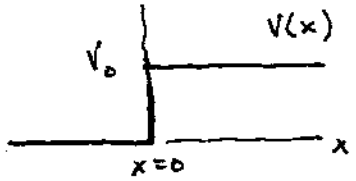
Scattering and barrier penetration

1st 1D examples, then 3D. Almost exclusively "potential scattering". ... soln of TISE with prescribed V + "scattering" boundary conditions

generic scat. problem: plane wave incident on scattering centers, what is the flux of scattered particles?

1st problem: potential "step"



incident particle(s) from l.h.s. $\psi = e^{ikx}$ — implicit $e^{-i\omega t}$ factor but we can ignore it for T.I.S.E.

we leave norm at 1 since we are interested in relative probabilities of scat or not scat.

flux of inc. particles $\vec{j} = \frac{\hbar}{2mi}(\psi^*\vec{\nabla}\psi - \psi\vec{\nabla}\psi^*)$

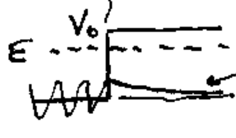
here $j_x = +\frac{\hbar k}{m} = +\frac{p_x}{m}$

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

or, $p_x\psi = -i\hbar\frac{\partial}{\partial x}e^{ikx} = \hbar k\psi$

so $\frac{\hbar^2 k^2}{2m} = E$ on l.h.s, $k = \frac{\sqrt{2mE}}{\hbar}$

let's assume $E < V_0$ initially . . .



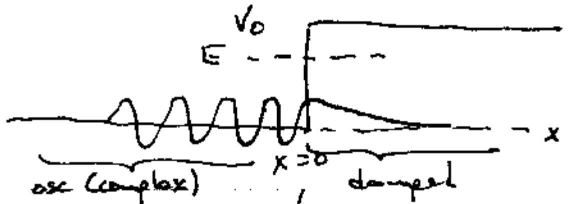
exp damped soln $\propto e^{-x/a}$

$$\psi_{rhs} = te^{-x/a} \xrightarrow[\text{Schrö}]{\text{soln}} \frac{\hbar^2}{2ma^2} = V_0 - E, \quad a = \frac{\hbar}{\sqrt{2m(V_0-E)}}$$

$$a = \frac{\hbar}{\sqrt{2mV_0}} \cdot \frac{1}{\sqrt{1-\epsilon}}$$

$\epsilon \equiv \frac{E}{V_0}$ = reduced energy

since there is no penetration to $x=\infty$, conservation of flux requires that the r.h.s. includes a reflected wave of equal magnitude to the incident one,



$$\underbrace{\psi_{lhs} = \underset{\uparrow \text{ incident}}{e^{ikx}} + r \underset{\uparrow \text{ reflected}}{e^{-ikx}}}$$

$$\underbrace{\psi_{rhs} = t e^{-x/a}}$$

$|r|^2 = 1$, so $r = e^{i\delta}$, a pure phase (for $E < V_0$, $\epsilon < 1$).

impose b.c. to find r, t (ψ & ψ' at $x=0$: 2 eqs & 2 unknowns)

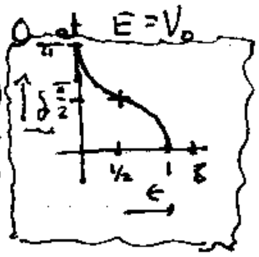
$$\left.\begin{aligned} \psi: &\quad 1 + r = t \\ \psi': &\quad ik(1-r) = -\tfrac{1}{a} t \end{aligned}\right\} \text{ solve } \quad \underline{r = -\frac{(1+ika)}{(1-ika)} \equiv e^{i\delta}}$$

or $\underline{\cos\delta} = -\dfrac{(1-k^2a^2)}{(1+k^2a^2)}$

$= \underline{-\left(1 - 2\frac{E}{V_0}\right) = -(1-2\epsilon)}$

$\therefore \delta$ runs from $+\pi$ at $E=0$ to 0 at $E = V_0$

$\underline{\delta = \cos^{-1}\left(-(1-2\epsilon)\right)}$



> note $\delta = \pi$ at $k=0$ makes sense,
> that is $E/V_0 = 0$ (∞ potential well),
> no penetration, $\psi = 0$ at bndy
> hence must be $e^{ikx} + \underbrace{(-1)}_{e^{i\pi}} \cdot e^{-ikx}$.

