(1) Charge and mass of electron, proton and neutron :⇒

Particle	Symbol	Mass		Charge	
		amu (approx)	grams	Charge units	Coulombs
Electron	e^-	1/1835	9.1×10^{-28}	−1	-1.60×10^{-19}
Proton	p	1	1.672×10^{-24}	+1	$+1.60\times10^{-19}$
Neutron	n	1	1.674×10^{-24}	0	0

(2) Balmer Equation : ⇒ (Emperical equation)

$$\frac{1}{\lambda} = R\left(\frac{1}{2^2} - \frac{1}{n^2}\right)$$

λ = wavelength of visible spectrum.

R = Rydberg constant = 109,677 cm^{-1}

n = 3, 4, 5, 6 etc.

If we substitute the values of 3, 4, 5, 6 for n we get respectively, the four wavelength of the for visible spectrum of H atom.

(3) Photo electric effect ⇒

$$h\nu = h\nu_0 + \frac{1}{2}mv^2$$

where, $h\nu$ = The energy of the incomming photon.

h = planck's constant = 6.626×10^{-27} erg sec.

$h\nu_0$ = minimum energy for an electron to escape from the metal.

ν = Frequency

$\frac{1}{2}mv^2$ = kinetic energy of the photo electron.

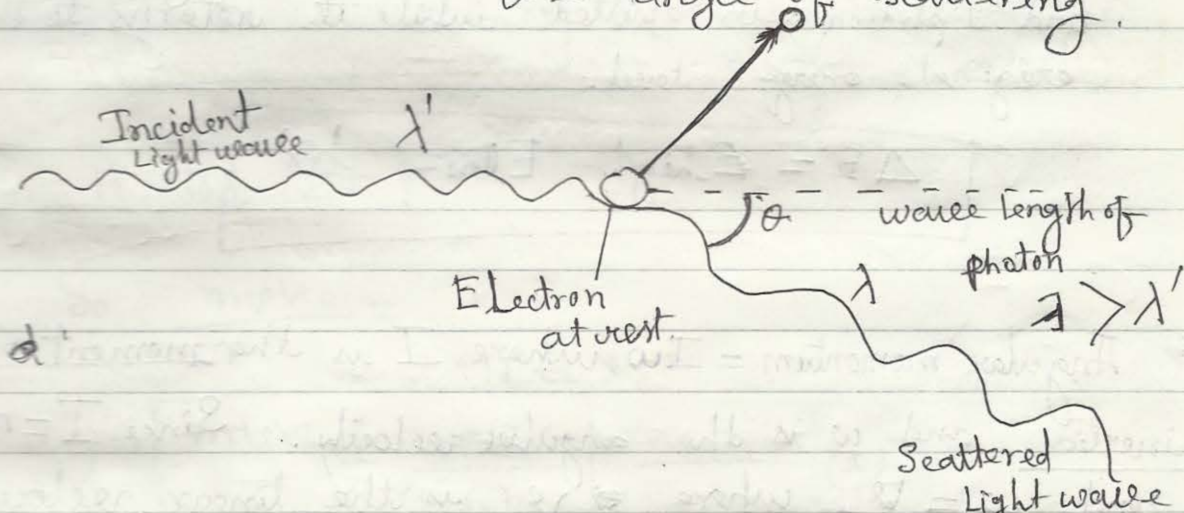
$h\nu_0$ is constant for a particular solid and is designated as W = Work function.

(4) **Compton effect** ⇒ By assuming photon-electron collisions to be perfectly elastic Compton found that the shift in wavelength, $d\lambda = \lambda' - \lambda$ was given by the expression —

$$d\lambda = \frac{2h}{mc} \sin^2 \theta/2$$

where, h = Planck's constant
$d\lambda = \lambda' - \lambda$ m = mass of an electron
c = velocity of light
θ = angle of scattering.

