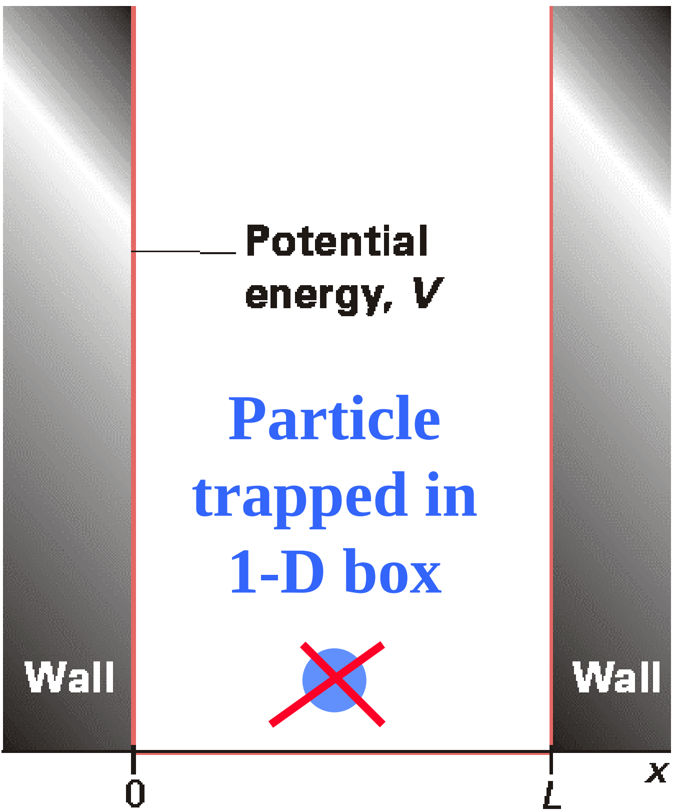
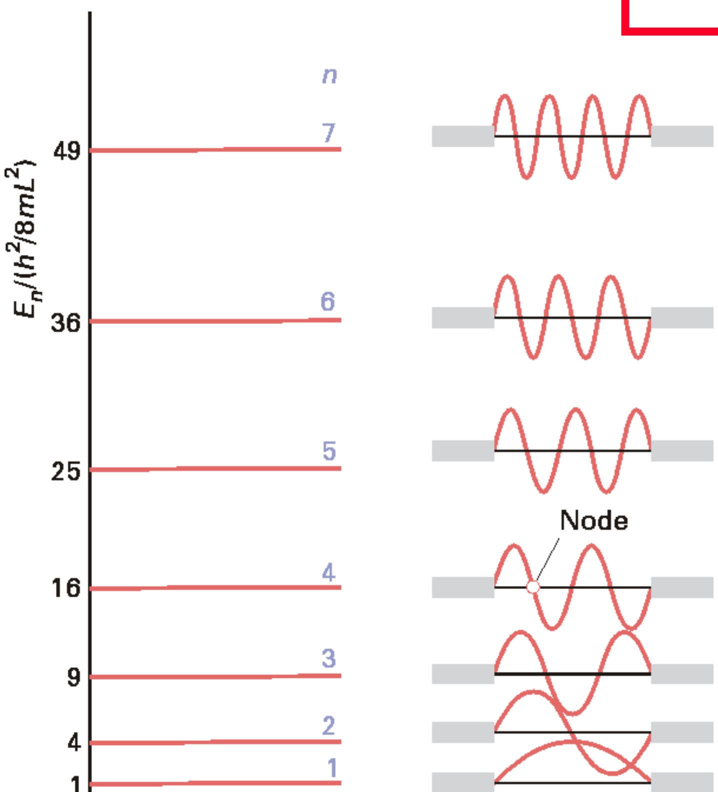
Application of Quantum Mechanics: Translational Motion of a Particle in a Box



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



$\Rightarrow$

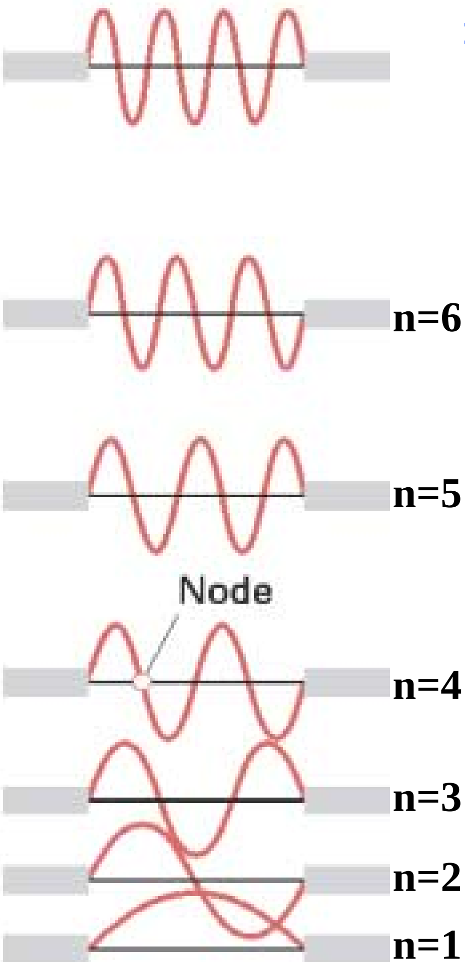
$$\lambda = 2L, L, \frac{2}{3}L, \ldots$$

