Application of Quantum Mechanics:
Translational Motion of a Particle in a Box

For L of same order of magnitude as $\lambda = \frac{h}{p}$:

$\Rightarrow \lambda = 2L, L, \frac{2}{3}L,...$

or $\lambda = \frac{2}{n}L$

$n = 1, 2, 3,...$
The Permitted Wavefunctions of a Particle in a Box

⇒ Permitted wavefunctions are:

\[ \Psi_n = N \sin \left( \frac{n\pi x}{L} \right); \quad n = 1, 2, \ldots \]

Normalization constant (for scaling)

\[ N = \sqrt{\frac{2}{L}} \]

According to Born’s interpretation:

\[ \int_0^L \Psi^2 \, dx = 1 \]

⇒ \( N^2 \int_0^L \sin^2 \left( \frac{n\pi x}{L} \right) \, dx = 1 = N^2 \frac{1}{2} L \)

b/c of

\[ \int_0^L \sin^2 \left( ax \right) \, dx = \frac{1}{2} x - \frac{\sin 2ax}{4a} \bigg|_0^L \]
The Permitted (Quantized!) Energies of a Particle in a Box

According to de Broglie

\[ p = \frac{h}{\lambda} = \frac{nh}{2L}; \quad n = 1, 2, \ldots \]

and

\[ E_{\text{total}} = E_{\text{kin}} = \frac{p^2}{2m} \]

\[ \Rightarrow E_n = \frac{n^2 \hbar^2}{8mL^2}; \quad n = 1, 2, \ldots \]

The same result is obtained when applying the Schrödinger equation to the wavefunction:

\[ -\frac{\hbar^2}{2m} \frac{d^2\Psi}{dx^2} + V\Psi = E\Psi; \quad \Psi_n = N \sin \frac{n\pi x}{L} \]

Only the \( n=1 \) state (lowest energy) has no nodes; state \( n \) has \( n-1 \) nodes.
The Behavior of a Particle in a Box

\[ E_n = \frac{n^2 \hbar^2}{8mL^2}; \quad n = 1, 2, \ldots \]

\[ \Delta E = E_{n+1} - E_n = (2n + 1) \frac{\hbar^2}{8mL^2} \]

Examples:

- electron in \( \text{NH}_3(\text{l}) \)
- conjugated polyenes

Zero-point energy (in accord with Heisenberg’s uncertainty principle!)
What about a Particle Travelling on a Ring?

Linear momentum $p \rightarrow$ angular momentum $J$

$$J = pr = mvr \quad \uparrow \uparrow$$

$$E_{total} = E_{kin} = \frac{1}{2} mv^2 = \frac{p^2}{2m} = \frac{J^2}{2mr^2}$$

$$J = pr = \frac{hr}{\lambda}$$

de Broglie

$$\Rightarrow \lambda = \frac{2\pi r}{n} ; \quad n = 0, 1, \ldots$$

Boundary condition:

unacceptable

acceptable

$$E_n = \frac{(nh/2\pi)^2}{2I} = \frac{n^2\hbar^2}{2I}$$

$n = 0, \pm 1, \pm 2, \ldots$