PYL 101

Electromagnetic waves and Quantum Mechanics

Tutorial sheet - 2

[L-3 & 4]

Ans. 2. Time independent Schrodinger's Equation -

$$-\frac{\hbar^2}{2m}\nabla^2\psi(r,t) + V(r,t)\psi(r,t) = i\hbar\frac{\partial\psi(r,t)}{\partial t}$$

For free particle $V(r,t) = 0$

$$\boxed{-\frac{\hbar^2}{2m}\nabla^2\psi(r,t) = i\hbar\frac{\partial\psi(r,t)}{\partial t}} \quad \text{--- (1)}$$

Now Time evolution of system -

$|\psi(t_0)\rangle \rightarrow$ initial state

$|\psi(t)\rangle \rightarrow$ at later time $t$

we can write $|\psi(t)\rangle = \hat{U}(t, t_0)|\psi(t_0)\rangle$ --- (2)

Substitute in above Equation -

$$-\frac{i}{\hbar} H\, U(t, t_0) = \frac{d}{dt}U(t, t_0)$$

where $\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + \hat{V}$

On integrating above Equation -

$$U(t, t_0) = e^{-i(t-t_0)H/\hbar}$$

$$\boxed{|\psi(t)\rangle = e^{-i(t-t_0)H/\hbar}\,|\psi(t_0)\rangle}$$

Ans.

Ans (3) Given wavefunction -

$$\psi(x,0) = \frac{A}{\sqrt{a}} \sin\left(\frac{\pi x}{a}\right) + \sqrt{\frac{3}{5a}} \sin\left(\frac{3\pi x}{a}\right) + \frac{1}{\sqrt{5a}} \sin\left(\frac{5\pi x}{a}\right)$$

compare above Equation by General Equation of wavefunction for 1 dim. Infinite potential well -

$$\phi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)$$

Above Equation can be written as -

$$\psi(x,0) = \frac{A}{\sqrt{2}} \phi_1(x) + \sqrt{\frac{3}{10}} \phi_3(x) + \frac{1}{\sqrt{10}} \phi_5(x)$$

as $\phi_1(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{\pi x}{a}\right)$

$\phi_3(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{3\pi x}{a}\right)$

$\phi_5(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{5\pi x}{a}\right)$

Now using Normalization condition -

$$\int_{-\infty}^{\infty} \psi^*(x,0)\, \psi(x,0)\, dx = 1$$

and orthonormalization condition -

$$\langle \phi_m(x) | \phi_n(x) \rangle = \delta_{mn} = \begin{cases} 1 & m=n \\ 0 & m \neq n \end{cases}$$

$$\left(\frac{A}{\sqrt{2}}\right)^2 + \left(\sqrt{\frac{3}{10}}\right)^2 + \left(\frac{1}{\sqrt{10}}\right)^2 = 1$$

$$\boxed{A = \sqrt{\frac{6}{5}}}$$

$$\boxed{\psi(x,0) = \sqrt{\frac{6}{5a}} \sin\left(\frac{\pi x}{a}\right) + \sqrt{\frac{3}{5a}} \sin\left(\frac{3\pi x}{a}\right) + \frac{1}{\sqrt{5a}} \sin\left(\frac{5\pi x}{a}\right)}$$

Ans (4)(8).
(4) Find state vector at time t by —

$$|\psi(t)\rangle = e^{-i(t-t_0)\frac{H}{\hbar}}|\psi(t_0)\rangle$$

$|\psi(t_0)\rangle =$

$$\psi(x,0) = \sqrt{\frac{6}{5a}}\sin\left(\frac{\pi x}{a}\right) + \sqrt{\frac{3}{5a}}\sin\left(\frac{3\pi x}{a}\right) + \frac{1}{\sqrt{5a}}\sin\left(\frac{5\pi x}{a}\right)$$

1st Excited state — 3rd E.S. — 5th E.S.

Energy value corresponding to 1st, 3rd, 5th Excited state will be $E_1, E_3$, and $E_5$ respectively.