(3)



(5) **Postulates of Bohr's Theory** ⇒ ORBIT-NO

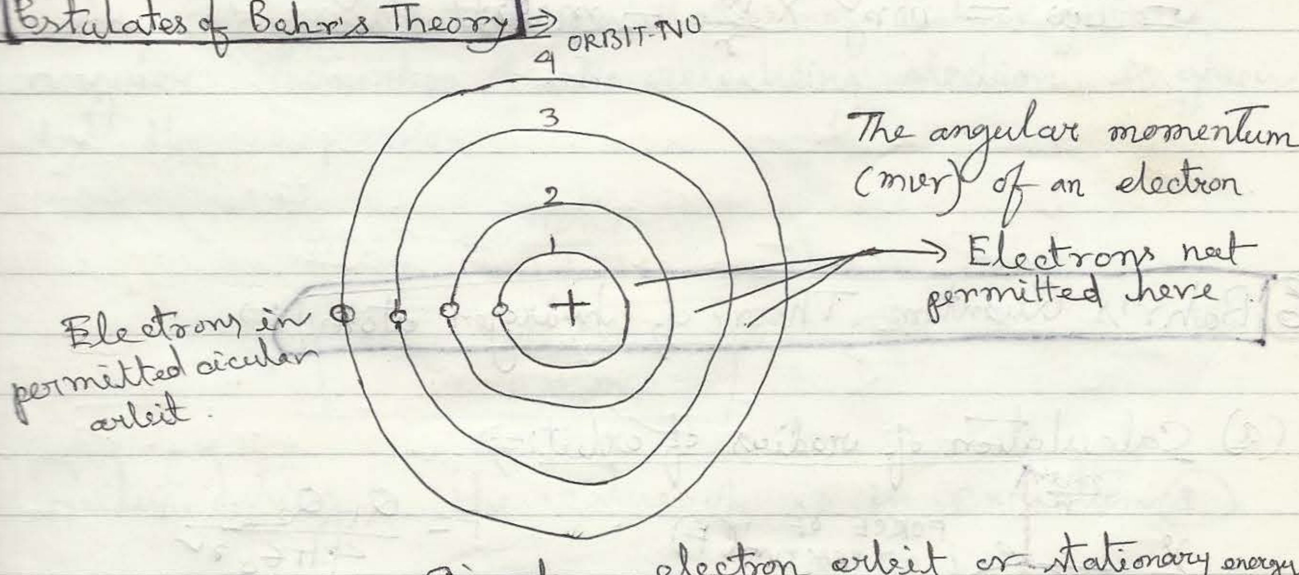


Fig:- Circular electron orbit or stationary energy levels in an atom.

* The angular momentum (mvr) of an electron orbiting around the nucleus is an integral multiple of Planck's constant divided by 2π

