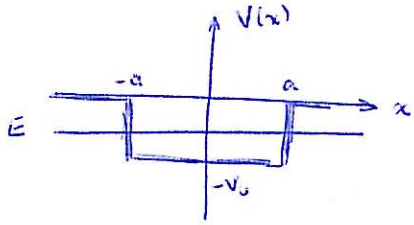
Finite Square Well

$$V(x) = \begin{cases} -V_0 & -a \le x \le a \\ 0 & |x| > a \end{cases}$$

⇝ Bound State $(E<0)$



classically the particle would be confined in the region $-a<x<a$ but in Q.M. it can be found in $x>a$ or $x<-a$

a) $x<-a$

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

$$\boxed{K = \frac{\sqrt{-2mE}}{\hbar}} \longrightarrow K \oplus \text{ and real, since } E \ominus$$

$$\frac{d^2\psi}{dx^2} = K^2\psi$$

$$\psi(x) = A e^{-Kx} + B e^{Kx}$$

$A e^{-Kx}$ blows up at $-\infty \Rightarrow A=0$

$$\longrightarrow \psi(x) = B e^{Kx} \quad \text{for } x<-a$$

there is a probability to find the particle at $x<-a$, but it decays as x approaches $-\infty$ (exponentially)

•) $-a < x < a$ $\qquad V(x) = -V_0$

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

$$l = \frac{\sqrt{2m(E+V_0)}}{\hbar}$$

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

E is $\ominus$, but $E+V_0$ is $\oplus$

$\Rightarrow$ l is real and $\oplus$

$\longrightarrow$ $\psi(x) = C\sin(lx) + D\cos(lx)$, for $-a < x < a$

•) $x > a$

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

$G=0$ because e^{Kx} blows up at $+\infty$

$\longrightarrow$ $\psi(x) = Fe^{-Kx}$, for $x > a$

•) To find $\cancel{A}$, $\underbrace{B, C, D, F}$, $\cancel{G}$ we use the <u>boundary</u> <u>conditions</u>

$$\left.\begin{array}{c}\psi(x)\\ \text{and}\\ \frac{d\psi}{dx}\end{array}\right\}$$ are continuous at $-a$ and $+a$

NOTE ① — Conditions on the wave function: (Remember $|\Psi(x,t)|^2$ is the prob. density)

1.) It must be twice differentiable (Schröd. eq.)

$\Downarrow$

$\Psi(x)$ and $\frac{d\Psi}{dx}$ must be continuous

$\frac{d\Psi}{dx}$ → continuous <u>except</u> at points where the potential is infinite

2.) To be normalizable, it must approach zero as x approaches infinity

NOTE ②

Here $V(x)$ is an <u>even</u> function

$$\boxed{V(x) = V(-x)}$$

$\Downarrow$

solutions are either

<u>even</u> $\Psi(x) = \Psi(-x)$

or

<u>odd</u> $\Psi(x) = -\Psi(-x)$

Proof: $\Psi(x)$ is a solution, ~~change~~

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

•) change $x \to -x$, we know that $V(x) = V(-x)$, for even $\Psi(x)$

$$-\frac{\hbar^2}{2m}\frac{d^2\Psi(-x)}{dx^2} + V(-x)\Psi(-x) = E\Psi(-x) \Rightarrow \Psi(-x) \text{ is also a solution}$$

•) change $x \to -x$, $V(x) = V(-x)$, for odd $\Psi(x)$

$$+\frac{\hbar^2}{2m}\frac{d^2\Psi(-x)}{dx^2} - V(-x)\Psi(-x) = -E\Psi(-x) \Rightarrow \Psi(-x) \text{ is also a solution}$$

Since $V(x) = V(-x)$ <u>even</u>

we can study just one side, for example $x \geq a$ and use

$$\psi(-x) = \pm \psi(x)$$

#) let us start with the <u>even</u> solution

$$\psi(x) = \psi(-x)$$

Keep the <u>cos</u>

$$\psi(x) = \begin{cases} F e^{-Kx} & x > a \\ D \cos(lx) & 0 < x < a \\ \psi(-x) & x < 0 \end{cases}$$

continuity at $x = a$

$$\begin{array}{l} \psi(x) \text{ at } x=a \longrightarrow \\ d\psi/dx \text{ at } x=a \longrightarrow \end{array} \begin{cases} F e^{-Ka} = D \cos(la) \\ -K F e^{-Ka} = -l D \sin(la) \end{cases}$$