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

$$n = 1, 2, 3, \ldots$$

Boundary condition:
Particle wave must fit into the box exactly

The Permitted Wavefunctions of a Particle in a Box



⇒ Permitted wavefunctions are:

$$\Psi_n = N \sin \frac{n\pi x}{L}; \quad n = 1, 2, \ldots \qquad N = \sqrt{\frac{2}{L}}$$

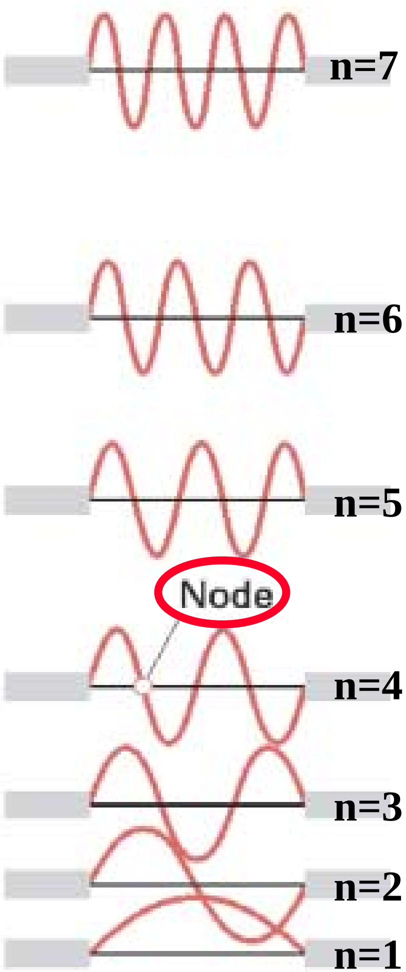
normalization constant (for scaling)

According to Born's interpretation: $\int_0^L \Psi^2 dx = 1$

$$\Rightarrow N^2 \int_0^L \sin^2 \frac{n\pi x}{L} dx = 1 = N^2 \frac{1}{2} L$$

b/c of $\int_0^L \sin^2(ax)\, dx = \frac{1}{2} x - \frac{\sin 2ax}{4a} \Big|_0^L$

The Permitted (Quantized!) Energies of a Particle in a Box



According to de Broglie $p = \dfrac{h}{\lambda} = \dfrac{nh}{2L}; \quad n = 1, 2, \ldots$

and $E_{total} = E_{kin} = \dfrac{p^2}{2m}$

$$\Rightarrow E_n = \frac{n^2 h^2}{8mL^2}; \quad n = 1, 2, \ldots$$

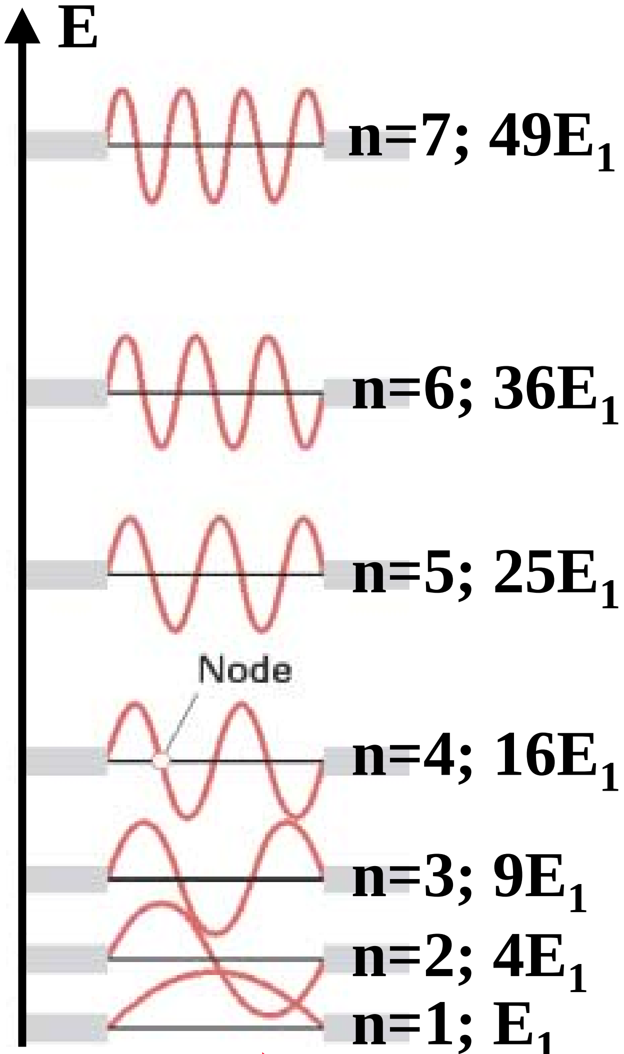
n is a quantum number specifying the energy of the particle

