Lecture 10: 1-D Bound States

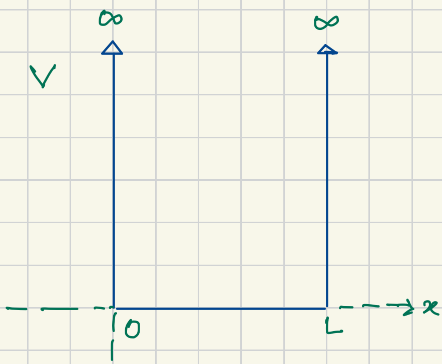
Ex. 10.1 Particle in a Box: 1-dim. Infinite Walls

Given $V(x) = 0, \quad 0 < x < L$

$\quad\quad\quad\;\; = \infty, \quad$ elsewhere

Infinite Potential Well (IPW)

Find p, E and $\psi(x)$ for all possible states.



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

Region I and III (i.e. $|x| > L$) $\psi = 0$

Region II:

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

$$\Rightarrow \frac{d^2\psi}{dx^2} + k^2\psi = 0, \quad k^2 \equiv \frac{2mE}{\hbar^2}$$

General Sol$^{\underline{n}}$: $\psi(x) = A' e^{ikx} + B' e^{-ikx}$.

or, $\psi(x) = A\sin(kx) + B\cos(kx)$ — (1)

Boundary Conditions:

$$\psi(0) = 0 \qquad —(2)$$
$$\psi(L) = 0 \qquad —(3)$$

Putting (2) i.e. $\psi(0) = 0$ in (1)

$$\psi(0) = A \sin(k \cdot 0) + B \cos(k \cdot 0) = 0$$

$$\Rightarrow \quad B = 0$$

Slly $\psi(L) = 0 \quad \Rightarrow \quad A \sin(kL) = 0$

$$\Rightarrow \quad kL = n\pi, \quad n = 1, 2, 3, \ldots$$

$$P_n = \hbar k_n, \qquad E_n = \frac{\hbar^2 k_n^2}{2m}, \quad k_n = \frac{\pi}{L} \cdot n$$

$$\therefore \; E_n = \frac{\hbar^2 \left(\frac{\pi}{L}\right)^2 \cdot n^2}{2m} =$$

$$\boxed{E_n = \frac{\hbar^2 \pi^2}{2mL^2} \cdot n^2, \qquad n = 1, 2, 3, \ldots}$$

- Energy is Quantized.
- Energy spectrum is discrete.
- Bound states.
- $E_n \propto n^2$ (spacing increases with $n\uparrow$)

L10: (3/13) ynm

Find $\psi(x)$. $\quad k_n = \frac{\pi}{L}\cdot n.$

$$\psi(x) \begin{cases} = A \sin\left(\frac{n\pi}{L}x\right), & 0 < x < L \\ = 0 , & \text{elsewhere.} \end{cases}$$

Need to normalize A.

$$\int_{-\infty}^{\infty} \psi^* \psi \, dx = 1$$

$$\Rightarrow A^2 \int_0^L \sin^2\left(\frac{n\pi}{L}x\right) dx = 1$$

$$\int \sin^2(ax)\, dx = \frac{x}{2} - \frac{\sin 2ax}{4a} + c$$

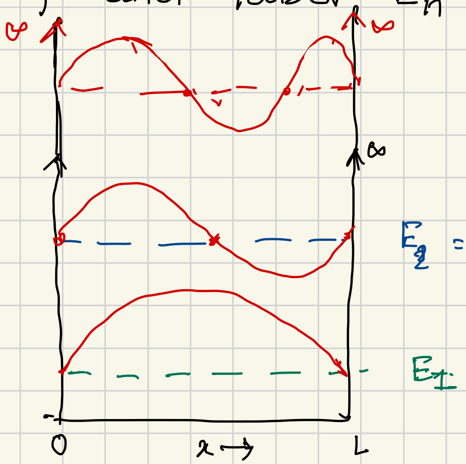
$$\boxed{E_n = \frac{h^2}{8mL^2} n^2}$$

$$\Rightarrow A = \sqrt{\frac{2}{L}}$$

$$\boxed{\psi(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right), \quad n = 1, 2, 3, \ldots}$$

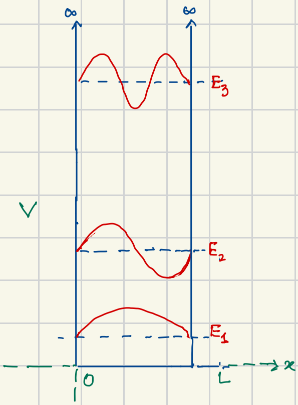
- Sketch $\psi(x)$ and label $E_n = E_1 n^2$

