- The Infinite Square Well

We have Schrödinger's equation as

$$\hat{H}|\psi\rangle = E|\psi\rangle$$

then in position basis, we have

$$\langle x|\hat{H}|\psi\rangle = E\langle x|\psi\rangle$$

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

Now for infinite wall we have $V(x) = \begin{cases} 0, & 0 \le x \le a \\ \infty, & \text{otherwise.} \end{cases}$, so we have

$$\frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi(x) \quad \Rightarrow \quad \frac{d^2\psi(x)}{dx^2} = -\frac{2mE}{\hbar^2}\psi(x)$$

so we have $k^2 = \frac{2mE}{\hbar^2}$, $\frac{d^2\psi(x)}{dx^2} = -k^2\psi(x)$, the solution of above equation is, $\psi(x) = A\sin(kx) + B\cos(kx)$, by using boundary condition we have $B=0$ as $\psi(x) \to 0$ on the boundary. So we have

$$\psi(x) = A\sin(kx)$$

Next step, $ka = n\pi \Rightarrow k = \frac{n\pi}{a}$ so we have

$$\psi(x) = A\sin\left(\frac{n\pi}{a}x\right)$$

By normalizing $\psi(x)$ we have

$$\int_0^a |\psi(x)|^2\,dx = 1.$$

$$\Rightarrow A = \sqrt{\frac{2}{a}}$$ so now we have,

$$\boxed{\psi(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right)}$$

now $\psi_n(x)$ are eigenfunction of the hamiltonian now we have for eigenvalues,

$$k = \frac{n\pi}{a} \Rightarrow \frac{2mE}{\hbar^2} = \frac{n^2\pi^2}{a^2}$$

$$\Rightarrow \boxed{E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}}$$

so our job is done we have all eigenvectors and the eigenvalues.

- The Harmonic Oscillator

Another very important problem we have in classical mechanics is of Hooke's law,

$$F = -kx$$

where

$$m\frac{d^2x}{dt} = -kx \Rightarrow x(t) = A\sin(\omega t) + B\cos(\omega t),$$

where $\omega = \sqrt{\frac{k}{m}}$ and the potential energy is $V = \frac{1}{2}kx^2$.

Now we should remember that any function $V(x)$ can be expanded x_0 where x_0 is a local minimum,

$$V(x) = V(x_0) + V'(x_0)(x-x_0) + \frac{V''(x_0)}{2}(x-x_0)^2 + O(x^3)$$

Now for x_0 be a minimum we have $V'(x_0) = 0$

$$V(x) \approx \frac{1}{2}V''(x_0)(x-x_0)^2$$

where $k \equiv V''(x_0)$.

Now we'll deal with the problem of quantum harmonic oscillator. So we have

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2}m\omega^2x^2\psi = E\psi.$$

Now there are two ways to solve this problem,

1. Algebraic Method
2. Analytical Method.

Algebraic Method

We have

$$\frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2 = \hat{H}$$

$$\Rightarrow \hat{H} = \frac{1}{2m}\left[\hat{p}^2 + m^2\omega^2x^2\right]$$

now by using $a^2+b^2 = (a-ib)(a+ib)$ for scalars but if $\hat{a}, \hat{b}$ are operators then,

$$a^2 + iab - iba + b^2 = a^2 + b^2 + i[a,b]$$

$$\hat{H} = \frac{1}{\sqrt{2m}}(m\omega\hat{x} - i\hat{p})\frac{1}{\sqrt{2m}}(m\omega\hat{x} + i\hat{p}] + \frac{i\omega}{2}[\hat{p},\hat{x}]$$

$$\hat{H} = \hbar\omega\left(\frac{1}{\sqrt{2\hbar m\omega}}(m\omega\hat{x} - i\hat{p})\frac{1}{\sqrt{2\hbar\omega m}}(m\omega\hat{x} + i\hat{p}) + \frac{1}{2}\right)$$

$$\boxed{\hat{H} = \hbar\omega\left(a^{+}a + \frac{1}{2}\right)}$$

so we have $\boxed{a^{+} \equiv \frac{1}{\sqrt{2\hbar m\omega}}(m\omega\hat{x} - i\hat{p})}$

Now we have everything as we want but now we would like to find how a^{+} and a works.

