Photon and Matter Waves

Quantization of Energy:-

In black body radiation it was considered that the radiation was emitted continuously. In 1902 Planck had shown that the energy from the body was emitted in separate packets of energy. The energy of each packet is equal to hf, called a quantum energy.

$i.e. E = hf$ Where, h = 6.67×10^{-34} JS is the Planck's constant. And f is the frequency of radiation. This theory is called Planck's quantum theory.

In general for n number of photons the total energy is;

$E_n = nhf$ Where, n =0,1,2,3,…

This means energy is emitted in the form of discrete amount. i.e. Energy is multiple of fundamental energy 'hf'. So energy is quantized.

De- Broglie Equation:-

De-Broglie suggested his hypothesis that there is "wave particle dualism" i.e. particle nature of electrons and wave nature of electrons.

To show the wave particle dualism he used Planck's theory of quantum radiation and Einstein's theory of relativity.

According to Planck's theory of quantum radiation energy of photon is given by;

$$E = hf = \frac{hC}{\lambda} \dots \dots \dots (i)$$

Again, According to Einstein mass energy relationship, energy of photon is given by;

$$E = mC^2 \dots \dots \dots (ii)$$

From equations (i) and (ii)

$$\frac{hC}{\lambda} = mC^2$$

$$\lambda = \frac{h}{mC} = \frac{h}{p}$$

Therefore according to De- Broglie, the wavelength of the wave associated with the moving particle having momentum $P = mv$ is given by; $\lambda = \frac{h}{mv}$.

The de-Broglie Electron wave:-

According to de-Broglie if an electron is accelerated to various velocities at various potential, different waves having different wave length are produced.

For de-Broglie matter wave we have,

$$\lambda = \frac{h}{p} = \frac{h}{mv} \dots \dots \dots \dots (1)$$

If an electron of mass 'm' is accelerated through the potential 'V' and velocity v then,

$$\frac{1}{2}mv^2 = eV \Rightarrow v = \sqrt{\frac{2eV}{m}} \ldots\ldots\ldots (2)$$

$$\therefore \lambda = \frac{h}{m\sqrt{\frac{2eV}{m}}} = \frac{h}{\sqrt{2meV}}$$

$$\therefore \text{Wave length of electron wave}, \lambda = \frac{h}{\sqrt{2meV}}$$

Wave and group Velocity:-

According to de-Broglie, each particle of matter in motion is associated with a group of wave or wave packet. The velocity of this group of wave which is quantitatively equal to mechanical velocity of the particle is called group velocity. It is given by

$$v = \frac{dw}{dk}$$

This group of wave consist of different component waves. The velocity with each component of the wave propagates is called phase or wave velocity. It is given by $u = f\lambda$.

Relation between group velocity and Phase velocity:-

We know wave vector $k = \frac{2\pi}{\lambda}$

$$\frac{dk}{d\lambda} = -\frac{2\pi}{\lambda^2}$$

And, $w = 2\pi f = \frac{2\pi u}{\lambda}$

$$\frac{dw}{d\lambda} = -\frac{2\pi u}{\lambda^2} + \frac{2\pi}{\lambda}\frac{du}{d\lambda}$$

$$\therefore \text{Group velocity}, v = \frac{dw}{dk} = \frac{dw/d\lambda}{dk/d\lambda}$$

$$= \frac{-\lambda^2}{2\pi}\left(\frac{-2\pi u}{\lambda^2} + \frac{2\pi}{\lambda}\frac{du}{d\lambda}\right)$$

$$v = u - \lambda\frac{du}{d\lambda}$$

This shows the relation between wave velocity (u) and group velocity (v). This shows that wave velocity is always greater than group velocity.

Wave Function and its significance:-

A simple harmonic wave is represented by the equation; $y = Asin(wt - kx)$. In such type of wave motion there is only the transfer of energy but in case of matter wave there is transfer of momentum in addition to the energy. The suitable function to represented wave function for matter wave is;

$$\psi(x,t) = Ae^{-i(wt-kx)} \ldots\ldots\ldots (i)$$

Science $E = hf = 2\pi\hbar f = w\hbar$

$$i.e\ w = \frac{E}{ħ}$$

$$\text{We have, } P = \frac{h}{\lambda} = \frac{2\pi ħ}{\lambda} = kħ$$

$$i.e.k = \frac{P}{ħ}$$

Therefore equation (i) can be represented as;

$$\psi(x,t) = Ae^{-\frac{i}{ħ}(Et-Px)} \ldots\ldots\ldots.(ii)$$

The wave function ψ has no physical meaning itself, when it is operated by Schrodinger wave equation; it describes the motion of the particle associated with it as done by second law of motion in classic mechanics.