$\div$ both $\Rightarrow$ $K = l \tan(la)$

$$\tan(la) = \frac{K}{l}$$

$$\tan(la) = \frac{K}{l} \qquad K = \frac{\sqrt{-2mE}}{\hbar} \qquad l = \frac{\sqrt{2m(E+V_0)}}{\hbar}$$

introduce

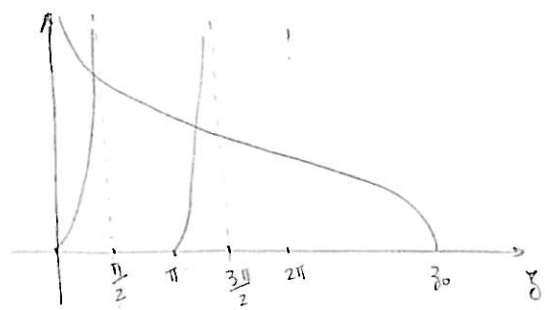
$$\gamma_0 = \frac{\sqrt{2mV_0}}{\hbar}\, a \qquad \text{and} \qquad \gamma = la$$

$$\tan(\gamma) = \frac{Ka}{la} \qquad Ka = \sqrt{\gamma_0^2 - l^2a^2} = \sqrt{\gamma_0^2 - \gamma^2}$$

$$\boxed{\tan(\gamma) = \sqrt{(\gamma_0/\gamma)^2 - 1}}$$

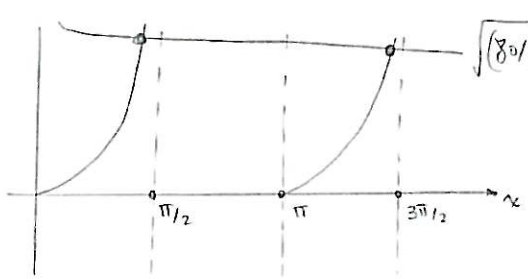
from here we find the energies

we know that
K, l are real $\oplus$ $\Rightarrow$ we only look at $\tan(la) > 0$



limits

1) wide, deep $\quad a, V_0 \to$ large $\Rightarrow \gamma_0 \to$ large



$\sqrt{(\gamma_0/\gamma)^2 - 1} \sim \gamma_0/\gamma$ and γ_0 is very large

$\Downarrow$

$\gamma_n \sim \frac{n\pi}{2}$ $\quad$ (n is odd) → half of the solutions

$$\Rightarrow la = \frac{n\pi}{2} \Rightarrow l^2 = \frac{n^2\pi^2}{(2a)^2} \Rightarrow \boxed{E_n + V_0 = \frac{n^2\pi^2\hbar^2}{2m(2a)^2}}$$

→ infinite square well energies

2.) shallow, narrow $\quad a, V_0$ — small, z_0 — very small

in the limit $z_0 < \pi/2 \rightarrow$ only <u>one</u> even state remain

↳ there is always <u>ONE</u> bound state no matter how weak the well becomes

#) <u>odd</u> solution

$$\psi(x) = -\psi(x)$$

Keep <u>sin</u>

$$\psi(x) = \begin{cases} F e^{-Kx} & x > a \\ C \sin(\ell x) & 0 < x < a \\ -\psi(-x) & x < 0 \end{cases}$$

$$\begin{cases} F e^{-Ka} = C \sin(\ell a) \\ -KF e^{-Ka} = \ell C \cos(\ell a) \end{cases}$$

$$\ell \operatorname{cotan}(\ell a) = -K$$

$$\boxed{-\operatorname{cotan}(\ell a) = \frac{K}{\ell}}$$

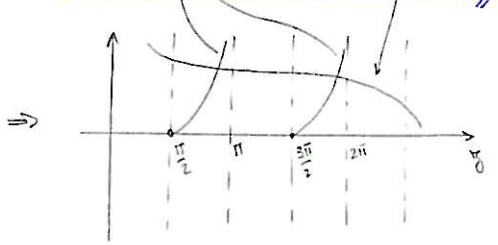
$$z_0 = \frac{\sqrt{2mV_0}\, a}{\hbar}$$

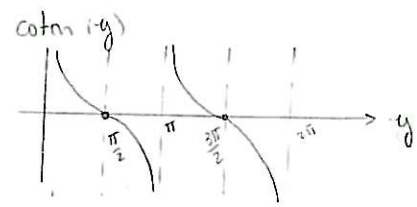
$$z = \ell a$$

$$Ka = \sqrt{z_0^2 - z^2}$$

$$-\operatorname{cotan}(z) = \frac{Ka}{\ell a} = \frac{\sqrt{z_0^2 - z^2}}{z}$$

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





Limits

1.) Wide deep

$\xi \sim \frac{n\pi}{2}$ $\quad$ n even → the other half of the solutions

$$\boxed{E_n + V_0 = \frac{n^2 \pi^2 \hbar^2}{2m\,(2a)^2}}$$

2.) Shallow, narrow

$\xi_0 < \pi/2 \Rightarrow$ no odd solution, so only ONE even solution remains

Therefore the solutions are:

$$\psi(x) = \begin{cases} F e^{-Kx} & x > a \\ D\cos(\ell x) & 0 < x < a \\ \psi(-x) & x < 0 \end{cases} \quad \text{AND} \quad \psi(x) = \begin{cases} F e^{-Kx} & x > a \\ D\sin(\ell x) & 0 < x < a \\ -\psi(-x) & x < 0 \end{cases}$$

