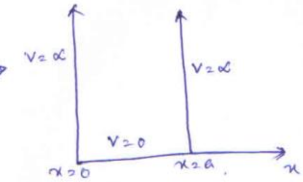
Solution of Tutorial-11

1(a) Given $V(x) = \begin{cases} 0 & \text{if } 0 \le x \le a \\ \infty & \text{otherwise} \end{cases}$ $\longrightarrow$



Schrödinger eqn. be, $-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + 0 = E\psi$.

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0 \qquad \text{where } k = \sqrt{\frac{2mE}{\hbar^2}}$$

The simbolic form of the eqn is $(D^2+k^2)\psi = 0$

$D = \pm ik$,

So complimentary function (C.F.) will be.

$$\psi = A\sin kx + B\cos kx \longrightarrow (i).$$

Boundary condition is at $x=0$, $\psi=0$. and at $x=a$, $\psi=0$.

using 1st Boundary condition. $0 = B$. so $\psi = A\sin kx$.

using 2nd " " $0 = A\sin ka$.

$$\text{So } \sin ka = \sin n\pi.$$

$$k = \frac{n\pi}{a}.$$

$$\text{So } \boxed{\psi = A\sin\frac{n\pi x}{a}.}$$

$$\text{and } k = \frac{n\pi}{a}$$

$$\Rightarrow k^2 = \frac{n^2\pi^2}{a^2}$$

$$\Rightarrow \frac{2mE}{\hbar^2} = \frac{n^2\pi^2}{a^2}$$

$$\Rightarrow \boxed{E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}}$$

ψ is not normalised here,

$$\int_0^a \psi^*\psi\, dx = 1.$$

$$\Rightarrow \int_0^a A^2\sin^2\frac{n\pi x}{a}dx = 1$$

$$\Rightarrow A^2\int_0^a \sin^2\frac{n\pi x}{a}dx = 1$$

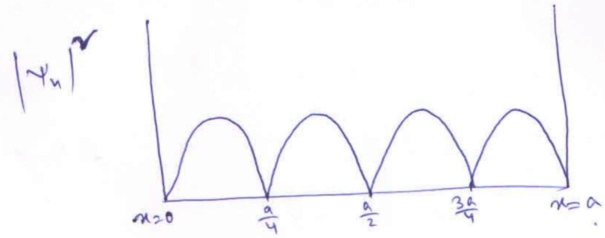
$$\Rightarrow A^2\cdot\frac{a}{2} = 1 \Rightarrow A = \sqrt{\frac{2}{a}}.$$

So normalised $\boxed{\psi_n = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}}$.

Energy eigen value $\boxed{E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}}$.

For, $n = 4$, $\psi_4 = \sqrt{\frac{2}{a}} \sin \frac{4\pi x}{a}$.

$|\psi_n|^2 = \psi_4^* \psi_4 = \frac{2}{a} \sin^2 \frac{4\pi x}{a}$.



For minima

$\frac{4\pi x}{a} = n\pi$.

$x = \frac{na}{4}$

$x_1 = 0, \frac{a}{4}, \frac{a}{2}, \frac{3a}{4}, a$.

It has 5-minima

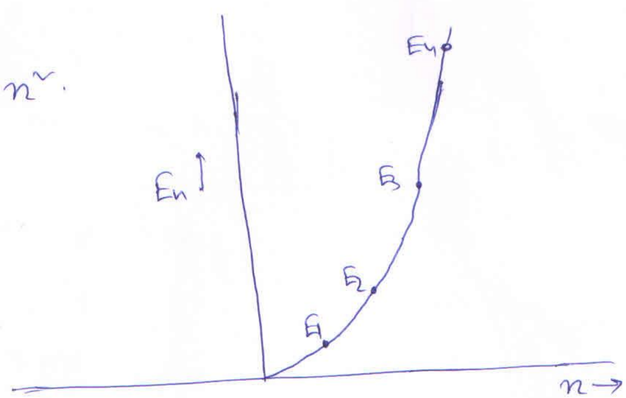
Now. $E_n \propto n^2$.