$$\text{Angular momentum} = mvr = \frac{nh}{2\pi}$$

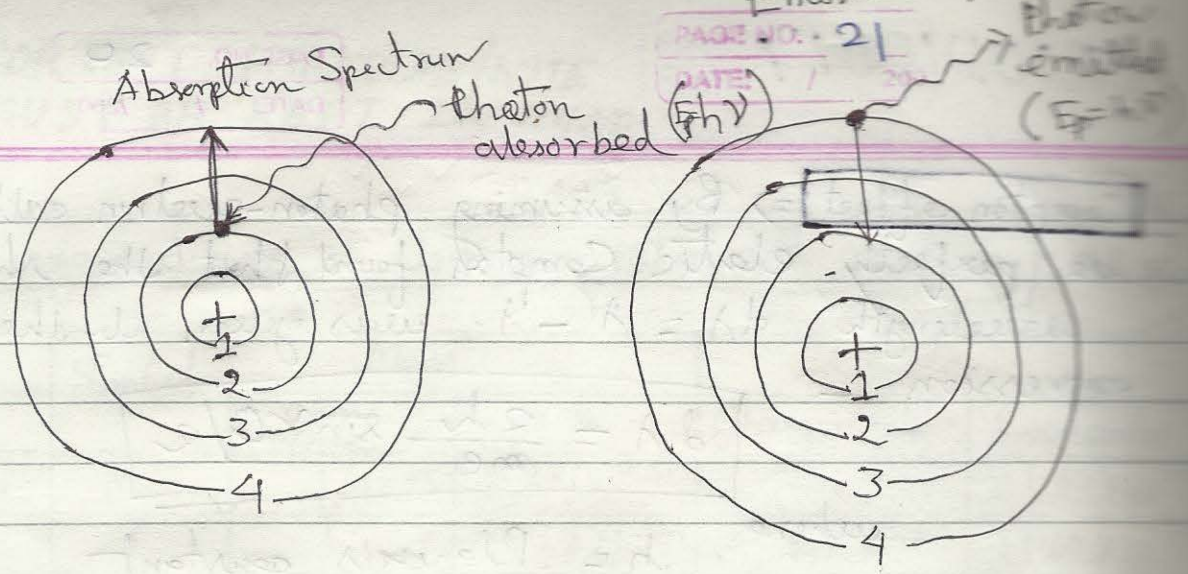


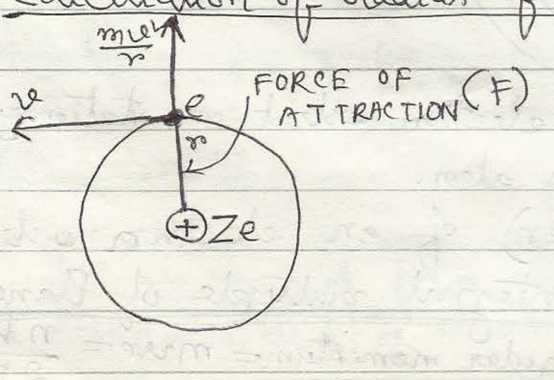
Fig:- An electron absorbes a photon of light while it jumps from a lower to a higher orbit and a photon is emitted while it returns to the original energy level.

$$\Delta E = E_{high} - E_{low} = h\nu$$

* Angular momentum = $I\omega$, where I is the <u>moment of inertia</u> and ω is the angular velocity. Since $I = mr^2$ and $\omega = \frac{v}{r}$ where v is the linear velocity and r is the radius. Therefore angular momentum $= I\omega = mr^2 \times \frac{v}{r} = mvr$

(6) Bohr's Quantum Theory of hydrogen atom :⇒

(a) <u>Calculation of radius of orbit</u> :⇒



$$F = \frac{Q_1 Q_2}{4\pi\epsilon_0 r^2}$$

Here $Q_1 = Ze$, $Q_2 = e$

ϵ_0 = Absolute permittivity of the medium $= 8.85 \times 10^{-12}$

F = The electrostatic force of attraction between the nucleus and the electron (Coulomb's law)

$$= \frac{Q_1 Q_2}{4\pi\epsilon_0 r^2} = \frac{Ze \cdot e}{4\pi\epsilon_0 r^2}$$

Centrifugal force acting on electron

$$= \frac{mv^2}{r}$$

Now, $\boxed{\frac{mv^2}{r} = \frac{Ze \cdot e}{4\pi\epsilon_0 r^2}}$ (According to Bohr's concept to keep the electron in orbit).

For H atom Z = 1

So, $\frac{mv^2}{r} = \frac{e \cdot e}{4\pi\epsilon_0 r^2}$

$$\Rightarrow \boxed{mv^2 = \frac{e^2}{4\pi\epsilon_0 r}} \text{ ——— (1)}$$

According to the postulates of Bohr's theory, angular momentum of the revolving electron is given by the expression

$$mvr = \frac{nh}{2\pi}$$

$$\Rightarrow \boxed{v = \frac{nh}{2\pi mr}} \text{ ——— (2)}$$

Substituting the value of v in equation (1)

we get, ~~$\frac{e^2}{4\pi\epsilon_0 r}$~~ $m\left(\frac{nh}{2\pi mr}\right)^2 = \frac{e^2}{4\pi\epsilon_0 r}$

$$\Rightarrow \frac{mn^2h^2}{4\pi^2m^2r^2} = \frac{e^2}{4\pi\epsilon_0 r}$$

$\Rightarrow$

$$\Rightarrow \frac{n^2h^2}{4m r} = \frac{e^2}{\epsilon_0}$$

$$\Rightarrow \boxed{r = \frac{\epsilon_0 n^2 h^2}{\pi e^2 m}} \quad \text{——— (3)}$$

~~The total energy~~, E

(b) Calculation of energy of electron in each orbit:→

The total energy (E) of the electron at any instant is given by the sum of kinetic energy and potential energy. Since the mass of an electron is taken as m and its velocity as v, the kinetic energy is given by $\frac{1}{2}mv^2$.

