Lecture 7 – Particle in an infinite Square Well potential

Wednesday, September 6, 2023 2:29 PM

1. Warm-up Quiz
2. HW3 due Friday (problems 1–5 only; prob 6 moved to HW4)
3. Today: • Consequences of TISE
   • Particle in a box

$$\int_{-\infty}^{\infty} P(x)\,dx = 1 \qquad \int_0^{\pi} A\sin(x)\,dx = 1$$

Last Time:

$$i\hbar\frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V\Psi$$

$$\Psi(x,t) = \psi(x)\phi(t) \quad \text{in } V \text{ time indep.}$$

$$\boxed{-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V\psi = E\psi} \qquad \text{TISE}$$

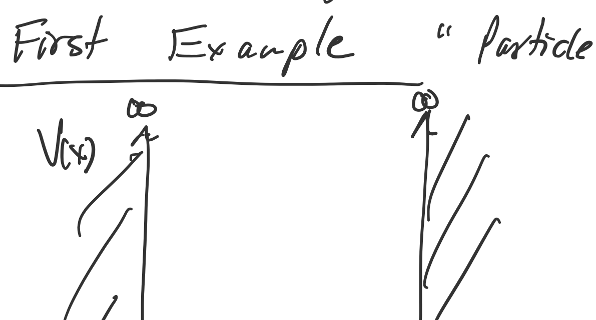
$$\boxed{\frac{\partial\phi}{\partial t} = \frac{-iE}{\hbar}\phi} \qquad \text{Time dependance}$$

simple solⁿ $\boxed{\phi(t) = e^{-iEt/\hbar}}$ phase evolution of wavefunction

Key Points:

- Total solⁿ $\Psi(x,t) = \psi(x)e^{-iEt/\hbar}$
  reduces main challenge to finding $\psi(x)$, E
  $$\hat{H}\psi = E\psi$$
- $\psi(x)$ are eigenfunctions of $\hat{H}$ (stationary states)
- E are the eigenvalues (may be quantized)
- There can be more than one ψ for each E
  $\Rightarrow$ degenerate solutions
- In general ψ are complex; $|\psi|^2$ is real

First Example "Particle in a box" – 1D infinite square well potential



$V = 0 \quad 0 < x < L$
$V = \infty \quad x \geq L$ or $x \leq 0$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \underbrace{V\psi}_{=0 \text{ inside box}} = E\psi$$

ψ cannot penetrate an ∞ potential $\left.\begin{array}{l}\psi(x \leq 0) = 0\\ \psi(x \geq L) = 0\end{array}\right\}$ b.c.

for $0 \leq x \leq L$

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

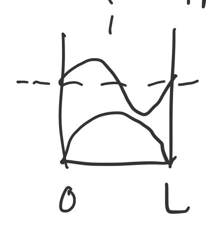
$$\boxed{k = \sqrt{\frac{2mE}{\hbar^2}}}$$

General Solⁿ

$$\psi(x) = A\sin(kx) + B\cos(kx)$$
$$\text{or } = A'e^{ikx} + B'e^{-ikx}$$

Solⁿ depends on if $E > 0$ or < 0

Suppose $E > 0 \Rightarrow$ 2 derivatives return $\psi \times$ negative const



Apply Boundary Conditions $\psi(x=0) = 0 \Rightarrow B = 0$

$$\psi(L) = 0 \Rightarrow \sin(k\cdot L) = 0 \Rightarrow kL = n\pi,\ n = 1, 2, \ldots$$

$$\therefore\ k_n = \frac{n\pi}{L} = \sqrt{\frac{2mE}{\hbar^2}}$$

$$\text{So } E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2}{2m}\left(\frac{n\pi}{L}\right)^2 = \frac{\pi^2\hbar^2 n^2}{2mL^2}$$

$$E_n = \frac{hn^2}{8mL^2}$$

- Only discrete energies are allowed.
  $\Rightarrow$ Comes from boundary Condition

