2}$$

$$\& \ \psi_n(x) = \psi_{n_1}(x_1)\, \psi_{n_2}(x_2)$$

Bosons are indistinguishable so there are 2 posibiliti



$$\psi(1,2) = \psi_1(x_1)\, \psi_2(x_2)$$
$$\psi(2,1) = \psi_1(x_2)\, \psi_2(x_1)$$

for Identical indisthguishable particles, superposition of these 2 w.fuc^{n}s $\quad \psi = \frac{1}{\sqrt{2}}\left[\psi(1,2) \pm \psi(2,1)\right]$

for Identical Bosons, total W.fuc^n must be symmetric

$$\psi_{Total} = \psi_{spac}\, \psi_{spin}$$
$$\left.\begin{aligned} &= \psi_{A\,spac}\, \psi_{A\,spin} \\ &= \psi_{S\,spac}\, \psi_{S\,spin} \end{aligned}\right\} \text{2 posibilities}$$

Spin ~~comp~~ state is same for both bosons so m_s is same.

spin State $\Rightarrow |s_1, s_2, m_{s_1}, m_{s_2}\rangle$

for $s=1$, $m_s = -1, 0, +1$

$(2s+1)^2 = (2\cdot1+1)^2 = 3^2 = 9$ states but we consider only symmetric spin states $\rightarrow$

$|1,1,+1,+1\rangle$, $|1,1,0,0\rangle$, $|1,1,-1,-1\rangle$

Bcoz of same spin state $\psi = \frac{1}{\sqrt{2}}\left[\psi(1,2) + \psi(2,1)\right]$

$$\psi = \frac{1}{\sqrt{2}}\left(\sqrt{\frac{2}{L}}\right)^2 \left[\sin\frac{\pi x_1}{L} \sin\frac{2\pi x_2}{L} + \sin\frac{2\pi x_1}{L} \sin\frac{\pi x_2}{L}\right].$$

same spin state will be symmetric alway but
different " " may be " or antisymmetric.

Problem:- Two identical fermions with spin $\frac{1}{2}$ are placed in 1-dim box of length L. Each particle has mass m. The energy of the system is $\frac{13\pi^2\hbar^2}{2mL^2}$. What is the space part of the wave fun

$$E = \frac{13\pi^2\hbar^2}{2mL^2} = \frac{n_1^2\pi^2\hbar^2}{2mL^2} + \frac{n_2^2\pi^2\hbar^2}{2mL^2}$$

$$\cancel{\psi(1,2) = \psi(1)\,\psi(2)} \qquad n^2 = n_1^2 + n_2^2$$

13

$$n_1 = 3, \; n_2 = 2 \quad \Big| \quad n_1 = 2, \; n_2 = 3$$

$$\psi_n = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$$

ψ depend on n. n is different so spin may be same

space part of W.fun

$$\left.\begin{aligned}\psi(x_1, x_2) &= \left(\sqrt{\frac{2}{L}}\right)^2 \sin\frac{2\pi x_1}{L} \sin\frac{3\pi x_2}{L} \\ &= \left(\sqrt{\frac{2}{L}}\right)^2 \sin\frac{3\pi x_1}{L} \sin\frac{2\pi x_2}{L}\end{aligned}\right\} \text{2 possiblities}$$

$$\psi(x_1, x_2) = \frac{1}{\sqrt{2}}\left(\sqrt{\frac{2}{L}}\right)^2 \left[\sin\frac{2\pi x_1}{L} \sin\frac{3\pi x_2}{L} \pm \sin\frac{3\pi x_1}{L} \sin\frac{2\pi x_2}{L}\right]$$

for 2 identical fermions →

$$\psi_{Total} = \psi_{space} \times \psi_{spin}$$

d
Antisy.

No idea of spin state so

$$\psi(x_1, x_2) = [\quad \pm \quad]$$

$$\left.\begin{aligned} S=1, \quad m_s &= +1 \quad && |\uparrow\uparrow\rangle \\ &= -1 && |\downarrow\downarrow\rangle \\ &= 0 && \tfrac{1}{\sqrt{2}}[|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle] \end{aligned}\right\} +$$

$$S=0, \quad m_s = 0 \qquad \left.\tfrac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)\right\} -$$

Problem, Consider the wave fun^n $\psi = \psi(\underline{r_1}, \underline{r_2})\chi_s$ for a fermion system consisting of 2 spin $\frac{1}{2}$ particles. The spacial part of the wave fun^n is given by

$$\psi(\underline{r_1}, \underline{r_2}) = \frac{1}{\sqrt{2}}\left[\phi_1(\underline{r_1})\,\phi_2(\underline{r_2}) + \phi_2(\underline{r_1})\,\phi_1(\underline{r_2})\right]$$

ϕ_1 & ϕ_2 are single particle states.

The spin part of wave fun^n with spin state α & β shou be

(a) $\frac{1}{\sqrt{2}}(\alpha\beta + \beta\alpha)$ ✓(b) $\frac{1}{\sqrt{2}}(\alpha\beta - \beta\alpha)$

(c) $\alpha\alpha$ (d) $\beta\beta$

Total W. fun^n ~~will~~ must be antisym. ~~So~~ space part is symmetr ~~so~~ spin part must be antisym.

Problem: Consider a 1-dim infinite square well pot^n defi as

$$V(x) = \begin{cases} 0, & \text{for } 0 < x < L \\ \infty, & \text{otherwise} \end{cases}$$

If 2 identical non-interacting bosons occupie the lowest 2 energy levels. The wave fun^n of the combined system is given by

(a) $\psi(x_1, x_2) = \sin\left(\frac{\pi x_1}{L}\right)\sin\left(\frac{2\pi x_2}{L}\right)$

(b) $\psi(x_1, x_2) = \sin\left(\frac{\pi x_1}{L}\right)\sin\left(\frac{\pi x_2}{L}\right)$

(c) $\psi(x_1, x_2) = \frac{1}{2}\left[\sin\left(\frac{\pi x_1}{L}\right)\sin\left(\frac{2\pi x_2}{L}\right) - \sin\left(\frac{\pi x_2}{L}\right)\sin\left(\frac{2\pi x_1}{L}\right)\right]$

(d) $\psi(x_1, x_2) = \frac{1}{2}\left[\sin\left(\frac{\pi x_1}{L}\right)\sin\left(\frac{\pi x_2}{L}\right) + \sin\left(\frac{2\pi x_1}{L}\right)\sin\left(\frac{2\pi x_2}{L}\right)\right]$

✓(e) $\psi(x_1, x_2) = \frac{1}{2}\left[\sin\left(\frac{\pi x_1}{L}\right)\sin\left(\frac{2\pi x_2}{L}\right) + \sin\left(\frac{2\pi x_1}{L}\right)\sin\left(\frac{\pi x_2}{L}\right)\right]$

Bosons are in general indistinguishable.

(a) & (b) → ✗ for distinguishable.

$n=2$

$n=1$

No idea of spin, (c) may be correct bcoz

$$\psi_s = \psi_{S\,spac}\,\psi_{S\,spin} \text{ or } \psi_{A\,spac}\,\psi_{A\,spin}$$

Problem :- 2 spin half fermions having spin $\vec{S_1}$ and $\vec{S_2}$ interact through a potⁿ. $V(r) = \vec{S_1}\cdot\vec{S_2}\, V_0(r)$. The contributio of this potⁿ in the siglet & triplet states respectively a

(a) $-\frac{3}{2} V_0(r)$ & $\frac{1}{2} V_0(r)$

(b) $-\frac{V_0(r)}{2}$ & $-\frac{3}{2} V_0(r)$

(c) $\frac{1}{4} V_0(r)$ & $-\frac{3}{4} V_0(r)$

(d) ~~$-\frac{3}{4} V_0(r)$ & $\frac{1}{4} V_0(r)$~~

$$V(r) = \vec{S_1}\cdot\vec{S_2}\, V_0(r)$$

$$S^2 = S_1^2 + S_2^2 + 2 S_1\cdot S_2$$

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

$$= \frac{S(S+1) - S_1(S_1+1) - S_2(S_2+1)}{2}$$

$$S = |S_1+S_2| \cdots\cdots |S_1-S_2|$$

$$S = 1, 0$$

for $S=0$ (singlet) $\Rightarrow \vec{S_1}\cdot\vec{S_2} = \frac{0 - \frac{3}{4} - \frac{3}{4}}{2} = -\frac{3}{4}$

for $S=1$ (triplet) $\Rightarrow \vec{S_1}\cdot\vec{S_2} = \frac{2 - \frac{3}{4} - \frac{3}{4}}{2} = \frac{1}{4}$

So $V(r)$ for singlet $\Rightarrow V(r) = -\frac{3}{4} V_0(r)$

$V(r)$ for triplet $\Rightarrow V(r) = \frac{1}{4} V_0(r)$

Qu:- Consider a system of 2 spin $\frac{1}{2}$ particles with total spin Q.No. $S=0$. The eigen value of the Hamiltonian $H = A\,\vec{S_1}\cdot\vec{S_2}$ ($A=+ve$) in this state is

(A) $\frac{A\hbar^2}{4}$ (B) $-\frac{A\hbar^2}{4}$ (C) $\frac{3A\hbar^2}{4}$ (d) $-\frac{3A\hbar^2}{4}$

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

$H = -\frac{3}{4} A\hbar^2$

$\vec{S_1}\cdot\vec{S_2}$ (above) $(S=0)$ $= -\frac{3}{4}$

Que:- Consider a system of 3 non-interacting particles that are confined to move in a 1-dim infinite potⁿ well of length a defined as $V(x) = \begin{cases} 0 & , 0<x<a \\ \infty & \text{otherwise} \end{cases}$

Determine the energy & w.funcⁿ of the ground, Ist excited & IInd excited state when the particles are

(a) spinless & distinguishable

(b) Identical bosons

(c) " spin half particles

(d) distinguishable spin half particles

(a) spinless & distinguishable

Not identical $\longrightarrow$ means masses are not same

given :- $m_1 < m_2 < m_3$

ground state :- $E = \frac{\hbar^2\pi^2}{2a^2}\left[\frac{n_1^2}{m_1} + \frac{n_2^2}{m_2} + \frac{n_3^2}{m_3}\right]$

$n_1 = n_2 = n_3 = 1$, $E_{111} = \frac{\hbar^2\pi^2}{2a^2}\left[\frac{1}{m_1} + \frac{1}{m_2} + \frac{1}{m_3}\right]$

Ist Excited state

$n_1 = 1,\ n_2 = 1,\ n_3 = 2$ $\quad E_{112} = \frac{\hbar^2\pi^2}{2a^2}\left[\frac{1}{m_1} + \frac{1}{m_2} + \frac{4}{m_3}\right]$

IInd Excited state

$n_1 = 1,\ n_2 = 2,\ n_3 = 1$ $\quad E_{121} = \frac{\hbar^2\pi^2}{2a^2}\left[\frac{1}{m_1} + \frac{4}{m_2} + \frac{1}{m_3}\right]$

Wave funcⁿ for ground state $\quad \psi_{111}(x_1, x_2, x_3) = \left(\sqrt{\frac{2}{a}}\right)^3 \sin\frac{\pi x_1}{a} \sin\frac{\pi x_2}{a} \sin\frac{\pi x_3}{a}$

Ist Excited $\quad \psi_{112}(x_1\, x_2\, x_3) = \left(\sqrt{\frac{2}{a}}\right)^3 \sin\frac{\pi x_1}{a} \sin\frac{\pi x_2}{a} \sin\frac{2\pi x_3}{a}$

IInd Excited $\quad \psi_{121}(x_1\, x_2\, x_3) = \left(\sqrt{\frac{2}{a}}\right)^3 \sin\frac{\pi x_1}{a} \sin\frac{2\pi x_2}{a} \sin\frac{\pi x_3}{a}$

(b) Identical Boson

$$m_1 = m_2 = m_3$$

$$E_{n_1 n_2 n_3} = \frac{\hbar^2 \pi^2}{2ma^2}(n_1^2 + n_2^2 + n_3^2)$$

$$E_{111} = \frac{\hbar^2 \pi^2}{2ma^2}(1+1+1) = \frac{3}{2}\frac{\pi^2 \hbar^2}{ma^2}$$

$$E_{112} = \frac{6}{2}\frac{\pi^2 \hbar^2}{ma^2}$$

$$E_{112} = E_{211} = E_{121} \quad (\because \text{Bosons are indistinguishable})$$

$$E_{122} = E_{212} = E_{221} = \frac{9\pi^2\hbar^2}{2ma^2}$$

ground

$$\psi_{111} = \left(\sqrt{\frac{2}{a}}\right)^3 \sin\left(\frac{\pi x_1}{a}\right)\sin\left(\frac{\pi x_2}{a}\right)\sin\left(\frac{\pi x_3}{a}\right)$$

$$\psi_{112} = \left(\sqrt{\frac{2}{a}}\right)^3 \sin\left(\frac{\pi x_1}{a}\right)\sin\left(\frac{\pi x_2}{a}\right)\sin\left(\frac{2\pi x_3}{a}\right)$$

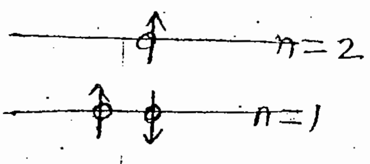
$$\psi_{121} = \left(\sqrt{\frac{2}{a}}\right)^3 \sin\left(\frac{\pi x_1}{a}\right)\sin\left(\frac{2\pi x_2}{a}\right)\sin\left(\frac{\pi x_3}{a}\right)$$

$$\psi_{211} = \left(\sqrt{\frac{2}{a}}\right)^3 \sin\left(\frac{2\pi x_1}{a}\right)\sin\left(\frac{\pi x_2}{a}\right)\sin\left(\frac{\pi x_3}{a}\right)$$

3 fold degenerate

$$\psi = \frac{1}{\sqrt{3}}\left[\psi_{112} + \psi_{121} + \psi_{211}\right]$$

(iii) 3 Identical spin $\frac{1}{2}$ particles ; Identical fermions



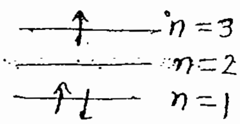
$$E_{112} = E_{121} = E_{211} \Rightarrow \text{3 fold degenerate}$$

$$E_{122} = \frac{9}{2}\frac{\pi^2\hbar^2}{ma^2}$$

$$E_{113} = \frac{11}{2}\frac{\pi^2\hbar^2}{ma^2}$$

g.s.

$$\begin{vmatrix} \psi_1(x_1)\uparrow & \psi_1(x_2)\uparrow & \psi_1(x_3)\uparrow \\ \psi_1(x_1)\downarrow & \psi_1(x_2)\downarrow & \psi_1(x_3)\downarrow \\ \psi_2(x_1) & \psi_2(x_2) & \psi_2(x_3) \end{vmatrix}$$



Slater determinant (only Antisym.)
for system of N particles

$$\frac{1}{\sqrt{N!}}\begin{vmatrix} \psi_{n_1}(x_1) & \psi_{n_1}(x_2) & \psi_{n_1}(x_3) & \cdots & \psi_{n_1}(x_n) \\ \psi_{n_2}(x_1) & \psi_{n_2}(x_2) & \psi_{n_2}(x_3) & \cdots & \psi_{n_2}(x_n) \\ \psi_{n_3}(x_1) & \psi_{n_3}(x_2) & & & \\ \vdots & & & & \\ \psi_{n_N}(x_1) & \psi_{n_N}(x_2) & \cdots & & \psi_{n_N}(x_n) \end{vmatrix}$$

(d) distinguishable spin $\frac{1}{2}$ particles
3 particles can't be distinguish by spin (↑↓) ; Not identical
⇒ dont follow Pauli's Exclusion principle. [3rd may be ↑ or ↓

$$\psi = \psi_{space}\,\psi_{spin}$$

Q. For Pauli's spin operators prove that,

$$(\vec{\sigma_1}\cdot\vec{\sigma_2})^2 + 2(\vec{\sigma_1}\cdot\vec{\sigma_2}) = 3$$

$$\vec{\sigma_1} = \sigma_{x_1}\hat{i} + \sigma_{y_1}\hat{j} + \sigma_{z_1}\hat{k}$$

$$\vec{\sigma_2} = \sigma_{x_2}\hat{i} + \sigma_{y_2}\hat{j} + \sigma_{z_2}\hat{k}$$

$$\vec{\sigma_1}\cdot\vec{\sigma_2} = \sigma_{x_1}\sigma_{x_2} + \sigma_{y_1}\sigma_{y_2} + \sigma_{z_1}\sigma_{z_2}$$

$$(\vec{\sigma_1}\cdot\vec{\sigma_2})^2 = \{ \cancel{\sigma_{x_1}\sigma_{x_2}}\sigma_{x_1}\sigma_{x_2} + \sigma_{x_1}\sigma_{x_2}\sigma_{y_1}\sigma_{y_2} + \sigma_{x_1}\sigma_{x_2}\sigma_{z_1}\sigma_{z_2}$$
$$+ \sigma_{y_1}\sigma_{y_2}\sigma_{x_1}\sigma_{x_2} + \sigma_{y_1}\sigma_{y_2}\sigma_{y_1}\sigma_{y_2} + \sigma_{y_1}\sigma_{y_2}\sigma_{z_1}\sigma_{z_2}$$
$$+ \sigma_{z_1}\sigma_{z_2}\sigma_{x_1}\sigma_{x_2} + \sigma_{z_1}\sigma_{z_2}\sigma_{y_1}\sigma_{y_2} + \sigma_{z_1}\sigma_{z_2}\sigma_{z_1}\sigma_{z_2}$$

$$\sigma_{x_2}\sigma_{x_1} = \sigma_{x_1}\sigma_{x_2}$$

so $(\vec{\sigma_1}\cdot\vec{\sigma_2})^2 = \sigma_{x_1}\sigma_{x_1}\sigma_{x_2}\sigma_{x_2} + \text{''} + \text{''}$
$+ \text{''} + \sigma_{y_1}\sigma_{y_1}\sigma_{y_2}\sigma_{y_2} + \text{''}$
$+ \text{''} + \text{''} + \sigma_{z_1}\sigma_{z_1}\sigma_{z_2}\sigma_{z_2}$

$$\sigma_{x_1}^2\sigma_{x_2}^2 = 1\cdot 1 = 1$$

so $(\vec{\sigma_1}\cdot\vec{\sigma_2})^2 = 1 + \sigma_{x_1}\sigma_{y_1}\sigma_{x_2}\sigma_{y_2} + \sigma_{x_1}\sigma_{z_1}\sigma_{x_2}\sigma_{z_2}$
$+ \sigma_{y_1}\sigma_{x_1}\sigma_{y_2}\sigma_{x_2} + 1 + \sigma_{y_1}\sigma_{z_1}\sigma_{y_2}\sigma_{z_2}$
$+ \sigma_{z_1}\sigma_{x_1}\sigma_{z_2}\sigma_{x_2} + \sigma_{z_1}\sigma_{y_1}\sigma_{z_2}\sigma_{y_2} + 1$

$= 3 + \sigma_{x_1}\sigma_{y_1}\sigma_{x_2}\sigma_{y_2} + \sigma_{x_1}\sigma_{z_1}\sigma_{x_2}\sigma_{z_2}$
$+ \sigma_{y_1}\sigma_{z_1}\sigma_{y_2}\sigma_{z_2} + \sigma_{z_1}\sigma_{x_1}\sigma_{z_2}\sigma_{x_2} + \sigma_{y_1}\sigma_{x_1}\sigma_{y_2}\sigma_{x_2} + \sigma_{z_1}\sigma_{y_1}\sigma_{z_2}\sigma_{y_2}$

$$\sigma_{x_1}\sigma_{y_1} = -\sigma_{y_1}\sigma_{x_1}$$

$$\sigma_{x_1}\sigma_{y_1} = i\sigma_{z_1}$$

$$(\sigma_1\cdot\sigma_2)^2 = 3 + (i\sigma_{z_1})(i\sigma_{z_2}) + (-i\sigma_{y_1})(i\sigma_{y_2}) + (-i\sigma_{z_1})(-i\sigma_{z_2})$$
$$+ (i\sigma_{x_1})(i\sigma_{x_2}) + (i\sigma_{y_1})(i\sigma_{y_2}) + (-i\sigma_{x_1})(-i\sigma_{x_2})$$

$$= 3 - \sigma_{z_1}\sigma_{z_2} - \sigma_{y_1}\sigma_{y_2} - \sigma_{z_1}\sigma_{z_2} - \sigma_{x_1}\sigma_{x_2} - \sigma_{y_1}\sigma_{y_2} - \sigma_{x_1}\sigma_{x_2}$$

$$= 3 - 2(\sigma_{x_1}\sigma_{x_2} + \sigma_{y_1}\sigma_{y_2} + \sigma_{z_1}\sigma_{z_2})$$

$$(\sigma_1\cdot\sigma_2)^2 + 2(\sigma_1\cdot\sigma_2) = 3$$

Another method, $\qquad S_1 = \frac{\hbar}{2}\sigma_1$

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

$$\frac{\hbar^2}{4}\vec{\sigma_1}\cdot\vec{\sigma_2} = \frac{[s(s+1) - s_1(s_1+1) - s_2(s_2+1)]\hbar^2}{2}$$

for singlet $s=0$,

$$\vec{\sigma_1}\cdot\vec{\sigma_2} = 2\left(0 - \frac{3}{4} - \frac{3}{4}\right) = 2\left(-\frac{3}{2}\right) = -3$$

for triplet $s=1$,

$$\vec{\sigma_1}\cdot\vec{\sigma_2} = 2\left(2 - \frac{3}{4} - \frac{3}{4}\right) = 2\left(\frac{1}{2}\right) = 1$$

So $\quad (\sigma_1\cdot\sigma_2)^2 + 2(\sigma_1\cdot\sigma_2) = (-3)^2 + 2(-3)$

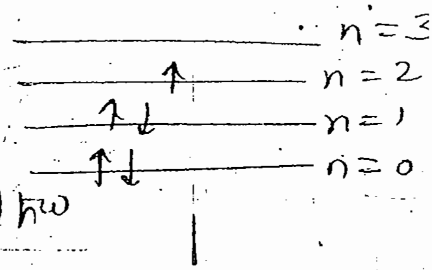
$= 9 - 6 = \underline{\underline{3}} \quad$ for $S=0$

$= (1)^2 + 2(1)$

$= 1 + 2 = \underline{\underline{3}} \quad$ for $S=1$

Problem:- The ground state energy ~~for~~ of 5 identical spin $\frac{1}{2}$ particle which are subject to a 1 dim harmonic oscillator potⁿ of freq. ω is

(a) $\frac{15}{2}\hbar\omega$ $\quad$ ✓(b) $\frac{13}{2}\hbar\omega$ $\quad$ (c) $\frac{1}{2}\hbar\omega$ $\quad$ (d) $5\hbar\omega$



$$E_n = \left(n+\tfrac{1}{2}\right)\hbar\omega$$

$$= \left(0+\tfrac{1}{2}\right)\hbar\omega + \left(0+\tfrac{1}{2}\right)\hbar\omega + \left(1+\tfrac{1}{2}\right)\hbar\omega + \left(1+\tfrac{1}{2}\right)\hbar\omega + \left(2+\tfrac{1}{2}\right)\hbar\omega$$

$$= \left(\frac{1}{2} + \frac{1}{2} + \frac{3}{2} + \frac{3}{2} + \frac{5}{2}\right)\hbar\omega = \frac{13}{2}\hbar\omega$$

for bosons,

$E_n = \frac{5}{2}\hbar\omega \quad$ all particles will be in ground state.