Prob. $|\psi(x)|^2$



L10: 4/13 ynm

Notice:



1. Bound States
2. Zero Energy not possible. Ground state $E_1 = \frac{\hbar^2}{2m}\left(\frac{\pi}{L}\right)^2$
3. $\psi_n(x)$ has $(n-1)$ nodes
4. Symmetry: $\left.\begin{array}{l}\psi_{2n}(x) \text{ are ODD} \\ \psi_{2n+1}(x) \text{ are EVEN}\end{array}\right\}$ wrt $x = \frac{L}{2}$.
5. For each n, there is a unique state with E_n. i.e. the states are non-degenerate.

(Recall for PoR example, each n was two-fold degenerate $k_n = \pm\sqrt{\frac{2mE_n}{\hbar^2}}$.)

These are stationary states with $E_n = n^2 E_1$

$$\Psi(x,t) = \sum_{n=1}^{\infty} \psi_n(x)\, e^{-i\frac{E_n}{\hbar}t}$$

$$= \sqrt{\frac{2}{L}} \sum_{n=1}^{\infty} \sin\left(\frac{n\pi}{L}x\right) e^{-i\frac{E_1}{\hbar}n^2 t}$$

Most General Solution.

Zero Point Energy:

Classically the particle can be at rest – NOT so quantum mechanically!

HUP: $\left.\begin{array}{l}\Delta x \sim L \\ \Delta p \sim \frac{\hbar}{L}\end{array}\right\} \Rightarrow E_{min} \sim \frac{\Delta p^2}{2m} \sim \frac{\hbar^2}{2mL^2}$

Significance of 'Particle in Box' Model

Simple yet powerful illustrator of QM.
Especially, relation between degree of confinement & Quantization.

- What happens if L is changed?

$L \uparrow \quad E_n \downarrow$

$L \to \infty$ Classical Regime

- $$\psi_n = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L} x\right) \quad , \quad n = 1, 2, 3, \ldots\ldots$$

Notice: $\int \psi_n^* \psi_m \, dx = \delta_{nm}$

Krönecker Delta

$$\delta_{nm} = \begin{cases} 0, & n \neq m \\ 1, & n = m \end{cases}$$

Indeed a special case of

$$\frac{1}{L} \int_0^L e^{ikx} e^{-ik'x} \, dx = \delta(k - k')$$

- Orthogonality of a set of basis functions.

- Fourier Expansion of any ψ can be done with this set.

  This infinite set is <u>COMPLETE</u>.

- Are the solutions progressive waves?

  Find $\langle \hat{p} \rangle$ for $|n\rangle$.

- Suppose we had chosen the walls at $x = -\frac{L}{2}$ and $x = \frac{L}{2}$.

What would solutions look like?
Sketch will not change, but math form will. (Physics does not change with choice of origin.)

Full symmetry (or, parity) is revealed.

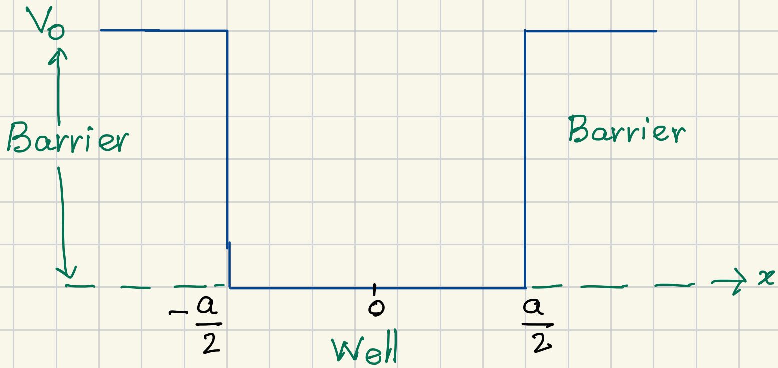
$\psi(-x) = \psi(x)$ Even Sol$^{\underline{n}}$.

$\psi(-x) = -\psi(x)$ Odd Sol$^{\underline{n}}$.