Let us try to get the commutation relation b/w the newly defined operators,

$$[a, a^{+}] = aa^{+} - a^{+}a = \frac{m^2\omega^2 x^2 - im\omega\hat{x}\hat{p} + im\omega\hat{p}\hat{x} + p^2}{2\hbar m\omega} - \frac{m\omega^2 x^2 + im\omega\hat{x}\hat{p} - im\omega\hat{p}\hat{x} + p^2}{2\hbar\omega m}$$

$$= -\frac{i}{2\hbar}[\hat{x}, \hat{p}] - \frac{i}{2\hbar}[\hat{x}, \hat{p}] = 1.$$

$\Rightarrow \boxed{[a, a^{+}] = 1.}$, now one can use this to get $\hat{H} = \hbar\omega\left(aa^{+} - \frac{1}{2}\right)$

Now an alternative formulation of $\hat{H}$ can be,

$$\boxed{\hat{H} = \hbar\omega\left(aa^{+} - \frac{1}{2}\right)}$$

<u>Claim</u>: For $|n\rangle$ be an eigenstate of $\hat{H}$ we have $\hat{H}(a^{+}|n\rangle) = (E + \hbar\omega)(a^{+}|n\rangle)$.

<u>Proof</u>:

$$\hat{H} = \hbar\omega\left(a^{+}a + \frac{1}{2}\right), \text{ so}$$

$$\hat{H}(a^{+}|n\rangle) = \hbar\omega\left(a^{+}aa^{+} + \frac{a^{+}}{2}\right)|n\rangle = a^{+}\hbar\omega\left(aa^{+} + \frac{1}{2}\right)|n\rangle$$

$$= a^{+}\hbar\omega\left(a^{+}a + 1 + \frac{1}{2}\right)|n\rangle = a^{+}\hbar\omega\left(a^{+}a + \frac{1}{2}\right)|n\rangle + \hbar\omega a^{+}|n\rangle$$

$$= E\, a^{+}|n\rangle + \hbar\omega a^{+}|n\rangle = (E + \hbar\omega)(a^{+}|n\rangle)$$

so we have

$\hat{H}(a^{+}|n\rangle) = (E + \hbar\omega)(a^{+}|n\rangle)$, which means it raises the level on the ladder.

Similarly we may prove $\hat{H}(a|n\rangle) = (E - \hbar\omega)(a|n\rangle)$.

So now we define $N \equiv a^{\dagger}a$, (number operator), now we have

$[N, H] = 0$ so eigenvectors of H are simultaneous eigenkets of $\hat{N}$, but what about eigenvalues.

So we have

$$\hat{H} = \hbar\omega\left(\hat{N} + \frac{1}{2}\right)$$

, so we have $|n\rangle$ are the eigenvectors of $\hat{H}$ and we showed $\hat{H}(a^{\dagger}|n\rangle) = (E_n + \hbar\omega)(a^{\dagger}|n\rangle)$ so we have

$$\hat{H}|n+1\rangle = (E_n + \hbar\omega)|n+1\rangle$$

So $E_{n+1} - E_n = \hbar\omega \implies E_n = \hbar\omega\left(n + \frac{1}{2}\right)$

Another thing become clear from here is that

- Algebra of Creation and Anhillcation operator

Now the above analysis talk about a single particle trapped in a harmonic oscillator like potential, now suppose we have multiple interacting via the following hamiltonian and they follow the following hamiltonian,

$$\hat{H} = \sum_k \omega\left(a_k^{\dagger}a_k + \frac{1}{2}\right)$$

This is the hamiltonian of light, and the following commutation relations follow from the fact that they are photon,

$$[a_k^{\dagger}, a_{k'}] = \delta_{kk'}$$

$$[a_k^{\dagger}, a_{k'}^{\dagger}] = 0, \quad [a_k, a_{k'}] = 0.$$

The free particle

A free particle is the case where $V(x) = 0$, $\forall x$. Classically this is a particle moving with a const. velocity but quantum mechanically its way different let us take a look,

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \Rightarrow \frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi.$$

so we have $k^2 = \frac{2mE}{\hbar^2} \Rightarrow \frac{d^2\psi}{dx^2} = -k^2\psi \Rightarrow \psi(x) = Ae^{ikx} + Be^{-ikx}.$

Now we have $E = \frac{\hbar^2 k^2}{2m}$ and the full solution will be like,

$$\Psi(x,t) = Ae^{ikx}e^{-i\frac{\hbar k^2}{2m}t} + Be^{-ikx}e^{-i\frac{\hbar k^2}{2m}t}$$
$$= Ae^{ik\left(x-\frac{\hbar k}{2m}t\right)} + Be^{-ik\left(x+\frac{\hbar k}{2m}t\right)}$$

So the full solution is,

$$\Psi(x,t) = A\exp\left(ik\left(x-\frac{\hbar k t}{2m}\right)\right) + B\exp\left(-ik\left(x+\frac{\hbar k t}{2m}\right)\right)$$

The above solution has a form of $f(x \pm vt)$ a traveling wave moving at a speed of v in $\pm x$-direction. Here the first term in the formula gives a right going wave and the second term gives a left going wave. So clearly the solution is a propagating wave moving left or right depending upon value of k.