Potential energy of a charged body at any point is given by the work ~~done~~ that has to be done to bring it from infinity to that point.

* Suppose, an electron carrying a charge −e, is at a distance r from the nucleus carrying a charge +e in the hydrogen atom. Then, according to the Coulomb's law of inverse squares, the force of attraction exerted by the nucleus on the electron is given by

$$\boxed{F = \frac{e \times e}{4\pi\epsilon_0 r^2} = \frac{e^2}{4\pi\epsilon_0 r^2}} \quad \text{——— (4)}$$

Suppose the electron, under this force of attraction, moves through a distance dr.

$$\text{Work done} = -\frac{e^2}{4\pi\epsilon_0 r^2}\,dr$$

Now, by diffinition, the patential energy of the electron when it is at a distance r from the nucleus is given by the work done in moveing the electron from infinity to that point. This work can be obtained integrating equation ⑤ between the limits r and infinity, keeping in view that when r is infinity, the potential energy of the electron is zero. Thus

$$\text{The required work done} = \frac{1}{4\pi\epsilon_0}\int_{r=\alpha}^{r=r}\frac{e^2}{r^2}\,dr = \frac{-e^2}{4\pi\epsilon_0 r}$$

Hence the potential energy of electron in the hydrogen atom, $U = \frac{-e^2}{4\pi\epsilon_0 r}$

The total energy of electron (E) is thus given by

~~$E = \frac{1}{2}mv^2$ (kinetic energy) $-e^2$~~

E = Kinetic energy + Potential energy (U)

$$= \frac{1}{2}mv^2 + \left(\frac{-e^2}{4\pi\epsilon_0 r}\right)$$

$$= \frac{1}{2}mv^2 - \frac{e^2}{4\pi\epsilon_0 r} \quad \text{——— (6)}$$

Knowing from equation ① that $mv^2 = \frac{e^2}{4\pi\epsilon_0 r}$

and substituting in equation ⑥ we get,

$$E = \frac{e^2}{8\pi\epsilon_0 r} - \frac{e^2}{4\pi\epsilon_0 r} = \frac{-e^2}{8\pi\epsilon_0 r} \quad \text{—— (7)}$$

Substituting the value of r from equation (3) into equation (7) follows that

$$E = -\frac{e^2}{8\pi\epsilon_0 \times \frac{\epsilon_0 n^2 h^2}{\pi e^2 m}}$$

$$= -\frac{e^2 \times \pi e^2 m}{8\pi \epsilon_0^2 n^2 h^2}$$

$$E = -\frac{m e^4}{8 \epsilon_0^2 n^2 h^2}$$

(7) de Broglie Equation :→

According to Planck, the photon energy 'E' is given by the equation

$$E = h\nu \quad \text{——— (1)}$$

h = Planck's constant
ν = Frequency of radiation

By applying Einstein's mass-energy principle / relationship, the energy association with photon of mass 'm' is given by

$$E = mc^2 \quad \text{——— (2)}$$

c = velocity of radiation.

Comparing equation (1) and (2)

$$mc^2 = h\nu = h\frac{c}{\lambda}$$

$$\boxed{mc = \frac{h}{\lambda}}$$

$$\Rightarrow \text{mass} \times \text{velocity} = \frac{h}{\text{wavelength}}$$

$$\Rightarrow \text{momentum}(p) = \frac{h}{\text{wavelength}}$$

$$\Rightarrow \boxed{\text{momentum} \propto \frac{1}{\text{wavelength}}} \quad \text{——— (3)}$$

The equation (3) is called de Broglie's equation

* The momentum of a particle in motion is inversely propotional to wavelength, Planck's constant 'h' being the constant of propotionality.

