One dimensional potential problems

Free particle :—

$$\hat{H}|\psi\rangle = i\hbar|\dot{\psi}\rangle = \frac{p^2}{2m}|\psi\rangle$$

Normal modes

$$|\psi\rangle = |E\rangle e^{-iEt/\hbar}$$

$$\hat{H}|E\rangle = E|E\rangle = \frac{p^2}{2m}|E\rangle$$

if $|\phi\rangle$ is eigenstate of p then it's of p^2 too.

$$\Rightarrow \frac{p^2}{2m}|p\rangle = E|p\rangle \Rightarrow \left(\frac{p^2}{2m} - E\right)|p\rangle = 0$$

$$\Rightarrow p = \pm\sqrt{2mE}$$

$$\Rightarrow |E\rangle = \alpha|p = \sqrt{2mE}\rangle + \beta|p = -\sqrt{2mE}\rangle$$

The degenerate eigenstates can be written as $|E,+\rangle, |E,-\rangle$;

$$|p, \tfrac{p^2}{2m}\rangle ; \}$$

Propogator :—

$$U(t) = \int_{-\infty}^{\infty} |p\rangle\langle p| e^{-iEt/\hbar} dp$$

$$p \to -i\hbar\frac{\partial}{\partial x} \Rightarrow |E\rangle = \alpha \frac{e^{i\sqrt{(2mE)}x/\hbar}}{\sqrt{2\pi\hbar}} + \beta\frac{e^{-i\sqrt{2mE}x/\hbar}}{\sqrt{2\pi\hbar}}$$

$$U(x,t,x') = \langle x|U(t)|x'\rangle = \int_{-\infty}^{\infty} \langle x|p\rangle\langle p|x'\rangle e^{\frac{-ip^2t}{2m\hbar}} dp$$

$$\langle x,t;x'\rangle = \left(\frac{m}{2\pi\hbar i t}\right)^{1/2} e^{\frac{im(x-x')^2}{2\hbar t}}$$

$$\psi(x,t) = \int U(x;t;x')\,\psi(x',0)\,dx'$$

... propogator

Time evolution: of Gaussian Packet.

$$\psi(x',0) = \frac{e^{\frac{i p_0 x'}{\hbar}} \cdot e^{\frac{-x^2}{2a^2}}}{\sqrt{\sqrt{(\pi a^2)}}}$$

$$\psi(x,t) = \int U(t)\, \psi(x',0)\, dx'$$

$$= \frac{1}{\sqrt{\sqrt{\pi}\left(a + \frac{i\hbar t}{ma}\right)}}\, e^{\left(\frac{-x^2}{2a^2\left(1+\frac{i\hbar t}{ma^2}\right)}\right)}$$

$$|\psi(t)\rangle = e^{-\frac{i\hat{H}t}{\hbar}} |\psi(0)\rangle$$

$$\langle x|\psi(t)\rangle = \psi(x,t) = \int dx' \langle x| e^{-\frac{i\hat{H}t}{\hbar}} |x'\rangle\langle x'|\psi(0)\rangle$$

$$U(t) = \exp\left[\frac{i}{\hbar}\left(\frac{\hbar^2 t}{2m}\frac{\partial^2}{\partial x^2}\right)\right] = \sum \frac{1}{n!}\left(\frac{i\hbar t}{2m}\right)^n \frac{d^{2n}}{dx^{2n}}$$

$$* \quad \psi(x',0) = \frac{e^{-\frac{x^2}{2}}}{(\pi)^{1/4}}$$

$$\psi(x,t) = \frac{1}{(\pi)^{1/4}}\int \sum \frac{1}{n!}\left(\frac{i\hbar t}{2m}\right)^t \frac{d^{2n}}{dx^{2n}} e^{-x^2/2}\, dx$$

$$\langle r_0|p'\rangle = e^{\frac{i r_0 p'}{\hbar}}, \quad \langle p'|r\rangle = e^{-\frac{i r_0' p}{\hbar}}$$