Ex. 10.2

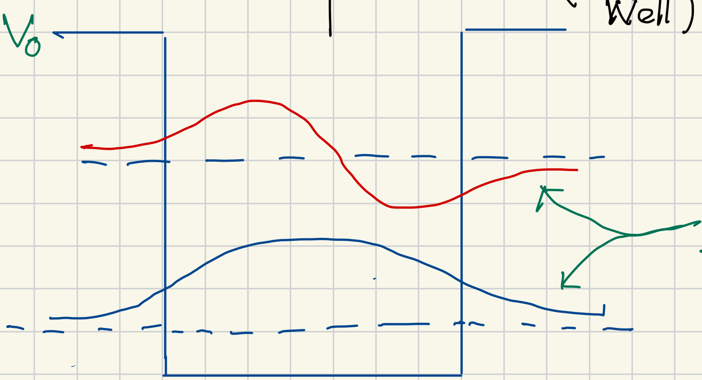
Finite Barrier 1-D Particle in a Box

Finite Potential Well (FPW)



$$V(x) = \begin{cases} 0 & |x| \leq \frac{a}{2} \\ V_0 & |x| \geq \frac{a}{2} \end{cases}$$

- What are our expectations (ref. 1-D Infinite Pot. Well) ?



Surprise! Surprise!!

classically not allowed here unless $E > V_0$.

Oscillatory inside & decaying exponential outside.

Correct slope & curvature!

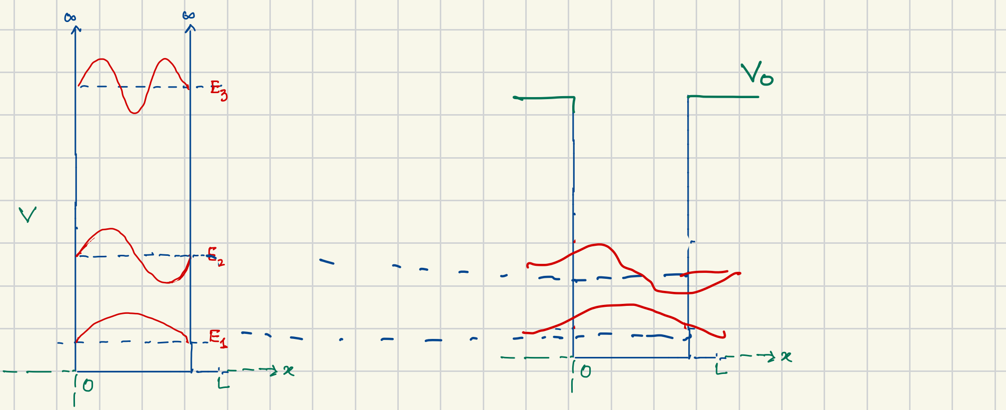
1. $\psi'' \propto \psi$
2. ψ is continuous
3. ψ' is continuous
4. $\psi(\infty) \to 0$
5. $\psi(-\infty) \to 0$

$$\frac{d^2\psi}{dx^2} = \underbrace{-\left[\frac{2m(E-V)}{\hbar^2}\right]}_{\text{sign of this quantity determines the nature of solution.}} \psi$$

$$\boxed{-\frac{2m}{\hbar^2}(E-V)}$$

proportionaity term

Region I and III Barrier Region	Region II
$E < V$, $\Rightarrow$ positive say, α^2 $\Downarrow$ decaying real exponentials $e^{-\alpha\lvert x\rvert}$	$V = 0$ negative $\Downarrow$ oscillatory (imaginary exponentials) e^{ikx}



Note: At the interface, slopes must match and curvature must be proportional to ψ at that point

Qualitative discussion:

Suppose the potential barrier was finite V_0, What changes would you expect in the previous solutions to our 1-D Infinite box?

- Energy E_n:

  $E_n' < E_n$

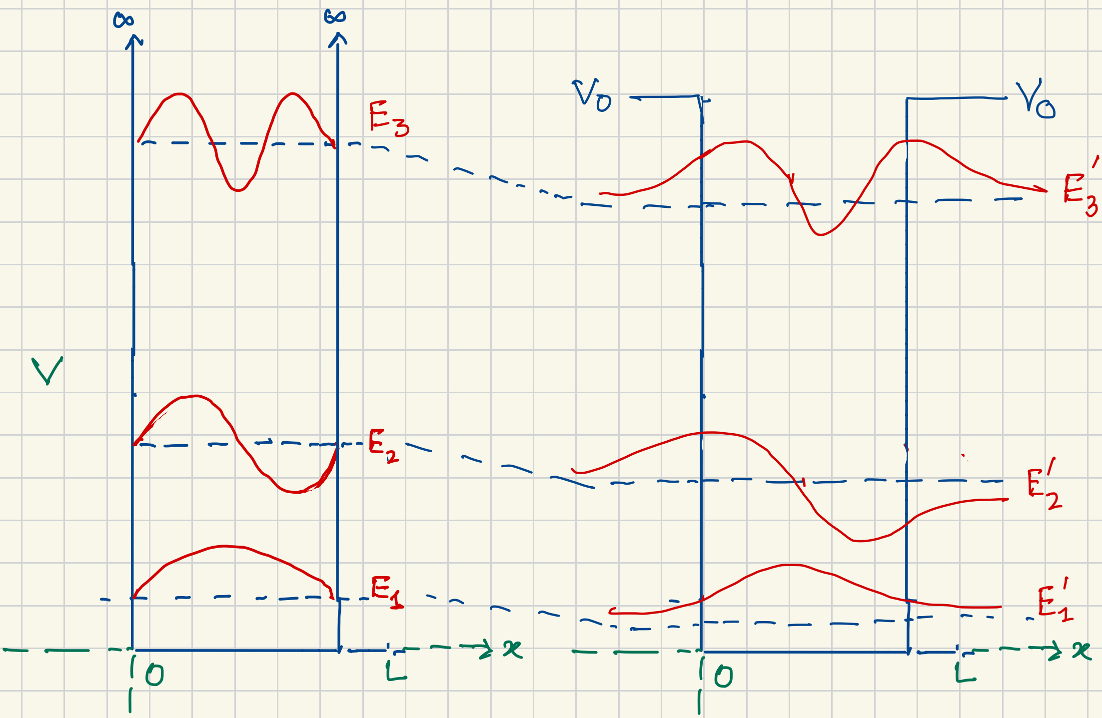
  finite V   Infinite V

General Moral:

More Confined, $E_n \uparrow$

Less Confined $\rightarrow$ classical

- Nature of $\psi(x)$:



$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x)\right]\psi = E\psi$$

$E < V_0$ OUTSIDE THE WELL

$$\psi(x) = \begin{cases} A\, e^{-\alpha\left(x-\frac{a}{2}\right)}, & x \geq \frac{a}{2} \\ B\, e^{\alpha\left(x+\frac{a}{2}\right)}, & x \leq -\frac{a}{2} \end{cases}$$

$$\alpha = \sqrt{\frac{2m(V-E)}{\hbar^2}}$$

INSIDE THE WELL

$$\psi(x) = C\cos(kx) + D\sin(kx), \quad |x| \leq \frac{a}{2}$$

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

MATCH ψ and ψ' at $\pm\frac{a}{2}$

$$C\cos\left(\frac{ka}{2}\right) = A \quad \& \quad Ck\sin\left(\frac{ka}{2}\right) = A\alpha$$

$$\Rightarrow \boxed{\tan\left(\frac{ka}{2}\right) = \frac{\alpha}{k}}$$

EVEN solutions.

Similarly Odd solutions

$$\boxed{\cot\left(\frac{ka}{2}\right) = -\frac{\alpha}{k}}$$

OR,

$$k\begin{cases}-\tan \\ \cot\end{cases}\left(\frac{ka}{2}\right) = -\alpha$$

For convenience, define $k_0 = \sqrt{\frac{2mV_0}{\hbar^2}}$

$$\cos\left(\frac{ka}{2}\right) = \pm\frac{k}{k_0}, \quad \text{for } \tan\left(\frac{ka}{2}\right) > 0$$

$$\sin\left(\frac{ka}{2}\right) = \pm\frac{k}{k_0}, \quad \text{for } \cot\left(\frac{ka}{2}\right) < 0$$

Even Sol$\underline{^n}$: $+, -$ chosen when $\cos\left(\frac{ka}{2}\right)$ is $+$ or $-$.

Odd Sol$\underline{^n}$; $+ -$ chosen when $\sin\left(\frac{ka}{2}\right)$ is $+$ $-$.

Effectively we are matching $\boxed{\frac{1}{\psi}\frac{d\psi}{dx} = \frac{d}{dx}\ln\psi}$

in which normalization cancels.

$$\tan\left(\frac{ka}{2}\right) = \frac{\alpha}{k}$$

$$\cot\left(\frac{ka}{2}\right) = -\frac{\alpha}{k}$$

$$\frac{\alpha}{k} = \frac{1}{k}\sqrt{\frac{2m}{\hbar^2}(V_0-E)}$$

$$= \sqrt{\frac{2mV_0}{\hbar^2 k^2} - 1}$$

Rewrite as

$$\boxed{\begin{matrix} \tan\left(\frac{ka}{2}\right) \\ -\cot\left(\frac{ka}{2}\right) \end{matrix} = \frac{\alpha}{k} = \sqrt{\frac{2mV_0}{\hbar^2 k_0^2} - 1}}$$