The only quantity having physical meaning is the square of its magnitude.

$P = \psi\psi^* = |\psi|^2$ where ψ^* is complex conjugate of ψ. The quantity $P = |\psi|^2$ evaluated at a particular point at particular time is proportional to the probability of finding the particle at that time.

Schrodinger time independent wave equation :-

Schrodinger wave equations describe a motion of quantum mechanical particle as Newton's second law in classic mechanics. The wave function for quantum mechanical particle is given by;

$$\psi(x,t) = Ae^{-\frac{i}{\hbar}(Et-Px)} \dots\dots\dots (1)$$

Now differentiating this equation with respect to x,

$$\frac{d\psi}{dx} = \frac{iP}{\hbar} Ae^{-\frac{i}{\hbar}(Et-Px)}$$

$$or\ P\psi = \frac{\hbar}{i}\frac{d\psi}{dx} = -i\hbar\frac{d\psi}{dx}$$

$$\therefore P\psi = -i\hbar\frac{d\psi}{dx} \dots\dots\dots (2)$$

Similarly, differentiating equation (1) two times w. r. t. x we get;

$$\therefore P^2\psi = -\hbar^2 \ \frac{d^2\psi}{dx^2} \dots\dots\dots. (3)$$

Consider a particle of mass m and potential energy V moving with velocity v, then total energy is given by;

$$E = \frac{1}{2}mv^2 + V$$

$$E = \frac{1}{2}\frac{m^2v^2}{m} + V$$

$$E = \frac{P^2}{2m} + V$$

Now multiplying this equation by ψ

$$E\psi = \frac{P^2\psi}{2m} + V\psi \dots\dots\dots (4)$$

Now from equation (3) and (4)

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

$$\therefore\ \frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + (E - V)\psi = 0$$

$$or\ \frac{d^2\psi}{dx^2} + \frac{2m(E-V)}{\hbar^2}\psi = 0$$

This is the time independent Schrodinger wave equation in one dimension. In three dimensions above equation can be written as;

$$\nabla^2\psi + \frac{2m(E-V)}{\hbar^2}\ \psi = 0$$

Schrodinger time dependent wave equation:-

The wave function for quantum mechanical particle is given by;

$$\psi(x,t) = Ae^{-\frac{i}{\hbar}(Et-Px)} \dots\dots\dots (1)$$

Now differentiating this equation with respect to t,

$$\frac{d\psi}{dt} = \frac{-iE}{\hbar}Ae^{-\frac{i}{\hbar}(Et-Px)} = \frac{-iE}{\hbar}\psi$$

$$or, E\psi = -\frac{\hbar}{i}\frac{d\psi}{dt} = i\hbar\frac{d\psi}{dt}$$

$$\therefore\ E\psi = i\hbar\frac{d\psi}{dt} \dots\dots\dots (2)$$

Consider a particle of mass m and potential energy V moving with velocity v, then total energy is given by;

$$E = \frac{1}{2}mv^2 + V$$

$$E = \frac{1}{2}\frac{m^2v^2}{m} + V$$

$$\therefore E = \frac{P^2}{2m} + V$$

Now multiplying this equation by ψ

$$E\psi = \frac{P^2\psi}{2m} + V\psi$$

$$\therefore i\hbar\frac{d\psi}{dt} = -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi$$

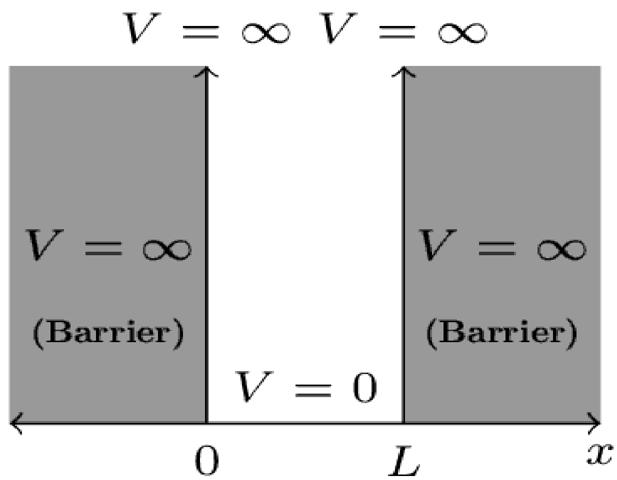
$$\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + i\hbar\frac{d\psi}{dt} - V\psi = 0$$