<u>What about the wfn within the potential?</u>

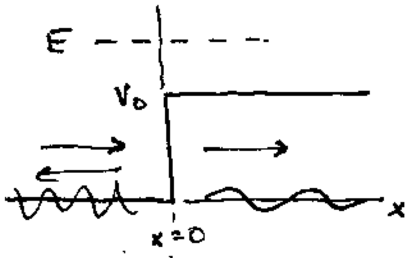
$$\underset{\overset{\shortparallel}{1+e^{i\delta}}}{t = 1 + r} = \frac{2}{\left(1 + \frac{i}{ka}\right)} \longrightarrow \begin{cases} 0 \cdot (-i)\ ka \to 0 & E \to 0 \\ 2 & E \to V_0 \ (ka \to \infty) \end{cases}$$

(matches 2 in-phase plane waves, $e^{ikx} + \underset{\hookrightarrow e^{i0}}{1} \cdot e^{-ikx}$)

$t \equiv |t| e^{i\delta_t}$ — <u>different phase than δ</u>

$\hookrightarrow |t| = 2\sqrt{\epsilon}$, $\tan\delta_t = -\frac{1}{ka}$

now consider $E > V_0$, so transmission is allowed



$$\underline{\psi_{lhs}} = \underline{e^{ikx} + r e^{-ikx}}$$

$$\underline{\psi_{rhs} = t e^{ipx}}$$

schrö' eqn:
$$\frac{\hbar^2 k^2}{2m} = E \qquad \frac{\hbar^2 p^2}{2m} = E - V_0$$

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

$$p = \frac{\sqrt{2m(E-V_0)}}{\hbar} < k$$

$$\frac{p}{k} = \sqrt{1 - \frac{V_0}{E}} < 1 \quad \text{for } E > V_0$$

b.c. at $x=0$
$$\psi: \quad 1 + r = t$$
$$\psi': \quad k(1-r) = p t$$

$$r = \frac{1 - \frac{p}{k}}{1 + \frac{p}{k}}$$

$$t = \frac{2}{1 + \frac{p}{k}}$$

purely real coeffs!

conservation of particle flux?

incident flux $j_x^i = + \frac{\hbar k}{m} \cdot |1|^2 = \frac{\hbar k}{m}$

reflected flux $j_x^r = + \frac{\hbar k}{m} \cdot |r|^2 = + \frac{\hbar k}{m} \cdot \left(\frac{1 - \frac{p}{k}}{1 + \frac{p}{k}} \right)^2$

this is ok because the cross-term flux vanishes.

transmitted flux $j_x^t = + \frac{\hbar p}{m} |t|^2 = + \frac{\hbar p}{m} \left(\frac{2}{1 + \frac{p}{k}} \right)^2$

