Free particle in 1 D box:

Here free particle refers to electron and 1D box can be an atom or a piece of metal wire. As the electron is completely free to move within the box, its potential energy is zero. And the electron moves only along x-axis, the following partial differential equation (from Schrodinger's time independent equation) will be written as compete differential equation.

$$\nabla^2\Psi + \frac{2m(E-V)}{\hbar^2}\Psi$$

As V=0 between the walls, the equation becomes

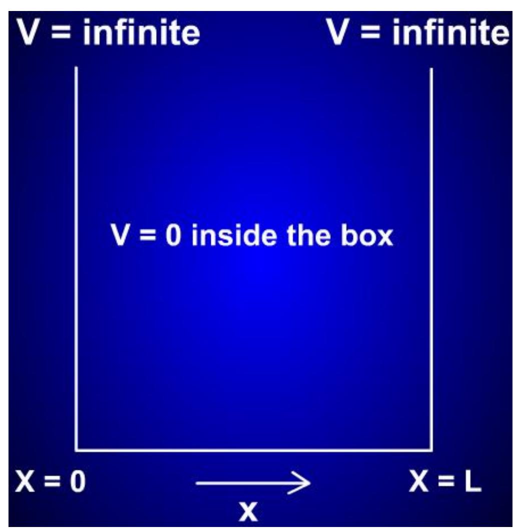
$$\frac{\partial^2\Psi}{\partial x^2} + \frac{2m}{\hbar^2}E\Psi = 0$$

$$\frac{d^2\Psi}{dx^2} + k^2 = 0 \text{ is the wave equation for electron's travel along one dimension.}$$

x=0 and x=L are the boundaries of the one dimensional potential box. In the following figure the potential energy inside the box is zero; and the electron may face up to infinite potential by the walls of the box in such a way that the electron never gets outside the box. Thus, the potential function is defined in the following way:

V(x)=0 for L>x>0
V(x)=∞ for x≥L, x≤0

$$\because k^2 = \frac{2mE}{\hbar^2}$$



The solution of the second order differential equation is as follows,

$$\Psi(x) = A\sin kx + B\cos kx$$

The wave function is zero at the boundaries so,

$$\Psi = 0 \text{ at } x = 0$$

After applying the first boundary condition,

$$0 = A \times 0 + B \times 1$$

$$= 0 + \mathrm{B}$$

$$\Longrightarrow \mathrm{B} = 0$$

Thus, $\Psi(\mathrm{x}) = \mathrm{A} \sin \mathrm{kx}$

$\Psi = 0$ at $\mathrm{x} = \mathrm{a}$ (the second boundary condition)

After applying the second boundary condition

$$0 = \mathrm{A} \sin \mathrm{ka}$$

$$\mathrm{ka} = \mathrm{n}\pi, \mathrm{n} = 1, 2, 3, \dots \dots$$

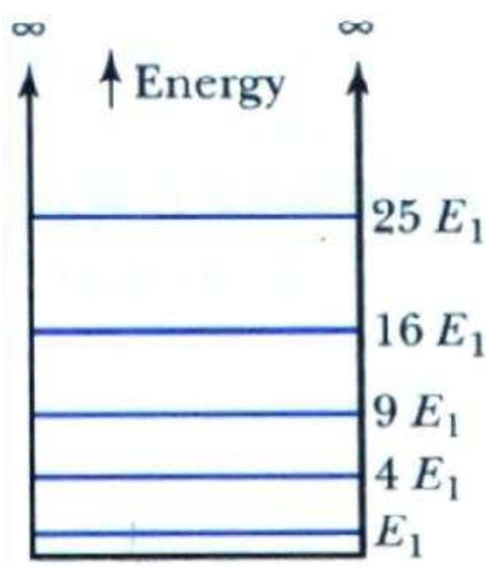
$$\mathrm{k} = \frac{\mathrm{n}\pi}{\mathrm{a}}$$

$$\mathrm{k} = \sqrt{\frac{2\mathrm{mE}}{\hbar^2}}, \text{and also } \mathrm{k} = \frac{\mathrm{n}\pi}{\mathrm{a}}$$

$$\mathrm{k}^2\mathrm{a}^2 = \frac{2\mathrm{mE_n}\mathrm{a}^2}{\hbar^2} = \mathrm{n}^2\pi^2$$

$$\mathrm{E_n} = \frac{\mathrm{n}^2\pi^2\hbar^2}{2\mathrm{ma}^2}, \mathrm{n} = 1,2,3 \dots$$