This is required time dependent Schrodinger wave equation in one dimension. In three dimensions above equation can be written as,

$$\frac{\hbar^2}{2m}\nabla^2\psi + i\hbar\frac{d\psi}{dt} - V\psi = 0 .$$

Applications of Schrodinger wave equation:-

A particle in an one dimensional infinitely deep potential well:-



Consider a particle restricted to move along $x = 0$ and $x = l$. The potential energy (V) of the particle is zero inside the box but raise to ∞ on the outside.

$i.e. V = 0$ for $0 < x < l$

and $V = \infty$ for $x \leq 0$ and $x \geq l$

In such case the particle is said to be moving in an infinitely deep potential well. The Schrodinger wave equation for the particle within the box is;

$$\frac{d^2\psi}{dx^2} + \frac{2m(E-V)}{\hbar^2}\psi = 0 \ldots\ldots\ldots (1)$$

$$\frac{d^2\psi}{dx^2} + \frac{2mE\psi}{\hbar^2} = 0 \ldots\ldots\ldots (2)$$

$$\text{Let, } k^2 = \frac{2mE}{\hbar^2} \ldots\ldots\ldots (3)$$

$$\therefore \frac{d^2\psi}{dx^2} + k^2\psi = 0 \ldots\ldots\ldots(4)$$

The solution of above equation is

$$\psi(x) = A\, sinkx + Bcoskx \ldots\ldots\ldots(5)$$

Where A and B are constants to be determine using Boundary condition. Science the particle cannot exist outside the box. Therefore the wave function ψ must be zero, outside the box and at the walls;

$$i.e. x = 0\ and\ x = l$$

$$for\ x = 0$$

$$\psi(x) = 0$$

$$\therefore 0 = 0 + B$$

$$\therefore B = 0$$

$$\text{Similarly, for } x = l$$

$$\psi(x) = 0$$

$$\therefore\ 0 = Asinkl + 0$$

$$or, \qquad sinkl = 0$$

$$or, \qquad sinkl = \sin n\pi$$

$$or, \qquad kl = n\pi$$

$$k = \frac{n\pi}{l} \ldots\ldots\ldots(6)$$

From equations (3) and (6)

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

$$or, \qquad \frac{n^2\pi^2}{l^2} = \frac{2mE}{\hbar^2}$$

$$\therefore E = \frac{n^2\pi^2\hbar^2}{2ml^2}$$

This means the energy of the particle in potential well is quantized. Each value of energy given by above relation is called Eigen value and corresponding function is called Eigen function.

Now substituting, $B = 0 \; and \; k = \frac{n\pi}{l}$ in equation (5), the allowed solutions of Schrodinger equation are;

$$\psi_n(x) = A \sin\left(\frac{n\pi x}{l}\right)$$

The coefficient A is called Normalizing constant and can be determined using Normalizing condition.

$$\int_0^l \psi\psi^* dx = 1$$

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

$$or, A^2 \int_0^l \frac{1}{2}(1 - cos2\frac{n\pi x}{l})dx = 1$$

$$or, A^2 \left[\frac{1}{2}\int_0^l dx - \frac{1}{2}\int_0^l \cos\frac{2n\pi x}{l}\, dx\right] = 1$$