$E_1 = \frac{\pi^2\hbar^2}{2ma^2}$

$E_2 = \frac{4\pi^2\hbar^2}{2ma^2} = \frac{2\pi^2\hbar^2}{ma^2}$

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

$E_4 = \frac{16\pi^2\hbar^2}{2ma^2} = \frac{8\pi^2\hbar^2}{ma^2}$.



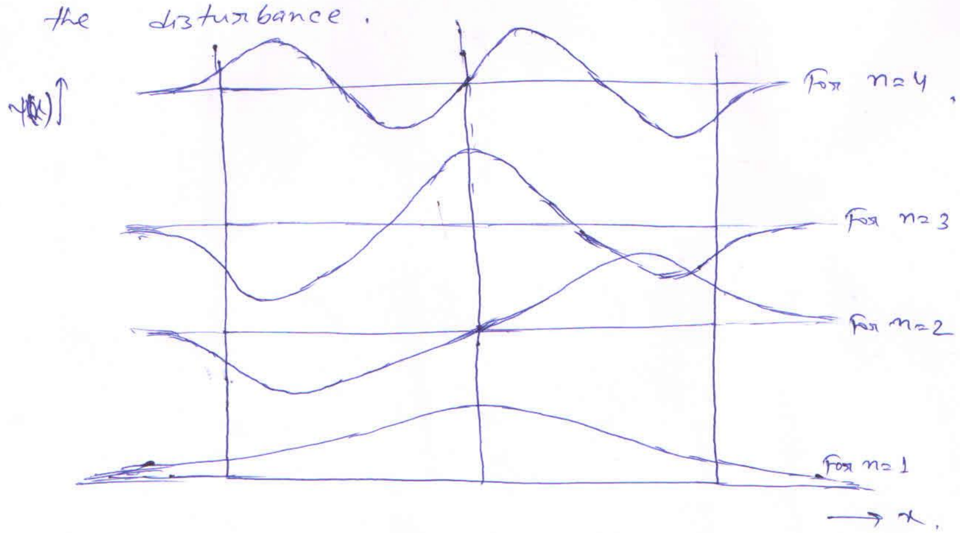
For $n = 4$, $E_4 = \frac{16\pi^2\hbar^2}{2ma^2}$

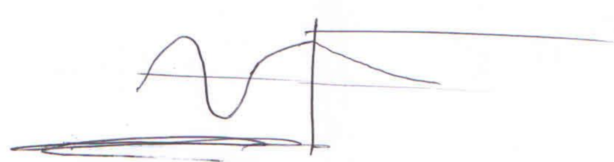
$n = 2$, $E_2 = \frac{4\pi^2\hbar^2}{2ma^2}$

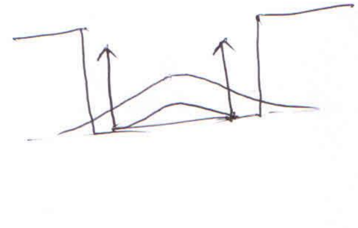
$\Delta E = \frac{12\pi^2\hbar^2}{2ma^2} = 12E_1$.

So the energy of emitted photon will be $12E_1$.

1) c) If $V(x) = V_0$ instead $V(x) = \infty$ then at $x = 0$ and $x = a$ there wavefunction will not be zero. There will be some penetration of the disturbance.







2) Given $\psi(x) = \left(\frac{\gamma^2}{\pi}\right)^{1/4} e^{-\frac{\gamma^2 x^2}{2}}$

$$E = \frac{\hbar^2 \gamma^2}{2m}$$

(a)

$$\langle x \rangle = \int_{-\infty}^{\infty} \psi^* x \psi \, dx.$$

$$= \left(\frac{\gamma^2}{\pi}\right)^{1/2} \int_{-\infty}^{\infty} x \, e^{-\gamma^2 x^2} \, dx.$$

$$= \left(\frac{\gamma^2}{\pi}\right)^{1/2} \left[x \left(-\frac{e^{-\gamma^2 x^2}}{2\gamma^2 x}\right) - (1) \left(\frac{e^{-\gamma^2 x^2}}{4\gamma^4 x^2}\right) \right]_{-\infty}^{\infty}$$

$$= \left(\frac{\gamma^2}{\pi}\right)^{1/2} \left[0 - 0 - 0 + 0 \right] = 0. \quad \text{Ans}$$