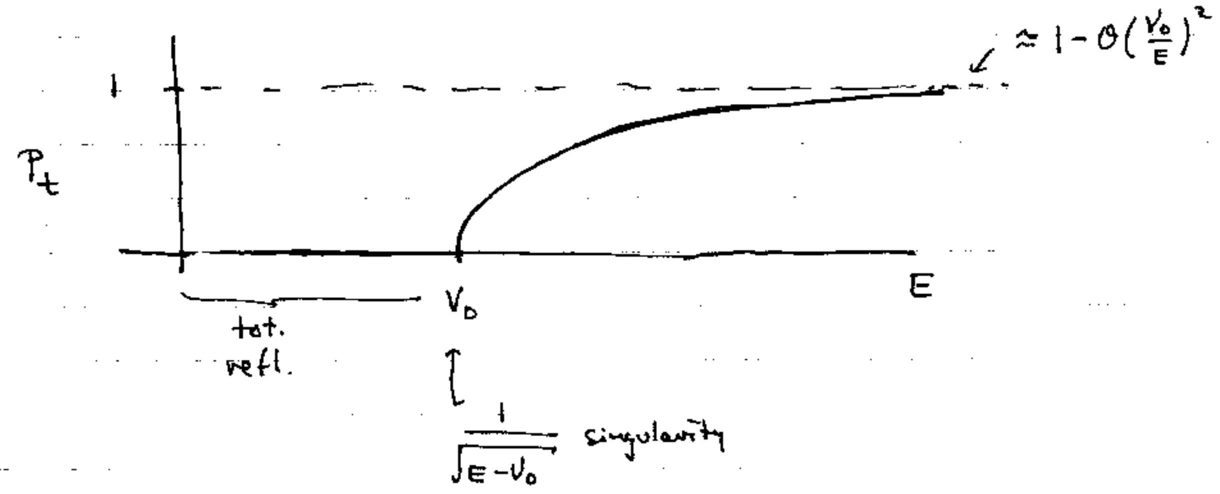
$$J_x^i \stackrel{?}{=} J_x^r + J_x^t$$

$$\frac{\hbar k}{m} \stackrel{?}{=} + \frac{\hbar k}{m} \cdot \left(\frac{1-\frac{p}{k}}{1+\frac{p}{k}}\right)^2 + \frac{\hbar p}{m}\left(\frac{2}{1+\frac{p}{k}}\right)^2$$

$$k\left(1+\frac{p}{k}\right)^2 \stackrel{?}{=} +k\cdot\left(1-\frac{p}{k}\right)^2 + 2^2 p \quad \checkmark$$

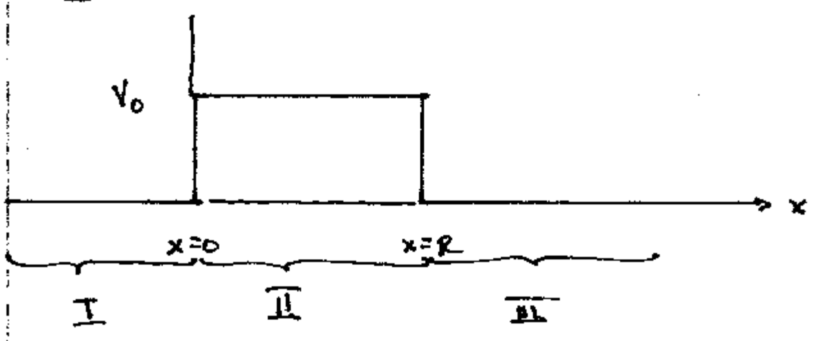
transmitted / incident flux :

$$\underbrace{P_t}_{\text{prob. of transmission}} = \frac{J_x^t}{J_x^i} = \frac{p}{k}\cdot\frac{|t|^2}{1} = \frac{p}{k}\cdot\frac{4}{\left(1+\frac{p}{k}\right)^2} = \frac{\sqrt{1-\frac{V_0}{E}}}{\left[\frac{1}{2}\left(1+\sqrt{1-\frac{V_0}{E}}\right)\right]^2}$$



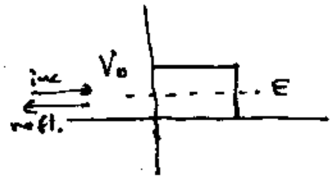
$P_r = 1 - P_t$ of course

Finite barrier



$$V(x) = \begin{cases} V_0 > 0 & R \geq x \geq 0 \\ 0 & \text{otherwise} \end{cases}$$

1st consider $E < V_0$. Classically would have total reflection



quantum mechanically there will be some transmission, since the exponential solutions will have some nonzero values at $x=R$.

