

## Modern Physics

- Valence electrons
- Crystal field splitting:  $d \xrightarrow{\text{tig}} \text{eg}$
- Stern and Gerlach expt.  $\rightarrow$  proved the  $e^-$  spin existence Ag source.
- Non-uniform magnetic field
- Photoelectric effect
- Radiation from an object
- Spectral lines in atoms
- Selection rules -

09/01/19

### Max Planck's law:

Power emitted per unit area per unit frequency

$$B_\gamma(\gamma, T) = \frac{2h\gamma^3}{c^2} \times \frac{1}{e^{\frac{hc}{k_B T}} - 1}$$

$k_B$  → Boltzmann constant

$h$  → Planck's constant

$c$  → speed of light

Rayleigh-Jeans law

Wein's Displacement law.

Black Body Radiation  
emits EM Radiations

$$\gamma = \frac{c}{\lambda}$$

$$\frac{\gamma^3}{c^2} = \frac{c^3}{\lambda^3 \cdot c^2}$$

$$= \frac{c}{\lambda^3}$$

$$B_\lambda(\lambda, T) = \frac{2hc^2}{\lambda^5} \times \frac{1}{e^{\frac{hc}{\lambda k_B T}} - 1} = \frac{2hc^2}{\lambda^5} \frac{1}{e^{\frac{hc}{\lambda k_B T}} - 1}$$

lower frequency (larger wavelength) → Rayleigh Jeans law

Higher frequency (smaller wavelength) → Wein's Displacement law.

Rayleigh & Jeans law

$$B_\lambda(T) = \frac{2c k_B T}{\lambda^4}$$

$B_\lambda$  = Spectral Radiance

$c$  → speed of light

$k_B$  → Boltzmann's Constant

$T$  → Temperature

$$B_\gamma(\gamma) = \frac{2\gamma^2 k_B T}{c^2} \rightarrow \text{larger wavelength (lower frequency).}$$

Ultraviolet catastrophe → Rayleigh Jeans catastrophe  
classical physics

Black body emit the radiation in all frequencies range.

$$\lambda = \frac{c}{\gamma}$$

$$B_\lambda(T) = \frac{2hc^2}{\lambda^5} \frac{1}{e^{\frac{hc}{\lambda k_B T}} - 1}$$

$$e^\lambda = 1 + \lambda + \frac{\lambda^2}{2!} + \frac{\lambda^3}{3!} + \dots$$

$$e^{\frac{hc}{\lambda k_B T}} \approx 1 + \frac{hc}{\lambda k_B T}$$

$$\frac{1}{e^{\frac{hc}{\lambda k_B T}} - 1} \leftarrow \frac{1}{\frac{hc}{\lambda k_B T}} = \frac{\lambda k_B T}{hc}$$

$$B_\lambda(T) = \frac{2ck_B T}{\lambda^4} \quad \text{which is identical to}$$

the classical physics Rayleigh Jeans law.

$$B_\gamma(T) = \frac{2h\nu^3}{c^2} \cdot \frac{1}{e^{\frac{h\nu}{k_B T}} - 1}$$

$$B_\gamma(T) = \frac{2h\nu^3}{c^2} \cdot \frac{k_B T}{h\nu} = \frac{2\nu^2 k_B T}{c^2}$$

~~Wien's~~ Wien's Displacement law

$$\frac{hc}{k_B T_{max}} = 4.965 \rightarrow \lambda_{max} = \frac{b}{T} \quad b = \text{Proportionality constant}$$

$\lambda$  is inversely proportional to temp. (T).  
It is directly proportional to temp (T).

There is a change in  $\lambda$  when we change the temp (T). Displacement is  $\Delta\lambda$  ...

Black Body radiation is a quantum physics phenomenon.  
- Classical phys is not adequate  
- Max Planck's law is universally accepted.

10/01/19

## Radiation Thermometers

- 1. Temperature sensor
- 2. Converting the same in numbers.

