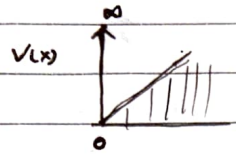
Assignment-10

Pg-1

Name: SUSNATA CHATTOPADHYAY
Roll: 22MS077 ; PH3102.

Date 9/11/2024
Page 1

Q.2) $$V(x) = \begin{cases} mgx & x > 0 \\ \infty & x < 0 \end{cases}$$



(a) Hamiltonian, $\hat{H} = \frac{\hat{p}_x^2}{2m} + V(x)$

At $x \to \infty$,

(i) Since, $V(x) = \infty$ for $x < 0$, we know that is not possible for a particle to exist in this region. (for particle experiences infinite force). so, $\psi(x) = 0$ (for $x < 0$)

To ensure continuity of the equations, we have $\lim_{x \to 0} \psi(x) = \psi(0^-) = 0$

$\therefore \boxed{\psi(0) = 0}$

(ii) Again, Normalisability (square integrability) condition for wavefunctions in Hilbert space, demands

$$\lim_{x \to \infty} \psi(x) = 0 \Rightarrow \boxed{\psi(\infty) = 0}.$$

The given wavefunction (Ansatz)

$$\psi(x) \propto \begin{cases} x e^{-ax} & x \geq 0 \\ 0 & x < 0 \end{cases}$$

succesfully satisfies the proposed boundary conditions. (Considering $a \in \mathbb{R}^+$)

$$\left(\lim_{x \to \infty} \frac{x}{e^{ax}} = \lim_{x \to \infty} \frac{1}{a e^{ax}} = 0 \right), \quad \lim_{x \to 0^-} \psi(x) = \lim_{x \to 0^+} \psi(x) = 0 !$$

$\therefore$ Consider,

$$\psi(x) = \begin{cases} A x e^{-ax} & x \geq 0 \\ 0 & x < 0 \end{cases}$$

Date / Page /

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

$$\therefore \int_{-\infty}^{\infty} \psi^*(x)\psi^*(x)\,dx = 0$$

$$\Rightarrow |A|^2 \int_0^{\infty} x^2 e^{-2ax}\,dx = 1.$$

using Int. by parts

	D	I
+	x^2	e^{-2ax}
−	$2x$	$\frac{-e^{-2ax}}{2a}$
+	2	$\frac{e^{-2ax}}{4a^2}$
−	0	$\frac{-e^{-2ax}}{(2a)^3}$

$$= \left(\frac{-x^2 e^{-2ax}}{2a} \right|_0^{\infty} - \left(\frac{+2x\, e^{-2ax}}{4a^2} \right|_0^{\infty} + \left(\frac{2 e^{-2ax}}{(2a)^3} \right|_0^{\infty}$$

$$\Rightarrow |A|^2 \left\{ \frac{2}{4a^3} \right\} = 1$$

$$\boxed{|A| = 2a^{3/2}}$$

$$\therefore \psi(x) = \begin{cases} 2a^{3/2} x e^{-ax} & x > 0 \\ 0 & x < 0 \end{cases}$$

$$\langle H \rangle_\psi = \langle \psi | H | \psi \rangle = \int_{-\infty}^{\infty} \psi^* H \psi \, dx$$

$$= \int_0^{\infty} 4a^3 x e^{-ax} \left(\frac{-\hbar^2}{2m} \frac{d^2}{dx^2} + mgx \right) x e^{-ax} \cdot dx$$

Date
Page

$$= 4a^3\left(-\frac{\hbar^2}{2m}\right)\int_0^\infty dx\; xe^{-ax}\frac{d^2}{dx^2}(xe^{-ax}) + 4a^3mg\int_0^\infty dx\, x^3e^{-ax\times 2}$$

$$= 4a^3\left(-\frac{\hbar^2}{2m}\right)\int_0^\infty dx\, x\,e^{-ax}\left[-ae^{-ax}(2-ax)\right] + 4a^3mg\int_0^\infty dx\, x^3e^{-2ax}$$

$$= 4a^3\left(-\frac{\hbar^2}{2m}\right)\left(-\frac{1}{4a^2}\right) + 4a^3mg\left(\frac{3}{8}\cdot\frac{1}{a^4}\right)$$

$$= \boxed{\frac{a^2\hbar^2}{2m} + \frac{3}{2}\frac{mg}{a}} = \langle H\rangle_\psi .$$

