1d potential problems

Time Independent Potentials:

Schrödinger eqn:

$$i\hbar \frac{\partial \Psi}{\partial t} = H \Psi$$

Let $H = -\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})$. NOTE: $V(\vec{r})$ is independent of time.

The wave function $\Psi(\vec{r},t)$ in such cases can be separated as follows:

$$\Psi(\vec{r},t) = \varphi(\vec{r})\,\chi(t)$$

Then:

$$i\hbar \frac{\partial}{\partial t}\left[\varphi(\vec{r})\,\chi(t)\right] = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})\right]\left(\varphi(\vec{r})\,\chi(t)\right)$$

or: $\div$ by $\varphi(\vec{r})\,\chi(t)$:

$$\underbrace{\frac{1}{\chi(t)}\, i\hbar \frac{\partial \chi(t)}{\partial t}}_{\text{function of } t} = + \underbrace{\frac{1}{\varphi(\vec{r})}\left[-\frac{\hbar^2}{2m}\nabla^2\varphi(\vec{r}) + V(\vec{r})\,\varphi(\vec{r})\right]}_{\text{function of } \vec{r}.}$$

This is possible iff the LHS & RHS is equal to a constant. Let us call this constant $\hbar\omega$.

Then: for the LHS:

$$\frac{i\hbar}{x(t)} \frac{dx(t)}{dt} = \hbar\omega$$

$$\frac{dx(t)}{x(t)} = \frac{\hbar\omega}{i\hbar} dt = -i\omega\, dt$$

$$\therefore \boxed{x(t) = A e^{-i\omega t}}$$

and: for the RHS:

$$\underbrace{-\frac{\hbar^2}{2m} \nabla^2 \varphi(\vec{r}) + V(\vec{r})\, \varphi(\vec{r}) = \hbar\omega\, \varphi(\vec{r})}_{\text{Eigenvalue eqn.}}$$

Then: $\Psi(\vec{r},t) = \varphi(\vec{r})\, e^{-i\omega t}$ [setting $A = 1$ → implies that we have absorbed the constant A in $\varphi(\vec{r})$].

$\Psi(\vec{r},t)$ which has the above form is called a stationary state solution of the Schrödinger eqn. This leads to time independent probabilities: $|\Psi(\vec{r},t)|^2 = |\varphi(\vec{r})|^2$

ω is related to E, the energy by: $E = \hbar\omega$. Therefore a stationary state has well defined energies. In classical Mechanics, when the potential is independent of time, then E is conserved. <u>In quantum mechanics, it leads to well determined energy states</u>

Symmetries ⟶ Conserved Qties ⟶ <u>Good quantum Numbers</u>

The radial eqn:

$$H\varphi(\vec{r}) = E\varphi(\vec{r})$$

leads to square integrable solutions : $\int_{-\infty}^{\infty} |\varphi(\vec{r})|^2 d\vec{r} < \infty$

only for some values of E leading to discretization of energies.

Although the radial eqn: $H\varphi(\vec{r}) = E\varphi(\vec{r})$ is called TISE and $i\hbar \frac{\partial \Psi}{\partial t} = H\Psi$ the TDSE, their essential difference lies in the fact that $\Psi(\vec{r},t)$ is the general solution, while TISE gives a subset which are stationary states.

Superposition of stationary states:

In order to distinguish between the various possible values of E, we label with an index n. ie:

$$H\varphi_n(\vec{r}) = E_n \varphi_n(\vec{r})$$

and the stationary state solution:

$$\Psi_n(\vec{r},t) = \varphi_n(\vec{r})\, e^{-i\omega_n t} = \varphi_n(\vec{r})\, e^{-iE_n t/\hbar}$$

Therefore the general solution:

$$\Psi(\vec{r},t) = \sum_n \cancel{\Psi_n(\vec{r},t)}^{\,\varphi_n(\vec{r})}\, e^{-iE_n t/\hbar} c_n$$

($\because$ the eqn is linear.

$\Rightarrow \hat{A}(\alpha|a\rangle + \beta|b\rangle) = \hat{A}\alpha|a\rangle + \hat{B}\beta|b\rangle$.

& c_n : are arbitrary complex coeffns: In particular:

$$\underbrace{\Psi(\vec{r},0) = \sum_n{}' c_n \varphi_n(\vec{r})}$$

Basis expansion of an arbitrary $|\Psi\rangle$.

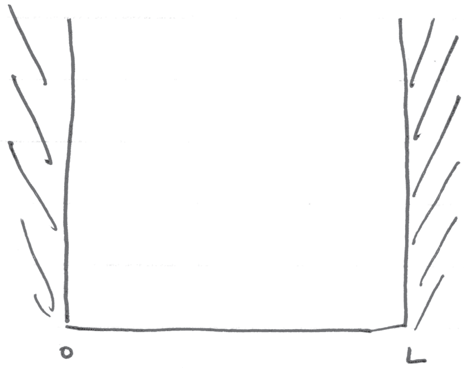
1) potential problems

We are going to solve the Schrödinger eqn for some standard cases:

(i) Particle in a box with infinite wall (1d)

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$$

where $V(x) = \begin{cases} 0 & \text{if } \quad 0 < x < L \\ \infty & \text{if } \quad x \leq 0 \,;\; x \geq L \end{cases}$



$\Psi(x = L) = \Psi(x = 0) = 0 \qquad$ (B.C)

$\Psi(x) = 0 \quad$ if $\quad x \leq 0, \; x \geq L.$

Solve for the Time independent eigenvalue eqn.

$$H\Psi = E\Psi$$

$$-\frac{\hbar^2}{2m}\frac{d^2\Psi}{dx^2} + V(x)\,\Psi(x) = E\Psi(x)$$

Choose: $\quad 0 < x < L$

$$\Rightarrow \; -\frac{\hbar^2}{2m}\frac{d^2\Psi(x)}{dx^2} = E\Psi(x)$$

$$\frac{d^2\Psi(x)}{dx^2} = -\frac{2mE}{\hbar^2}\Psi(x)$$

or: $$\frac{d^2\Psi(x)}{dx^2} + \frac{2mE}{\hbar^2}\Psi(x) = 0$$

$\Rightarrow \ \Psi(x) = A \sin(ax) + B \cos(ax)$

where

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

$\Psi(0) = 0 = \Psi(L)$

$\Rightarrow \ B = 0$ (using $x = 0$)

$A \sin(aL) = 0$

$\Rightarrow \ aL = n\pi \qquad n = \cancel{0}, 1, 2 \dots$

$$a = \frac{n\pi}{L}$$

Conventional to call $a \equiv k = \frac{n\pi}{L}$.