Ansatz:

$$\psi(x) = \begin{cases} e^{ikx} + \underset{\sim}{r}\, e^{-ikx} & \text{region I} \\ \underset{\sim}{c}\, e^{-r/a} + \underset{\sim}{d}\, e^{+r/a} & \text{II} \\ \underset{\sim}{t}\, e^{ikx} & \text{III} \end{cases}$$

V_0, E, R given

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

$$\frac{\hbar^2}{2ma^2} = V_0 - E$$

from Schrö eqn.

4 unknowns r, c, d, t — most interesting (observable at ∞)

4 eqs (ψ & ψ' cont at $x=0$, $x=R$)

eqs:

	at $x=0$	at $x=R$
ψ:	$1 + r = c + d$	$c e^{-R/a} + d e^{R/a} = t e^{ikR}$
ψ':	$ik(1-r) = -\frac{1}{a}(c-d)$	$-\frac{1}{a}\left(c e^{-R/a} - d e^{R/a}\right) = ik\, t e^{ikR}$

proceed by solving for c & d & eliminating them

$\underline{x=0:}$

$$c = \frac{1}{2}\left[(1-ika) + r(1+ika)\right]$$

$$d = \frac{1}{2}\left[(1+ika) + r(1-ika)\right] \qquad (\neq c^* \text{ because } r \neq r^* \text{ in general})$$

$\underline{x=R:}$

$$c = \frac{1}{2}(1-ika)\, t\, e^{ikR + R/a}$$

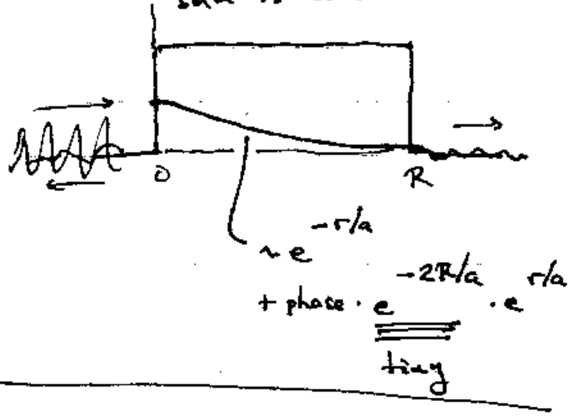
$$d = \frac{1}{2}(1+ika)\, t\, e^{ikR - R/a}$$

before we proceed, note $\quad \dfrac{d}{c} = \dfrac{1+ika}{1-ika}\, e^{-2R/a}$

so

$$\frac{|d|}{|c|} = e^{-2R/a}$$

$\therefore$ for a "long" barrier, $R \gg a$, the decaying soln is dominant



now eliminate c & d & solve for $\underset{\sim}{t}$ & $\underset{\sim}{r}$. introduce abbreviations

$$f = \frac{1+ika}{1-ika} \quad \text{(a pure phase)},$$

$$s = e^{R/a}$$

& we find

$$\underset{\sim}{r} = -f\left(\frac{s^2-1}{s^2-f^2}\right) \qquad\qquad \underset{\sim}{t} = \left(\frac{s}{s^2-f^2}\right)(1-f^2)\,e^{-ikR}$$

n.b. limit of "step" is $\frac{R}{a} \to \infty$, hence $s \to \infty$. $\; r \to -f = -\dfrac{(1+ika)}{(1-ika)}$ ✓ $\;,\; t \to 0$ ✓.

soln for $|t|^2 = P_t$,
general case. transmission probability $P_t = |t|^2$ is, after considerable algebra,

$$\boxed{P_t = \left[1 + \frac{1}{4\epsilon(1-\epsilon)} \sinh^2\left(\xi \sqrt{1-\epsilon} \right) \right]^{-1} \quad E < V_0}$$

$\epsilon \equiv E/V_0 < 1$

$\xi \equiv \dfrac{\sqrt{2mV_0}\,R}{\hbar}$

= dimensionless well parameter.