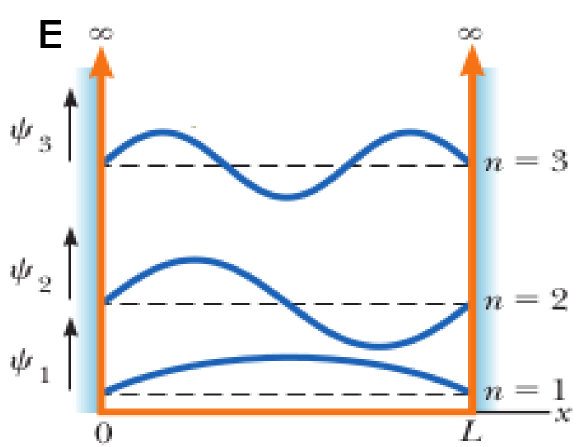
$$or, A^2.\frac{l}{2} = 1$$

$$or, A = \sqrt{\frac{2}{l}}$$

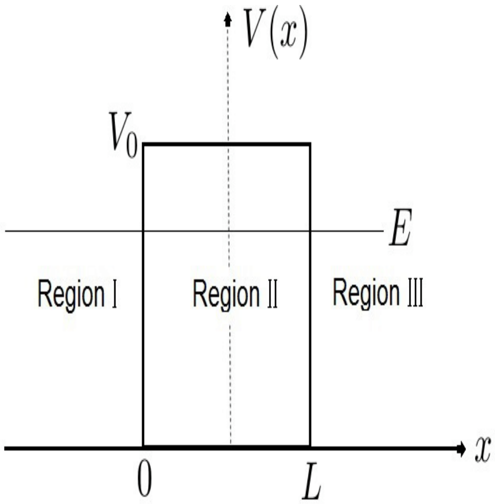
∴ The normalized wave functions of the particles are therefore

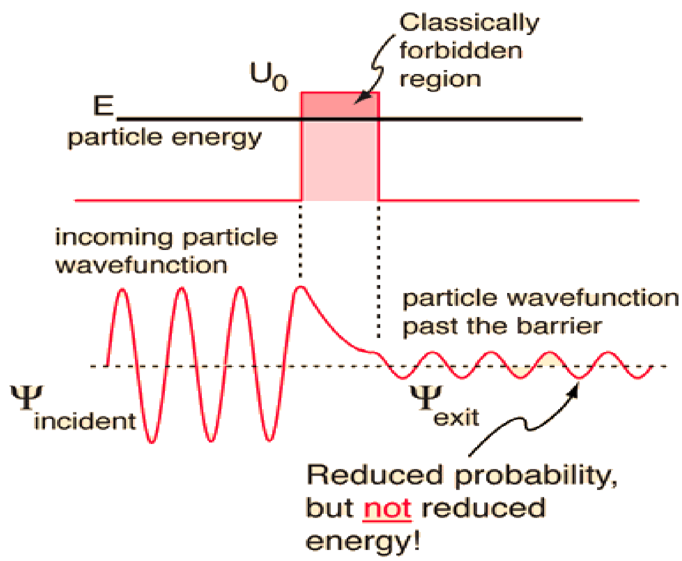
$$\psi_n(x) = \sqrt{\frac{2}{l}}\sin\left(\frac{n\pi x}{l}\right)$$

The first three Eigen functions, ψ_1, ψ_2, ψ_3 and Eigen values are shown in figure below.



Barrier Tunneling:-





Tunneling is a quantum mechanical phenomenon when a particle is able to penetrate through a potential energy barrier that is higher in energy than the particle's kinetic energy. The probability of finding the particle in third region by penetrating the barrier is known as barrier tunneling. Consider a barrier of potential V having width L. When a moving particle of energy $E < V$ be incident on the barrier from the left of region I, classically region II and III are forbidden to particle. But for quantum mechanics all region are accessible to the particle. This is because for relatively narrow barrier, in short time, the particle can allow to cross it. This effect of quantum mechanical particle is called barrier tunneling.

The potential function for barrier tunneling can be expressed as;

$\mathrm{V(x) = 0, for\ x < 0}$

$= V_0$ for $0 < x < L$ and

$= 0$ for $x > L$

The Schrodinger wave equation in region I, II and III are

$$\frac{d^2\psi_I}{dx^2} + \frac{2mE\psi_I}{\hbar^2} = 0 \quad \text{or,} \qquad \frac{d^2\psi_I}{dx^2} + \beta^2\psi_I = 0$$

where $\beta^2 = \frac{2mE}{\hbar^2}$

$$\frac{d^2\psi_{II}}{dx^2} + \frac{2m(E-V_0)\psi_{II}}{\hbar^2} = 0 \quad \text{or,} \qquad \frac{d^2\psi_{II}}{dx^2} + \alpha^2\psi_{II} = 0$$

where $\alpha^2 = \frac{2m(E-V_0)}{\hbar^2}$

$$\frac{d^2\psi_{III}}{dx^2} + \frac{2mE\psi_{III}}{\hbar^2} = 0 \quad \text{or,} \qquad \frac{d^2\psi_{III}}{dx^2} + \beta^2\psi_{III} = 0$$

where $\beta^2 = \frac{2mE}{\hbar^2}$

The wave functions in these regions are;

$\psi_I = Ae^{i\beta x} + Be^{-i\beta x}$, where A is the amplitude of the incident wave and B is the amplitude of the reflected wave.