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

A: fixed through normalization

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

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

$$= \frac{A^2}{2} L - \underbrace{\int_0^L \cos\left(\frac{2n\pi x}{L}\right) dx}_{= 0}$$

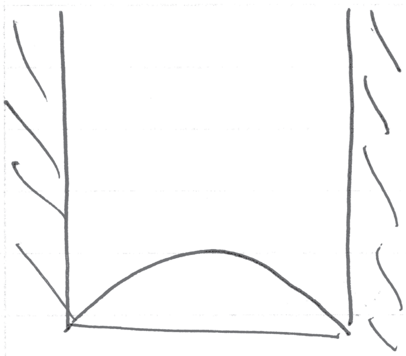
$$\Rightarrow \ A = \sqrt{\frac{2}{L}}$$

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

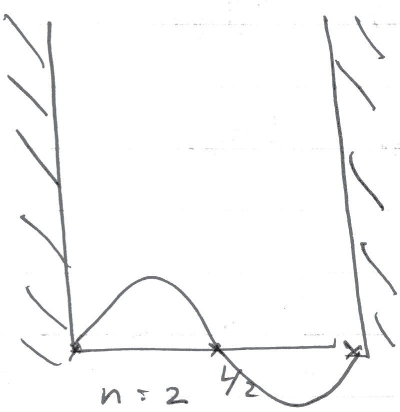
Energies: $k = \sqrt{\frac{2mE}{\hbar^2}} = \frac{n\pi}{L} \quad \Rightarrow \quad \frac{2mE}{\hbar^2} = \frac{n^2\pi^2}{L^2}$

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

$E \propto n^2$ (Notice that not all values of n are allowed!)



$n = 1$



$n = 2$

etc...

$\Psi(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{\cancel{2n}\,\pi x}{2}\right)$

$= \cancel{\sqrt{\frac{2}{L}} \sin}$ $\quad x = L/2$

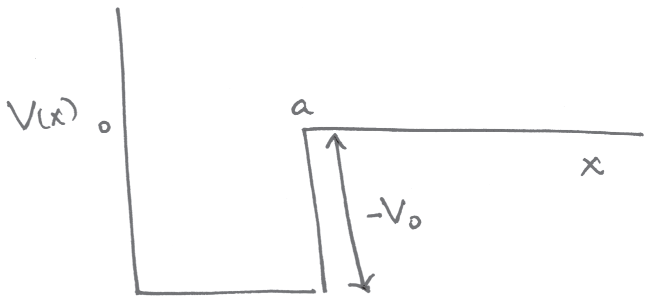
Square Wells: Stationary States

Square well potential is defined by $V(x) = V$ in certain regions of space. In such regions: we have the following eqn:

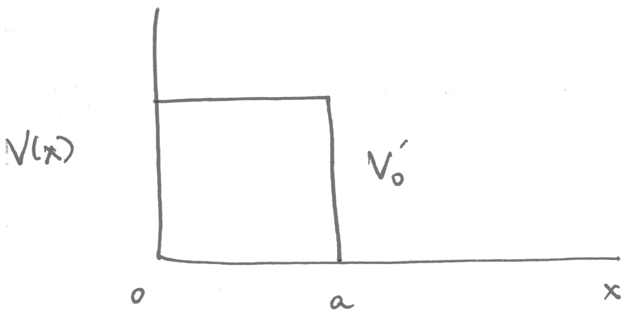
$$\frac{d^2}{dx^2}\varphi(x) + \frac{2m}{\hbar^2}(E-V)\varphi(x) = 0$$

Examples:

$$V(x) = \begin{cases} -V_0 & 0 \leq x < a \\ 0 & \text{otherwise.} \end{cases}$$



$$V(x) = \begin{cases} V_0' & 0 < x \leq a \\ 0 & \text{otherwise.} \end{cases}$$



We shall distinguish two cases:

(i) $E > V$

Then set ~~E-V~~ $E - V = \frac{\hbar^2 k^2}{2m}$ (positive Const k).

Then: $\frac{d^2\varphi(x)}{dx^2} + k^2\varphi(x) = 0$ or: $\varphi(x) = A e^{ikx} + A' e^{-ikx}$

A, A' are complex constants.

(ii) $E < V$ (classically forbidden region)

Then: define: $V - E = \frac{\hbar^2 \rho^2}{2m}$ $(\rho > 0)$

Then: $\frac{d^2\varphi(x)}{dx^2} - \rho^2\varphi(x) = 0$

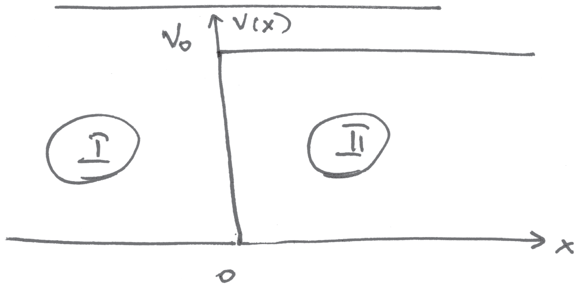
$\Rightarrow \varphi(x) = B e^{\rho x} + B' e^{-\rho x}$

B, B' : Complex Constants

(iii) $E = V$ $\Rightarrow \frac{d^2\varphi(x)}{dx^2} = 0$ $\varphi(x)$: linear fn of x.

