Table of Contents

Introduction Quantum Mechanics

"The branch of mechanics that deals with the mathematical description of motion and interaction of sub-atomic particles incorporating the concepts of quantization of energy, wave-particle duality, the uncertainity principle and the correspondence principle is <u>quantum mechanics</u>."

At the scale of atoms and electrons many of the equations of classical mechanics, which describe how things move at every day sizes and speeds, cease to be useful. In classical mechanics objects exist in specific place at a time. However, in quantum mechanics objects instead exist in a haze of probability; they have a certain chance being at point A another chance of being at point B and so on.

Light can sometimes behave as a **particle**. Added wave crests results in brighter lighter spectral lines while waves cancel out to give darkness. **Matter** can also behave as a **wave**.

Quantum mechanics is also known as <u>quantum physics</u>.

→ **While studying Quantum Mechanics or Quantum Physics must keep in view the following six points:**

(i) Every thing is made of waves.

Every thing in the universe is having both particle and wave nature at the same time.

"All is waves, with nothing waving, over no distance at all"

The objects depticed in Quantum Mechanics are neither particles nor waves but a third ~~categgory~~ category that share properties of waves (a frequency and a wavelength) and some properties of particles (they can be counted and can be localized).

(ii) Quantum Physics is Discrete.

The word quantum comes from Latin word "quantum" meaning "how much". Quantum model always include models coming in discrete amounts. For light of higher frequency and shorter wavelenght has a large energy and vice versa. The energy comes in integer multiples of energy 1, 2, ... 137 times. This property is also been seen in discrete energy levels of atoms and energy bands of solids.

(iii) Quantum Physics is Probabilistic.

It is impossible to predict the outcome of some experiments in Quantum physics with certainity. The mathematical description of quantum system is represented by Ψ. The probability of finding an outcome is not given directly by the wavefunction and the operation to get probability is slightly more involved but

but "square of the wavefunction" is enough good. Some particles may be at multiple states in one time. All we can predict is probability and prior to a measurement that describes a particular outcome, in which a system being measured in superposition of all possible probabilities.

(iv) Quantum Physics is non-local

The EPR paper argued that quantum physics allowed the existence of systems where measurements made at widely separated locations could be correlated. Quantum mechanics must be in-complete a mere approximation. Quantum mechanics is non-local that results of the measurements made at a particular location can depend on the properties of distant objects in a way that cannot be explained using signals moving at speed of light.

(V) Quantum physics is very small

The wavelenght of the macroscopic objects is very small that it can be considered as a single atom in a the entire solar system. Quantum phenomena is confined to the scale of atoms and fundamental particles where masses and velocities are relatively small so that the wavelenghts can be observed.

(Vi) Quantum Physics is not magic

The things quantum physics predicts are really odd but they are well understood by laws of the mathematics. We can find some practical work in quantum but it will remain in certain condition.

DeBrogile used theory of special relativity to show particle also have wave nature and that wave also have particle like nature. Heisenberg proposed a "matrix mechanics" showing how electron whized around in the atoms and Schrödinger proposed "wave mechanics".

The Heisenberg-Schrödinger model in which electron acts as a wave replaced Rutheford's model of atom. Unlike Rutherford's model atomic orbitals have a variety of shapes.

Schrödinger's wave mechanics

Schrödinger was guided by a mathematical formulation of optics in which the straight line travelling of light rays can be derived from wave motion when the wavelenght is small. In classical mechanics if a particle is subjected to force with potential energy is $V(x,y,z)$ at position x, y, z then the sum of potential energy and Kinetic energy $P^2/2m$ is equal to constant; the total energy E of particle.

$$\frac{P^2}{2m} + V(x,y,z) = E$$

Postulating a wave function in quantum mechanics $\Psi(x,y,z)$ that varies with position Schrödinger replaced potential energy in above energy equation with a differential operator.