(8) Heisenberg's uncertainty principle →

It is impossible to Know simultaneously both the conjugate properties accurately. For example the position and momentum of a moving particle are independent and thus conjugate properties also. Both the position and momentum of the particle at any instant cannot be determined with absolute exactness or certainty. If the momentum (or velocity) be ~~determined~~ measured very accurately, a measurement of the position of the particle correspondingly becomes less precise.

On the otherhand if position is determined with accuracy or ~~precian~~ precision, the momentum becomes less accurately known or uncertain. Thus certainty of determination of one property introduces uncertainty of determination of the other property.

The uncertainty of measurement of position

Δx and the uncertainty of determination of momentum, Δp (or Δmv), are related by Heisenberg's relationship as.

$$\Delta x \times \Delta p \geq \frac{h}{2\pi}$$

7 $$\Delta x \times \Delta mv \geq \frac{h}{2\pi}$$

where h = Planck's constant $= 6.625 \times 10^{-27}$ erg sec.

* Thus in view of the uncertainty principle, Bohr's model of definite orbits has no meaning. It is not possible to know exactly the position of an electron as is implied in Bohr's model. Instead, it is possible only to state or predict the probability of locating an electron of a particular energy in a given region of space at a given time.

* It may be noted that there exists a clear difference between the behavior of large objects like a stone and small particles like electrons. The uncertainty product is negligible in case of large object.

Ex:- For a moving ball of iron weighing 500g, the uncertainty expression assumes the form

$$\Delta x \times \Delta mv \geqslant \frac{h}{2\pi}$$

$$\Rightarrow \Delta x \times \Delta v \geqslant \frac{h}{2\pi m}$$

$$\Rightarrow \Delta x \times \Delta v \geqslant \frac{6.625 \times 10^{-27}}{2 \times 3.14 \times 500}$$

$$\approx 5 \times 10^{-31} \text{ erg. sec. gm}^{-1}$$

which is very small and thus negligible. Therefore for large objects the uncertainty of measurements is practically nil.

But for an electron of mass $m = 9.1091 \times 10^{-28}$ g the product of the uncertainty of measurements is quite large as.

$$\Delta x \times \Delta v \geqslant \frac{h}{2\pi m}$$

$$\geqslant \frac{6.625 \times 10^{-27}}{2 \times 3.14 \times 9.1091 \times 10^{-28}}$$

$$\approx 0.3 \text{ erg. sec. gm}^{-1}$$ (approx)

DATE: / /200

* This value is large enough in comparison with the size of the electron and is thus in no way is negligible. If position is known quite accurately i.e. Δx is very small, the uncertainty regarding velocity Δv becom immensely large and vice versa. It is therefore, very clear that the uncertainty principle is only important is considering measurements of small particles comprising an atomic system.

(9) SCHRODINGER'S WAVE EQUATION

In order to provide sense and meaning to the probability approach, Schrodinger's ~~wave~~ derived an equation known after his name as Schrodinger's wave equation. His equation is key note of wave mechanics and is based upon the idea of the electron as 'standing wave' around the nucleus.

* The equation for the standing wave, comparable with that of a stretched string is

$$\boxed{\psi = A \sin 2\pi \frac{x}{\lambda}} \quad \text{—— (1)}$$

where ψ (pronounced as sigh) is a mathematical function representing the amplitude of wave (called wave function) x, the displacement in a given direction, and λ, the wave length and A is constant

* By differentiating equation (1) twice with respect to x, we get

$$\frac{d\psi}{dx} = A \frac{2\pi}{\lambda} \cos 2\pi \frac{x}{\lambda} \quad \text{—— (2)}$$

and $$\frac{d^2\psi}{dx^2} = -\frac{4\pi^2 A}{\lambda^2} \sin 2\pi \frac{x}{\lambda} \quad \text{—— (3)}$$

But $A \sin 2\pi \frac{x}{\lambda} = \psi$ (From eqn (1))

$$\therefore \frac{d^2\psi}{dx^2} = -\frac{4\pi^2\psi}{\lambda^2} \quad \text{---} (4)$$