Perturbation Theory

This is an approximation method

Hamiltonian. $H = H_0 + H_P$ $\boxed{(H_P << H_0)}$

$H_0 \rightarrow$ unperturbed
$H_P \rightarrow$ Perturbed

If $H_P \rightarrow$ time independent $\Rightarrow$ Time Independent perturbation theory
$H_P \rightarrow$ " dependent $\Rightarrow$ " dependent " "

In Time dependent P.T., Transition will be calculated i.e. on applying the perturbation what is the probability of transition.

In Time Independent P.T., shifting of energy level.

$\hat{H}_P = \lambda H'$, $\boxed{\lambda << 1} \rightarrow$ unitless parameter.

Sch^r eq^n for Unperturbed H,

$$\boxed{H_0 | n > = E_n^{(0)} | n >}$$

for perturbed, $H|n> = E_n|n>$

$$(H_0 + \lambda H')|n> = E_n|n>$$

$$E_n = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \cdots\cdots + \lambda^k E_n^{(k)} + \cdots\cdots$$

$$|\psi_n> = |\phi_n> + \lambda|\psi_n^{(1)}> + \lambda^2|\psi_n^{(2)}> + \cdots\cdots \lambda^k|\psi_n^{(k)}> + \cdots$$

$E_n^{(k)}$ = Kth order Energy correction
$|\psi_n^{(k)}>$ = " " correction in wave fue^n.

$$(H)|\psi_n> = E_n|\psi_n>$$

$$\Rightarrow (H_0 + \lambda H')|\psi_n> = E_n|\psi_n>$$

λ^0 : $H_0|\phi_n> = E_n^{(0)}|\phi_n>$ ——— (1)

λ^1 : $H_0|\psi_n^{(1)}> + H'|\phi_n> = E_n^{(0)}|\psi_n^{(1)}> + E_n^{(1)}|\phi_n>$ ——— (2)

λ^2 : $H_0|\psi_n^{(2)}> + H'|\psi_n^{(1)}> = E_n^{(0)}|\psi_n^{(2)}> + E_n^{(1)}|\psi_n^{(1)}> + E_n^{(2)}|\phi_n>$

→ First order energy correction = ?

from (2),

$$\langle \phi_n | H_0 | \psi_n^{(1)} \rangle + \langle \phi_n | H' | \phi_n \rangle = E_n^{(0)} \langle \phi_n | \psi_n^{(1)} \rangle + E_n^{(1)} \langle \phi_n | \phi_n \rangle$$

$$\langle \phi_n | \phi_n \rangle = 1$$

$$\langle \phi_n | \psi_n^{(1)} \rangle = 0$$

$$\left\{ \begin{array}{l} \langle \psi | \psi \rangle = 1, \; \langle \phi_n | \phi_n \rangle = \\ \langle \phi_n | \psi_n^{(1)} \rangle = \langle \phi_n | \psi_n^{(2)} \rangle = \end{array} \right.$$

$H_0 \longrightarrow$ hermitian operator

$$\Rightarrow \cancel{\langle \phi_n | E_n^{(0)} | \psi_n^{(1)} \rangle} + \cancel{\langle \phi_n | H' | \phi_n \rangle} = \cancel{E_n^{(1)}}(1) + 0$$

$$\Rightarrow E_n^{(0)} \langle \phi_n | \psi_n^{(1)} \rangle + \langle \phi_n | H' | \phi_n \rangle = E_n^{(1)}$$

$$\Rightarrow \boxed{E_n^{(1)} = \langle \phi_n | H' | \phi_n \rangle}$$

First order energy correction in energy is equal to the expectation value of perturbed hamiltonian over unperturbed state

If wave funcⁿ is not normalised to unity then

$$E_n^{(1)} = \frac{\langle \phi_n | H' | \phi_n \rangle}{\langle \phi_n | \phi_n \rangle}$$

→ Energy corrected to Ist order → means

$$E_n = E_n^{(0)} + \lambda E_n^{(1)}$$

$$E_n = E_n^{(0)} + \langle \phi_n | H_P | \phi_n \rangle$$

→ First Order correction in wave funcⁿ :-

$$H_0 | \psi_n^{(1)} \rangle + H' | \phi_n \rangle = E_n^{(0)} | \psi_n^{(1)} \rangle + E_n^{(1)} | \phi_n \rangle$$

$$| \psi_n^{(1)} \rangle = \hat{I} | \psi_n^{(1)} \rangle$$

$$= \sum_m | \phi_m \rangle \langle \phi_m | \psi_n^{(1)} \rangle$$

$$= \sum_{m \neq n} \langle \phi_m | \psi_n^{(1)} \rangle | \phi_m \rangle$$

Now, multiply by $\langle \phi_m |$,

$$\langle \phi_m | H_0 | \psi_n^{(1)} \rangle + \langle \phi_m | H' | \phi_n \rangle = \langle \phi_m | E_n^{(0)} | \psi_n^{(1)} \rangle + \langle \phi_m | E_n^{(1)} | \phi_n \rangle$$

$$\langle \phi_m | E_m^{(0)} | \psi_n^{(1)} \rangle + \langle \phi_m | H' | \phi_n \rangle = \langle \phi_m | E_n^{(0)} | \psi_n^{(1)} \rangle + E_n^{(1)} \langle \phi_m | \phi_n \rangle$$

$\langle \phi_m | \phi_n \rangle = 0$ by orthonormality

$$\Rightarrow \langle \phi_m | \psi_n^{(1)} \rangle \left(E_n^{(0)} - E_m^{(0)}\right) = \langle \phi_m | H' | \phi_n \rangle$$

$$\langle \phi_m | \psi_n^{(1)} \rangle = \frac{\langle \phi_m | H' | \phi_n \rangle}{E_n^{(0)} - E_m^{(0)}}$$

$$\boxed{|\psi_n^{(1)}\rangle = \sum_m{}' \frac{\langle \phi_m | H' | \phi_n \rangle}{E_n^{(0)} - E_m^{(0)}} |\phi_m\rangle}$$

$\left\{ \sum_m{}' = \sum_{m \neq n} \right.$

→ Second Order Energy Correction,

$$E_n^{(2)} = \sum_m{}' \frac{|\langle \phi_m | H' | \phi_n \rangle|^2}{E_n^{(0)} - E_m^{(0)}}$$

→ Energy Corrected to IInd order,

$$E_n = E_n^{(0)} + \langle \phi_n | \hat{H}_p | \phi_n \rangle + \sum_{m \neq n} \frac{|\langle \phi_m | \hat{H}_p | \phi_n \rangle|^2}{E_n^{(0)} - E_m^{(0)}}$$

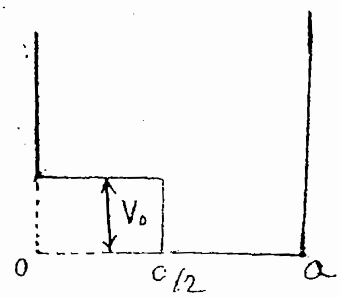
→ Wave fucn corrected to Ist order,

$$|\psi_n\rangle = |\phi_n\rangle + \sum_{m \neq n} \frac{\langle \phi_m | H_p | \phi_n \rangle}{E_n^{(0)} - E_m^{(0)}} |\phi_m\rangle$$

Problem:- The unperturbed wavefucn for the infinite square well is given by $\psi_n^{0}(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)$

suppose we perturbed the system by simply raising the floor of the well by a constant amount only half way across the well. Calculate the energy of the nth state correcting to first order.

$$V_p(x) = H_p(x) = V_0 \quad , 0 < x < a/2$$
$$= 0 \quad , \text{otherwise}$$



$$H_p(x) = \int \psi_n^{0}(x)\, H_p\, \psi_n^{0}(x)\, dx$$

$$E_n^{(1)} = \int_0^{a/2} \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) V_0 \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) dx$$

$$E_n^{(1)} = H_p(x) = \int_0^{a/2} \frac{2}{a} \sin^2\left(\frac{n\pi x}{a}\right) V_0 \, dx$$

$$= \frac{2}{a} V_0 \int_0^{a/2} \frac{1}{2}\left[1 - \cos\frac{2n\pi x}{a}\right] dx$$

$$= \frac{2V_0}{a} \cdot \frac{1}{2}\left[\frac{a}{2} - 0\right] = \frac{V_0}{2}$$

$$E_n^{(1)} = \frac{V_0}{2}$$

Energy corrected to Ist order,

$$E_n = E_n^{(0)} + E_n^{(1)}$$

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2} + \frac{V_0}{2}$$

Problem:- Calculate the energy of the nth ~~excited~~ state to first order perturbation theory for a spinless particle of mass m moving in an infinite potential well of length 2L defined as,

$$V(x) = \begin{cases} 0 , & 0 < x < 2L \\ \infty , & \text{otherwise} \end{cases}$$

which is modified at the bottom by the following perturbations,

(i) $V_p(x) = \lambda V_0 \delta(x-L)$

(ii) $V_p(x) = \lambda V_0 \sin\left(\frac{\pi x}{2L}\right)$, $\lambda << 1$

(i) $V_p(x) = \lambda V_0 \delta(x-L)$

$$E_n^{(1)} = \int \psi_n^0(x) H_p \psi_n^0(x) \, dx$$

$$= \int_0^{2L} \sqrt{\frac{2}{2L}} \sin\left(\frac{n\pi x}{2L}\right) \lambda V_0 \delta(x-L) \sqrt{\frac{2}{2L}} \sin\left(\frac{n\pi x}{2L}\right) dx$$

$$= \frac{\lambda V_0}{L} \int_0^{2L} \sin^2\left(\frac{n\pi x}{2L}\right) \delta(x-L) \, dx$$

$$\boxed{\int_{x_1}^{x_2} f(x)\,\delta(x-a)\,dx = \begin{cases} f(a) , & x_1 < a < x_2 \\ 0 , & \text{otherwise} \end{cases}}$$

$$E_n^{(1)} = \frac{\lambda V_0}{L} \int_0^{2L} \sin^2\left(\frac{n\pi \cancel{L}}{2\cancel{L}}\right) \cdot 1 \, dL = \frac{\lambda V_0}{L} \sin^2\frac{n\pi}{2}$$

$$E_n^{(1)} = \frac{\lambda V_0}{L} \sin^2\frac{n\pi}{2}$$

if $n \to$ odd , $E_n^{(1)} = \frac{\lambda V_0}{L}$ (as $\sin\frac{n\pi}{2} = 1$)

$n \to$ even , $E_n^{(1)} = 0$ ($\because \sin\frac{n\pi}{2} = 0$)

(ii) $V_p(x) = \lambda V_0 \sin\left(\frac{\pi x}{2L}\right)$

$$E_n^{(1)} = \int \psi^{\circ}(x) H_p \psi_n^{(0)}(x)\,dx$$

$$= \int_0^{2L} \frac{1}{L}\sin^2\frac{n\pi x}{2L}\,\lambda V_0 \sin\left(\frac{\pi x}{2L}\right)dx$$

$$= \frac{\lambda V_0}{L}\int_0^{2L}\sin^2\frac{n\pi x}{2L}\sin\left(\frac{\pi x}{2L}\right)dx$$

$$= \frac{\lambda V_0}{L}\int_0^{2L}\frac{1}{2}\left(1-\cos\frac{2n\pi x}{2L}\right)\sin\left(\frac{\pi x}{2L}\right)dx$$

$$= \frac{\lambda V_0}{2L}\int_0^{2L}\left(\sin\frac{\pi x}{2L} - \cos\frac{2n\pi x}{2L}\sin\frac{\pi x}{2L}\right)dx$$

$$= \frac{\lambda V_0}{2L}\int_0^{2L}\left[\sin\frac{\pi x}{2L} - \frac{1}{2}\sin\left(\frac{\pi x}{2L}(2n+1)\right) + \frac{1}{2}\sin\left(\frac{\pi x}{2L}(2n-1)\right)\right]dx$$

$$= \frac{\lambda V_0}{2L}\left[-\cos\frac{\pi x}{2L}\left[\frac{2L}{\pi}\right] + \frac{1}{2}\frac{2L}{\pi(2n+1)}\cos\left\{\frac{\pi x}{2L}(2n+1)\right\} - \frac{1}{2}\frac{2L}{\pi(2n-1)}\cos\left\{\frac{\pi x}{2L}(2n-1)\right\}\right]_0^{2L}$$

$$= \frac{\lambda V_0}{2L}\left[-\frac{2L}{\pi}\cos\pi + \frac{L}{\pi(2n+1)}\cos\pi(2n+1) - \frac{L}{\pi(2n-1)}\cos\pi(2n-1) + \frac{2L}{\pi}\cos 0 - \frac{L}{\pi(2n+1)}\cos 0 + \frac{L}{\pi(2n-1)}\cos 0\right]$$

$$= \frac{\lambda V_0}{2L}\left[-\frac{2L}{\pi}(-1) + \frac{L}{\pi(2n+1)}(-1) - \frac{L}{\pi(2n-1)}(-1) + \frac{2L}{\pi} - \frac{L}{\pi(2n+1)} + \frac{L}{\pi(2n-1)}\right]$$

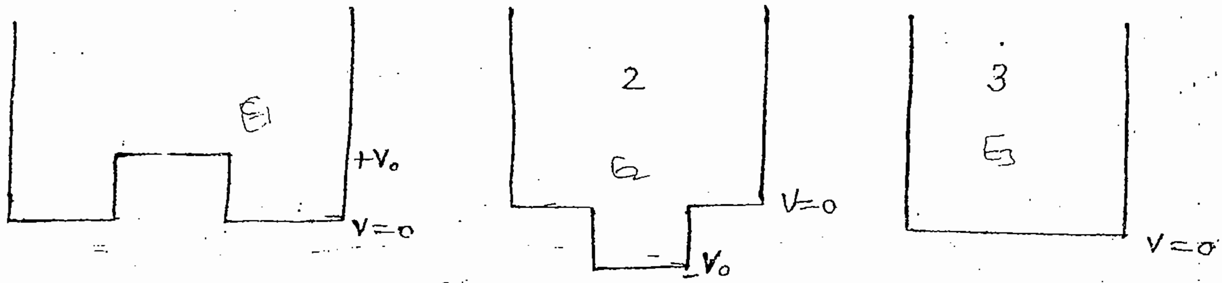
$$= \frac{\lambda V_0}{2L}\left[\frac{4L}{\pi} - \frac{2L}{\pi(2n+1)} + \frac{2L}{\pi(2n-1)}\right]$$

$$= \frac{\lambda V_0}{2L}\frac{2L}{\pi}\left[2 - \frac{1}{2n+1} + \frac{1}{2n-1}\right] = \frac{\lambda V_0}{\pi}\left[\frac{8n^2-2-2n+1+2n+1}{4n^2-1}\right]$$

$$= \frac{\lambda V_0}{\pi}\frac{8n^2}{4n^2-1} = \frac{2\lambda V_0}{\pi}\left(\frac{4n^2}{4n^2-1}\right)$$

Ans

Problem:- Let E_1, E_2, E_3 be the respective ground state energies of the following potential



which one of the following option is correct:-

(a) $E_1 < E_2 < E_3$ (b) $E_3 < E_1 < E_2$

(c) $E_2 < E_3 < E_1$ (d) $E_2 < E_1 < E_3$

Let width of potⁿ a. Ground state energy of 3 potⁿ is

$$E_3 = \frac{\pi^2 \hbar^2}{2ma^2} \quad (n=1 \text{ for G.S.})$$

for (1) potⁿ ⇒ $E_1 = \frac{\pi^2 \hbar^2}{2ma^2} + \frac{V_0}{3}$

for (2) potⁿ ⇒ $E_2 = \frac{\pi^2 \hbar^2}{2ma^2} - \frac{V_0}{3}$

So $\underline{E_2 < E_3 < E_1}$ Ans

Prob:- If the perturbation $H' = ax$ where a is a constant, is added to infinite square well potⁿ

$$V(x) = \begin{cases} 0 & , \text{ for } 0 < x < \pi \\ \infty & , \text{ otherwise} \end{cases}$$

The Ist order correction to ground state energy is

(a) $\frac{a\pi}{2}$ (b) $a\pi$ (c) $\frac{a\pi}{4}$ (d) $\frac{a\pi}{\sqrt{2}}$

$$H' = ax$$

$$E_n^{(1)} = \int_0^{\pi} \psi_n^{0*} H' \psi_n^0 \, dx$$

$$\psi_n^0(x) = \sqrt{\frac{2}{\pi}} \sin \frac{n\pi x}{\pi}$$

$$E_n^{(1)} = \int_0^{\pi} \frac{2}{\pi} \sin^2 \frac{n\pi x}{\pi} \; ax\,dx$$

$$= \frac{2}{\pi} a \int_0^{\pi} \frac{x}{2}\left[1 - \cos \frac{2n\pi x}{\pi}\right] dx$$

$$= \frac{a}{\pi} \int_0^{\pi} (x - x\cos 2nx)\, dx$$

$$= \frac{a}{\pi}\left[\frac{x^2}{2} - x\frac{\sin 2nx}{2n} - \frac{\cos 2nx}{(2n)^2}\right]_0^{\pi}$$

$$= \frac{a}{2}\left[\frac{\pi^2}{2} - 0 - \frac{1}{4n^2}\left\{\cos 2n\pi - \cos 0\right\}\right]$$

$$= \frac{a}{2}\left[\frac{\pi^2}{2} - 0 - \frac{1}{4n^2}(1-1)\right] = \frac{a}{2}\left[\frac{\pi^2}{2} - 0\right]$$

$$\boxed{E_n^{(1)} = \frac{a\pi}{2}} \text{ Ans}$$

Prob:- A particle of mass m is confined in a infinite ~~square~~ pot^n well $V(x) = \begin{cases} 0, & \text{for } 0 < x < L \\ \infty, & \text{otherwise} \end{cases}$

It is subjected to a perturbing pot^n $V_p(x) = V_0 \sin\left(\frac{2\pi x}{L}\right)$ within the well. Let $E^{(1)}$ & $E^{(2)}$ be the corrections to ground state energy in the Ist & IInd order in V_0 respectively. Which of the following are true?

(a) $E^{(1)} = 0$, $E^{(2)} < 0$

(b) $E^{(1)} > 0$, $E^{(2)} = 0$

(c) $E^{(1)} = 0$, $E^{(2)}$ depends on the sign of V_0

(d) $E^{(1)} < 0$, $E^{(2)} < 0$

$$E_n^{(1)} = \frac{2V_0}{L}\int_0^L \sin^2 \frac{\pi x}{L} \sin\frac{2\pi x}{L} dx = \frac{2V_0}{L}\int_0^L \sin\frac{2\pi x}{L} \frac{1}{2}\left[1 - \cos\frac{2\pi x}{L}\right] dx$$

$$= \frac{V_0}{L}\int_0^L \left(\sin\frac{2\pi x}{L} - \sin\frac{2\pi x}{L}\cos\frac{2\pi x}{L}\right) dx$$

($n = 1$ for G.S.)

$$= \frac{V_0}{L}\left[-\frac{\cos\frac{2\pi x}{L}}{2\pi/L} - 0\right]_0^L = \frac{V_0}{L}\frac{L}{2\pi}\left[\cos 2\pi - \cos 0\right]$$

$$= \frac{V_0}{2\pi}[1-1]$$

$$= 0$$

$$E_n^{(2)} = \sum_{m \neq n} \frac{|\langle \phi_m | H_P | \phi_n \rangle|^2}{E_n^{(0)} - E_m^{(0)}}$$

Prob :- Let E_n' ($n = 0, 1, 2 \ldots$) be the energy eigen value for a partic of mass m placed in an anharmonic potⁿ

$$V(x) = \frac{1}{2} m \omega^2 x^2 + a x^4 \quad (a > 0)$$

Let $E_n = \left(n + \frac{1}{2}\right) \hbar \omega$ then acc. to Ist order perturbation the

(a) $E_0' = E_0$ (c) $E_0' < E_0$

(b) $E_0' > E_0$, $E_n' > E_n$ for all n (d) $E_n' < E_n$ for all n

$$E_n' = E_n + E_n^{(1)}$$

$$E_n^{(1)} = \langle n | a x^4 | n \rangle$$

$$\langle x^4 \rangle = \frac{\hbar^2}{4 m^2 \omega^2} (6n^2 + 6n + 3)$$

$$E_n^{(1)} = \frac{a \hbar^2}{4 m^2 \omega^2} (6n^2 + 6n + 3)$$

$$E_0' = E_0^{(0)} + E_0^{(1)}$$

& $E_n' = E_n^{(0)} + E_n^{(1)}$ for all n.