Now clearly, the wave length of the moving wave is $\lambda = \frac{2\pi}{|k|}$ and corresponding momentum given as $p = \hbar k$.

and speed of the wave is

$$v_{quan} = \frac{\hbar k}{2m} = \sqrt{\frac{E}{2m}}$$

on the other hand for a classical particle, $v_{cla} = \sqrt{\frac{2E}{m}} = 2v_{quan}$. But how is this possible?

Let us look at $\Psi(x,t)$ clearly $\int_{-\infty}^{\infty}\Psi_k^*\Psi_k\,dx = \infty$ (Not normalizable)

So its not a physically realizable state. In short, there is no such thing as a free particle with a definite energy.

So solutions from method of separation of var is waste? No!! we can still talk about linear combination of these solution and get something.

So we have,

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\phi(k)\,e^{-ik\left(x-\frac{\hbar k t}{2m}\right)}\,dk.$$

Now we can normalize the above solution but it contain a number of ks hence it is not a wave but a wavepacket.

In QM, most of the time we are given $\Psi(x,0)$ and we aim to determine $\Psi(x,t)$.

So we have,

$$\Psi(x,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k)\, e^{ikx}\, dk$$

This is fourier's transform.

So we have

$$\phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(x,0)\, e^{-ikx}\, dx.$$

Now let us try to resolve the paradox

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k)\, e^{-i(kx-\omega t)}\, dk$$

where $\omega = \frac{\hbar k^2}{2m}$, dispersion relation. Now $\phi(k)$ peaks at k_0 so we can taylor expand $\omega(k)$ as,

$$\omega(k) \simeq \omega_0 + \omega'(k)(k-k_0)$$

let $s = k-k_0$ so we have $s+k_0 = k$. So we have,

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(s+k_0)\, e^{i((s+k_0)x - (\omega_0+\omega' s)t)}$$

$$= \frac{1}{\sqrt{2\pi}} \underbrace{e^{+ik_0x - i\omega_0 t}}_{\text{Travelling wave}} \underbrace{\int_{-\infty}^{\infty} \phi(s+k_0)\, e^{is(x-\omega' t)}\, ds.}_{\text{Amplitude}}$$

Now $v_{phase} = \frac{\omega}{k}$ and $v_{group} = \frac{d\omega}{dk} \Rightarrow v_{group} = v_{classical}.$

So a single particle is not a single solution but a linear combination of multiple stationary state solution.

Example: A free particle has the initial wave function form as

$$\Psi(x,0) = A e^{-a|x|}$$

a) Normalize it. b) Find $\phi(k)$ c) Construct $\Psi(x,t)$ d) Discuss limiting case

Sol^n

a) $|A|^2 \int_{-\infty}^{\infty} e^{-2a|x|} = 1 \Rightarrow 2|A|^2 \int_0^{\infty} e^{-2ax} dx = -\frac{\cancel{2}|A|^2}{\cancel{2}a} \int_0^{-\infty} e^u du = -\frac{|A|^2}{a} |0-1| = 1$

$\Rightarrow |A|^2 = a \Rightarrow |A| = \sqrt{a}$, So we have, $\Psi(x,0) = \sqrt{a}\, e^{-a|x|}$

b) $$\phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(x,0) e^{-ikx} dx = \sqrt{\frac{a}{2\pi}} \int_{-\infty}^{+\infty} e^{-a|x|} e^{-ikx} dx$$

$$= \sqrt{\frac{a}{2\pi}} \left(\int_{-\infty}^{0} e^{ax-ikx} dx + \int_0^{\infty} e^{-ax-ikx} dx \right)$$

$$= \sqrt{\frac{a}{2\pi}} \left(\frac{1}{a-ik} + \frac{1}{a+ik} \right) = \sqrt{\frac{a}{2\pi}} \left(\frac{2a}{a^2+k^2} \right)$$

$\therefore$

$$\phi(k) = \sqrt{\frac{a}{2\pi}} \left(\frac{2a}{a^2+k^2} \right)$$

c) $$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{+ikx - \frac{\hbar^2 k^2}{2m} t} \sqrt{\frac{a}{2\pi}} \left(\frac{2a}{a^2+k^2} \right) dx.$$

d) limiting case, $a \to 0$.