(b) We have

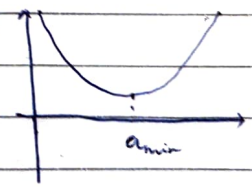
$$\psi(x) = \begin{cases} 2a^{3/2}x\,e^{-ax} & x \geq 0 \\ 0 & x < 0 \end{cases}$$

∴ According to Variational principle formulation, we try to minimize ~~the Ansatz $\psi(x)$ wrt to parameter 'a'~~ $E(a) = \langle\psi|H(a)|\psi\rangle$ wrt parameter 'a', on which the Hamiltonian $(H(a))$ and matrix element $E(a)$ are dependent since the true ~~value~~ energy,

$$E_0 \leq \langle\psi|H|\psi\rangle .$$

by minimizing the expression we can obtain a more tighter upper bound on E_0, ground state energy.

$$E(a) = \frac{a^2\hbar^2}{2m} + \frac{3}{2}\frac{mg}{a}$$



$$\frac{dE}{da} = 0 \Rightarrow \frac{2a\hbar^2}{2m} + \frac{-3}{2}\frac{mg}{a^2} = 0$$

$$\frac{a\hbar^2}{m} = \frac{3}{2}\frac{mg}{a^2} \Rightarrow a_{min} = \left(\frac{3}{2}\frac{m^2g}{\hbar^2}\right)^{1/3}$$

$$\therefore E_0 \leq E(a_{min}) = \frac{\hbar^2}{2m}\left(\frac{3m^2g}{2\hbar^2}\right)^{2/3} + \frac{3mg}{2}\left(\frac{2\hbar^2}{3m^2g}\right)^{1/3}$$

$$= \left[\frac{\hbar^2}{8m^3}\,\frac{9}{4}\,m^4 g^2\right]^{1/3} + 3\left[\frac{9}{8}\,m^4 g^2\,\frac{2^3}{4^3}\,\frac{\hbar^2}{m^3}\right]^{1/3}$$

$$= \left[\frac{9\hbar^2 m g^2}{32}\right]^{1/3} + 2\left[\frac{9}{32}\hbar^2 m g^2\right]^{1/3}$$

$$\Rightarrow \boxed{E_0 \leq 3\left(\frac{9}{32}\hbar^2 g^2 m\right)^{1/3}}$$

□

Q1)

$$H = \frac{1}{2m}(p_x^2 + p_y^2) + \frac{1}{2}m\omega^2(x^2+y^2) = H_x + H_y$$

(a) H, H_x.

We make use $[p_i, p_j] = 0 \quad i \neq j$

$[x_i, x_j] = 0 \quad i \neq j$

$\therefore$

Let $H \sim (p_x^2 + p_y^2) + (x^2+y^2)$

$H_x \sim p_x^2 + x^2$ (upto constants).

$$\therefore [H, H_x] = [p_x^2 + p_y^2 + x^2 + y^2,\ p_x^2 + x^2]$$

$$= [p_x^2 + x^2, p_x^2] + [p_x^2 + x^2, x^2]$$

(commute) (commute)

$$= [x^2, p_x^2] + [p_x^2, x^2] = 0$$

Hence proved.

(b) Hence we can choose eigenstates of H to be eigenstates of H_x.

The normalised w.f in ground st, 1st E.S is

$$\psi_0(x) = N_0 e^{-\alpha x^2/2}; \quad \psi_1(x) = \sqrt{2\alpha}\, x \psi_0(x)$$

Let $\Phi_{nm}(x,y) = \phi_n(x)\,\phi_m(y)$

(b) $L_z := x p_y - y p_x$ (x-y plane).

similarly (cyclic constants)

$$[L_z, H_x] = [x p_y - y p_x,\ p_x^2 + x^2]$$

$$= [x p_y, p_x^2] - [y p_x, x^2]$$

$$= [x, p_x^2]\, p_y - y\,[p_x, x^2]$$

$$= 2p_x(it)p_y + y\,(2x(it))$$

$$= 2it\,(p_x p_y + xy) \neq 0$$

D.