The kinetic energy of particle of mass m and velocity v is given by the relation

$$K.E = \frac{1}{2}mv^2 = \frac{1}{2}\frac{m^2v^2}{m} \quad \text{---} (5)$$

According to de Broglie equation

$$\lambda = \frac{h}{mv}$$

$$\Rightarrow \lambda^2 = \frac{h^2}{m^2v^2}$$

$$\Rightarrow m^2v^2 = \frac{h^2}{\lambda^2} \quad \text{---} (6)$$

Substituting the value of m^2v^2, we have

$$K.E. = \frac{1}{2} \times \frac{h^2}{m\lambda^2} \quad \text{---} (7)$$

From equation (4), we have

$$\lambda^2 = \frac{-4\pi^2\psi}{\frac{d^2\psi}{dx^2}} \quad \text{---} (8)$$

Substituting the value of λ^2 in equation ⑦ we get,

$$K.E. = -\frac{1}{2m} \cdot \frac{h^2}{4\pi^2\psi} \cdot \frac{d^2\psi}{dx^2}$$

$$\boxed{K.E = -\frac{h^2}{8\pi^2 m\psi} \cdot \frac{d^2\psi}{dx^2}} \quad \text{— (9)}$$

* The total energy E of a particle is the sum of kinetic energy and the potential energy (P.E)

$$E = K.E + P.E$$

$$\boxed{K.E = E - P.E} = -\frac{h^2}{8\pi^2 m\psi} \cdot \frac{d^2\psi}{dx^2}$$

$$\Rightarrow \frac{d^2\psi}{dx^2} = -\frac{8\pi^2 m}{h^2}(E - P.E.)\psi$$

$$\Rightarrow \boxed{\frac{d^2\psi}{dx^2} + \frac{8\pi^2 m}{h^2}(E - P.E.)\psi = 0} \quad \text{— (10)}$$

* This is Schrodinger wave equation in one dimension. It need to be generalised for a particle whose motion is described by three space co-ordinates x, y and z.

Thus (11)

$$\frac{d^2\psi}{dx^2} + \frac{d^2\psi}{dy^2} + \frac{d^2\psi}{dz^2} + \frac{8\pi^2 m}{h^2}(E - P.E)\psi = 0$$

This equation is called the Schrodinger wave Equation.

The first three terms on the left hand side are ~~seperated by a~~ represended by $\nabla^2\psi$ (pronounced as del-square sigh).

$$\boxed{\Delta^2\psi + \frac{8\pi^2 m}{h^2}(E - P.E.)\psi = 0} \quad (12)$$

Δ^2 is known as Laplacian Operator.

* Schrodinger wave equation

↓

Second order differential equation

↓

has innumerable solutions.

Many of them being without any significance.

The solutions will have significance

↓

only for certain definite values of total energy E.

definite values → Eigen values

↓

corresponds to discrete set of energy values postulated by Bohr's theory

⇒ The occurrence of definite energy levels in an atom follows directly from the wave mechanical concepts.

~~The~~ The solutions of the Schrodinger's wave equation

↓ On substituting proper values of E

give values of the wave functions (Ψ) or eigen functions

(10) Application of Schrodinger wave equation :⇒

applied to

identify the energy of a moving particle (e.g. an electron)

- when it is free to move in any direction in
- when it is enclosed in a box

introduces concept of atomic orbital

yield and expression for describing the energy of electron in case of H atom

The Free particle: ⇒ Consider a particle of mass m moving with velocity u under conditions where the potential energy (P.E/U) of the particle is zero, i.e. $U=0$.

The equation (11) becomes

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} + \frac{8\pi^2 m}{h^2} E\psi = 0$$

⇒ Dividing by ψ we get,

$$\Rightarrow \frac{1}{\psi}\left(\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2}\right) + \frac{8\pi^2 m}{h^2} E = 0 \quad (12)$$

The total energy of the particle (E) ⇒ can be considered to consists of three components, E_x, E_y and E_z along the three axes X, Y, and Z, respectively such that

$$\boxed{E = E_x + E_y + E_z} \quad (14)$$

The wave function may be taken as

$$\boxed{\psi = \psi_x \psi_y \psi_z} \quad (15)$$

(* Why? needs to be explained)

Where, ψ_x is a function of x only, ψ_y is a function of y only and ψ_z is function of z only.