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

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

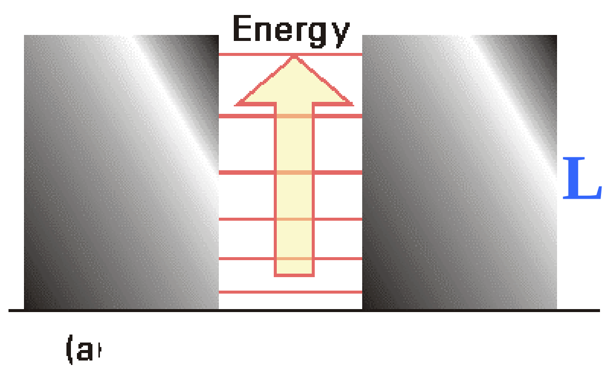
Only the n=1 state (lowest energy) has no nodes; state n has n-1 nodes

The Behavior of a Particle in a Box

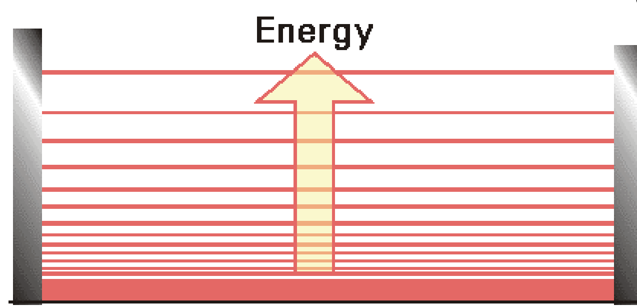


$$\boxed{E_n = \frac{n^2h^2}{8mL^2}; \quad n = 1, 2, \ldots}$$

$$\boxed{\begin{aligned}\Delta E &= E_{n+1} - E_n \\ &= (2n+1)\frac{h^2}{8mL^2}\end{aligned}}$$



L small



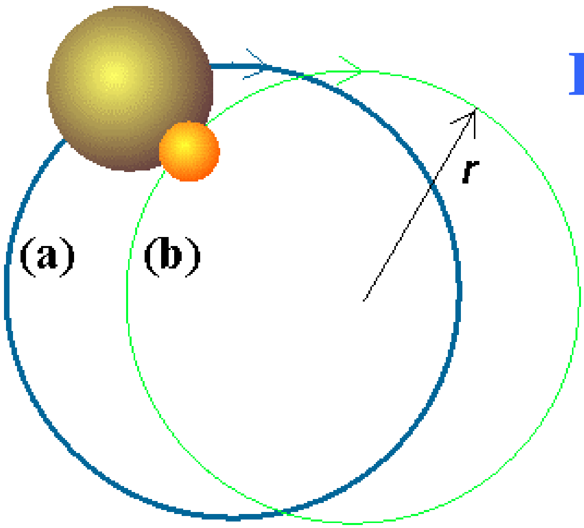
L large

Examples:

- **electron in NH_3(l)**
- **conjugated polyenes**

Zero-point energy (in accord with Heisenberg's uncertainty principle!)

What about a Particle Travelling on a Ring?



Linear momentum p → angular momentum J

$$J = pr = m\mathrm{v}r \qquad \mathbf{m\uparrow, v\uparrow \Rightarrow J\uparrow}$$

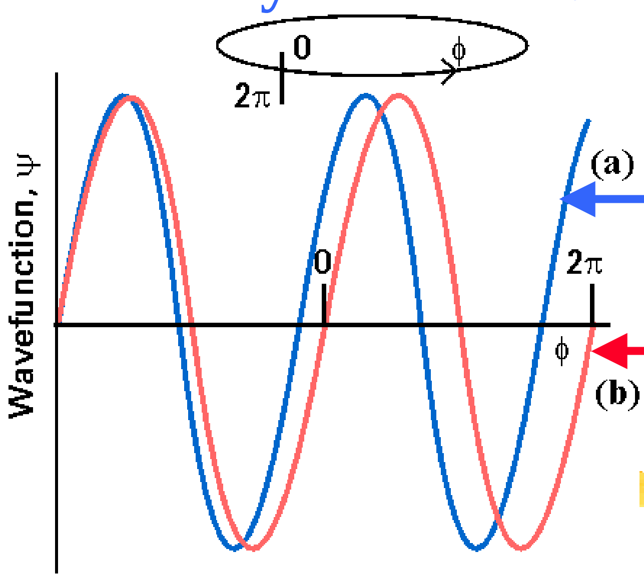
$$E_{total} = E_{kin} = \frac{1}{2}m\mathrm{v}^2 = \frac{p^2}{2m} = \frac{J^2}{2mr^2}$$

moment of inertia I

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

de Broglie

Boundary condition:



unacceptable

acceptable

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

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

Nils

n = 0, ±1, ±2,...