The Free Particle

$V(x)=0$ everywhere

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}=E\psi, \quad \frac{d^2\psi}{dx^2}=-\frac{2mE}{\underbrace{\hbar^2}_{k^2}}\psi, \quad \psi(x)=Ae^{ikx}+Be^{-ikx} \qquad E=\frac{\hbar^2k^2}{2m}$$

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

$$=Ae^{i(kx-\frac{\hbar k^2}{2m}t)}$$

phase velocity $V_p=\frac{\hbar k}{2m}$

$V_c=\frac{\hbar k}{m}=2V_p$

$$\int_{-\infty}^{+\infty}\Psi^*(x)\Psi(x)dx=|A^2|\int_{-\infty}^{+\infty}e^{-ikx}e^{ikx}dx=|A|^2\infty \Rightarrow \text{not normalizable}$$

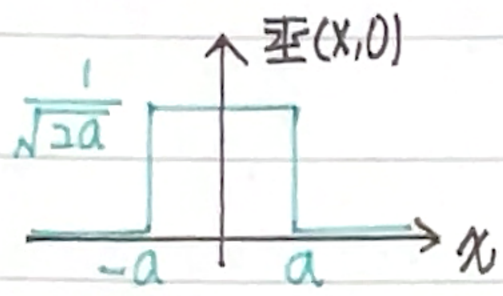
$$\psi=\sum_n C_n\psi_n$$

$$\Psi(x,t)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}\underbrace{\phi(k)}_{C_n}\underbrace{e^{i(kx-\frac{\hbar k^2}{2m}t)}}_{\psi_n(x,t)}dk, \quad \Psi(x,0)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}\phi(k)e^{ikx}dk$$

Plancherel's theorem: $f(x)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}F(k)e^{ikx}dk \Leftrightarrow F(k)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}f(x)e^{-ikx}dx$

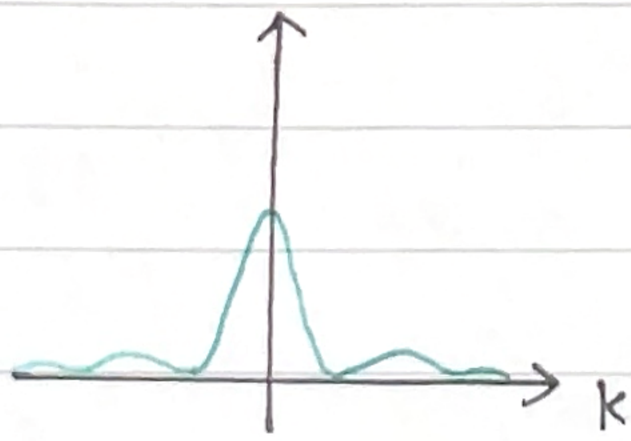
$$\phi(k)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}\Psi(x,0)e^{-ikx}dx$$

Example



$$\phi(k)=\frac{1}{\sqrt{2\pi}}\frac{1}{\sqrt{2a}}\int_{-a}^{a}e^{-ikx}dx=\frac{1}{2\sqrt{\pi a}}\frac{1}{-ik}e^{-ikx}\Big|_{-a}^{a}=\frac{1}{\sqrt{\pi a}}\frac{\sin(ka)}{k}$$

$$\Psi(x,t)=\frac{1}{\pi\sqrt{2a}}\int_{-\infty}^{\infty}\frac{\sin(ka)}{k}e^{i(kx-\frac{\hbar k^2}{2m}t)}dk$$



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

$\omega(k) \approx \omega_0 + \omega_0' \underbrace{(k - k_0)}_{s}$

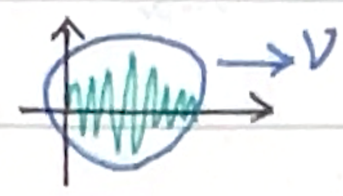
$$\Psi(x,t) \approx \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k_0+s) e^{i[(k_0+s)x - (\omega_0 + \omega_0' s)t]} ds$$

