* Some solutions of SE are un-normalizable:
UNBOUND or SCATTERING solutions; usually of plane-wave form:

$$\psi(x) = Ae^{+ikx} \quad \text{or} \quad \psi(x) = B\sin kx + C\cos kx$$

$$\text{or} \quad \psi(x) = De^{-ikx}$$

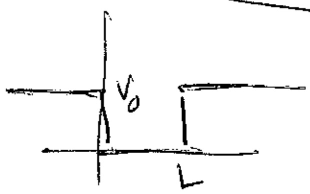
→ A special case, doesn't fit comfortably in mathematical formulation; not member of a Hilbert space. ☹ Nevertheless important.

We will formulate "scattering" questions using such w.f.'s.

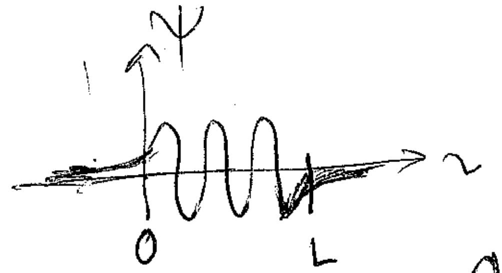
* continue FINITE SQUARE WELL

defined on p. 40

Two types of solutions:



Ⓐ $E < V_0$ bound state



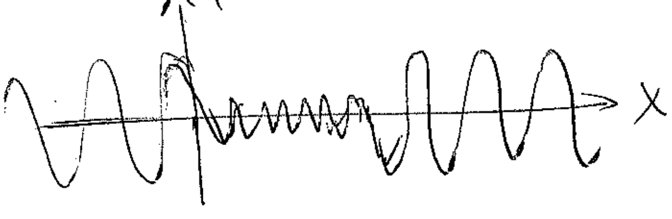
Inside: similar as infinite well.

Outside: falls of EXPONENTIALLY, but not strictly zero, although classically forbidden.

[Classically: when $E < V_0$, kin. energy < 0
$\rightarrow$ not possible]

Can be regarded as a basic example of quantum tunneling.

Ⓑ $E > V_0$ unbound state



Different wavelengths inside and outside.
Hence also different amplitudes.

Inside: $k = \sqrt{\frac{2mE}{\hbar^2}}$ $\longleftarrow$ k larger inside

Outside: $\tilde{k} = \sqrt{\frac{2m(E-V_0)}{\hbar^2}}$ $\Rightarrow$ wavelength smaller inside.

Can solve inside and outside, and then match boundary conditions.

Theorem. If $V(x)$ is everywhere finite [e.g., finite square well], then both $\psi(x)$ and $\psi'(x)$ are continuous everywhere.

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

$\Rightarrow$ ψ'' must be finite & well-defined everywhere

$\Rightarrow$ ψ, ψ' must be continuous everywhere.

Ⓐ Bound state solutions of finite square well

$\boxed{0 < E < V_0}$

Region II:

$$\frac{d^2}{dx^2}\psi_n(x) + \overbrace{\left(\frac{2mE_n}{\hbar^2}\right)}^{k_n^2}\psi_n(x)$$

Same as for infinite square well. Solutions

$$\psi_n(x) = A_{II}e^{ik_nx} + B_{II}e^{-ik_nx} = C\cos(k_nx) + D\sin(k_nx)$$

Outside?
$$\frac{d^2}{dx^2}\psi_n(x) - \underbrace{\frac{2m}{\hbar^2}(V_0 - E_n)}_{\text{positive}}\psi_n(x) = 0$$

Define $\alpha = \sqrt{\frac{2m(V_0-E)}{\hbar^2}}$

Common to use K

avoid confusion K & k

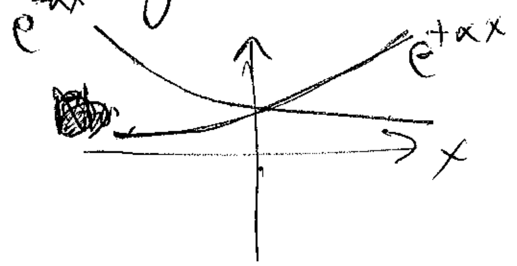
real because $V_0 > E$

$$\frac{d^2\psi_n}{dx^2} - \alpha^2 \psi_n = 0$$

Solutions are $e^{+\alpha x}$ and $e^{-\alpha x}$

Region I: $\psi_n(x) = A_I e^{\alpha x} + B_I e^{-\alpha x}$

Region III: $\psi_n(x) = A_{III} e^{\alpha x} + B_{III} e^{-\alpha x}$



Makes no sense for $\psi(x)$ to diverge. So,

Region I $\psi_n(x) = A_I e^{\alpha x}$ $(B_I = 0)$

II $\psi_n(x) = B_{III} e^{-\alpha x}$ $(A_{III} = 0)$

Thus we have:

Region I: $\psi_n(x) = A_I e^{\alpha x}$

Reg. II: $\psi_n(x) = C \cos kx + D \sin kx$

Reg. III: $\psi_n(x) = B_{III} e^{-\alpha x}$

with $k = \sqrt{\frac{2mE}{\hbar^2}}$, $\alpha = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$

We have 5 constants: A_I, C, D, B_{III}, E

and 5 conditions: $\psi_I(0) = \psi_{II}(0)$, $\psi_I'(0) = \psi_{II}'(0)$

$\psi_{II}(L) = \psi_{III}(L)$, $\psi_{II}'(L) = \psi_{III}'(L)$, normalization: $\int_{-\infty}^{\infty} |\psi|^2 dx = 1$

$\Rightarrow$ consistent solutions can be found, in principle.

Five equations (nonlinear):

$$
\begin{cases}
A_I = C, \quad \alpha A_I = kD \\
C\cos(kL) + D\sin(kL) = B_{III} e^{-\alpha L} \\
-kC\sin(kL) + kD\cos kL = -\alpha B_{III} e^{-\alpha L} \\
\text{and} \quad \int_{-\infty}^{0} dx\, |A_I|^2 e^{2\alpha x} + \int_0^L dx\, |C\cos kx + D\sin kx|^2 + \int_L^{\infty} dx\, |B_{III}|^2 e^{-2\alpha x} = 1
\end{cases}
$$

Solutions can be obtained numerically or graphically. (Some details in Nash.)

Finite number of solutions.

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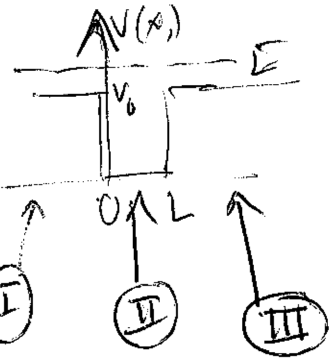
(B) Unbound states. $E > V_0$



Define $k = \sqrt{\frac{2mE}{\hbar^2}}$, $\alpha = \sqrt{\frac{2m}{\hbar^2}(E - V_0)}$

definition changed from $E < V_0$ case

Solutions in regions ↑ :

(I) $\psi_I(x) = A_I e^{i\alpha x} + B_I e^{-i\alpha x}$

Can also be written as: $\psi_I(x) = A_I' \sin \alpha x + B_I' \cos \alpha x$

Either would be "complete", i.e., all solutions included.

(II) $\psi_{II}(x) = A_{II} e^{ikx} + B_{II} e^{-ikx}$

(III) $\psi_{III}(x) = A_{III} e^{i\alpha x} + B_{III} e^{-i\alpha x}$

\# constants? $A_I, B_I, A_{II}, B_{II}, A_{III}, B_{III}$ (6)

E is arbitrary; solutions exist for every E.

equations / # conditions?

4 boundary conditions:

$$\begin{cases} \psi_I(0) = \psi_{II}(0) \\ \psi_I'(0) = \psi_{II}'(0) \\ \psi_{II}(L) = \psi_{III}(L) \\ \psi_{II}'(L) = \psi_{III}'(L) \end{cases}$$

No normalization condition ☹

but overall magnitude can be chosen arbitrarily. (E.g., set $A_I = 1$.)

Total 5.

5 constants, 4 equations! $\Rightarrow$ for every E, there is an infinite # of solutions.

* Can reformulate to study transmission/reflection:

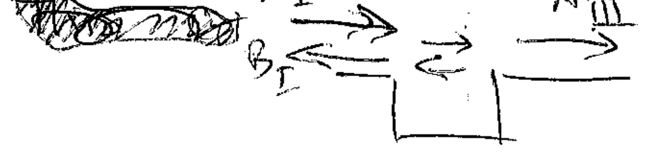
Choose

$$\psi_I = A_I e^{i\alpha x} + B_I e^{-i\alpha x}$$

$$\psi_{II} = A_{II} e^{ikx} + B_{II} e^{-ikx}$$

$$\psi_{III} = A_{III} e^{i\alpha x} \quad [\text{no } e^{-i\alpha x} \text{ term}]$$

Interpreting $e^{\pm i\alpha x}$ as right(left)-moving waves,



and the A_I term as INCIDENT wave,

B_I represents REFLECTION, A_{III} represents TRASMISSION.

