Photon and matter wave :-

Syllabus:-

photon, group velocity and phase velocity, de-Broglie's wavelength, Schrodinger wave eqn, 1-d potential well, tunnelling effect.

Q. Explain the physical significance of wave function (Ψ). Discuss the Eigen function of the particle travelling in 1-D box of infinite height. [9 marks].

Q. What is the physical significance of wave function (Ψ)? Derive the Schrodinger time independent wave equation for a free particle like electron. [9 marks].

Q. What is the wave function. Derive the Schrodinger time independent wave equation for free particle like electron.

Quantization of energy:-

Energy of electromagnetic radiation is quantized. Electromagnetic radiation has photons each of energy $= hf$; where $h =$ plank's constant $= 6.63 \times 10^{-34}$ J s

f is frequency.

i.e. energy of a photon.

$E = hf$.

Also, $E = \hbar\omega$. where, $\hbar = \frac{h}{2\pi}$.

$\omega = 2\pi f$. , angular frequency.

If there are 'n' no. of photons than total energy is given by.

$E_n = n\,hf$

De-Broglie wave:-

Since, a light or electromagnetic wave shows particle nature, matter in motion should also resemble wave nature. This is De-Broglie hypothesis. This kind of wave associated with the matter in motion is called De-Broglie wave or matter wave.

From Einstein's mass energy relation

$$E = mc^2 \quad \text{—— (I)}$$

Also, a photon has energy, $E = hf$ —— (II).

From (I) + (II),

$$mc^2 = hf = \frac{hc}{\lambda}.$$

or, $mc = \frac{h}{\lambda}$.

or, $p = \frac{h}{\lambda}$, p = momentum = mc.

$$\boxed{\therefore \lambda = \frac{h}{p}}$$

Here, λ is called de-Broglie wavelength.

For a particle, moving with velocity v,

$p = mv$.

$$\boxed{\lambda = \frac{h}{p} = \frac{h}{mv}}$$

De-Broglie wavelength for an electron :-

For electron, $\lambda = \frac{h}{p}$, where m = mass of electron.

v = velocity of electron.

To find v :-

let the electron be accelerated through p.d. such that it gains K.E. $K.E = \frac{1}{2}mv^2$

Then,

P.E. = K.E. gained

or, $eV = \frac{1}{2}mv^2$, V = potential

$$\therefore v = \sqrt{\frac{2eV}{m}} \quad \text{——— (II)}$$

From (I) & (II),

$$\lambda = \frac{h}{m\sqrt{\frac{2eV}{m}}} = \frac{h}{\sqrt{2m \times K.E.}}$$

$$\boxed{\therefore \lambda \propto \frac{1}{\sqrt{V}}}$$

Heisenberg's uncertainity principle :-

It states that canonically conjugate pairs or variable cannot be determined simultaneously and accurately. linear momentum and position (or linear displacement); energy & time; Angular momentum & angular displacement are called conjugate pairs or variable. The more accurately one tries to determine one quantity, the less accurately the other will be and vice-versa.

In case of position and momentum, when position is determined accurately, there will be inaccuracy for the simultaneous measurement of momentum.

By Heisenberg's uncertainity principle,

$$\Delta x \cdot \Delta p \geq \hbar \left(\text{or } \frac{h}{2\pi} \right).$$

$I = \frac{e}{t} = ef$

$\Delta E \cdot \Delta t \geq \hbar \left(\text{or } \frac{h}{2\pi} \right)$.

$\Delta L \cdot \Delta \theta \geq \hbar \left(\text{or } \frac{h}{2\pi} \right)$

Q. In the Bohr's model of hydrogen atom, the electron circulates around nucleus in the path of radius 5.1×10^{-11} m. atom at a frequency of 6.8×10^{15} rev/sec. What is the value of magnetic field?

Q. What are phase velocity and group velocity. Derive the relation between them.

⇒ The displacement of a vibrating particle is given by.

$y = A\cos(\omega t - Kx)$ —— (I)

where, $\omega = 2\pi f = \frac{2\pi}{\lambda} \times \lambda f$.

$= K v_p$.

where, $v_p = \lambda f$ is the phase or wave velocity.

Also, $K = \frac{2\pi}{\lambda}$

$v_p = \frac{\omega}{K}$.