$$\frac{-h^2}{2m}\left(\frac{\partial^2\Psi}{\partial x^2} + \frac{\partial^2\Psi}{\partial y^2} + \frac{\partial^2\Psi}{\partial z^2}\right) + V(x,y,z)\Psi = E\Psi \quad -(1)$$

Different forms of Schrödinger Wave Equation

Let us Take ψ as a common form of differentiation then;

$$\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\psi+\frac{8\pi^2 m}{h^2}(E-P)\psi=0 \longrightarrow (1)$$

where as, $\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}=\nabla^2$

Laplacian operator $=\nabla^2$ so (1) con

written as;

$$\nabla^2\psi+\frac{8\pi^2 m}{h^2}(E-P)\psi=0 \longrightarrow (2)$$

By rearranging the equation (2) we bring E on L.H.S of the equation.

$$\nabla^2\psi = -\frac{8\pi^2 m}{h^2}(E-P)\psi$$

$$\frac{-h^2}{8\pi^2 m}\nabla^2\psi = E\psi - P\psi$$

$$-\frac{h^2}{8\pi^2 m}\nabla^2\psi + P\psi = E\psi$$

$$E\psi = \left(\frac{-h^2}{8\pi^2 m}\nabla^2+P\right)\psi \longrightarrow (3)$$

where as,

$$E\psi = H\psi \longrightarrow (4)$$

where H is the Hamailtonian operator which is the sum of total energies possessed by a particle. eq (3) becomes;

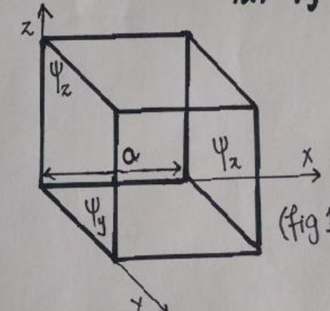
$$H\psi = \left[\left(-\frac{h^2}{8\pi^2 m}\nabla^2\right)+P\right]\psi$$

$$H = \frac{-h^2}{8\pi^2 m}\nabla^2 + P \text{ — (5)}$$

Equation (4) is the simplest form of Schrödinger wave equation and the advantage of this equation is that no arbitrary quantum conditions need to be postulated.

Derivation of the Schrödinger wave equation for a particle in three-dimensional box.

Consider a particle in 3-dimensional box (3-D) of length 'a' (fig 1). The box has 3 coordinates x, y and z so the wave function for the three coordinates in which a particle can move can written as Ψ_x, Ψ_y and Ψ_z respectively.



(fig 1)

If particle is supposed to be an electron then it is seemed to be entrapped in potential energy well. But in our case the potential energy V is zero inside the box and at boundary and outside the box it is infinity.

The Schrödinger wave equation for the particle in 3-coordinates can be written as,

$$\nabla^2 \Psi_{xyz} + \frac{8\pi^2 m}{h^2}(E - V)\Psi_{xyz} = 0 \longrightarrow (1)$$

The potential energy inside the box was zero; as described earlier

So,

$$V=0$$

The the equation (1) is written as;

$$\nabla^2 \Psi_{xyz} + \frac{8\pi^2 m (E-0)}{h^2} \Psi_{xyz} = 0$$

$$\nabla^2 \Psi_{xyz} + \frac{8\pi^2 m}{h^2} E \, \Psi_{xyz} = 0 \longrightarrow (2)$$

Where in eq (2)

Ψ_{xyz} = wave function of Total particle moving in a 3-dimensional box.

∇^2 = Laplacian operator

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \longrightarrow (3)$$

If we put value of ∇^2 from (3) in (2) we will get,

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) \Psi_{xyz} + \frac{8\pi^2 m}{h^2} E \left(\Psi_{xyz}\right) = 0 \longrightarrow (4)$$

As we have $\Psi_{xyz} = \Psi_x \cdot \Psi_y \Psi_z$

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) \Psi_x \Psi_y \Psi_z + \frac{8\pi^2 m}{h^2} E(\Psi_x \Psi_y \Psi_z) = 0 \longrightarrow (5)$$

In equation (4) Ψ_{xyz} is replaced by the product of $\Psi_x . \Psi_y . \Psi_z$ because Ψ_{xyz} is a probable value and is therefore the product of the individual probabilities available.