$\Psi(x,t) \to 0$

limiting case, $a \to \infty$

$\Psi(x,t) \to 0$ (Use L' hospital Rule)

Just a note,

$$\begin{cases} E < V(-\infty) \text{ and } V(+\infty) & , \text{ bound state} \\ E > V(-\infty) \text{ and } V(\infty+) & , \text{ scattering state} \end{cases}$$

In real life as most of potentials $V(-\infty) = V(+\infty) = 0$, so we have

$$\begin{cases} E < 0 & , \text{ bound state} \\ E > 0 & , \text{ scattering state.} \end{cases}$$

Till now we looked into examples of bound state potentials as infinite well and simple harmonic oscillator and scattering potentials as free particle, but there are potentials which support both.

◦ <u>Delta function potential</u>

Consider a potential of the form,

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

Now let us try to solve the schrödinger's equation, here,

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

Now this can give rise to both bound state solution and scattering solution.

Bound State Solution, $(E<0)$,

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

$$\Rightarrow \quad \frac{d^2\psi}{dx^2} = \frac{-2mE}{\hbar^2}\psi(x) = k^2\psi(x)$$

Now $k^2 = \frac{-2mE}{\hbar^2}$, so we have, $\psi(x) = Ae^{kx} + Be^{-kx}$, for $x>0$ Be^{-kx} is a valid solution and for $x<0$ Ae^{kx} is a valid solution, so to write it more clearly.

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

how do we determine the coefficients? Now note, standard boundary condition for $\psi(x)$ are

→ $\psi(x)$ is continuous.

→ $\frac{d\psi}{dx}$ is continuous at all points except where potential blows up.

Now first boundary condition tell us that.

1) $A e^{-k(0)} = B e^{k(0)} \Rightarrow A = B.$

So

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

Now let use second boundary condition,

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

$$\Rightarrow \quad \frac{-\hbar^2}{2m^2}\left[\left.\frac{d\psi}{dx}\right|_{+\epsilon} - \left.\frac{d\psi}{dx}\right|_{-\epsilon}\right] = -\int_{-\epsilon}^{+\epsilon} V(x)\,\psi(x)\, dx$$

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

$$\Rightarrow \quad \Delta\left(\frac{d\psi}{dx}\right) = \frac{-2m\alpha\,\psi(0)}{\hbar^2}$$

Now we know $\psi(x) = \begin{cases} Be^{-kx}, & x \geq 0 \\ Be^{kx}, & x \leq 0 \end{cases}$, so $\Delta\left(\frac{d\psi}{dx}\right) = -2Bk$, $\psi(0) = B.$

So we have

$$+\cancel{2}\cancel{B}k = +\frac{\cancel{2}m\alpha\,\cancel{B}}{\hbar^2} \Rightarrow \boxed{k = \frac{m\alpha}{\hbar^2}}$$

So we have

$$E = \frac{-\hbar^2 k^2}{2m} = -\frac{\cancel{\hbar^2}}{2\cancel{m}}\,\frac{m^{\cancel{2}}\alpha^2}{\hbar^{\cancel{4}\,2}} = -\frac{m\alpha^2}{2\hbar^2}$$

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

Now we have by normalization,

$$2\int_0^\infty |B|^2 e^{-2kx}\, dx = 1 \Rightarrow \frac{|B|^2}{k} = 1, \text{ so } \boxed{B = \sqrt{k} = \frac{\sqrt{m\alpha}}{\hbar}}$$

So we have,

$$\boxed{\psi(x) = \frac{\sqrt{m\alpha}}{\hbar}\, e^{-m\alpha|x|/\hbar^2}\ ; \quad E = -\frac{m\alpha^2}{2\hbar^2}}$$

For Scattering States, $(E>0)$

We had. for $x \geq 0$

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

The solution looks like, $\psi(x) = Ae^{-ikx} + Be^{ikx}$

and for $(x \leq 0)$ we have.

