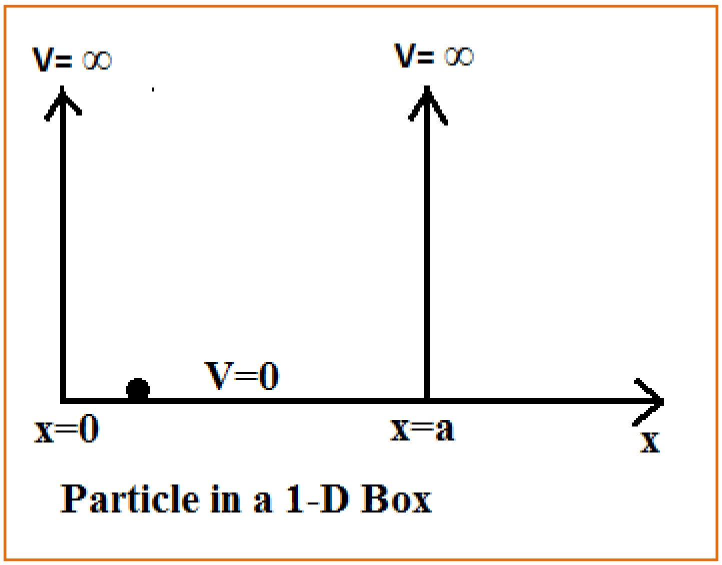
Application of Schrodinger Equation to One Dimensional System

- We need to solve Schrodinger Equation for some simple one dimensional systems to obtain the energy eigenvalues, eigenfunctions and their physical significance.
- The potential energy function V(x) will be different for different systems.
- Different systems will have different boundary conditions.
- The boundary conditions are imposed on the wavefunction.
- These are the predefined values of the wave function at the boundary of the system under consideration.

1. Particle in an infinitely rigid box

Suppose a particle is moving inside an infinitely rigid box of length ***a*** in one dimension like the following figure.



The potential is infinite everywhere except for $0 \leq x \leq a$ where it is zero. So,

$V(x) = 0$ for $0 \leq x \leq a$

$= \infty$ elsewhere.

As the particle is confined within the $0 \leq x \leq a$, we need to solve Schrodinger equation in the region $0 \leq x \leq a$. The solution is zero outside the region. Time independent Schrodinger equation reads

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = (E - V)\psi$$

Putting V=0

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi$$

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi,$$

$$or, \boldsymbol{\frac{d^2\psi}{dx^2} = -k^2\psi} \quad ----(1)\ where\ k^2 = \frac{2mE}{\hbar^2}$$

The general of the second order differential equation (1) is

$$\psi = A\sin kx + B\cos kx ------(2)$$

The constants A and b can be determined using proper boundary conditions. Note that the value of the wave function must be zero at the endpoints of the box. So

i) $\psi=0$ at x=0
ii) $\psi=0$ at x=a.

Putting the boundary condition (i) in equation (2), we get B=0. Then equation (ii) reduces to

$$\psi = A\sin kx ----(3)$$

Putting the boundary condition (ii) in equation (3), we get $A\sin ka = 0$. The constant A cannot be zero as it would make the wave function zero everywhere. So

$$\sin ka = 0, \quad or, \quad ka = n\pi \quad where\ n = 1,2,3, \ldots.$$

The value n=0 is left out as it leads to ψ=0. Thus $k = \frac{n\pi}{a}$.