Thus, for each value of n, the possible energy of the particle is given by the above equation



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

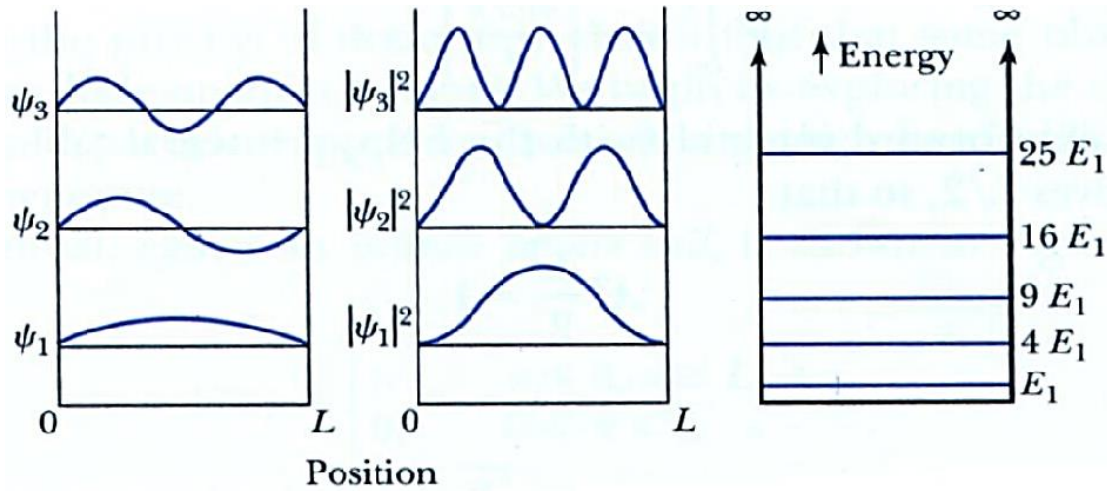
$$\mathrm{E_2} = 4\frac{\pi^2\hbar^2}{2\mathrm{mL}^2} = 4\mathrm{E_1}$$