Now generalising;

$$\langle r|\psi(t)\rangle = \langle r|U(t)|\psi(0)\rangle$$

$$= \int dr' \underbrace{\langle r|U(t)|r'\rangle}_{\text{propogator}}\langle r'|\psi_0\rangle$$

$$K(r,r';t) = \langle r|U(t)|r'\rangle$$

$$= \int \langle r|p'\rangle dp' \langle p'| e^{-\frac{i p^2 t}{2m\hbar}} |p\rangle dp \langle p'|r\rangle$$

$$= \left(\frac{m}{2\pi i\hbar t}\right)^{1/2} e^{\frac{im}{2\hbar t}(r-r')^2}$$

for free particle

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General scheme,

if $\psi(0) = \psi(x,0) = \langle x|\psi(0)\rangle$

then

$$\psi(x,t) = \int dp\, e^{-i\frac{p^2 t}{2m}} \langle x|p\rangle \langle p|\psi(0)\rangle$$

$$\langle p|\psi(0)\rangle = \int dx\, \langle p|x\rangle \langle x|\psi_0\rangle$$

$$\langle p|x\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{-i\frac{px}{\hbar}}$$

better yet, $\psi(r,t) = \left(\frac{m}{2\pi i\hbar t}\right)^{1/2} \int dr' e^{\frac{im(r-r')^2}{2\hbar t}} \psi(r',0)$

For free particle

Propogator can also be represented as

$$\langle x',t'|x_0,t_0\rangle$$

$$= \lim_{N\to\infty} \int dx_1 \int dx_2 \cdots \int dx_{N-1} \left(\frac{m}{2\pi\hbar i\Delta t}\right)^{N/2} \exp\left[\frac{i}{\hbar}\Delta t \sum \frac{m}{2}\left(\frac{x_i - x_{i-1}}{\Delta t}\right)^2\right]$$

for $y_i = x_i \sqrt{\frac{m}{2\hbar\Delta t}}$;

$$= \int dy_1 \int dy_2 \cdots \int dy_{n-1} \exp\left[i \sum (y_i - y_{i-1})^2\right]$$

$$\langle x',t'|x_0,t_0\rangle = \sqrt{\frac{m}{2\pi\hbar i(t-t_0)}} \exp\left[\frac{im}{2\hbar} \frac{(x-x_0)^2}{(t'-t_0)}\right]$$

From path integrals.

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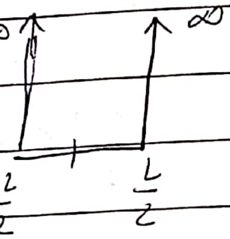
$$* \quad \langle x | \psi(0) \rangle = \begin{cases} \sin\left(\frac{\pi x}{L}\right) & |x| < L/2 \\ 0 & \end{cases}$$

Not a solution of Schro. eq.

<u>Particle in a box</u> :—

$$V(x) = \begin{cases} 0 & |x| < \frac{L}{2} \\ \infty & |x| > \frac{L}{2} \end{cases}$$



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

$$\psi = Ae^{ikx} + Be^{-ikx}$$

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

$$\psi\left(-\frac{L}{2}\right) = \psi(L/2) = 0$$

$$Ae^{-ikL/2} + Be^{ikL/2} = 0$$
$$Ae^{ikL/2} + Be^{-ikL/2} = 0$$

$$\begin{pmatrix} e^{-ikL/2} & e^{ikL/2} \\ e^{ikL/2} & e^{-ikL/2} \end{pmatrix} \begin{bmatrix} A \\ B \end{bmatrix} = 0$$

$$e^{-ikL} \cancel{\phi} - e^{ikL} = -2i\sin(kL) = 0$$

$$kL = n\pi \qquad k = \frac{n\pi}{L}$$

$$\Rightarrow \psi_n(x) = \begin{cases} \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right) & n \text{ is even} \\ \sqrt{\frac{2}{L}}\cos\left(\frac{n\pi x}{L}\right) & n \text{ is odd.} \end{cases}$$

$$E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2\pi^2 n^2}{2mL^2}$$

* The uncertainty principle dictates the lowest energy state,

For initial state

$$|\psi(0)\rangle = \sum_{n=1}^{\infty} a_n |n\rangle$$

$$|\psi(t)\rangle = \sum_{n=1}^{\infty} a_n |n\rangle e^{-\frac{i}{\hbar} E_n t}$$

$$|n\rangle = \varphi_n(x), \quad |\psi(t)\rangle = \psi(x,t)$$

5.2.1

$$\psi(x,0) = \sqrt{\frac{2}{L}} \cos\left(\frac{\pi x}{L}\right)$$

New basis :— $\begin{cases} \sqrt{\frac{1}{L}} \sin\left(\frac{n\pi x}{2L}\right) & n \text{ even} \\ \sqrt{\frac{1}{L}} \cos\left(\frac{n\pi x}{2L}\right) & n \text{ odd} \end{cases}$