Prob :- A quantum harmonic oscillator is in the energy eigen state $|n\rangle$. A time independent perturbation $\lambda (\hat{a}^+ a)^2$ acts on a particle where λ is constant of suitable dimension. a & a^+ are lowering & raising operator respectively. Then the first order energy shift is given by

(a) λn (b) $\lambda^2 n$ (c) λn^2 (d) $(\lambda n)^2$

$$E_n^{(1)} = \langle n | \lambda (a^+ a)^2 | n \rangle$$

$$= \cancel{\lambda a^{+2} a}\, \lambda \langle n | a^{+2} a^2 | n \rangle = \lambda \langle n | a^+ a a^+ a | n \rangle$$

$$E^{(1)} = \lambda n \langle n | a^+ a | n \rangle$$
$$= \lambda n \cdot n$$
$$E^{(1)} = \underline{\underline{\lambda n^2}}$$

Prob :- An unperturbed 2 level system has energy eigen value E_1 & E_2 & has energy eigen func's $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ & $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$, when perturbed its Hamiltonian is repⁿ by $\begin{pmatrix} E_1 & A \\ A^* & E_2 \end{pmatrix}$.

(i) The Ist order correction to E_1 is

(a) 4A (b) 2A (c) A ✓(d) 0

(ii) The IInd order correction to energy E_1 is

(a) 0 (b) A (c) $\frac{A^2}{E_2 - E_1}$ ✓(d) $\frac{A^2}{E_1 - E_2}$

(iii) The Ist order correction to wave func $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$

(a) ✓ $\begin{pmatrix} 0 \\ \frac{A^*}{E_1 - E_2} \end{pmatrix}$ (b) $\begin{bmatrix} 0 \\ 1 \end{bmatrix}$ (c) $\begin{pmatrix} \frac{A^*}{E_1 - E_2} \\ 0 \end{pmatrix}$ (d) $\begin{bmatrix} 1 \\ 1 \end{bmatrix}$

Total Hamiltonian $H = \begin{pmatrix} E_1 & A \\ A^* & E_2 \end{pmatrix}$

$$E_1 = \langle \phi | \hat{H}_P | \phi \rangle$$

$$E_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad E_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

Unperturbed Hamiltonian, $H_0 = \begin{bmatrix} E_1 & 0 \\ 0 & E_2 \end{bmatrix}$

Perturbed " $H_P = \begin{pmatrix} 0 & A \\ A^* & 0 \end{pmatrix}$ $\{ H_P = H - H^0$

check which is the wave func for which e-value E_1 & E_2 by $H\psi = E\psi$

(i) $E_1 = \langle \phi_1 | \hat{H}_P | \phi_1 \rangle$

$$= (\phi \;\; 0) \begin{bmatrix} 0 & A \\ A^* & 0 \end{bmatrix} \begin{bmatrix} \cancel{\phi} \\ \cancel{\phi} \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

$\therefore E' = (\phi \; 0)\begin{pmatrix} 0 \\ A^* \end{pmatrix} = 0$

$E' = 0$

(ii) $$E^{(2)} = \sum_m \frac{|\langle \phi_m | H_p | \phi_n \rangle|^2}{E_n^0 - E_m^0}$$

There are 2 possible values of m bcoz 2 ε-values are gi

Only possibility is $$E_1^{(2)} = \cancel{\Sigma} \frac{|\langle \phi_2 | H_p | \phi_1 \rangle|^2}{E_1 - E_2}$$

$$\langle \phi_2 | H_p | \phi_1 \rangle = (0 \;\; 1)\begin{bmatrix} 0 & A \\ A^* & 0 \end{bmatrix}\begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

$$= (0 \;\; 1)\begin{bmatrix} 0 \\ A^* \end{bmatrix} = A^*$$

$$E^2 = \frac{|A^*|^2}{E_1 - E_2} = \frac{A^2}{E_1 - E_2}$$

(iii) $$\psi^{(1)}\rangle = \frac{\langle \phi_2 | H_p | \phi_1 \rangle}{E_1 - E_2} |\phi_2\rangle$$

$$= \frac{1}{E_1 - E_2} A^* \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \frac{A^*}{E_1 - E_2}\begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

$$= \begin{bmatrix} 0 \\ \frac{A^*}{E_1 - E_2} \end{bmatrix}$$

<u>Prob</u>:- A particle of mass m & charge q which is moving in a 1-D harmonic oscillator potn of freq. ω is subjec to a constant electric field $E = E_0 \hat{x}$. Calculate the energy of the n^{th} state corrected to Ist Non-zero correction.

$F = -\nabla V = -\nabla W \Rightarrow W = -\int F \cdot d\gamma$ $\quad V \to$ Potn energy

$E = -\nabla V \Rightarrow V = +\int E \cdot d\gamma$ $\quad V \to$ Potentia

$V \propto \frac{1}{\gamma}$, $E \propto \frac{1}{\gamma^2}$

$V = +\int E_0 \hat{x} (dx\,\hat{x} + dy\,\hat{y} + dz\,\hat{z})$

$V = +\int E_0 \, dx$

$V = E_0 \hat{x}$

Potential Energy, $W = qE_0\hat{x} = \hat{H}_p$

$$E_n^{(1)} = \langle n|H_p|n\rangle$$
$$= qE_0\langle n|\hat{x}|n\rangle = 0$$

$$E_n^{(2)} = \sum_{m\neq n} \frac{|\langle m|qE_0\hat{x}|n\rangle|^2}{E_n^{(0)} - E_m^{(0)}}$$

$$= q^2E_0^2 \sum_{m\neq n} \frac{\left|\langle m|\sqrt{\frac{\hbar}{2m\omega}}(a^\dagger + a)|n\rangle\right|^2}{E_n^{(0)} - E_m^{(0)}}$$

$$= \frac{q^2E_0^2\hbar}{2m\omega} \sum_{m\neq n} \cancel{\frac{\langle m|(a^2 + a^{\dagger 2} + 2a^\dagger a + 1)|n\rangle}{E_n^0 - E_m^0}}$$

$$= \frac{q^2E_0^2\hbar}{2m\omega\,\cancel{(E_n^0 - E_m^0)}} \sum_{m\neq n} \frac{|\langle m|(a^\dagger + a)|n\rangle|^2}{E_n^{(0)} - E_m^{(0)}}$$

$$= \frac{q^2E_0^2\hbar}{2m\omega\,\cancel{(E_n^{(0)} - E_m^{(0)})}} \sum_{m\neq n} \frac{\left[\langle m|\sqrt{n+1}|n+1\rangle + \langle m|\sqrt{n}|n-1\rangle\right]^2}{(E_n^{(0)} - E_m^{(0)})}$$

$$E_n^{(2)} = \frac{q^2E_0^2\hbar}{2m\omega} \sum_{m\neq n} \frac{|\sqrt{n}\,\delta_{m,n-1} + \sqrt{n+1}\,\delta_{m,n+1}|^2}{E_n^{(0)} - E_m^{(0)}}$$

$$= \frac{q^2E_0^2\hbar}{2m\omega}\left[\frac{|\sqrt{n}|^2}{E_n^{(0)} - E_{n-1}^{(0)}} + \frac{|\sqrt{n+1}|^2}{E_n^0 - E_{n+1}^0}\right] = \frac{q^2E_0^2\hbar}{2m\omega}\left[\frac{n}{\hbar\omega} + \frac{n+1}{(-\hbar\omega)}\right]$$

$$= \frac{q^2E_0^2\hbar}{2m\omega}\left[\frac{\cancel{n} - \cancel{n} - 1}{\hbar\omega}\right]$$

$$\boxed{E_n^{(2)} = \frac{-q^2E_0^2}{2m\omega^2}}$$

Note:- $V_p = \frac{1}{2}m\omega^2x^2 \pm qE_0x$

Only for $V = qE_0x$ i.e. $V \propto x$

$$E_n^{(2)} = \frac{(\text{coff of } x)^2}{4(\text{coff of } x^2)}$$

$$\left[E_n^{(2)} = \frac{-(qE_0)^2}{4\,\frac{1}{2}m\omega^2} \right\}$$

Prob :- The wave fuen of a 1-Dim Harmonic oscillator is

$$\psi_0 = A \exp\left(-\frac{\alpha^2 x^2}{2}\right)$$

for ground state energy $E_0 = \frac{1}{2}\hbar\omega$ where $\alpha^2 = \frac{m\omega}{\hbar}$

In the presence of a purturbing pot^n $E_0 \left(\frac{\alpha x}{10}\right)^4$. The Ist order change in the ground state energy is

(a) $\frac{1}{2} E_0 \cancel{\alpha^4} 10^{-4}$ (b) $3 E_0 \cancel{\alpha^4} 10^{-4}$

(c) $\frac{3}{4} E_0 \cancel{\alpha^4} 10^{-4}$ ✓ (d) $E_0 \cancel{\alpha^4} 10^{-4}$

$$E^{(1)} = \frac{\cancel{|A|^2} \int_0^\infty e^{-\alpha^2 x^2} E_0 \left(\frac{\alpha x}{10}\right)^4 dx}{\cancel{|A|^2} \int_0^\infty e^{-\alpha^2 x^2} dx}$$

$$= \frac{\alpha^4 E_0}{(10)^4} \frac{\int_0^\infty x^4 e^{-\alpha^2 x^2} dx}{\int_0^\infty x^0 e^{-\alpha^2 x^2} dx}$$

$$\left\{ \int_0^\infty e^{-\alpha x^2} x^n dx = \frac{\Gamma\frac{n+1}{2}}{2\alpha^{\frac{n+1}{2}}} \right.$$

$$= \frac{\alpha^4 E_0}{(10)^4} \frac{\Gamma\frac{5}{2} \Big/ 2(\alpha^2)^{\frac{5}{2}}}{\Gamma\frac{1}{2} \Big/ 2(\alpha^2)^{\frac{1}{2}}}$$

$$= \frac{\cancel{\alpha^4} E_0}{(10)^4} \frac{\frac{3}{2}\cdot\frac{1}{2}\cancel{\sqrt{\tfrac{1}{2}}}}{\cancel{2}\cancel{\alpha^5}} \times \frac{\cancel{2}\cancel{\alpha}}{\cancel{\sqrt{\tfrac{1}{2}}}}$$

$$\boxed{E^{(1)} = \frac{3}{4} E_0 (10^{-4})}$$ Ans

Prob :- Consider an e^- in a box of length L with pereodic boundary condition $\psi(x) = \psi(x+L)$ ~~with energy~~

If the e^- is in the state $\psi_k(x) = \frac{1}{\sqrt{L}} e^{ikx}$ with energy $\epsilon_k = \frac{\hbar^2 k^2}{2m}$

What is the correction to its energy to IInd order of perturbation theory when it is subjected to a weak pereodic pot^n,

$V(x) = V_0 \cos gx$ where g is an integral multiple of $\frac{2\pi}{L}$.

(a) $V_0^2 \epsilon_g / \epsilon_k^2$ ✓(b) $-\frac{mV_0^2}{2\hbar^2}\left[\frac{1}{g^2+2kg}+\frac{1}{g^2-2kg}\right]$

(c) $\frac{V_0^2(\epsilon_k-\epsilon_g)}{\epsilon_g^2}$. (d) $\frac{V_0^2}{\epsilon_k+\epsilon_g}$

$$E_k^{(2)} = \sum_{m\neq k} \frac{|\langle \psi_m | V(x) | \psi_k \rangle|^2}{\epsilon_k - \epsilon_m}$$

$$\langle \psi_m | V(x) | \psi_k \rangle = \int_{-\infty}^{+\infty} \frac{1}{\sqrt{L}} e^{-imx} V_0 \cos gx \frac{1}{\sqrt{L}} e^{ikx} dx$$

$$= \frac{V_0}{L}\int_0^L e^{-imx} \cos gx \; e^{ikx} dx$$

$$= \frac{V_0}{L}\int_0^L e^{i(k-m)x}\left(\frac{e^{igx}+e^{-igx}}{2}\right) dx$$

$$= \frac{V_0}{2L}\int_0^L \left[e^{x(k-m+g)i} + e^{x(k-m-g)i}\right] dx$$

$$= \frac{V_0}{2L}\left[\frac{e^{x(k-m+g)i}}{(k-m+g)i} + \frac{e^{x(k-m-g)i}}{(k-m-g)i}\right]_0^L$$

$$= \frac{V_0}{2L}\left[\frac{e^{L(k-m+g)i}}{(k-m+g)i} + \frac{e^{L(k-m-g)i}}{(k-m-g)i} - \frac{1}{(k-m+g)i} - \frac{1}{(k-m-g)i}\right]$$

Prob:- Consider a system whose hamiltonian is given by

$$\hat{H} = E_0 \begin{pmatrix} 1+\lambda & 0 & 0 & 0 \\ 0 & 8 & 0 & 0 \\ 0 & 0 & 3 & -2\lambda \\ 0 & 0 & -2\lambda & 7 \end{pmatrix} \qquad (\lambda << 1)$$

Using Ist & IInd order perturbation theory. Find the energy corrected to IInd order & w.fuc^n corrected to Ist order.

$$\hat{H} = \underbrace{E_0 \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 8 & 0 & 0 \\ 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 7 \end{pmatrix}}_{\text{unperturbed Hamiltonian}} + \underbrace{E_0 \begin{pmatrix} \lambda & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -2\lambda \\ 0 & 0 & -2\lambda & 0 \end{pmatrix}}_{\text{perturbed Hamilt}}$$

Energy eigen values are $\Rightarrow$ E_0, $8E_0$, $3E_0$, $7E_0$

So corresponding eigen fuc^n,

$$|\phi_1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad |\phi_2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \quad |\phi_3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \quad |\phi_4\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

$$E_0^{(1)} = \langle \phi_1 | H_p | \phi_1 \rangle = \lambda E_0$$

$$(8E_0)^{(1)} = \langle \phi_2 | H_p | \phi_2 \rangle = 0$$

$$(3E_0)^{(1)} = \langle \phi_3 | H_p | \phi_3 \rangle = 0$$

$$(7E_0)^{(1)} = \langle \phi_4 | H_p | \phi_4 \rangle = 0$$

$$E_n^{(2)} = \sum_{m \neq n} \frac{|\langle \phi_m | H_p | \phi_n \rangle|^2}{E_n^{(0)} - E_m^{(0)}} = \sum_{m \neq 1} \frac{|\langle \phi_m | H_p | \phi_1 \rangle|^2}{E_1^{(0)} - E_m^{(0)}} \qquad [E_0^{\prime} = E_1^{(}$$

$$= \frac{\langle \phi_2 | H_p | \phi_1 \rangle|^2}{E_1^{(0)} - E_2^{(0)}} + \frac{|\langle \phi_3 | H_p | \phi_1 \rangle|^2}{E_1^{(0)} - E_3^{(0)}} + \frac{|\langle \phi_4 | H_p | \phi_1 \rangle|^2}{E_1^{(0)} - E_4^{(0)}}$$

$\langle \phi_2 | H_p | \phi_1 \rangle = 0$ | $\langle \phi_2 | H_p | \phi_3 \rangle = 0$

$\langle \phi_3 | H_p | \phi_1 \rangle = 0$ | $\langle \phi_2 | H_p | \phi_4 \rangle = 0$

$\langle \phi_4 | H_p | \phi_1 \rangle = 0$ | $\langle \phi_3 | H_p | \phi_4 \rangle = -2\lambda E_0$

$$E_1^{(1)} = \langle \phi_1 | H_P | \phi_1 \rangle$$

$$= [1\ 0\ 0\ 0]\begin{bmatrix} \lambda E_0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -2\lambda E_0 \\ 0 & 0 & -2\lambda E_0 & 0 \end{bmatrix}\begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

$$= [1\ 0\ 0\ 0]\begin{bmatrix} \lambda E_0 \\ 0 \\ 0 \\ 0 \end{bmatrix} = \lambda E_0$$

$$E_2^{(1)} = (8E_0)^{(1)} = \langle \phi_2 | H_P | \phi_2 \rangle$$

$$= [0\ 1\ 0\ 0]\begin{bmatrix} \lambda E_0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -2\lambda E_0 \\ 0 & 0 & -2\lambda E_0 & 0 \end{bmatrix}\begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}$$

$$= [0\ 1\ 0\ 0]\begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} = 0$$

$$E_3^{(1)} = \cancel{8}\,(3E_0)^{(1)} = \langle \phi_3 | H_P | \phi_3 \rangle = [0\ 0\ 1\ 0]\begin{bmatrix} \lambda E_0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -2\lambda E_0 \\ 0 & 0 & -2\lambda E_0 & 0 \end{bmatrix}\begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}$$

$$= [0\ 0\ 1\ 0]\begin{bmatrix} 0 \\ 0 \\ 0 \\ -2\lambda E_0 \end{bmatrix} = 0$$

$$E_4^{(1)} = (7E_0)^{(1)} = \langle \phi_4 | H_P | \phi_4 \rangle = (0\ 0\ 0\ 1)\begin{bmatrix} \lambda E_0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -2\lambda E_0 \\ 0 & 0 & -2\lambda E_0 & 0 \end{bmatrix}\begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$$

$$= [0\ 0\ 0\ 1]\begin{bmatrix} 0 \\ 0 \\ -2\lambda E_0 \\ 0 \end{bmatrix} = 0$$

$$E_n^{(2)} = \sum_{m \neq n} \frac{|\langle \phi_m | H_P | \phi_n \rangle|^2}{E_n^0 - E_m^0} = \sum_{m=2,3,4} \frac{|\langle \phi_m | H_P | \phi_1 \rangle|^2}{E_1^0 - E_m^0}$$

$$E_1^2 = \frac{|\langle \phi_2 | H_P | \phi_1 \rangle|^2}{E_1^0 - E_2^0} + \frac{|\langle \phi_3 | H_P | \phi_1 \rangle|^2}{E_1^0 - E_3^0} + \frac{|\langle \phi_4 | H_P | \phi_1 \rangle|^2}{E_1^0 - E_4^0} \quad \text{①}$$

$$\langle \phi_2 | H_P | \phi_1 \rangle = [0\ 1\ 0\ 0]\begin{bmatrix} \lambda E_0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -2\lambda E_0 \\ 0 & 0 & -2\lambda E_0 & 0 \end{bmatrix}\begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

$$= [0\ 1\ 0\ 0]\begin{bmatrix} \lambda E_0 \\ 0 \\ 0 \\ 0 \end{bmatrix} = 0$$

$$\langle \phi_3 | H_P | \phi_1 \rangle = [0\ 0\ 1\ 0]\begin{bmatrix} \lambda E_0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -2\lambda E_0 \\ 0 & 0 & -2\lambda E_0 & 0 \end{bmatrix}\begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} = 0$$

$$\langle \phi_4 | H_p | \phi_1 \rangle = [0\ 0\ 0\ 1]\begin{bmatrix} \lambda E_0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -2\lambda E_0 \\ 0 & 0 & 0 & -2\lambda E_0 \\ 0 & 0 & -2\lambda E_0 & 0 \end{bmatrix}\begin{bmatrix}1\\0\\0\\0\end{bmatrix} = 0$$

① $\Rightarrow$

$$E_1^{(2)} = 0 + 0 + 0$$

$$\boxed{E_1^{(2)} = 0}$$

$$E_2^{(2)} = \sum_{m=1,3,4} \frac{|\langle \phi_m | H_p | \phi_2 \rangle|^2}{E_2^0 - E_m^0}$$

$$= \frac{|\langle \phi_1 | H_p | \phi_2 \rangle|^2}{E_2^0 - E_1^0} + \frac{|\langle \phi_3 | H_p | \phi_2 \rangle|^2}{E_2^0 - E_3^0} + \frac{|\langle \phi_4 | H_p | \phi_2 \rangle|^2}{E_2^0 - E_4^0} = \boxed{0 = E}$$

$$E_3^{(2)} = \sum_{m=1,2,4} \frac{|\langle \phi_m | H_p | \phi_3 \rangle|^2}{E_3^0 - E_m^0} = \frac{|\langle \phi_1 | H_p | \phi_3 \rangle|^2}{E_3^0 - E_1^0} + \frac{|\langle \phi_2 | H_p | \phi_3 \rangle|^2}{E_3^0 - E_2^0} + \frac{|\langle \phi_4 | H_p | \phi_3 \rangle}{E_3^0 - E_4^0}$$

$$= 0 + 0 + \frac{|-2\lambda E_0|^2}{(3-7)E_0} = \frac{4\lambda^2 E_0^2}{-4E_0} = \boxed{-\lambda^2 E_0 = E_3^{(2)}}$$

$$E_4^{(2)} = \sum_{m=1,2,3} \frac{|\langle \phi_m | H_p | \phi_4 \rangle|^2}{E_4^0 - E_m^0} = \frac{|\langle \phi_1 | H_p | \phi_4 \rangle|^2}{E_4^0 - E_1^0} + \frac{|\langle \phi_2 | H_p | \phi_4 \rangle|^2}{E_4^0 - E_2^0} + \frac{|\langle \phi_3 | H_p | \phi_4 \rangle|}{E_4^0 - E_3^0}$$

$$= 0 + 0 + \frac{|-2\lambda E_0|^2}{(7-3)E_0} \Rightarrow \boxed{E_4^{(2)} = \lambda^2 E_0}$$

Energy corrected to IInd order.