If a group of waves superimpose to eachother, we define the group velocity, denoted by v_g.

It is defined by $v_g = \frac{d\omega}{dK}$.

The new displacement equation superimpose with (I) may be of the type

$y' = A\cos[(\omega + d\omega)t - (K + dK)x]$ —— (II)

The resultant wave is given by

$y = y + y'$

$= 2A\cos(\omega t - Kx) \cdot \cos\frac{1}{2}(d\omega t - dKx)$ —— (III)

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This represents a wave of angular frequency ω and wave number k_0 that has superimpose with modulation of angular frequency $\frac{d\omega}{2}$ and wave number $\frac{dk}{2}$

Relation between v_p + v_g :-

Since, $v_p = \frac{\omega}{k}$ + $v_g = \frac{d\omega}{dk}$

where, $\omega = 2\pi f = \frac{2\pi}{\lambda} \times \lambda f = k v_p$.

Here, $v_p = f(\lambda)$

$v_g = f(\lambda)$

Now, Differentiating $\omega = \frac{2\pi}{\lambda} v_p$ w.r.t. λ, we get

$$\frac{d\omega}{d\lambda} = 2\pi \left[\frac{d\lambda^{-1}}{d\lambda} v_p + \frac{1}{\lambda} \frac{dv_p}{d\lambda} \right]$$

$$= \frac{-2\pi}{\lambda^2} \left[v_p - \lambda \frac{dv_p}{d\lambda} \right]$$

And, $\frac{dk}{d\lambda} = \frac{-2\pi}{\lambda^2}$ $\left[\because k = \frac{2\pi}{\lambda} \right]$

Since, $v_g = \frac{d\omega}{dk}$

$$= \frac{d\omega/d\lambda}{dk/d\lambda}$$

$$\boxed{\therefore v_g = v_p - \lambda \frac{dv_p}{d\lambda}}$$

This is the required relation between group velocity and phase velocity.

$e^{i\theta} = \cos\theta + i\sin\theta$
$e^{-i\theta} = \cos\theta - i\sin\theta.$

Cases:-

① For the dispersive medium,

$$v_p = f(\lambda)$$

& usually, $\frac{dv_p}{d\lambda}$ is +ve

$\therefore v_g < v_p.$

This is the case with de-broglie waves or matter waves.

② For the non-dispersive medium,

$$v_p \neq f(\lambda)$$

$$\frac{dv_p}{d\lambda} = 0$$

$\therefore v_g = v_p$

This is the case with electromagnetic wave with vaccum.

Significance of wave function:-

A wave function or state function or the eigen function is denoted by ψ (psi). It describes the state of particle. It may be displacement, energy, momentum, etc. The product of ψ with it's complex conjugate (ψ^*) gives the probability density i.e. $\psi^*\psi = |\psi|^2$ gives the probability of finding the particle like an electron in a certain region in a certain time. This is the statistical interpretation of the wave function (ψ) i.e.

$$\text{probability} = \int \psi^* \psi \, dx \quad (\text{in } 1\text{-d}).$$

In 3-d,

$$\text{probability} = \int \psi^* \psi \, dV.$$

If the particle is certain to be found in a region from a to b.

$$\int_a^b \psi^* \psi \, dx = 1.$$

This is the normalization condition.
The wave function obtained from above condition is called Normalized wave function.

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Schroendiger wave equation :-

① Time independent equation:-

let, the wave function be
$$\psi = A e^{-i(\omega t - Kx)} \quad \text{—— (I)}.$$

Now, differentiating (I) w.r.t. 'x', we get,
$$\frac{d\psi}{dx} = A \cdot e^{-i(\omega t - Kx)} (-i) \cdot (-K)$$
$$= (iK) A e^{-i(\omega t - Kx)}.$$

Again, diff w.r.t. 'x', we get.
$$\frac{d^2\psi}{dx^2} = (iK)^2 A e^{-i(\omega t - Kx)}$$
$$= -K^2 \psi. \quad [\because i^2 = -1] \quad \text{—— (II)}$$

Since, momentum of the particle is given by
$$p = \hbar K \quad [\because p = \hbar K]$$
$$= \frac{h}{\lambda}$$

Then, eqn (II) becomes,
$$\frac{d^2\psi}{dx^2} = -K^2 \psi.$$
$$= \frac{-\hbar^2 K^2}{\hbar^2} \psi.$$
$$= \frac{-p^2 \psi}{\hbar^2}$$
$$= -\frac{p^2 \psi}{\hbar^2}$$

$$\therefore \boxed{p^2\psi = -\hbar^2 \frac{d^2\psi}{dx^2}} \quad \text{——— (III)}$$

Now,

The total energy of the particle is given by

$$E = K.E + P.E$$

$$= \frac{p^2}{2m} + V \quad \left[\because K.E = \frac{1}{2}mv^2 = \frac{1}{2}\frac{p^2}{m}\right]$$

Now, operating this eqn with ψ.