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

By continuity condition we have,

$$A+B = F+G.$$

and as shown earlier,

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

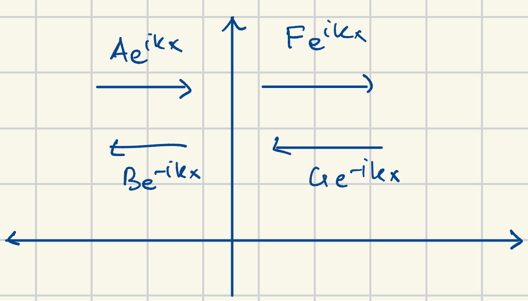
Now $\Delta\left(\frac{d\psi}{dx}\right) = -ik(A-B) + ik(F-G) = ik(F-G-A+B)$

So we have,

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

$$\Rightarrow \boxed{F-G = A(1+2i\beta) - B(1-2i\beta)} \quad , \quad \boxed{\beta = \frac{m\alpha}{\hbar^2 k}}$$

Now normalization won't work, so let us get some physical intuition.



Now one can assume. $G=0$ say incoming wave pass ahead the barrierer. and there is no wave in $(x>0)$ going backward and hence we can put $G=0$, So from above equations.

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

Now let us try to find some quantities of interest. One is reflection coefficient and other is transmission coefficient.

Now By using relation $A+B = F + \cancel{G}^{0}$

Now

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

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

$$A(\cancel{1}-\cancel{1}-2i\beta) = -B(2-2i\beta) \Rightarrow 2i\beta A = B\,2(1-i\beta)$$

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

Now $\frac{|B|^2}{|A|^2} = \frac{i\beta}{(1-i\beta)} \frac{-i\beta}{(1+i\beta)} = \frac{\beta^2}{1+\beta^2}$ $\left(\beta = \frac{m\alpha}{\hbar^2 k} \right)$

$$R = \frac{\beta^2}{1+\beta^2}$$, the reflectance coefficient.

Now for transmission coefficient,

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

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

Again by using $F = A+B$,

$$F = A + \frac{i\beta A}{(1-i\beta)} \Rightarrow \frac{F}{A} = \frac{1+i\beta}{1-i\beta}$$

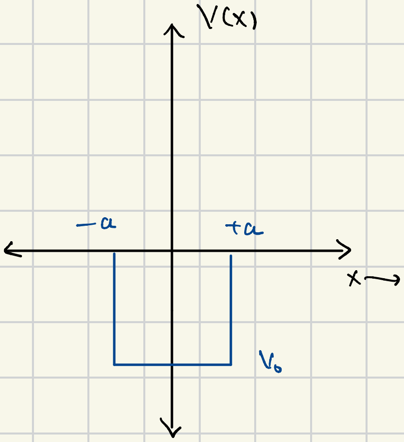
and $R+T = 1$ then we have,

$$T = \frac{1}{1+\beta^2}$$, transmission coefficient.

Finite square well

Consider a particle in a finite square well as,

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



Now consider Schrödinger's eqn as

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

① Bound state solution, ($E<0$).

In region $(x<-a)$, we have

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi$$

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

$\Rightarrow \dfrac{d^2\psi}{dx^2} = +k^2\psi$, where $k = \sqrt{\dfrac{-2mE}{\hbar}}$, then in region-I the solution look like

$$\psi_1(x) = Ae^{-kx} + Be^{kx}$$

In region $(-a<x<a)$

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

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

$\Rightarrow \dfrac{d^2\psi}{dx^2} = -l^2\psi(x)$, where $l = \sqrt{\dfrac{2m(E+V_0)}{\hbar}}$

and we have

$$\psi_{II}(x) = C\sin(lx) + D\cos(lx)$$

For region II $(x>a)$:

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

$$\Rightarrow \frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi(x) \Rightarrow \psi_{III}(x) = Ee^{kx} + Fe^{-kx}$$

Now we have in three regions the wavefunction as,

$$\psi_1(x) = Ae^{kx} + Be^{-kx}$$
$$\psi_2(x) = C\sin(lx) + D\cos(lx)$$
$$\psi_3(x) = Ee^{kx} + Fe^{-kx}$$

Now for $x<-a$ we have

$$\psi_1(x) = Ae^{kx}$$

let us take up even solutions first since the potential is even.

$$\psi_2(x) = D\cos(lx)$$
$$\psi_3(x) = Fe^{-kx}$$

Now since the potential is even the boundary conditions applied for $x>a$ goes as $\psi(-x)$. So we have,