$$E_1 = E_1^0 + E_1^1 + E_1^2 = (1+\lambda)E_0 \qquad E_2 = E_2^0 + E_2^1 + E_2^2 = 8E_0$$

$$E_3 = E_3^0 + E_3^1 + E_3^2 = (3-\lambda^2)E_0 \qquad E_4 = E_4^0 + E_4^1 + E_4^2 = (7+\lambda^2)E_0$$

$$|\psi_1^{(1)}\rangle = \sum_{m=2,3,4} \frac{\langle \phi_m | H_p | \phi_1 \rangle}{E_1^0 - E_m^0} |\phi_m\rangle = \frac{\langle \phi_2 | H_p | \phi_1 \rangle}{E_1^0 - E_2^0}\begin{bmatrix}0\\1\\0\\0\end{bmatrix} + \frac{\langle \phi_3 | H_p | \phi_1 \rangle}{E_1^0 - E_3^0}\begin{bmatrix}0\\0\\1\\0\end{bmatrix} + \frac{\langle \phi_4 | H_p | \phi_1 \rangle}{E_1^0 - E_4^0}$$

$$|\psi_1^{(1)}\rangle = 0 = \begin{bmatrix}0\\0\\0\\0\end{bmatrix} \quad \text{So } |\psi_1\rangle = |\phi_1\rangle + |\psi_1^{(1)}\rangle = \begin{bmatrix}1\\0\\0\\0\end{bmatrix}$$

$$|\psi_2^{(1)}\rangle = \sum_{m=1,3,4} \frac{\langle \phi_m | H_p | \phi_2 \rangle}{E_2^0 - E_m^0} |\phi_m\rangle = \frac{\langle \phi_1 | H_p | \phi_2 \rangle}{E_2^0 - E_1^0}\begin{bmatrix}1\\0\\0\\0\end{bmatrix} + \frac{\langle \phi_3 | H_p | \phi_2 \rangle}{E_2^0 - E_3^0}\begin{bmatrix}0\\0\\1\\0\end{bmatrix} + \frac{\langle \phi_4 | H_p | \phi_2 \rangle}{E_2^0 - E_4^0}\begin{bmatrix}0\\0\\0\\1\end{bmatrix}$$

$$= 0$$

$$|\psi_2\rangle = |\phi_2\rangle + |\psi_2^{(1)}\rangle = \begin{bmatrix}0\\1\\0\\0\end{bmatrix}$$

$$|\psi_3^{(1)}\rangle = \frac{\langle \phi_1 | H_p | \phi_3 \rangle}{E_3^0 - E_1^0}|\phi_1\rangle + \frac{\langle \phi_2 | H_p | \phi_3 \rangle}{E_3^0 - E_2^0}|\phi_2\rangle + \frac{\langle \phi_4 | H_p | \phi_3 \rangle}{E_3^0 - E_4^0}|\phi_4\rangle = 0 + 0 - \frac{2\lambda E_0}{(3-7)E_0}\begin{bmatrix}0\\0\\0\\1\end{bmatrix}$$

$$= \begin{bmatrix}0\\0\\0\\\lambda/2\end{bmatrix}$$

$$|\psi_3\rangle = |\phi_3\rangle + |\psi_3^{(1)}\rangle = \begin{bmatrix}0\\0\\1\\\lambda/2\end{bmatrix}$$

$$|\psi_4^{(1)}\rangle = \begin{bmatrix}0\\0\\-\lambda/2\\0\end{bmatrix} \quad \text{So } |\psi_4\rangle = |\phi_4\rangle + |\psi_4^{(1)}\rangle = \begin{bmatrix}0\\0\\-\lambda/2\\1\end{bmatrix}$$

Degenerate Perturbation Theory :-

Hamiltonian $\hat{H} = \hat{H}_o + \hat{H}_P$

$$H_o|\phi_n\rangle = E_n^{(0)}|\phi_n\rangle$$

If $E_n^{(0)}$ is f-fold degenerate then purturbition will be degenerate perturbation, & wave fuc^n

$$|\psi_n\rangle = \sum_{i=1}^{f} c_i|\phi_n^{(i)}\rangle \quad \Rightarrow \quad \langle\psi_n| = \sum_{j=1}^{j} c_j^*\langle\phi_n^{(1)}|$$

$$H|\psi_n\rangle = E_n|\psi_n\rangle$$

$$\Rightarrow (\hat{H}_o + \hat{H}_P)\sum_{i=1}^{f} c_i|\phi_n^{(i)}\rangle = E_n\sum_{i=1}^{f} c_i|\phi_n^{(i)}\rangle$$

$$E_n^{(0)} + \hat{H}_P\sum_{i=1}^{f} c_i|\phi_n^{(i)}\rangle = E_n\sum_{i=1}^{f} c_i|\phi_n^{(i)}\rangle$$

$$\hat{H}_P\sum_{i=1}^{f} c_i|\phi_n^{(i)}\rangle = (E_n - E^{(0)})\sum_{i=1}^{f} c_i|\phi_n^{(i)}\rangle \qquad E_n - E^{(0)} = E^{(1)}$$

$$\Rightarrow \boxed{\sum_{i=1}^{f}\sum_{j=1}^{f}\left[H_{P\,ij} - E_n^{(1)}\delta_{ij}\right]c_i = 0}$$

Secular Determinent :-

$$\begin{vmatrix} H_{P11} - E_n^{(1)} & H_{P12} & \cdots & H_{P1f} \\ H_{P21} & H_{P22} - E_n^{(1)} & \cdots & H_{P2f} \\ H_{P31} & H_{P32} & \cdots & H_{P3f} \\ \vdots & & & \\ H_{Pf1} & H_{Pf2} & \cdots & H_{Pff} - E_n^{(1)} \end{vmatrix}_{f\times f} = 0$$

$$\Rightarrow E_n^{(1)} = f \text{ values}$$

→ If all f values are same ⇒ correction term = 0

→ " " " " different ⇒ degeneracy removed

e.g. If 3 roots are diffrent then 3 fold degeneracy will be removed.

Total Energy = Sum of all the correction terms

$$E_n = E_n^{\circ} + E_n^{(1)}$$

The removal of degeneracy may be complete or partial, depanding upon the different roots of $E_n^{(1)}$ or values of $E_n^{(1)}$.

Note :- In degenerate case, only upto Ist order energy correction is calculated.

Que :- Consider a system in the unperturbed state described by the hamiltonian $H_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ the system is subjected to a Perterbation $H' = \begin{pmatrix} \delta & \delta \\ \delta & \delta \end{pmatrix}$ where $\delta << 1$. The Energy eigen values of the perturbed system using the Ist order perturbatio approximation are

(a) 1 & $1+2\delta$ (b) $(1+\delta)$ & $(1-\delta)$

(c) $(1+2\delta)$ & $(1-2\delta)$ (d) $(1+\delta)$ & $(1-2\delta)$

for unperturbed Hamiltonian,

eigen Values $= 1, 1 \Rightarrow E_1^{\circ} = 1, \ E_2^{\circ} = 1$

eigen states $= \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

Same E. value for 2 diff. states $\Rightarrow$ 2 fold degenerate

$$\begin{vmatrix} \langle \phi_1 | H_P | \phi_1 \rangle - E' & \langle \phi_1 | H_P | \phi_2 \rangle \\ \langle \phi_2 | H_P | \phi_1 \rangle & \langle \phi_2 | H_P | \phi_2 \rangle - E' \end{vmatrix} = 0$$

$$\langle \phi_1 | H_P | \phi_1 \rangle = (1, 0) \begin{pmatrix} \delta & \delta \\ \delta & \delta \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = (1, 0) \begin{pmatrix} \delta \\ \delta \end{pmatrix} = \delta$$

$$\langle \phi_2 | H_P | \phi_2 \rangle = (0, 1) \begin{pmatrix} \delta & \delta \\ \delta & \delta \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = (0, 1) \begin{pmatrix} \delta \\ \delta \end{pmatrix} = \delta$$

$$\langle \phi_1 | H_P | \phi_2 \rangle = (1 \ 0) \begin{pmatrix} \delta & \delta \\ \delta & \delta \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = (1 \ 0) \begin{pmatrix} \delta \\ \delta \end{pmatrix} = \delta$$

$$\langle \phi_2 | H_P | \phi_1 \rangle = (0 \ 1) \begin{pmatrix} \delta & \delta \\ \delta & \delta \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = (0 \ 1) \begin{pmatrix} \delta \\ \delta \end{pmatrix} = \delta$$

$$\begin{vmatrix} \delta - E' & \delta \\ \delta & \delta - E' \end{vmatrix} = 0 \Rightarrow (\delta - E')^2 - \delta^2 = 0$$

$$\cancel{\delta^2} + E'^2 - 2\delta E' - \cancel{\delta^2} = 0$$

$$E'(E' - 2\delta) = 0 \Rightarrow \boxed{E' = 0, 2\delta}$$

$$E_1 = E_1^0 + E_1' \Rightarrow E_1 = 1+0 \Rightarrow E_1 = 1$$
$$E_2 = E_2^0 + E_2' \Rightarrow E_2 = 1+2\delta \Rightarrow E_2 = 1+2\delta$$

Problem:- Calculate the energy of $n=1$ & $n=2$ level of a hydrogen atom placed in a external uniform electric field directed along the +ve z-axis by using time independent perturbation theory.

$n=1,\ l=0,\ m=0$

$$\psi_{1s} = \left(\frac{1}{\pi a_0^3}\right)^{1/2} e^{-r/a_0}$$

for $n=1$; degeneracy $= n^2 = 1^2 = 1$ i.e. Non-degenerate
first order energy correction, $g_1 = 1$

$E_n^{(1)} \neq$ first Unperturbed hamiltonian,

$$H_0 = \frac{-\hbar^2\nabla^2}{2m} - \frac{1}{4\pi\epsilon_0}\frac{e^2}{r}$$

electric field is along +z axis. So $E = E\hat{z}$
$W = qEz$

$$H_0 = \frac{-\hbar^2\nabla^2}{2m} - \frac{1}{4\pi\epsilon_0}\frac{e^2}{r} - eE_0 r\cos\theta \qquad z = r\cos\theta$$

So $E_n^{(1)'} = -eE_0 \int \psi_{1s}^* r\cos\theta\, \psi_{1s}\, r^2 dr \sin\theta\, d\theta\, d\phi$

$$= -eE_0\, 2\pi \int_0^r \int_0^\pi \left(\frac{1}{\pi a_0^3}\right) e^{-2r/a_0} r^3 \cos\theta \sin\theta\, d\theta$$

$$E_n^{(1)} = 0$$

i.e. there is no splitting because correction term is zero.
There is No first Order Stark Effect for the ground state of hydrogen atom. (Linear Stark effect bcoz single power of E)

for $n=2$;
$g_2 = 2^2 = 4$, $E_2^{(0)} = \frac{-13.6}{4}$ eV
$l = 0, 1 \Rightarrow m = 0, +1, 0, -1$

There will be 4 levels having same energy

$|2,0\,0\rangle$, $|2\,1\,0\rangle$, $|2\,1\,1\rangle$, $|2\,1\,-1\rangle$

Seccular determinent,

$$\begin{vmatrix} \langle 200|H_P|200\rangle - E_2^{(1)} & \langle 200|H_P|210\rangle & \langle 200|H_P|211\rangle & \langle 200|H_P|21\text{-}1\rangle \\ \langle 210|H_P|200\rangle & \langle 210|H_P|210\rangle - E_2^{(1)} & \langle 210|H_P|211\rangle & \langle 210|H_P|21\text{-}1\rangle \\ \langle 211|H_P|200\rangle & \langle 211|H_P|210\rangle & \langle 211|H_P|211\rangle - E_2^{(1)} & \langle 211|H_P|21\text{-}1\rangle \\ \langle 21\text{-}1|H_P|200\rangle & \langle 21\text{-}1|H_P|210\rangle & \langle 21\text{-}1|H_P|211\rangle & \langle 21\text{-}1|H_P|21\text{-}1\rangle \end{vmatrix}_4 = 0$$

All the integrals are of the form

$$-eE_0\int \psi^*_{nl'm'}\, r\cos\theta\, \psi_{nlm}\, d\tau$$

$$\Rightarrow \int_0^{2\pi} e^{-im'\phi}\, e^{im\phi}\, d\phi = 2\pi\, \delta_{mm'}$$

$$= 2\pi \quad \text{if } m = m'$$
$$= 0 \quad \text{if } m \neq m'$$

Part $(r\cos\theta)$ is odd, if total integrant is odd then integra will be zero.

If Parity of $\psi_{nl'm'}$ & ψ_{nlm} are different i.e. l & l' are different then integral $\rightarrow$ Non zero [Parity $= (-1)^l$]

$$\cancel{\int_0^{2\pi} e^{-im\phi}\, d}\ -eE_0\int \psi^*_{nl'm'}\, r\cos\theta\, \psi_{nlm}\, d\tau \neq 0 \quad \text{if } l \neq l'$$
$$= 0 \quad \text{if } l = l'$$

So

$$\begin{vmatrix} -E_2^{(1)} & \langle 200|H_P|210\rangle & 0 & 0 \\ \langle 210|H_P|200\rangle & -E_2^{(1)} & 0 & 0 \\ \cancel{\langle 211|H_P|200\rangle} & \cancel{\langle 211|H_P|210\rangle} & \cancel{-E_2^{(1)}} & \\ 0 & 0 & -E_2^{(1)} & 0 \\ 0 & 0 & 0 & -E_2^{(1)} \end{vmatrix} = 0$$

$$\psi_{200} = \psi_{2s} = \left(\frac{1}{32\pi a_0^3}\right)^{1/2} e^{-\frac{r}{2a_0}}\left(2-\frac{r}{a_0}\right)$$

$$\psi_{210} = \psi = \left(\frac{1}{32\pi a_0^3}\right)^{1/2}\left(\frac{r}{\cancel{2}a_0}\right) e^{-\frac{r}{2a_0}} \cos\theta$$

$$\langle 200|H_p|210\rangle = -\left(\frac{1}{32\pi a_0^3}\right)\int_0^{r}\int_0^{\pi}\int_0^{2\pi} e^{-\frac{r}{\cancel{2}a_0}}\left(2-\frac{r}{a_0}\right)\cos\theta \cdot \frac{r}{a_0}\, eE_0 r\cos\theta \cdot r^2 dr \sin\theta\, d\theta\, d\phi$$

$$= -\frac{2\pi\, eE_0}{32\pi a_0^3 a_0}\int_0^{\pi}\cos^2\theta\sin\theta\, d\theta\int_0^{\infty} e^{-\frac{r}{a_0}}\left(2-\frac{r}{a_0}\right) r^4\, dr$$

$$= \frac{-2\pi\, eE_0}{32\pi a_0^3 a_0}\int_0^{\pi}\cos^2\theta\sin\theta\, d\theta\left[2\int_0^{\infty} e^{-\frac{r}{a_0}} r^4\, dr - \frac{1}{a_0}\int_0^{\infty} e^{-\frac{r}{a_0}} r^5\, dr\right]$$

$$= \frac{-2\pi\, eE_0}{32\pi a_0^3 a_0}\int_0^{\pi}\left(\frac{1+\cos 2\theta}{2}\right)\sin\theta\, d\theta\left[2\cdot\frac{\Gamma 5}{\left(+\frac{1}{a_0}\right)^5} - \frac{1}{a_0}\,\frac{\Gamma 6}{\left(+\frac{1}{a_0}\right)^6}\right]$$

$$= \frac{-2\pi\, eE_0}{32\pi a_0^4}\int_0^{\pi}\frac{1}{2}\left(\sin\theta + 2\frac{(\sin 3\theta - \sin\theta)}{2}\right) d\theta\left[\frac{2\,\lfloor 4}{(1/a_0)^5} - \frac{1}{a_0}\,\frac{\lfloor 5}{(1/a_0)^6}\right]$$

$$= \frac{-2\pi\, eE_0}{32\pi a_0^4}\,\frac{1}{2}\left[-\cos\theta - \frac{(3\cos 3\theta + \cos\theta)}{2}\right]_0^{\pi}\left[48 a_0^5 - 120 a_0^5\right]$$

$$= \frac{-\cancel{2}\cancel{\pi} eE_0}{24\times\cancel{16}a_0^4}\,\frac{1}{\cancel{2}}\left[\frac{\cancel{64}}{6}\right]\left[-\cancel{72}a_0^5\right]$$

$$= -3\, eE_0 a_0$$

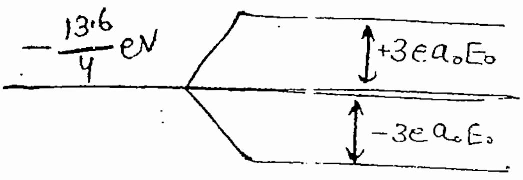
So

$$\begin{vmatrix} -E_2^{(1)} & 3eE_0a_0 & 0 & 0 \\ 3ea_0E_0 & -E_2^{(1)} & 0 & 0 \\ 0 & 0 & -E_2^{(1)} & 0 \\ 0 & 0 & 0 & -E_2^{(1)} \end{vmatrix} = 0$$

$$\Rightarrow \left(E_2^{(1)}\right)^2\left[\left(E_2^{(1)}\right)^2 - \left(3ea_0E_0\right)^2\right] = 0$$

$$E_2^{(1)} = 0, 0$$

$$E_2^{(1)} = \pm\, 3ea_0E_0$$



So out of 4 fold degeneracy, 2 fold degeneracy is removed.

$$\boxed{W = -p\cdot E}$$

In the presence of electric field H_2 atom behave like perma[nent] dipole, that can be rep^n by 3 ways

$W = -pE = -3ea_oE$ i.e. dipole mom. $\parallel$ to E-field

$W = pE = 3ea_oE$ i.e. " ". oriented opposite (antiparallel) ~~to E. field~~

$W = 0$ dipole mom. $\perp$ to E_o

So in presence of E field, H_2 atom behave as dipole having dipole mom. $3ea_oE$ which is oriented in abou[t] 3 different ways.

Total state can be rep^n as a linear superposition of 4 ~~3~~ diferent states.

$$|\psi\rangle = \alpha_1\psi_{200} + \alpha_2\psi_{210} + \alpha_3\psi_{211} + \alpha_4\psi_{21-1}$$

$$= \alpha_1|200\rangle + \alpha_2|210\rangle + \alpha_3|211\rangle + \alpha_4|21-1\rangle$$

$$= \begin{pmatrix} \alpha_1\psi_{200} \\ \alpha_2\psi_{210} \\ \alpha_3\psi_{211} \\ \alpha_4\psi_{21-1} \end{pmatrix}$$

$$|H-\lambda I|\psi = 0 \Rightarrow \begin{vmatrix} -E_2^{(1)} & 3ea_oE_o & 0 & 0 \\ 3ea_oE_o & -E_2^{(1)} & 0 & 0 \\ 0 & 0 & -E_2^{(1)} & 0 \\ 0 & 0 & 0 & -E_2^{(1)} \end{vmatrix} \begin{bmatrix} \alpha_1\psi_{200} \\ \alpha_2\psi_{210} \\ \alpha_3\psi_{211} \\ \alpha_4\psi_{21-1} \end{bmatrix} =$$

Substitute $\underline{E_2^{(1)} = +3eE_oa_o}$

$$\Rightarrow \begin{vmatrix} -3ea_oE_o & 3ea_oE_o & 0 & 0 \\ 3ea_oE_o & -3ea_oE_o & 0 & 0 \\ 0 & 0 & -3ea_oE_o & 0 \\ 0 & 0 & 0 & -3ea_oE_o \end{vmatrix} \begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \\ \alpha_4 \end{bmatrix} = 0$$

$$\Rightarrow 0\alpha_1 + 0\alpha_2 + 0\alpha_3 + (-3ea_oE_o)\alpha_4 = 0 \Rightarrow \boxed{\alpha_4 = 0}$$

$0\alpha_1 + 0\alpha_2 + (-3ea_0E_0)\alpha_3 + 0\alpha_4 = 0$

$$\Rightarrow \boxed{\alpha_3 = 0}$$

$-3ea_0E_0\,\alpha_1 + 3ea_0E_0\,\alpha_2 = 0 \quad \Rightarrow \quad \alpha_1 = \alpha_2$

$|\alpha_1|^2 + |\alpha_2|^2 = 1$ (Normalised to unity → Total W. fun^n).

$\Rightarrow 2|\alpha_1|^2 = 1$

$\Rightarrow \quad \alpha_1 = \alpha_2 = \pm \frac{1}{\sqrt{2}}$

So $\quad |\psi\rangle = \frac{1}{\sqrt{2}}|200\rangle + \frac{1}{\sqrt{2}}|210\rangle$

for $E_2^{(1)} = -3ea_0E_0$, We get

$$\alpha_1 = -\alpha_2$$

So $\quad |\psi\rangle = \frac{1}{\sqrt{2}}|200\rangle - \frac{1}{\sqrt{2}}|210\rangle$

Now for $E_2^{(1)} = 0$

$$\begin{vmatrix} 0 & 3ea_0E_0 & 0 & 0 \\ 3ea_0E_0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{vmatrix} \begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \\ \alpha_4 \end{bmatrix} = 0$$

$\Rightarrow \quad \alpha_1 = 0 \quad \& \quad \alpha_2 = 0$

But α_3 & α_4 are Non-zero.

$|\alpha_3|^2 + |\alpha_4|^2 = 1$

By assuming α_3, we can calculate α_4 & then we get 2 linearly independent solution bcoz there is 2 fold degeneracy.