Solving equation (5) we get;

$$\cancel{\psi_{xyz}}\,\psi_x \psi_y \psi_z \frac{\partial^2}{\partial x^2} + \psi_x \psi_y \psi_z \frac{\partial^2}{\partial y^2} + \psi_x \psi_y \psi_z \frac{\partial^2}{\partial z^2} + \frac{8\pi^2 m E}{h^2} \psi_x \psi_y \psi_z = 0. \rightarrow (6)$$

Rearranging equation (6) for the seperate variables;

$$\psi_y \psi_z \frac{\partial^2}{\partial x^2}(\psi_x) + \psi_x \psi_z \frac{\partial^2}{\partial y^2}(\psi_y) + \psi_y \psi_x \frac{\partial^2}{\partial z^2}(\psi_z) + \frac{8\pi^2 m E}{h^2} \psi_x \psi_y \psi_z = 0.$$

Dividiving above equation by '$\psi_x \psi_y \psi_z$' on both sides;

$$\frac{1}{\psi_x \psi_y \psi_z}\left[\psi_y \psi_z \frac{\partial^2}{\partial x^2}(\psi_x) + \psi_x \psi_z \frac{\partial^2}{\partial y^2}(\psi_y) + \psi_y \psi_x \frac{\partial^2}{\partial z^2}(\psi_z) + \frac{8\pi^2 m E}{h^2} \psi_x \psi_y \psi_z\right] = 0$$

$$\frac{1}{\cancel{\psi_x}\cancel{\psi_y}\cancel{\psi_z}} \cancel{\psi_y} \cancel{\psi_z} \frac{\partial^2}{\partial x^2}\psi_x + \frac{1}{\cancel{\psi_x}\cancel{\psi_y}\cancel{\psi_z}} \cancel{\psi_x} \cancel{\psi_z} \frac{\partial^2}{\partial y^2}\psi_y + \frac{1}{\cancel{\psi_x}\cancel{\psi_y}\cancel{\psi_z}} \cancel{\psi_x} \cancel{\psi_y} \frac{\partial^2}{\partial z^2}\psi_z + \frac{8\pi^2 m E}{h^2} \frac{\cancel{\psi_x}\cancel{\psi_y}\cancel{\psi_z}}{\cancel{\psi_x}\cancel{\psi_y}\cancel{\psi_z}} = 0$$

$$\frac{1}{\psi_x}\frac{\partial^2\psi_x}{\partial x^2}+\frac{1}{\psi_y}\frac{\partial^2\psi_y}{\partial y^2}+\frac{1}{\psi_z}\frac{\partial^2\psi_z}{\partial z^2}+\frac{8\pi^2 m}{h^2}E=0 \rightarrow (7)$$

Inorder to seperate E from eq we ~~divide~~ multiply eq (7) by $\frac{h^2}{8\pi^2 m}$ on both sides;

$$\frac{h^2}{8\pi^2 m}\left[\frac{1}{\psi_x}\frac{\partial^2\psi_x}{\partial x^2}+\frac{1}{\psi_y}\frac{\partial^2\psi_y}{\partial y^2}+\frac{1}{\psi_z}\frac{\partial^2\psi_z}{\partial z^2}\right]+\frac{h^2}{8\pi^2 m}\cdot\frac{8\pi^2 m}{h^2}E=0$$

$$\frac{h^2}{8\pi^2 m}\frac{1}{\psi_x}\frac{\partial^2\psi_x}{\partial x^2}+\frac{h^2}{8\pi^2 m}\frac{1}{\psi_y}\frac{\partial^2\psi_y}{\partial y^2}+\frac{h^2}{8\pi^2 m}\frac{1}{\psi_z}\frac{\partial^2\psi_z}{\partial z^2}=-E_{xyz} \rightarrow (8)$$