(b)

$$\langle p \rangle = \int_{-\infty}^{\infty} \psi^* \left(-i\hbar \frac{\partial}{\partial x}\right) \psi \, dx.$$

$$= \left(\frac{\gamma^2}{\pi}\right)^{1/2} (-i\hbar) \int_{-\infty}^{\infty} e^{-\frac{\gamma^2 x^2}{2}} \frac{\partial}{\partial x} \left(e^{-\frac{\gamma^2 x^2}{2}}\right) dx.$$

$$= \left(\frac{\gamma^2}{\pi}\right)^{1/2} (-i\hbar) \int_{-\infty}^{\infty} e^{-\gamma^2 x^2} \left(-\frac{\gamma^2}{2} 2x\right) dx.$$

$$= \left(\frac{\gamma^2}{\pi}\right)^{1/2} (+i\hbar)\gamma^2 \int_{-\infty}^{\infty} x \, e^{-\gamma^2 x^2} \, dx.$$

$$= \left(\frac{\gamma^2}{\pi}\right)^{1/2} (i\hbar \gamma^2) \left[0 \right] \quad \left[\text{see previous part} \right].$$

$$= 0 \quad \text{Ans}$$

(c) $H\psi = E\psi$.

$\left(\frac{p^2}{2m} + V\right)\psi = E\psi$.

$$\langle K.E.\rangle = \int_{-\infty}^{\infty} \psi^* \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right)\psi \, dx$$

$$= \int_{-\infty}^{\infty} \left(-\frac{\hbar^2}{2m}\right) e^{-\frac{\gamma^2x^2}{2}} \cdot \frac{d^2}{dx^2}\left(e^{-\frac{\gamma^2x^2}{2}}\right) . dx.$$

$$= -\frac{\hbar^2}{2m}\left[\int_{-\infty}^{\infty} e^{-\frac{\gamma^2x^2}{2}} \frac{d}{dx}\left(e^{-\frac{\gamma^2x^2}{2}} \cdot \left(-\frac{\gamma^2}{2}2x\right)\right) dx\right].$$

$$= -\frac{\hbar^2}{2m}(-\gamma^2)\left[\int_{-\infty}^{\infty} e^{-\frac{\gamma^2x^2}{2}}\left(e^{-\frac{\gamma^2x^2}{2}} - x.\left(-\frac{\gamma^2}{2}2x\right)e^{-\frac{\gamma^2x^2}{2}}\right)dx\right]$$

$$= -\frac{\hbar^2}{2m}(-\gamma^2) \int_{-\infty}^{\infty} e^{-\gamma^2x^2}\left(1+\gamma^2x^2\right) dx.$$

$$= +\frac{\hbar^2\gamma^2}{2m}\left[\int_{-\infty}^{\infty} e^{-\gamma^2x^2} dx + \gamma^2\int_{-\infty}^{\infty} x^2 e^{-\gamma^2x^2} dx.\right]$$

$$= \frac{\hbar^2\gamma^2}{2m}\left[\sqrt{\frac{\pi}{\gamma^2}} + \frac{1}{2}\gamma^2\sqrt{\frac{\pi}{\gamma^6}}\right].$$

$$= \frac{\hbar^2}{2m}\gamma\sqrt{\pi} + \frac{\hbar^2}{2m}.\gamma\sqrt{\pi}.$$

$$= \frac{\hbar^2}{2m}.(2\gamma\sqrt{\pi})$$

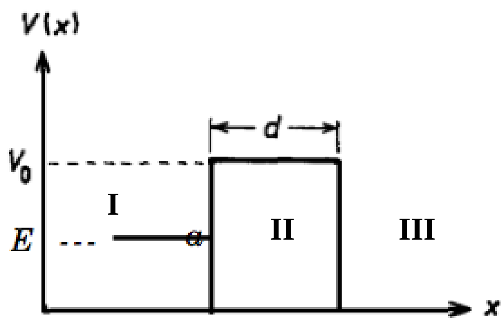
* Formula, $\int_{-\infty}^{\infty} x^2 e^{-ax^2}dx = \frac{1}{2}\sqrt{\frac{\pi}{a^3}}$