So we get $|\psi\rangle = \frac{1}{\sqrt{2}}[\psi_{211} + \psi_{21\bar{1}}]$ & $\frac{1}{\sqrt{2}}[\psi_{21} - \psi_{21\bar{1}}]$

Prob :- A system with an unperturbed hamiltonian H_0,

$$H_0 = E_0 \begin{pmatrix} 15 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 \\ 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 3 \end{pmatrix}$$

is subjected to a perturbation H_P,

$$H_P = \frac{E_0}{100} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

Find the eigen energies corrected to Ist order.

$$H = H_0 + H_P$$

Energy eigen value , $\overset{E_1^{(0)}}{15E_0}$, $\overset{E_2^{(0)}}{3E_0}$, $\overset{E_3^{(0)}}{3E_0}$, $\overset{E_4^{(0)}}{3E_0}$

& Eigen states are (Normalised) i.e. $E_2^{(0)} = E_3^{(0)} = E_4^{(0)} = 3$

$$|\phi_1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad |\phi_2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \quad |\phi_3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} \quad |\phi_4\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

$E_1^{(0)}$ is Non-degenerate

$\cancel{E_1^{(1)} = \langle\phi_1|H_P|\phi_1\rangle =}$ $E_2^{(0)}$, $E_3^{(0)}$, $E_4^{(0)}$ are Degenerate.

$$E_1^{(1)} = \langle\phi_1|H_P|\phi_1\rangle = [1\ 0\ 0\ 0]\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}\begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}\frac{E_0}{100}$$

$$= \frac{E_0}{100}\begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} = 0$$

So $E_1 = E_1^0 + E_1^1 = 15E_0 + 0$ $\cancel{\Rightarrow E_1 = 0}$

$$\Rightarrow \boxed{E_1 = 15E_0}$$

Now, for 3 degenerate states,

$$\begin{vmatrix} \langle\phi_2|H_0|\phi_2\rangle - E_2^{(1)} & \langle\phi_2|H_P|\phi_3\rangle & \langle\phi_2|H_P|\phi_4\rangle \\ \langle\phi_3|H_0|\phi_2\rangle & \langle\phi_3|H_P|\phi_3\rangle - E_2^{(1)} & \langle\phi_3|H_P|\phi_4\rangle \\ \langle\phi_4|H_0|\phi_2\rangle & \langle\phi_4|H_P|\phi_3\rangle & \langle\phi_4|H_P|\phi_4\rangle - E_2^{(1)} \end{vmatrix}_{3\times3} = 0$$

$$\langle\phi_2|H_0|\phi_2\rangle = 0$$

$$\langle \phi_2 | H_P | \phi_3 \rangle = \frac{E_0}{100} \quad , \quad \langle \phi_3 | H_P | \phi_2 \rangle = \frac{E_0}{100}$$

$$\Rightarrow \begin{vmatrix} -E_2^{(1)} & \frac{E_0}{100} & 0 \\ \frac{E_0}{100} & -E_2^{(1)} & 0 \\ 0 & 0 & -E_2^{(1)} \end{vmatrix} = 0$$

$$\Rightarrow E_2^{(1)} \left[(E_2^{(1)})^2 - \left(\frac{E_0}{100}\right)^2 \right] = 0$$

$$\Rightarrow E_2^{(1)} = 0 \quad , \quad E_2^{(1)} = \pm \frac{E_0}{100}$$

$$E_2 = E_2^{(0)} + E_2^{(1)}$$

For $E_2^{(1)} = 0$ $\quad E_2 = 3E_0 + 0$

$$E_2 = 3E_0$$

$$E_2^{(1)} = +\frac{E_0}{100} \Rightarrow E_2 = 3E_0 + \frac{E_0}{100} = \frac{301}{100} E_0$$

$$E_2^{(1)} = -\frac{E_0}{100} \Rightarrow E_2 = 3E_0 - \frac{E_0}{100} = \frac{299}{100} E_0$$

So $\boxed{E_1 = 15E_0 \ \& \ E_2 = 3E_0 , \frac{301}{100}E_0 , \frac{299}{100}E_0}$ Ans

Que :- Consider the 3-D infinite potential well defined as

$$V(x,y,z) = \begin{cases} 0 & \text{if } 0<x<a \\ & \quad 0<y<a \\ & \quad 0<z<a \\ \infty & , \text{otherwise} \end{cases}$$

The unperturbed states are

$$\psi(x,y,z) = \left(\frac{2}{a}\right)^{3/2} \sin\left(\frac{n_x \pi x}{a}\right) \sin\left(\frac{n_y \pi y}{a}\right) \sin\left(\frac{n_z \pi z}{c}\right)$$

$$\& \quad E^{(0)}_{n_x n_y n_z} = \frac{\hbar^2 \pi^2}{2ma^2} \left[n_x^2 + n_y^2 + n_z^2 \right]$$

Find the energy corrected to Ist order for the ground state and Ist excited state in the perturbation

$$H_P = \begin{cases} V_0 & \text{if } 0<x<a/2 , \ 0<y<a/2 \\ 0 & \text{otherwise} \end{cases}$$

ground state;..

$\psi_{111}(x,y,z)$

$n_x = 1 = n_y = n_z$, $E_{111} = \frac{\hbar^2\pi^2}{2ma^2}(1+1+1) = \frac{3}{2}\frac{\hbar^2\pi^2}{ma^2} = E_0^{\circ}$ (ground state)

(1) $E_{111}^{(1)} = \langle \psi_{111} | H_p | \psi_{111} \rangle$

$$= \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} \psi_{111}^* \, H_p \, \psi_{111} \, dx\,dy\,dz$$

$$= \int_{-\infty}^{+\infty} \psi_1^*(x) H_{p_x} \psi_1(x)\,dx \int_{-\infty}^{+\infty} \psi_1^*(y) H_{p_y} \psi_1(y)\,dy \int_{-\infty}^{+\infty} \psi_1^*(z) \psi_1(z)$$

No perturbation on z

$$= \left(\frac{2}{a}\right)^3 \int_0^{a/2} \sin^2\frac{n_x\pi x}{a} V_0\,dx \int_0^{a/2} \sin^2\frac{n_y\pi y}{a} V_0\,dy \times \int_0^{a} \sin^2\frac{n_z\pi z}{a}$$

$$= \frac{8}{a^3} V_0 \int_0^{a/2} \sin^2\frac{\pi x}{a}\,dx \int_0^{a/2} \sin^2\frac{\pi y}{a}\,dy \int_0^{a} \sin^2\frac{\pi z}{a}\,dz$$

$$= \frac{8}{a^3} V_0 \int_0^{a/2} \frac{1}{2}\left(1-\cos\frac{2\pi x}{a}\right)dx \int_0^{a/2} \frac{1}{2}\left(1-\cos\frac{2\pi y}{a}\right)dy \int_0 \frac{1}{2}\left(1-\cos\frac{2\pi z}{a}\right)$$

$$= \frac{8}{a^3} V_0 \; \frac{1}{2}\left[x - \frac{a}{2\pi}\sin\frac{2\pi x}{a}\right]_0^{a/2} \frac{1}{2}\left[y - \frac{a}{2\pi}\sin\frac{2\pi y}{a}\right]_0^{a/2} \frac{1}{2}\left[z - \frac{a}{2\pi}\cos\frac{2\pi z}{a}\right]_0$$

$$= \frac{8}{a^3} V_0 \left(\frac{1}{2}\frac{a}{2} \times \frac{1}{2}\frac{a}{2} \times \frac{1}{2} a\right) = \frac{\cancel{8} V_0}{\cancel{a^3}} \frac{\cancel{a^3}}{\cancel{8} \times 4}$$

$$= \frac{V_0}{4}$$

$$E_0 = E_0^{(0)} + E_0^{1} = \frac{3}{2}\frac{\hbar^2\pi^2}{ma^2} + \frac{V_0}{4}$$

(2) $\psi_{112} = |\phi_1\rangle$, $\psi_{121} = |\phi_2\rangle$, $\psi_{211} = |\phi_3\rangle$

$$\begin{vmatrix} \langle\phi_1|H_p|\phi_1\rangle - E_2^{(1)} & \langle\phi_1|H_2|\phi_2\rangle & \langle\phi_1|H_2|\phi_3\rangle \\ \langle\phi_2|H_p|\phi_1\rangle & \langle\phi_2|H_p|\phi_2\rangle - E_2^{(1)} & \langle\phi_2|H_2|\phi_3\rangle \\ \langle\phi_3|H_p|\phi_1\rangle & \langle\phi_3|H_p|\phi_2\rangle & \langle\phi_3|H_p|\phi_3\rangle - E_2^{(1)} \end{vmatrix} = 0$$

$$\langle\phi_1|H_p|\phi\rangle = \left(\frac{2}{a}\right)^3 V_0 \int \sin^2\left(\frac{\pi x}{a}\right)\sin^2\left(\frac{\pi y}{a}\right)\sin^2\left(\frac{2\pi z}{a}\right)dx\,dy\,dz$$

$$= \left(\frac{2}{a}\right)^3 V_0 \int_0^{a/2} \sin^2\frac{\pi x}{a}\,dx \int_0^{a/2} \sin^2\frac{\pi y}{a}\,dy \int_0^{a} \sin^2\frac{2\pi z}{a}\,dz$$

$$= \frac{8V_0}{a^3}\cdot\frac{a}{4}\cdot\frac{a}{4}\cdot\frac{a}{2} = \frac{V_0}{4}$$

$$\langle\phi_2|H_p|\phi_2\rangle = \frac{V_0}{4} = \langle\phi_3|H_p|\phi_3\rangle$$

$$\langle\phi_1|H_p|\phi_2\rangle = \left(\frac{2}{a}\right)^3 V_0 \int_0^{a/2}\int_0^{a/2}\int_0^{a} \sin\frac{\pi x}{a}\,\sin\frac{\pi y}{a}\,\sin\frac{2\pi z}{a}\,\sin\frac{\pi x}{a}\,\sin\frac{2\pi y}{a}\,\sin\frac{\pi z}{a}\,dx\,dy\,dz$$

$$= \frac{8}{a^3}V_0\int_0^{a/2}\sin^2\frac{\pi x}{a}\,dx\int_0^{a/2}\sin\frac{\pi y}{a}\sin\frac{2\pi y}{a}\,dy\int_0^{a}\sin\frac{2\pi z}{a}\sin\frac{\pi z}{a}\,dz$$

$$= \frac{8}{a^3}V_0\,(0) = 0$$

$$\langle\phi_2|H_p|\phi_3\rangle = \left(\frac{2}{a}\right)^3 V_0\int_0^{a/2}\sin\frac{\pi x}{a}\sin\frac{2\pi x}{a}\,dx\int_0^{a/2}\sin\frac{2\pi y}{a}\sin\frac{2\pi y}{a}\,dy\int_0^{a}\sin^2\frac{\pi z}{a}\,dz$$

$$= \frac{16}{9\pi^2}V_0$$

$$\Rightarrow \begin{vmatrix} \frac{V_0}{4}-E_2^{(1)} & 0 & 0 \\ 0 & \frac{V_0}{4}-E_2^{(1)} & \frac{16V_0}{9\pi^2} \\ 0 & \frac{16V_0}{9\pi^2} & \frac{V_0}{4}-E_2^{(1)} \end{vmatrix} = 0$$

$$\Rightarrow \left(\frac{V_0}{4}-E_2^{(1)}\right)\left[\left(\frac{V_0}{4}-E_2^{(1)}\right)^2-\left(\frac{16V_0}{9\pi^2}\right)^2\right] = 0$$

$$\Rightarrow E_2^{(1)} = \frac{V_0}{4},\quad \frac{V_0}{4}+\frac{16V_0}{9\pi^2},\quad \frac{V_0}{4}-\frac{16V_0}{9\pi^2}$$

$$E_2 = E_2^0 + E_2^1 \qquad \text{(Ist Excited state)}$$

$$\cancel{= \frac{2\hbar^2\pi^2}{ma^2} + \frac{V_0}{4}}$$

$$= \frac{6\hbar^2\pi^2}{2ma^2} + \frac{V_0}{4}$$

$$= \frac{6\hbar^2\pi^2}{2ma^2} + \frac{V_0}{4} + \frac{16V_0}{9\pi^2}$$

$$= \frac{6\hbar^2\pi^2}{2ma^2} + \frac{V_0}{4} - \frac{16V_0}{9\pi^2}$$

VARIATIONAL METHOD

Variational method is the approximation method to calcul the energy of ground state of the system if Hamiltonian is known but Eigen fuc^n and eigen energies for the unpertu hamiltonian are unknown.

Need of Variational method :-

~~By perturbation theory, higher order terms are difficult~~ to calculate & lower order terms are not sufficient so we need this method.

$$\langle E \rangle = \langle H \rangle = \frac{\langle \psi_0 | H | \psi_0 \rangle}{\langle \psi_0 | \psi_0 \rangle}$$

This integral is known as Variational Integral.

If we choose a wave fuc^n, $\psi = e^{-r^2}$
then, the properties which are unknown, include in Variational parameter (α).

i.e. $\boxed{\psi = e^{-\alpha r^2}}$

To calculate α,

$$\frac{\partial \langle E \rangle}{\partial \alpha} = 0 \quad \Rightarrow \alpha = ?$$

for Symmetric pot^n, consider W.fuc^n of the form $f(x) = \pm f$

Again put the value of α in $\langle E \rangle$ to calculate the expectation value of energy.

In Q.M., K.E. term is always Non zero.

$$\boxed{H = \underset{\neq 0}{T} + V}$$

→ If P.E. $=0$ then $(V=0)$ calculate only $\langle K.E. \rangle$
If $V=0$, $\langle H \rangle = \langle K.E. \rangle$

→ If $V \neq 0$ then $\alpha \neq 0$ $(E \geq E_0)$

This Variational method gives the upper bound values of energy.

→ Energy calculated by Variation method ~~may~~ will be equal or larger than the exact energy. $E \geq E_0$

→ ~~If~~ $\langle E \rangle = E_0$

$$|\psi\rangle = \sum_n C_n |\phi_n\rangle$$

$$\langle H \rangle = \langle E \rangle = \langle \psi | H | \psi \rangle$$

$$= \sum_n E_n |C_n|^2$$

$$\langle E \rangle - E_0 = \sum_n E_n |C_n|^2 - E_0$$

$$\Rightarrow \boxed{\langle E \rangle \geq E_0} \qquad E_0 \rightarrow \text{Exact Energy}$$

- for symmetric pot^n, wave fun^n must be symmetric or antisymmetric i.e. w. fun^n must have definate parity.

Que :- Calculate the ground state energy of 1-dim Harmonic oscillator

$$H = \frac{p^2}{2m} + \frac{1}{2} k x^2$$

Assume a wave func^n,

Pot^n is symmetric. So $\psi = A e^{-\alpha |x|}$

or $\psi = A e^{-\alpha x^2}$

Take $\psi = A e^{-\alpha |x|^2}$

$$\langle H \rangle = \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle}$$

$$= \frac{|A|^2 \int_{-\infty}^{+\infty} e^{-\alpha x^2} \left(\frac{p^2}{2m} + \frac{1}{2} k x^2 \right) e^{-\alpha x^2} dx}{|A|^2 \int_{-\infty}^{+\infty} e^{-2\alpha x^2} dx}$$

$$= \frac{\frac{1}{2m} \int_{-\infty}^{+\infty} e^{-\alpha x^2} \left(-\hbar^2 \frac{\partial^2}{\partial x^2} \right) e^{-\alpha x^2} dx + \int_{-\infty}^{\infty} e^{-\alpha x^2} \frac{1}{2} k x^2 e^{-\alpha x^2} dx}{\int_{-\infty}^{\infty} e^{-2\alpha x^2} dx}$$

$$\cancel{\Rightarrow -\frac{\hbar^2}{2m}\int_{-\infty}^{\infty} e^{-\alpha x} e^{-\alpha x^2}\alpha^2\, dx + \frac{K}{2}\int_{-\infty}^{\infty} x^2}$$

$$= \frac{-\frac{\hbar^2}{2m}\int_{-\infty}^{\infty} e^{-2\alpha x^2}(-2\alpha x)^2\, dx + \frac{K}{2}\int_{-\infty}^{\infty} x^2 e^{-2\alpha x^2}\, dx}{\int_{-\infty}^{\infty} e^{-2\alpha x^2}\, dx}$$

$$= \frac{+\frac{-\hbar^2}{2m}(2\alpha)^2\int_{-\infty}^{\infty} e^{-2\alpha x^2} x^2\, dx + \frac{K}{2}\int_{-\infty}^{\infty} x^2 e^{-2\alpha x}}{\int_{-\infty}^{\infty} e^{-2\alpha x^2}\, dx}$$

$$= -\frac{2\alpha^2\hbar^2}{m}\left[x^2\,\frac{e^{-2\alpha x^2}}{-2\times 2\alpha x} + \int \cancel{2x}\cdot\frac{e^{-2\alpha x^2}}{-2\cdot\cancel{2\alpha x}}\, dx\right]$$

$$\frac{\partial \langle E \rangle}{\partial \alpha} = 0$$

$$\Rightarrow \quad \frac{\hbar^2}{2m} - \frac{m\omega^2}{8\alpha^2} = 0 \quad \Rightarrow \quad \frac{m\omega^2}{8\alpha^2} = \frac{\hbar^2}{2m}$$

$$\Rightarrow \quad \alpha = \frac{m\omega}{2\hbar}$$

Now substitute α in $\langle E \rangle$,

$$\langle E \rangle = \frac{\hbar^2}{2m}\alpha + \frac{m\omega^2}{8\alpha}$$

$$= \frac{\hbar^2}{2m}\,\frac{m\omega}{2\hbar} + \frac{m\omega^2\, 2\hbar}{8\, m\omega} = \frac{\omega\hbar}{4} + \frac{\omega\hbar}{4}$$

$$\boxed{\langle E \rangle = \frac{\hbar\omega}{2}}$$

so $\quad \psi = A e^{-\frac{m\omega}{2\hbar}x^2}$

(i) अगर variation न दिया हो तो केवल expectation value निकालो हो तो Ans.

Qu:— A variation calculation is done with the normalised trail wave fuc^n $\psi(x) = \frac{\sqrt{15}}{4a^{5/2}}(a^2 - x^2)$ for the 1-dim potential well.
$$V(x) = \begin{cases} 0 & \text{if } |x| \le a \\ \infty & \text{if } |x| > a \end{cases}$$
The ground state ~~property~~ Energy is estimated to be

(a) $\frac{5}{3}\frac{\hbar^2}{ma^2}$ (b) $\frac{3}{2}\frac{\hbar^2}{ma^2}$ (c) $\frac{3}{5}\frac{\hbar^2}{ma^2}$ (d) $\frac{5}{4}\frac{\hbar^2}{ma^2}$ ✓

$$\langle E \rangle = \int_{-\infty}^{+\infty} \psi^* H \psi \, dx$$

$$= \int_{-a}^{a} \psi^* \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right)\psi \, dx \qquad \left\{ V = 0 \text{ for } -a < x < +a \right.$$

$$\langle E \rangle = \int_{-a}^{a} \frac{\sqrt{15}}{4a^{5/2}}(a^2 - x^2)\left(\frac{-\hbar^2}{2m}\right)\frac{d^2}{dx^2}\,\frac{\sqrt{15}}{4a^{5/2}}(a^2 - x^2)\, dx$$

$$= \frac{15}{(4)^2 a^5}\left(\frac{-\hbar^2}{2m}\right)\int_{-a}^{a}(a^2 - x^2)\,(-2)\, dx$$

$$= \frac{15\hbar^2}{16\, a^5 m}\int_{-a}^{a}(a^2 - x^2)\, dx$$

$$= \frac{15\hbar^2}{16a^5 m}\left[a^2x - \frac{x^3}{3}\right]_{-a}^{+a}$$

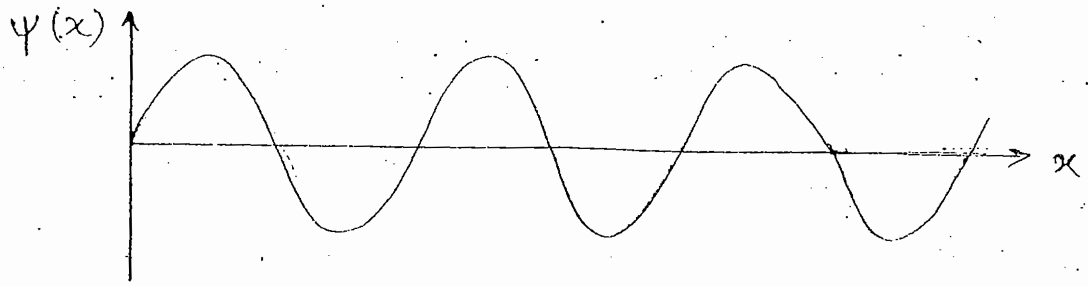
$$= \frac{15\hbar^2}{16a^5 m}\left[\cancel{a^3} - \frac{a^3}{3} + \cancel{a^3} - \frac{a^3}{3}\right] = \frac{\overset{5}{\cancel{15}}\hbar^2}{\underset{8}{\cancel{16}}a^5 m}\left(+\frac{\cancel{4}a^3}{\cancel{3}}\right)$$

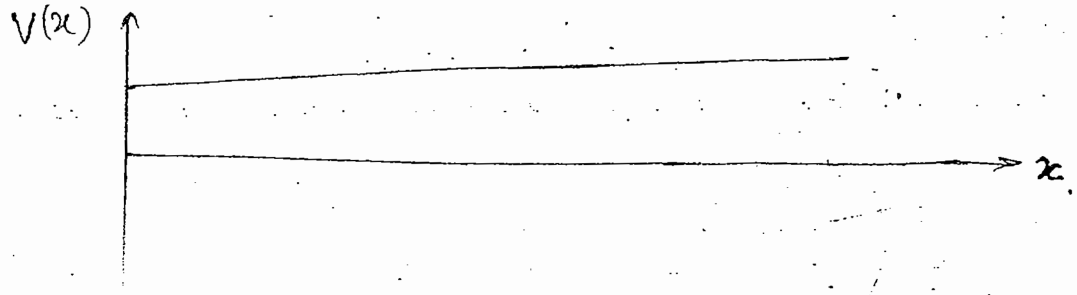
$$= \frac{5\hbar^2}{48a^2 m}$$

W.K.B Method :-

This W.K.B approximation is valid only for a ~~slightbely vari~~ potentials (The variation is very small).

If variation is almost constant over a region of several de-broglei wavelength.





This W.K.B. approximation is also known as semi-classical approximation.

for classical system, de-broglei W.L. $\Rightarrow 0$ (neglesible)

Any pat^n in this region ($\lambda \to 0$) can be located as slightely varing pat^n.