① By continuity of wavefunction, at $x=a$ we have,

$$Fe^{-ka} = D\cos(la)$$

and by continuity of derivative of wavefunction at $x=a$ we have,

$$-Fke^{-ka} = -lD\sin(la)$$

Now from above two eqns we have

$$\frac{-1}{k} = \frac{-1}{l}\cot(la)$$

$$\Rightarrow \quad \boxed{\frac{k}{l} = \tan(la)}$$

Now let $z \equiv la$, Now

$$k^2 + l^2 = \frac{2mV_0}{\hbar^2}$$

let $z_0 = a\sqrt{\frac{2mV_0}{\hbar}}$

$$1 + \frac{k^2}{l^2} = \frac{1}{l^2}\frac{2mV_0}{\hbar^2}$$

$$\Rightarrow \quad 1 + \frac{k^2}{l^2} = \frac{a^2}{z^2}\frac{2mV_0}{\hbar^2}$$

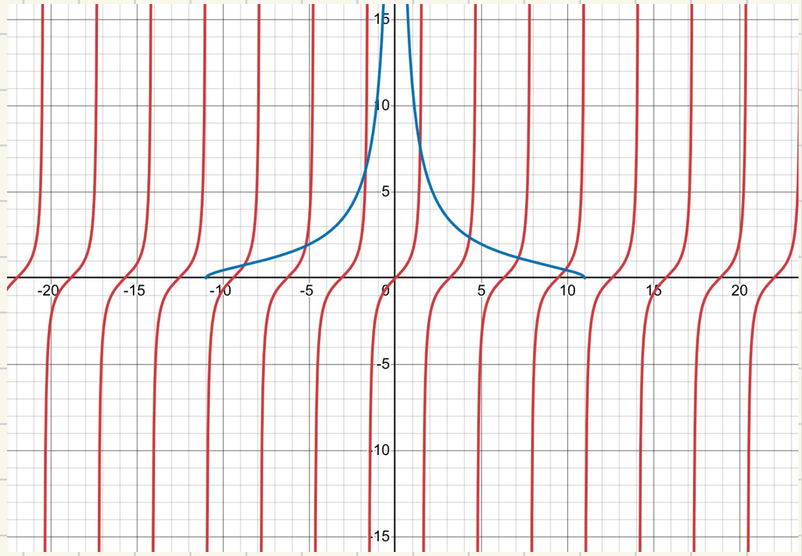
$$\Rightarrow \quad 1 + \frac{k^2}{l^2} = \frac{z_0^2}{z^2} \Rightarrow \frac{k}{l} = \sqrt{\left(\frac{z_0}{z}\right)^2 - 1}$$

$$\therefore \quad \tan(z) = \sqrt{\frac{z_0^2}{z^2} - 1}$$

Now the above eqn is a transcedental equation hence can be solved by plotting the two curves.

Now one can change value of z_0 and play with graph.

Let us try to understand the system of equations by some mathematics.



Now from the curve we have

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

$$\frac{n\pi}{2a} = \sqrt{\frac{2m(E+V_0)}{\hbar}}$$

$$\Rightarrow \quad \frac{n^2\pi^2}{4a^2} = \frac{2m(E+V_0)}{\hbar} \Rightarrow \boxed{E+V_0 \simeq \frac{n^2\pi^2\hbar^2}{2m4a^2}}$$

Now $V_0 \to \infty$ we have half of infinite solutions of infinite deep well. Other half comes from odd-solutions. Let us consider them.

So we had the most general solution as.

$$\psi(x) = \begin{cases} Ae^{kx} + Be^{-kx} \\ C\sin(la) + D\cos(la) \\ E\, e^{kx} + Fe^{-kx} \end{cases}$$

Now again using the same boundary conditions we have,

$$Fe^{-kx} = C\sin(la)$$

$$\Rightarrow -kFe^{-kx} = lC\cos(la)$$

$$\Rightarrow \quad -\frac{1}{k} = \frac{1}{l}\tan(la) \quad \Rightarrow \quad \frac{k}{l} = -\cot(la)$$

let $la \equiv z$ and we have

$$k^2a^2 + l^2a^2 = a^2\frac{2mV_0}{\hbar^2}$$

$$\Rightarrow \quad k^2a^2 = z_0^2 - z^2 \Rightarrow \quad ka = \sqrt{z_0^2 - z^2}, \quad \text{now} \quad ka = -la\cot(la).$$

$$-\cancel{z}\cot(z) = \cancel{z}\sqrt{\frac{z_0^2}{z} - 1} \quad \Rightarrow \quad \boxed{-\cot(z) = \sqrt{\frac{z_0^2}{z^2} - 1}}$$