In eq (8) $E=E_{xyz}$ because the particle is moving in three dimensional box so the energy is also taken along three coordinate axes;

$$E_{xyz}=E_x+E_y+E_z \rightarrow (9)$$

The total energy E_{xyz} is the sum of individual energies E_x, E_y and E_z along x, y and z axes respectively;

Putting eq (9) in eq (8) we get,

$$\frac{h^2}{8\pi^2 m}\frac{1}{\psi_x}\frac{\partial^2\psi_x}{\partial x^2}+\frac{h^2}{8\pi^2 m}\frac{1}{\psi_y}\frac{\partial^2\psi_y}{\partial y^2}+\frac{h^2}{8\pi^2 m}\frac{1}{\psi_z}\frac{\partial^2\psi_z}{\partial z^2}=-(E_x+E_y+E_z)$$

$$\frac{h^2}{8\pi^2 m}\frac{1}{\psi_x}\frac{\partial^2\psi_x}{\partial x^2}+\frac{h^2}{8\pi^2 m}\frac{1}{\psi_y}\frac{\partial^2\psi_y}{\partial y^2}+\frac{h^2}{8\pi^2 m}\frac{1}{\psi_z}\frac{\partial^2\psi_z}{\partial z^2}=-E_x-E_y-E_z \rightarrow (10)$$

eq (10) is having three variables in right hand side i.e it has three parts so, by seperating the parts we compare the coefficients then we get;

$$\frac{h^2}{8\pi^2 m}\frac{1}{\psi_x}\frac{\partial^2\psi_x}{\partial x^2} = -E_x \quad \text{— (11)a}$$

$$\frac{h^2}{8\pi^2 m}\frac{1}{\psi_y}\frac{\partial^2\psi_y}{\partial y^2} = -E_y \quad \text{— (11)b}$$

$$\frac{h^2}{8\pi^2 m}\frac{1}{\psi_z}\frac{\partial^2\psi_z}{\partial z^2} = -E_z \quad \text{— (11) c}$$

Solving equation (11 a) which is in the variable 'x'

$$\frac{h^2}{8\pi^2 m}\frac{1}{\psi_x}\frac{\partial^2\psi_x}{\partial x^2} = -E_x$$

$$\frac{1}{\psi_x}\frac{\partial^2\psi_x}{\partial x^2} = \frac{-8\pi^2 m}{h^2} E_x$$

$$\frac{\partial^2\psi_x}{\partial x^2} = -\psi_x \frac{8\pi^2 m}{h^2} E_x .$$

$$\frac{\partial^2\psi_x}{\partial x^2} + \frac{8\pi^2 m}{h^2} E_x \psi_x = 0 \longrightarrow (12)$$

equation (12) is a second order differential equation in variable 'x' having wave function ψ_x.

So, from above equation;

$\frac{8\pi^2 m}{h^2} E_x$ is a constant term where,

m = mass of particle

h = Plank's constant

E_x = Energy of particle along x-axis

Therefore,

$$\frac{8\pi^2 m}{h^2} E_x = K^2$$

eq (12) becomes;

$$\frac{\partial^2\psi_x}{\partial x^2} + K^2\psi_x = 0 \quad \text{— (13 a)}$$

For y-axis we have;

$$\frac{\partial^2 \psi_y}{\partial y^2} + K^2 \psi_y = 0 \longrightarrow (13b)$$

Similarly for z-axis,

$$\frac{\partial^2 \psi_z}{\partial z^2} + K^2 \psi_z = 0 \longrightarrow (13c)$$

Hence, (13 a), (13b) and (13c) are the second order differential equations along x, y and z respectively, These equations have their solution in exponential forms; By solving (13 a) we get;

$$\psi_x = Ae^{mx} \text{ — (14)}$$

∴ x shows the direction in which particle is moving.