$$\langle x | E_1^{L\text{-width}} \rangle = \sqrt{\frac{2}{L}} \cos\left(\frac{\pi x}{L}\right)$$

$$\langle x | E_1^{2L\text{-width}} \rangle = \sqrt{\frac{1}{L}} \cos\left(\frac{\pi x}{2L}\right)$$

$$\langle E_1^{2L} | E_1^{L} \rangle = \int_{-a/2}^{a/2} \frac{\sqrt{2}}{L} \cos\left(\frac{\pi x}{L}\right) \cos\left(\frac{\pi x}{2L}\right) dx$$

$$= \frac{8}{3\pi}$$

$$P = |\langle E_1^{2L} | E_1^{L} \rangle|^2 = \left(\frac{8}{3\pi}\right)^2$$

S.2.2

(a) Expand $|\psi\rangle$ in $|E_n\rangle$ basis.

$$|\psi_0\rangle = \sum |E_n\rangle\langle E_n|\psi_0\rangle$$

$$|\psi(t)\rangle = \sum e^{-\frac{i}{\hbar}E_n t}|E_n\rangle\langle E_n|\psi_0\rangle$$

$$H|\psi(t)\rangle = \sum e^{-\frac{i}{\hbar}E_n t} E_n |E_n\rangle\langle E_n|\psi_0\rangle$$

$$\langle\psi(t)| = \sum e^{+\frac{i}{\hbar}E_n t}\langle E_n|\psi_0\rangle\langle E_n|$$

$$\Rightarrow \langle\psi(t)|H|\psi(t)\rangle = \sum E_n|\langle E_n|\psi_0\rangle|^2 > E_0\sum|\langle E_n|\psi_0\rangle|^2 = E_0$$

(b) "Every attractive potential has a bound state."

$$V(\infty) = 0, \quad V(x) = -|V(x)| \quad \forall x$$

take some $\psi_a(x) = \left(\frac{a}{\pi}\right)^{1/4} e^{-ax^2/2}$

$$H|\psi\rangle = \left(\frac{a}{\pi}\right)^{1/4}\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}(e^{-ax^2/2}) - |V(x)|e^{-ax^2/2}\right)$$

$$= \left(\frac{a}{\pi}\right)^{1/4}\left(\frac{\hbar^2}{2m}e^{-ax^2/2}\cdot(xa) - |V(x)|e^{-ax^2/2}\right)$$

$$\langle\psi|H|\psi\rangle = \int_{-\infty}^{\infty}dx\sqrt{\frac{a}{\pi}}\cdot e^{-ax^2/2}\left(\frac{\hbar^2}{2m}\cdot(xa)e^{-ax^2/2} - |V(x)|e^{-ax^2/2}\right)$$

$$= < \infty$$

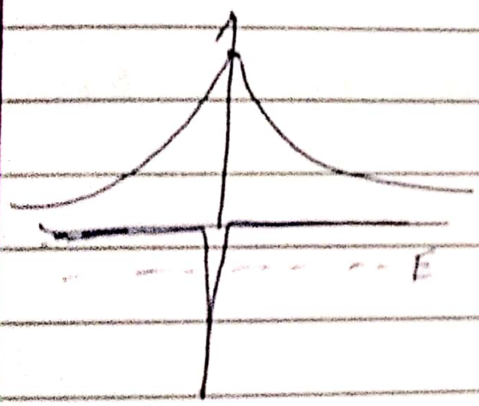
5.2.3

$$V(x) = -aV_0\,\delta(x)$$

Negative energy states are most plausible

$$\psi(x) = \begin{cases} Ae^{kx} & x<0 \\ Ae^{-kx} & x>0 \end{cases}$$

$$k = \sqrt{\frac{-2mE}{\hbar^2}}$$; (for positive energy, this becomes free particle)



Derivative is discontinuous at $x=0$,

$$\frac{\partial\psi}{\partial x}_{+\epsilon} - \frac{\partial\psi}{\partial x}_{-\epsilon} = \frac{-2maV_0}{\hbar^2}\psi(0)$$

$$-k-k = \frac{-2maV_0}{\hbar^2}$$

($A=1$, normalisation)

$$\therefore k = \frac{maV_0}{\hbar^2} \Rightarrow E = -\frac{ma^2V_0^2}{2\hbar^2}$$

Only one bound state.