$$\therefore \frac{2mE}{\hbar^2} = \frac{n^2\pi^2}{a^2}$$

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

These are the energy eigenvalues for different energy levels denoted by the value of n. Now the wave function becomes

$$\psi(x) = A\sin\frac{n\pi x}{a}$$

The normalization condition requires

$$\int_0^a \psi^2(x)dx = 1$$

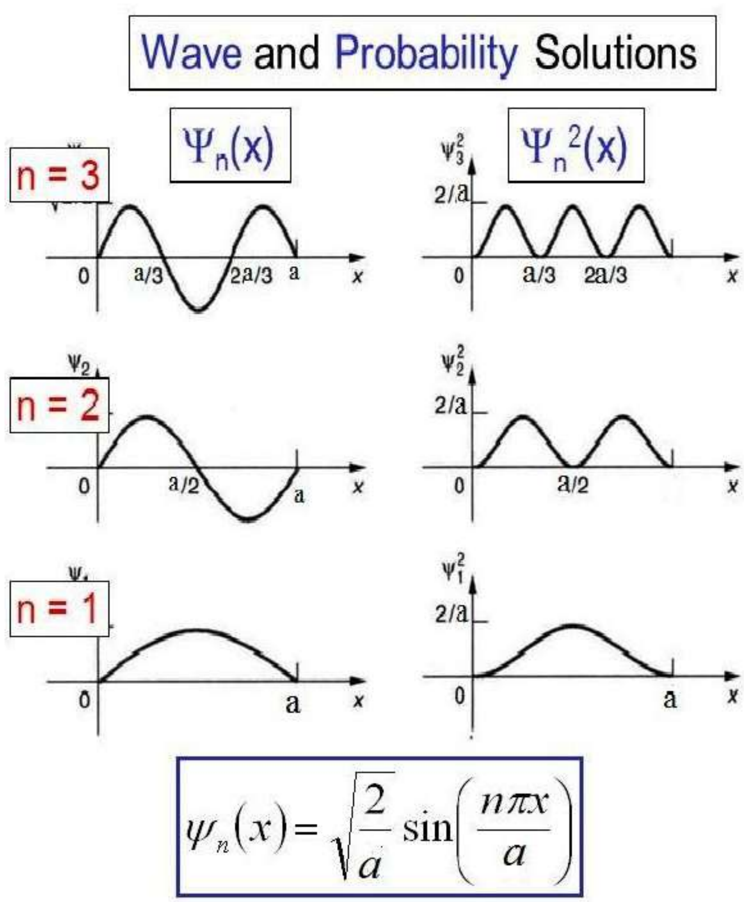
$$|A^2| \int_0^a \sin^2 \frac{n\pi x}{a} dx = 1$$

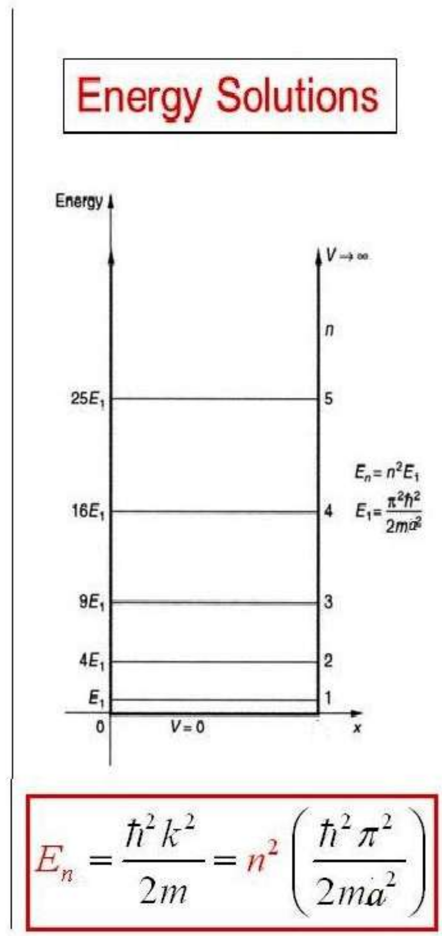
$$|A^2| \frac{a}{2} = 1$$

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

Thus the stationary state wave functions for the particle in an infinitely rigid box is given by

$$\boldsymbol{\psi_n(x) = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}} \qquad n = 1,2,3, \ldots$$