Put value of ψ_x from (14) in eq (13 a)

$$\frac{\partial^2}{\partial x^2} Ae^{mx} + K^2 Ae^{mx} = 0$$

$$Am^2 e^{mx} + K^2 Ae^{mx} = 0$$

$$Ae^{mx}(m^2 + K^2) = 0$$

∴ $\frac{\partial^2}{\partial x^2}$ is the double derivative

$$\frac{\partial}{\partial x} Ae^{mx} = A\frac{\partial}{\partial x} e^{mx}$$

$$= A(me^{mx})$$

$$\frac{\partial}{\partial x}\left(\frac{\partial}{\partial x} Ae^{mx}\right) = \frac{\partial}{\partial x}\left[Ame^{mx}\right]$$

$$= A\frac{\partial}{\partial x}(me^{mx})$$

$$= Am \cdot me^{mx}$$

$$\boxed{\frac{\partial^2}{\partial x^2} Ae^{mx} = Am^2 e^{mx}}$$

$Ae^{mx} \neq 0$; $m^2 + K^2 = 0$ — (15)

↓

exponentials never give zero answer moverover it has a variable x.

m and K are both constants

eq (15)

$m^2 + K^2 = 0$ is an auxillary equation and cannot be factorized.

$m^2 = -K^2$

Taking $\sqrt{\ }$:

$\therefore \sqrt{m^2} = \sqrt{-K^2} \Rightarrow m = \sqrt{(-1)K^2}$

$\therefore (-1) = i^2$

$\sqrt{-1} = i$

$m = \sqrt{(i^2 K^2)}$

$$\boxed{m = \pm iK}$$

Putting value of 'm' in eq. (14)

$$\psi_x = Ae^{(\pm iK)x}$$

$\therefore e^{\pm iKx} = e^{iKx} \cdot e^{-iKx}$

$$\boldsymbol{\psi_x = Ae^{iKx} + Be^{-iKx}} \quad \text{—— (16)}$$

Where A and B are constants in eq (16) and it has real and imaginary part.

It can be written as in polar form:

$\because e^{i\theta} = \cos\theta + i\sin\theta \longrightarrow (a)$

or $e^{-i\theta} = \cos\theta - i\sin\theta$ (b) then eq (16) becomes as in two parts;

$Ae^{iKx} = A[\cos(Kx) + i\sin(Kx)]$ as in (a) $(\theta = Kx)$

$Be^{-iKx} = B[\cos(Kx) - i\sin(Kx)]$ as in (b)

So, we get;

$$\boldsymbol{\psi_x = A[\cos(Kx) + i\sin(Kx)] + B[\cos(Kx) - i\sin(Kx)]}$$

$= A\cos(Kx) + i\sin(Kx)A + B\cos(Kx) - i\sin(Kx)B.$

$= A\cos(Kx) + B\cos Kx + Ai\sin(Kx) - Bi\sin(Kx)$

$\psi_x = (A+B)\cos Kx + i\sin(Kx)(A-B)$ —— (17)

Let

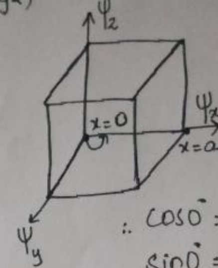
$A+B=D$

and $i(A-B)=C$ then eq (17) becomes,

$$\psi_x = D\cos Kx + C\sin(Kx) \rightarrow (17a)$$

Applying the boundary conditions in equation (17a) (fig2)

$\psi_x = 0$ at $x=0$ (at origin)



fig(2)

$0 = D\cos K(0) + C\sin K(0)$

$0 = D\cos(0^\circ) + C\sin(0)$

$0 = D(1) + C(0)$

$\therefore \cos 0^\circ = 1$

$\sin 0^\circ = 0$

$\boxed{0 = D}$

By putting $D=0$ eq (17a) becomes;

$\psi_x = (0)\cos Kx + C\sin Kx$

$$\psi_x = C\sin(Kx) \rightarrow (18)$$

This wave function has a limitation towards sine wave

Applying secondary boundary condition on eq(18)

i.e $\psi_x = 0$, $x=a$

$\psi_x = C\sin(Ka)$

$$0 = C\sin(Ka) \rightarrow (19)$$

This condition is only true if $K = n\pi$

$$K = \frac{n\pi}{a} \rightarrow (20)$$

In eq (19) $Ka = \theta$ which makes the equatio[n] equals to 0.