Define coefficients $T = \left|\dfrac{A_{III}}{A_I}\right|^2$, $R = \left|\dfrac{B_I}{A_I}\right|^2$

---

* Why is e^{+ikx} (e^{-ikx}) interpreted as right- (left-) moving?

If e^{ikx} is a solution of Time-indep. SE, then corresponding sol^n of TDSE is

$$e^{ikx}e^{-iEt/\hbar} = \exp\left[i\left(kx - \frac{E}{\hbar}t\right)\right]$$

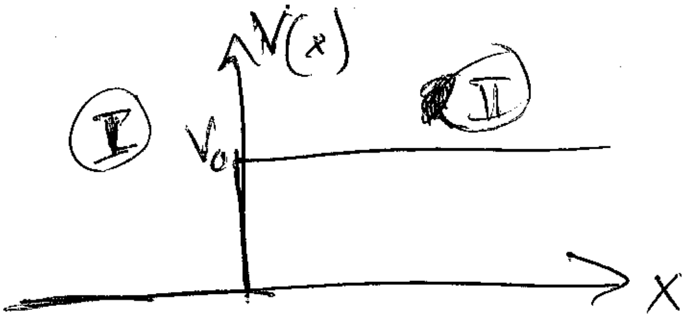
$$= \cos\left(kx - \frac{E}{\hbar}t\right) + i\sin\left(kx - \frac{E}{\hbar}t\right)$$

These are right-moving waves. (Slight increase of t represents slight decrease of phase, i.e., slight shift of wave rightward.)

Similarly, $e^{-ikx}e^{-iEt/\hbar} = \cos\left(kx + \frac{E}{\hbar}t\right) - i\sin\left(kx + \frac{E}{\hbar}t\right)$

~~FIRST ... PROBABILITY CURRENT DENSITY~~
~~FIRST, CURRENT (next page)~~

* The Potential Step : reflection & Transmission



We consider matter wave (particle or particle current) incident from left,

Solutions :
(A) $E > V_0$

$$\Psi_I(x) = A_I e^{ik_1x} + B_I e^{-ik_1x}$$

$$\Psi_{II}(x) = A_{II} e^{ik_2x}$$ no leftmoving/incoming in (II)

$$k_1 = \sqrt{\frac{2mE}{\hbar^2}}, \quad k_2 = \sqrt{\frac{2m}{\hbar^2}(E-V_0)}$$

previously $\propto$ RATIO of CURRENTS

Let's set $A_I = 1$, then $R = |B_I|^2$, $\boxed{T = |A_{II}|^2 \frac{k_2}{k_1}}$

Boundary conditions : $\Psi_I(0) = \Psi_{II}(0)$, $\Psi_I'(0) = \Psi_{II}'(0)$

$$\Rightarrow \quad 1 + B_I = A_{II}, \quad k_1 - k_1 B_I = k_2 A_{II}$$

$$\Rightarrow \quad B_I = \frac{k_1 - k_2}{k_1 + k_2} \qquad A_{II} = \frac{2k_1}{k_1 + k_2}$$

$$\boxed{R = \left(\frac{k_1 - k_2}{k_1 + k_2}\right)^2 \qquad T = \frac{4k_1k_2}{(k_1+k_2)^2}}$$

Probability Current Density

For a single particle in 1D,

$$j = \frac{i\hbar}{2m}\left(\psi\,\partial_x\psi^* - \psi^*\partial_x\psi\right) = \frac{\hbar}{m}\,\mathrm{Im}\left[\psi^*\partial_x\psi\right]$$

is the probability current density. The TDSE can be rewritten as (Nash, footnote, p. 42-43)

$$\frac{\partial\rho}{\partial t} + \frac{\partial j}{\partial x} = 0$$

where $\rho = |\psi|^2$

A continuity equation for prob^y

In 3D, $\vec{j} = \frac{i\hbar}{2m}\left(\psi\vec{\nabla}\psi^* - \psi^*\vec{\nabla}\psi\right)$ (a vector)

obeys the 3D continuity eq.

$$\frac{\partial}{\partial t}|\psi(\vec{r},t)|^2 + \vec{\nabla}\cdot\vec{j}(\vec{r},t) = 0$$

Similar eq. for charge in classical EM, & for mass in fluid dynamics.

prob. currents INTERLUDE contd.