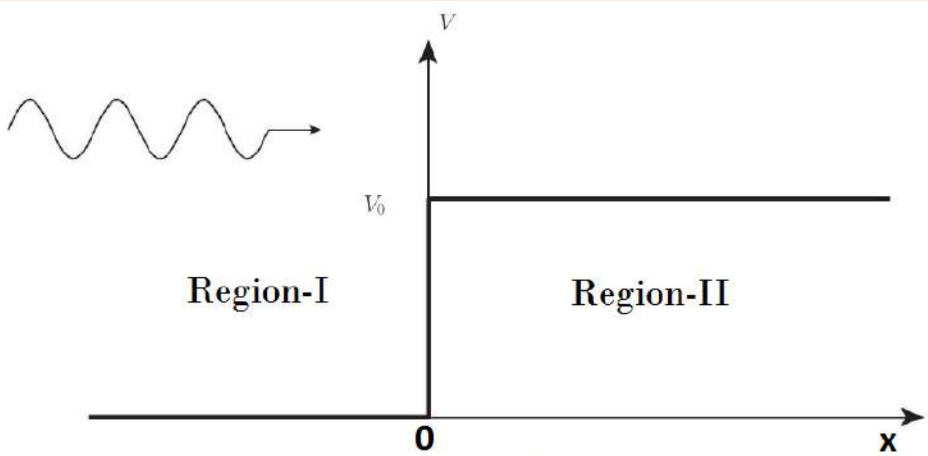
2. One Dimensional Step Potential

Consider a particle of mass m and energy E moving along X axis acted upon by a constant potential V_0 at all points x>0. The potential is zero for all x<0. A step potential of this type is given by

$V(x) = V_0, \ x>0$

$\quad\quad = 0, \ x<0$

Two cases may arise: (1) $E>V_0$ (Classically no reflection is possible towards region I) and (2) $E<V_0$ (Classically no transmission is possible in region II)



Step Potential

Case 1. $E>V_0$

First Part: General solution of Schrodinger Equation

For region I, (*x<0*) where *V(x)=0*, the time independent Schrodinger equation is

$$\frac{d^2\psi_1}{dx^2} + \frac{2mE}{\hbar^2}\psi_1 = 0, or, \frac{d^2\psi_1}{dx^2} + \alpha^2\psi_1 = 0 - (1)$$

$\alpha^2 = \frac{2mE}{\hbar^2}$ (a real quantity) and ψ_1 is the wave function in region I.

The general solution to equation (1) is

$$\psi_1(x) = Ae^{i\alpha x} + Be^{-i\alpha x} - (2)$$

The term $Ae^{i\alpha x}$ represents the incident particles and $Be^{-i\alpha x}$ represents the reflected particles.

For region II, (*x>0*) where *V(x)=V₀*, the time independent Schrodinger equation is

$$\frac{d^2\psi_2}{dx^2} + \frac{2m(E-V_0)}{\hbar^2}\psi_2 = 0, or, \frac{d^2\psi_2}{dx^2} + \beta^2\psi_2 = 0 - (3)$$

$\beta^2 = \frac{2m(E-V_0)}{\hbar^2}$ (a real quantity) and ψ_2 is the wave function in region II.

The general solution to equation (3) is

$$\psi_2(x) = Ce^{i\beta x} - (4)$$

Since in region II, the wave propagates to right only, there is no question of reflecting back and thus $e^{-i\alpha x}$ term is absent.