normalizing to find D and F

$$1 = 2\int_0^\infty |\psi|^2\,dx = 2\int_0^a |D|^2 \cos^2(\ell x)\,dx + 2\int_a^\infty |F|^2 e^{-2Kx}\,dx$$

$$\cos^2 x \longrightarrow \cos 2x = \cos^2 x - \sin^2 x = 2\cos^2 x - 1 \Rightarrow \cos^2 x = \frac{1+\cos 2x}{2}$$

$$= \cancel{2}\,|D|^2 \left(\frac{a}{\cancel{2}} + \frac{\sin 2\ell x}{\underset{2}{\cancel{4}}\ell}\Big|_0^a \right) + \cancel{2}\,|F|^2 \frac{e^{-2Ka}}{\cancel{2}K} \Rightarrow |D|^2 \left(a + \frac{\sin 2\ell a}{2\ell} \right) + \frac{|F|^2 e^{-2Ka}}{K} = 1$$

but $F = D e^{Ka} \cos(\ell a)$ (from continuity)

$$\Rightarrow |D|^2 \left(a + \frac{\sin 2la}{2l} \right) + \frac{|D|^2 \cos^2 la}{K} = 1 \qquad \text{use} \quad \underline{K = l \tan(la)}$$

$$|D|^2 \left(a + \frac{\sin la \cos la}{l} + \frac{\cos^3 la}{l \sin(la)} \right) = 1$$

$$|D|^2 \left(a + \frac{\cos la \left(\sin^2 la + \cos^2 la \right)}{l \sin(la)} \right) = 1$$

$$|D|^2 \left(a + \frac{1}{l \tan(la)} \right) = 1 \quad \Rightarrow \quad |D|^2 \left(a + \frac{1}{K} \right) = 1$$

$$\boxed{D = \frac{1}{\sqrt{a + 1/K}}}$$

$$\boxed{F = \frac{e^{Ka} \cos(la)}{\sqrt{a + 1/K}}}$$

⇝ Scattering States $(E>0)$

we don't use symmetry anymore

scattering problem is intrinsically asymmetric

waves come from one side only

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

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

$$\psi(x) = \underbrace{Ae^{ikx}}_{\text{comes from } -\infty} + \underbrace{Be^{-ikx}}_{\text{reflected to } -\infty}$$

- $-a < x < a$

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

$$\psi(x) = C\sin(\ell x) + D\cos(\ell x)$$

- $x > a$

there is no incoming wave, only transmission

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

$$\begin{cases} A \rightarrow \text{amplitude of the incident wave} \\ B \rightarrow \text{amplitude of the reflected wave} \\ F \rightarrow \text{amplitude of the transmitted wave} \end{cases}$$

$$R = \frac{|B|^2}{|A|^2}$$ reflection coefficient
(prob that an incident particle is reflected)

$$T = \frac{|F|^2}{|A|^2}$$ transmission coefficient
(prob of transmission)

$$\boxed{R + T = 1}$$

boundary conditions

at $x = -a$
$$\begin{cases} Ae^{-ika} + Be^{+ika} = -C\sin(la) + D\cos(la) \\ ik\left(Ae^{-ika} - Be^{ika}\right) = l\left(C\cos(la) + D\sin(la)\right) \end{cases}$$

at $x = a$
$$\begin{cases} C\sin(la) + D\cos(la) = Fe^{ika} \\ l\left(C\cos(la) - D\sin(la)\right) = ikFe^{ika} \end{cases}$$

$$T = \frac{|F|^2}{|A|^2}$$

$$T = \frac{(2kl)^2}{\cos^2(2la)\,(2kl)^2 + (k^2+l^2)^2\sin^2(2la)}$$

$$T = \frac{(2kl)^2}{(2kl)^2 + (k^2-l^2)^2\sin^2(2la)}$$

$T = 1$ when $\underline{2la = n\pi}$

$$B = i\,\frac{\sin(2la)}{2kl}\,(l^2 - k^2)\,F$$

$$F = \frac{e^{-2ika}\,A}{\cos(2la) - i\,\frac{(k^2+l^2)}{2kl}\sin(2la)}$$

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

$$= \frac{+\sin^2(2la)\,(l^4 - 2l^2k^2 + k^4) + (2kl)^2}{(2kl)^2\cos^2(2la) + \sin^2(2la)\,(k^4 + 2l^2k^2 + l^4)} = \frac{+\overbrace{(l^4 - 2l^2k^2 + k^4) + (2kl)^2}^{2l^2k^2} - \cos^2(2la)\,(l^4 - 2l^2k^2 + k^4)}{+(l^4 + 2l^2k^2 + k^4) - \cos^2(2la)\left[k^4 + \underbrace{2l^2k^2 + l^4 - (2kl)^2}_{-2l^2k^2}\right]}$$

$$= \boxed{1}$$