$\psi_{II} = Ce^{-\alpha x} + De^{\alpha x}$, where C is the amplitude of the incident wave and D is the amplitude of the reflected wave.

And $\psi_{III} = Fe^{i\beta x}$ where F is the amplitude of the transmitted wave.

The transmission coefficient represents the probability that the particle penetrates to the other side of the barrier. It is

$$T = \frac{|F|^2}{|A|^2} = \frac{16E(V_0 - E)}{V_0^2} e^{-2k_2 L}$$

where, $$k_2 = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$$

Numerical Examples:-

1. **Calculate the wavelength associated with an electron subjected to a potential difference of 1.25 KV.**

Solution:-

We have; $\frac{1}{2}mv^2 = eV$

$$or, v = \sqrt{\frac{2eV}{m}}$$

$$\text{Now; } \lambda = \frac{h}{mv} = \frac{h}{\sqrt{2meV}}$$

$$= \frac{6.62 \times 10^{-34}}{\sqrt{2 \times 1.6 \times 10^{-19} \times 9.1 \times 10^{-31} \times 1.25 \times 10^{3}}}$$

$$\therefore \lambda = 0.347 A^0$$

2. **Find the energy of the neutron in units of eV. Which de-Broglie wavelength is 1 A^0. Given mass of neutron = $1.67 \times 10^{-27}\ Kg$.**

Solution:-

wavelength $(\lambda) = 1\ \mathrm{A}^0 = 1 \times 10^{-10}$ m

Mass of neutron $= 1.67 \times 10^{-27}\ Kg$

We know that; $\lambda = \dfrac{\mathrm{h}}{\mathrm{mv}}$

$$\therefore \mathrm{v} = \frac{\mathrm{h}}{\mathrm{m}\lambda} = \frac{6.62 \times 10^{-34}}{1.67 \times 10^{-27} \times 1 \times 10^{-10}}$$
$$= 3964.07\ m/sec$$

$$\therefore E = \frac{1}{2}\ mv^2 = \frac{1}{2}\ 1.67 \times 10^{-27} \times (3964.07)^2$$
$$= 1.31 \times 10^{-20}\ Joule$$

$= 8.13 \times 10^{-2}\ eV$

3. **What voltage must be applied to an electron microscope to produce electron of wavelength $0.50\ A^0$.**

Solution:-

Charge of electron (e) $= 1.6 \times 10^{-19}$

Wavelength $(\lambda) = 0.50\ \mathrm{A}^0 = 0.50 \times 10^{-10}$ m

Mass of electron (m) $= 9.1 \times 10^{-31}\ Kg$

We have; $\frac{1}{2}\mathrm{mv}^2 = \mathrm{eV}$

$$or, \mathrm{eV} = \frac{1}{2}\mathrm{m}(\frac{\mathrm{h}}{\mathrm{m}\lambda})^2$$

$$= \frac{1}{2} \times \frac{(6.62 \times 10^{-34})^2}{9.1 \times 10^{-31} \times (0.50 \times 10^{-10})^2}$$

$\therefore$ V = 597.89 volts

4. An electron is confined to an infinite height box of size $0.1\ nm$. Calculate the ground state energy of the electron. How this electron can be put to the third energy level?

Solution:-

Width (l) = 0.1 nm = 0.1×10^{-9} m

$$\text{We have; Energy } (E) = \frac{n^2\pi^2\hbar^2}{2ml^2} = \frac{n^2h^2}{8ml^2}$$

$$= \frac{n^2(6.62 \times 10^{-34})^2}{8 \times 9.1 \times 10^{-31} \times 0.1 \times 10^{-9}}$$

$= 6.05 \times 10^{-18}\ n^2\ Joule$

$= 37.7\ n^2\ eV$

In ground state; n = 1, $E_1 = 37.7\ eV$

In third energy state; n = 3, $E_3 = 37.7 \times 3^2\ eV$

$$= 37.7 \times 9\ eV$$

$\therefore E_3 - E_1 = (9-1) \times 37.7 = 301.5\ eV$

Hence to put the electron to third energy level an extra energy of 301.5 eV is to be given.

5. The wave function of a particle confined in a box of length $\boldsymbol{l}$ is $\psi(x) = \sqrt{\frac{2}{l}}\ \boldsymbol{sin}\frac{\pi x}{l}$. Calculate the probability of finding the particle in length 0 to $\frac{l}{2}$.