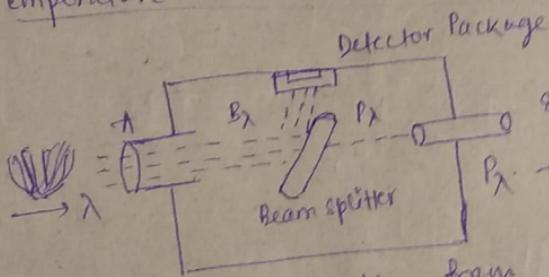
When we heat an iron bar, there are 3 range in colour:

- (i) Red-hot
- (ii) Red-Orange
- (iii) White

### Radiation Thermometer

measures the thermal energy emitted by a source using Planck's law

### Temperature Measurement using Radiation

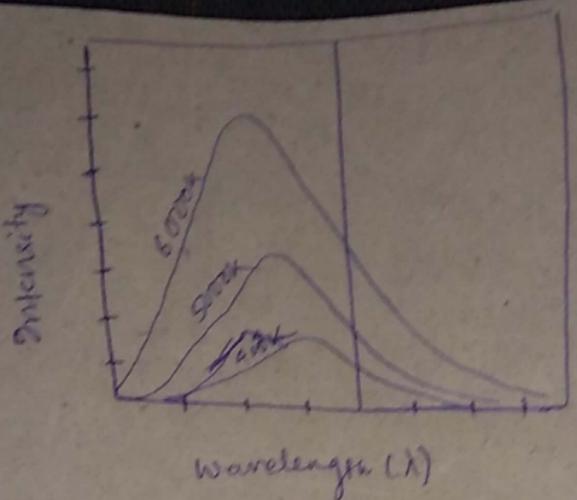


The Intensity of radiation from black body is a function of

$$I_b = f(r, \theta, \phi)$$

from Planck's Law,

$$B_\lambda(T) = \frac{2hc^2}{\lambda^5} \cdot \frac{1}{e^{\frac{hc}{kT}} - 1}$$



The area under the curve grows with temperature.

### Bark's Ideas for Radiation Thermometre

- $10^{-6} \mu\text{m}$  at  $0^\circ\text{C}$  and  $1.5 \mu\text{m}$  at  $200^\circ\text{C}$
  - Radiation predominantly lies in visible region, sometimes near and middle infrared regions
  - collect radiation from target and produces output signal (electrical)
- $V \Rightarrow$  Potential  
 $E \Rightarrow$  spectral radiance  
 $dV \Rightarrow$  output in response to  
 the radiant flux  
 $dE_\lambda$
- $$R_\lambda = \frac{dV}{dE_\lambda}$$
- $$dV = R_\lambda dE_\lambda$$

$$dV = R_\lambda I_\lambda A B_\lambda P_\lambda d\lambda$$

$$V = \int_0^{\infty} R_\lambda I_\lambda A B_\lambda P_\lambda d\lambda \rightarrow \text{Radiometer measurement equation.}$$

$$I_{b,\lambda}(\lambda, T) = \frac{2hc^2}{\lambda^5} \frac{1}{e^{\frac{hc}{\lambda k_B T}} - 1}$$

Differentiate this w.r.t temp  $T$ :

$$\frac{dI}{dT} = \frac{2hc^2}{\lambda^5}$$

$$dI_{b,\lambda}(\lambda, T) = \frac{2hc^2}{\lambda^6 T^2} \frac{1}{e^{\frac{hc}{\lambda k_B T}} - 1} dT$$

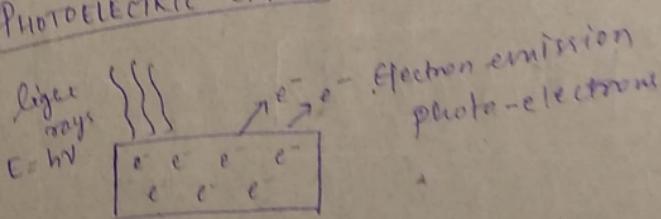
$$\frac{dI_{b,\lambda}(\lambda, T)}{I_{b,\lambda}(\lambda, T)} = \frac{hc}{k_B} \frac{dT}{\lambda T^2}$$

$$\frac{d}{ds} \frac{dT}{T} = \frac{dI_{b,\lambda}(\lambda, T)}{I_{b,\lambda}(\lambda, T)} \times \frac{\lambda T}{\frac{hc}{k_B}}$$