Now using time evolution operator — wavefunction can be written at time t —

$$\psi(x,t) = \sqrt{\frac{6}{5a}}\sin\left(\frac{\pi x}{a}\right)e^{-i\frac{E_1 t}{\hbar}} + \sqrt{\frac{3}{5a}}\sin\left(\frac{3\pi x}{a}\right)e^{-iE_3 t/\hbar} + \frac{1}{\sqrt{5a}}\sin\left(\frac{5\pi x}{a}\right)e^{-iE_5 t/\hbar}$$

Now $\boxed{\text{Probability density} = \psi^*(x,t)\cdot\psi(x,t).}$

above wavefunction can be written as —

$$\psi(x,t) = \sqrt{\frac{3}{5}}\phi_1(x)e^{-iE_1 t/\hbar} + \sqrt{\frac{3}{10}}\phi_3(x)e^{-iE_3 t/\hbar} + \sqrt{\frac{1}{10}}\phi_5(x)e^{-iE_5 t/\hbar}$$

$$\rho = \psi^*(x,t)\,\psi(x,t)$$

$$\begin{aligned}
\rho = {} & \left(\frac{3}{5}\right)\phi_1^2(x) + \sqrt{\frac{3}{5}}\sqrt{\frac{3}{10}}\phi_1(x)\phi_3(x)e^{i(E_3-E_1)t/\hbar} \\
& + \sqrt{\frac{3}{5}}\sqrt{\frac{1}{10}}\phi_1(x)\phi_5(x)e^{i(E_5-E_1)t/\hbar} \\
& + \sqrt{\frac{3}{10}}\sqrt{\frac{3}{5}}\phi_3(x)\phi_1(x)e^{-i(E_3-E_1)t/\hbar} + \frac{3}{10}\phi_3^2(x) \\
& + \sqrt{\frac{3}{10}}\sqrt{\frac{1}{10}}\phi_3(x)\phi_5(x)e^{i(E_5-E_3)t/\hbar} \\
& + \sqrt{\frac{1}{10}}\sqrt{\frac{3}{5}}\phi_5(x)\phi_1(x)e^{-i(E_5-E_1)t/\hbar} \\
& + \sqrt{\frac{1}{10}}\sqrt{\frac{3}{10}}\phi_3(x)\phi_5(x)e^{-i(E_5-E_3)t/\hbar} + \frac{1}{10}\phi_5^2(x).
\end{aligned}$$

Now using Relation $E_n = \frac{n^2\pi^2\hbar^2}{(2ma)^2}$

$E_1 = \frac{\hbar^2\pi^2}{2ma^2} \quad E_3 = \frac{9\hbar^2\pi^2}{2ma^2} \quad E_5 = 25\frac{\pi^2\hbar^2}{2ma^2}$

$E_3 = 9E_1$

$E_5 = 25E_1$

Using above Relation and we can rewrite the Equation as

$$\rho = \left(\frac{3}{5}\right)\phi_1^2(x) + \left(\frac{3}{10}\right)\phi_3^2(x) + \left(\frac{1}{10}\right)\phi_5^2(x) + \sqrt{\frac{3}{5}}\sqrt{\frac{3}{10}}\,\phi_1\phi_3\left[e^{i8E_1t/\hbar} + e^{-i8E_1t/\hbar}\right]$$
$$+ \sqrt{\frac{1}{10}}\sqrt{\frac{3}{5}}\,\phi_1(x)\phi_5(x)\left[e^{i24E_1t/\hbar} + e^{-i24E_1t/\hbar}\right]$$
$$+ \sqrt{\frac{1}{10}}\sqrt{\frac{3}{10}}\,\phi_3(x)\phi_5(x)\left[e^{i16E_1t/\hbar} + e^{-i16E_1t/\hbar}\right]$$

$$\rho = \frac{3}{5}\phi_1^2(x) + \frac{3}{10}\phi_3^2(x) + \frac{1}{10}\phi_5^2(x) + \sqrt{\frac{3}{10}}\sqrt{\frac{3}{5}}\,\phi_1\phi_3\;2\cos\left(\frac{8E_1t}{\hbar}\right)$$
$$+ \sqrt{\frac{1}{10}}\sqrt{\frac{3}{5}}\,\phi_1(x)\phi_5(x)\;2\cos\left(\frac{24E_1t}{\hbar}\right)$$
$$+ \sqrt{\frac{1}{10}}\sqrt{\frac{3}{10}}\,\phi_3(x)\phi_5(x)\;2\cos\left(\frac{16E_1t}{\hbar}\right)$$