This is cal $H\psi = E\psi$

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]\psi = E\psi(x)$$

$$\frac{d^2}{dx^2}\psi(x) + \frac{2m}{\hbar^2}\left[E - V(x)\right]\psi(x) = 0$$

$$k = \sqrt{\frac{2m}{\hbar^2}(E-V)} \quad , E>V$$

$$= \sqrt{\frac{2m}{\hbar^2}(V-E)} \qquad E<V$$

& solutions are $\psi = Ae^{ikx} + Be^{-ikx}$

$$= Ce^{kx} + De^{-kx}$$

for constant Pot^n

But when pot^n is not constant i.e. varing then

$$p_x(x) = \sqrt{2m\,[E - V(x)]}$$

& solution,

$$\psi = \frac{A}{\sqrt{p(x)}} e^{\frac{i}{\hbar}\int p(x)dx} + \frac{B}{\sqrt{p(x)}} e^{-\frac{i}{\hbar}\int p(x)dx}$$

$$= \frac{C}{\sqrt{p(x)}} e^{\frac{1}{\hbar}\int p(x)dx} + \frac{D}{\sqrt{p(x)}} e^{-\frac{1}{\hbar}\int p(x)dx}$$

Probability density will be of the form

$$|\psi|^2 \propto \frac{1}{p(x)}$$

If mom. is large then $|\psi|^2$ will be small.

$$\psi = \frac{1}{\sqrt{p(x)}}\left[Ae^{i\alpha} + Be^{-i\alpha}\right]$$

$$= \frac{1}{\sqrt{p(x)}}\left[A(\cos\alpha + i\sin\alpha) + B(\cos\alpha - i\sin\alpha)\right]$$

$$= \frac{1}{\sqrt{p(x)}}\left[(A+B)\cos\alpha + i(A-B)\sin\alpha\right]$$

$$= \frac{1}{\sqrt{p(x)}}\left[C_1\cos\alpha + C_2\sin\alpha\right]$$

Let $C_1 = A\sin\beta$

$C_2 = A\cos\beta$

then $\psi = \frac{1}{\sqrt{p(x)}}\left[A\sin\beta\cos\alpha + A\cos\beta\sin\alpha\right]$

$$\psi = \frac{A}{\sqrt{p(x)}}\left[\sin(\alpha+\beta)\right]$$

$$\boxed{\psi(x) = \frac{A}{\sqrt{p(x)}}\sin\left\{\frac{1}{\hbar}\int p(x)dx + \beta\right\}}$$

This is the form of wave func^n for classically allow region $(E>V)$

β can take 2 values. $\boxed{\beta \rightarrow \text{phase factor}}$

$\beta = 0$, if turning points lies on the rigid walls $(V=\infty)$

$= \frac{\pi}{4}$ if turning points lies in non-rigid wall $(V \neq \infty)$

At turning pt., $P.E. = K.E.$ i.e. mom. $p = 0$.

$$K.E. = 0$$

$$\boxed{E_{total} = V}$$

Boundary cond^n,

$$\psi_1 = \psi_2$$

$$\sin\theta_1 = \sin\theta_2 \qquad \theta = \frac{1}{\hbar}\int p(x)dx + \beta$$

$$\Rightarrow \boxed{\theta_1 + \theta_2 = n\pi} \longrightarrow \text{Quantization Condition}$$

$$n = 1, 2, 3, \ldots$$

or

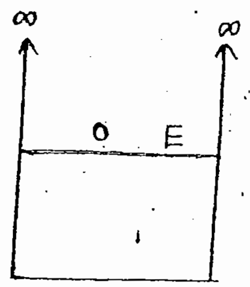
$$\boxed{\theta_1 + \theta_2 = (n+1)\pi} \quad , \quad n = 0, 1, 2, \ldots$$

<u>Condition of Validity for W.K.B. Approximation</u> :-

$$\left|\frac{d}{dx}\left(\frac{\hbar}{p}\right)\right| << 1$$

$$\left|\frac{d\lambda}{dx}\right| << 1$$

<u>Prob</u> :- Use the W.K.B. Approximation to calculate the energy of a spinless particle of mass m moving in the 1-dim box, with walls at $x=0$ & $x=L$.



$$\psi(x) = \frac{A}{\sqrt{p(x)}} \sin\left[\frac{1}{\hbar}\int p(x)dx + \beta\right]$$

There are 2 turning points,

$$\underbrace{\frac{1}{\hbar}\int_0^x p(x)dx + 0}_{\text{from 1 turning pt. to an}} + \underbrace{\frac{1}{\hbar}\int_x^L p(x)dx + 0}_{\text{from } x \text{ to another}} = n\pi \text{ or } (n+1)\pi \quad , \quad n = 1, 2, 3 \ldots \quad n = 0, 1, 2 \ldots$$

$$\Rightarrow \frac{1}{\hbar}\int_0^L p(x)\,dx = n\pi \text{ or } (n+1)\pi$$

$$\Rightarrow \int_0^L p(x)\,dx = n\pi\hbar \text{ or } (n+1)\pi\hbar$$

$p = \sqrt{2m(E-V)}$ $(V=0)$

$$\Rightarrow \sqrt{2mE}\,L = n\pi\hbar \text{ or } (n+1)\pi\hbar$$

$$\Rightarrow 2mE\,L^2 = n^2\pi^2\hbar^2 \text{ or } (n+1)^2\pi^2\hbar^2$$

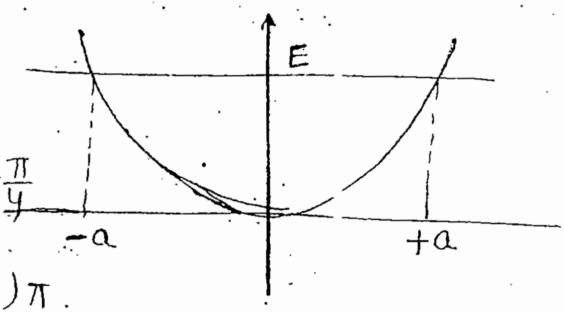
$$\Rightarrow \boxed{\begin{aligned} E &= \frac{n^2\pi^2\hbar^2}{2mL^2} \\ E &= \frac{(n+1)^2\pi^2\hbar^2}{2mL^2} \end{aligned}}$$

$\cancel{n = 1, 2, 3}$ …

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

<u>Que</u>:- Calculate the energy of the nth level for a particle of mass m moving in the potⁿ $V = \frac{1}{2}kx$

There are 2 turning points at $x = -a$ & $x = +a$.



$$\frac{1}{\hbar}\int_{x_1}^{x_B} p(x)\,dx + \frac{\pi}{4} + \frac{1}{\hbar}\int_{x_B}^{x_2} p(x)\,dx + \frac{\pi}{4} = n\pi \text{ or } (n+1)\pi$$

$$\frac{1}{\hbar}\int_{x_1}^{x_B} p(x)\,dx + \frac{1}{\hbar}\int_{x_B}^{x_2} p(x)\,dx + \frac{\pi}{2} = n\pi \text{ or } (n+1)\pi$$

$$\frac{1}{\hbar}\int_{x_1}^{x_2} p(x)\,dx = \left(n-\frac{1}{2}\right)\pi \text{ or } \left(n+\frac{1}{2}\right)\pi$$

$n\pi - \pi/2$

$(n+1)\pi - \frac{\pi}{2}$

$$\int_{x_1}^{x_2} p(x)\,dx = \left(n-\frac{1}{2}\right)\pi\hbar \text{ or } \left(n+\frac{1}{2}\right)\pi\hbar$$

$$\Rightarrow \int_{-a}^{+a} \sqrt{2m\left[E-\frac{1}{2}kx^2\right]}\,dx = \left(n-\frac{1}{2}\right)\pi\hbar \text{ or } \left(n+\frac{1}{2}\right)\pi\hbar$$

At turning point, $E = V = \frac{1}{2}ka^2$

$$\int_{-a}^{+a} \sqrt{2m\left(\frac{1}{2}ka^2 - \frac{1}{2}kx^2\right)}\,dx =$$

$$\int_{-a}^{+a}\sqrt{mK(a^2-x^2)}\,dx = 2\int_0^a \sqrt{mK(a^2-x^2)}\,dx$$

Put $x = a\cos\theta \Rightarrow dx = -a\sin\theta\,d\theta$

$$2\int_0^\pi \sqrt{mK}\;a\,(\sin\theta)\,(-a\sin\theta)\,d\theta$$

$$2\int_0^\pi \sqrt{mK}\;a^2\left[\frac{1-\cos 2\theta}{2}\right]d\theta \qquad \left\{\begin{array}{l} E = \frac{1}{2}Ka^2 \\ a^2 = 2E/K \end{array}\right.$$

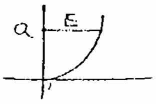
$$\frac{\cancel{2}}{\cancel{2}}\sqrt{mK}\,a^2\left[\theta - \frac{\sin 2\theta}{2}\right]_0^\pi$$

$$\sqrt{mK}\cdot\frac{2E}{K}\cdot\pi \Rightarrow \sqrt{\frac{\cancel{m}}{\cancel{m}\omega^2}}\cdot 2E\cdot\cancel{\pi} = \left(n-\frac{1}{2}\right)\cancel{\pi\hbar}\ \text{or}\ \left(n+\frac{1}{2}\right)$$

$$\Rightarrow \frac{2E}{\omega} = \left(n-\frac{1}{2}\right)\hbar \ \text{or}\ \left(n+\frac{1}{2}\right)\hbar$$

$$E = \frac{\omega}{2}\left(n-\frac{1}{2}\right)\hbar \ \text{or}\ \frac{\omega}{2}\left(n+\frac{1}{2}\right)\hbar$$

Que:- What is the Quantisation condition for a particle of mass m moving in potⁿ $V(x) = \begin{cases} \frac{1}{2}m\omega^2x^2, & x>0 \\ \infty, & x<0 \end{cases}$



2 turning pt.

$$\frac{1}{\hbar}\int_0^{x_1} p(x)\,dx + \beta_1(0) + \frac{1}{\hbar}\int_{x_1}^{x_2} p(x)\,dx + \frac{\pi}{4} = n\pi \ \text{or}\ (n-1)\pi$$

$$\int_0^a p(x)\,dx = \left(n-\frac{1}{4}\right)\pi\hbar \ \text{or}\ \left(n+\frac{3}{4}\right)\pi\hbar$$

$$\int_0^a \sqrt{2m(E-V)}\,dx = \left(n-\frac{1}{4}\right)\hbar\pi \ \text{or}\ \left(n+\frac{3}{4}\right)\pi\hbar$$

$$\int_0^a \sqrt{2m\,\tfrac{1}{2}K(a^2-x^2)}\,dx$$

Put $n = a\sin\theta$ — at $a \Rightarrow E = P.E. = \frac{1}{2}m\omega^2 a^2$

$$\int_0^{\pi/2}\sqrt{mK}\;a\cos\theta\;a\cos\theta\,d\theta \qquad a^2 = \frac{2E}{K}$$

$$\int_0^{\pi/2}\sqrt{mK}\;a^2\left(\frac{1+\cos 2\theta}{2}\right)d\theta$$

$$\sqrt{mK}\;\frac{2E}{K}\left[\theta + \frac{\sin 2\theta}{2}\right]_0^{\pi/2}$$

$$\sqrt{\frac{m}{K}}\;E\cdot\pi/2$$

$$\sqrt{\frac{m}{m\omega^2}}\;E\;\pi/2 = \left(n-\frac{1}{4}\right)\hbar\pi \ \text{or}\ \left(n+\frac{3}{4}\right)\pi\hbar$$

$$\boxed{\frac{E}{2\omega} = \left(n-\frac{1}{4}\right)\hbar \ \text{or}\ \left(n+\frac{3}{4}\right)\hbar}$$

Que :- Consider a particle of mass m that is bouncing vertically & elastically on a reflecting hard floor where

$$V(z) = \begin{cases} mgz & , z > 0 \\ +\infty & , z \le 0 \end{cases}$$

$g \rightarrow$ accⁿ due to gravity

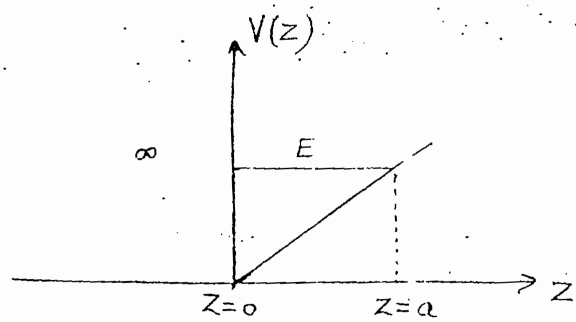
Use WKB method to estimate the ground state energy of the particle

$\theta_1 + \theta_2 = n\pi$ or $(n+1)\pi$

$$\frac{1}{\hbar}\int_{x_1}^{x_0} p(x)\,dx + \beta_1 + \frac{1}{\hbar}\int_{x}^{x_2} p(x)\,dx + \beta_2 = n\pi \text{ or } (n+1)\pi.$$

At ∞ potⁿ, $\beta = 0$

finite " , $\beta = \frac{\pi}{4}$



So,

$$\frac{1}{\hbar}\int_0^z p(z)\,dz + 0 + \int_z^a p(z)\,dz + \frac{\pi}{4} = n\pi \text{ or } (n+1)\pi$$

$$\int_0^a p(z)\,dz = \left(n - \frac{1}{4}\right)\pi\hbar \text{ or } \left(n + \frac{3}{4}\right)\pi\hbar$$

$$\int_0^a \sqrt{2m(E - mgz)}\,dz = \left(n - \frac{1}{4}\right)\pi\hbar \text{ or } \left(n + \frac{3}{4}\right)\pi\hbar$$

$$\Rightarrow \left\{ \sqrt{2mE}\int_0^a \sqrt{1 - \frac{mgz}{E}}\,dz = \text{"} \right\}$$

OR put $E = mga$ (at turning pt. T.E. = P.E.)

$$\text{So } \int_0^a \sqrt{2m(mga - mgz)}\,dz = \left(n - \frac{1}{4}\right)\pi\hbar \text{ or } \left(n + \frac{3}{4}\right)\pi\hbar$$

$$\Rightarrow \sqrt{2m(mg)} \int_0^a \sqrt{a-z}\, dz = \quad \text{Put } z = a\sin^2\theta$$
$$dz = 2a\sin\theta\cos\theta = a\sin 2\theta\, d\theta$$

$$= \sqrt{2m\,mg} \int_0^{\pi/2} \sqrt{a}\, a \cos\theta \sin 2\theta\, d\theta$$
$$= \sqrt{2m\,mg}\,\sqrt{a}\; a\, \frac{1}{2}\int_0^{\pi/2} (\cos\theta + \cos 3\theta)\, d\theta$$
$$= \sqrt{2mE}\; \frac{2E}{mg}\left[\sin\theta + \frac{\sin 3\theta}{3}\right]_0^{\pi/2} = \sqrt{2mE}\;\frac{2E}{mg}\left[1 + \tfrac{1}{3} + 0 + 0\right]$$
$$= \sqrt{2mE}\;\frac{2E}{2mg}\left(\frac{4}{3}\right) = \sqrt{2mE}\;\frac{2E}{3mg}$$

$$\Rightarrow \sqrt{2mE} \times \frac{2E}{3mg} = \left(n - \frac{1}{4}\right)\pi\hbar \quad \text{or} \quad \left(n + \frac{3}{4}\right)\pi\hbar$$

$$\Rightarrow E = \left[\frac{9\pi^2}{8} mg^2\hbar^2 \left(n - \frac{1}{4}\right)^2\right]^{1/3}$$

or

$$\left[\frac{9\pi^2}{8} mg^2\hbar^2 \left(n + \frac{3}{4}\right)^2\right]^{1/3}$$

Q. A particle in 1 dim moves under the influence of a pot^n $V(x) = ax^6$ where a is a real constant. For large n, the quantised energy levels E_n depends on n as

(a) $E_n \sim n^3$ (b) $E_n \sim n^{4/3}$ (c) $E_n \sim n^{6/5}$ (d) $E_n \sim n^{3/2}$ ✓

$V(x) = ax^6$ even (symmetric) pot^n

Both turning pt's will be on finite boundary

$$\frac{1}{\hbar}\int_{-a}^{x} \sqrt{2m(E - ax^6)}\, dx + \frac{\pi}{4} + \frac{1}{\hbar}\int_{x}^{+a} \sqrt{2m(E - ax^6)}\, dx + \frac{\pi}{4} = n\pi \text{ or } (n+1)\pi$$

$$\Rightarrow \int_{-a}^{a} \sqrt{2m(E - ax^6)}\, dx = \left(n - \frac{1}{2}\right)\pi\hbar$$
$$\text{or } \left(n + \frac{1}{2}\right)\pi\hbar$$

$$\Rightarrow \sqrt{2mE}\int_{-a}^{a} \sqrt{\left(1 - \frac{ax^6}{E}\right)}\, dx = \text{''}$$

Suppose $\frac{ax^6}{E} = t \Rightarrow x = \left(\frac{Et}{a}\right)^{1/6}$

$dx = \ldots$

$$\Rightarrow \underset{\downarrow\; E^{1/2}}{\sqrt{2mE}} \int_{-a}^{a} \sqrt{\left(1-\frac{ax^6}{E}\right)}\, \underset{\downarrow\; E^{1/6}}{dx}$$

$$dx = \underbrace{\left(\frac{E}{a}\right)^{1/6} \frac{1}{6}}_{\text{const.}} t^{\frac{1}{6}-1}\, dt$$

$$E^{1/2} E^{-1/6} \propto (n-\tfrac{1}{2}) \text{ or } (n+\tfrac{1}{2})$$

$$E^{2/3} \propto n \quad \text{(for large } n\text{, neglect } \tfrac{1}{2} \text{ factor)}$$

$$\boxed{E_n \propto n^{3/2}}$$

Q:- Use the WKB approximation to find the allowed energies of a particle of mass m moving in the pot^n $V(x) = \alpha|x|^{\nu}$ where $\nu = +$ve no.

$$V(x) = \alpha|x|^{\nu}$$

Suppose turning pt $\rightarrow x = +a$ or $-a$

$$\frac{1}{\hbar}\int_{-a}^{x} p(x)\,dx + \beta_1 + \frac{1}{\hbar}\int_{x}^{a} p(x)\,dx + \beta_2 = n\pi \text{ or } (n+1)\pi$$

$$\frac{1}{\hbar}\int_{-a}^{x} \sqrt{2m(E-\alpha|x|^{\nu})}\,dx + \frac{\pi}{4} + \frac{1}{\hbar}\int_{x}^{+a} \sqrt{2m(E-\alpha|x|^{\nu})}\,dx + \frac{\pi}{4} = n\pi \text{ or } (n+1)\pi$$

$$\Rightarrow \int_{-a}^{+a} \sqrt{2m[E-\alpha|x|^{\nu}]}\,dx = (n-\tfrac{1}{2})\pi\hbar \text{ or } (n+\tfrac{1}{2})\pi\hbar$$

$$\Rightarrow 2\sqrt{2mE}\int_{0}^{a} \sqrt{\left(1-\frac{\alpha (x)^{\nu}}{E}\right)}\,dx =$$

suppose $\dfrac{\alpha x^{\nu}}{E} = t$

$$\Rightarrow x = \left(\frac{Et}{\alpha}\right)^{1/\nu} \Rightarrow dx = \left(\frac{E}{\alpha}\right)^{1/\nu} \frac{1}{\nu} t^{\frac{1}{\nu}-1}\,dt$$

- If turning pt's are at finite boundry then $(n-\frac{1}{2})^{3/2}$ or $(n+\frac{1}{2})^{3/2}$ then factor with n will be same but if turning pt's are at diff boundry i.e. one is at finite & other is at ∞ boundry then this factor will be diff. i.e. $(n-\frac{1}{4})^{3/2}$ or $(n+\frac{3}{4})^{3/2}$ but power of n will be same.

$\Rightarrow$ dependancy,

(just cheak the depandency)

$$E^{1/2}\, E^{1/\nu} \propto (n-\tfrac{1}{2}) \text{ or } (n+\tfrac{1}{2})$$

$$E^{\frac{\nu+2}{2\nu}} \propto (n-\tfrac{1}{2}) \text{ or } (n+\tfrac{1}{2})$$

$$\boxed{E \propto (n-\tfrac{1}{2})^{\frac{2\nu}{\nu+2}} \text{ or } (n+\tfrac{1}{2})^{\frac{2\nu}{\nu+2}}}$$

Ans

Exact solⁿ :-

$$E_n = \alpha\left[(n-\tfrac{1}{2})\hbar\sqrt{\frac{\pi}{2m\alpha}}\;\frac{\Gamma(\frac{1}{\nu}+\frac{3}{2})}{\Gamma(\frac{1}{\nu}+1)}\right]^{\frac{2\nu}{\nu+2}}$$

$$= \alpha\left[(n+\tfrac{1}{2})\hbar\sqrt{\frac{\pi}{2m\alpha}}\;\frac{\Gamma(\frac{1}{\nu}+\frac{3}{2})}{\Gamma(\frac{1}{\nu}+1)}\right]^{\frac{2\nu}{\nu+2}}$$

Full harmonic Oscillator, $V = \frac{1}{2}m\omega^2x^2$

Here $\nu = 2$, $\alpha = \frac{1}{2}m\omega^2$

So $$E_n = \frac{1}{2}m\omega^2\left[(n-\tfrac{1}{2})\hbar\sqrt{\frac{\pi\,\cancel{2}}{\cancel{2}m\, m\omega^2}}\;\frac{\Gamma(\frac{1}{2}+\frac{3}{2})}{\Gamma(\frac{1}{2}+1)}\right]^{\frac{2\times2}{2+2}}$$

$$= \frac{1}{2}m\omega^2\left[(n-\tfrac{1}{2})\hbar\sqrt{\frac{\pi}{m^2\omega^2}}\;\frac{\Gamma 2}{\Gamma\frac{3}{2}}\right]^1$$

$$= \frac{1}{\cancel{2}}\cancel{m}\omega^2\left[(n-\tfrac{1}{2})\hbar\frac{\sqrt{\pi}}{\cancel{m}\omega}\;\frac{1}{\frac{1}{\cancel{2}}\sqrt{\pi}}\right]$$

$$\left.\begin{aligned} E_n &= (n-\tfrac{1}{2})\hbar\omega \\ \& \quad E_n &= (n+\tfrac{1}{2})\hbar\omega \end{aligned}\right\}$$

Half H.O. :- Only n factor will change.

Time Dependent Perturbation Theory :-

$$H = H_0 + V(t)$$ (Hamiltonian depent on time)

In Time dep. Per. Theory, No need to calculate correction term Only calculate the probability of transition from one stat to another.

Perturbation should be applied for a limited time.

$$\cancel{V(t)} = \begin{cases} V(t) & 0 \le t \le \tau \\ 0 & t > \tau \end{cases}$$

$$\boxed{H\psi = i\hbar \frac{\partial \psi}{\partial t}}$$

Expression for Probability of Transition :-

$$P_{if} = \left| \langle \psi_f | \psi_i \rangle - \frac{i}{\hbar} \int_0^t e^{\frac{i(E_f - E_i)t'}{\hbar}} \langle \psi_f | V(t') | \psi_i \rangle dt' \right|^2$$

$$\boxed{P_{if} = \left| \frac{-i}{\hbar} \int_0^t e^{i\omega_{fi} t'} \langle \psi_f | V(t') | \psi_i \rangle dt' \right|^2}$$ Imp

Case. 1 :- Constant Perturbation (Fermi-Golden Rule) :-

$V(t') = V_0 \Rightarrow$ Perturbation potn is not depending on time.

$$P_{if} = \frac{1}{\hbar^2} |\langle \psi_f | V_0 | \psi_i \rangle|^2 \left| \int_0^t e^{i\omega_{fi} t'} dt' \right|^2$$

$$= \frac{1}{\hbar^2} |\langle \psi_f | V_0 | \psi_i \rangle|^2 \left| \frac{(e^{i\omega_{fi} t} - 1)}{\omega_{fi}^2} \right|^2$$

$$= \frac{1}{\hbar^2} |\langle \psi_f | V_0 | \psi_i \rangle|^2 \frac{(e^{i\omega_{fi} t} - 1)(e^{-i\omega_{fi} t} + 1)}{\omega_{fi}^2}$$

$$\left\{ (1 - e^{i\omega_{fi} t} - e^{-i\omega_{fi} t} + 1) \Rightarrow (2 - 2\cos\omega_{fi} t) \right\}$$

$$= \frac{1}{\hbar^2 \omega_{fi}^2} |\langle \varphi_f | V_0 | \varphi_i \rangle|^2 (2 - 2\cos \omega_{fi} t)$$

$$= \frac{2}{\hbar^2 \omega_{fi}^2} |\langle \varphi_f | V_0 | \varphi_i \rangle|^2 (1 - \cos \omega_{fi} t)$$

$$\boxed{P_{if} = \frac{4}{\hbar^2 \omega_{fi}^2} |\langle \varphi_f | V_0 | \varphi_i \rangle|^2 \sin^2\left(\frac{\omega_{fi} t}{2}\right)}$$

i.e. prob. of transition is a sinusoidal func^n.

