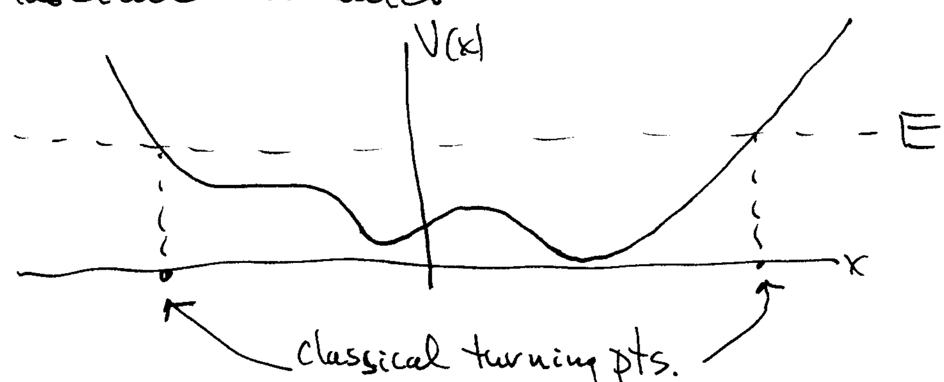
IIc) Bound & Scattering States:

The δ-function Potential

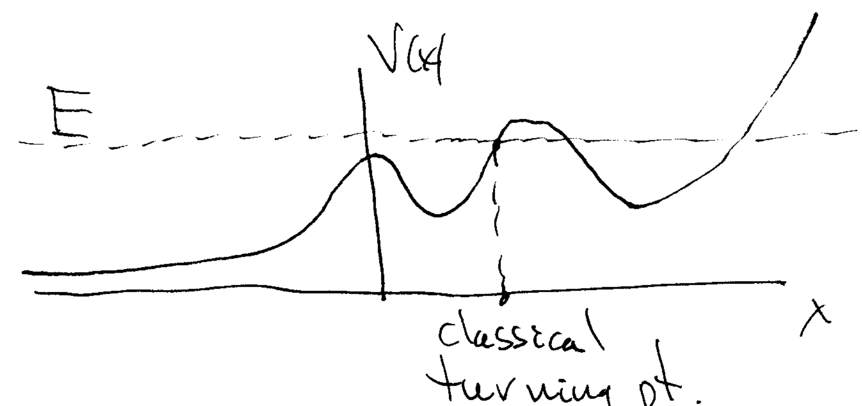
Classical Mechanics:

a)



i.e. $\frac{1}{2}mv^2 = E - V \geq 0 \Rightarrow$ no motion past turning points — The particle just oscillates between the turning pts. → Bound State

b)



particle with E comes initially from $x \to -\infty$ to turning pt. — stops at $E = V(x = \text{turning pt})$ reverses velocity and goes back out to infinity ($x \to -\infty$) → Scattering State

II C) In Quantum Mechanics the 2-types of states - bound & scattering - correspond to the 2 classes of wavefunctions we have found. The ∞-square well and the harmonic oscillator had normalizable stationary states labelled by an integer - these are bound states. The free particle or plane wave wavefunction was not normalizable, the different states were labelled by a continuous variable k - these were scattering states. The plane waves do not correspond to physically realizable states - but linear combinations (integrals over k) do - they are normalizable.

Further in QM there is tunneling a particle has a probability to penetrate and go through any finite width potential barrier (barrier has $V > E$) Hence only the potential at $x \to \pm\infty$ matters in determining if the potential leads to bound and/or scattering states.

$$E < V(x \to +\infty) \text{ and } V(x \to -\infty)$$
$$\Rightarrow \text{Bound State}$$

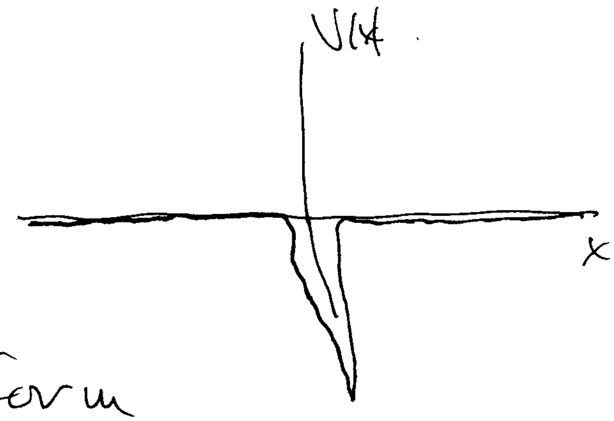
$$E > V(x \to \infty) \text{ \& } V(x \to -\infty) \Rightarrow \text{Scattering State}$$