$$V(x) = E - K.E.$$

$$= \frac{\hbar^2\gamma^2}{2m} - \frac{\hbar^2}{2m}.\left(2\gamma\sqrt{\pi}\right)$$

$$= \frac{\hbar^2}{2m}\left[\gamma^2 - 2\gamma\sqrt{\pi}\right] \quad \text{Ans.}$$

3) An electron with energy E = 1 eV is incident upon a rectangular barrier of potential energy V_o= 2 eV (see Figure). About how wide must the barrier be so that the transmission probability is 10^{-3} ?



Solution:

In Region I and III, V_0 = 0, Schrodinger Equation:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} = E\psi$$

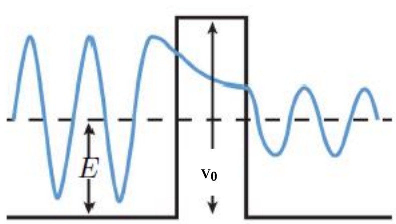
$\therefore$ In region I : $\psi_I = Ae^{ik_Ix} + Be^{-ik_Ix}$ $\quad k_I{}^2 = \frac{2mE}{\hbar^2}$

In region III : $\psi_{III} = Fe^{ik_Ix}$ (Negative solution is rejected as the particle cannot come from infinity).

In region II, E < V_0, Schrodinger Equation:

$$\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} = (V_0 - E)\psi$$

$\therefore \psi_{II} = Ce^{-k_{II}x} + De^{k_{II}x}$ $\quad k_{II}{}^2 = \frac{2m(V_0-E)}{\hbar^2}$



Coefficients A,B,C,D,F can be obtained by applying the boundary conditions at the two boundaries, but transmission coefficient can be approximated as:

$$T = \left|\frac{F}{A}\right|^2 \sim \frac{16e^{-2k_{II}d}}{\left(\frac{k_I}{k_{II}} + \frac{k_{II}}{k_I}\right)^2}$$

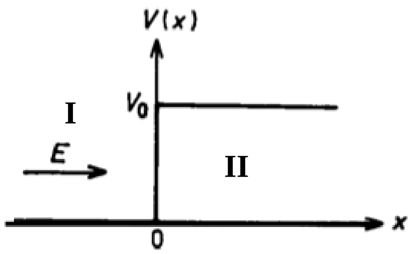
As, E=V_0/2, $k_I = k_{II} = k = \sqrt{\frac{mV_0}{\hbar^2}}$ ~ 5.11 x 10^{-9} m.

$$T = \sim 4e^{-2kd}$$

But, T~ 10^{-3} (given). $\therefore \boxed{d \sim -\frac{1}{2k}\ln\frac{T}{4} \sim 8.1\, x 10^{-10} m \sim 8\text{ Å}}$

4. Consider a one-dimensional system with potential energy (see Fig.)

$$V(x) = V_0, \quad x > 0,$$
$$V(x) = 0, \quad x < 0,$$



where V_o is a positive constant. If a beam of particles with energy E is incident from the left (i.e., from x = - ∞), what fraction of the beam is transmitted and what fraction reflected? Consider all possible values of E (i.,e. $E < V_o$ as well as $E > V_o$).

Solution:

a) $E > V_o$

$\therefore$ In region I : $\psi_I = Ae^{ik_1x} + Be^{-ik_2x}$ $\qquad k_1{}^2 = \frac{2mE}{\hbar^2}$

In region II : $\psi_{II} = Ce^{ik_2x}$ $\qquad k_2{}^2 = \frac{2m(E-V_0)}{\hbar^2}$

(Negative solution is rejected as the particle cannot come from infinity).