CONTINUED FROM P.G ⇒ 42

Substituting the values of equation (14) and (15) in equation (13) we get,

$$\frac{1}{\psi_x\psi_y\psi_z}\left(\frac{\partial^2 \psi_x\psi_y\psi_z}{\partial x^2} + \frac{\partial^2 \psi_x\psi_y\psi_z}{\partial y^2} + \frac{\partial^2 \psi_x\psi_y\psi_z}{\partial z^2}\right.$$

$$\left. + \frac{8\pi^2 m(E_x+E_y+E_z)}{h^2}\right) = 0$$

~~$$\Rightarrow \frac{\psi_y\psi_z\,\partial^2\psi_x}{\psi_x\psi_y\psi_z} + \frac{\psi_x\cdot\psi_z}{\psi_x\psi_y\psi_z}\frac{\partial^2\psi_y}{\partial^2 y}$$~~

$$\Rightarrow \frac{\psi_y\psi_z}{\psi_x\cdot\psi_y\psi_z}\cdot\frac{\partial^2\psi_x}{\partial x^2} + \frac{\psi_x\cdot\psi_z}{\psi_x\cdot\psi_y\cdot\psi_z}\frac{\partial^2\psi_y}{\partial y^2}$$

$$+ \frac{\psi_x\cdot\psi_y}{\psi_x\cdot\psi_y\cdot\psi_z}\cdot\frac{\partial^2\psi_z}{\partial z^2}$$

$$+ \frac{8\pi^2 m}{h^2}E_x + \frac{8\pi^2 m}{h^2}E_y$$

$$+ \frac{8\pi^2 m}{h^2}E_z = 0$$

$$\Rightarrow \left(\frac{1}{\psi_x}\frac{\partial^2\psi_x}{\partial x^2} + \frac{8\pi^2 m}{h^2}E_x\right) + \left(\frac{1}{\psi_y}\cdot\frac{\partial^2\psi_y}{\partial y^2} + \frac{8\pi^2 m}{h^2}\cdot E_y\right)$$

$$+ \left(\frac{1}{\psi_z}\frac{\partial^2\psi_z}{\partial z^2} + \frac{8\pi^2 m}{h^2}E_z\right) = 0 \quad \text{——(16)}$$

In the above equation, each term in the brackets is a function of one variable only. Since each variable can be varied independently, each of these terms must be equal to zero. We thus have three differential equations, viz.

Not understood

$$\frac{1}{\psi_x}\frac{\partial^2 \psi_x}{\partial x^2} + \frac{8\pi^2 m}{h^2}E_x = 0 \quad \text{— (17)}$$

$$\frac{1}{\psi_y}\frac{\partial^2 \psi_y}{\partial y^2} + \frac{8\pi^2 m}{h^2}E_y = 0 \quad \text{— (18)}$$

$$\frac{1}{\psi_z}\frac{\partial^2 \psi_z}{\partial z^2} + \frac{8\pi^2 m}{h^2}E_z = 0 \quad \text{— (19)}$$

(7)

The solution of these equations yield the following expressions.

Not understood

$$E_x = \frac{1}{2} m v_x^2 \quad \text{—— (20)}$$

$$E_y = \frac{1}{2} m v_y^2 \quad \text{—— (21)}$$

$$E_z = \frac{1}{2} m v_z^2 \quad \text{—— (22)}$$

where v_x, v_y, v_z are the component of the velocity v along the three co-ordinate axes X, Y and Z, respectively.