5.2.4

$$|n\rangle = \begin{cases} \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) & n \text{ even} \\ \sqrt{\frac{2}{L}} \cos\left(\frac{n\pi x}{L}\right) & n \text{ odd} \end{cases}$$

$$F = -\frac{\partial E}{\partial L} \qquad E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2}$$

$$\frac{\partial E_n}{\partial L} = \frac{-n^2\pi^2\hbar^2}{\cancel{2}mL^3}$$

$$\Rightarrow F = \frac{n^2\pi^2\hbar^2}{mL^3}$$

For classical particle, of energy E_n,

$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}$$

$$\frac{p^2}{2m} = \frac{n^2\pi^2\hbar^2}{2mL^2}$$

$$p = \frac{n\pi\hbar}{L} \Rightarrow V = \frac{n\pi\hbar}{mL}$$

momentum transfer = $\Delta p = \frac{2n\pi\hbar}{L}$

$$\Delta t = \frac{2L}{V} = \frac{2mL^2}{n\pi\hbar}$$

$$F = \frac{\Delta p}{\Delta t} = \frac{2n\pi\hbar}{L} \cdot \frac{n\pi\hbar}{2mL^2} = \frac{\cancel{2}n^2\pi^2\hbar^2}{\cancel{2}mL^3}$$

* Weird, ~~this~~ agrees the quantum result.

Probability and Continuity equation :—

Time evolution is Unitary :—

$$\langle \psi(t) | \psi(t) \rangle = \langle \psi(0) | U^{\dagger} U | \psi(0) \rangle$$
$$= \langle \psi(0) | \psi(0) \rangle$$

$$\Rightarrow \langle \psi(t) | \psi(t) \rangle = \text{constant}$$
$$= \iiint \psi^{*}(r,t)\, \psi(r,t)\, d^3 r$$
$$= \iiint \rho(r,t)\, d^3 r.$$

extract from Schrodinger's equation :—

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

$$-i\hbar \frac{\partial \psi^{*}}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi^{*} + V\psi^{*}$$

$$\Rightarrow i\hbar \frac{\partial}{\partial t}(\psi^{*}\psi) = -\frac{\hbar^2}{2m}\left(\psi^{*}\nabla^2\psi - \psi \nabla^2 \psi^{*}\right)$$

$$\Rightarrow \frac{d\rho}{dt} = -\nabla \cdot J$$

$$\vec{J} = \frac{\hbar}{2mi}\left(\psi^{*}\nabla\psi - \psi\nabla\psi^{*}\right)$$

if $V = V_r + iV_i$

then

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + V\psi \;;\; -i\hbar\frac{\partial \psi^{*}}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi^{*} + \tilde{V}\psi^{*}$$

$$\Rightarrow i\hbar\left(\frac{\partial \psi}{\partial t}\right)\psi^{*} = -\frac{\hbar^2}{2m}(\nabla^2\psi)\psi^{*} + V\psi\psi^{*} \;;\; -i\hbar\left(\frac{\partial \psi}{\partial t}\right)^{*}\psi = -\frac{\hbar^2}{2m}(\nabla^2\psi^{*})\psi + \tilde{V}\psi^{*}\psi$$

$$\Rightarrow i\hbar\frac{\partial(\psi\psi^{*})}{\partial t} = -\frac{\hbar^2}{2m}\left(\psi^{*}\nabla^2\psi - \psi\nabla^2\psi^{*}\right) + (V - \tilde{V})\psi^{*}\psi$$

$$= -\frac{\hbar^2}{2mi}\nabla\cdot\left(\psi^{*}\nabla\psi - \psi\nabla\psi^{*}\right) - \frac{2V_i}{i}\psi^{*}\psi$$