$-\omega_0 t + k_0 \omega_0' t + (x - \omega_0' t)(k_0 + x)$

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

$$\Psi(x,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k_0+s) e^{i(k_0+s)x} ds$$

$$\Rightarrow \Psi(x,t) = e^{-i(\omega_0 - k_0 \omega_0')t} \Psi(x - \underbrace{\omega_0' t}_{v_g}, 0)$$



$$\left[\begin{array}{l} \omega_0' = v_{group} = \left.\frac{d\omega}{dk}\right|_{k=k_0} \\ v_{phase} = \frac{\omega}{k} \end{array} \right.$$

$$\left[\begin{array}{l} p = \hbar k \\ E = \hbar \omega \end{array} \right. \qquad v_{group} = \frac{d\omega}{dk} = \frac{d\frac{E}{\hbar}}{d\frac{p}{\hbar}} = \frac{p}{m} = v_{classical}$$

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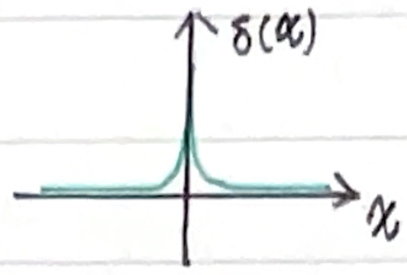
The Delta-Function Potential

$V(x) = -\alpha\delta(x) \quad \alpha > 0$

$\delta(x) \begin{cases} 0 & x = 0 \\ \infty & x \neq 0 \end{cases} \qquad \int_{-\infty}^{+\infty} \delta(x)\,dx = 1$



$\int_{-\infty}^{+\infty} \delta(x-a) f(x)\,dx = f(a)$

$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} - \alpha\delta(x)\psi = E\psi$ looking for bound states, $E<0$

(I) $x>0$

$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi, \quad \frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi \qquad$ let $k = \frac{\sqrt{-2mE}}{\hbar}$

$\Rightarrow \frac{d^2\psi}{dx^2} = k^2\psi, \quad \psi(x) = Ae^{kx} + Be^{-kx} \quad \because x\to\infty, \psi(x)$ is finite $\therefore A=0$

$\Rightarrow \psi(x) = Be^{-kx}$

(II) $x<0$

$\Rightarrow \psi(x) = Fe^{kx}$

at $x=0$, $\psi(0^+) = \psi(0^-)$ boundary condition

$B = F \qquad \psi(x) \begin{cases} Be^{-kx}, & x>0 \\ Be^{kx} & x<0 \end{cases} \qquad \int_{-\infty}^{+\infty} |\psi(x)|^2 dx = 1$

Is $\left.\frac{d\psi}{dx}\right|_{x=0^+} = \left.\frac{d\psi}{dx}\right|_{x=0^-}$?

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

$-\frac{\hbar^2}{2m}\left(\left.\frac{d\psi}{dx}\right|_{x=+\epsilon} - \left.\frac{d\psi}{dx}\right|_{x=-\epsilon}\right) = \underbrace{-\int_{-\epsilon}^{+\epsilon} V(x)\psi(x)dx}_{\to 0,\infty \ \epsilon\to 0} + \underbrace{E\int_{-\epsilon}^{+\epsilon}\psi(x)dx}_{\to 0 \text{ as } \epsilon\to 0}$

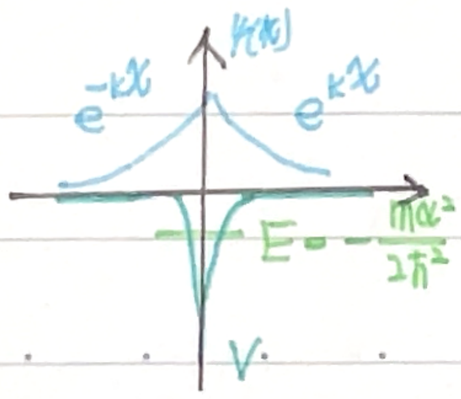
$\Rightarrow \frac{d\psi}{dx}$ is continuous as long as $V(x)$ is finite

$\text{right} = -\int_{-\epsilon}^{+\epsilon} -\alpha\,\delta(x)\psi(x)dx = \alpha\int_{-\epsilon}^{+\epsilon}\delta(x)\psi(x)dx = \alpha\psi(0)$

$\Rightarrow \left.\frac{d\psi}{dx}\right|_{x=0^+} - \left.\frac{d\psi}{dx}\right|_{x=0^-} = -\frac{2m\alpha}{\hbar^2}\psi(0), \quad \underbrace{-Bke^{-kx}\Big|_{x=0^+} - Bke^{kx}\Big|_{x=0^-}}_{-2Bk} = -\frac{2m\alpha}{\hbar^2}B$

