# Modern Physics:Lecture 05: Particle in a BOX

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# Outline


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2. Time-Independent Schrödinger Equation
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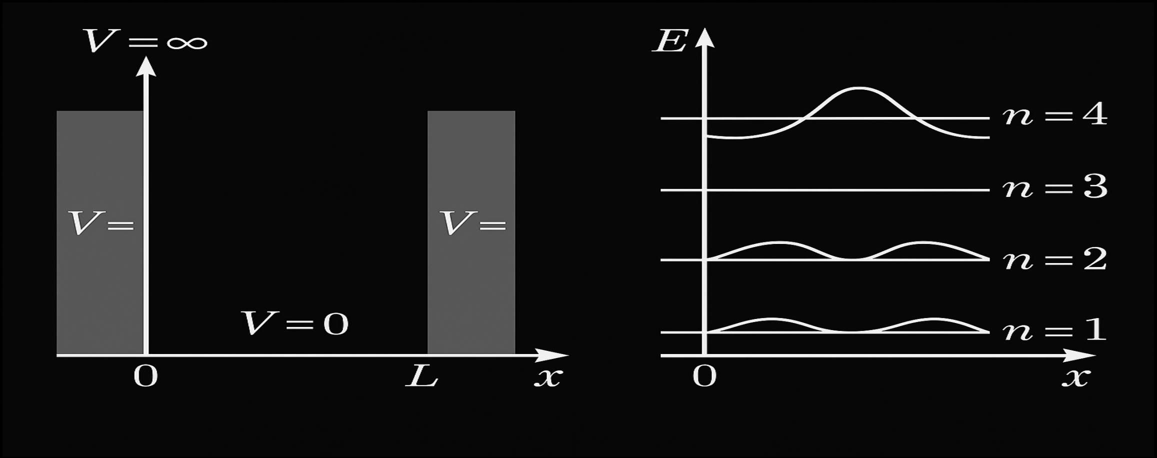
# particle in a box potential



# Physical Setup

- A particle of mass $m$ is confined to a one-dimensional box of length $L$.
- The potential energy is defined as:

$$V(x) = \begin{cases} 0 & \text{if } 0 < x < L \\ \infty & \text{if } x \leq 0 \text{ or } x \geq L \end{cases}$$

- The particle cannot exist outside the box.
- This is an idealized model but captures essential features of quantization.

# Solving the Schrödinger Equation

We solve the time-independent Schrödinger equation in the region $0 < x < L$:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi(x) \Rightarrow \frac{d^2\psi(x)}{dx^2} + k^2\psi(x) = 0$$

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

- General solution: $\psi(x) = A\sin(kx) + B\cos(kx)$

# Applying Boundary Conditions

Boundary conditions:

- At $x = 0$: $\psi(0) = B = 0$
- At $x = L$: $\psi(L) = A\sin(kL) = 0 \Rightarrow \sin(kL) = 0 \Rightarrow kL = n\pi$

$$\Rightarrow k = \frac{n\pi}{L}, \quad n = 1, 2, 3, \ldots$$

Therefore,

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

# Normalization

Require:

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

Using:

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

Thus,

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$$

# Energy Quantization

Substituting $k = \frac{n\pi}{L}$ into the energy expression:

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

- Energies are discrete (quantized) and increase as $n^2$.
- The ground state ($n = 1$) has non-zero energy — the zero-point energy:

$$E_1 = \frac{\pi^2 \hbar^2}{2mL^2}$$

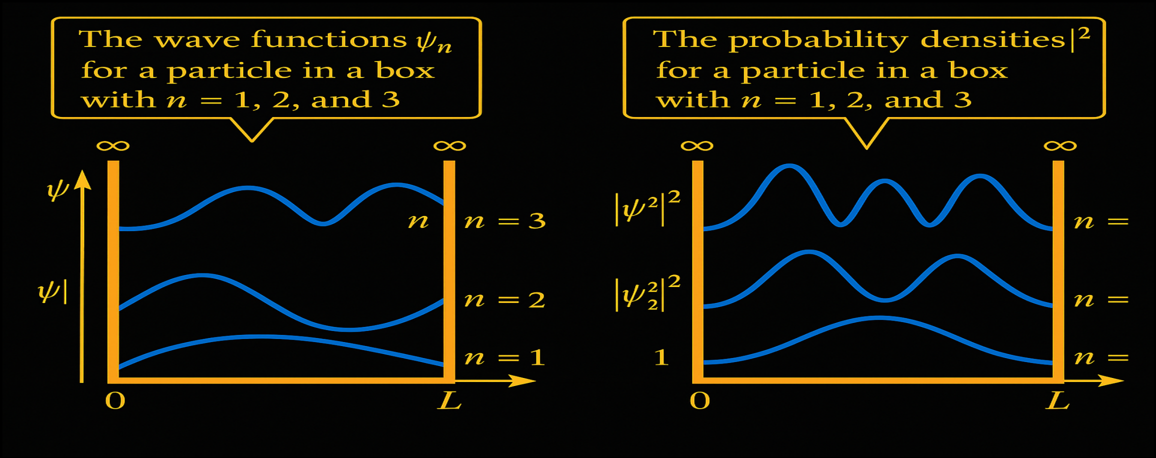
# Wavefunction Properties

- $\psi_n(x)$ has $(n-1)$ nodes (zero crossings) inside the box.
- All wavefunctions are orthogonal:

$$\int_0^L \psi_m(x)\psi_n(x)dx = \delta_{mn}$$

- They form a complete set — any function satisfying the boundary conditions can be expanded in this basis.

# Visualizing Wavefunctions



# Time-Dependent Solutions

Time evolution:

$$\Psi_n(x,t) = \psi_n(x) e^{-iE_n t/\hbar}$$

- Each eigenstate evolves with a phase factor.
- A general state:

$$\Psi(x,t) = \sum_n c_n \psi_n(x) e^{-iE_n t/\hbar}$$

- Coefficients $c_n$ determined by initial condition.

# Expectation Value of Position

$$\langle x \rangle_n = \int_0^L x|\psi_n(x)|^2 dx = \frac{L}{2}$$

- Due to symmetry of the potential and wavefunctions.

# Expectation Value of Momentum

$$\langle p \rangle_n = \int_0^L \psi_n^*(x) \left( -i\hbar \frac{d}{dx} \right) \psi_n(x) dx = 0$$

$$\langle p^2 \rangle_n = \int_0^L \psi_n^*(x) \left( -\hbar^2 \frac{d^2}{dx^2} \right) \psi_n(x) dx = \left( \frac{n\pi\hbar}{L} \right)^2$$

# Uncertainty Principle

- Compute:

$$\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}, \quad \Delta p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2}$$

- For $n = 1$, one finds:

$$\Delta x \approx 0.18L, \quad \Delta p \approx \frac{\pi\hbar}{L} \Rightarrow \Delta x \Delta p \approx 0.18\pi\hbar > \frac{\hbar}{2}$$

# Applications of the Model

- Electron in a quantum dot or nanowire.
- Modeling of particle confinement in nanostructures.
- Insight into quantization and boundary effects.

# Conclusion

- Analytic solution of particle in a box illustrates core quantum concepts.
- Quantized energy, wavefunctions, and expectations obey physical principles.
- Model serves as foundation for understanding more complex systems.

# Slide 1: Basic Wavefunction and Energy

1. Given a 1D infinite potential well of width $L$, find the normalized wavefunction $\psi_n(x)$ for the $n^{\text{th}}$ energy level.
2. Derive the expression for the energy levels $E_n$ of a particle in the box.

# Slide 2: Expectation Values

1. Compute the expectation value $\langle x \rangle$ for the ground state $n = 1$.
2. Calculate the expectation value $\langle x^2 \rangle$ and hence find the standard deviation $\Delta x$.

# Slide 3: Momentum and Uncertainty

1. Show that $\langle p \rangle = 0$ for any state $n$ in the infinite potential well.
2. Find $\langle p^2 \rangle$ and compute the momentum uncertainty $\Delta p$.

# Slide 4: Orthogonality and Superposition

1. Prove that the wavefunctions $\psi_n(x)$ and $\psi_m(x)$ are orthogonal for $n \neq m$.
2. Consider the superposition $\Psi(x,t) = \frac{1}{\sqrt{2}}(\psi_1(x)e^{-iE_1 t/\hbar} + \psi_2(x)e^{-iE_2 t/\hbar})$. Find the probability density $|\Psi(x,t)|^2$.

# Slide 5: Numerical and Applied Problems

1. For an electron in a box of width $L = 1$ nm, compute the energy of the first three quantum states.
2. If a particle in a box is in a superposition of $\psi_1$ and $\psi_3$ with equal probability amplitudes, what is the expected value $\langle x \rangle$ at $t = 0$?

# Slide 6: Advanced Challenge

**Deep Conceptual Problem:**

A particle is placed in a 1D infinite potential well of width $L$. At $t = 0$, its wavefunction is given by:

$$\Psi(x,0) = \begin{cases} \sqrt{\frac{30}{L^5}}x(L-x) & \text{for } 0 < x < L, \\ 0 & \text{otherwise} \end{cases}$$

1. Show that this wavefunction is normalized.
2. Expand $\Psi(x,0)$ in terms of the stationary states $\psi_n(x)$.
3. Compute the probability of finding the particle in the first excited state.
4. Determine $\Psi(x,t)$.
5. Discuss the time-dependence of the probability density $|\Psi(x,t)|^2$ and whether it exhibits any periodicity.

# References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