By substituting values of $\phi_1, \phi_3, \phi_5$ we get –

$$\rho = \frac{6}{5a}\sin^2\left(\frac{\pi x}{a}\right) + \frac{3}{5a}\sin^2\left(\frac{3\pi x}{a}\right) + \frac{1}{5a}\sin^2\left(\frac{5\pi x}{a}\right)$$
$$+ \frac{6\sqrt{2}}{5a}\sin\left(\frac{\pi x}{a}\right)\sin\left(\frac{3\pi x}{a}\right)\cos\left(\frac{8E_1t}{\hbar}\right)$$
$$+ \frac{2\sqrt{6}}{5a}\sin\left(\frac{\pi x}{a}\right)\sin\left(\frac{5\pi x}{a}\right)\cos\left(\frac{16E_1t}{\hbar}\right)$$
$$+ \frac{2\sqrt{3}}{5a}\sin\left(\frac{3\pi x}{a}\right)\sin\left(\frac{5\pi x}{a}\right)\cos\left(\frac{24E_1t}{\hbar}\right)$$

Ans

Ans (5).

$$\psi(x,t) = \sin\left(\frac{\pi x}{4}\right)e^{-i\omega t}$$

Find $\frac{d\psi}{dx}$, $\frac{d^2\psi}{dx^2}$ and $\frac{d\psi}{dt}$ and substitute all the values in time dependent schrodinger's Equation –

$$\frac{\partial\psi}{\partial t} = (-i\omega)\,\psi(x,t) =$$

$$\frac{\partial\psi}{\partial x} = \left(\frac{\pi}{4}\right)\cos\left(\frac{\pi x}{4}\right)e^{-i\omega t}$$

$$\frac{\partial^2\psi}{\partial x^2} = -\frac{\pi^2}{(4)^2}\sin\left(\frac{\pi x}{4}\right)e^{-i\omega t}.$$

Time dep. Schrodinger Equation in 1 dim –

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = \frac{-\hbar^2}{2m}\left[\frac{\partial^2\psi(x,t)}{\partial x^2}\right] + \hat{V}(x,t)\,\psi(x,t)$$

Now

$$i\hbar(-i\omega)\,\psi(x,t) = -\frac{\hbar^2}{2m}\left[-\frac{\pi^2}{(4)^2}\psi(x,t)\right] + \hat{V}(x,t)\,\psi(x,t)$$

$$\hbar\omega\,\psi(x,t) = \frac{\pi^2\hbar^2}{2m(4)^2}\psi(x,t) + \hat{V}\,(\psi(x,t))$$

$$\left(\hbar\omega - \frac{\pi^2\hbar^2}{2m(4)^2}\right)\psi(x,t) = \hat{V}(x,t)\,\psi(x,t)$$

$$\boxed{\hat{V}(x,t) = \left[\hbar\omega - \frac{\pi\hbar^2}{32m}\right]}$$ Ans.

Ans (6) Probability of finding the particle in given region –

$$P = \frac{\int_1^3 |\psi(x)|^2\,dx}{\int_0^4 |\psi(x)|^2\,dx} \quad \text{where } |\psi(x)|^2 = \psi^*(x)\,\psi(x).$$

Denominator function is used to Normalize the wavefunction.

Ans (7). $\Delta x . \Delta p \geq \frac{\hbar}{2}$ Uncertainity Relation.