Second Part: Applying Boundary Conditions

The three co-efficients A, B, C can be obtained by applying boundary conditions at *x=0*. The boundary conditions are-

i) Wave function ψ is continuous at x=0

$$(\psi_1)_{x=0} = (\psi_2)_{x=0}$$

ii) $\frac{d\psi}{dx}$ is continuous at x=0.

$$(\frac{d\psi_1}{dx})_{x=0} = (\frac{d\psi_2}{dx})_{x=0}$$

Applying the boundary condition (i) at x=0 in equations (2) and (4) we get

$$A + B = C \dots (5)$$

Applying the boundary condition (ii) at x=0 in equations (2) and (4) we get

$$A - B = \frac{\beta}{\alpha} C \ldots (6)$$

Solution:

Solving 5 and 6 we get,

$$A = \frac{C}{2}\left(1 + \frac{\beta}{\alpha}\right) \ldots (7)$$

$$B = \frac{C}{2}\left(1 - \frac{\beta}{\alpha}\right) \ldots (8)$$

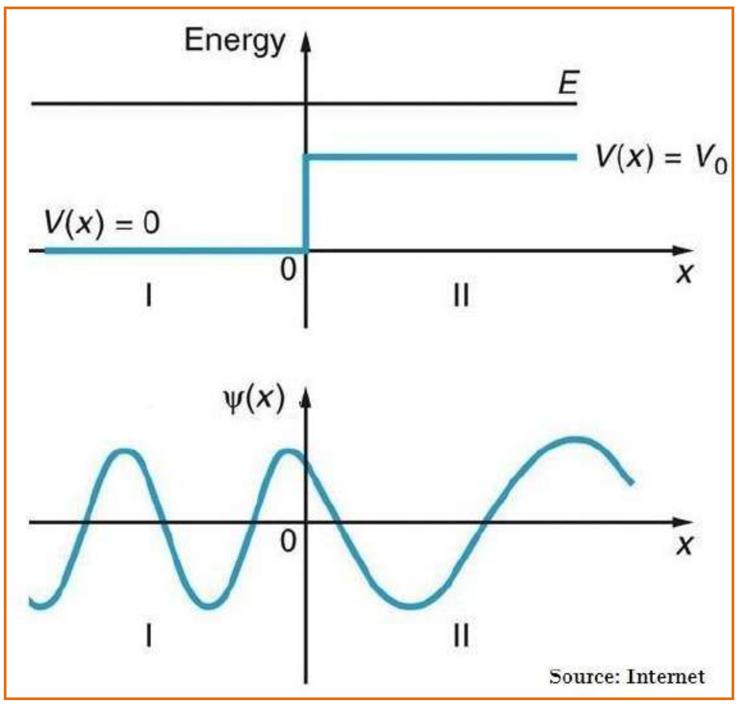
Hence we have

$$\frac{B}{A} = \frac{\alpha - \beta}{\alpha + \beta} \ldots \ldots (9)$$

$$\frac{C}{A} = \frac{2\alpha}{\alpha + \beta} \ldots \ldots (10)$$

Remember: A represents incident particles, B represents reflected particles, C represents transmitted particles.

According to equation 10, C>A as α>β. So the amplitude of the transmitted wave is greater than the amplitude of incident wave. Nature of the wave function is shown in the following figure.



Transmission co-efficient is defined as

$$T = \frac{Probability\ current\ density\ for\ transmitted\ wave}{Probability\ current\ density\ for\ incident\ wave}$$

$$= \frac{S_t}{S_i}$$

$$= \frac{\frac{\hbar\beta}{m}|C|^2}{\frac{\hbar\alpha}{m}|A|^2}$$

$$= \frac{\beta}{\alpha}\frac{|C|^2}{|A|^2}$$

$$= \frac{\beta}{\alpha}(\frac{2\alpha}{\alpha+\beta})^2$$

$$= \frac{4\alpha\beta}{(\alpha+\beta)^2}$$

Reflection co-efficient is defined as

$$R = \frac{Probability\ current\ density\ for\ reflected\ wave}{Probability\ current\ density\ for\ incident\ wave}$$

$$= \frac{S_r}{S_i}$$

$$= \frac{\frac{\hbar\alpha}{m}|B|^2}{\frac{\hbar\alpha}{m}|A|^2}$$

$$= (\frac{\alpha-\beta}{\alpha+\beta})^2$$

$$Thus, R + T = 1$$

This also shows there is a non-zero, finite probability of reflection at the step.

