

$$\textcircled{1} a) \quad H\psi = E\psi \Rightarrow \left(-\frac{\hbar^2}{2m} \nabla^2 + V(x,y,z) \right) \psi = E\psi$$

Separation of variables: $\psi(x,y,z) = X(x)Y(y)Z(z)$

$$-\frac{\hbar^2}{2m} \left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right] XYZ = E XYZ \quad \text{for } 0 \leq x, y, z \leq d$$

$$-\frac{\hbar^2}{2m} \left[YZ \frac{\partial^2 X}{\partial x^2} + XZ \frac{\partial^2 Y}{\partial y^2} + XY \frac{\partial^2 Z}{\partial z^2} \right] = E XYZ$$

$$-\frac{\hbar^2}{2m} \left[\frac{1}{X} \frac{\partial^2 X}{\partial x^2} + \frac{1}{Y} \frac{\partial^2 Y}{\partial y^2} + \frac{1}{Z} \frac{\partial^2 Z}{\partial z^2} \right] = E$$

Solving for X :

$$-\frac{\hbar^2}{2m} \frac{1}{X} \frac{\partial^2 X}{\partial x^2} = \text{constant} = E_x \Rightarrow \frac{\partial^2 X}{\partial x^2} = -k_x^2 X$$

$$k_x = \frac{\sqrt{2mE_x}}{\hbar}$$

Solutions:

$$X(x) = A' \sin(k_x x) + B' \cos(k_x x)$$

$$X(x=0) = 0 \Rightarrow B' = 0$$

$$X(x=d) = 0 \Rightarrow A' \sin(k_x d) = 0 \Rightarrow k_x d = n\pi \Rightarrow k_x = n\pi/d$$

$$\text{So: } X = A' \sin\left(\frac{n\pi x}{d}\right) \quad \text{and similar for } Y \text{ and } Z.$$

$$\Rightarrow \psi(x,y,z) = A \sin\left(\frac{n\pi x}{d}\right) \sin\left(\frac{m\pi y}{d}\right) \sin\left(\frac{l\pi z}{d}\right)$$

To find the constant A (normalization):

$$\iiint |\psi|^2 d^3r = 1 \Rightarrow A^2 \int_0^d \sin^2\left(\frac{n\pi x}{d}\right) dx \int_0^d \sin^2\left(\frac{m\pi y}{d}\right) dy \int_0^d \sin^2\left(\frac{l\pi z}{d}\right) dz = 1$$

$$b) E_T = E_x + E_y + E_z = \frac{\hbar^2 \pi^2}{2md^2} (n^2 + m^2 + l^2) \quad n, m, l = 1, 2, 3, 4, \dots$$

$$E_1 \Rightarrow n=m=l=1 \Rightarrow E = \frac{3}{2} \frac{\hbar^2 \pi^2}{md^2} \quad \text{degeneracy } 1$$

$$E_2 \quad \begin{array}{ccc} n & m & l \\ 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{array}$$

$$E_2 = \frac{6}{2} \frac{\hbar^2 \pi^2}{md^2} \Rightarrow E_2 = 3 \frac{\hbar^2 \pi^2}{md^2}$$

deg. 3

$$E_3 \quad \begin{array}{ccc} n & m & l \\ 2 & 2 & 1 \\ 2 & 1 & 2 \\ 1 & 2 & 2 \end{array}$$

$$E_3 = \frac{9}{2} \frac{\hbar^2 \pi^2}{md^2}$$

deg. 3

$$E_4 \quad \begin{array}{l} n=m=l=2 \\ \text{deg. } 1 \end{array}$$

$$E_4 = \frac{12}{2} \frac{\hbar^2 \pi^2}{md^2} \Rightarrow E_4 = 6 \frac{\hbar^2 \pi^2}{md^2}$$

c) Possible spin states:

$$|s=0 \ m_s=0\rangle = \frac{1}{\sqrt{2}} [|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle] \quad \text{singlet (antisymmetric)}$$

$$|1 \ 1\rangle = |\uparrow\uparrow\rangle$$

$$|1 \ 0\rangle = \frac{1}{\sqrt{2}} [|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle]$$

$$|1 \ -1\rangle = |\downarrow\downarrow\rangle$$

} triplet (symmetric)

$$d) \psi_{a,b} = \psi_{11}^a \psi_{21}^b - \psi_{21}^a \psi_{11}^b$$

Upon particle exchange: $a \rightarrow b \quad b \rightarrow a$

$$\psi_{b,a} = \psi_{11}^b \psi_{21}^a - \psi_{21}^b \psi_{11}^a = -\psi_{a,b}$$

Antisymmetric.