From right side,

$$\cancel{\frac{d^2\psi}{dx^2}} \quad E\psi = \frac{1}{2m} p^2\psi + V\psi$$

$$\text{or,} \quad E\psi = \frac{1}{2m}\left(-\hbar^2 \frac{d^2\psi}{dx^2}\right) + V\psi \quad [\because \text{using (III)}]$$

$$\therefore \boxed{E\psi = \frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi}$$

This is the schorendiger time independent equation.

Also,

$$\frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi = E\psi$$

$$\text{or,} \quad \boxed{\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E - V)\psi = 0}$$

This is the Schroendiger's time independent equation in the standard form in 1-D.

For 3-d,

$$\boxed{\nabla^2\psi + \frac{2m}{\hbar^2}(E - V)\psi = 0}$$

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(II) Schrodinger time dependent equation.

let, the wave function be.

$$\psi = Ae^{-i(\omega t - kx)} \quad \text{---} \text{(I)}$$

Diff w.r.t 'x'

$$\frac{d\psi}{dx} = Ae^{-i(\omega t - kx)}(-i)(-k).$$

$$= (ik)Ae^{-i(\omega t - kx)}$$

Differentiating w.r.t. (x)

$$\frac{d^2\psi}{dx^2} = (ik)^2 Ae^{-i(\omega t - kx)}$$

$$= -k^2 Ae^{-i(\omega t - kx)} \quad \text{---} \text{(II)}$$

Since, momentum of particle is given by

$$p = \hbar k$$

$\therefore$ eq^n (II) becomes

$$\frac{d^2\psi}{dx^2} = -k^2\psi$$

$$= \frac{-\hbar^2 k^2 \psi}{\hbar^2}$$

$$= \frac{-p^2\psi}{\hbar^2}$$

$$\therefore \quad -p^2\psi = \frac{-\hbar^2 d^2\psi}{dx^2} \quad \text{---} \text{(III)}$$

From (I),

$$\psi = Ae^{-i(\omega t - kx)}$$

Since, $E = \hbar\omega$

$$\therefore \omega = \frac{E}{\hbar}$$

and, $p = \hbar k$, momentum of particle.

$$\therefore k = \frac{p}{\hbar}$$

$\therefore \psi = Ae^{-i\left[(E/\hbar)t - (P/\hbar)x\right]}$

$= Ae^{-i/\hbar(Et - Px)}$

Now, differentiating w.r.t. time 't', we get

$$\frac{d\psi}{dt} = Ae^{-i/\hbar(Et-Px)}\left(-\frac{i}{\hbar}E\right).$$

$$= \frac{-i}{\hbar}E\psi$$

or, $E\psi = -\frac{\hbar}{i}\frac{d\psi}{dt}$

$$\boxed{\therefore E\psi = \frac{i^2\hbar}{i} \times \frac{d\psi}{dt}} \Rightarrow \boxed{E\psi = i\hbar \times \frac{d\psi}{dt}}$$

Now, the total energy of the particles is given by

$E = K.E + P.E$

$= \frac{p^2}{2m} + V.$

Operating by ψ from R.H.S,

$E\psi = \frac{1}{2m}p^2\psi + V\psi.$

$$E\psi = \frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi$$

or, $$\boxed{i\hbar\frac{d\psi}{dt} = -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi.}$$