2. One Dimensional Step Potential *(Continued)*

Case 2. $E<V_0$

First Part: General solution of Schrodinger Equation

For region I, (*x<0*) where *V(x)=0*, the time independent Schrodinger equation is

$$\frac{d^2\psi_1}{dx^2}+\frac{2mE}{\hbar^2}\psi_1=0, or, \frac{d^2\psi_1}{dx^2}+\alpha^2\psi_1=0-(1)$$

$\alpha^2=\frac{2mE}{\hbar^2}$ (a real quantity) and ψ_1 is the wave function in region I.

The general solution to equation (1) is

$$\psi_1(x)=Ae^{i\alpha x}+Be^{-i\alpha x}-(2)$$

The term $Ae^{i\alpha x}$ represents the incident particles and $Be^{-i\alpha x}$ represents the reflected particles.

For region II, (*x>0*) where $V(x)=V_0$, the time independent Schrodinger equation is

$$\frac{d^2\psi_2}{dx^2}+\frac{2m(E-V_0)}{\hbar^2}\psi_2=0, or, \frac{d^2\psi_2}{dx^2}-\beta^2\psi_2=0-(3)$$

$\beta^2=\frac{2m(V_0-E)}{\hbar^2}$ and ψ_2 is the wave function in region II. *Notice the change in β to keep it positive*

The general solution to equation (3) is

$$\psi_2(x)=Ce^{-\beta x}-(4)$$

In region II, $Ce^{-\beta x}$ is an exponentially decreasing function, which penetrates the potential barrier for some finite distance in positive X direction. $De^{\beta x}$ term is an exponentially increasing wave function. But according to physical interpretation of wave function, a wave function must remain finite when $x\to\infty$. So d must be zero, hence this term is omitted.

Second Part: Applying Boundary Conditions

The three co-efficients A, B, C can be obtained by applying boundary conditions at *x=0*. The boundary conditions are-

i) Wave function ψ is continuous at x=0

$$(\psi_1)_{x=0} = (\psi_2)_{x=0}$$

ii) $\frac{d\psi}{dx}$ is continuous at x=0.

$$(\frac{d\psi_1}{dx})_{x=0} = (\frac{d\psi_2}{dx})_{x=0}$$

Applying the boundary condition (i) at x=0 in equations (2) and (4) we get

$$A + B = C \ldots (5)$$

Applying the boundary condition (ii) at x=0 in equations (2) and (4) we get

$$A - B = \frac{i\beta}{\alpha} C \ldots (6)$$

Solution:

Solving 5 and 6 we get,

$$A = \frac{C}{2}\left(1 + \frac{i\beta}{\alpha}\right) \ldots (7)$$

$$B = \frac{C}{2}\left(1 - \frac{i\beta}{\alpha}\right) \ldots (8)$$

Hence we have

$$\frac{B}{A} = \frac{\alpha - i\beta}{\alpha + i\beta} \ldots\ldots (9)$$

$$\frac{C}{A} = \frac{2\alpha}{\alpha + i\beta} \ldots\ldots (10)$$

Reflection Co-efficient

$$R = \frac{|B|^2}{|A|^2}$$

$$= \frac{|\alpha - i\beta|^2}{|\alpha + i\beta|^2} = 1$$

Since T+R=1, T=0. The conclusions from the result are-

i) There is a finite probability of finding the particle in region II represented by the factor $e^{-\beta x}$ in equation (4).

ii) There is no absorption in region II, 100% reflection at the boundary. The wave penetrating a small distance into region II is continuously reflected till all the incident energy is reflected back to region 1.

iii) According to classical mechanics a particle of energy $E<V_0$ can never penetrate into region II. But in quantum mechanics, there is a finite probability of finding the particle at region II within a short distance.