Once we have solved for different regions (and cases) we match the solutions at the discontinuities and fix the constants. Let us see examples where this strategy becomes clear.

a. POTENTIAL STEP:



$$V(x) = \begin{cases} 0 & x < 0 \\ V_0 & x \geq 0 \end{cases}$$

(i) $E > V_0$

In region I:

$$-\frac{\hbar^2}{2m}\frac{d^2\varphi_1(x)}{dx^2} + \underbrace{V(x)}_{=0}\varphi_1(x) = E\,\varphi_1(x)$$

$$\Rightarrow \frac{d^2\varphi_1(x)}{dx^2} + \left(\sqrt{\frac{2mE}{\hbar^2}}\right)^2 \varphi_1(x) = 0$$

Let $\sqrt{\frac{2mE}{\hbar^2}} = k_1^2$

$$\therefore \frac{d^2\varphi_1(x)}{dx^2} + k_1^2\,\varphi_1(x) = 0$$

or $\varphi_1(x) = A_1 e^{ik_1 x} + A_1' e^{-ik_1 x}$

<u>In region II</u>:

$$-\frac{\hbar^2}{2m}\frac{d^2\varphi_2}{dx^2} + V_0\,\varphi_2(x) = E\,\varphi_2(x)$$

$$-\frac{\hbar^2}{2m}\frac{d^2\varphi_2}{dx^2}\ \cancel{+}\ - (E-V_0)\,\varphi_2(x) = 0$$

or: $$\frac{d^2\varphi_2}{dx^2} + \frac{2m}{\hbar^2}(E-V_0)\,\varphi_2(x) = 0$$

Let $k_2 = \sqrt{\frac{2m}{\hbar^2}(E-V_0)}$

$$\Rightarrow \frac{d^2\varphi_2}{dx^2} + k_2^2\,\varphi_2 = 0$$

or $\varphi_2(x) = A_2 e^{ik_2 x} + A_2' e^{-ik_2' x}$

Match at $x = 0$

$$\varphi_1(x=0) = \varphi_2(x=0)$$

$$\varphi_1'(x=0) = \varphi_2'(x=0)$$

$\Rightarrow \cancel{A_1 + A_2}$

Two eqns. 4 unknowns! Set $A_2' = 0$ (Physical requirement particle coming from $-\infty$ $\vec{k}$ along $\vec{x}$)

$$\therefore \varphi_1(x) = A_1 e^{ik_1 x} + A_1' e^{-ik_1 x}$$

$$\varphi_2(x) = A_2 e^{ik_2 x}$$

$$\varphi_1(0) = \varphi_2(0)$$

$$A_1 + A_1' = A_2$$

$$\varphi_1'(0) = \varphi_2'(0)$$

$$k_1(A_1 - A_1') = k_2 A_2$$

$$\text{or: } A_2 = \frac{k_1}{k_2}(A_1 - A_1')$$

$$\therefore A_1 + A_1' = \frac{k_1}{k_2}(A_1 - A_1')$$

$$A_1\left(1 - \frac{k_1}{k_2}\right) = -A_1'\left(1 + \frac{k_1}{k_2}\right)$$

$$\therefore \frac{A_1'}{A_1} = -\frac{(1 - k_1/k_2)}{1 + k_1/k_2} = -\frac{k_2 - k_1}{k_1 + k_2} = \frac{k_1 - k_2}{k_1 + k_2}$$

$$\frac{A_2}{A_1} = 1 + \frac{A_1'}{A_1} = 1 + \frac{k_1 - k_2}{k_1 + k_2} = \frac{k_1 + \cancel{k_2} + k_1 - \cancel{k_2}}{k_1 + k_2}$$

$$= \frac{2k_1}{k_1 + k_2}$$

In order to make sense: let us understand $\varphi_1(x)$ and $\varphi_2(x)$.

$$\varphi_1(x) = A_1 e^{ik_1 x} + A_1' e^{-ik_1 x}$$

$e^{ik_1 x}$: particle moving from $-\infty \to \infty$ (left to right)
$(\hbar k_1 = p_1)$

$e^{-ik_1 x}$: particle moving from right to left. $(-\hbar k_1 = p_1)$

$\varphi_2(x) = A_2 e^{ik_2 x}$: Outgoing particle left to right.

Define ~~transmission~~ Reflection coeffn

$$\cancel{T = A_2} \quad R = \left|\frac{A_1'}{A_1}\right|^2$$

Then transmission coeffn: $1 - R = T$

Physical meaning: For a particle traveling from left to right, it sees the barrier at $x = 0$. A part of it gets reflected and a part transmitted. (Think of waves).

$$R = \left|\frac{A_1'}{A_1}\right|^2 = \left|\frac{k_1 - k_2}{k_1 + k_2}\right|^2 \quad \text{(prob. of being reflected)}$$

$$T = 1 - \left|\frac{k_1 - k_2}{k_1 + k_2}\right|^2 = \frac{\cancel{k_1^2} + \cancel{k_2^2} + 2k_1k_2 - \cancel{k_1^2} - \cancel{k_2^2} + 2k_1k_2}{(k_1 + k_2)^2}$$

$$= \frac{4k_1k_2}{(k_1 + k_2)^2} = \frac{k_2}{k_1}\left|\frac{A_2}{A_1}\right|^2$$

~~Tot~~ Case (ii) $E < V_0$: total reflection

Region 1: Same:

$$\varphi_1(x) = A_1 e^{ik_1 x} + A_1' e^{-ik_1 x}$$

Region 2: $\rho_2 = \sqrt{\dfrac{2m(V_0 - E)}{\hbar^2}} > 0$

Ren: $\dfrac{d^2\varphi_2(x)}{dx^2} - \rho_2(x)\,\varphi_2(x) = 0$

$$\therefore \varphi_2(x) = \underbrace{B_2}_{0} e^{\rho_2 x} + B_2' e^{-\rho_2 x}$$

(since $x \to \infty$ $\int |\varphi_2(x)|^2 dx < \infty$.