This is the Schorendiger time dependent equation

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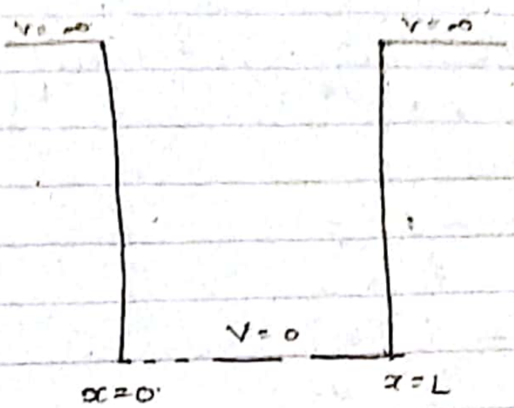
Particle in a 1-D potential well (or box):-

Consider, an infinite potential well or box of length L for which the potential is given by

$V = 0$ for $0 < x < L$

$= \infty$ for $x < 0$, $x \geq L$



Now,

For the well, schrodinger time independent equation is

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E-V)\psi = 0$$

But, $V = 0$

$$\therefore \frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}E\psi = 0$$

or, $\boxed{\dfrac{d^2\psi}{dx^2} + K^2\psi = 0}$, where, $K^2 = \dfrac{2mE}{\hbar^2}$

$$\therefore K = \sqrt{\frac{2mE}{\hbar^2}}$$

The solution of this eq^n is

$$\psi(x) = A\sin Kx + B\cos Kx \quad \text{——— (I)}$$

At $x = 0$, $\psi(x) = 0$.

$\therefore$ eq^n (I) becomes,

$$0 = A\sin 0 + B\cos 0$$

$$0 = A \cdot 0 + B \cdot 1$$

$$\therefore B = 0$$

So, eq^n (I) becomes,

$$\psi(x) = A\sin Kx \quad \text{——— (II)}$$

Again, at $x = L$, $\psi(x) = 0$

$\psi(x) = e^{ix}$
$\psi^*(x) = e^{-ix}$.

$\therefore 0 = A\sin KL$

$\therefore \sin KL = 0 = \sin n\pi$, $n = 1, 2, \ldots$

$\therefore KL = n\pi$

So, $\therefore K = \frac{n\pi}{L}$ — (ii).

Hence, the wave function is

$$\boxed{\psi(x) = A\sin\left(\frac{n\pi}{L}\right)x}$$

Since, the particle is sured to be found between 0 to L. Then, probability of finding the particle from $x = 0$ to $x = L$.

$$\int_0^L \psi^*(x)\,\psi(x)\,dx = 1 \qquad \left[\because \int_a^b |\psi|^2\,dx = 1\right].$$

or, $\displaystyle\int_0^L A^2\sin^2\left(\frac{n\pi}{L}\right)x\,dx = 1$

or, $\displaystyle\frac{A^2}{2}\int_0^L \left[1 - \cos\left(\frac{2n\pi}{L}\right)x\right]dx = 1 \qquad \left(\because \cos 2\theta = 1 - 2\sin^2\theta\right)$.

or, $\displaystyle\frac{A^2}{2}\left[\int_0^L dx - \int_0^L \cos\left(\frac{2n\pi}{L}\right)x\,dx\right] = 1$.

or, $\displaystyle\frac{A^2}{2}\left[L - \left|\frac{\sin\left(\frac{2n\pi}{L}\right)x}{\frac{2n\pi}{L}}\right|_0^L\right] = 1$.

or, $\frac{A^2}{2}\cdot L = 1$.

or, $A = \sqrt{\frac{2}{L}}$

Hence, the normalized wave function is

$$\boxed{\psi(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}\right)x}$$

And now energy of particle is given by

$$k^2 = \frac{2mE}{\hbar^2}$$

or, $$\left(\frac{n\pi}{L}\right)^2 = \frac{2mE}{\hbar^2}$$

or, $$\frac{n^2\pi^2}{L^2} = \frac{2mE}{\hbar^2}$$

$$\boxed{\text{or, } E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}}$$

or, $$E_n = \frac{n^2h^2}{8mL^2} \quad \left[\because \hbar = \frac{h}{2\pi}\right]$$

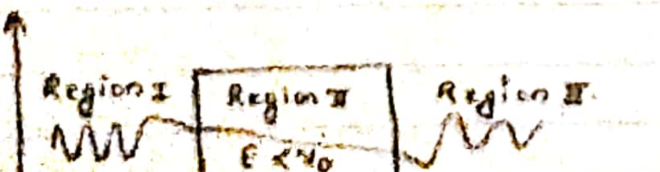
This is the required energy of the particle in the well or box of length (L)

Here, $E_n \propto n^2$, $n = 1, 2, 3, \ldots$

Hence the energy of the particle is quantized.