5.3.4

$$\psi = Ae^{\frac{ipx}{\hbar}} + \beta e^{\frac{-ipx}{\hbar}}$$

$$\psi^* = Ae^{-ip\frac{x}{\hbar}} + \beta e^{ip\frac{x}{\hbar}}$$

$$J = \frac{\hbar}{2mi}\left(\psi^*\frac{\partial\psi}{\partial x} - \psi\frac{\partial\psi^*}{\partial x}\right)$$

$$\frac{\partial\psi}{\partial x} = \frac{Aip}{\hbar}e^{i\frac{px}{\hbar}} \cancel{+} - \frac{\beta ip}{\hbar}e^{-i\frac{px}{\hbar}}$$

$$\frac{\partial\psi^*}{\partial x} = -\frac{Aip}{\hbar}e^{-i\frac{px}{\hbar}} + \frac{\beta ip}{\hbar}e^{i\frac{px}{\hbar}}$$

$$\frac{A^2ip}{\hbar} - \frac{ABip}{\hbar}e^{-2i\frac{px}{\hbar}} + \frac{\beta Aip}{\hbar}e^{2i\frac{px}{\hbar}} - \frac{B^2ip}{\hbar}$$

$$-\left(-\frac{A^2ip}{\hbar} + \frac{A\beta ip}{\hbar}e^{2i\frac{px}{\hbar}} - \frac{\beta Aip}{\hbar}e^{-2i\frac{px}{\hbar}} + \beta^2\frac{ip}{\hbar}\right)$$

$$= \left[\frac{2A^2ip}{\hbar^2} - \frac{2\beta^2ip}{\hbar^2} + \frac{2ABip}{\hbar^2}\left(e^{2i\frac{px}{\hbar}} - e^{-2i\frac{px}{\hbar}}\right)\right]$$

$$\vec{J} = \frac{1}{m}\left(\frac{A^2p}{\hbar} - \frac{\beta^2p}{\hbar} + \frac{\cancel{B}ABp}{\hbar}\left(e^{2i\frac{px}{\hbar}} - \cancel{2}e^{-2i\frac{px}{\hbar}}\right)\right)$$

$$= \frac{(A^2-\beta^2)p}{m\hbar} + \frac{ABp}{m\hbar}(2i$$

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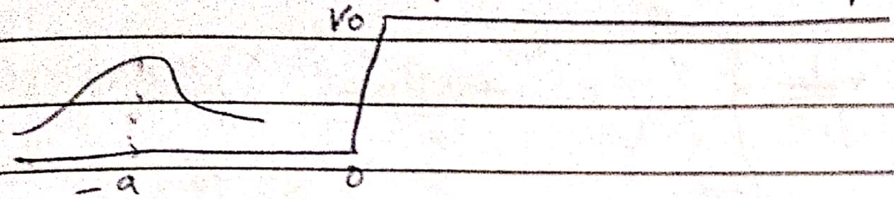
Step function potential analysis :-



take initial to be
$$\psi(x,0) = (\pi\Delta^2)^{-1/4} e^{ik_0(x+a)} e^{-\frac{(x+a)^2}{2\Delta^2}}$$

Reflection coeff $= R = \int |\psi_R|^2 dx \quad t \to \infty$.
Transmission $= T = \int |\psi_T|^2 dx \quad t \to \infty$

Solving scheme :-

1. Find $\psi_E(x)$ as in energy eigen funcs.
2. Then find $\psi(x,0)$ projection along each $\psi_E(x) = a(E)$.
3. Recreate $\psi(x,t)$ from $a(E) e^{-\frac{i}{\hbar}Et}$.
4. Find ψ_R, ψ_T

① $$\psi_E(x) = \begin{cases} Ae^{ik_1x} + Be^{-ik_1x} & k_1 = \sqrt{\frac{2mE}{\hbar^2}} \;;\; x<0 \\ Ae^{ik_2x} + Be^{-ik_2x} & k_2 = \sqrt{\frac{2m}{\hbar^2}(E-V_0)} \;;\; x>0 \end{cases}$$

let $D = 0$ -- (right going only)

$\Rightarrow A+B = C, \quad ik_1(A-B) = ik_2 C$

$\Rightarrow B = \left(\frac{k_1-k_2}{k_1+k_2}\right)A, \quad C = \left(\frac{2k_1}{k_1+k_2}\right)A$

$\Rightarrow \psi_E(x) = \psi_{k_1}(x) \quad \ldots$ (writing $k_2 = \phi(k_1)$)

$$= A\left[\left(e^{ik_1x} + \frac{B}{A}e^{-ik_1x}\right)\theta(-x) + \frac{C}{A}e^{i\sqrt{k_1^2 - \frac{2mV_0}{\hbar^2}}\,x}\,\theta(x)\right]$$