Put eq (20) in (18)

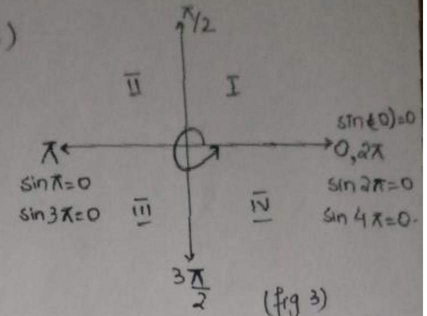
$$\psi_x = C \sin\left(\frac{n\pi x}{a}\right) \quad \text{--- (21 a)}$$

Similarly,

$$\psi_y = C \sin\left(\frac{n\pi y}{a}\right) \quad \text{--- (21 b)}$$

and,

$$\psi_z = C \sin\left(\frac{n\pi z}{a}\right) \quad \text{--- (21 c)}$$



(fig 3)

where n = Quantum number.

Value of n is not permitted to be zero. So, $n=0$ then $\psi_x = 0$ everywhere within the box. In other words value of n, which are acceptable are $n = 1, 2, 3 \ldots\ldots$ and as $\sin\theta$ has a zero value after every π (fig 3).

$\sin 0 = 0$

$\sin 1\pi = 0$

$\sin 2\pi = 0 \ldots\ldots\ldots \sin(n\pi) = 0.$

In equations (21 a), (21 b) and (21 c) there is a constant 'C' If we found value 'C' then Total wave function of the particle can be determined.

Determination of value of 'C'.

Overlape between two waves to get larger amplitude So, inorder to get maximum amplitude we must apply condition of normalization,

Two waves are said to be normal to each other, if they satisfy the following relation,

$$\int_0^a \Psi_x \Psi_x^* d\Psi_x = 1 \rightarrow (22)$$

$d\Psi_x$ = differential of the Ψ_x.

We know that from eq

$$\Psi_x = c\sin\left(\frac{n\pi x}{a}\right) \text{ Put in eq (22)}$$

we get;

$$\int_0^a c\sin\left(\frac{n\pi x}{a}\right) . c\sin\left(\frac{n\pi x}{a}\right) d\Psi_x = 1.$$

$$\int_0^a c^2 \sin^2\left(\frac{n\pi x}{a}\right) d\Psi_x = 1$$

$\therefore \sin\theta . \sin\theta = \sin^2\theta$.

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

we know that

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

$$\sin^2\theta = \frac{1-\cos 2\theta}{2}$$

Therefore, above equation can also be written as,

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

$$\frac{c^2}{2} \int_0^a \left[1 - \cos 2\left(\frac{n\pi x}{a}\right)\right] dx = 1.$$

$$\frac{c^2}{2} \left[\int_0^a dx - \int_0^a \cos 2\left(\frac{n\pi x}{a}\right) dx\right] = 1.$$

$$\frac{c^2}{2} \left[|x|_0^a - \left| \frac{\sin 2\left(\frac{n\pi x}{a}\right)}{\frac{2n\pi}{a}} \right|_0^a \right] = 1.$$

$$\frac{c^2}{2}\left[(a-0)-\frac{a}{2n\pi}\left\{\sin 2\left(\frac{n\pi a}{a}\right)-\sin 2\left(\frac{n\pi(0)}{a}\right)\right\}\right]=1$$

$$\frac{c^2}{2}\left[a-\frac{a}{2n\pi}\left(\sin 2(n\pi)-\sin 2(0)\right)\right]=1$$