$\Rightarrow k = \frac{m\alpha}{\hbar^2} = \frac{\sqrt{-2mE}}{\hbar^2}$

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



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

$$\int_{-\infty}^{+\infty} |\psi(x)|^2 dx = 2|A|^2 \int_0^{\infty} e^{-2kx} dx = \frac{|A|^2}{k} = 1, \quad A = \sqrt{k} = \frac{\sqrt{m\alpha}}{\hbar}$$

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

For scattering states $E>0$

for $x<0$

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

$$\psi(x) = \underbrace{\overrightarrow{A} e^{ikx}}_{\text{incident}} + \underbrace{\overleftarrow{B} e^{-ikx}}_{\text{reflected}}$$

for $x>0$

$$\psi(x) = \underbrace{\overrightarrow{F} e^{ikx}}_{\text{transmitted}} \leftarrow$$

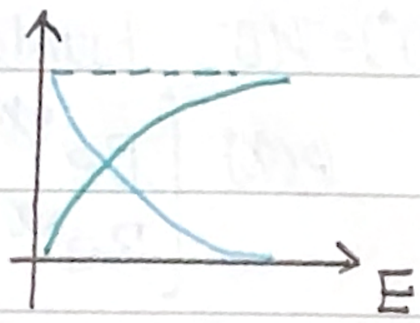
$$\psi(0^+) = \psi(0^-) \Rightarrow A + B = F$$

$$\left.\frac{d\psi}{dx}\right|_{x=0^+} - \left.\frac{d\psi}{dx}\right|_{x=0^-} = ikA - ikB - ikF = -\frac{2m\alpha}{\hbar^2}(A+B)$$

$$\underbrace{T(E)}_{\text{transmission coefficient}} = \frac{|F|^2}{|A|^2} \qquad \underbrace{R(E)}_{\text{reflection coefficient}} = \frac{|B|^2}{|A|^2}$$

by (i), (ii), $B = \frac{i\beta}{1-i\beta} A \quad F = \frac{1}{1-i\beta} A \quad \beta = \frac{m\alpha}{\hbar^2 k}$

$$\Rightarrow R = \frac{\beta^2}{1+\beta^2} = \frac{1}{1+\frac{2\hbar E}{m\alpha^2}} \qquad T = \frac{1}{1+\beta^2} = \frac{1}{1+\frac{m\alpha^2}{2\hbar^2 E}}$$



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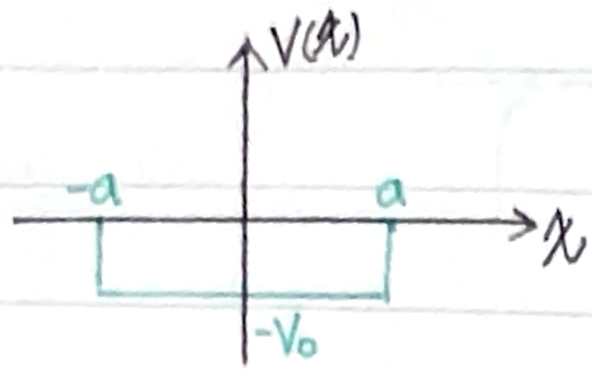
The Finite Square Well



look first at the bound states
$0 > E > -V_0$

(I) $x < -a$

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

$$\psi(x) = Ae^{-kx} + Be^{kx} = Be^{kx} \qquad \frac{d\psi}{dx} = kBe^{kx}$$

(II) $x > a$

$$\psi(x) = Fe^{-kx} \qquad \frac{d\psi}{dx} = -kFe^{-kx}$$

(III) $-a < x < a$

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

$$\Rightarrow \psi(x) = \underbrace{C\sin(lx)}_{\text{even}} + \underbrace{D\cos(lx)}_{\text{odd}}$$

$$\frac{d\psi}{dx} = lC\cos lx - lD\sin lx$$

at $x = -a$, $Be^{-ka} = -C\sin la + D\cos la$ —— (1)

$kBe^{-ka} = lC\cos la + lD\sin la$ —— (2)

at $x = a$ $Fe^{ka} = C\sin la + D\cos la$ —— (3)

$-kFe^{ka} = lC\cos la - lD\sin la$ —— (4)