Q. Find the lowest ~~energy~~ energy of an electron confined to move in a 1-D potential box of length 1 Å

<u>Barrier Tunneling or Barrier penetration :-</u>



let, us consider a 1-dimensional potential barrier given below:-

$V = 0$ for $x < a$ (region I)

$= V_0$ for $a < x < b$ (region II).

$= 0$ for $x > b$

For region I:-

Schrodinger time independent wave equation becomes ~~time / ...~~

$$\frac{d^2\psi_I}{dx^2} + \frac{2m}{\hbar^2} E \psi_I = 0 \quad [\because V = 0 \text{ for region I}].$$

Or, $$\frac{d^2\psi_I}{dx^2} + \alpha^2\psi_I = 0 \quad \left(\text{where } \alpha^2 = \frac{2mE}{\hbar^2}\right).$$

whose sol^n is

$$\psi_I = Ae^{i\alpha x} + Be^{-i\alpha x}$$

The first term represents the incident wave and second wave represents the reflected wave.

For region II:-

SWE becomes

$$\frac{d^2\psi_{II}}{dx^2} - \frac{2m}{\hbar^2}(V_0 - E)\psi_{II} = 0 \quad (\text{since, } E < V_0).$$

whose solution is

$$\psi_{II} = Ce^{\beta x} + De^{-\beta x}.$$

where, $\beta^2 = \frac{2m}{\hbar^2}(V_0 - E)$

For region III:-

SWE becomes

$$\frac{d^2\psi_{II}}{dx^2} + \frac{2m}{\hbar^2} E \cdot \psi_{III} = 0 \quad (\text{since, } V = 0)$$

whose solution is

$\psi_{III} = E e^{i\alpha x}$

where, $\alpha^2 = \frac{2mE}{\hbar^2}$.

In this case, there is no reflecting surface or medium, so no reflected wave is present. The values of constants A, B, C, D and E are obtained by using boundary condition.

$$\frac{d\psi_I}{dx} = \frac{d\psi_{II}}{dx} = \frac{d\psi_{III}}{dx} \quad \text{at } x=0 \text{ \& } x=b.$$

The probability of tunneling is described with transmission coefficients (T) and reflection coefficients (R) which are given by

$$T = \left|\frac{E}{A}\right|^2$$

$$\boxed{T = 16\frac{E}{V_0}\left(1-\frac{E}{V_0}\right)e^{-2K.L}}$$ ~~V.V.Imp~~

where K is beta i.e. $K=\beta$, L be the length of barrier.

and. $R = \left|\frac{B}{A}\right|^2$

Among all the particles incident on the barrier only few get transmitted through it. This phenomenon is called Tunneling effect or Barrier tunneling or Barrier penentration. This phenomenon can't be explained by classic mechanics. This is purly a quantum mechanics phenomenon which can be best described in α-particle decay, β-decay, tunneling diode, etc.

Q. Calculate the probability of transmission of α-particle through the rectangular barrier indicated below

$V_0 = 2eV$

$E = 1eV$ & barrier width, $L = 1A°$

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$\alpha = \sqrt{mp}\ 2e$

$V_0 = 2 \times 1.6 \times 10^{-19}\ J$

$E = 1.6 \times 10^{-19}\ J.$

$L = 10^{-10}\ m.$

$B: K = \sqrt{\frac{2m}{\hbar^2}(V_0 - E)}$

$= \sqrt{\frac{2 \times 4 \times 1.67 \times 10^{-19}}{\left(\frac{6.62 \times 10^{-34}}{2\pi}\right)^2} \times (1.6 \times 10^{-19})}$

$= \cancel{\sqrt{2.662 \times 10^{-67}}}$

$= \sqrt{\frac{2 \times 6.68 \times 10^{-27}}{1.11 \times 10^{-68}} \times 1.6 \times 10^{-19}}$

$= \sqrt{1.9 \times 10^{23}}$

$= 4.38 \times 10^{11}\ m^{-1}.$

$T = 16 \times \frac{1.61}{2}\left(1 - \frac{1.8}{2}\right) e^{-2 \times 4.38 \times 10^{11} \times 10^{-10}}$

$= 4.2 \times 0.21\ e^{-86}.$

$= \cancel{2.8 \times 10^{-38}}$

$= \cancel{3.18 \times 10^{-38}}\ 1.79 \times 10^{-37}.$

Q. A beam of electrons having energy of each 3eV is inci[dent] on a potential barrier of height 4eV. If the width of the barrier is 20Å, calculate the % of Transmission through the barrier.

