Quantum Mechanics in Medicine
Lecture 7: The Free Particle and Box Normalization

Presented by:
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Third-Year Students

Outline

Starting Point and Assumptions

Physical Problem: A single particle (mass m) is free to move along one dimension, but confined between two impenetrable walls at $x = -L/2$ and $x = +L/2$.

Assumptions:

- The motion is one-dimensional along x.
- Potential inside the region is zero ($V(x) = 0$).
- Outside this region, $V(x) \to \infty$ so that the particle can never exist there.
- The particles total energy is purely kinetic:

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

- The system is stationary time dependence can be separated as $e^{-iEt/\hbar}$.

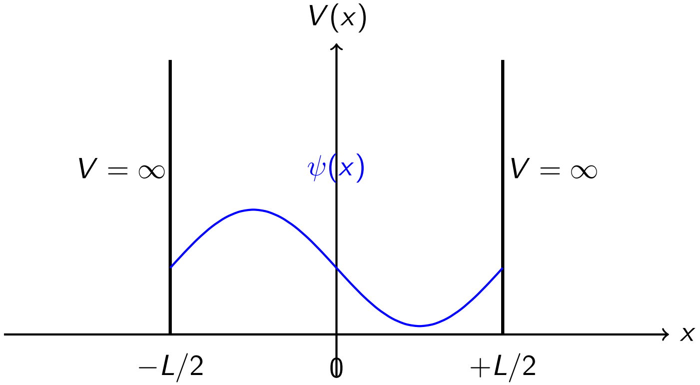
Potential Well Representation

$$V(x) = \begin{cases} 0, & -\frac{L}{2} < x < +\frac{L}{2}, \\ \infty, & |x| \geq \frac{L}{2}. \end{cases}$$

Meaning:

- Inside $(V = 0)$: the particle behaves as a *free* particle.
- Outside $(V = \infty)$: the wavefunction must vanish, $\psi(x) = 0$.
- The walls represent absolute confinement the particle cannot leak out.

Figure: Infinite Potential Well from $-L/2$ to $+L/2$



Interpretation: The particle is free inside the well but cannot exist beyond the infinite boundaries.

Time-Independent Schrödinger Equation

Inside the well, where $V(x) = 0$:

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

The general solution is:

$$\psi(x) = Ae^{ikx} + Be^{-ikx},$$

where $k = \sqrt{2mE}/\hbar$.
Alternatively, we can write:

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

using the trigonometric form for real k.

Boundary Conditions and Quantization

Since $\psi(x)$ must vanish at the infinite walls:

$$\psi(-L/2) = 0, \qquad \psi(+L/2) = 0.$$

Applying these to $\psi(x) = C\sin(kx) + D\cos(kx)$:

$$\psi(-L/2) = 0 \Rightarrow C\sin(-kL/2) + D\cos(-kL/2) = 0,$$
$$\psi(+L/2) = 0 \Rightarrow C\sin(kL/2) + D\cos(kL/2) = 0.$$

Adding and subtracting leads to:

$$D = 0, \qquad \sin(kL/2) = 0.$$

Hence, $kL/2 = n\pi$, giving:

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

Allowed Energies

The energy eigenvalues follow from $E_n = \hbar^2 k_n^2/(2m)$:

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

Features:

- Energy is quantized: only discrete values are allowed.
- E_n increases with n^2 higher states require more energy.
- The lowest state $(n = 1)$ is not zero: $E_1 = \pi^2\hbar^2/(2mL^2)$.

Physical meaning: Even in its lowest state, the particle cannot be at rest due to the Heisenberg uncertainty principle.

Normalized Wavefunctions

Inside the well, the general solution satisfying $\psi(\pm L/2) = 0$ is:

$$\psi_n(x) = A_n \sin\left[\frac{n\pi(x + L/2)}{L}\right].$$

Normalization requires:

$$\int_{-L/2}^{L/2} |\psi_n(x)|^2 dx = 1.$$

Performing the integration gives:

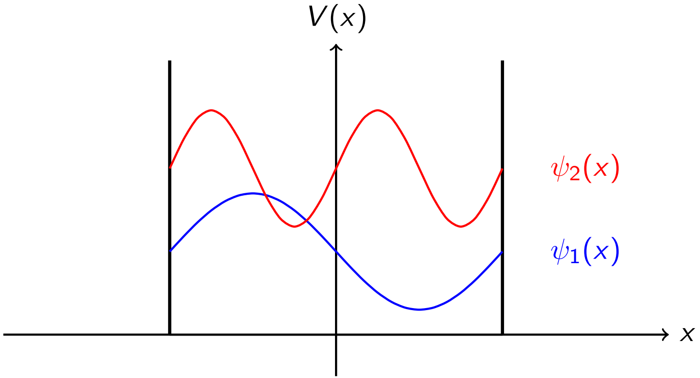
$$A_n = \sqrt{\frac{2}{L}}.$$

Final normalized wavefunction:

$$\boxed{\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left[\frac{n\pi(x + L/2)}{L}\right]}.$$

Graphical Representation

- Each wavefunction $\psi_n(x)$ forms a standing wave with n half-wavelengths inside the well.
- The number of nodes (points where $\psi = 0$) increases with n.
- Higher n corresponds to shorter wavelength and higher energy.