$$\frac{c^2}{2}\left[a-\frac{a}{2n\pi}\left(\sin(2n\pi)-0\right)\right]=1 \quad \because \sin 0=0$$

$$\frac{c^2}{2}\left[a-\frac{a}{2n\pi}\left(\sin(0)-0\right)\right]=1 \quad \because \sin 2n\pi=0$$

$$\frac{c^2}{2}\left[a-\frac{a}{2n\pi}(0)\right]=1$$

$$\frac{c^2}{2}(a-0)=1.$$

$$\frac{c^2 a}{2}=1.$$

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

$$c=\sqrt{\frac{2}{a}} \longrightarrow (A)$$

Put value of '(C)' from (A) in (21 a), (21 b) and (22 C) where C = constant of normalization.

$$\psi_x=\sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right) \rightarrow (23\,a)$$

$$\psi_y=\sqrt{\frac{2}{a}}\sin\left(\frac{n\pi y}{a}\right) \rightarrow (23\,b)$$

$$\psi_z=\sqrt{\frac{2}{a}}\sin\left(\frac{n\pi z}{a}\right) \rightarrow (23\,c)$$

As we have ψ_{xyz} the total probability of the particle as

$$\psi_{xyz} = \psi_x \cdot \psi_y \cdot \psi_z$$

Putting values from (23a), (23b) and (23c) we get

$$\psi_{xyz} = \sqrt{\frac{2}{a}}\sqrt{\frac{2}{a}}\sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) \sin\left(\frac{n\pi y}{a}\right) \sin\left(\frac{n\pi z}{a}\right) \longrightarrow (24)$$

The eq (24) gives the total wave function of the particle placed in three dimensional box.

Calculation of Energies.

By using eq (24) we can find probability of the total wave function of particle in a 3-D box. We can also find the total energies of the particle using Schrödinger wave equation;

We have a constant;

$$K^2 = \frac{8\pi^2 m}{h^2} E_x \longrightarrow (i)$$

also we know that

$$K = \frac{n\pi}{a} \longrightarrow (ii)$$

Taking square of eq(ii)

$$K^2 = \frac{n^2\pi^2}{a^2} \longrightarrow (iii)$$

Comparing eq (i) & (iii)

$$\frac{8\pi^2 m}{h^2} E_x = \frac{n^2\pi^2}{a^2}$$

or $$E_x = \frac{n^2\cancel{\pi^2}}{a^2}\frac{h^2}{8\cancel{\pi^2}m}$$

$$E_x = \frac{n_x^2 h^2}{8a^2m} \quad \text{—(iv)}$$ Total Energy of the particle along x axis.

m = mass of particle
a = length of box
h = Plank's constant.
n_x = quantum number along 'x'.

Similarly, $$E_y = \frac{n_y^2 h^2}{8a^2m} \quad \text{— (V)}$$

$$E_z = \frac{n_z^2 h^2}{8a^2m} \quad \text{— (VI)}$$

The Energy is an absoulte value so E_{xyz} is the sum of three Energies along x, y and z.

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

From eq (IV), (V) and (vi).

$$= \frac{n_x^2 h^2}{8a^2m} + \frac{n_y^2 h^2}{8a^2m} + \frac{n_z^2 h^2}{8a^2m}$$

$$E_{xyz} = \frac{h^2}{8a^2m}(n_x^2 + n_y^2 + n_z^2) \quad \text{— (vii)}$$

With the equation (vii) we can find the Total energy of the particle entrapped in three-dimensional box.

Factors upon which total energy depends:-

→ $E_{Total} \propto \frac{1}{a^2}$

a = lenght of the box

Energy depends upon the structure of box.

→ $E_{Total} \propto \frac{1}{m}$

m = mass of particle.

We can also calculate the **ground state energies**.

n_x, n_y and n_z depends upon Principle Quantum numbers i.e how far is electron from the nucleus.

Physical quantum states are never zero.