$$\mathrm{E_3} = 9\frac{\pi^2\hbar^2}{2\mathrm{mL}^2} = 9\mathrm{E_1}$$

$$\mathrm{E_4} = 16\frac{\pi^2\hbar^2}{2\mathrm{mL}^2} = 16\mathrm{E_1}$$

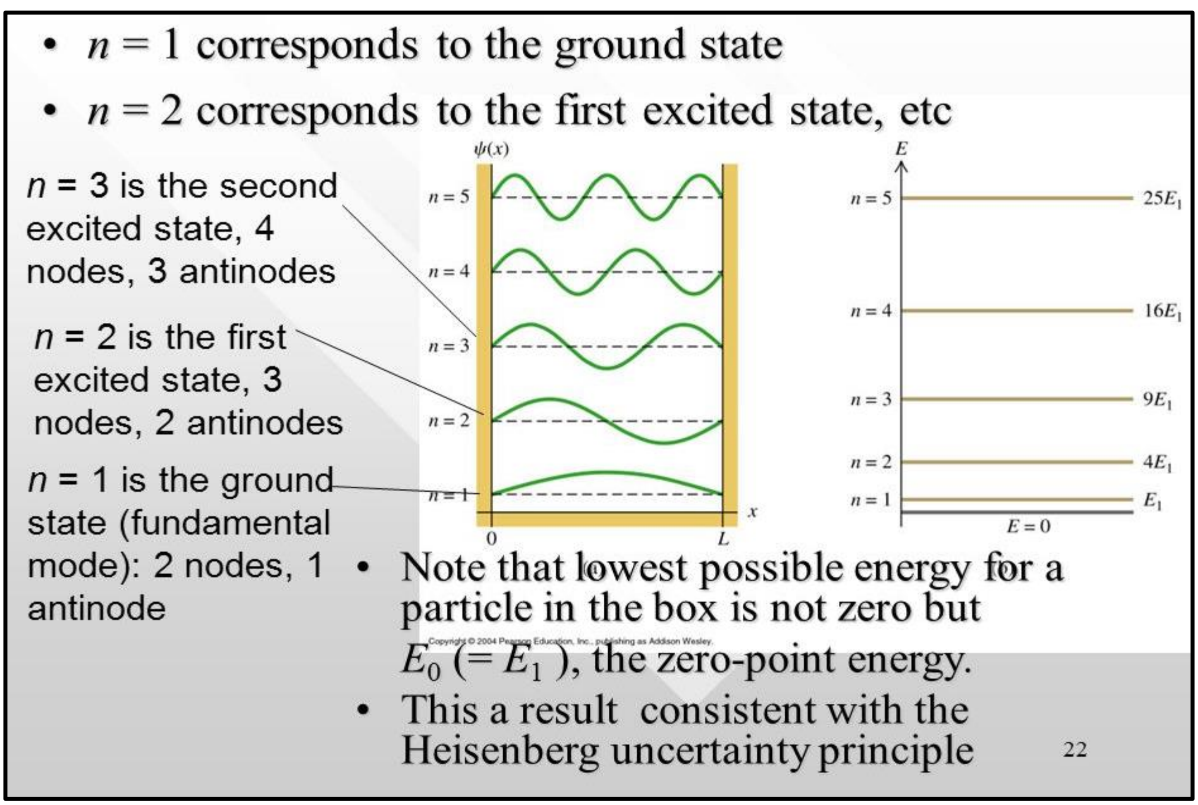
$$\mathrm{E_5} = 25\frac{\pi^2\hbar^2}{2\mathrm{mL}^2} = 25\mathrm{E_1}$$

The following figure explains the wave functions, probability densities and energy values of the particle at different energy levels.



At a particular point, the probability of the particle being present is different for different quantum numbers. For example, $|\Psi_1|^2$ has its maximum value at L/2 in the middle. Thus, a particle in the lowest energy level of n=1 is most likely to be in the middle while a particle in the next higher state of n=2 is never there.

Nodes and Antinodes:



Eigen functions:

Eigen means special or particular. After including particular energy value function, the wave function is called as Eigen function.

$$\Psi_n = A\sin kx = A\sin\sqrt{\frac{2mE_n}{\hbar^2}}x\,,\text{where}, n = 1,2,3 \ldots.$$

$$\Psi_n = A\sin\frac{n\pi x}{a}$$

$\int_{-\infty}^{+\infty}|\Psi_n|^2 dx = 1$ (within the box, the hundred percentage of the particle is existing, since boundaries prevent them strongly from escaping outside)

$$\int_0^a |\Psi_n|^2 dx = \int_0^a A^2 \sin^2\left(\frac{n\pi x}{a}\right) dx = 1$$

$$\int_0^a \sin^2\left(\frac{n\pi x}{a}\right) dx = \frac{a}{2} \text{ (standard integral)}$$

$$\int_0^a |\Psi_n|^2 dx = A^2\frac{a}{2} = 1$$

$$A^2 = \frac{2}{a}$$

$$A = \sqrt{\frac{2}{a}} \text{ is the normalised constant}$$

Thus by applying the normal condition (100% existence of the particle within the box) the constant A has been found out. So the constant A is called as normalised constant.

Normalised Eigen functions:

Eigen function with the normalised constant is called as normalized Eigen function.

$$\Psi_n(x) = A \sin kx = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a} x\right), \text{where}, n = 1,2,3 \ldots.$$