Solution:-

The probability of finding the particle in length 0 to $\frac{l}{2}$ is;

$$P = \int_0^{\frac{l}{2}} |\psi|^2 dx$$

$$= \int_0^{l/2} \frac{2}{l} sin^2 \frac{\pi x}{l}\ dx = \frac{2}{l}\int_0^{l/2} (1 - cos\frac{2\pi x}{l})dx$$

$$\therefore P = \frac{2}{l} . \frac{l}{4} = \frac{1}{2} = 50\ \%$$

6. Calculate the probability of transmission of α particle through the rectangular barrier indicated below. Height of the barrier $(\boldsymbol{V}) = \boldsymbol{2\ eV}$, energy of α particle

$(E) = 1\ eV$ barrier width $(L) = 1\ A^0$, mass of α particle $(m) = 6.4 \times 10^{-27}\ kg$.

Solution:-

$$\hbar = \frac{h}{2\pi} = \frac{6.62 \times 10^{-34}}{2\pi} = 1.0557 \times 10^{-34} \text{ J sec}$$

$$K_2 = \sqrt{\frac{2m(V-E)}{\hbar^2}}$$

$$= \sqrt{\frac{2 \times 6.4 \times 10^{-27}(2-1) \times 1.16 \times 10^{-19}}{(1.0557 \times 10^{-34})^2}}$$

$$\therefore K_2 = 4.2867 \times 10^{11}$$

$$And, \quad \frac{16E(V-E)}{V^2}$$

$$= \frac{16 \times 1 \times 1.16 \times 10^{-19}(2-1) \times 1.16 \times 10^{-19}}{(2 \times 1.16 \times 10^{-19})^2}$$

$$= 4$$

$$\therefore \text{Transmission coefficient (T)} = \frac{16E(V-E)}{V^2}.e^{-2K_2L}$$

$$= 4 \times e^{-2\times 4.2867\times 10^{11}\times 1\times 10^{-10}}$$

$$= 1.47 \times 10^{-37}$$

Exercise:-

1. What are the significance of wave function? Using the wave function derive and expression for the dependent Schrodinger wave equation.
2. Write down Schrodinger time dependent and time independent wave equations. Prove that the energy levels are quantized when the electron is confined in an infinite potential well of width ‘a’.
3. A free particle is confined in a box of width L. Using Schrodinger wave equation find an expression for the energy Eigen value.
4. Derive Schrodinger time independent wave equation. A particle is moving in one dimensional potential well of infinite height and width ‘a’. Find the expression for energy of the particle.
5. Determine the total energy of a particle using Schrodinger equation, when the potential energy has value V = 0 for $0 < x < a, and\ V = \infty\ for\ x \leq 0\ and\ x \geq a$.
6. What is barrier tunneling? Discuss and write the Schrodinger wave equation in each region. Also write the formula of transmission coefficient, T in this case.
7. Prove that the energy level are quantized , when the electron is confined in an infinite potential well of width ‘a’
8. A beam of electrons having energy of each 3eV is incident on a potential barrier of height 4eV. If the width of the barrier is $20A^0$, calculate the transmission coefficient of the beam through the barrier.

9. A non relativistic particle is moving three times as fast as an electron. The ratio of the de- Broglie wavelength of the particle to that of the electron is 1.813×10^{-4}. Calculate the mass of the particle.

10. Using the uncertainty principle, calculate the minimum uncertainty in velocity when an electron is confined to a length $\Delta x = 1nm$. Given, $\mathrm{m} = 9.1 \times 10^{-31}$ Kg, $\mathrm{h} = 6.6 \times 10^{-34}$ Js.

(Formula:- $\Delta x \Delta p \geq \frac{h}{4\pi}$, where Δx is uncertainty in position and Δp is uncertainty of momentum)

11. An electron is confined in an one dimensional infinite potential well of width a, the potential energy is $\mathrm{V} = 0$ for $0 \leq \mathrm{x} \leq a$ and $\mathrm{V} = \infty$ for $\mathrm{x} \leq 0$ and $\mathrm{x} \geq a$. Find the Eigen functions $\psi_n(x) = A \sin\left(\frac{n\pi x}{a}\right)$ and energy Eigen values $E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$.

12. Calculate the permitted energy levels of an electron in one dimensional potential well of width 0.2nm.