Now note, for large z_0 we have

$$\frac{2n\pi}{2} = z \Rightarrow \frac{n^2\pi^2}{a^2} = \frac{2m}{\hbar^2}(E_0+V)$$

$$\Rightarrow \boxed{E_0+V \simeq \frac{(2n)^2\pi^2\hbar^2}{2m(2a)^2}}$$, all even solutions.

How many bound states are there?

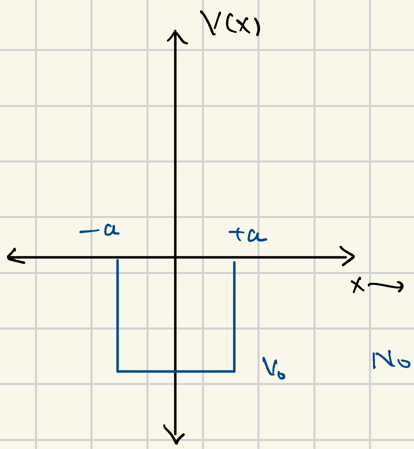
For even solutions we have, there is always a bound state solution but for odd solutions we don't have a bound state solution always. but how to show it? one way, look at graph.

Note that z_0 controls the value of number of bound state but $z_0 \to \infty$ we have some infinite number of solutions now let us see as $z_0 \to 0$.

Scattering State Solution $(E>0)$

Consider the solution for the part for where $(E>0)$ now we have,

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



Now for $x < -a$, we have

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

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi = -k^2\psi(x), \text{ where } k^2 = \frac{2mE}{\hbar^2}$$

Now we have, $\psi_I(x) = Ae^{ikx} + Be^{-ikx}$

$\psi_{II}(x) = C\sin(lx) + D\cos(lx)$, where $l = \frac{\sqrt{2m(E+V)}}{\hbar}$

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

Now $x < -a$ by continuity of wavefunction we have,

$$Ae^{-ika} + Be^{ika} = -C\sin(la) + D\cos(la)$$

$$\Rightarrow \quad -ik\left[Ae^{-ika} - Be^{ika}\right] = -l\left[C\cos(la) + D\sin(la)\right]$$

Now for $x > a$ by continuity of wavefunction we have,

$$Fe^{ika} = C\sin(la) + D\cos(la)$$

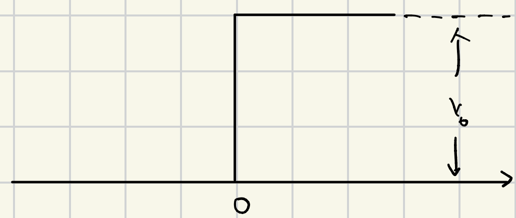
$$\Rightarrow \quad ikFe^{ika} = l\left[C\cos(la) - D\sin(la)\right]$$

Step potential

Consider a particle of mass m, and energy E, moving under potential V_0 and we would like to study it for both bound state and scattering state.

We have,

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



For scattering state $(E > V)$.

For $(x<0)$ we have,

$$\frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi$$

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

Now we have, $\boxed{\psi_I(x) = Ae^{+ikx} + Be^{-ikx}}$, $\quad -(1)$

For $x \geq 0$ we have,

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

$$= -l^2\psi(x)$$

So we have $\boxed{\psi_{II}(x) = Ce^{+ilx} + De^{-ilx}}$ $\quad -(2)$

Now by continuity at $x=0$ we have

$$\boxed{A+B = C+D} \quad -(3)$$

Now by putting $D=0$, for left going wave to be zero. We have

$$\boxed{A+B = C} \quad -(4)$$

By using continuity of first derivative.

$$+ikA - ikB = +il\,C - il\,D$$

$$\Rightarrow \boxed{A-B = \frac{l}{k}C} \quad -(5)$$

Now associated prob. density is.

$$\boxed{\vec{J} = \frac{-i\hbar}{2m}\left(\psi^*\nabla\psi - \psi\nabla\psi^*\right)} \quad -(6)$$