→ Limiting case :- $\omega_{fi} \to 0$

$$\lim_{\theta \to 0} \frac{\sin^2\theta}{\theta^2} = 1$$

$$\therefore \lim_{\omega_{fi} \to 0} \frac{\sin^2\left(\frac{\omega_{fi} t}{2}\right)}{\left(\frac{\omega_{fi} t}{2}\right)^2} = 1$$

$$\Rightarrow \lim_{\omega_{fi} \to 0} \frac{\sin^2\left(\frac{\omega_{fi} t}{2}\right)}{\left(\frac{\omega_{fi}}{2}\right)^2} = t^2$$

→ In terms of Dirac Delta func^n,

$$\lim_{g \to \infty} \frac{\sin^2 g x}{\pi g x^2} = \delta(x)$$

$$\lim_{t \to \infty} \frac{\sin^2\left(\frac{\omega_{fi} t}{2}\right)}{\cancel{\sin}\, \pi t \left(\frac{\omega_{fi}}{2}\right)^2} = \delta\left(\frac{\omega_{fi}}{2}\right)$$

$$\Rightarrow \lim_{t \to \infty} \frac{\sin^2\left(\frac{\omega_{fi} t}{2}\right)}{\left(\frac{\omega_{fi}}{2}\right)^2} = \pi t\, \delta\left(\frac{\omega_{fi}}{2}\right)$$

Use $\delta(x-a) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{ik(x-a)} dx$ then

$$\lim_{t \to \infty} \frac{\sin^2\left(\frac{\omega_{fi} t}{2}\right)}{\left(\frac{\omega_{fi}}{2}\right)^2} = 2\pi t\, \delta(\omega_{fi})$$

In the limit $t \to \infty$, Prob. of transition,

$$\boxed{P_{if} = \frac{2\pi t}{\hbar^2} |\langle \psi_f | V_0 | \psi_i \rangle|^2 \delta(\omega_{fi})}$$

Rate of transition,

$$W_{if} = \frac{dP_{if}}{dt}$$

$$W_{if} = \frac{2\pi}{\hbar^2} |\langle \psi_f | V_0 | \psi_i \rangle|^2 \delta\left(\frac{E_f - E_i}{\hbar}\right)$$

$$\boxed{W_{if} = \frac{2\pi}{\hbar} |\langle \psi_f | V_0 | \psi_i \rangle|^2 \delta(E_f - E_i)}$$

$\Rightarrow$ $\delta(E_f - E_i) = \infty \qquad E_f = E_i$

$\qquad\qquad\quad = 0 \quad , \quad E_f \neq E_i$

$\Rightarrow$ In case of Const. perturbation,

The probability of transition in the limit $t \to \infty$ is non-vanishing only b/w states of same energy. Hence a constant perturbation in neither removes energy from the system nor supplies energy to the system. It simply causes energy conserving transitions.

Let us now consider the transition of the system from initial state $|\psi_i\rangle$ to a continuum of a final state or group of states. $|\psi_f\rangle$

$\Rightarrow$ If $\rho_f(E_f)$ is the density of final states

No. density of state $\to$ density of state in unit interval,

$\rho_f(E_f)\, dE_f \Rightarrow$ density of state in b/w E_f to $E_f + dE_f$

So Total Transition Rate,

$$W_{if} = \int \frac{2\pi}{\hbar} |\langle \psi_f | V_0 | \psi_i \rangle|^2 \rho_f(E_f)\, dE_f \;\; \delta(E_f - E_i)$$

$$W_{if} = \frac{2\pi}{\hbar}\int |\langle\psi_f|V_0|\psi_i\rangle|^2 \rho_f(E_f)\,\delta(E_f - E_i)\,dE_f$$

$$\int_{-\infty}^{\infty} f(x)\,\delta(x-a)\,dx = f(a)$$

$$\boxed{W_{if} = \frac{2\pi}{\hbar} |\langle\psi_f|V_0|\psi_i\rangle|^2 \rho_f(E_i)}$$

$$\left\{\begin{array}{l} E_f - E_i = 0 \\ \delta(0) = 1 \\ E_f = E_i \end{array}\right.$$

In Fermi Golden Rule,

Transition Rate $W_{if} \propto |\langle\psi_f|V_0|\psi_i\rangle|^2 \rightarrow$ Matrix element

W_{if} depend on density of final state at energy of initial state $\propto \rho_f(E_i) \rightarrow$ density of states

$\Downarrow$

It is non-zero b/w two continuum states of same energy.

- Fermi-Golden Rule shows Energy Conservation

For constant perturbation, transition will be in degenerate states

2. Harmonic Perturbation :-

$$V(t) = V_0 e^{i\omega t} + V_0^{+} e^{-i\omega t}$$

Probability of transition,

$$P_{if} = \left| \frac{-i}{\hbar}\int_0^t e^{i\omega_{fi}t'} \langle\psi_f|(V_0 e^{i\omega t'} + V_0^{+} e^{-i\omega t'})|\psi_i\rangle dt' \right|^2$$

$$= \frac{1}{\hbar^2}\left| \int_0^t \langle\psi_f|V_0|\psi_i\rangle e^{i(\omega_{fi}+\omega)t'} dt' + \int_0^t \langle\psi_f|V_0^{+}|\psi_i\rangle e^{i(\omega_{fi}-\omega)t'} dt' \right|^2$$

In the limit $t \longrightarrow 0$

$$P_{if} = \frac{2\pi t}{\hbar^2}\left[|\langle\psi_f|V_0|\psi_i\rangle|^2 \delta(\omega_{fi}+\omega) + |\langle\psi_f|V_0^{+}|\psi_i\rangle|^2 \delta(\omega_{fi}-\omega) \right]$$

P_{if} = maxi. when $\boxed{\omega_{fi} = \pm\omega}$

In the limit $t \to \infty$

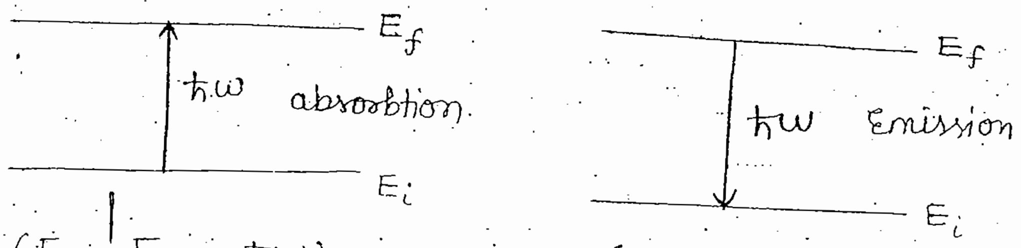
$$P_{if} = \frac{2\pi t}{\hbar}\left[|\langle\psi_f|V_0|\psi_i\rangle|^2 \delta(E_f - E_i + \hbar\omega) + |\langle\psi_f|V_0^{+}|\psi_i\rangle|^2 \delta(E_f - E_i - \hbar\omega)\right]$$

$\boxed{E_f - E_i + \hbar\omega = 0} \Rightarrow E_f - E_i = -\hbar\omega$

$\boxed{E_f - E_i - \hbar\omega = 0} \Rightarrow E_f - E_i = \hbar\omega$

In these 2 cond^{n}s ; P_{if} = Non zero.

& In all other cases $P_{if} = 0$



$(E_f - E_i = \hbar\omega)$

$E_f > E_i$ Absorption

$(E_f - E_i = -\hbar\omega)$

i.e. $E_f < E_i$ Emission

In $V(t) = V_0 e^{i\omega t} + V_0^{+} e^{-i\omega t}$

from these 2 terms, we observe that for which term we get emission & for which we get absorption.

$e^{i(\omega_{fi} \pm \omega)}$

If add $\longrightarrow$ emission $(\omega_{fi} + \omega)$

subs. $\longrightarrow$ absorption $(\omega_{fi} - \omega)$

) <u>Adiabatic Approximation</u> :-

$$P_{if} = \left| \frac{-i \times \omega_{fi}}{i\hbar\omega_{fi}} \int_0^t (e^{i\omega_{fi} t'}) \langle \psi_f | V(t') | \psi_i \rangle dt' \right|^2$$

$$P_{if} = \left| \frac{-i}{i\hbar\omega_{fi}} \int_0^t \left(\frac{\partial}{\partial t'}(e^{i\omega_{fi} t'}\right) \langle \psi_f | V(t') | \psi_i \rangle dt' \right|^2$$

$$V(t) = V(t) \quad 0 < t' < t$$
$$= 0 \quad \text{otherwise}$$

$$P_{if} = \left| \frac{-1}{\hbar\omega_{fi}} \langle \psi_f | V(t') | \psi_i \rangle \frac{e^{i\omega_{fi}t'}}{i\omega_{fi}} \Big|_0^{t} + \frac{1}{\hbar\omega_{fi}} \right.$$

$$= \left| \frac{1}{\hbar\omega_{fi}} \int_0^t e^{i\omega_{fi}t'} \frac{\partial}{\partial t} \langle \psi_f | V(t') | \psi_i \rangle \, dt' \right|^2$$

for adeabatic app.,

$$\boxed{\frac{\partial}{\partial t} \langle \psi_f | V(t) | \psi_i \rangle = \text{constant}}$$

$$P_{if} \simeq \frac{4}{\hbar^2 \omega_{fi}^2} \left| \frac{\partial}{\partial t} \langle \psi_f | V(t) | \psi_i \rangle \right|^2 \sin^2\left(\frac{\omega_{fi} t}{2}\right)$$

$\because \frac{\partial}{\partial t} \langle \psi_f | V(t) | \psi_i \rangle << (E_f - E_i)$

$\therefore \boxed{P_{if} << 1}$

Prob. of transition is very-2 less i.e chance of transition is less. So on applying adiabatic perturbation, energy will be changed but state will be same. i.e. if unperturbed state is E_3 then after applying pert^n state will remain E_3 but energy will be different.

- When the perturbation is turne ON & OFF adiabatically No transition occur.

i.e. If a system is in n^{th} state initially $(t=0)$ with energy $E_n^{(0)}$ then after applying the adiabatic perturbation $\hat{V}(t)$, the system will be in the n^{th} state of new Hamiltonian.

$$\boxed{\hat{H} = \hat{H}_0 + V(t)}$$

4.) Sudden Approximation :-

When the perturbation is turn ON & OFF suddenly then the term $e^{i\omega_{fi}t}$ does not change much during switching ON time.

$$P_{if} = \frac{1}{\hbar^2 \omega_{fi}^2} \left| e^{i\omega_{fi}t} \right|^2 \left| \int_0^t \frac{\partial}{\partial t'} \langle \psi_f | V(t') | \psi_i \rangle dt' \right|^2 .$$

$$\boxed{P_{if} \simeq \frac{1}{\hbar^2 \omega_{fi}^2} \left| \langle \psi_f | V(t) | \psi_i \rangle \right|^2} \longrightarrow \text{approximate}$$

$$\psi = \sum_n C_n \phi_n \Rightarrow P_n = |\langle \phi_n | \psi \rangle|^2 \longrightarrow \text{Exact}$$

Semi Classical Theory of Radiation :-

In semi classical theory of radiation, P_{if} depend on $e^{ik\cdot r}$ & $\langle \psi_f | A e^{ik\cdot r} | \psi_i \rangle$ → matrix element

$$P_{if} = \frac{2\pi t}{\hbar} \langle \psi_f | A e^{ik\cdot r} | \psi_i \rangle \, \delta$$

$$E = E_0 \, e^{i(k\cdot r - \omega t)}$$

$$B = B_0 \, e^{i(k\cdot r - \omega t)}$$

Harmonic term variation $e^{-i\omega t}$

Selection Rules :- $\boxed{\begin{array}{l} \Delta l = \pm 1 \\ \Delta m_l = 0, \pm 1 \end{array}}$

Scattering :-

Diff b/w collision & Sca :-

for collision, incident & target both particles should be structure particle.

for Scattering, target particle will be structure particle, incident particle will be structureless.

Scattering means deviation from incident dirⁿ.

- Elastic $\longrightarrow$ L.M., total Energy, K.E. conserved
- Inelastic $\longrightarrow$ L.M., total Energy $\rightarrow$ conserved

  K.E. $\nrightarrow$ Not conserved.

from $|\psi|^2 \Rightarrow$ No. of scattered particle can be found.

Differential Cross-Section :-

The No. of particles scattered per unit ~~area~~ incident flux per unit time per unit scattering centres, per unit solid angle.

$$d\Omega = \frac{dA}{r^2}$$

$$= \frac{\sin\theta\, d\theta\, d\phi\, r^2}{r^2} = \sin\theta\, d\theta\, d\phi$$

No. of particle scatter

$dN \propto n J_{in} d\Omega$

$dN = \frac{d\sigma}{d\Omega} n J_{in} d\Omega$

Total Cross-Section :-

The total no. of particles scattered per unit incident flux per unit time into whole solid angle.

$$\boxed{\sigma_t = \int \left(\frac{d\sigma}{d\Omega}\right) d\Omega}$$

$$\boxed{\frac{d\sigma}{d\Omega} = \frac{dN}{n J_{in} d\Omega}} \longrightarrow \text{Diff. Cross section}$$

Unit $\rightarrow$ unit of area of cross-section

$J_{in} \rightarrow$ incident flux

n = scattering centres (or targets)

In scattering prob:, we take the asymptotic form of wave func^n [asymptotic means variation from 0 to ∞].

$$\psi \xrightarrow[r\to\infty]{} \psi_{in} + \psi_{sca}$$

$$\boxed{\psi \xrightarrow[r\to\infty]{} Ae^{ikz} + \frac{Af(\theta,\phi)\, e^{ikr}}{r}}$$

or,
$$\boxed{\psi \xrightarrow[r\to\infty]{} \underbrace{Ae^{i\underline{k}\cdot\underline{r}}}_{\text{plane wave}} + \underbrace{\frac{Af(\theta,\phi)e^{ikr}}{r}}_{\text{spherical wave}}}$$

$e^{ikr} \rightarrow$ gives spherical wavefronts.

Wavefront → locus of all point that have same phase.

$e^{+ikr} \longrightarrow$ + for outgoing

$e^{-ikr} \longrightarrow$ − for incoming

No. of scattered particles are independent on area so spherical wave is also independent on $\frac{1}{r}$.

<u>Relation b/w Scattering amplitude & differential Cross section</u> :-

$$\psi \xrightarrow[r\to\infty]{} \underbrace{Ae^{ik_1 z}}_{\psi_{in}} + \underbrace{\frac{Af(\theta,\phi)}{r}\, e^{ik_2 r}}_{\psi_{sca}}$$

$$\psi_{in} = Ae^{ik_1 z}$$

$$\psi_{sca} = Af(\theta,\phi)\frac{e^{ik_2 r}}{r}$$

$$J_{in} = -\frac{i\hbar}{2m}\left[\psi^*\nabla\psi - \psi\nabla\psi^*\right] = \psi^*\psi v$$

$$= -|A|^2\frac{i\hbar}{2m}\left[e^{-ik_1 z}\, ik_1 e^{ik_1 z} - e^{ik_1 z}(-ik)e^{-ik_1 z}\right]$$

$$= -|A|^2\frac{i\hbar}{2m}\left[2ik_1\right]$$

$$J_{in} = |A|^2 \frac{\hbar K_1}{m}$$

$$J_{sca} = \frac{|A|^2 |f(\theta,\phi)|^2}{r^2} \frac{\hbar K_2}{m}$$

diff. Cross section, $\frac{d\sigma}{d\Omega} = \frac{dN}{n J_{in} d\Omega}$

$$\frac{d\sigma}{d\Omega} = \frac{1}{n J_{in}} \cdot \frac{dN}{d\Omega}$$

$n=1$, $\frac{d\sigma}{d\Omega} = \frac{1}{J_{in}} \frac{dN}{d\Omega}$

$\because dN = J_{sc} \times dA$

$dN = J_{sc} \times r^2 d\Omega$

$\frac{dN}{d\Omega} = J_{sc} r^2$

$$\therefore \frac{d\sigma}{d\Omega} = \frac{1}{J_{in}} J_{sc} r^2$$

$$\frac{d\sigma}{d\Omega} = \frac{\cancel{m}\, \cancel{r^2}}{\cancel{|A|^2} \cancel{\hbar} K_1} \frac{\cancel{|A|^2} |f(\theta,\phi)|^2 \cancel{\hbar} K_2}{\cancel{r^2}\, \cancel{m}}$$

$$\boxed{\frac{d\sigma}{d\Omega} = \frac{|K_2|}{|K_1|} |f(\theta,\phi)|^2}$$ $\Rightarrow$ Valid for any type of sc

for elastic, $|K_1| = |K_2|$, $\boxed{\frac{d\sigma}{d\Omega} = |f(\theta,\phi)|^2}$

Total cross section, $\sigma_t = \int |f(\theta,\phi)|^2 d\Omega$

$$\boxed{\sigma_t = \int_0^{\pi} \int_0^{2\pi} |f(\theta,\phi)|^2 \sin\theta \, d\theta \, d\phi}$$

Note :- for scattering problem, No need to check the wave func^n is normalised or not i.e. no need to calculate normalisation constant.

L-System :- The frame of reference in which target is at rest initially (i.e. before sca.)

C-System :- The frame of reference in which C.M. of the system is at rest always.

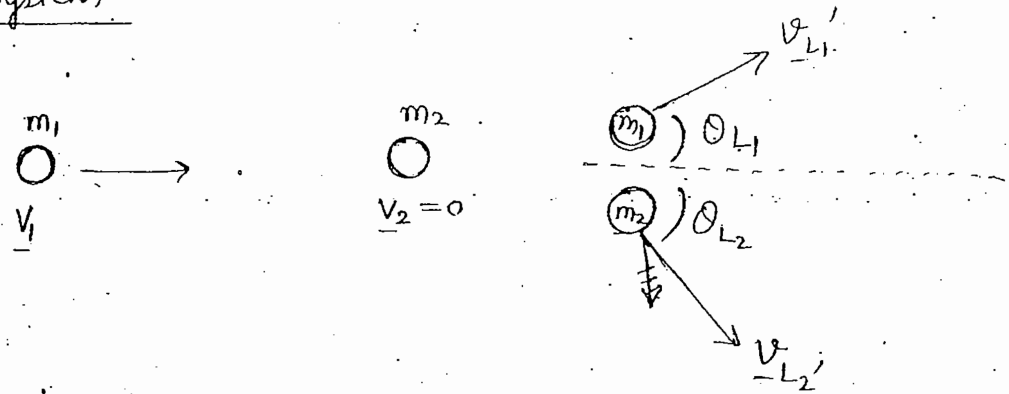
for 1 particle → d.o.f. = 3
2 particle → d.o.f. = 6
~~break 6 into~~ ⇒ 6 = 3 D.o.f. of C.M. + 3 relative motion
C.M. is always at rest so 6 = 0 + 3 relative motion

→ In C-system, 6 d.o.f. reduces to 3 d.o.f. but In L-system D.o.f. remain 6.

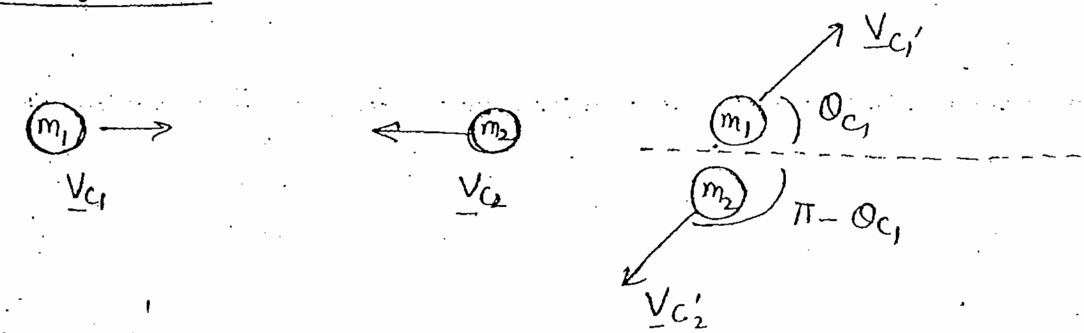
→ More D.o.f. ⇒ More chance of accuracy.