$\therefore$ Match:

$$\varphi_2(0) = \varphi_1(0)$$

$$\Rightarrow B_2' = A_1 + A_1'$$

$$\varphi_2'(0) = \varphi_1'(0)$$

$$\Rightarrow -\rho_2 B_2' = ik_1 (A_1 - A_1')$$

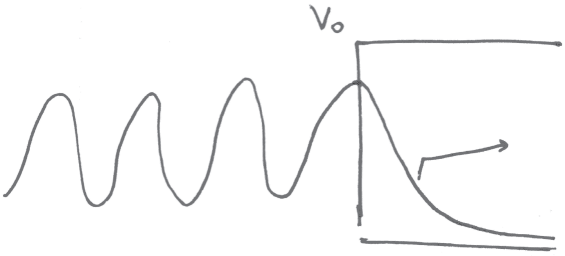
$$B_2' = \frac{k_1}{i\rho_2}(A_1 - A_1')$$

$$2B_2' = \left(\frac{k_1}{i\rho_2} + 1\right) A_1 + A_1' \left(1 - \frac{k_1}{i\rho_2}\right)$$

$$\therefore \cancel{B_2}\ \frac{A_1'}{A_1} = \frac{k_1 - i\rho_2}{k_1 + i\rho_2} \qquad R = \left|\frac{A_1'}{A_1}\right|^2 = 1$$

$$\frac{B_2'}{A_1} = \frac{2k_1}{k_1 + i\rho_2} \qquad T = 0.$$

The particle gets entirely reflected. But if one sketches the wave function for $x > 0$

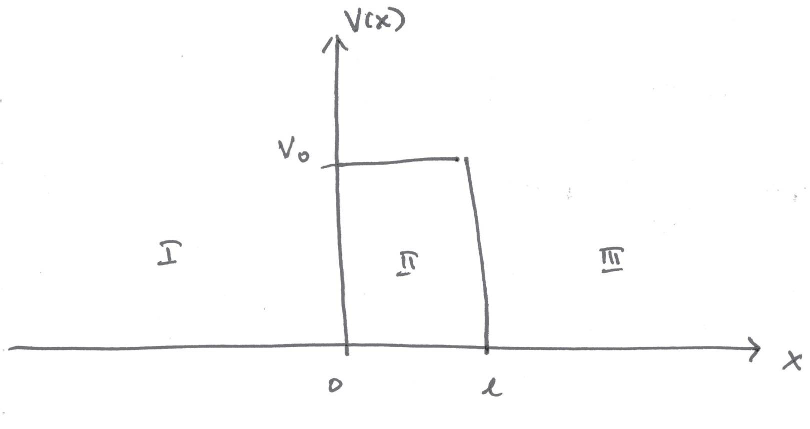


decaying tail fall off. $1/\rho_2$.

Since $\frac{A_1'}{A_1}$ is complex, there is a phase shift that appears upon reflection. (due to the fact that the particle is delayed due to penetration in the $x>0$ region).

→ This has no classical analogue.

b. POTENTIAL BARRIER



Case (i) $E > V_0$

Region I:

$$\frac{d^2\varphi_1}{dx^2} = -\frac{2mE}{\hbar^2}\varphi_1(x) \quad \text{or} \quad \frac{d^2\varphi_1}{dx^2} + \frac{2mE}{\hbar^2}\varphi_1(x) = 0$$

Use: $k_1 = \sqrt{\frac{2mE}{\hbar^2}}$

$$\Rightarrow \frac{d^2\varphi_1(x)}{dx^2} + k_1^2 \varphi_1(x) = 0$$

$$\Rightarrow \varphi_1(x) = A_1 e^{ik_1 x} + A_1' e^{-ik_1 x}$$

Region II:

$$-\frac{\hbar^2}{2m}\frac{d^2\varphi_2(x)}{dx^2} + V_0 \varphi_2(x) = E\varphi_2(x)$$

or: $$\frac{d^2\varphi_2(x)}{dx^2} + \frac{2m}{\hbar^2}(E - V_0)\varphi_2(x) = 0$$

Define $k_2 = \sqrt{\frac{2m(E-V_0)}{\hbar^2}}$

$$\therefore \frac{d^2\varphi_2(x)}{dx^2} + k_2^2 \varphi_2(x) = 0$$

$$\varphi_2(x) = A_2 e^{ik_2 x} + A_2 e^{-ik_2 x}$$

Region 3:

$$-\frac{\hbar^2}{2m}\frac{d^2\varphi_3}{dx^2} = E\varphi_3(x)$$

$$\therefore \varphi_3 = A_3 e^{ik_1 x} + A_3' e^{-ik_1 x}$$

Set $A_3 = 0$ (No reflection going from left to right).

Match at $x = 0$

$\varphi_1(x=0) = \varphi_2(x=0)$

$\varphi_1'(x=0) = \varphi_2'(x=0)$

$$\therefore A_1 + A_1' = A_2 + A_2' \quad \text{——(i)}$$

$$ik_1(A_1 - A_1') = ik_2(A_2 - A_2') \quad \text{——(ii)}$$

Match at $x = l$:

$$\varphi_2(x=l) = \varphi_3(x=l)$$
$$\varphi_2'(x=l) = \varphi_3'(x=l)$$

$$\Rightarrow \quad A_3 e^{ik_1 l} = A_2 e^{ik_2 l} + A_2' e^{-ik_2 l} \quad \text{——— (iii)}$$

$$ik_1 A_3 e^{ik_1 l} = ik_2 \left[A_2 e^{ik_2 l} - A_2' e^{-ik_2 l} \right] \quad \text{—— (iv)}$$

Using (i), (ii), (iii) and (iv) Can show:

$$A_1 = \left[\cos k_2 l - i \frac{k_1^2 + k_2^2}{2k_1 k_2} \sin k_2 l \right] e^{ik_1 l} A_3$$

and

$$A_1' = i \frac{k_2^2 - k_1^2}{2k_1 k_2} \sin k_2 l \; e^{ik_1 l} A_3$$

Matching currents, it is easy to show that

$$R = \left| \frac{A_1'}{A_1} \right|^2 \quad \text{and} \quad T = \left| \frac{A_3}{A_1} \right|^2.$$

$$\Rightarrow R = \frac{(k_1^2 - k_2^2)^2 \sin^2 k_2 l}{4k_1^2 k_2^2 + (k_1^2 - k_2^2)^2 \sin k_2 l}$$

and

$$T = \frac{4k_1^2 k_2^2}{4k_1^2 k_2^2 + (k_1^2 - k_2^2)^2 \sin^2 k_2 l} = \frac{4E(E-V_0)}{4E(E-V_0) + V_0^2 \sin^2\left(\sqrt{2m(E-V_0)}\, l/\hbar\right)}$$

Max value of $T = 1$ when $k_2 l = n\pi$, min $= \dfrac{1}{\left[1 + \dfrac{V_0^2}{4E(E-V_0)}\right]}$

(when $\sin^2() = 1$)

$T = 1 \Rightarrow R = 0$ so the barrier is transparent!