We have

$$\vec{J}_i = \frac{-i\hbar}{2m}\left(Ae^{ikx}(-ik)Ae^{-ikx} - ikAe^{ikx}Ae^{-ikx}\right) = \frac{\hbar k}{m}|A|^2 \quad -(7)$$

$$\vec{J}_r = \frac{-i\hbar}{2m}\left(Be^{ikx}(-ik)Be^{-ikx} - ikBe^{ikx}Be^{-ikx}\right) = \frac{\hbar k}{m}|B|^2 \quad -(8)$$

$$\vec{J}_t = \frac{\hbar l}{m}|C|^2 \quad -(9)$$

Now we have.

$$2A = \left(\frac{k+l}{k}\right)C \Rightarrow \frac{|C|^2}{|A|^2} = \frac{4k^2}{(k+l)^2}$$

$$\Rightarrow T = \frac{J_t}{J_i} = \frac{l}{k}\left(\frac{|C|^2}{|A|^2}\right) = \frac{l}{\cancel{k}}\frac{4k^{\cancel{2}}}{(k+l)^2} = \frac{4kl}{(k+l)^2}$$

So we have

$$\boxed{T = \frac{4kl}{(k+l)^2}} \quad -(10)$$

For reflection we have

$$R+T = 1 \Rightarrow R = 1 - \frac{4kl}{(k+l)^2} = \frac{k^2+l^2-2kl}{(k+l)^2} = \left(\frac{k-l}{k+l}\right)^2$$

$$\boxed{R = \left(\frac{k-l}{k+l}\right)^2} \quad -(11)$$

For Bound State $(E<V)$:

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

For $x>0$ we have,

$$\frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi$$

$$\Rightarrow \psi(x) = Ae^{+ikx} + Be^{-ikx}, \quad \text{where} \quad k = \frac{\sqrt{2mE}}{\hbar} \quad -(13)$$

Incident ↙ ↘ reflected.

For $x>0$,

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

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

So we have

$$\psi_2(x) = Ce^{-lx} + De^{lx}$$

Now for $x>0$, we have $D=0$.

$$\boxed{\psi_2(x) = Ce^{-lx}} \quad -(14)$$

Now by continuity of wavefunction we have,

$$\boxed{A+B = C} \quad -(15)$$

By continuity of first derivative we have,

$$ikA - ikB = -lC$$

$$\Rightarrow \boxed{A-B = \frac{il}{k}C} \quad -(16)$$

Now

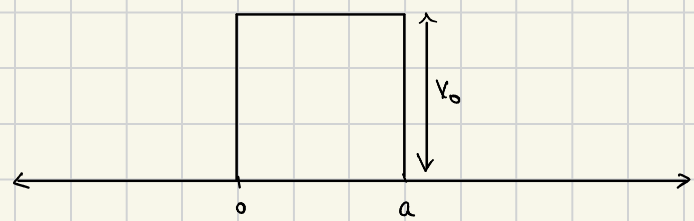
$$T = \frac{J_t}{J_i}; \qquad J_t = \frac{i\hbar}{2m}\left(\psi^* \nabla\psi - \psi \nabla\psi^*\right) \quad \text{as } \psi \in R, \; J_t = 0$$

So we have $T=0$, So $R=1$.

$\Rightarrow$ Note, there is still a finite prob. of finding particle $x\geq 0$.

Step potential of finite width 'a'.

Consider a potential well V of finite width 'a' and we want to analyse this situation. A particle of mass m is moving with energy E and we want to analyse the situation.



We have two types of solutions.

(1) Scattering State ($E > V_0$)

We have, for $x < 0$.

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

$$\Rightarrow \psi_I(x) = Ae^{ikx} + Be^{-ikx} \qquad -(1)$$

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

For $0 \le x \le a$, we have.

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

$$\Rightarrow \frac{d^2\psi}{dx^2} = -\frac{2m}{\hbar^2}(E-V)\psi(x) = -l^2\psi(x)$$

$$\psi_2(x) = Ce^{ilx} + De^{-ilx} \qquad -(2)$$

For $x > a$ we have,

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi$$

$$\Rightarrow \psi_3(x) = Ee^{ikx} + Fe^{-ikx} \qquad -(3)$$

From Eq (1), (2) & (3) we have

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx}, & x \le 0 \\ Ce^{ilx} + De^{-ilx}, & 0 \ge x \ge a \\ Ee^{ikx} + Fe^{-ikx}, & x > a \end{cases}$$

Applying the condition of continuity of function and first derivative on the above function

Now we have the following conditions placed.