$k = l\tan z$
$ka = la\tan z$
$= z\tan z$

let $C = 0$ first:

$$\frac{(1)}{(2)} = \frac{1}{k} = \frac{\cos la}{l\sin la} = \frac{1}{l}\frac{1}{\tan la}, \quad k = l\tan la$$

let $z = la$ $\quad z_0 \equiv \frac{a}{\hbar}\sqrt{2mV_0}$ $\quad k^2 + l^2 = -\frac{2mE}{\hbar^2} + \frac{2m(E+V_0)}{\hbar^2} = \frac{2mV_0}{\hbar^2} = \frac{z_0^2}{a^2}$

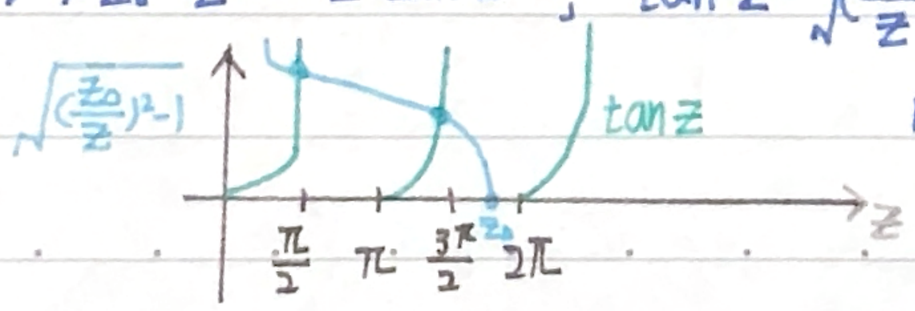
$(ka)^2 + (la)^2 = z_0^2$ $\quad ka = \sqrt{z_0^2 - z}$

$$\Rightarrow \sqrt{z_0^2 - z^2} = z\tan z, \quad \tan z = \sqrt{\left(\frac{z_0}{z}\right)^2 - 1}$$

$\sqrt{\left(\frac{z_0}{z}\right)^2 - 1} = 0$

$\frac{z_0^2}{z^2} = 1$

$z_0 = z$



must have one solution

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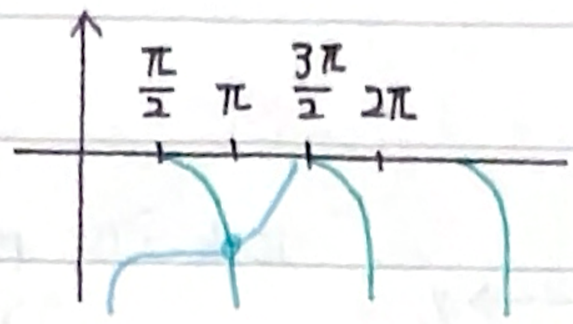
let $D=0$

$\Rightarrow C_0 + Z = -\sqrt{\left(\frac{Z_0}{Z}\right)^2 - 1}$



Scattering State ($E>0$)

$x<-a, \quad \psi(x) = Ae^{ikx} + Be^{-ikx} \qquad k = \frac{\sqrt{2mE}}{\hbar}$

$-a<x<a \quad \psi(x) = C\sin(lx) + D\cos(lx) \qquad l = \frac{\sqrt{2m(E+V_0)}}{\hbar}$

$x>a \quad \psi(x) = Fe^{ikx}$

four boundary:

$$\left.\begin{aligned} &Ae^{-ika} + Be^{ika} = -C\sin(la) + D\cos(la) \\ &\frac{d\psi}{dx} = ik\left[Ae^{-ika} - Be^{ika}\right] = l\left[C\cos(la) + D\sin(la)\right] \\ &C\sin(la) + D\cos(la) = Fe^{ika} \\ &l\left[C\cos(la) - D\sin(la)\right] = ikFe^{ika} \end{aligned}\right\} \begin{aligned} &F = \frac{e^{-2ika}A}{\cos(2la) - i\frac{(k^2+l^2)}{2kl}\sin(2la)} \\ &B = i\frac{\sin(2la)}{2kl}(l^2-k^2)F \end{aligned}$$

$$T^{-1} = \frac{|A|^2}{|F|^2} = 1 + \frac{V_0^2}{4E(E+V_0)}\sin^2\left[\frac{2a}{\hbar}\sqrt{2m(E+V_0)}\right]$$

if $T=1$, mean sine is zero, $\frac{2a}{\hbar}\sqrt{2m(E_n+V_0)} = n\pi$. $E_n + V_0 = \frac{n^2\pi^2\hbar^2}{2m(2a)^2}$