$\Rightarrow$ Waves scattering from $x=0$, $x=l$ interfere constructively in Region II leading to standing waves $\Rightarrow$ what gets transmitted is 1.

Off resonance, the waves reflected at $x=0$, $x=l$ this is not true and what is transmitted is small.

If $E < V_0$:

$$\psi_2(x) = B_2 e^{\rho_2 x} + B_2' e^{-\rho_2 x}$$

$\Rightarrow$ $ik_2 = \rho_2$ replace $k_2 = -i\rho_2$

$$\Rightarrow T = \left|\frac{A_3}{A_1}\right|^2 = \frac{4E(V_0-E)}{4E(V_0-E) + V_0^2 \sinh^2\left[\sqrt{2m(V_0-E)}\, l/\hbar\right]}$$

$$\sinh^2(\rho_2 l) \sim \frac{\left[e^{\rho_2 l} - e^{-\rho_2 l}\right]^2}{4} \quad \text{limit } \rho_2 l >> 1$$

$$\sim \frac{e^{2\rho_2 l}}{4}$$

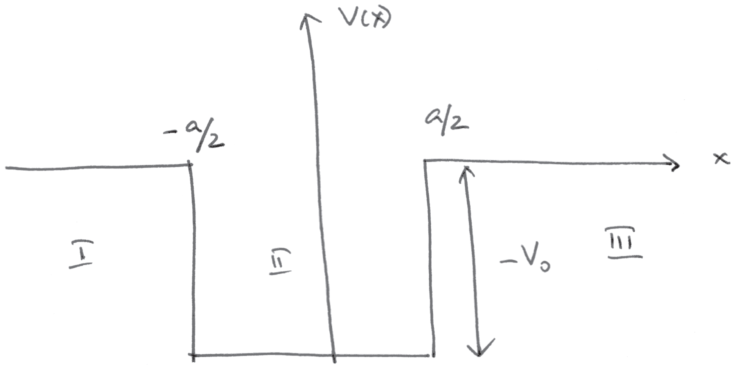
$$\therefore T \sim \frac{1}{1 + \dfrac{V_0^2}{16E(V_0-E)} e^{2\rho_2 l}} \sim \frac{16E(V_0-E)}{V_0^2} e^{-2\rho_2 l}$$

$\rightarrow$ finite prob. for tunneling

If $\rho_2 l \rightarrow \infty$ $T \rightarrow 0$

If $\rho_2 \ell$ is small: T is significantly large!

Bound states: Square well potential



$$\varphi_1(x) = B_1 e^{\rho_1 x} \qquad \rho = \sqrt{\frac{2m|E|}{\hbar^2}}$$

[$\because$ $$-\frac{\hbar^2}{2m}\frac{d^2\varphi_1(x)}{dx^2} = E\varphi_1(x)$$

or: $$\frac{d^2\varphi_1(x)}{dx^2} + \frac{2mE}{\hbar^2}\varphi_1(x) = 0$$

$-V_0 < E < 0$ range. Replace $E = -|E|$

$$\Rightarrow \frac{d^2\varphi_1(x)}{dx^2} - \frac{2m|E|}{\hbar^2}\varphi_1(x) = 0$$

Define $\rho^2 = \dfrac{2m|E|}{\hbar^2} > 0$]

Region II:

$$-\frac{\hbar^2}{2m}\frac{d^2\varphi_2(x)}{dx^2} - V_0\varphi_2(x) = -|E|\varphi_2(x)$$

$$\frac{d^2\varphi_2(x)}{dx^2} + \frac{2m}{\hbar^2}\left[V_0 - |E|\right]\varphi_2(x) = 0$$

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

$$\varphi_2(x) = A_2 e^{ikx} + A_2' e^{-ikx}$$

Region III : $V = 0$

$$\Rightarrow \varphi_3(x) = B_3' e^{-\rho x}$$

Match at $x = -a/2$

$$\varphi_1(-a/2) = \varphi_2(-a/2)$$

$$B_1 e^{-\rho a/2} = A_2 e^{-ika/2} + A_2' e^{ika/2}$$

$$\varphi_1'(-a/2) = \varphi_2'(-a/2)$$

$$\Rightarrow \rho B_1 e^{-\rho a/2} = ik\left[A_2 e^{-ika/2} - A_2' e^{ika/2}\right]$$

Can show:

$$\boxed{\begin{aligned} A_2 &= e^{(ik-\rho)a/2}\left(\frac{\rho + ik}{2ik}\right) B_1 \\ A_2' &= -\, e^{(ik+\rho)a/2}\, \frac{(\rho - ik)\, B_1}{2ik} \end{aligned}}$$

Match at $x = a/2$

$$\varphi_2(a/2) = \varphi_3(a/2) \quad \text{and} \quad \varphi_2'(a/2) = \varphi_3'(a/2)$$

$$A_2\, e^{ika/2} + A_2'\, e^{-ika/2} = B_3'\, e^{-\rho a/2}$$

$$\frac{-ik}{\rho}\left[A_2\, e^{ika/2} - A_2'\, e^{-ika/2}\right] = B_3'\, e^{-\rho a/2}$$

$$\therefore\ A_2\, e^{ika/2} + A_2'\, e^{-ika/2} = \frac{-ik}{\rho}\left[A_2\, e^{ika/2} - A_2'\, e^{-ika/2}\right]$$

Use the expressions for A_2, A_2' in terms of B_1.