Substituting the values of E_x, E_y and E_z in equation (14) we get

$$E = \frac{1}{2}m(v_x^2 + v_y^2 + v_z^2) \quad \text{——— (23)}$$

$$\boxed{E = \frac{1}{2}mv^2 = \text{Kinetic energy}} \quad \text{——— (24)}$$

Since the total energy $E = P.E + K.E$, It is expected that when $P.E = 0$, the total energy, $\boxed{E = K.E = \frac{1}{2}mv^2}$ ——— (25)

* **The particle in a Box** :⇒ consider the same particle (of mass m moving with velocity v) to be contained in a rectangular box of dimension a, b and c in length. Let U is the potential energy and E be the total energy of the particle. In the present case the potential energy U comprise of three components, U_x, U_y and U_z, along the three co-ordinates X, Y and Z respectively so that

$$U = U_x + U_y + U_z \quad \text{——— (26)}$$

From equation (14) we get

$$E = E_x + E_y + E_z \quad \text{——— (27)}$$

Subtracting (26) from (27) we get,

$$(E - U) = (E_x - U_x) + (E_y - U_y) + (E_z - U_z) \quad \text{——— (28)}$$

Proceeding in the same manner as above, it is possible to separate the Schrodinger wave equation into the following equations.

$$\frac{1}{\psi_x}\frac{\partial^2 \psi_x}{\partial x^2} + \frac{8\pi^2 m}{h^2}(E_x - U_x) = 0 \quad \text{--- (29)}$$

$$\frac{1}{\psi_y}\frac{\partial^2 \psi_y}{\partial y^2} + \frac{8\pi^2 m}{h^2}(E_y - U_y) = 0 \quad \text{--- (30)}$$

$$\frac{1}{\psi_z}\frac{\partial^2 \psi_z}{\partial z^2} + \frac{8\pi^2 m}{h^2}(E_z - U_z) = 0 \quad \text{--- (31)}$$

The solution of these equations yield following expressions.

Not understood ←

$$E_x = \frac{n_x^2 h^2}{8ma^2} \quad \text{--- (32)}$$

$$E_y = \frac{n_y^2 h^2}{8mb^2} \quad \text{--- (33)}$$

$$E_z = \frac{n_z^2 h^2}{8mc^2} \quad \text{--- (34)}$$

where n_x, n_y, n_z are the quantum numbers = 1, 2, 3 etc. and a, b and c as already mentioned are the dimensions of the box.

Total energy, $E = E_x + E_y + E_z$

$$= \frac{h^2}{8m}\left[\frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} + \frac{n_z^2}{c^2}\right] \quad (35)$$

It is evident ~~that~~ from equation (35) that energies of a particle contained in a box are quantized. This is not so in the case of a free particle. In the latter case the ~~energy~~ energies can vary continuously with variation in velocity.

(11) Concept of Atomic Orbital :-

The wave function ψ in Schroedinger wave equation (represents the amplitude of the electron wave)

↓

has no physical significance.

However ⇒ Square (ψ^2) of wave function

↓ gives.

The probability of finding an electron of a given energy E, from place to place in a given region around the nucleus.

It is thus possible

↓

to identify regions of (space) around the nucleus

↓

where there is high probability of locating an electron associated with specific energy.

This space → (atomic orbital.)

↓

represents → a definite region in three dimensional space around the nucleus where there is high probability of finding an electron of a specific energy E.

Energy of electron in Hydrogen atom:-

A single electron of charge $-e$ is revolving round the nucleus of charge $+e$. So potential energy

$$U = -\frac{e^2}{r} \quad \text{——— (36)}$$

Therefore for H-atom the applied Schrodinger wave equation takes the form

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} + \frac{8\pi^2 m}{h^2}\left(E + \frac{e^2}{r}\right)\psi = 0 \quad \text{——— (37)}$$

This equation when solved advanced mathematical treatment gives the following expression for energy of electron in the nth level of H atom

$$E_n = -\frac{me^4}{8\epsilon_0^2 h^2 n^2} \qquad \text{—— (38)}$$

↓

Identical expression with Bohr's equation for H atom derived from basis of classical mechanics.

a) Classical mechanics
b) Wave mechanical treatment

} → energy of electron in H atom

↓

both values agrees with the experimental values.

(Wave mechanical treatment) ↓

Superior for more complicated atom.