- II c) Usually the potential vanishes as $x \to \pm\infty$ so that these criteria simply become

$$E<0 \Rightarrow \text{bound state}$$
$$E>0 \Rightarrow \text{scattering state}$$

Consider the example of a Dirac Delta function potential well

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



V is time independent hence solutions to Sch. eq. have the form

$$\Psi(x,t) = \psi(x)\, e^{-i\frac{E}{\hbar}t}$$

where

$\psi(x)$ obeys the time indep. Sch. eq.

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

This potential will have both bound states $E<0$, and scattering states $E>0$.

II c) Consider Bound States First $E<0$.

For $x<0$ $V(x)=0 \Rightarrow$

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi = \kappa^2\psi$$

$$\kappa \equiv \frac{\sqrt{-2mE}}{\hbar} > 0, \ (E<0)$$

The general solution is

$$\psi(x) = Ae^{-\kappa x} + Be^{+\kappa x}$$

but as $x \to -\infty$ the first term $\to \infty$ hence $A=0$:

$$\psi(x) = Be^{+\kappa x} \qquad x<0.$$

Likewise for $x>0$; $V(x)=0$ and Sch. Eq. becomes again $\frac{d^2\psi}{dx^2} = \kappa^2\psi$

with general solution

$$\psi(x) = Fe^{-\kappa x} + Ge^{+\kappa x}$$

as $x \to +\infty$ the second term blows up $\Rightarrow G=0$

$$\Rightarrow \quad \psi(x) = Fe^{-\kappa x} \qquad x>0.$$

-II c) Now we must match the 2 solution regions where they meet $x=0$. We always have that ψ is finite & <u>continuous</u> hence

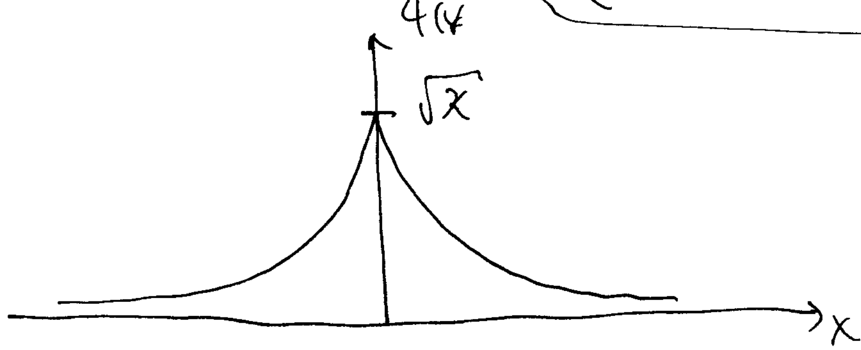
$$\psi(x=0^-) = \psi(x=0^+)$$

$$\begin{aligned} &\| \\ &B e^{0} = F e^{0} \end{aligned}$$

$$\Rightarrow \quad \boxed{B = F}$$

hence

$$\boxed{\psi(x) = \begin{cases} B e^{\kappa x} & \text{for } x \leq 0 \\ B e^{-\kappa x} & \text{for } x \geq 0 \end{cases}}$$



In addition we have Sch. Eq.: (recall since $V(x)$ is singular at $x=0$ we must determine the BC for $\frac{d\psi}{dx}$ by explicitly integrating Sch-Eq).