(2) $a(k_1) = \langle \psi_{k_1} | \psi_i \rangle$

$$= \frac{1}{\sqrt{2\pi}} \left\{ \int_{-\infty}^{\infty} \left(e^{-ik_1 x} + \left(\frac{B}{A}\right)^* e^{ik_1 x} \right) \theta(-x)\, \psi_i(x)\, dx + \int_{-\infty}^{\infty} \left(\frac{C}{A}\right)^* e^{-ik_2 x}\, \theta(x)\, \psi_i(x)\, dx \right\}$$

$$\Rightarrow a(k_1) = \left(\frac{\Delta^2}{\pi}\right)^{1/4} e^{-\frac{(k_1 - k_0)^2 \Delta^2}{2}} e^{ik_1 a}$$

(3) $$\psi(x,t) = \int_{-\infty}^{\infty} a(k_1)\, e^{-\frac{iE(k_1)t}{\hbar}} \cdot \psi_{k_1}(x)\, dk_1$$

$$\Rightarrow R = \frac{|B|^2}{|A|^2}, \quad T = \frac{|C|^2}{|A|^2} \frac{(E_0 - V_0)^{1/2}}{E_0^{1/2}}$$

For $E < V_0$,

$$\psi_{region-2}(x) = C e^{-kx}.$$

$$R = \left| \frac{\sqrt{E_0} - \sqrt{E_0 - V_0}}{\sqrt{E_0} + \sqrt{E_0 + V_0}} \right|^2 = 1$$

$T = 0$

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5.4.2

$V(x) = V_0 a\, \delta(x)$ | I | II

initial conditions

$$\psi_I(0) = \psi_{II}(0)$$

$$\psi'_{II}(0) - \psi'_I(0) = \frac{2m}{\hbar} V_0 a\, \psi(0)$$

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

$$\psi_I(x) = e^{ikx} + r e^{-ikx}$$

$$\psi_{II}(x) = t e^{ikx}$$

$$\Rightarrow \quad 1 + r = t$$

$$ikt - ik + ikr = \frac{2m}{\hbar^2} V_0 a t.$$

$$\Rightarrow \quad t = \frac{1}{1 + \frac{imV_0 a}{k\hbar^2}}, \quad r = \frac{-\frac{imV_0 a}{k\hbar^2}}{1 + \frac{imV_0 a}{k\hbar^2}}$$

$$R = |r|^2 = \frac{\frac{m^2 V_0^2 a^2}{\hbar^4 k^2}}{1 + \frac{m^2 V_0^2 a^2}{k^2 \hbar^4}} = \frac{1}{1 + \frac{2\hbar^2 E}{ma^2 V_0}}$$

$$T = 1 - R = \frac{1}{1 + \frac{ma^2 V_0^2}{2\hbar^2 E}}$$

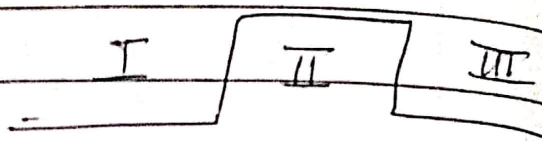
5.4.3 (b)

Scattering from barrier :-

$\psi_I(x) = e^{ikx} + r e^{-ikx}$

$\psi_{III}(x) = t e^{ikx}$

$\psi_{II} = A e^{k_1 x} + B e^{-k_1 x}$



$\psi_I(-a) = \psi_{II}(-a) \Rightarrow e^{-ika} + r e^{ika} = A e^{-ka} + B e^{ka}$

$\psi_I'(-a) = \psi_{II}'(-a) \quad ik e^{-ika} - ikr e^{ika} = kA e^{-ka} - kB e^{ka}$

$\psi_{II}(a) = \psi_{III}(a) \Rightarrow t e^{ika} = A e^{ka} + B e^{-ka}$

$\psi_{II}'(a) = \psi_{III}'(a) \quad ikt e^{ika} = k_1 A e^{ka} - kB e^{-ka}$

$E < V_0 \Rightarrow T = \dfrac{1}{1 + \frac{1}{4}\sinh^2(2ka)\cdot\left(\frac{k^2+k_1^2}{k_1 k}\right)^2}$

$R = 1 - T$

For $E > V_0$,

$T = \dfrac{1}{1 + \frac{1}{4}\left(\frac{k^2-k_1^2}{kk_1}\right)^2 \cdot \sin^2(k_2 a)}$

For $E = V_0$,

$T \approx 1 - \dfrac{mV_0a^2}{2\hbar^2}$