The lowest energy of the particle which it possesses in 3-dimensional box is known to be has ground state energy.

Hydrogen atom has the least mass for inorder to calculate the Energy of Hydrogen we should know value of 'm' and 'a'

Since we have,

$$n_x = n_y = n_z = 1$$

Then

$$E_{Total} = \frac{h^2}{8ma^2}(n_x^2 + n_y^2 + n_z^2)$$

$$= \frac{h^2}{8ma^2}(1^2 + 1^2 + 1^2)$$

$$= \frac{h^2}{8ma^2}(3)$$

other values of energies at different levels

$$E_{TOTAL} = \frac{3h^2}{8ma^2}$$

Let, $n_x = 2$, $n_y = n_z = 1$

$$E_{TOTAL} = \frac{h^2}{8ma^2}(n_x^2 + n_y^2 + n_z^2)$$

$$= \frac{h^2}{8ma^2}(2^2 + 1^2 + 1^2)$$

$$= \frac{h^2}{8ma^2}(4+1+1)$$

$$= \frac{h^2}{{}_4\cancel{8}ma^2}(\cancel{6}^{3})$$

$$E_{TOTAL} = \frac{3h^2}{4ma^2}$$

Let $n_x = 1 = n_y$ and $n_z = 2$

$$E_{TOTAL} = \frac{h^2}{8ma^2}(n_x^2 + n_y^2 + n_z^2)$$

$$= \frac{h^2}{8ma^2}(1^2 + 1^2 + 2^2)$$

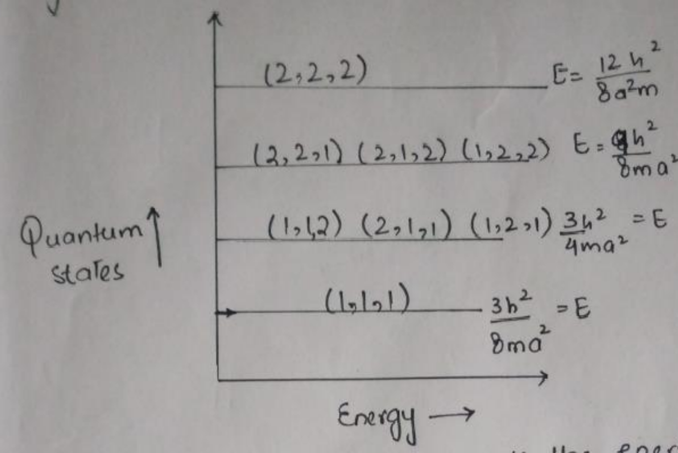
$$= \frac{h^2}{8ma^2}(1+1+4)$$

$$= \frac{h^2}{{}_4\cancel{8}ma^2}(\cancel{6}^{3})$$

$$E_{TOTAL} = \frac{3h^2}{4ma^2}$$

We can also find the Quantum states more for the other atoms or particles;

The following distribution is shown for the hydrogen atom;



The more quantum states the more is the energy. The more quantum states are actually the no. of ways of the Quantum states are actually the no. of ways of the distribution of the energies and macro state is referred to the energy possession.

Similarly, degeracy of these quantum states can also be found by the solving of the Schrödinger ware equation.

Significance of the Schrödinger wave Equation.

- The structure of atoms and molecules can be well explained.
- The solution of the equation results in quantized properties of quantum particles.
- Most of the semi-conductor properties are well explained from the results of Schrödinger's equation.
- It describes the majority of mircoscopic situations.
- Schrödinger's equation is used to find the allowed energy levels of quantum mechanical systems. The associated wave-function gives the probability of finding the particle of at a certain position.
- It shows all of the wave-like properties of matter.
- In classical mechanics Newton's laws of motion describe future state of system whereas in quantum mechanics wave function ψ defines the state of system

  $$\text{Probability} = \int_a^b \psi^2 dx$$

  These have exception values and wave function is needed to find these values and Schrödinger's equation is solved to get wave functions.