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

II c) Integrate around $x=0$ letting $\epsilon \to 0$

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

$$\parallel$$

$$-\frac{\hbar^2}{2m}\left[\frac{d\psi}{dx}(x=0^+) - \frac{d\psi}{dx}(x=0^-)\right] - \alpha\psi(0)$$

$$= E\,\psi(0)\,2\epsilon \to 0$$

So we have that the "jump" or discontinuity in $\frac{d\psi}{dx}$ is given by ψ at $x=0$.

$$\boxed{\frac{d\psi}{dx}(x=0^+) - \frac{d\psi}{dx}(x=0^-) = -\frac{2m\alpha}{\hbar^2}\psi(0)}$$

Now $\frac{d\psi}{dx}(x=0^+) = -\kappa B e^{-\kappa x}\Big|_{x=0^+} = -\kappa B$

$\frac{d\psi}{dx}(x=0^-) = +\kappa B e^{\kappa x}\Big|_{x=0^-} = +\kappa B$

$$\Rightarrow \quad -2\kappa B = -\frac{2m\alpha}{\hbar^2}\psi(0) = -\frac{2m\alpha}{\hbar^2}B$$

$$\Rightarrow \quad \boxed{\kappa = \frac{m\alpha}{\hbar^2}}$$ The only allowed κ!

II C) Thus we find only one allowed energy

$$\boxed{E = -\frac{\hbar^2 \kappa^2}{2m} = -\frac{m\alpha^2}{2\hbar^2}}$$

There is only one bound state!

Finally we can normalize ψ

$$1 \equiv \int_{-\infty}^{+\infty} dx\, |\psi|^2 = 2|B|^2 \int_0^\infty dx\, e^{-2\kappa x}$$

$$= 2|B|^2 \left(\frac{-1}{2\kappa}\right) e^{-2\kappa x}\Big|_{x=0}^{\infty}$$

$$1 = \frac{|B|^2}{\kappa}$$

$\Rightarrow$ (taking B positive & real)

$$\boxed{B = \sqrt{\kappa}} = \frac{\sqrt{m\alpha}}{\hbar}$$

Hence we have the normalized stationary state

$$\psi(x) = \frac{\sqrt{m\alpha}}{\hbar} e^{-\frac{m\alpha}{\hbar^2}|x|}$$

with energy $E = -\frac{m\alpha^2}{2\hbar^2}$

c) Next consider the scattering states $E>0$ as before for $x<0$ the Sch.-eq. becomes

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi \equiv -k^2\psi$$

$$k = \frac{\sqrt{2mE}}{\hbar} > 0, \; E>0.$$

The general solution is

$$\boxed{\psi(x) = Ae^{ikx} + Be^{-ikx} \quad ; \; x<0}$$

neither term blows up, hence they cannot be ruled out.

Likewise for $x>0$; $\frac{d^2\psi}{dx^2} = -k^2\psi$

and in general $\boxed{\psi(x) = Fe^{ikx} + Ge^{-ikx} \; ; \; x>0}$

BC: Continuity of ψ across $x=0 \Rightarrow$

$$\boxed{A+B = F+G}$$

The jump in $\frac{d\psi}{dx}$ is given by again by

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

II-c) So $\frac{d\psi}{dx}(x=0^+) = ik\left(Fe^{ikx} - Ge^{-ikx}\right)\Big|_{x\to 0^+}$

$$= ik(F-G)$$

$$\frac{d\psi}{dx}(x=0^-) = ik\left(Ae^{ikx} - Be^{-ikx}\right)\Big|_{x\to 0^-}$$

$$= ik(A-B)$$

Thus $$\boxed{ik[F-G-A+B] = -\frac{2m\alpha}{\hbar^2}(A+B)}$$

This may be written as

$$\boxed{\begin{array}{l} F-G = A(1+2i\beta) - B(1-2i\beta) \\ \text{where } \beta = \frac{m\alpha}{\hbar^2 k} \end{array}}$$

Thus we have 2 equations for the 4 unknowns A, B, F, G. We are left with 2 free constants. These are not normalizable states — so we cannot fix the constants by normalizing the wavefunctions.