1. Wavelength
2. shortest possible wavelength
3. wavelength  $\propto$  Temp

16/01/19

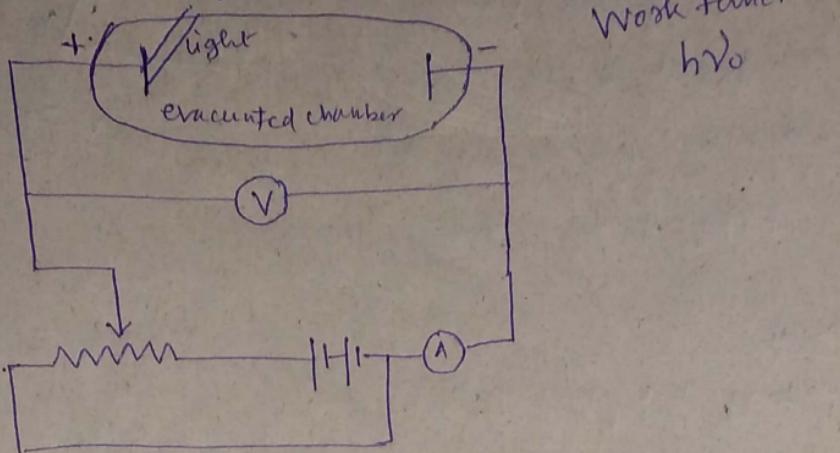
### PHOTOELECTRIC EFFECT



- \* The inter-band transition exists in semi-conductor and insulators. optical absorption

On metals, there is no band gap; optical conductivity due to intra-band transition.

### Experimental Setup



NOTE: (i) Constant P.D is not maintained between cathode and anode.

(ii) Not all the  $e^-$  ejected will move to cathode as cathode is -vely charged.

(iii) When the intensity of light is increased, the probability of  $e^-$  which reaches cathode increases.

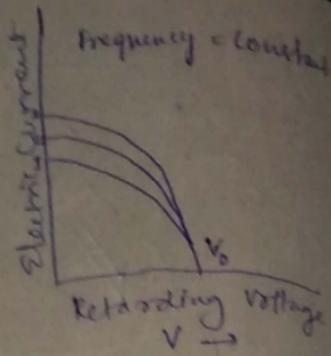
(iv) A min threshold energy called work function ( $\phi = h\nu_0$ ) is required for an  $e^-$  to get ejected.

(v) stopping Potential is the potential difference needed to prevent the most energetic  $e^-$  from reaching the other electrode.

(vi) Electric dipole approximation

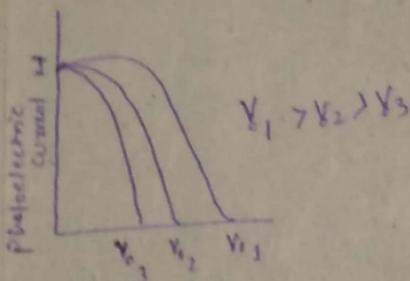
Kinetic Energy of Intensity of Incident light

\* The energy from photons are transferred to the  $e^-$  and they attain the K.E. to come out of the metal surface.

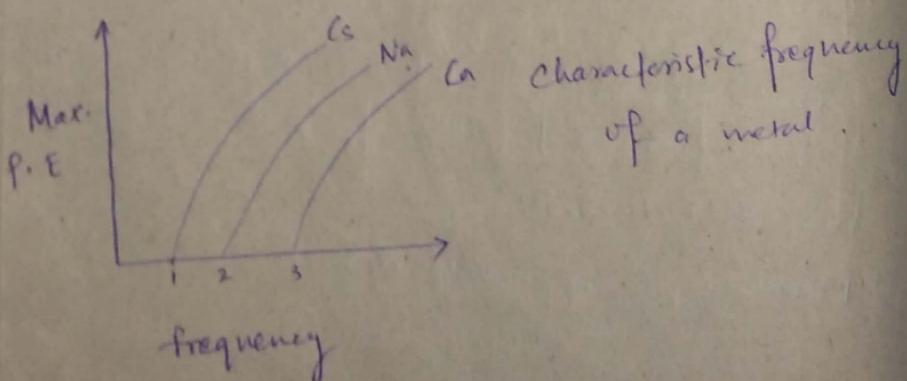


### Note:

- (I) Large K.E. when they can travel & reach the cathode
- (II) No time interval between light falling and photoelectron coming out of the surface  $-10^{-6}$  sec
- (III) A layer of sodium 1 atom thick - each atom releases an energy  $10^{-25}$  W.