Equating the boundary conditions $\psi_I(0) = \psi_{II}(0)$

$\frac{d\psi_I}{dx} = \frac{d\psi_{II}}{dx}$ at x = 0 we get,

$$A+B=C \text{ and } k_1(A-B) = k_2C$$

$$\boxed{\begin{aligned} \text{Reflection} = R &= \left|\frac{B}{A}\right|^2 = \left|\frac{k_1-k_2}{k_1+k_2}\right|^2 \\ \text{Transmission} = T &= 1-R \\ &= \frac{4k_1k_2}{|k_1+k_2|^2} \end{aligned}}$$

b) ***E* < *V*$_o$**

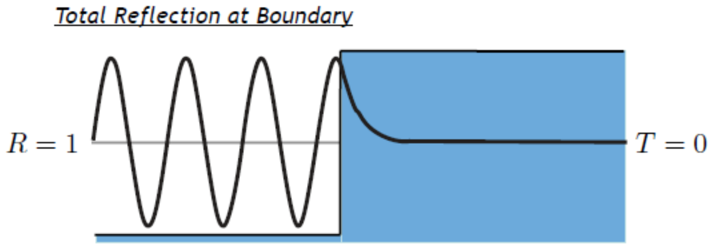
$\therefore$ In region I : $\psi_I = Ae^{ik_1x} + Be^{-ik_2x}$ $\qquad k_1{}^2 = \frac{2mE}{\hbar^2}$

In region II : $\psi_{II} = Ce^{-k_2x}$ $\qquad k_2{}^2 = \frac{2m(V_0-E)}{\hbar^2}$

(Growth solution is not feasible and hence rejected).

The solution beyond the barrier decays, there is no periodic wave solution. Hence there is no transmission.

$\boxed{\therefore \text{T= 0, so R = 1 (total reflection)}}$



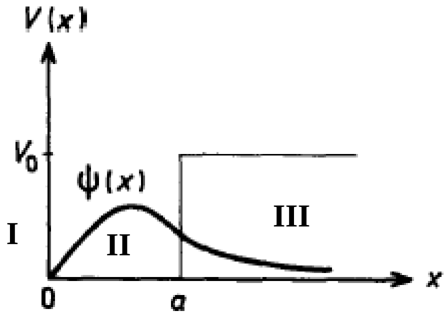
5. Consider the one-dimensional problem of a particle of mass *m* in a potential

$$\begin{aligned} &V=\infty, && x<0, \\ &v = 0, && 0 \le x \le a, \\ &V=V_0, && x>a. \end{aligned}$$

Show that the bound state energies (*E* < *V*$_o$) are given by the equation

$$\tan\frac{\sqrt{2mE}a}{\hbar} = -\sqrt{\frac{E}{V_0-E}}.$$

Solution:



In Region I: $\Psi_I = 0$ (Particle cannot get out of the well)

In Region II: V= 0 → $\psi_{II} = A\sin k_{II}x + B\cos k_{II}x,\ \ {k_{II}}^2 = \frac{2mE}{\hbar^2}$

In region III : $\psi_{III} = Ce^{-k_{III}x}$, V_0>E $\ \ {k_{III}}^2 = \frac{2m(V_0-E)}{\hbar^2}$

(Exponential growth solution is rejected as it is not feasible).

Using boundary conditions

at x = 0, we get $\Psi_I(0) = \Psi_{II}(0) = 0 \rightarrow B = 0$

at x = a, $\Psi_{II}(a) = \Psi_{III}(a)$ → $A\sin k_{II}a = Ce^{-k_{III}a}$

$$\frac{d\psi_{II}}{dx} = \frac{d\psi_{III}}{dx} \rightarrow A\,k_{II}\cos k_{II}a = -k_{III}Ce^{-k_{III}a}$$

Taking the ratio of the above equations, we get,

$$\tan k_{II}a = -\frac{k_{II}}{k_{III}}$$

Substituting the values

$$\boxed{\tan\left(\frac{\sqrt{2mE}}{\hbar}\right) = -\sqrt{\frac{E}{V_0 - E}}}$$