II.C) Hence we must interpret the solutions. Recall

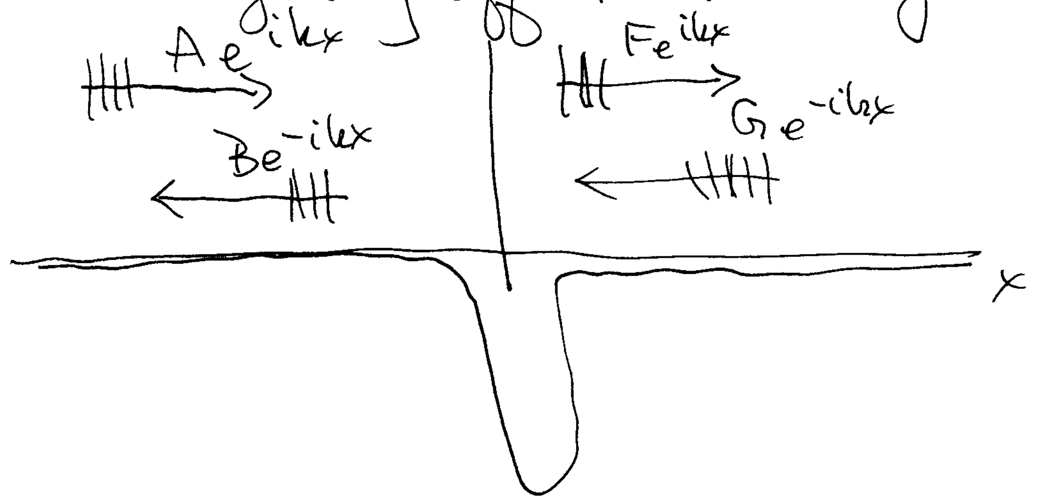
$$e^{ikx - i\frac{E}{\hbar}t}$$

corresponds to a plane wave moving from left to right while

$$e^{-ikx - i\frac{E}{\hbar}t}$$

corresponds to a plane wave moving from right to left.

A then is the amplitude of a wave coming in from the left moving to the right while B is the amplitude of the wave returning to the left. Similarly G is the amplitude of a wave coming in from the right while F is the amplitude of the wave going off to the right.



-II c) In a typical scattering experiment the particles are initially projected in from one direction say from the left towards the right. Hence the wave coming in from the right is set to ~~zero~~ zero $\Rightarrow$ $\boxed{G=0}$ for incident beam from the left.

A is then the amplitude of the <u>incident wave</u>. B is the amplitude of the <u>reflected</u> wave and F is the amplitude of the <u>transmitted</u> wave.

We may then solve for B, F in terms of A

$$F = A + B$$

$$F = A(1+2i\beta) - B(1-2i\beta)$$

$$\Rightarrow \quad F = A(1+2i\beta) - (F-A)(1-2i\beta)$$

$$\Rightarrow \quad 2F(1-i\beta) = 2A \quad \Rightarrow \quad \boxed{F = \frac{1}{1-i\beta}A}$$

$$\Rightarrow \quad B = \left[\frac{1}{1-i\beta} - \frac{1-i\beta}{1-i\beta}\right]A = \frac{i\beta}{1-i\beta}A$$

$$\boxed{B = \frac{i\beta}{1-i\beta}A}$$

IIc) Since the wavefunction is the prob. amplitude of the particles presence we can find the relative probabilities by taking the ratios of |amplitudes|^2

The relative prob. that an incident particle is reflected back is

$$R \equiv \frac{|B|^2}{|A|^2} = \frac{\beta^2}{1+\beta^2} .$$

R = reflection coefficient.

The relative prob. that the incident particle is transmitted to the right is

$$T \equiv \frac{|F|^2}{|A|^2} = \frac{1}{1+\beta^2}$$

T = transmission coefficient.

Since the particle is either transmitted or reflected we have $R+T=1$, and it is by direct calculation. Plugging in β we have

$$R = \frac{\frac{m^2\alpha^2}{\hbar^4 k^2}}{1+\frac{m^2\alpha^2}{\hbar^4 k^2}} = \frac{1}{1+\frac{\hbar^4 k^2}{m^2\alpha^2}}$$

$$= \frac{1}{1+2\hbar^2 E/m\alpha^2}$$

II C) And
$$T = \frac{1}{1+\frac{m\alpha^2}{2\hbar^2 E}} .$$

Hence as E increases the higher the transmission probability — as is reasonable.

