

② Region I ($0 < x < L$)

Since $U(x) = 0$ here,

the time-independent Schrödinger eq

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

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

for convenience, let's make the following definition.

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

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

Solution: $\psi(x) = A \sin kx$ & $\psi(x) = B \cos kx$

$$\Rightarrow \psi(x) = A \sin kx + B \cos kx$$

General solution for region I

$$\frac{2m \cdot \frac{1}{2} \hbar^2 k^2}{\hbar^2} = \frac{m \hbar^2 k^2}{\hbar^2}$$

$$p = \hbar k$$

$$k = \frac{p}{\hbar}$$

③ Region II ($x < 0$)

Here, $U(x) = U_0$,

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi(x)}{dx^2} + U_0 \psi(x) = E \psi(x)$$

$$\rightarrow \frac{d^2 \psi(x)}{dx^2} = \frac{2m(U_0 - E)}{\hbar^2} \psi(x), \quad \alpha = \sqrt{\frac{2m(U_0 - E)}{\hbar^2}}$$

$$\rightarrow \frac{d^2 \psi(x)}{dx^2} = \alpha^2 \psi(x)$$

A pair of independent solutions?

$$\psi(x) = ce^{+\alpha x}, \quad \psi(x) = de^{-\alpha x}$$

and the general solution is the sum

$$\psi(x) = ce^{+\alpha x} + de^{-\alpha x}$$

diverges as $x \rightarrow -\infty$
i.e. mathematically
but physically
unacceptable
so $D = 0$

③ Region II ($x > L$)

Same as Region I (since $u(x)$ is the same)

$$\psi(x) = F e^{+ax} + G e^{-ax}$$

must be "zero"

$$x \rightarrow \pm \infty$$

$$\psi \rightarrow 0$$

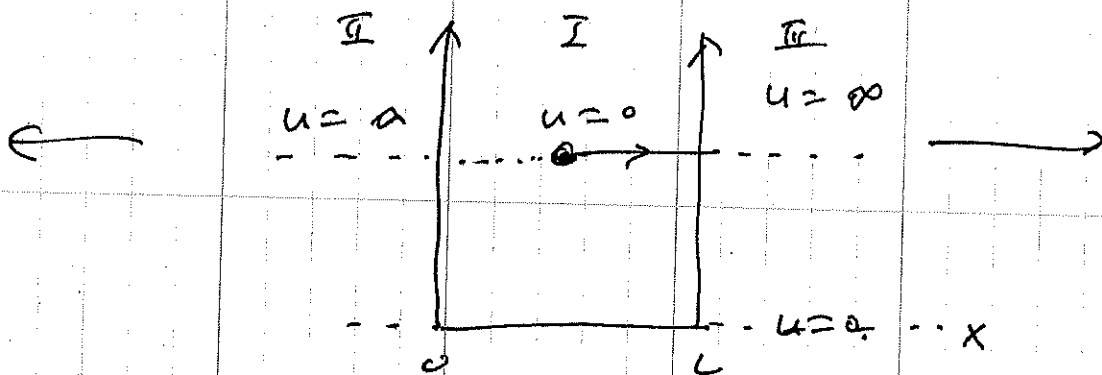
$$\Rightarrow F = 0 = G$$

$$\psi(x) = \begin{cases} C e^{+ax} & x < 0 \\ A \sin kx + B \cos kx & 0 < x < L \\ G e^{-ax} & x > L \end{cases}$$

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

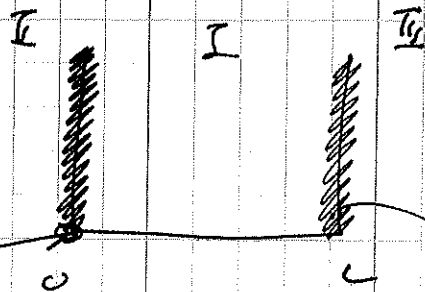
$$L = \sqrt{\frac{2m(U_0 - E)}{\hbar^2}}$$