* For $\psi = A e^{i(kx-\omega t)}$, (plane wave, right moving. $\omega = \frac{E}{\hbar}$

time-dependence

$$j = \frac{\hbar}{m} \operatorname{Im} \left[\left(A e^{i(kx-\omega t)}\right)^* \partial_x \left(A e^{ikx}\right) \right]$$

$$= \frac{\hbar}{m} |A|^2 \operatorname{Im} \left[e^{-i(kx-\omega t)} \, ik \, e^{i(kx-\omega t)} \right]$$

$$= |A|^2 \frac{\hbar k}{m}$$

$\longrightarrow$ proportional to wavenumber k, momentum $\hbar k$

$\longrightarrow$ prop. to particle density / probability $\boxed{|A|^2 = |\psi|^2}$

* Think of $\psi = Ae^{ikx}$ as a steady beam/stream of ptcles, with density $|A|^2$

Classical interpretation : $j = |A|^2 \times \frac{\hbar k}{m}$

current density = particle density × velocity

* For bound state, $\psi = \phi(x)\, e^{-i\omega t}$ $\omega = \frac{E}{\hbar}$

with $\phi(x)$ a real function $\left[\sin \frac{\pi x}{L}, \; e^{-x^2/\sigma^2}, \; \text{etc} \right]$

$\Rightarrow j(x,t) = 0$ No current. Makes sense?

(55)

Potential step continued : $\boxed{T = \frac{j_T}{j_I} = \frac{|A_{II}|^2 \frac{\hbar k_2}{m}}{|A_I|^2 \frac{\hbar k_1}{m}} = |A_{II}|^2 \frac{k_2}{k_1}}$

$R + T = 1$ makes sense ? particles either reflected or conserved!

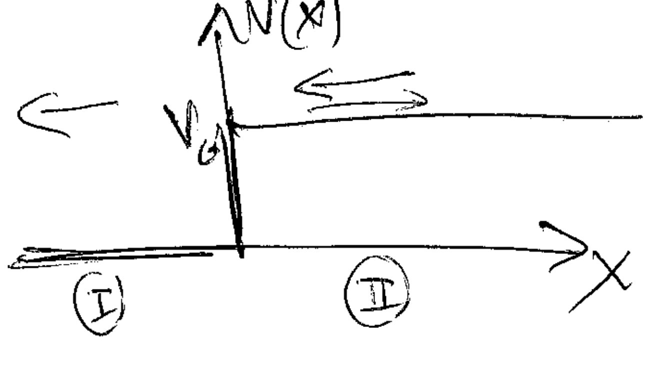
For $V_0 \to 0$, $k_2 = \sqrt{\frac{2m}{\hbar^2}(E - V_0)} \to \sqrt{\frac{2m}{\hbar^2}E} = k_1$

$\Rightarrow$ $R \to 0$, $T \to \frac{4k_1k_1}{(k_1+k_1)^2} = 1$

If no potential barrier, no reflection, complete, transmission.

Do after $E < V_0$ (next page)

* Negative potential step, or pole from right



$\psi_I(x) = A_I e^{ik_1x} + B_I e^{-ik_1x}$

$\psi_{II}(x) = A_{II} e^{ik_2x} + B_{II} e^{-ik_2x}$

Now, set $B_I = 1$, $A_{II} = 0$.

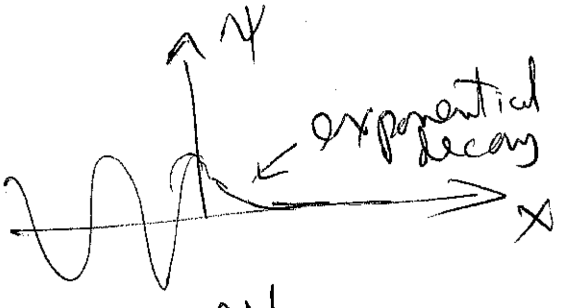
$R = |A_I|^2$, $T = |B_{II}|^2 \frac{k_1}{k_2}$