Note in general $\psi = \psi_{incident} + \psi_{scattered}$

$\psi_{scattered}$ consists of a piece due to reflection and a piece due to transmission

$$\psi_{scatt.} = \psi_{refl.} + \psi_{trans.}$$

In the laboratory we will project a beam of particles at a certain rate — that is an incident probability ~~flux rate~~ we will then measure the ratio of the scattered probability fluxes to the incident prob. ~~flux~~. rates

The prob. flux is given by the prob. current:

$$J = \frac{\hbar}{2im}\left[\psi^* \frac{d\psi}{dx} - \frac{d\psi^*}{dx}\psi\right]$$

IIc) For the incident particles (from left to right)

$$\psi_{inc} = A e^{ikx} \text{ ; hence}$$

$$J_{inc} = \frac{\hbar}{2im}\left[A^* e^{-ikx}\left(ik A e^{+ikx}\right) - A^*(-ik)e^{-ikx} A e^{ikx}\right]$$

$$\boxed{J_{inc} = |A|^2 \frac{\hbar k}{m}}$$. This is just the prob. density $\rho = |\psi_{inc}|^2 = |A|^2$ times the free incident particle's velocity $\frac{\hbar k}{m}$.

We can measure the probability current density that is reflected or transmitted by measuring the particle flux in the region to the left of the potential and to the right of the potential (i.e. by putting particle counters at $x = \pm\infty$)

II c) We measure the reflection coefficient

$$R = \left| \frac{J_{\text{reflection}}}{J_{\text{incident}}} \right|$$

and the transmission coefficient

$$T = \left| \frac{J_{\text{transmission}}}{J_{\text{incident}}} \right|$$

with

$$J_{\text{refl.}} = \frac{\hbar}{2im}\left(\psi^*_{\text{refl.}} \frac{d\psi_{\text{refl.}}}{dx} - \frac{d\psi^*_{\text{refl.}}}{dx} \psi_{\text{refl.}} \right)$$

and

$$J_{\text{trans.}} = \frac{\hbar}{2im}\left(\psi^*_{\text{trans.}} \frac{d\psi_{\text{trans}}}{dx} - \frac{d\psi^*_{\text{trans.}}}{dx} \psi_{\text{trans.}} \right)$$

For our problem each of these were plane waves with

$$\psi_{\text{refl.}} = Be^{-ikx}$$

$$\psi_{\text{trans.}} = Fe^{+ikx}$$

-II c.) So

minus indicates traveling to the left

$$J_{refl.} = -|B|^2 \frac{\hbar k}{m}$$

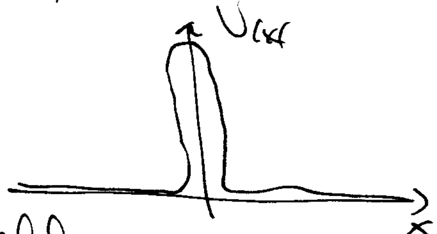
$$J_{trans.} = |F|^2 \frac{\hbar k}{m}.$$

Hence we find, as when using probabilities since all speeds were the same,

$$R = \frac{|B|^2}{|A|^2} \; ; \; T = \frac{|F|^2}{|A|^2}.$$

Finally, we may consider the δ-function barrier

$$V(x) = +\alpha\,\delta(x) \qquad \alpha > 0$$



This is obtained by letting $\alpha \to -\alpha$ in our δ-function well problem.

First $\alpha \to -\alpha$ eliminates the bound state — as is physically reasonable. Specifically we required the jump BC for $d\psi/dx$ $\Rightarrow$

$$\kappa = \frac{m\alpha}{\hbar^2} \xrightarrow{\alpha\to-\alpha} -\frac{m\alpha}{\hbar^2}$$

but $\kappa > 0$! hence

#c) There is no solution for $E < 0$.
Generally this comes from Problem 2.2
$E > V_{min.} \Rightarrow E > 0$ only.

For the scattering states then $\alpha \to -\alpha$
$\Rightarrow \beta \to -\beta$ and we have

$$B = \frac{-i\beta}{1+i\beta} A \; ; \; F = \frac{1}{1+i\beta} A$$

But R & T only depend on β^2 and hence remain unchanged!! The particle is as likely to cross the barrier as the well!!

Classically the particle cannot make it through a barrier if its energy is less than the maximum of the potential i.e. if $E > V_{max} \Rightarrow T=1, R=0$ if $E < V_{max} \Rightarrow T=0, R=1$.

In QM there is the possibility for the particle to <u>tunnel</u> through the barrier even when $E < V_{max}$!!
(Also if $E > V_{max}$ there is a non-zero reflection probability.)