** p.t.l in a Box: The Infinite Well



$$\psi(x) = \begin{cases} A \sin kx + B \cos kx & 0 < x < L \\ 0 & x < 0, x > L \end{cases}$$

$A = ?$
 $B = ?$



If wave f.t is to be continuous,
its pieces must have the same value @ $x=0$,

$$\psi_{II}(0) = \psi_I(0)$$

or

using $\psi(x) = A \sin kx + B \cos kx$

$$\Rightarrow \psi = \underbrace{A \sin kx}_{\substack{\uparrow \\ \text{must be 0}}} + \underbrace{B \cos kx}_{\substack{\uparrow \\ \text{must be 0}}} \rightarrow \textcircled{!} B = 0$$

now $x=L$,

$$\psi_I(L) = \psi_{III}(L)$$

or

$$\psi(x) = A \sin kx + B \cos kx$$

$$0 = A \sin kL$$

B is already zero
now forget about B here

① The only the wave f.t can be continuous is if the following condition hold:

$$kL = n\pi$$

②

$$\sqrt{\frac{2mE}{\hbar^2}} L = n\pi \Rightarrow E = \frac{\hbar^2 \pi^2 n^2}{2mL^2}$$

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

$$\psi_n(x) = A \sin \frac{n\pi}{L} x \quad (0 < x < L)$$

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2} \leftarrow \text{only certain } E\text{-levels are allowed!!}$$

★★ The wave f.t is a typical standing-wave form!!
QMally, bound states are standing wave!!

Thus, we have the normalized, continuous W.f representing the allowed states of p.tl in an infinite well and their corresponding E_n !!

$$\psi_n(x) = \begin{cases} \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L} & 0 < x < L \\ 0 & x < 0, x > L \end{cases}$$

A we will see this soon

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2}$$

A = ?

★ Normalization of $\psi(x, t)$

$$\int_{\text{all space}} |\psi(x, t)|^2 dx = 1$$

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

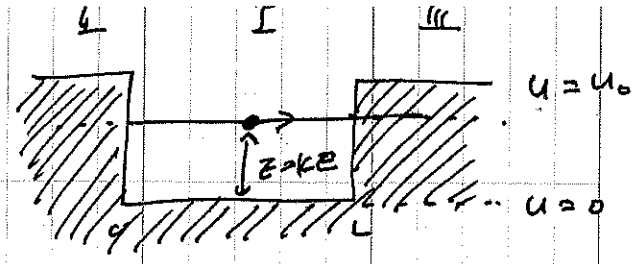
See Appendix C-5

$$\frac{x}{2} - \frac{L}{4n\pi} \sin \left(\frac{2n\pi x}{L} \right) \Big|_0^L$$

$$\int_{\text{all space}} |\psi(x, t)|^2 dx = \int_{-\infty}^{\infty} |\psi(x)|^2 dx = \int_0^L \left(A \sin \frac{n\pi}{L} x \right)^2 dx = 1$$

$$\therefore A^2 \frac{L}{2} = 1 \rightarrow A = \sqrt{\frac{2}{L}}$$

Finite Potential Well



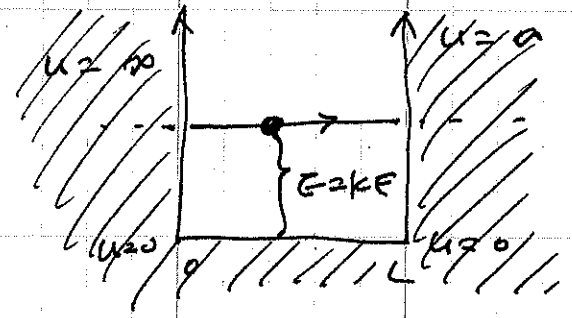
$$\psi(x) = \begin{cases} \psi_{II}(x) & x < 0 \\ A \sin kx + B \cos kx & 0 < x < L \\ \psi_{III}(x) & x > L \end{cases}$$

$$\psi_{II}(x) = Ce^{+kx}$$

$$\psi_{III}(x) = Ge^{-dx}$$

where $k \equiv \sqrt{\frac{2mE}{\hbar^2}}$, $d \equiv \sqrt{\frac{2m(U_0 - E)}{\hbar^2}}$

Infinite Potential Well



$$\psi_n(x) = \begin{cases} \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L} & 0 < x < L \\ 0 & x < 0, x > L \end{cases}$$

$$E_n(x) = \frac{n^2 \pi^2 \hbar^2}{2m L^2}$$

DON'T!!