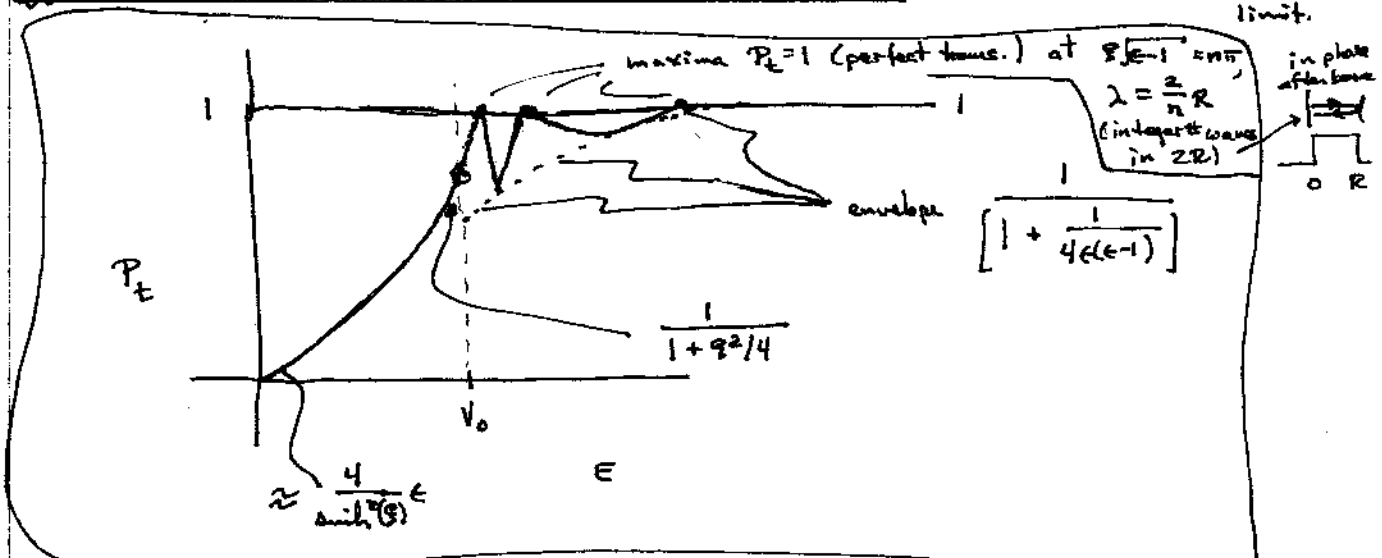
"$\hbar$ large" $\xi \to 0$ extreme quantum limit

"$\hbar$ small" $\xi \to \infty$ classical limit.

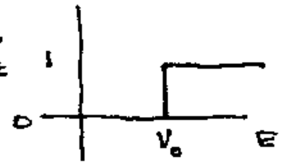
+ repeating this exercise for osc. solns in barrier,

$$\boxed{P_t = \left[1 + \frac{1}{4\epsilon(\epsilon-1)} \sin^2\left(\xi \sqrt{\epsilon - 1} \right) \right]^{-1} \quad E > V_0}$$

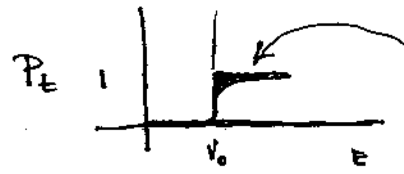
$P_r = 1 - P_t$ of course



The classical result is



note we do not recover this as $\xi \to \infty$, in stead we approach a rapidly osc. limit



with osc between 1 and $\dfrac{1}{\left(1 + \frac{1}{4\epsilon(\epsilon-1)}\right)}$

QM $\not\to$ classical !? (perhaps because of the discontinuous $V(x)$?).

barrier phase shifts.

reflected wave $\quad r = \underbrace{\underbrace{-f}_{\text{step result}}}_{e^{i\delta^{(0)}}} \underbrace{\underbrace{\left(\frac{s^2-1}{s^2-f^2}\right)}_{\text{correction for finite barrier}}}_{\cdot |r| e^{i\delta^{(1)}}} = |r| e^{i\delta}$