Therefore, spin state should be one of the triplet states.

$$(2) a) \hat{A} \rightarrow \begin{pmatrix} a_1 & 0 \\ 0 & a_2 \end{pmatrix}$$

b) The system collapses to state $|\psi_1\rangle$.

$$c) |\phi_1\rangle = \frac{3}{5}|\psi_1\rangle + \frac{4}{5}|\psi_2\rangle \quad |\phi_2\rangle = \frac{4}{5}|\psi_1\rangle - \frac{3}{5}|\psi_2\rangle$$

Matrix elements given by: $\langle\psi_{1,2}|\hat{B}|\psi_{1,2}\rangle$

$$3|\phi_1\rangle + 4|\phi_2\rangle = \frac{9}{5}|\psi_1\rangle + \frac{12}{5}|\psi_2\rangle + \frac{16}{5}|\psi_1\rangle - \frac{12}{5}|\psi_2\rangle$$

$$3|\phi_1\rangle + 4|\phi_2\rangle = \frac{25}{5}|\psi_1\rangle \Rightarrow |\psi_1\rangle = \frac{3}{5}|\phi_1\rangle + \frac{4}{5}|\phi_2\rangle$$

$$4|\phi_1\rangle - 3|\phi_2\rangle = \frac{16}{5}|\psi_1\rangle - \frac{9}{5}|\psi_2\rangle - \frac{12}{5}|\psi_1\rangle + \frac{12}{5}|\psi_2\rangle$$

$$\langle\psi_1|\hat{B}|\psi_1\rangle = \frac{1}{25} [3\langle\phi_1| + 4\langle\phi_2|] \hat{B} [3|\phi_1\rangle + 4|\phi_2\rangle] = \frac{9}{25}b_1 + \frac{16}{25}b_2$$

$$\langle\psi_1|\hat{B}|\psi_2\rangle = \frac{1}{25} [3\langle\phi_1| + 4\langle\phi_2|] \hat{B} [4|\phi_1\rangle - 3|\phi_2\rangle] = \frac{12}{25}b_1 - \frac{12}{25}b_2$$

$$\langle\psi_2|\hat{B}|\psi_1\rangle = \frac{1}{25} [4\langle\phi_1| - 3\langle\phi_2|] \hat{B} [3|\phi_1\rangle + 4|\phi_2\rangle] = \frac{12}{25}b_1 - \frac{12}{25}b_2$$

$$\langle\psi_2|\hat{B}|\psi_2\rangle = \frac{1}{25} [4\langle\phi_1| - 3\langle\phi_2|] \hat{B} [4|\phi_1\rangle - 3|\phi_2\rangle] = \frac{16}{25}b_1 + \frac{9}{25}b_2$$

$$\hat{B} \rightarrow \begin{matrix} & \begin{matrix} |\psi_1\rangle & |\psi_2\rangle \end{matrix} \\ \begin{matrix} \langle\psi_1| \\ \langle\psi_2| \end{matrix} & \frac{1}{25} \begin{pmatrix} 9b_1 + 16b_2 & 12b_1 - 12b_2 \\ 12b_1 - 12b_2 & 16b_1 + 9b_2 \end{pmatrix} \end{matrix}$$

$$d) |\psi_2\rangle = \frac{4}{5}|\phi_1\rangle - \frac{3}{5}|\phi_2\rangle \Rightarrow \begin{matrix} b_1 \text{ with prob } \frac{16}{25} \\ b_2 \text{ with prob } \frac{9}{25} \end{matrix}$$

$$(3) a) a_{\pm} = \frac{1}{\sqrt{2\hbar m \omega}} (\mp i p + m \omega x)$$

$$a_{+} + a_{-} = \frac{2}{\sqrt{2\hbar m \omega}} m \omega x$$

$$a_{-} - a_{+} = \frac{2}{\sqrt{2\hbar m \omega}} i p$$

$$\Rightarrow x = \sqrt{\frac{\hbar}{2m\omega}} (a_{+} + a_{-})$$

$$\Rightarrow p = i \sqrt{\frac{\hbar m \omega}{2}} (a_{+} - a_{-})$$

Important!
 $a_{+} a_{-} \neq a_{-} a_{+}$

↓

$$x^2 = \left(\sqrt{\frac{\hbar}{2m\omega}} \right)^2 (a_{+} + a_{-})(a_{+} + a_{-}) = \left(\frac{\hbar}{2m\omega} \right) [a_{+}^2 + a_{+} a_{-} + a_{-} a_{+} + a_{-}^2]$$

$$p^2 = - \left(\frac{\hbar m \omega}{2} \right) [a_{+}^2 - a_{+} a_{-} - a_{-} a_{+} + a_{-}^2]$$

$$H = \frac{p^2}{2m} + \frac{m \omega^2 x^2}{2}$$

$$= - \frac{\hbar \omega}{4} [a_{+}^2 - a_{-} a_{+} - a_{+} a_{-} + a_{-}^2] + \frac{\hbar \omega}{4} [a_{+}^2 + a_{+} a_{-} + a_{-} a_{+} + a_{-}^2]$$