Similarly

$$[L, H_y] = [x p_y - y p_x,\ p_y^2 + y^2]$$

$$= [x p_y, y^2] - [y p_x, p_y^2]$$

$$= x\,[p_y, y^2] - [y, p_y^2]\,p_x$$

$$= x\,(2y(-it)) - [2p_y(it)]\,p_x$$

$$= -2it\,(xy + p_x p_y) \neq 0$$

Commutes

So,

$$[L, H] = [L, H_x] + [L, H_y] = 2it\,(p_x p_y + xy) - 2it\,(xy + p_x p_y)$$

$$= 0 \;!!$$

D.

$\Rightarrow$ L and H will have the same eigenstates

$\Rightarrow$ Eigenstates of H_r will have to be azimuthally symmetric (wrt X-Y plane). rotationally invariant).

(c) Note that, $\phi(x)$, $\phi(y)$ are 1D SHO, ~~solutions of~~ action under operator $\hat{H}$ of which, we already know.

~~$\hat{H}\,\Phi(x)$~~

$$H\,\Phi_{nm}(x,y) = (H_x + H_y)\,\Phi_n(x)\,\phi_m(y)$$

$$= \phi_m(y)\,H_x\,\phi_n(x) + \phi_n(x)\,H_y\,\phi_m(y)$$

$$= (n+\tfrac{1}{2})\hbar\omega\;\phi_m(y)\,\phi_n(x) + (m+\tfrac{1}{2})\hbar\omega\;\phi_n(x)\,\phi_m(y)$$

$$= (n+\tfrac{1}{2})\hbar\omega\;\Phi_{nm}(x,y) + (m+\tfrac{1}{2})\hbar\omega\;\Phi_{nm}(x,y)$$

$$= (n+m+1)\,\hbar\omega\;\Phi_{nm}(x,y)$$

$$= E_{nm}\,\Phi_{nm}(x,y).$$

$n,m \in \{0,1,2,3,\dots\} \equiv N_0$

Clearly $E_{00} = \hbar\omega \le E_{nm}$ $\forall\, n,m \in N_0$.

And so, $|0;0\rangle$ or $\Phi_{00}(x,y)$ is the ground state.

Now,

$E_{10} = E_{01} = 2\hbar\omega$

∴ we have a doubly ~~excited~~ degenerate 1st Excited state. $\equiv$ $\Phi_{10}(x,y)$ & $\Phi_{01}(x,y)$

2.

(d) Now, $H \longrightarrow H + H_1$

$H_1 = \lambda xy$ (Perturbation)

Excluding constants from 1-D SHO we can write,

$$\hat{a}_x \sim \hat{x} + i\hat{p}_x$$

$$\hat{a}_x^\dagger \sim \hat{x} - i\hat{p}_x$$

$$\therefore \hat{x} \sim a_x + a_x^\dagger \quad \& \quad \hat{y} \sim a_y + a_y^\dagger$$

∴ The Perturbing potential can be written as

$$H_1 V = \lambda' (a_x + a_x^\dagger)(a_y + a_y^\dagger)$$

Date
Page

The ground state is non-degenerate. ∴ The first order correction to the energy is

$$E_0^{(1)} = \langle 0,0|H_1|0,0\rangle$$

$$= \lambda' \langle 0,0|(a_x + a_x^\dagger)(a_y + a_y^\dagger)|0,0\rangle$$

a_y, a_x will annihilate $|0,0\rangle$ & $a_y^\dagger, a_x^\dagger$ will annihilate $\langle 0,0|$

$$= \lambda' (\langle 0,0| (a_x a_y + a_x a_y^\dagger + a_x^\dagger a_y + a_x^\dagger a_y^\dagger) |0,0\rangle)$$

$$= \lambda' (\langle 0,0| a_x a_y^\dagger |0,0\rangle)$$

$$\sim \langle 0,0| a_x |0,1\rangle = 0 ,$$

clearly, also all the terms in perturbing potential change both m and n, so their overlap must be zero.

Hence, upto 1st order in λ, the perturbed ground state energy does not change.

Degenerate Perturbation Theory

Let $H = H_0 + H_1$ (perturbed Hamiltonian).

~~where~~

$= H_0 + \lambda V$ $\quad V = xy$

$H_0 = H_x + H_y$

Let the wavefunction(s) of the 1st excited state (degenerate subspace) in this ~~perturbed~~ new Hamiltonian (H) be

$|\psi\rangle = \alpha \Phi_{10}(x,y) + \beta \Phi_{01}(x,y)$.

$|\psi\rangle = \alpha |1,0\rangle + \beta |0,1\rangle \Rightarrow$ This vectors span the subspace which has $E_{nm} = 2\hbar\omega$.