$f = \frac{1+ika}{1-ika}$

$s = e^{R/a}$

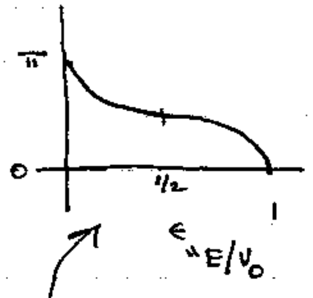
$ka = \sqrt{\frac{E}{V_0 - E}} = \sqrt{\frac{\epsilon}{1-\epsilon}}$

$$\delta^{(1)} = \tan^{-1}\left\{\frac{4\sqrt{\epsilon(1-\epsilon)}\,(1-2\epsilon)}{s^2-1+8\epsilon(1-\epsilon)}\right\}$$

$$\delta^{(0)} = \tan^{-1}\left\{\frac{2\sqrt{\epsilon(1-\epsilon)}}{1-2\epsilon}\right\} \rightarrow$$ (have to be careful which branch we are on!)

$\epsilon \to 0$, $\delta^{(0)} \to \pi$.

or $\delta^{(0)} = \cos^{-1}(2\epsilon - 1)$ better!



$\therefore$ total refl. phase is

$$\delta = \delta^{(0)} + \delta^{(1)} = \cos^{-1}(2\epsilon-1) + \underbrace{\tan^{-1}\left\{\frac{4(1-2\epsilon)\sqrt{\epsilon(1-\epsilon)}}{s^2-1+8\epsilon(1-\epsilon)}\right\}}_{\text{vanishes at } \epsilon = 0,\, 1/2}$$

$$\xrightarrow[\epsilon \to 1]{} -\tan^{-1}\left(\frac{2}{9}\right)$$

$$f = \frac{1+ika}{1-ika}$$

... phase shifts.

transmitted wave $(E<V_0)$

$$t = \frac{s}{(s-f^2)}(1-f^2)e^{-ikR}$$

$$\equiv |t|e^{i\delta_t} \quad = \underbrace{\frac{s}{(s^2-f^2)(s^2-f^{*2})}}_{\text{real}} \underbrace{(s-f^{*2})(1-f^2)}_{\text{complex, } |t_1|e^{i\delta_t^{(1)}}} \underbrace{e^{-ikR}}_{e^{i\delta_t^{(0)}}}$$

(no-barrier phase)

solve for the phase, using $\epsilon \equiv E/V_0$, $ka = \sqrt{\frac{\epsilon}{1-\epsilon}}$;

$$\tan\delta_t \quad \delta_t = -kR$$

$$\underset{\sim}{\delta_t} = \delta_t^{(0)} + \delta_t^{(1)}$$

$$\delta_t^{(0)} \to -kR = -\xi\sqrt{\epsilon}$$

$$\xi \equiv \frac{\sqrt{2mV_0}\,R}{\hbar}$$

$$\delta_t^{(1)} \to -\tan^{-1}\left\{\frac{(1-2\epsilon)}{2\sqrt{\epsilon(1-\epsilon)}}\tanh\left(\xi\sqrt{1-\epsilon}\right)\right\}$$

limits: $\epsilon \to 0$, $\delta_t \to -\frac{\pi}{2} + \sqrt{\epsilon}\left(\frac{2}{\xi} - \xi\right)$

$\epsilon \to 1_-$, $\delta_t \to -\xi + \tan^{-1}(\xi/2)$

repeating this exercise for $E > V_0$, we find

$$\delta_t = -\xi\sqrt{\epsilon} + \tan^{-1}\left\{\frac{(2\epsilon-1)}{2\sqrt{\epsilon(\epsilon-1)}}\tan\left(\xi\sqrt{\epsilon-1}\right)\right\}$$

$$\text{or} \quad -kR + \tan^{-1}\left\{\frac{p^2+k^2}{2pk}\tan(pR)\right\}$$

limits: $\xi \to 0$, $\delta_t \to -\frac{1}{2\sqrt{\epsilon}}\xi$. $\quad \epsilon \to 1_+$, $\delta_t \to -\xi + \tan^{-1}(\xi/2)$