Light intensity constant  
Higher the frequency, more energy of the electrons.



Quantum Theory of Light:  
Light is not spread as wavefront, small packet called photons.

- Total Energy is concentrated on photons
- All photons have same freq.  $\nu$ .
- Intensity change will change the no. of  $e^-$  ejected but energy remains unchanged.
- The higher the freq  $\nu$ , the greater the photon energy  $h\nu$ .
- Work function,  $\Phi = h\nu_0$
- Total Energy =  $K \cdot E_{max} + \Phi$   
 $h\nu =$  photoelectric energy.

$K \cdot E_{max}$  = Maximum photoelectron energy  
(which is proportional to stopping potential).

$\Phi$  = Max energy required for an  $e^-$  to leave the metal.

$$h\nu = K \cdot E_{max} + h\nu_0$$
$$\boxed{K \cdot E_{max} = h(\nu - \nu_0)}$$

1. What are the energy and momentum of a photon of a red light of wavelength 650nm?  
 What is the wavelength of a photon of energy 2.40 eV?

$$\underline{\text{Ans}} \quad E = \frac{hc}{\lambda} = \frac{6.63 \times 10^{-34} \times 3 \times 10^8}{650 \times 10^{-9}}$$

$$E = 0.031 \times 10^{-17} \text{ J.}$$

$$1 \text{ J} = 6.24 \times 10^{18} \text{ eV}$$

$$0.031 \times 10^{-17} \text{ J} = 0.193 \times 10^{-17} \text{ eV}$$

$$= 1.93 \text{ eV}$$

$$\text{Momentum } p = \frac{E}{c} = \frac{0.031 \times 10^{-17}}{3 \times 10^8}$$

$$= 0.01 \times 10^{-9}$$

$$= 0.01 \text{ nm}$$

$$\text{Now, } \frac{2.4}{6.24 \times 10^{18}} = \frac{6.63 \times 10^{-34} \times 3 \times 10^8}{\lambda}$$

$$\lambda = \frac{6.63 \times 3 \times 10^{-34} \times 6.24 \times 10^{18} \times 10^8}{2.4}$$

$$= 517 \text{ nm.}$$

2. The work function of tungsten metal is 4.52 eV
- What is the cut-off wavelength?
  - What is the max kinetic energy of the  $e^-$  when radiation wavelength 198nm is used?
  - What is the stopping potential in this case?

Ans - (a)  $\frac{4.52}{6.24 \times 10^{18}} = \frac{6.63 \times 10^{-34} \times 3 \times 10^8}{\lambda}$

$$\therefore \lambda = \frac{6.63 \times 10^{-34} \times 3 \times 10^8 \times 6.24 \times 10^{18}}{4.52}$$

$$\begin{aligned}\lambda &= 4.4 \times 10^{-26} \text{ nm/eV} \\ &= 27.45 \times 10^{-8} \text{ nm} \\ &= 275 \text{ nm.}\end{aligned}$$

(b)  $E - \frac{4.52}{6.24 \times 10^{18}} = \frac{6.63 \times 10^{-34} \times 3 \times 10^8}{198 \times 10^{-9}}$

$$\begin{aligned}E &= (0.1 \times 10^{-17}) + (0.72 \times 10^{-18}) \\ &= 0.73 \times 10^{-18} \text{ J}\end{aligned}$$

$$\therefore E = 4.055 \text{ eV}$$

(c)  $V = -4.055 \text{ eV}$

3. The wavelength of the photo-electric threshold for silver is  $3.250 \times 10^{-10}$  m. Determine the velocity of the  $e^-$  ejected from silver surface by UV light of wavelength  $2.536 \times 10^{-10}$  m.