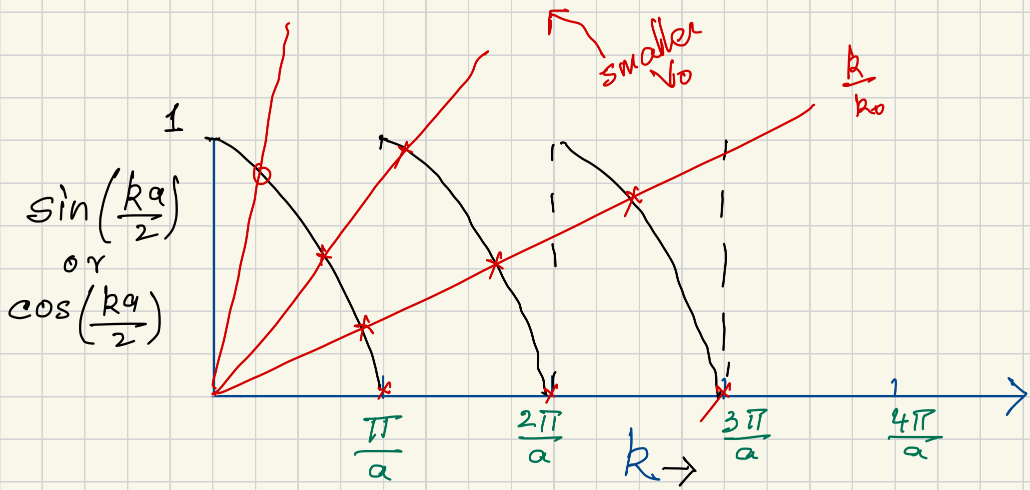
These are TRANSCENDENTAL Equations.
Need to solve graphically or numerically.

For convenience, define $k_0 = \sqrt{\dfrac{2mV_0}{\hbar^2}}$

$$\cos\left(\frac{ka}{2}\right) = \pm \frac{k}{k_0}, \quad \text{for } \tan\left(\frac{ka}{2}\right) > 0$$

$$\sin\left(\frac{ka}{2}\right) = \pm \frac{k}{k_0}, \quad \text{for } \cot\left(\frac{ka}{2}\right) < 0$$

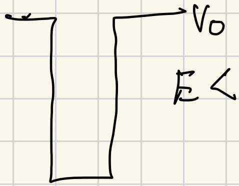
This sets the scale in the problem. → $k_0 = \sqrt{\dfrac{2mV_0}{\hbar^2}}$



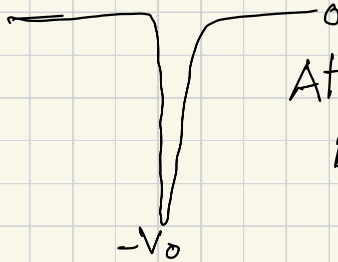
- $V_0 \downarrow$ larger is the slope, less interaction with curves, hence less number of bound states.
- $k_0 \to \infty$, i.e. $V_0 \to \infty$, Infinite number of bound states at $k = \frac{\pi}{a} \cdot n$ (Recovering Infinite Potential Well results.
- There is always ONE bound state! Prove.

Potential Wells, $E < V$, Bound States

Examples:



$E < V$,



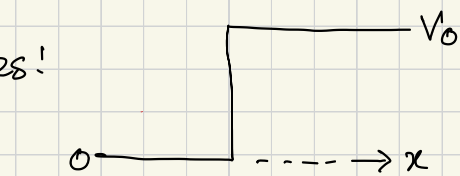
Attractive $\delta(x)$

$E < 0$

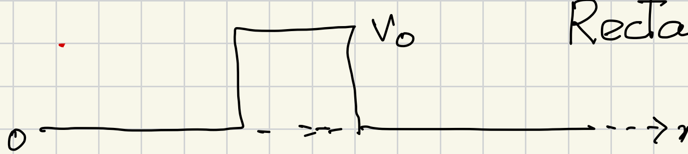
Potential Barriers, or, $E > V$, Scattering states.

(We will study them with care later.)

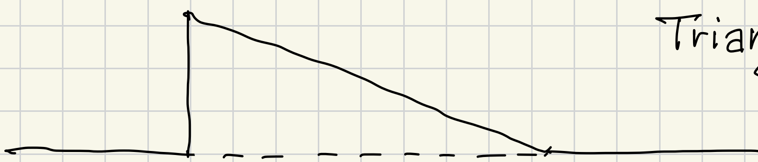
Examples:



Step potential barrier.



Rectangular Barrier.



Triangular

$V_0 a = \text{constant}$ δ- barrier.

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