$$e^{ika}(\rho+ik)^2 - e^{-ika}(\rho-ik)^2 = 0$$

$$\Rightarrow\ \left(\frac{\rho-ik}{\rho+ik}\right)^2 = e^{2ika}$$

or: $$\boxed{\left(\frac{\rho-ik}{\rho+ik}\right) = \pm\, e^{ika}}$$

(i) choose −ve root:

$$\boxed{\frac{\rho-ik}{\rho+ik} = -e^{ika}}$$

$$\rho - ik = -e^{ika}(\rho+ik)$$

$$\rho(1+e^{ika}) = ik\left[1-e^{ika}\right]$$

Multiply by $e^{-ika/2}$

$$\rho\left(e^{-ika/2} + e^{ika/2}\right) = ik\left[e^{-ika/2} - e^{ika/2}\right]$$

$$\Rightarrow\ 2\rho\cos\left(\frac{ka}{2}\right) = 2k\sin\left(\frac{ka}{2}\right)$$

or: $$\boxed{\frac{\rho}{k} = \tan\left(\frac{ka}{2}\right)}$$

Set $k_0 = \sqrt{\dfrac{2mV_0}{\hbar^2}}$

Then:

$$k^2 = \frac{2m(V_0 - |E|)}{\hbar^2} = k_0^2 - \rho^2$$

or: $k_0^2 = k^2 + \rho^2$

Now: $\dfrac{\rho}{k} = \tan\left(\dfrac{ka}{2}\right)$

$$\frac{\rho^2}{k^2} = \tan^2\left(\frac{ka}{2}\right)$$

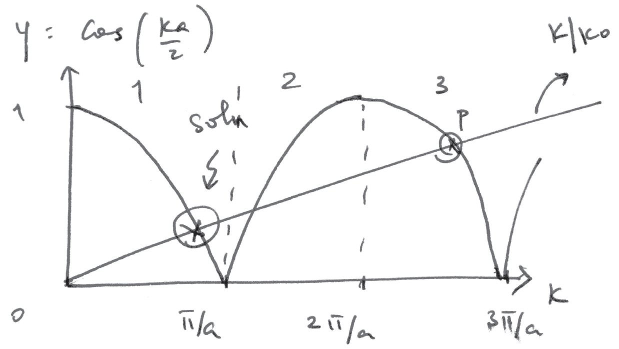
or $$1 + \frac{\rho^2}{k^2} = 1 + \tan^2\left(\frac{ka}{2}\right) = \sec^2\left(\frac{ka}{2}\right) = \frac{1}{\cos^2\left(\frac{ka}{2}\right)}$$

or: $$\frac{1}{\cos^2\left(\frac{ka}{2}\right)} = \frac{k^2+\rho^2}{k^2} = \left(\frac{k_0}{k}\right)^2$$

$$\Rightarrow \left|\cos\frac{ka}{2}\right| = \frac{k}{k_0}$$

$\therefore \dfrac{\rho - ik}{\rho + ik} = -e^{ika} \longrightarrow$ is equivalent to: $\tan\left(\frac{ka}{2}\right) > 0 \quad \left(\frac{\rho}{k} > 0\right)$

$\left|\cos\left(\frac{ka}{2}\right)\right| = \frac{k}{k_0} \rightarrow$ [transcendental eqn.]



$\frac{ka}{2} = n\pi$

$k = \frac{2n\pi}{a}$ } max

$\frac{ka}{2}$ $k = \frac{(2n+1)\pi}{a}$ } min.

tan is positive : 1, 3 quadrants

Now: $A_2' = -e^{-(\rho+ik)a/2} \dfrac{\rho-ik}{\rho+ik} B_1$

Using $\dfrac{\rho-ik}{\rho+ik} = -e^{ika}$

One can show that $\dfrac{A_2}{A_2'} = -\dfrac{e^{-(\rho-ik)a/2}}{e^{-(\rho+ik)a/2}}\left(\dfrac{\rho+ik}{\rho-ik}\right) = 1$

$\Rightarrow A_2 = A_2'$

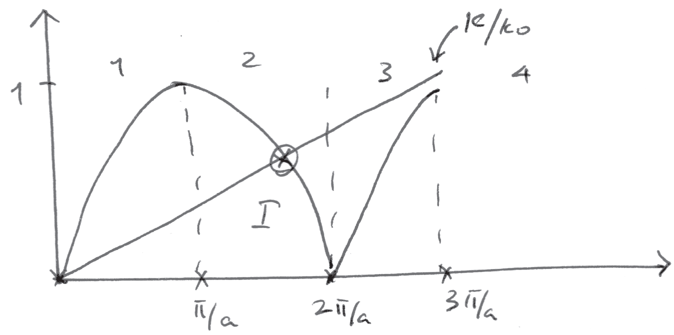
III^{ly} $B_3' = B_1$.

$$\left.\begin{aligned} \therefore\ \varphi_1(x) &= B e^{-\rho x} \\ \varphi_2(x) &= A(e^{ikx} + e^{-ikx}) \\ \varphi_3(x) &= B e^{\rho x} \\ \Rightarrow \varphi(-x) &= \varphi(x) \end{aligned}\right\} \text{ Even solutions :}$$

Case(ii) $\dfrac{\rho-ik}{\rho+ik} = e^{ika}$ leads to :

$$\left|\sin\left(\frac{ka}{2}\right)\right| = \frac{k}{k_0}$$

and $\tan\left(\dfrac{ka}{2}\right) < 0$



tan is <0 in 2nd and 4th quadrent.

One can check that these soln. lead to odd wave fns.

If V_0 increases k_0 increases $\Rightarrow \dfrac{1}{k_0}$ decreases. $\Rightarrow$ More B. states

Delta fn potential

$$V(x) = -\alpha\delta(x) \quad \Rightarrow \quad \begin{cases} 0 & \text{if } x \neq 0 \\ \infty & \text{if } x = 0 \end{cases} \qquad \text{with } \int_{-\infty}^{\infty} \delta(x)\,dx = 1.$$

α : positive constant.