Clearly, $|\psi\rangle$ will also be an eigenvector of H_0.

Now, $(H_0 + \lambda V)|\psi\rangle = (E^{(0)} + \lambda E^{(1)} + \dots)|\psi\rangle$

$E^{(0)} = E_{nm}$

$V = xy$

Date | Page |

This leads to · (comparing coeff. of λ)

$$H_0|\psi\rangle = E_{nm}|\psi\rangle = E^{(0)}|\psi\rangle \quad \cdots ①$$

And

$$V|\psi\rangle = E^{(1)}|\psi\rangle \quad \cdots ①$$

$E^{(1)} \rightarrow$ 1st order correction in (E_{10} or E_{01}) 1st

The eq ① is satisfied for any value of α, β. excited state energy eigenvalue.

Taking inner product of eq① with $|1,0\rangle$ and $|0,1\rangle$ yields. (to find comp. α, β)

$$\langle 1,0| \left(V(\alpha|1,0\rangle + \beta|0,1\rangle) \right) = E^{(1)} \langle 1,0| \left(\alpha|1,0\rangle + \beta|0,1\rangle \right)$$

$$\Rightarrow \alpha \langle 1,0|V|1,0\rangle + \beta \langle 1,0|V|0,1\rangle = \alpha E^{(1)}$$

[$\because \langle 1,0|0,1\rangle = 0$ orthogonal!]

Similarly

$$\alpha \langle 0,1|V|1,0\rangle + \beta \langle 0,1|V|0,1\rangle = \beta E^{(1)}$$

The equations can be written as.

$$\begin{bmatrix} \langle 1,0|V|1,0\rangle & \langle 1,0|V|0,1\rangle \\ \langle 0,1|V|1,0\rangle & \langle 0,1|V|0,1\rangle \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = E^{(1)} \begin{bmatrix} \alpha \\ \beta \end{bmatrix}$$

$\Rightarrow$ Let us denote

$$|\psi_a\rangle = |1,0\rangle$$
$$|\psi_b\rangle = |0,1\rangle.$$

We can write the matrix elements as $W_{ab} = \langle \psi_a|V|\psi_b\rangle = \langle \psi_a|V\psi_b\rangle$

So, we have a familiar eigen problem,

$$\begin{bmatrix} W_{aa} & W_{ab} \\ W_{ba} & W_{bb} \end{bmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = E^{(1)} \begin{bmatrix} \alpha \\ \beta \end{bmatrix}$$

Clearly $V = xy$ is Hermitian!

$$\therefore W_{ab} = \langle \psi_a | V \psi_b \rangle = \langle V\psi_a | \psi_b \rangle = \langle \psi_b | V \psi_a \rangle^*$$

$$= W_{ba}^*$$

implying the matrix W is Hermitian

and hence $E^{(1)}$ should be real.

$\therefore$ Non-trivial solutions for $E^{(1)}$ require that.

$$\begin{vmatrix} W_{aa} - E^{(1)} & W_{ab} \\ W_{ba} & W_{bb} - E^{(1)} \end{vmatrix} = 0$$

$$(W_{aa} - E^{(1)})(W_{bb} - E^{(1)}) = W_{ab} \cdot W_{ba}.$$

$$E^{(1)2} - E^{(1)}(W_{aa} + W_{bb}) + W_{aa}W_{bb} = W_{ab}W_{ba}$$

$$\therefore E^{(1)} = \frac{W_{aa} + W_{bb} \pm \sqrt{(W_{aa} - W_{bb})^2 + 4 W_{ab}W_{ba}}}{2}.$$

Now, it remains to compute the matrix elements.

we have, $\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}\,(a_x + a_x^\dagger)$

$$\hat{y} = \sqrt{\frac{\hbar}{2m\omega}}\,(a_y + a_y^\dagger)$$

$V = \hat{x}\hat{y}$.