Back to Finite Potential Well problem.

A, B, C, G, E?

Let's look at "Continuity" at $x=0$ and $x=L$

$\Rightarrow \psi(x)$ continuous @ $x=0$: $\psi_{II}(0) = \psi_I(0)$

(i) $Ce^{+kx} = A \sin kx + B \cos kx \Rightarrow C = B$

$\Rightarrow \frac{\partial \psi(x)}{\partial x}$ continuous @ $x=0$: $\frac{\partial \psi_{II}}{\partial x} \Big|_{x=0} = \frac{\partial \psi_I}{\partial x} \Big|_{x=0}$

(ii) $dCe^{+dx} = kA \cos kx - kB \sin kx \Rightarrow dC = kA$

→ $\psi(x)$ continuous @ $x=L$: $\psi_I(L) = \psi_{II}(L)$

$$A \sin kL + B \cos kL = G e^{-\alpha L}$$

→ $\frac{\partial \psi(x)}{\partial x}$ continuous @ $x=L$: $\left. \frac{\partial \psi_I}{\partial x} \right|_{x=L} = \left. \frac{\partial \psi_{II}}{\partial x} \right|_{x=L}$

$$kA \cos kL - kB \sin kL = -\alpha G e^{-\alpha L}$$

we know two things:

$$\begin{cases} G = B \\ \alpha G = kA \end{cases} \rightarrow A = \frac{\alpha C}{k}$$

$$\frac{\alpha}{k} C \sin kL + C \cos kL = G e^{-\alpha L} \quad \text{--- ①}$$

$$\left(k \frac{\alpha C}{k} \cos kL - k C \sin kL \right) = (-\alpha G e^{-\alpha L}) \quad \text{--- ②}$$

to make equal b/w ①-②

$$\frac{\alpha}{k} \cancel{C} \sin kL + \cancel{C} \cos kL = -\cancel{C} \cos kL + \frac{k}{\alpha} \cancel{C} \sin kL$$

$$\frac{\alpha}{k} \sin kL + \cos kL = -\cos kL + \frac{k}{\alpha} \sin kL$$

$$\cancel{\frac{k}{\alpha}} \left(\frac{k}{\alpha} - \frac{\alpha}{k} \right) \sin kL$$

$$= \cos kL + \cos kL$$

(= 2 cos kL)

$$\left(\frac{k}{\alpha} - \frac{\alpha}{k} \right) = \frac{2 \cos kL}{\sin kL} \quad \text{Bsp.}$$

$$= 2 \cot kL$$

$$2 \cot kL = \frac{k}{\alpha} - \frac{\alpha}{k}$$

Transcendental Eq.

impossible to solve analytically !!

numerical solution is possible

⇒ e.g. graphing solution !!

$$2 \cot KL = \frac{k}{d} - \frac{d}{k}$$

$$\cos \theta = \cos^2\left(\frac{\theta}{2}\right) - \sin^2\left(\frac{\theta}{2}\right)$$

$$\sin \theta = 2 \sin\left(\frac{\theta}{2}\right) \cos\left(\frac{\theta}{2}\right)$$

~~sec~~ / secant
 $\sec x = \frac{1}{\cos x}$
 $\csc x = \frac{1}{\sin x}$
 cosecant

$$2 \cot KL = 2 \cdot \frac{\cos KL}{\sin KL} = 2 \cdot \frac{\cos^2\left(\frac{KL}{2}\right) - \sin^2\left(\frac{KL}{2}\right)}{2 \sin\left(\frac{KL}{2}\right) \cos\left(\frac{KL}{2}\right)}$$

$$\left(\cot\left(\frac{KL}{2}\right) - \tan\left(\frac{KL}{2}\right)\right) = \frac{k}{d} - \frac{d}{k}$$