For Ground state of Hydrogen Atom –

$$\Delta x . \Delta p \sim \hbar$$

maximum uncertainity in position is $r$ (radius of orbit)

$$\Delta x \rightarrow r$$

$$r . \Delta p \sim \hbar$$

$$\Delta p \sim \frac{\hbar}{r} \quad \text{[uncertainity in momentum]}$$

The minimum value of momentum cannot be less than the uncertainity of momentum thus

$$p \sim \frac{\hbar}{r}$$

Now Electron proton Energy –

$$E(r) = \frac{p^2}{2m_e} - \frac{e^2}{4\pi\epsilon_0 r} = \frac{\hbar^2}{2m_e r^2} - \frac{e^2}{4\pi\epsilon_0 r}.$$

At ground state, electron proton energy must be minimum Thus –

$$\frac{dE(r)}{dr} = 0 \quad \text{at } r = r_0.$$

After solving this $\boxed{r_0 = 0.53 \text{ nm}}$

Now Energy value can be calculated by above Energy relation –

$$\boxed{E(r) = -13.6 \text{ eV}}$$

Ans. (8). Energy of Electron in hydrogen atom -

$$\boxed{E_n = -\frac{R_H}{(n)^2}}$$ where $R_H \rightarrow$ Rydberg constant -

Ground state Energy $E_0 = -\frac{R_H}{(1)^2}$

$$E_0 = -13.6\ eV$$

First Excited state energy $E_1 = -\frac{R_H}{(2)^2} = -3.4\ eV$.

Now De Broglie wavelength -

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2mE}}$$

$$\lambda_0 = \frac{h}{\sqrt{2mE_0}}$$

mass of electron -

$m_e = 9.109 \times 10^{-31}$ kg

Plank's constant -

$h = 6.63 \times 10^{-34}\ m^2 kg/s$.

$$\boxed{\lambda_0 = 3.329\ A^\circ}$$

Ans (9).

Energy for First Excited state

$$\boxed{E_1 = -3.4\ eV}$$

De - Broglie wavelength for First Excited state -

$$\lambda_1 = \frac{h}{\sqrt{2mE_1}} = 6.659\ A^\circ$$

$$\boxed{\lambda_1 = 6.659\ A^\circ}$$ Ans

# Harmonic Oscillator

Ans. (10). Energy Eigen Value -

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

where $n = 0, 1, 2, 3 \ldots$

As. $\omega = \sqrt{\frac{k}{m}} \rightarrow \omega \propto \frac{1}{\sqrt{m}}$

For mass m particle -

$\omega_1 \propto \frac{1}{\sqrt{m}}$

$E_n = \left(n+\frac{1}{2}\right)\hbar\omega_1$

$E_1 = \frac{1}{2}\hbar\omega$

$E_2 = \frac{3}{2}\hbar\omega$

$\vdots$

$\Delta E = \hbar\omega$

For mass 4m particle -

$\omega_2 \propto \frac{1}{\sqrt{4m}} \rightarrow \frac{1}{2\sqrt{m}} \rightarrow \frac{\omega_1}{2}$

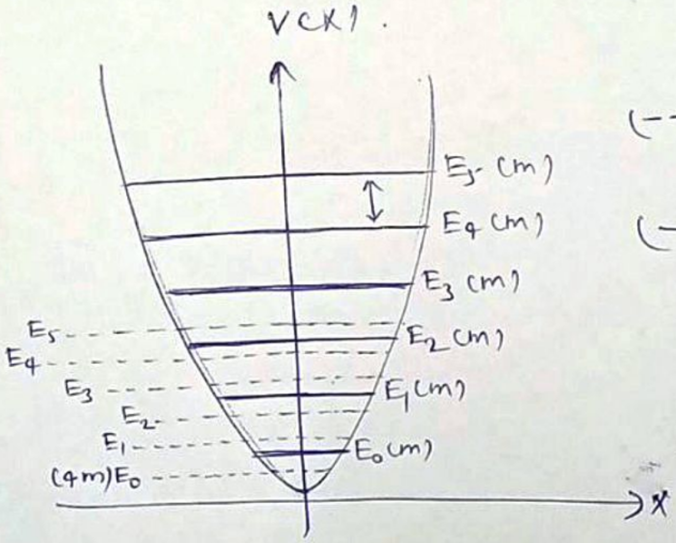
$E_n = \left(n+\frac{1}{2}\right)\hbar\frac{\omega_1}{2}$

$E_1 = \frac{1}{4}\hbar\omega$

$E_2 = \frac{3}{4}\hbar\omega$

$\vdots$

$\Delta E = \frac{1}{2}\hbar\omega.$




(-----) Represent - Energy For mass 4m

(——) Energy For mass m. particle