→ observation will be done in Lab frame & calculations " " " C.M. "

L-System :-



C-System :-



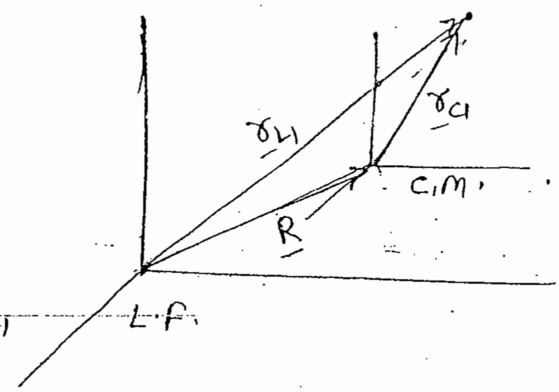
Centre of mass, $\underline{R} = \dfrac{m_1 r_1 + m_2 r_2}{m_1 + m_2}$

~~$V_{cm} = \frac{m_1 V_1}{}$~~

Velocity of C.M. $\boxed{\underline{V}_{cm} = \dfrac{m_1 \underline{V}_{L_1}}{m_1+m_2}}$

$$\underline{r}_{L_1} = \underline{R} + \underline{r}_{c_1}$$

$$\underline{V}_{L_1} = \underline{v}_{cm} + \underline{v}_{c_1}$$



Angle :-

$$|V'_{L_1}| \cos\theta_{L_1} = v_{cm} + |v'_{c_1}| \cos\theta_{c_1}$$

$$|V'_{L_1}| \sin\theta_{L_1} = |v'_{c_1}| \sin\theta_{c_1}$$

deviding,
$$\tan\theta_{L_1} = \frac{\sin\theta_{c_1}}{\cos\theta_{c_1} + \dfrac{|V_{cm}|}{|V'_{c_1}|}}$$

On applying K.E conservation & Lineare mom. conservation

$$\frac{|V_{cm}|}{|V'_{c_1}|} = \frac{m_1}{m_2} \quad \text{then}$$

$$\boxed{\tan\theta_{L_1} = \frac{\sin\theta_{c_1}}{\cos\theta_{c_1} + \dfrac{m_1}{m_2}}}$$

<u>Relation b/w cross-section in L-system & C-system</u> :-

$$\left(\frac{d\sigma}{d\Omega}\right)_L d\Omega_L = \left(\frac{d\sigma}{d\Omega}\right)_c d\Omega_c$$

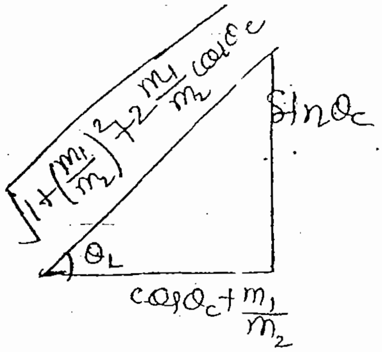
$$\left(\frac{d\sigma}{d\Omega}\right)_L = \left(\frac{d\sigma}{d\Omega}\right)_c \frac{\sin\theta_c \, d\theta_c \, d\phi_c}{\sin\theta_L \, d\theta_L \, d\phi_L}$$

for beam, there is cylendrical symmetry so $d\phi_c = d\phi_L$

$$\text{so} \quad \left(\frac{d\sigma}{d\Omega}\right)_L = \left(\frac{d\sigma}{d\Omega}\right)_c \frac{\sin\theta_c \, d\theta_c}{\sin\theta_L \, d\theta_L}$$

We know $\quad \tan\theta_L = \dfrac{\sin\theta_c}{\cos\theta_c + \dfrac{m_1}{m_2}}$

$$\cos\theta_c = \frac{\cos\theta_c + \frac{m_1}{m_2}}{\sqrt{1+\left(\frac{m_1}{m_2}\right)^2 + 2\frac{m_1}{m_2}\cos\theta_c}}$$



$$\left(\frac{d\sigma}{d\Omega}\right)_L = \left(\frac{d\sigma}{d\Omega}\right)_c \frac{\left(1+\left(\frac{m_1}{m_2}\right)^2 + 2\frac{m_1}{m_2}\cos\theta_c\right)^{3/2}}{\left(1+\frac{m_1}{m_2}\cos\theta_c\right)}$$

Relation b/w velocity in L & C system:-

$$\vec{V}_{cm} = \frac{m_1\vec{v}_{1L}}{(m_1+m_2)}$$

$$\vec{v}_{1L} = \vec{v}_{cm} + \vec{v}_{1c}$$

$$\vec{v}_{1c} = \vec{v}_{1L} - \vec{v}_{cm} = \vec{v}_{1L} - \frac{m_1 v_{1L}}{(m_1+m_2)}$$

$$\vec{v}_{1c} = \frac{m_2\vec{v}_{1L}}{(m_1+m_2)}$$

$$\boxed{\vec{v}_{1L} = \left(\frac{m_1+m_2}{m_2}\right)\vec{v}_{1c}}$$

Momentum, $\boxed{\vec{P}_{1L} = \left(\frac{m_1+m_2}{m_2}\right)\vec{P}_{1c}}$

Kinetic Energy :- $T = K.E. = \frac{p^2}{2m}$

$$\frac{P_{1L}^2}{2m_1} = \left(\frac{m_1+m_2}{m_2}\right)^2 \frac{P_{1c}^2}{2m_1}$$

$$\boxed{T_{1L} = \left(\frac{m_1+m_2}{m_2}\right)^2 T_{1c}}$$

K.E. of total system in Lab frame,

$$T_L = \frac{1}{2}m_1V_{1L}^2 = \frac{p_{1L}^2}{2m} = T_{1L}$$

In C.M. frame, $T_c = \frac{1}{2}m_1V_{1c}^2 + \frac{1}{2}m_2V_{2c}^2$

$$T_c = T_{1c}$$

$$\boxed{T_L = \left(\frac{m_1+m_2}{m_2}\right) T_c}$$

First Born Approximation :-

When scattering potⁿ is small & incident energy is ~~small~~ lar then there will be Born App.

In Ist B.A., there will be direct scattering (i.e. particle sca. one time)

[If particle In IInd B.A., consider 2 sca
" IIIrd " " 3 "]

Scattering Amplitude in Ist Born approximation,

$$\boxed{f(\theta,\phi) = \frac{-m}{2\pi\hbar^2}\int e^{i(\vec{k}-\vec{k}')\cdot r}\, V(\vec{r})\, d\tau}$$ → for any kir of potⁿ

$k \rightarrow$ propogation vector of incident wave

$k' \rightarrow$ " " " scattered "

$$\boxed{\vec{K} = \vec{k} - \vec{k}'} \Rightarrow \boxed{|\vec{K}| = K = 2k\sin\frac{\theta}{2}}$$

$$f(\theta,\phi) = \frac{-m}{2\pi\hbar^2}\int e^{iK\cdot r}\, V(\vec{r})\, r^2 dr \sin\theta\, d\theta\, d\phi$$

$\because V(\vec{r}) = V(r) \Rightarrow$ Sherically sym. potⁿ

$$\therefore f(\theta,\phi) = \frac{-m\times 2\pi}{2\pi\hbar^2}\int_0^\infty\int_0^\pi e^{iKr\cos\theta}\, V(r)\, r^2 dr \sin\theta\, d\theta$$

$$\boxed{f(\theta,\phi) = \frac{-2m}{\hbar^2 K}\int_0^\infty r \sin Kr\, V(r)\, dr}$$ → for spherical symmetric potⁿ

where $K = 2k\sin\frac{\theta}{2}$

Problem :- A free particle described by a plane wave & moving in the +ve z-dirⁿ undergoes scattering by a potⁿ

$$V(r) = \begin{cases} V_0, & \text{if } r \le R \\ 0, & \text{if } r > R \end{cases}$$

If V_0 is changed to $2V_0$, keeping R fixed then the differential sca. cros-section in the born Approximation,

(1) increases to 4 times the original value
(2) " " " 2 " " " "
(3) decreases to half of " " "
(4) decreases " $\frac{1}{4}$ " " "

$$f(\theta,\phi) = \frac{-2m}{\hbar^2 k}\int_0^{\infty} r \sin kr \, V(r)\, dr$$

$$= \frac{-2m V_0}{\hbar^2 k}\int_0^{R} r \sin kr \, dr$$

$$\frac{f_2(\theta)}{f_1(\theta)} = \frac{\left(\frac{-2m}{\hbar^2 k}\right) 2V_0 \int_0^R r \sin kr\, dr}{\left(\frac{-2m}{\hbar^2 k}\right) V_0 \int_0^R r \sin kr\, dr}$$

$$f_2(\theta) = 2 f_1(\theta)$$

$$\frac{\left(\frac{d\sigma}{d\Omega}\right)_2}{\left(\frac{d\sigma}{d\Omega}\right)_1} = \frac{|f_2(\theta)|^2}{|f_1(\theta)|^2} = \underline{\underline{4}}$$

Partic Problems on Born App.

Q.1 :- Find the total scattering cross section using Ist Born approximation for the scattering of an e^- by the pot^n $V(r) = -V_0 e^{-r/a}$ where a is +ve constant.

Result

$$f(\theta) = \frac{4 m V_0 a^3}{\hbar^2(1+4k^2a^2\sin^2\theta/2)^2}$$

$$\sigma_t = \int_0^{\pi}\int_0^{2\pi} |f(\theta)|^2 \sin\theta \, d\theta \, d\phi = \frac{16 m^2 V_0^2 a^4}{3\hbar^2 k^2}\left[1 - \frac{1}{(1+4k^2a^2)^3}\right]$$

Q.2 :- Calculate the differential cross-section for the coulomb pot^n $V(r) = \frac{Z_1 Z_2 e^2}{r}$ by using Ist Born App. where $Z_1 e$ & $Z_2 e$ are the charges of projectile & target particles respectively.

Result $f(\theta\phi) = \dfrac{-2mZ_1Z_2e^2}{\hbar^2K^2}$

$$\frac{d\sigma}{d\Omega} = |f(\theta,\phi)|^2 = \left(\frac{2mZ_1Z_2e^2}{\hbar^2K^2}\right)^2 , \quad K = 2k\sin\frac{\theta}{2}$$

Energy $E = \dfrac{\hbar^2k^2}{2m} = \left(\dfrac{Z_1Z_2e^2}{4E}\right)^2 \operatorname{cosec}^4(\theta/2)$

Partial Wave Analysis :-

$$\psi = \psi_{in} + \psi_{sc}$$

$$\psi_{in} = Ae^{ik\cdot r} \quad \text{(plane wave)}$$

$$= \sum_l (2l+1) \quad , \quad l = 0, 1, 2, \dots\dots \infty$$

(in terms of partial wave)

For each value of l, there is a partial wave.

Scattering Amplitude,

$$\boxed{f(\theta) = \frac{1}{k}\sum_l (2l+1)\, e^{i\delta_l} \sin\delta_l\, P_l(\cos\theta)}$$

diff cross section, $\dfrac{d\sigma}{d\Omega} = |f(\theta)|^2 = f^*(\theta)\,f(\theta)$

Total cross section, $\boxed{\sigma_t = \dfrac{4\pi}{K^2}\sum_l (2l+1)\sin^2\delta_l} \rightarrow$ Partial cross section

$$\boxed{\sigma_t = \frac{4\pi}{K}\, \mathrm{Im} f(0)}$$

If $\theta = 0$ dirn then no deflection i.e. no contribution of sca

Im $f(0)$ means the particles which are not going in $\theta = 0$ dirn.

i.e. No of scattered particles.

This eqn shows the conservation of particle flux.

unscattered + scattered Particles = Incident particles

(46):- $V(x) = 0 \quad , 0 \le x \le a$
$\quad\quad\quad = \infty \quad ,$ otherwise

$$\psi(x,0) = \sqrt{\frac{8}{5a}}\left[1+\cos\left(\frac{\pi x}{a}\right)\right]\sin\frac{\pi x}{a}$$

$$\psi(x,t) = \sqrt{\frac{8}{5a}}\, e^{-\frac{iHt}{\hbar}}\left[\sin\frac{\pi x}{a} + \frac{1}{2}\times\sin\frac{2\pi x}{a}\right]$$

$=$

(b)

(47):- $\psi = \frac{1}{\sqrt{4\pi}}\left(e^{i\phi}\sin\theta + \cos\theta\right) g(r)$

$$Y_{00} = \frac{1}{\sqrt{4\pi}}$$

$$Y_{10} = \sqrt{\frac{3}{4\pi}}\cos\theta$$

$$Y_{11} = \sqrt{\frac{3}{8\pi}}\sin\theta\, e^{i\phi}$$

$$Y_{1\bar{1}} = \sqrt{\frac{3}{8\pi}}\sin\theta\, e^{-i\phi}$$

$$\psi = g(r)\left[-\sqrt{\frac{2}{3}}\,Y_{11} + \frac{1}{\sqrt{3}}Y_{10}\right]$$

Prob. in Y_{10} state, $P = \left|\frac{1}{\sqrt{3}}\right|^2 = \frac{1}{3}$

(48):- $f = a + b\,\sigma_1\cdot\sigma_2$

$$S = \frac{\hbar}{2}(\sigma_1+\sigma_2)$$

$[S^2, S_z] = 0$

S^2, S_z commute always.

$f = \underset{\text{const.}}{a} + \underbrace{b\,\sigma_1\cdot\sigma_2}$ → check this part,

const.
so always commute

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

$\Rightarrow \sigma_1\cdot\sigma_2$

(d)

(49) :- $V = \frac{1}{2}Kx^2$, $V = qE_x$

$E' = \langle x \rangle = 0$

✓(d)

(50) :- $V(r) = -\frac{a}{r}$

$\left|\frac{d\lambda}{dr}\right| << 1$ → cond^n of validity

$\left|\frac{d\left(\frac{h}{p}\right)}{dr}\right| << 1$

✓(c)

(51) :- $|\phi_1\rangle, |\phi_2\rangle$, $B = |\phi_1\rangle\langle\phi_2|$

Involuntory ; $\hat{B}^2 = I$

$\hat{B}^2 = |\phi_1\rangle\underbrace{\langle\phi_2|\phi_1\rangle}_{0}\langle\phi_2| = 0 \neq I$

$BB^+ = |\phi_1\rangle\underbrace{\langle\phi_2|\phi_2\rangle}_{1}\langle\phi_1| = |\phi_1\rangle\langle\phi_1|$

ϕ_1 → normalised to unit so projection o/p.

✓(b)

$(BB^+ - B^+B)^+ (\quad) = 1$ ⇒ Not unitory

$\neq 1 = -1$

(52) :- $V(x,y) = \frac{1}{2}m\omega^2x^2 + 8m\omega^2y^2$

$= \frac{1}{2}m\omega^2x^2 + \frac{1}{2}16m\omega^2y^2 = \frac{1}{2}m\omega^2x^2 + \frac{1}{2}m(4\omega)^2 y^2$

$\omega \qquad 4\omega$

$E = (n_x + \frac{1}{2})\hbar\omega + (n_y + \frac{1}{2})\hbar(4\omega)$

$= \left[n_x + 4n_y + \frac{5}{2}\right]\hbar\omega$

$= (n + \frac{5}{2})\hbar\omega$ ✓(d)

(53) :- $V(x) = 0$ if $|x| < L$

$= \infty$ otherwise

Variance = Mean square deviation

$= \langle(x - \langle x\rangle)^2\rangle = \langle x^2\rangle - \langle x\rangle^2$, $\langle x\rangle = 0$

$= \frac{L^2}{6}$

✓(c)

Q.1 :- The product of 2 hermitian operators $\hat{A}$ & $\hat{B}$ is also Hermitian.
$\therefore$ $\hat{A} \to$ Herm & $\hat{A}$ & $\hat{B}$ should commute.
✓(c) $\hat{A}$ & $\hat{B}$ $\to$ Hermitian & $[\hat{A}\ \hat{B}] = 0$

Q.2 :- $\lambda = \frac{h}{p} = \frac{h}{\sqrt{2mE}}$

In 3-Dim
$E = \frac{3}{2}KT$
$\lambda = \frac{h}{\sqrt{2m\frac{3}{2}KT}} = \frac{h}{\sqrt{3mKT}}$ ✓(b)

Q.3 :- $\sigma_i\ (i = 1, 2, 3)$
For Pauli spin matrices, $\sigma_i\sigma_j + \sigma_j\sigma_i = 2\delta_{ij}$
$Tr(\sigma_i) = 0$
Eigen value of σ_i are ± 1

So $\det(\sigma_i) \neq 1$
✓(d)

Q.4 :- $R_{10} = \frac{2}{a_0^{3/2}} \exp\left(\frac{-r}{a_0}\right)$ $n = 1,\ l = 0$
Most probable value of $r = n^2 a_0$ $(l = n-1)$
$= (1)^2 a_0 = a_0$ ✓(a)

Q.5 :- (a) $\psi = \left(\frac{1}{\pi a_0^3}\right)^{1/2} e^{-r/a_0}$
$m = 0$ So $L_z = m\hbar = 0$
$[L_x\ L_y] = i\hbar L_z$

Q.6 :- $[x\ p] = i\hbar$
$[x^3\ p] = 3x^2 p - p x^3$
$[x^3, p] = [x^2 x . p] = x[\underbrace{x^2}_{= x x} p] + [x\ p]x^2$
$= x\{x[x\ p] + [x\ p]x\} + [x\ p]x^2$
$= x\{x i\hbar + i\hbar x\} + i\hbar x^2$
$= x^2 i\hbar + i\hbar x^2 + i\hbar x^2$
$= 3 i\hbar x^2$
✓(c)

(9) $S = \frac{i\hbar}{2m}\left[\psi^* \nabla \psi - \psi \nabla \psi^*\right]$

$\psi = A e^{ikx}$

$S = |A|^2 \frac{\hbar k}{m}$

(15) $\langle z \rangle = \int \psi_{100}^* \, z \, \psi_{100} \, d$

(17) $S_x S_y S_z = \frac{\hbar}{2}\sigma_x \frac{\hbar}{2}\sigma_y \frac{\hbar}{2}\sigma_z = \frac{\hbar^3}{8}\sigma_x \sigma_y \sigma_z$

$= \frac{\hbar^3}{8} i\sigma_z \sigma_z = \frac{i\hbar^3}{8}\sigma_z^2 = \frac{i\hbar^3}{8}$

(18) $p(x)\,dx = a e^{-ax}$

$\int_{x_1}^{x_2} p(x)\,dx = \int_{x_1}^{x_2} a e^{-ax}\,dx$

$= a\left[\frac{e^{-ax}}{-a}\right]_{x_1}^{x_2} = -\left(e^{-ax_2} - e^{-ax_1}\right) = e^{-ax_1} - e^{-a}$

(19) $[L_z \, Y_{lm}(\theta, \phi)] = m\hbar$ ← (c)

(20) $|\psi\rangle = c_1 |\alpha_1\rangle + c_2 |\alpha_2\rangle$

$|c_1|^2 + |c_2|^2 = 1$ ← (d)

(21) $[x, p^2] = [x, pp]$

$= p[x, p] + [x\, p]\, p$

$= p\, i\hbar + i\hbar\, p$

$= 2i\hbar\, p$

(24) $\langle L_+ L_- \rangle = ?$

$L_+ L_- = (L_x + iL_y)(L_x - iL_y)$

$= L_x^2 - iL_x L_y + iL_y L_x + L_y^2$

$= L_x^2 + L_y^2 - i[L_x L_y - L_y L_x]$

$= L_x^2 + L_y^2 - i \cdot i\hbar L_z = L_x^2 + L_y^2 + \hbar L_z$

$\langle l m | L_+ L_- | l m \rangle = \cancel{l(l+1)\hbar^2 + l(l+1)\hbar^2 + m\hbar^2}$, $L^2 - L_z^2 + \hbar L_z$

$= l(l+1)\hbar^2 - l^2\hbar^2 + \hbar^2 l = l(l+1)\hbar^2 - l(l-1)\hbar$

$= l\hbar^2 + l\hbar^2 - 2l\hbar^2$

(42) Energy of IInd excited state $= \frac{13.6}{n^2}$

$= \frac{13.6}{9} = -1.5$

(43) $[L_x L_y, L_z]$ $= [\cancel{i\hbar L_z}, \cancel{L_z}] = i\hbar[\cancel{L_z}, \cancel{L_z}]$

$L_x[L_y L_z] + [L_x L_z]L_y$

$L_x\, i\hbar L_x + (-i\hbar L_y)L_y = i\hbar(L_x^2 - L_y^2)$

(44) $\omega(\lambda) \propto 1/\sqrt{\lambda}$

$\cancel{\omega(\lambda)}$ $v_p = \frac{\omega}{k} = \frac{1}{k\sqrt{\lambda}} = \frac{1}{\frac{2\pi}{\lambda}\sqrt{\lambda}} = \frac{\sqrt{\lambda}}{2\pi}$

$\boxed{v_g = v_p - \lambda \frac{dv_p}{d\lambda}}$

$= \frac{1}{k\sqrt{\lambda}} - \cancel{\frac{\lambda}{k}\left(\frac{-1}{2}\right)\sqrt{\lambda}}\,\lambda \frac{1}{\frac{2\pi}{\lambda}} \frac{1}{2} \frac{1}{\sqrt{\lambda}}$

$v_g = v_p - \frac{1}{2k\sqrt{\lambda}}\lambda = v_p - \frac{v_p}{2}$

$\boxed{v_g = v_p/2}$

(45) $\Delta x\, \Delta p = \left[\sqrt{\frac{1}{12} - \frac{1}{2n^2\pi^2}}\right] n\pi\hbar$

$n=1$ $\Delta x\, \Delta p = \pi\hbar\sqrt{\frac{1}{12} - \frac{1}{2\pi^2}} = \pi\hbar\sqrt{\frac{2\pi^2 - 12}{24\pi^2}}$

$= \hbar\sqrt{\frac{\pi^2 - 6}{12}}$

(46)

(46) $E_{(eV)} = \frac{1240}{\lambda(nm)} = \frac{1240}{200} = 6.2\ eV$

(53) $\phi(x) = Nx\, e^{-\alpha^2 x^2/2}$

$\int \phi^*(x)\phi(x)dx = |N|^2\int_{-\infty}^{+\infty} x^2 e^{-\alpha^2x^2} dx$

$= 2|N|^2\int_0^\infty x^2 e^{-\alpha^2x^2} dx = 2|N|^2 \frac{\Gamma\frac{3}{2}}{2(\alpha^2)^{3/2}}$

$$\cancel{2}|N|^2 \frac{\frac{1}{2}\sqrt{\pi}}{\cancel{2}\alpha^3} = 1$$

$$|N|^2 = \frac{2\alpha^3}{\sqrt{\pi}} \Rightarrow \# \; N = \sqrt{\frac{2\alpha^3}{\sqrt{\pi}}}$$

(54) $[L_x L_z] = L_x L_z - L_z L_x$

$$[L_+ L_z] = [L_x + iL_y, L_z]$$
$$= [L_x L_z] + i[L_y L_z]$$
$$= -i\hbar L_y + i \; i\hbar L_x$$
$$= -i\hbar L_y - \hbar L_x \Rightarrow -\hbar (L_x + iL_y)$$
$$= -\hbar L_+$$

(55) $J_+ \psi_{jm} = \sqrt{(j-m)(j+m+1)}\,\hbar\, \psi_{jm'}$

$$= \sqrt{(j^2 - jm + j - mj - m^2 + m)}\,\hbar\, \psi_{jm'}$$
$$= \sqrt{j^2 + j - m^2 + m}\,\hbar\, \psi_{jm+1}$$

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