$\therefore W_{aa} = \frac{\hbar}{2m\omega}\left(\langle 1,0 | (a_x + a_x^\dagger)(a_y + a_y^\dagger) | 1,0 \rangle\right)$

(By inspection)

$= 0$

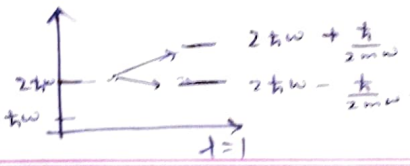
$$W_{bb} = \frac{\hbar}{2m\omega}\left(\langle 0,1 | (a_x + a_x^\dagger)(a_y + a_y^\dagger) | 0,1 \rangle\right)$$

$= 0$

$$W_{ab} = \frac{\hbar}{2m\omega}\left(\langle 1,0 | (a_x + a_x^\dagger)(a_y + a_y^\dagger) | 0,1 \rangle\right)$$

$$= \frac{\hbar}{2m\omega} = W_{ba}.$$

So, $E^{(1)}_{\pm} = \pm \frac{\hbar}{2m\omega}$ $\neq 0$ Thus the degeneracy is lifted!!



Along with Normalisability condition: $\sqrt{\alpha^2 + \beta^2} = 1$

For $E_+ = \frac{\hbar}{2m\omega}$	$E_- = -\frac{\hbar}{2m\omega}$.
$\alpha = \beta = \frac{1}{\sqrt{2}}$.	$\alpha = -\beta = \frac{-1}{\sqrt{2}}$.

So, the energy eigenstates of the perturbed Hamilton is

So, $|\psi_\pm\rangle = \frac{1}{\sqrt{2}}(|0,1\rangle \pm |1,0\rangle)$

$E'_\pm = 2\hbar\omega \pm \frac{\hbar}{2m\omega}$.

Degeneracy of 1st E-S is lifted

(f) Consider, $H_x \sim p_x^2 + x^2$

$H_1 \simeq \lambda xy$

$\therefore$

$[H_x, H_1] \simeq \lambda[p_x^2 + x^2, xy] = \lambda[p_x^2, x]y + [x^2, x]y$

$= \lambda 2p_x(-i\hbar)y$

$\neq 0$.

$[x^2, x] = 0$ $\because$ commute.

And

$[L, H_1] = [xp_y - yp_x, \lambda xy]$

$= \lambda([xp_y, xy] - [yp_x, xy])$

$= \lambda(x[p_y, xy] - y[p_x, xy])$.

$= \lambda(x^2[p_y, y] - y[p_x, x]y)$

$= \lambda(x^2(-i\hbar) + y^2(+i\hbar))$

$= \lambda i\hbar(y^2 - x^2) \neq 0$.

So, neither the eigenstates of H_x, nor L, will make diagonalisation of H_1 possible for $\lambda \neq 0$.

pg-4

Date
Page

1)f) Now, we consider the operation S of reflection about the line $x=y$

$Sx = yS, \quad Sy = xS.$

Then, $[S, H_1] = \lambda [S, xy]$

$= \lambda (Sxy - xyS)$

$= \lambda (ySy - xyS)$

($\because \hat{x}, \hat{y}$ commute!). $= \lambda (yxS - xyS) = 0$

Now, consider action of S on eigenstate.

$S \Phi_{01}(x,y) = \Phi_{01}(y,x)$

and

$S \Phi_{10}(x,y) = \Phi_{10}(y,x)$.

$\therefore S\Phi_{01}(x,y) = \phi_0(y)\phi_1(x)$

$= N_0 e^{-\alpha y^2/2} \left(\sqrt{2\alpha}\, x\, N_0 e^{-\alpha x^2/2}\right)$

$= N_0^2 \sqrt{2\alpha}\, x e^{-\frac{\alpha}{2}(y^2+x^2)} \quad \therefore = \Phi_{10}(x,y)$

Similarly,

$S \Phi_{10}(x,y) = N_0^2 \sqrt{2\alpha}\, y e^{-\frac{\alpha}{2}(y^2+x^2)} = \Phi_{01}(x,y)$.

Hence,

$S \frac{1}{\sqrt{2}} \left(\Phi_{01}(x,y) + \Phi_{10}(x,y)\right) = \frac{1}{\sqrt{2}} \left(\Phi_{10}(x,y) + \Phi_{01}(x,y)\right)$

$\therefore \Psi_+(x,y)$ is an eigenfunction of S with eigenvalue = 1

And

$S \frac{1}{\sqrt{2}} \left(\Phi_{01}(x,y) - \Phi_{10}(x,y)\right) = \frac{-1}{\sqrt{2}} \left(\Phi_{01} - \Phi_{10}\right)$

$= -\Psi_-$

So, $\Psi_-(x,y)$ is an eigenfunction of S, with eigenvalue -1