$$\text{Ans} - T = h\nu - h\nu_0 \quad \lambda = 2.536 \times 10^{-10} \text{ m.}$$

$$\lambda_0 = 3.250 \times 10^{-10} \text{ m}$$

$$T = \frac{6.63 \times 10^{-34}}{3 \times 10^8} \times \left( \frac{1}{2.536} - \frac{1}{3.250} \right) \times 10^{20}$$

$$= 6.63 \times 3 \times 9.23 \times 10^{-20}$$

$$= 183.58 \times 10^{-20}$$

$$183.58 \times 10^{-20} = \frac{1}{2} \times 9.1 \times 10^{-27} \times v^2$$

$$\therefore v = \sqrt{40.34 \times 10^7}$$

$$v = 20.08 \times 10^3 \text{ m s}^{-1}$$

24/01/19

1. An ultraviolet light of wavelength 350nm and intensity  $1.00 \text{ W/m}^2$  is directed at a potassium surface. E =  $1.00 \times 10^{-4} \text{ m}^2$

(a) Find the max kinetic energy of the photoelectrons.

(b) If 0.5% of incident photons produce photo-electrons; how many are emitted

per second if the potassium surface has an area  $1.00 \text{ cm}^2$ ?  $\nu_0 = 2.2 \text{ eV}$

$$\text{Ans } (a) \frac{hc}{\lambda} = E$$

$$E = \frac{6.63 \times 10^{-39} \times 3 \times 10^8}{350 \times 10^{-9}}$$

$$= \frac{6.63 \times 3}{350} \times 10^{-34+8+9}$$

$$= 0.056 \times 10^{-17} \text{ J}$$

$$0.056 \times 10^{-17} \text{ J} = 0.056 \times 6.24 \times 10^{-19} \text{ J}$$

$$= 0.349 \times 10^{-19} \text{ J}$$

$$= 3.49 \text{ eV}$$

$$E = 3.5 \text{ eV}$$

$$K.E_{\max} = E - h\nu_0$$

$$= 3.5 - 2.2$$

$$K.E_{\max} = 1.3 \text{ eV}$$

~~(b) Total energy of photoelectrons =  $0.056 \times 10^{-17} \text{ J}$~~

~~No. of  $e^-$  incident at area  $1 \text{ cm}^2 = \frac{0.056 \times 10^{-17}}{(10^{-4} \text{ m}^2)} \text{ J}$~~

~~$= 0.056 \times 10^{-13} \text{ eV}$~~

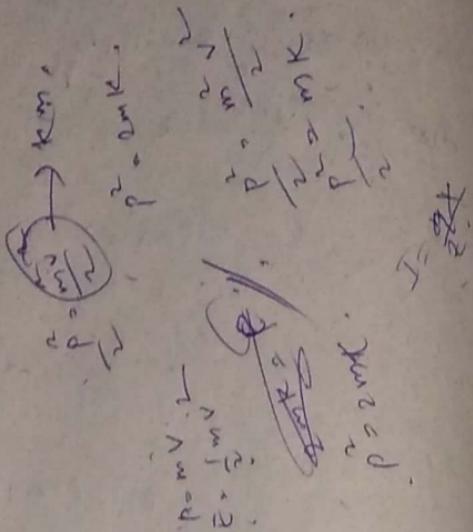
~~6.5% of incident photons~~

$$= 0.056 \times 10^{-13} \times 0.5 \times 10^{-2}$$

$$= 0.056 \times 0.5 \times 10^{-15}$$

$$=$$

Electrons emitted



Q. Show that photo electric effect cannot take place with a free  $e^-$ ?

$$E = h\nu$$

$$E^2 = h^2 \nu^2$$

$$P = h\nu/c$$

$$E = P^2 c^2$$

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

$$= h^2 \nu^2$$

place w

$$\boxed{E = CP}$$

$$P = \sqrt{\frac{2h\nu}{2mKE}}$$

$$2h\nu \cdot mc^2 = 0$$

$$E = C\sqrt{2mKE}$$

$$E^2 = C^2 2mKE$$

$$KE^2 = C^2 2mKE$$

$$KE = C^2 m$$

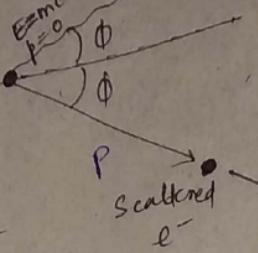
$$\boxed{KE = 2mc^2}$$

6-02-19

## Compton Effect

Inelastic scattering

(Light-matter interaction)  
(K.E. is not conserved)