$$= \frac{\hbar \omega}{2} [a_{+} a_{-} + a_{-} a_{+}]$$

$$= \frac{\hbar \omega}{2} [a_{+} a_{-} + a_{+} a_{-} + 1]$$

Using $[a_{+}, a_{+}] = 0 \Rightarrow a_{+} a_{+} - a_{+} a_{+} = 0$
 $\Rightarrow a_{-} a_{+} = a_{+} a_{-} + 1$

$$\Rightarrow \hat{H} = \hbar \omega (a_{+} a_{-} + \frac{1}{2})$$

$$b) a_- \psi_0 = 0$$

$$\frac{1}{\sqrt{2\hbar m\omega}} \left(\hbar \frac{d}{dx} + m\omega x \right) \psi_0 = 0$$

$$\hbar \frac{d\psi_0}{dx} + m\omega x \psi_0 = 0 \Rightarrow \frac{d\psi_0}{dx} = -\frac{m\omega x}{\hbar} \psi_0$$

$$\int \frac{d\psi_0}{\psi_0} = -\frac{m\omega}{\hbar} \int x dx \Rightarrow \ln \psi_0 = -\frac{m\omega}{\hbar} \frac{x^2}{2} + C$$

$$\psi_0 = A e^{-\frac{m\omega}{2\hbar} x^2}$$

$$c) \langle H \rangle = ? \quad |\psi\rangle = \sqrt{\frac{2}{3}} |\psi_0\rangle + \sqrt{\frac{1}{3}} e^{i\pi/3} |\psi_1\rangle$$

$$\langle H \rangle = \langle \psi | \hat{H} | \psi \rangle \quad \text{or} \quad \int \psi^* \hat{H} \psi dx \quad (\text{dif. notation, same results})$$

$$= \left(\sqrt{\frac{2}{3}} \langle \psi_0 | + \sqrt{\frac{1}{3}} e^{-i\pi/3} \langle \psi_1 | \right) \left(\hbar\omega (a_+ a_- + \frac{1}{2}) \right) \left(\sqrt{\frac{2}{3}} |\psi_0\rangle + \sqrt{\frac{1}{3}} e^{i\pi/3} |\psi_1\rangle \right)$$

$$a_+ a_- |\psi_0\rangle = 0 \quad (\text{since } a_- |\psi_0\rangle = 0)$$

$$a_+ a_- |\psi_1\rangle = a_+ (\sqrt{1} |\psi_0\rangle) = \sqrt{0+1} |\psi_1\rangle = |\psi_1\rangle$$

$$\text{So: } \langle H \rangle = \left(\sqrt{\frac{2}{3}} \langle \psi_0 | + \sqrt{\frac{1}{3}} e^{-i\pi/3} \langle \psi_1 | \right) \left(\hbar\omega \left[\frac{1}{2} \sqrt{\frac{2}{3}} |\psi_0\rangle + \sqrt{\frac{1}{3}} e^{i\pi/3} \left(|\psi_1\rangle + \frac{1}{2} |\psi_1\rangle \right) \right] \right)$$

$$= \hbar\omega \left(\frac{1}{2} \frac{2}{3} \langle \psi_0 | \psi_0 \rangle + \frac{1}{3} \frac{3}{2} \langle \psi_1 | \psi_1 \rangle \right) = \hbar\omega \left(\frac{1}{3} + \frac{1}{2} \right)$$

$$\Rightarrow \boxed{\langle H \rangle = \frac{5}{6} \hbar\omega}$$

d) t-ev. operator $\hat{U} = e^{i\hat{H}t/\hbar}$

$$\Psi(x, t=0) = \sqrt{\frac{2}{3}} \Psi_0 + \sqrt{\frac{1}{3}} e^{i\pi/3} \Psi_1$$

$$E_n = \hbar\omega(n + 1/2) \quad n = 0, 1, 2, \dots$$

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

$$\Psi(x, t) = \sqrt{\frac{2}{3}} e^{iE_0 t/\hbar} \Psi_0 + \sqrt{\frac{1}{3}} e^{i\pi/3} e^{iE_1 t/\hbar} \Psi_1$$

$$= \sqrt{\frac{2}{3}} e^{i\frac{\hbar\omega t}{2\hbar}} \Psi_0 + \sqrt{\frac{1}{3}} e^{i(\pi/3 + \frac{3}{2}\hbar\omega t/\hbar)} \Psi_1$$

$$\boxed{\Psi(x, t) = \sqrt{\frac{2}{3}} e^{i\frac{\omega}{2}t} \Psi_0 + \sqrt{\frac{1}{3}} e^{i(\frac{3\omega}{2}t + \pi/3)} \Psi_1}$$