Engineering Physics

(PHY1701)

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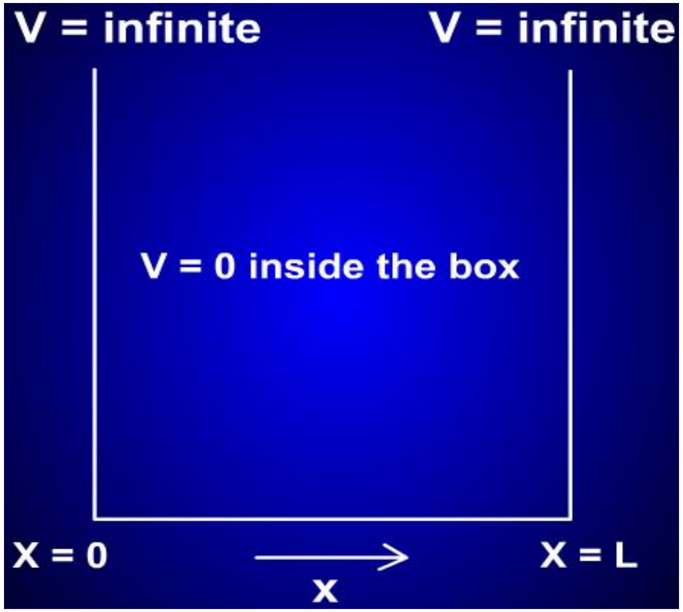
Contents

- Particle in a 1-D box (Eigen Value and Eigen Function) (AB 198-202),
- 3-D Analysis (Qualitative),
- Tunneling Effect (Qualitative) (AB 205), &
- Scanning Tunneling Microscope (STM)*

❖ Concepts of Modern Physics, Arthur Beiser et al., Sixth Edition, Tata McGraw Hill (2013) (AB)

Particle in 1D box



$V(x)=0$ for $L>x>0$

$V(x)=\infty$ for $x \geq L$, $x \leq 0$

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

- 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.
- 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.

Particle in 1D box

Schrödinger Time Independent Equation for a particle is given by

$$\nabla^2\Psi + \frac{2m(E-V)}{\hbar^2}\Psi = 0 \qquad \text{-------eq. 1}$$

As V=0 between the walls, the equation becomes

$$\frac{d^2\Psi}{dx^2} + \frac{2m}{\hbar^2}E\Psi = 0 \qquad \text{-------eq. 2}$$

Let, $\frac{2m}{\hbar^2}E = k^2$, eq. 2 becomes

$$\frac{d^2\Psi}{dx^2} + k^2\Psi = 0 \qquad \text{-------eq. 3}$$

Eq. 3 is the wave equation for electron′s travel along one dimension.

This is similar to the general differential equation:

$$-\frac{d^2\psi(x)}{dx^2} = k^2\psi \longrightarrow \psi = A\sin kx + B\cos kx$$

Finding the Wave Function.

The solution for this second order differential equation is as follows,

$$\Psi(x) = A\sin kx + B\cos kx \quad \text{-------eq. 4}$$

Where A and B are arbitrary constants.

Boundary conditions:

When $x = 0$, Ψ=0
$x = L$, Ψ=0

So we can start applying boundary conditions:

x=0, ψ=0

$$0 = A\sin 0k + B\cos 0k \longrightarrow 0 = 0 + B*1 \therefore B = 0$$

x=L, ψ=0

$$0 = A\sin kL \qquad A \neq 0 \longrightarrow kL = n\pi \ \text{(where n =0, 1,2,3,....)}$$

Calculating Energy Levels:

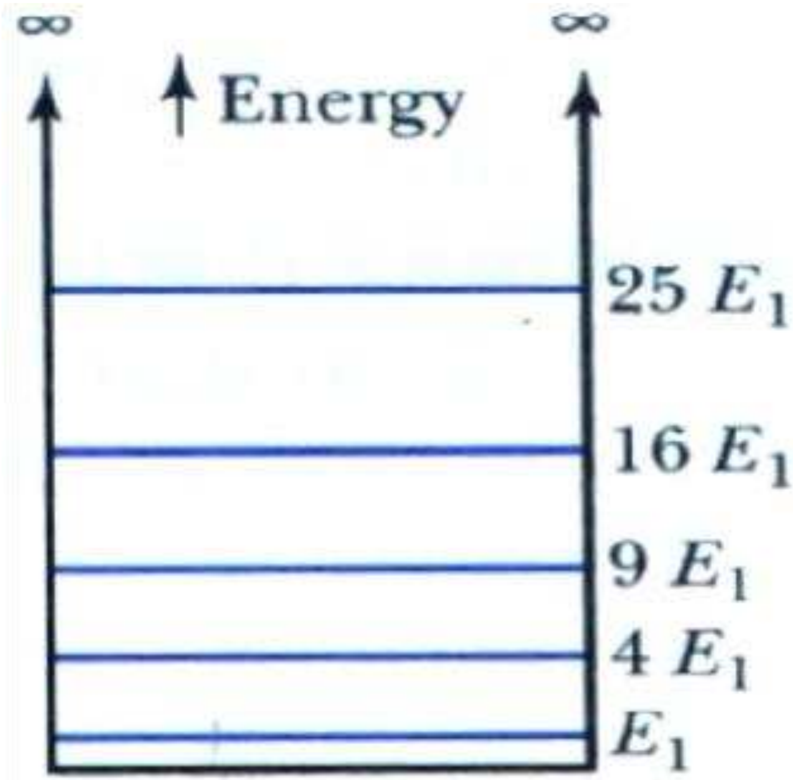
$$\frac{2m}{\hbar^2}E = k^2 \longrightarrow E = \frac{k^2\hbar^2}{2m} \longrightarrow E = \frac{k^2h^2}{2m4\pi^2}$$

Finding the Wave Function

$$E=\frac{n^2\pi^2}{L^2}\frac{h^2}{2m4\pi^2} \longrightarrow E=\frac{n^2h^2}{8mL^2} \longrightarrow \mathrm{E}_1=n^2\frac{\pi^2\hbar^2}{2\mathrm{mL}^2} \text{ -------eq. 5} \quad \left[\because \hbar=\frac{\mathrm{h}}{2\pi}, k=\frac{\mathrm{n}\pi}{\mathrm{L}}\right]$$

(where, n = 1,2,3,…)

Thus, for each value of n, the possible energy of the particle is given by eq. 5



Energy level of the particle inside an infinite potential well

$$\mathrm{E}_1=\frac{\pi^2\hbar^2}{2\mathrm{mL}^2}$$

$$\mathrm{E}_2=4\frac{\pi^2\hbar^2}{2\mathrm{mL}^2}=4\mathrm{E}_1$$

$$\mathrm{E}_3=9\frac{\pi^2\hbar^2}{2\mathrm{mL}^2}=9\mathrm{E}_1$$

$$\mathrm{E}_4=16\frac{\pi^2\hbar^2}{2\mathrm{mL}^2}=16\mathrm{E}_1$$

$$\mathrm{E}_5=25\frac{\pi^2\hbar^2}{2\mathrm{mL}^2}=25\mathrm{E}_1$$

Finding the Wave Function

Eigen functions:

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

$$\psi_n = A\sin\frac{n\pi x}{L}$$

Normalizing wave function:

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

The value of A in eq. 4 can be obtained by normalization condition,

$$|\Psi_n|^2 = \Psi^*\Psi = 1$$

$$\int_0^a |\Psi_n|^2 dx = 1$$

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

$$\because \cos 2\theta = 1 - \sin^2\theta$$

$$A^2 \int_0^L \frac{1}{2}\left(1 - \cos\frac{2n\pi x}{a}\right) dx = 1$$

$$\frac{A^2}{2}\left[x - \frac{a}{2\pi n}\sin\frac{2n\pi x}{a}\right]_0^L dx = 1$$

$$|A|^2\left(\frac{L}{2}\right) = 1 \quad \rightarrow \quad |A| = \sqrt{\frac{2}{L}}$$