Orthogonality of States

For any two distinct states $m \neq n$:

$$\int_{-L/2}^{L/2} \psi_m^*(x)\psi_n(x)\,dx = 0.$$

This can be shown by direct integration using:

$$\psi_m(x)\psi_n(x) = \frac{2}{L}\sin\left(\frac{m\pi(x + L/2)}{L}\right)\sin\left(\frac{n\pi(x + L/2)}{L}\right).$$

Implication:

- Each eigenfunction is independent.
- Together, they form an orthonormal basis for representing any confined wavefunction.

MCQ 12

Q1. Inside the box, potential energy $V(x)$ is:
A) Constant and nonzero
B) Zero
C) Infinite
D) Negative

Q2. At the boundaries $x = \pm L/2$, $V(x)$ equals:
A) Zero
B) Finite
C) Infinite
D) Undefined

MCQ 34

Q3. The wavefunction outside the box is:
A) Constant
B) Zero
C) Oscillating
D) Infinite

Q4. The particles total energy is:
A) Potential
B) Zero
C) Kinetic only
D) Thermal

MCQ 56

Q5. Schrödinger equation inside the box:

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

B) $\frac{d^2\psi}{dx^2} = 0$

C) $E = \psi$

D) $\psi = E$

Q6. General wavefunction inside the box:

A) $\psi = Ae^{kx} + Be^{-kx}$

B) $\psi = Ae^{ikx} + Be^{-ikx}$

C) $\psi = A + Bx$

D) $\psi = \sin x$

Q7. Quantization condition from boundary values:
A) $kL/2 = n\pi$
B) $kL = n\pi/2$
C) $k = L/n$
D) $k = \pi n^2$

Q8. Allowed wavenumbers are:
A) $k_n = \frac{2\pi n}{L}$
B) $k_n = \frac{n\pi}{L}$
C) $k_n = \frac{\pi}{2L}$
D) None

MCQ 910

Q9. Energy eigenvalues are:

A) $E_n = \dfrac{\hbar^2 k_n^2}{2m}$
B) $E_n = \hbar k_n$
C) $E_n = m k_n^2$
D) $E_n = k_n^2/\hbar$

Q10. Energy depends on:

A) n
B) n^2
C) $1/n$
D) $1/n^2$

Q11. Ground-state energy is not zero because:

A) Heisenberg uncertainty principle

B) Coulomb attraction

C) Temperature effects

D) Friction

Q12. Normalized eigenfunction is:

A) $\sqrt{\frac{2}{L}}\sin\left[\frac{n\pi(x+L/2)}{L}\right]$

B) $\sin(kx)$

C) e^{ikx}

D) $\cos(kx)$

MCQ 1314

Q13. Normalization constant A_n equals:
A) $1/L$
B) $\sqrt{L/2}$
C) $\sqrt{2/L}$
D) $2L$

Q14. The number of nodes in $\psi_n(x)$ is:
A) $n-1$
B) n
C) 1
D) 0

MCQ 1516

Q15. For $n = 2$, the wavefunction has:
A) One half-wavelength
B) Two half-wavelengths
C) Three half-wavelengths
D) Infinite half-wavelengths

Q16. Orthogonality means:
A) $\psi_m^*\psi_n$ is constant
B) $\int_{-L/2}^{L/2} \psi_m^*\psi_n \, dx = 0$ for $m \neq n$
C) $\psi_m = \psi_n$
D) Energies are equal

Q17. Orthogonality ensures:
A) States overlap completely
B) States are independent
C) States are identical
D) Normalization fails

Q18. $|\psi_n(x)|^2$ represents:
A) Uniform probability
B) Standing-wave probability pattern
C) Traveling wave
D) Decaying exponential

MCQ 1920

Q19. Confinement of the particle results in:
A) Continuous energy levels
B) Discrete quantized energies
C) Negative energies
D) Zero energy

Q20. The infinite potential well model is most useful for understanding:
A) Electron confinement in quantum dots and nanodevices
B) The motion of planets around the Sun
C) Radioactive decay inside the nucleus
D) Chemical bonding in large organic molecules