Multiplying by dk

$$dk \left(\cot\left(\frac{KL}{2}\right) - \tan\left(\frac{KL}{2}\right)\right) = dk \left(\frac{k}{d} - \frac{d}{k}\right)$$

$$= k^2 - d^2$$

$$d^2 + dk \left(\cot\left(\frac{KL}{2}\right) - \tan\left(\frac{KL}{2}\right)\right) - k^2 = 0$$

Factoring, $(d + k \cot\left(\frac{KL}{2}\right)) (d - k \tan\left(\frac{KL}{2}\right)) = 0$

$$\rightarrow d = -k \cot\left(\frac{KL}{2}\right) \text{ or } k \tan\left(\frac{KL}{2}\right)$$

~~we have to be a solution~~

~~we have to be a solution~~

$$d = \frac{\sqrt{2m(U_0 - E)}}{\hbar}, \quad k = \frac{\sqrt{2mE}}{\hbar}$$

$$d = -k \cot\left(\frac{KL}{2}\right)$$

$$\frac{\sqrt{2m(U_0 - E)}}{\hbar} = -\frac{\sqrt{2mE}}{\hbar} \cot\left(\frac{KL}{2}\right)$$

$$U_0 - E = E \cot^2\left(\frac{KL}{2}\right)$$

$$U_0 = E \left(\cot^2\left(\frac{KL}{2}\right) + 1\right) = E \csc^2\left(\frac{KL}{2}\right)$$

$$d = +k \tan\left(\frac{KL}{2}\right) \Rightarrow \frac{\sqrt{2m(U_0 - E)}}{\hbar} = \frac{\sqrt{2mE}}{\hbar} \tan\left(\frac{KL}{2}\right)$$

$$U_0 - E = E \tan^2\left(\frac{KL}{2}\right)$$

$$U_0 = E \left(\tan^2\left(\frac{KL}{2}\right) + 1\right) = E \sec^2\left(\frac{KL}{2}\right)$$

Replacing E w/ $\frac{\hbar^2 k^2}{2m}$

become (5-23)

$$U_0 = \begin{cases} \frac{\hbar^2 k^2}{2m} \sec^2 \frac{KL}{2} \\ \frac{\hbar^2 k^2}{2m} \csc^2 \frac{KL}{2} \end{cases}$$

$n=1, 3, 5, \dots$
 $(n-1)\pi < KL < n\pi$
 $n=2, 4, 6, \dots$
 $(n-1)\pi < KL < n\pi$

* Graphing Solution

$$2 \cot kL = \frac{k}{a} - \frac{1}{k}$$



Volunteer work

$$a = \begin{cases} k \tan \frac{1}{2} kL \\ -k \cot \frac{1}{2} kL \end{cases}$$

$$2n\pi < kL < 2n\pi + \pi$$

$$2n\pi - \pi < kL < 2n\pi$$

$$\sqrt{\frac{2m(U_0 - E)}{\hbar^2}}$$

$$U_0 = \begin{cases} \frac{\hbar^2 k^2}{2m} \sec^2 \frac{1}{2} kL \\ \frac{\hbar^2 k^2}{2m} \csc^2 \frac{1}{2} kL \end{cases}$$

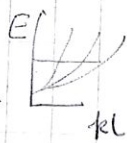
$$(n-1)\pi < kL < n\pi \quad n=1, 3, 5, \dots$$