Energy eigenstates $\psi_n(x) = A\sin\left(\frac{n\pi x}{L}\right)$

Need to find A such that

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1 \Rightarrow A = \sqrt{\frac{2}{L}}$$

Total wavefunction:

$$\Psi_n(x,t) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)e^{-iE_n t/\hbar}$$

On your own $\Rightarrow$ show this has the form of a plane wave

$$\Psi_n \rightarrow e^{\pm i(kx \mp \omega t)}$$

Go back: what about $E < 0$ solutions?

$$\cancel{+}\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = \cancel{+}|E|\psi \rightarrow \frac{d^2\psi}{dx^2} = \frac{2m|E|}{\hbar^2}\psi$$

$$\psi(x) = Ae^{\varkappa x} + Be^{-\varkappa x} \qquad \varkappa = \sqrt{\frac{2m|E|}{\hbar^2}}$$

@ Boundaries $\psi(x=0) = 0 \Rightarrow A + B = 0 \Rightarrow B = -A$

$$\psi(x=L) = 0 \Rightarrow A(e^{\varkappa L} - e^{-\varkappa L}) = 0$$

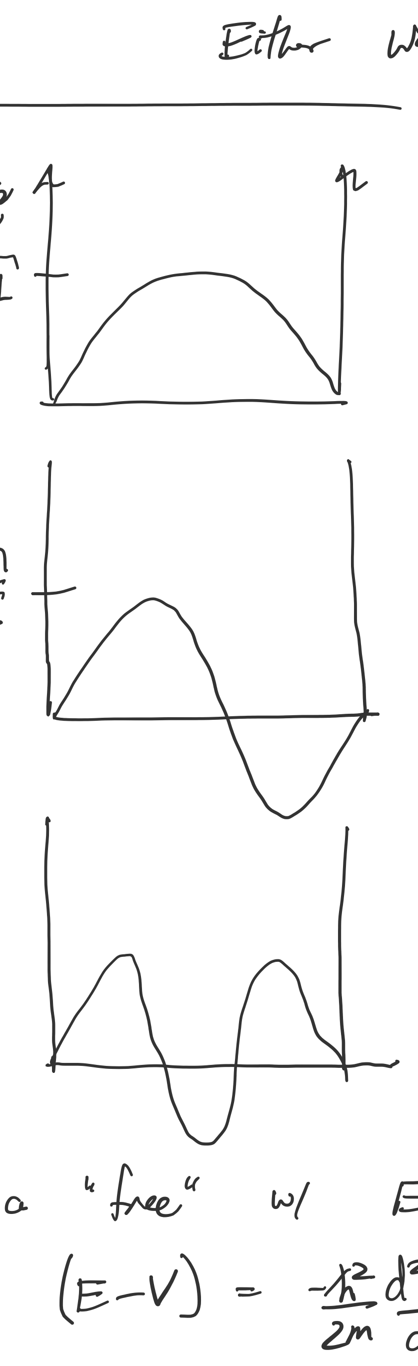
Possible solⁿ $A = 0$ or $\varkappa = 0$ $(E = 0)$

Either way $\psi(x) = 0$ for all x

$E_1 = \frac{h^2}{8mL^2}$

$E_2 = \frac{h^2(2)^2}{8mL^2}$

$E_3 = \frac{h^2(3)^2}{8mL^2}$



no nodes

1 node

2 nodes

① For a "free" w/ $E > V$

$$(E - V) = \frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2}\frac{1}{\psi} \Rightarrow \text{Energy is related to the Curvature of the wave function.}$$

recall $\hat{p}\psi(x) = -i\hbar\frac{\partial}{\partial x}\psi$

② the n^{th} solⁿ in 1D has $n-1$ nodes (zero-crossings)
alternately even/odd $\Rightarrow$ mutually orthogonal

more explicitly $\int_{-\infty}^{\infty}\psi_m^*\psi_n\,dx = \delta_{nm}$ ← kroenicker delta

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