The wave function of the particle confined in a box of length is $\psi(x) = \sqrt{\frac{2}{L}} \sin \frac{\pi x}{L}$. Calculate the probability of finding the particle in the region $0 < x < \frac{L}{2}$ and $-\frac{L}{2} < x < \frac{L}{2}$

Solution:-

Probability of finding particle for $0 < x < \frac{L}{2}$ is

$$P = \int_0^{L/2} \psi^*(x)\, \psi(x)\, dx.$$

$$= \int_0^{L/2} |\psi(x)|^2 \, dx.$$

$$= \int_0^{L/2} \left(\sqrt{\frac{2}{L}} \sin \frac{\pi x}{L}\right)^2 dx$$

$$= \int_0^{L/2} \frac{2}{L} \sin^2 \frac{\pi x}{L} \, dx.$$

or, $\frac{1}{L} \int_0^{L/2} 2\sin^2 \frac{\pi x}{L} \, dx$

or, $\frac{1}{L} \int_0^{L/2} 1 - \cos \frac{2\pi x}{L} \, dx$

or, $\frac{1}{L} \left[\int_0^{L/2} 1 \, dx - \int_0^{L/2} \cos \frac{2\pi x}{L} \, dx \right]$

or, $\frac{1}{L} \left[[x]_0^{L/2} - \left[\frac{\sin \frac{2\pi x}{L}}{\frac{2\pi}{L}} \right]_0^{L/2} \right]$

the barrier.

$$T = 16\frac{E}{V_0}\left(1 - \frac{E}{V_0}\right)e^{-2kL}$$

A ground state electron is trapped in a 1-d infinite potential well with length $L = 100\ pm$.
What is the probability that electron can be detected in the left $\frac{1}{3}$rd
i.e. 0 to $\frac{L}{3}$.

Solution:-

$$\psi(x) = \sqrt{\frac{2}{L}}\sin\frac{n\pi x}{L}$$

$$|\psi(x)|^2 = \frac{2}{L}\sin^2\frac{\pi x}{L}$$

$$\therefore P = \int_0^{L/3}\frac{2}{L}\sin^2\frac{\pi x}{L}\,dx$$

$$= \frac{1}{L}\int_0^{L/3} 2\sin^2\frac{\pi x}{L}\,dx$$

$$= \frac{1}{L}\int_0^{L/3} 1 - \cos\frac{2\pi x}{L}\,dx$$

$$= \frac{1}{L}\left[\int_0^{L/3} 1\,dx - \int_0^{L/3}\cos\frac{2\pi x}{L}\,dx\right]$$

$$= \frac{1}{L}\left[[x]_0^{L/3} - \frac{L}{2\pi}\left[\sin\frac{2\pi x}{L}\right]_0^{L/3}\right]$$

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$$= \frac{1}{L}\left[\left(\frac{L}{2}-0\right) - \frac{L}{2\pi}\left(\sin\frac{\cancel{2}\pi\cdot\cancel{L}}{\cancel{2}\cdot\cancel{L}} - \sin 0\right)\right]$$

$$= \frac{1}{L}\left[\frac{L}{2} - \frac{L}{2\pi}\times 0\right]$$

$$= \frac{1}{\cancel{L}}\times\frac{\cancel{L}}{2}$$

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

For second region II,

$$P = \frac{1}{L}\int_{-L/2}^{L/2} |\psi(x)|^2\,dx.$$

Q. A particle is moving in 1-dimensional potential box of width 25Å. Calculate the probability of finding the particle within an interval of 5Å at the center of the box when it is at the state of least energy.

$$P = \int_a^b |\psi_n(x)|^2\,dx.$$

$$= \int_a^b |\psi(x)|^2\,\Delta x$$

Q. Suppose that the electron having total energy of 5.1eV approaches a barrier of height 6.8 eV and thickness 750pm. What is the approximate probability that electron will be transmitted through