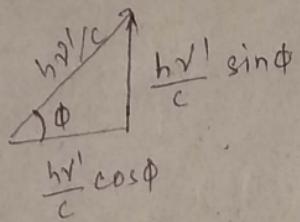


Arthur Holly  
Compton

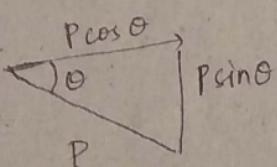
→ When the photon hits the  $e^-$ , the K.E. of photon increases and the wavelength of photon decreases.

## Scattering of $e^-$

Energy - Momentum conservation



Vector diagram of the momenta and their components of incident scattered photon.



$\gamma$  = Initial photon  
 $\gamma'$  = lower than the initial.

Loss in photon energy = Gain in electron energy

$$h\nu - h\nu' = KE \quad \text{--- (1)}$$

*Initial P*

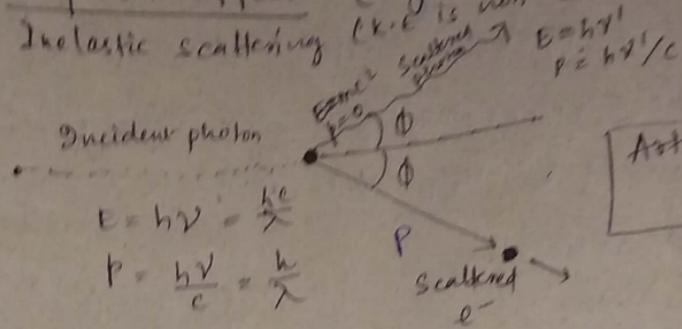
$$E = pc \Rightarrow p = E/c = \frac{h\nu}{c} \quad (\text{Initial photon momentum})$$

$$\text{Scattered Photon Momentum} = \frac{h\nu'}{c}$$

Initial Momentum = Final Momentum.

6-02-19

Compton Effect (Light-matter interaction)  
 Inelastic scattering ( $K.E$  is not conserved)

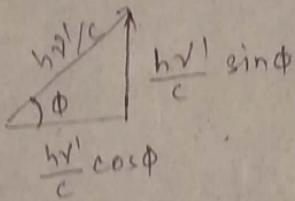


Arthur Holly  
Compton

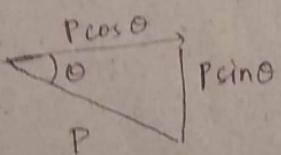
→ when the photon hits the  $e^-$ , the  $K.E$  of photon decreases and the wavelength of photon increases

Scattering of  $e^-$

Energy - Momentum conservation



Vector diagram of the momenta and their components of incident scattered photon.



$\nu$  = Initial photon

$\nu'$  = lower than the initial.

Loss in photon energy = Gain in electron energy

$$h\nu - h\nu' = KE \quad \text{--- (1)}$$

~~$O$  and  $P$   
Initial final~~

$$E = P c \Rightarrow P = E/c = \frac{h\nu}{c} \quad (\text{Initial photon momentum})$$

$$\text{Scattered Photon Momentum} = \frac{h\nu'}{c}$$

Initial Momentum = Final Momentum.

$$\frac{h\nu}{c} + \theta = \frac{h\nu'}{c} \cos\phi + p \cos\theta \rightarrow ②$$

$$1^{\text{st}} \text{ direction: } \theta = \frac{h\nu'}{c} \sin\phi - p \sin\theta \rightarrow ③$$

$\phi$ : Angle between the direction of initial and scattered photon

$\theta$ : Angle between the direction of initial photon and scattered  $e^-$ .