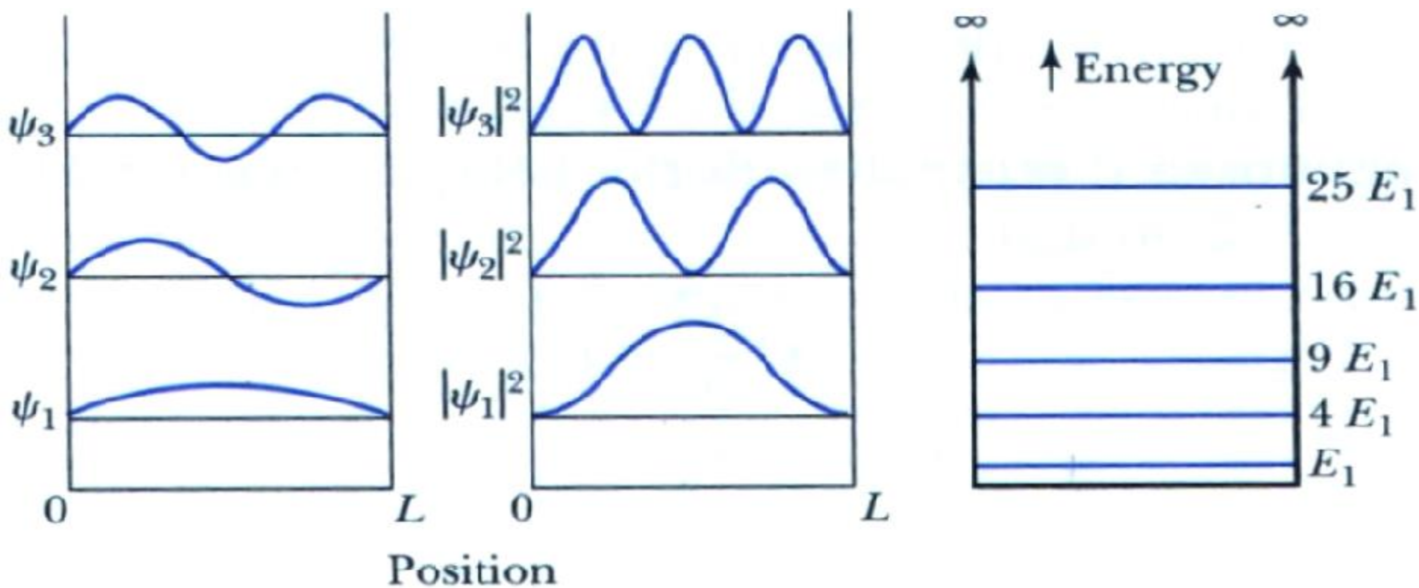
$A = \sqrt{\dfrac{2}{L}}$ is the normalized constant

Wave Functions & Probability densities

Our normalized wave function is:

$$\Psi_n = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{a}\right) \qquad n = 1,2,3,\ldots$$

Wave function Ψ_n is called as Eigen function of the free particle and their corresponding energies eq.5 is called Eigen values.



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

Inference

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

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

1) Difference b/w adjacent energy levels:

$$\Delta E = E_{n+1} - E_n$$
$$= (2n + 1)\, E_1$$

2) zero point energy: As "n" is quantum number, the total energy is quantized and the lowest possible energy is never zero. This called zero-point energy.

3) Probability density is structure with regions of space demonstrating enhanced probability. At very high n values, spectrum becomes continuous convergence with CM **(Bohr's correspondence principle)**

Particle in a 2D Box

A similar argument can be made:

$$\frac{-\hbar^2}{2m}\left(\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}\right)=E\psi$$

$$\psi(x,y)=X(x)Y(y)$$

$$\downarrow$$

Our Wave Equations:

$$\frac{-\hbar^2}{2m}\frac{\partial^2 X}{\partial x^2}=E_x\psi$$

$$\frac{-\hbar^2}{2m}\frac{\partial^2 Y}{\partial y^2}=E_y\psi$$

Particle in a 2D box

Doing the same thing do these differential equations that we did in one dimension we get:

$$X = \sqrt{\frac{2}{L}} \sin \frac{n_x \pi x}{L_x} \qquad\qquad Y = \sqrt{\frac{2}{L}}_{y} \sin \frac{n_y \pi y}{L_y}$$

In one dimension we needed only one ‘n’, But in two dimensions we need an ‘n’ for the x and y component.

Since $\psi = X(x)Y(y)$

$$\psi_{n_x n_y} = \sqrt{\frac{4}{L_x L_y}} \sin \frac{n_x \pi x}{L_x} \sin \frac{n_y \pi y}{L_y} \longrightarrow \psi_{n_x} = \sqrt{\frac{2}{L}} \sin \frac{n \pi x}{L}$$

For energy levels:

$$E_{n_x} = \frac{n^2 h^2}{8mL^2} \longrightarrow E_{n_x n_y} = \frac{h^2}{8m}\left[\left(\frac{n_x}{L_x}\right)^2 + \left(\frac{n_y}{L_y}\right)^2\right]$$

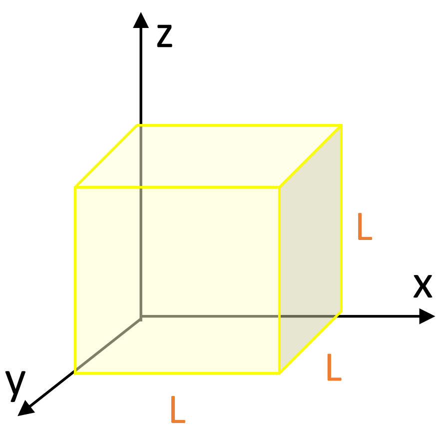
Particle in a 3D box

The extension of the Schrödinger Equation to 3D is straightforward in Cartesian (x,y,z) coordinates:

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}\right)+U(x,y,z)\psi = E\psi \quad \text{where } \psi \equiv \psi(x,y,z)$$

Kinetic energy term: $\frac{1}{2m}\left(p_x^2+p_y^2+p_z^2\right)$

Let's solve this SEQ for the particle in a 3D cubical box:



$$U(x,y,z) = \begin{cases} \infty & \text{outside box, } x \text{ or } y \text{ or } z < 0 \\ 0 & \text{inside box} \\ \infty & \text{outside box, } x \text{ or } y \text{ or } z > L \end{cases}$$

This U(x,y,z) can be "separated":
U(x,y,z) = U(x) + U(y) + U(z)

U = ∞ if any of the three terms = ∞.

Particle in a 3D box

If quantum numbers corresponding to x, y, z axes are n_x, n_y, n_z respectively for a rectangular box of sides a, b, c.

Each function contributes to the energy.
The total energy is the sum:

$E_{total} = E_x + E_y + E_z$

$$E_{Total} = E_{n_x n_y n_z} = \frac{h^2}{8m}\left[\frac{{n_x}^2}{a^2} + \frac{{n_y}^2}{b^2} + \frac{{n_z}^2}{c^2}\right]$$

Corresponding normalized wave function is

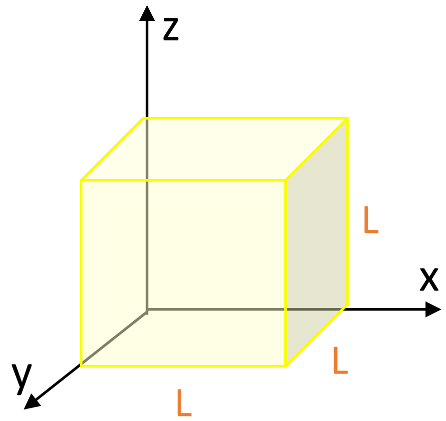
$$\psi_{n_x n_y n_z} = \sqrt{\frac{8}{a.b.c}}\left[Sin\frac{n_x \pi x}{a} Sin\frac{n_y \pi y}{b} Sin\frac{n_z \pi z}{c}\right]$$

Particle in a 3D box

The energy eigenstates and energy values in a 3D cubical box are:

$$\psi = N \sin\left(\frac{n_x \pi}{L_x} x\right) \sin\left(\frac{n_y \pi}{L_y} y\right) \sin\left(\frac{n_z \pi}{L_z} z\right)$$

$$E_{n_x n_y n_z} = \frac{h^2}{8m}\left(\frac{n_x^2}{L_x^{\ 2}} + \frac{n_y^2}{L_y^{\ 2}} + \frac{n_z^2}{L_z^{\ 2}}\right)$$



where n_x, n_y, and n_z can each have values 1,2,3,….

This one illustrates two important points:

- Three quantum numbers (n_x,n_y,n_z) are needed to identify the state of this three-dimensional system.

  That is true for every 3D system.

- More than one state can have the same energy: "Degeneracy".
  Degeneracy reflects an underlying symmetry in the problem.
  3 equivalent directions, because it's a cube, not a rectangle.

Summary

Energy Eigen value | Eigen Wave function

1D

$$E = \frac{n^2 h^2}{8mL^2}$$

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

2D

$$E_{n_x n_y} = \frac{h^2}{8m}\left[\left(\frac{n_x}{L_x}\right)^2 + \left(\frac{n_y}{L_y}\right)^2\right]$$

$$\psi_{n_x n_y} = \sqrt{\frac{4}{L_x L_y}} \sin\frac{n_x \pi x}{L_x} \sin\frac{n_y \pi y}{L_y}$$

3D

$$E_{n_x n_y n_z} = \frac{h^2}{8m}\left(\frac{n_x^2}{L_x^{\;2}} + \frac{n_y^2}{L_y^{\;2}} + \frac{n_z^2}{L_z^{\;2}}\right)$$

$$\psi = \sqrt{\frac{8}{L_x L_y L_z}} \sin\left(\frac{n_x \pi}{L_x} x\right) \sin\left(\frac{n_y \pi}{L_y} y\right) \sin\left(\frac{n_z \pi}{L_z} z\right)$$