$$(n-1)\pi < kL < n\pi \quad n=2, 4, 6, \dots$$

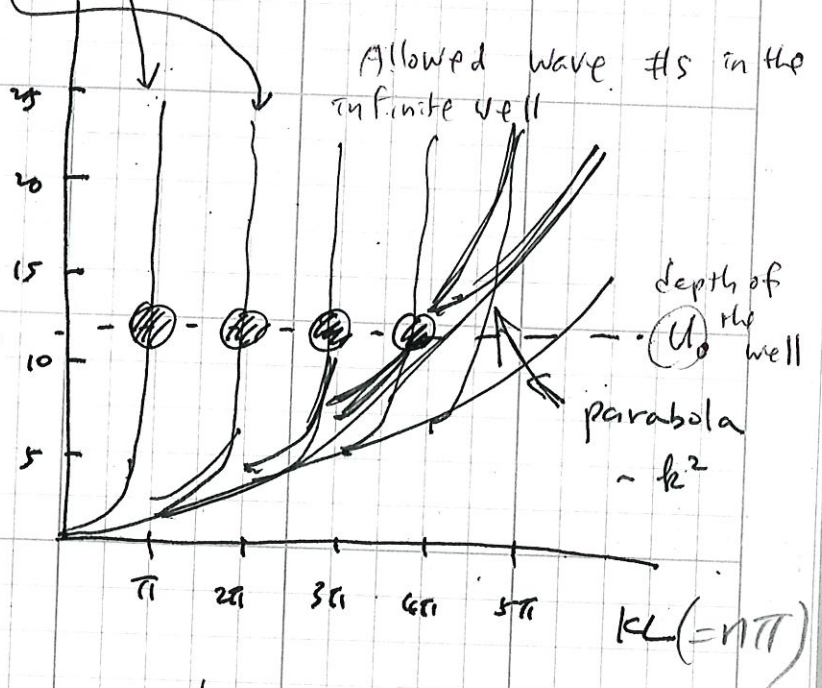
$$U_0 = E \sec^2 \frac{kL}{2}$$

$$E = \frac{U_0}{\sec^2 \frac{kL}{2}}$$

$$E = \frac{U_0}{\sec^2 \frac{kL}{2}}$$



$$E_n = \left(\frac{\pi^2 \hbar^2}{2mL^2} \right) n^2$$



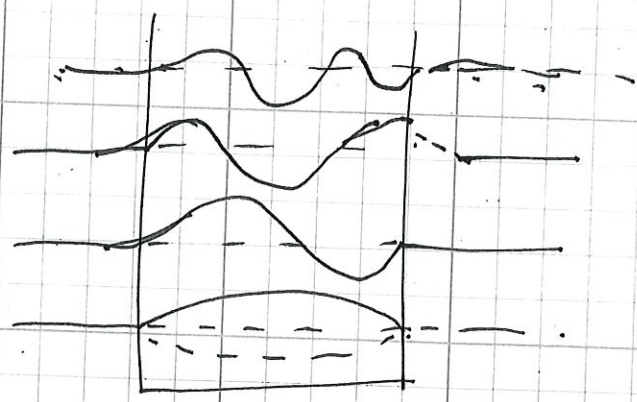
Finite Well			Infinite Well	
$U_0 = 12 \frac{\pi^2 \hbar^2}{2mL^2}$			$U_0 = \infty$	
n	k^*	E	k^*	E
1	↓	↓	↓	↓
2	↓	↓	↓	↓
3	↓	↓	↓	↓
4	↓	↓	↓	↓

$$E = \frac{\hbar^2 k^2}{2m}$$

$$E = \left(\frac{\pi^2 \hbar^2}{2mL^2} \right) n^2$$

$$kL = n\pi$$

$$= 0, \pi, 2\pi, 3\pi, \dots$$



$$2 \cot kL = \frac{k}{\alpha} - \frac{\alpha}{k}$$

$$k \equiv \sqrt{\frac{2mE}{\hbar^2}}$$

$$\alpha \equiv \sqrt{\frac{2m(U_0 - E)}{\hbar^2}}$$

$$\text{limit } U_0 \rightarrow \infty \Rightarrow \alpha \rightarrow \infty$$

$$\text{then } 2 \cot kL = \frac{k}{\alpha} - \frac{\alpha}{k} \text{ becomes } \cot kL = -\alpha$$

this requires

$$kL = n\pi$$

Same as

infinite

well condition.

$\Rightarrow$ the infinite well is indeed a limiting case of the finite well. ($U_0 \rightarrow \infty$)