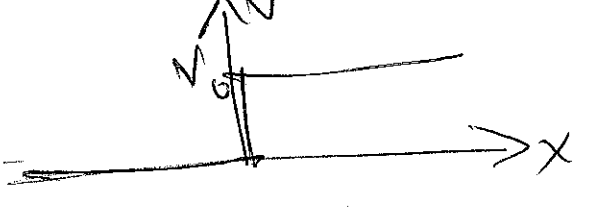
Problem is identical to previous, with $k_1 \longleftrightarrow -k_2$

Thus $R = \left(\frac{k_1 - k_2}{k_1 + k_2}\right)^2$, $T = \frac{4 k_1 k_2}{(k_1 + k_2)^2}$

i.e., there is reflection also from a potential drop. Surprising? Doesn't happen in classical mechanics.

(B) $E < V_0$





$$\psi_I(x) = A_I e^{ik_1 x} + B_I e^{-ik_1 x}$$

$$\psi_{II}(x) = C e^{-\alpha x} + D e^{+\alpha x}$$

$$k_1 = \sqrt{\frac{2m}{\hbar^2} E}, \quad \alpha = \sqrt{\frac{2m}{\hbar^2}(V_0 - E)}$$

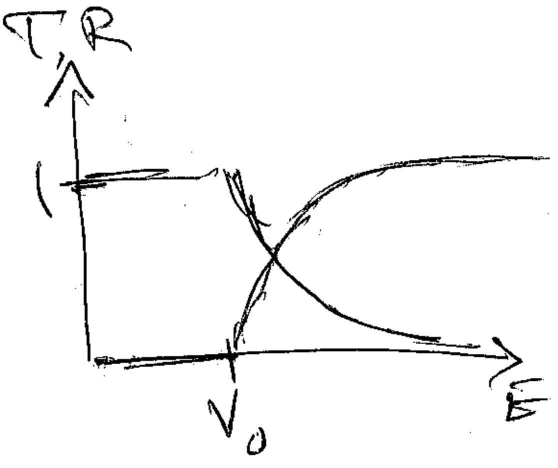
$D = 0$, exploding w.f. makes no sense

Set $A_I = 1$, use boundary conditions:

$$B_I = -\frac{\alpha + ik}{\alpha - ik} \qquad C = \frac{-2ik}{\alpha - ik}$$

$$R = |B_I|^2 = \frac{\alpha^2 + k^2}{\alpha^2 + k^2} = 1$$ NO TRANSMISSION, COMPLETE REFLECTION

Transmission & reflection as f^n of E



$$T = \begin{cases} 0 & E < V_0 \\ \dfrac{4k_1k_2}{(k_1+k_2)^2} & E > V_0 \end{cases}$$

$$R = \begin{cases} 1 & E < V_0 \\ \left(\dfrac{k_1-k_2}{k_1+k_2}\right)^2 & E > V_0 \end{cases}$$

NOW DO NEGATIVE POTENTIAL STEP, p.55

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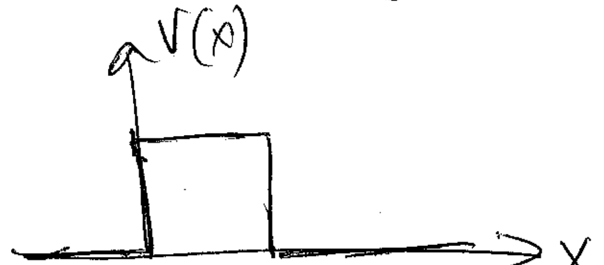
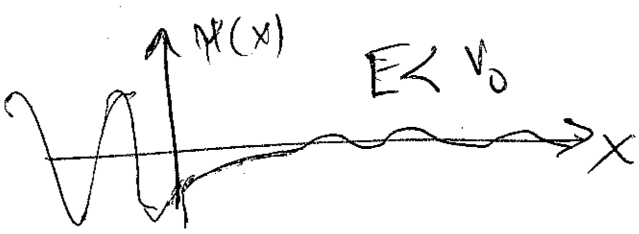
* The finite potential barrier





Finite transmission even for $E < V_0$

Can get complicated but explicit formulas for $|R|^2$ and T

$A_I = 1$

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

$\psi_{II}(x) = Ce^{\alpha x} + De^{-\alpha x}$

$\psi_{III}(x) = A_{III} e^{ikx}$ no incident from right