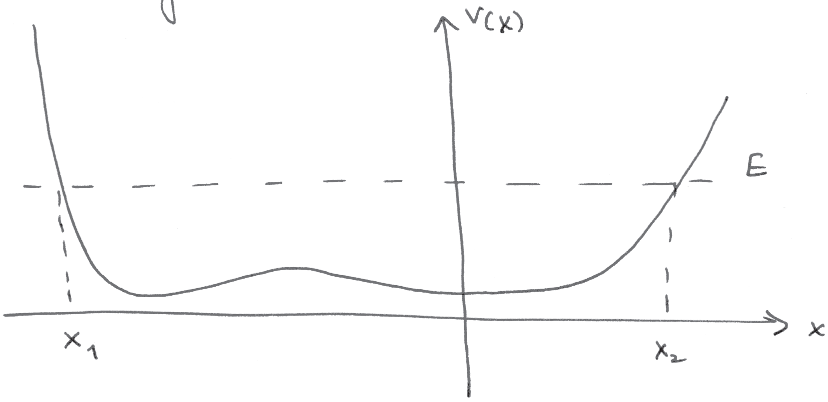
S. eqn.:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} - \alpha\,\delta(x)\,\psi = E\psi$$

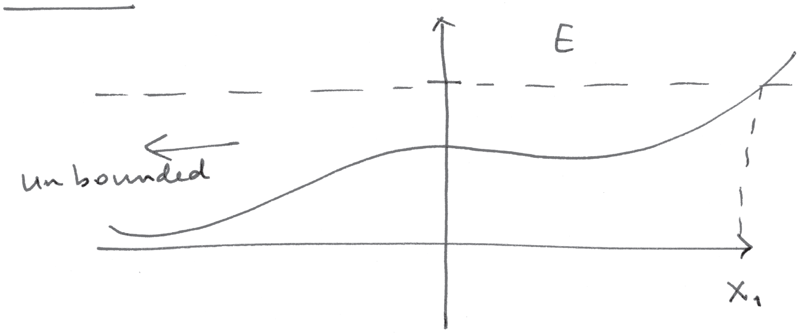
$E<0$ yields B. states $\quad E>0$ scattering states.

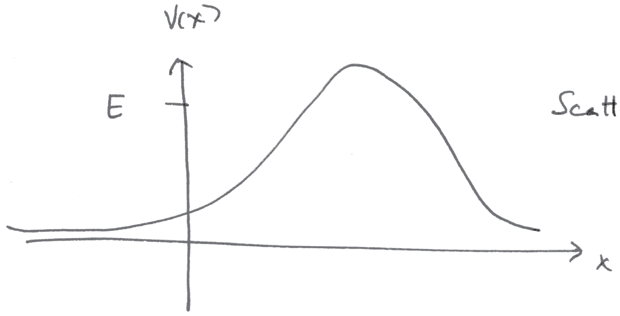
Digression: What are Bound states and scattering states?

Classically:



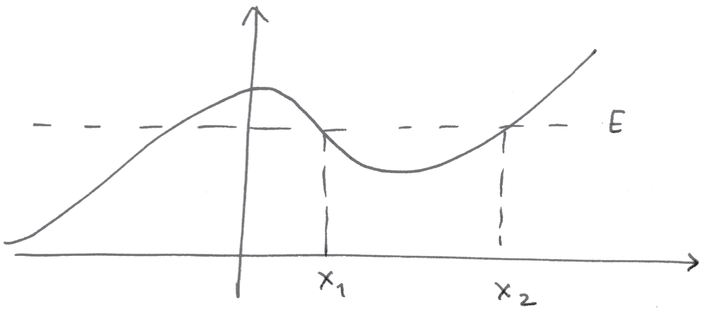
If E is the energy of the particle, then it is stuck between the classical turning points x_1, x_2. $\Rightarrow$ The particle is bound.





Scattering state.

Now:



$x_1, x_2 \to$ classical turning points

Q. Mechanically, the particle can tunnel beyond x_1.

$\Rightarrow$ Classical B. states $E < V_0$

Scattering states $E > V_0$.

But quantum Mechanical Bound states

$\Rightarrow$ $E < V(-\infty)$ and $V(+\infty)$

and scattering states:

$E > V(-\infty)$ or $V(+\infty)$.

Usually $V(\pm\infty) = 0$

$\Rightarrow$ $E > 0$ Scattering states

$E < 0$ Bound states.

<u>Particle in a Box</u> $E < V(-\infty) \,\&\, V(+\infty)$ $\Rightarrow$ Bound.

<u>Barriers and steps</u> : $E > V(\infty)$ or $V(+\infty)$ $\to$ Scattering states.

<u>In Square well:</u> Look B. states by requiring $E < 0$.

<u>Look at B. states for δ fn potential:</u>

$x < 0 \qquad V(x) = 0$

$$\Rightarrow \frac{d^2\varphi}{dx^2} + \underbrace{\frac{2m|E|}{\hbar^2}}_{\rho^2}\varphi = 0$$

$$\therefore \varphi_1(x) = B_1 e^{+\rho x} + B_1' e^{-\rho x}$$

$B_1' = 0$ (as $x \to -\infty$ $\varphi_1(x)$ should be bounded).

$$\therefore \varphi_1(x) = B_1 e^{\rho x}$$

$x > 0$

$$\varphi_2(x) = B_2' e^{-\rho x}$$

at $x = 0$

$$\varphi_1(0) = \varphi_2(0)$$

$$\Rightarrow B_1 = B_2'$$

$$\therefore \varphi(x) = \begin{cases} B e^{\rho x} & x < 0 \\ B e^{-\rho x} & x > 0 \end{cases}$$

<u>Next integrate the S. eqn:</u> $-\epsilon$ to $+\epsilon$ and take the limit $\epsilon \to 0$

$$-\frac{\hbar^2}{2m}\int_{-\epsilon}^{\epsilon}\frac{d^2\varphi}{dx^2}dx + \int_{-\epsilon}^{\epsilon}V(x)\varphi(x)\,dx = \underbrace{E\int_{-\epsilon}^{\epsilon}\varphi(x)\,dx}_{0} \to 0 \text{ in the limit } \epsilon \to 0$$

$$\cancel{\varphi(-\epsilon) = \varphi(\epsilon)}\Big|_{\epsilon \to 0}$$

$$\left.\frac{d\varphi}{dx}\right|_{\epsilon} - \left.\frac{d\varphi}{dx}\right|_{-\epsilon} = \frac{2m}{\hbar^2}\lim_{\epsilon\to 0}\int_{-\epsilon}^{\epsilon}V(x)\varphi(x)\,dx$$

