Particle in a 1-D box

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Particle in One–Dimensional Box

$$V(x) = 0; 0 < x < L,$$
$$= \infty; x \leq 0 \text{ and } x \geq L$$

Schrodinger equation will reduce to:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial^2 x^2} = E\psi(x); 0 \leq x \leq L$$

Solution:

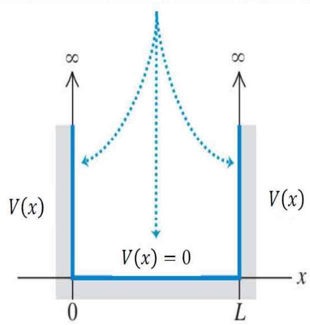
$$\psi(x) = A\cos\frac{\sqrt{2mE}}{\hbar} + B\sin\frac{\sqrt{2mE}}{\hbar}$$

Boundary conditions:

$$\psi(0) = 0 \Rightarrow A = 0$$

$$\psi(L) = 0 \Rightarrow \sin\frac{\sqrt{2mE}}{\hbar}L = 0$$

The potential energy V is zero in the interval 0<x<L and is infinite else where.



- Classical Physics: The particle can exist anywhere in the box and follow a path in accordance to Newton's Laws.
- Quantum Physics: The particle is expressed by a wave function and there are certain areas more likely to contain the particle within the box.

$$\sin\frac{\sqrt{2mE}}{\hbar}L = 0 \Rightarrow \frac{\sqrt{2mE}}{\hbar} = n\pi \Rightarrow En = \frac{n^2\pi^2\hbar^2}{2mL^2}$$

Eigen value

Wave Function:

$$\psi_n(x) = B\sin\frac{\sqrt{2mE_n}}{\hbar} = B\sin\frac{n\pi}{L}$$

Wave function must be normalizable

$$\int_{-\infty}^{+\infty}|\psi(x)|^2dx = 1 \Rightarrow \int_{-\infty}^{+\infty}B^2\sin^2(\frac{n\pi}{L}x)dx = 1 \Rightarrow B = \sqrt{\frac{2}{L}}$$

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

Wave Function for a Particle in One-Dimensional Box

- Energy is quantized
- Solving for the energy yields

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

- Note that the energy depends on the integer values of *n*. Hence the energy is quantized and nonzero.

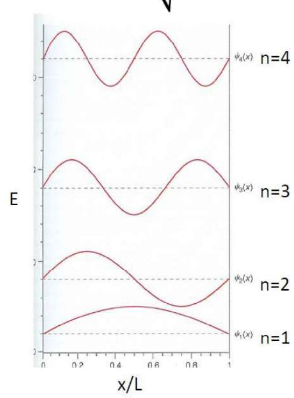
$$E_1 = \frac{\pi^2 \hbar^2}{2mL^2}$$

Quantized Energy

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

Applying the Born Interpretation

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



- The quantized wave number now becomes
- Solving for the energy yields

$$E_n = n^2 \frac{\pi^2 h^2}{2mL^2} \qquad (n = 1, 2, 3, \ldots)$$

- Note that the energy depends on the integer values of *n*. Hence the energy is quantized and nonzero.
- The special case of *n* = 1 is called the ground state energy.

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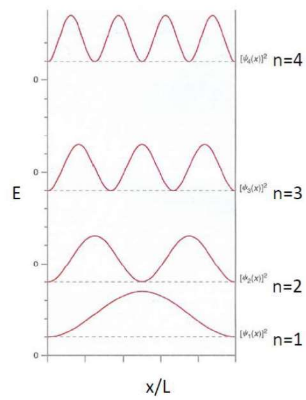

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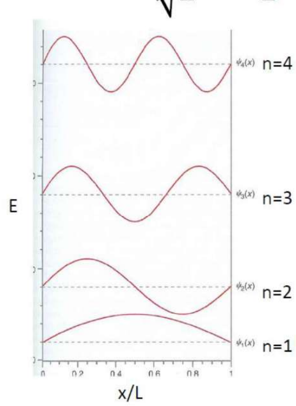

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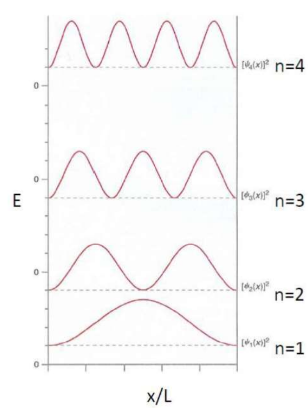

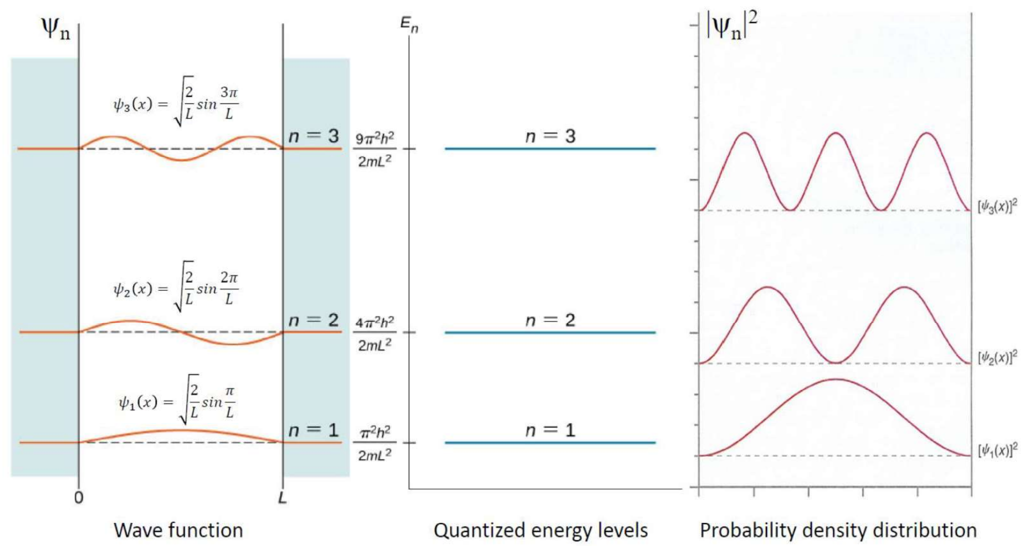

ψ_n
$\psi_3(x) = \sqrt{\frac{2}{L}} sin \frac{3\pi}{L}$
$\psi_2(x) = \sqrt{\frac{2}{L}} sin \frac{2\pi}{L}$
$\psi_1(x) = \sqrt{\frac{2}{L}} sin \frac{\pi}{L}$
$n = 3$
$n = 2$
$n = 1$
0
L
E_n
$\frac{9\pi^2\hbar^2}{2mL^2}$
$\frac{4\pi^2\hbar^2}{2mL^2}$
$\frac{\pi^2\hbar^2}{2mL^2}$
$|\psi_n|^2$
$[\psi_3(x)]^2$
$[\psi_2(x)]^2$
$[\psi_1(x)]^2$
Wave function
Quantized energy levels
Probability density distribution