$$= \frac{2m}{\hbar^2}\lim_{\epsilon\to 0}\int_{-\epsilon}^{\epsilon}-\alpha\,\delta(x)\varphi(x)\,dx = -\frac{2m\alpha}{\hbar^2}\varphi(0)$$

$$\varphi(x) = \begin{cases} B e^{\rho x} & x < 0 \\ B e^{-\rho x} & x > 0 \end{cases}$$

$$\Rightarrow \left.\frac{d\varphi}{dx}\right|_{+\epsilon} = \left. -\rho B e^{-\rho x}\right|_{+\epsilon \to 0} = -\rho B$$

$$\left.\frac{d\varphi}{dx}\right|_{-\epsilon} = \left. +\rho B e^{-\rho x}\right|_{-\epsilon \to 0} = \rho B .$$

$$\therefore \; -\cancel{2}\rho \cancel{B} = -\frac{\cancel{2} m \alpha}{\hbar^2} \cancel{B}$$

$$\rho = \sqrt{\frac{2m|E|}{\hbar^2}} \quad \therefore \; \rho^2 = \frac{m^{\cancel{2}} \alpha^2}{\hbar^{\cancel{4}\,2}} = \frac{2\cancel{m}}{\hbar^{\cancel{2}}} |E|$$

$$\Rightarrow \boxed{|E| = \frac{m\alpha^2}{2\hbar^2}} \longrightarrow 1 \text{ Bound state.}$$

<u>$E > 0$: Scattering states</u> :

$$\left.\begin{aligned} \varphi_1(x) &= A_1 e^{ik_1 x} + A_1' e^{-ikx} \\ \varphi_2(x) &= A_2 e^{ikx} + A_2' e^{-ikx} \end{aligned}\right\} \quad k = \sqrt{\frac{2mE}{\hbar^2}}$$

Match at $x = 0$

$$\Rightarrow \; A_1 + A_1' = A_2 + A_2'$$

$$\frac{d\varphi_1}{dx} = ik\left[A_1 e^{ikx} - A_1' e^{-ikx}\right]$$

$$\frac{d\varphi_2}{dx} = +ik\left[A_2 e^{ikx} - A_2' e^{-ikx}\right]$$

$$\Rightarrow \left.\frac{d\varphi_1}{dx}\right|_{+\epsilon} - \left.\frac{d\varphi_2}{dx}\right|_{-\epsilon} = ik\left[A_1 - A_1'\right] - ik\left[A_2 - A_2'\right]$$

$$\Rightarrow \left.\frac{d\varphi_1}{dx}\right|_{x=+\epsilon} - \left.\frac{d\varphi_2}{dx}\right|_{x=-\epsilon} = -\frac{2m}{\hbar^2}\alpha\,\varphi(0)$$

$$\Rightarrow ik\left[A_2 - A_2' - A_1 + A_1'\right] = -\frac{2m}{\hbar^2}\alpha\,(\cancel{A_2+A_2'}) \quad (A_1+A_1')$$

$$(A_1 + A_1' = A_2 + A_2')$$

Define $\beta = \frac{m\alpha}{\hbar^2 k}$. $\beta^2 = \frac{m^2\alpha^2}{\hbar^4 k^2}$ $E = \frac{\hbar^2 k^2}{2m} \Rightarrow \cancel{\frac{\beta^2}{E} = \frac{m\alpha^2/\hbar^2 k^2}{\hbar^2 k^2/2m}}$

$$A_2 - A_2' - A_1 + A_1' + \frac{2\beta}{i}(A_1 + A_1') = 0$$

$$\beta^2 = \frac{m\alpha^2}{2\hbar^2}\left[\frac{2m}{\hbar^2 k^2}\right] = \frac{m\alpha^2}{2E\hbar^2}$$

~~or $A_1 - A_1' - A_2\left(1 + \frac{1}{i\beta}\right)$~~

$$A_2 - A_2' - A_1(1+2i\beta) + A_1'(1-2i\beta) = 0$$

$$A_2 - A_2' = A_1(1+2i\beta) + A_1'(1-2i\beta)$$

$A_2' = 0$ No scattering to the rt. of the Barrier (No reflection)

$$A_2 = A_1(1+2i\beta) + A_1'(1-2i\beta).$$

and $A_2 = A_1 + A_1'$

We get: $R = \left|\frac{A_1'}{A_1}\right| = \frac{\beta^2}{1+\beta^2} = \frac{1}{1+1/\beta^2}$

~~$A_2 =$~~

and $T = \left|\frac{A_2}{A_1}\right|^2 = \frac{1}{1+\beta^2}$.

$$\therefore R = \frac{1}{1 + \left(\frac{2\hbar^2}{m\alpha^2}E\right)} \qquad T = \frac{1}{1 + \frac{m\alpha^2}{2\hbar^2 E}} \qquad \left(\text{Using } \beta^2 = \frac{m\alpha^2}{2E\hbar^2}\right)$$

What happens if we have a δ fn barrier?

NOTE on Scattering states: Consider the soln. to the S-eqn for $V = 0$

Then: $$-\frac{\hbar^2}{2m}\frac{d^2\varphi}{dx^2} = E\varphi$$

$$\Rightarrow \varphi(x) = A e^{ikx} + \underbrace{A' e^{-ikx}}_{\overset{\shortparallel}{0}\ (\text{No reflection})} \quad \text{where } k^2 = \frac{2mE}{\hbar^2}$$

Then: $$|\varphi(x)|^2 = |A|^2 \Rightarrow \int_{-\infty}^{\infty} |\varphi(x)|^2 dx \Rightarrow \infty \text{ diverges!}$$

$\Rightarrow$ A free particle cannot be represented by a Stationary state!! $\Rightarrow$ No definite energy.

However if we have $\Psi(x,t) = \varphi(x)\, e^{iEt/\hbar}$

Then the general solution: $$\alpha(x,t) = \int_{-\infty}^{\infty} dk\, \underbrace{e^{ikx - iEt/\hbar}}_{\Psi(x,t)}\, \alpha(k)$$

represents a superposition of stationary states and "Represents" a particle. This can be normalized. $\Rightarrow$ A free particle is represented by ~~Scatt~~ Wave packets and carries a range of k's.