Multiplying ② and ③ by  $c$ .

$$② \times c : h\nu = h\nu' \cos\phi + p \cos\theta$$

$$\Rightarrow p \cos\theta = h\nu - h\nu' \cos\phi$$

$$③ \times c : \theta = h\nu' \sin\phi - p \sin\theta$$

$$\Rightarrow p \sin\theta = h\nu' \sin\phi$$

Squaring and adding,

$$p^2 c^2 = h^2 \nu^2 + (h\nu')^2 \cos^2\phi - 2h^2 \nu \nu' \cos\phi + (h\nu')^2 \sin^2\phi.$$

$$p^2 c^2 = h^2 \nu^2 + h^2 \nu'^2 - 2h^2 \nu \nu' \cos\phi \rightarrow ④$$

$$E = K \cdot E + M c^2 \rightarrow ⑤$$

$$E = \sqrt{M^2 c^4 + p^2 c^2} \rightarrow ⑥$$

We know,

$$(K \cdot E + M c^2)^2 = M^2 c^4 + p^2 c^2$$

$$p^2 c^2 = K \cdot E + 2mc^2 K \cdot E$$

$$K.E = h\nu - h\nu'$$

$$P^2 c^2 = (h\nu)^2 - 2(h\nu)(h\nu') + (h\nu')^2 + 2mc^2(h\nu - h\nu')$$

Sub  $P^2 c^2$  in ④,

$$2mc^2(h\nu - h\nu') = 2(h\nu)(h\nu')(1 - \cos\phi) \quad \text{--- ⑤}$$

Dividing by  $2h^2 c^2$ ,

$$\frac{mc}{h} (\gamma/c - \gamma'/c) = \frac{\gamma}{c} \cdot \frac{\gamma'}{c} (1 - \cos\phi)$$

$$\gamma/c = \frac{1}{\lambda}, \quad \gamma'/c = \frac{1}{\lambda'}$$

$$\frac{mc}{h} \left( \frac{1}{\lambda} - \frac{1}{\lambda'} \right) = \frac{1 - \cos\phi}{\lambda\lambda'}$$

$$\boxed{(\lambda - \lambda') = \frac{h}{mc}(1 - \cos\phi)} \Rightarrow \text{Compton effect}$$

$\lambda \rightarrow$  initial wavelength

$\lambda' \rightarrow$  scattering wavelength

$h \rightarrow$  Planck's constant

$m \rightarrow$  mass of  $e^-$

$c \rightarrow$  speed of light

$\phi \rightarrow$  scattering angle

07/02/19

## compton scattering

$$E = \sqrt{m^2 c^4 + p^2 c^2}$$

## Mass and Energy

Work done on an object by constant force  $F$ :

$$W = \vec{F} \cdot \vec{s}$$

$$K.E = \vec{F} \cdot \vec{s}$$

$F$  is not constant

$$K.E = \int_0^s \vec{F} \cdot d\vec{s}$$

$$K.E = \frac{1}{2} m v^2$$

$$p = \cancel{m} v \quad (\text{Relativistic Momentum})$$

$$F = \frac{dp}{dt} = \frac{d}{dt} (\cancel{m} v)$$

$$\text{Here } \gamma = \frac{1}{\sqrt{1 - \frac{v^2}{c^2}}}$$

$$K.E = \int_0^v \frac{d}{dt} (\cancel{m} v) ds = \int_0^v v \frac{d(\cancel{m} v)}{ds} ds$$

$$= \int_0^v v \frac{d}{ds} \left( \frac{mv}{\sqrt{1 - v^2/c^2}} \right) ds$$

Integration by part:

$$K.E = \frac{mv^2}{\sqrt{1 - v^2/c^2}} - m \int_0^v \frac{vdv}{\sqrt{1 - v^2/c^2}}$$

$$= \frac{mv^2}{\sqrt{1 - v^2/c^2}} + \left[ m c^2 \sqrt{1 - v^2/c^2} \right]_0^v$$

$$= \frac{mc^2}{\sqrt{1-v^2/c^2}} - mc^2$$

$$\Rightarrow K.E = \gamma mc^2 - mc^2$$

$$| K.E = (\gamma - 1) mc^2 |$$

$$\text{Total Energy, } E = \frac{mc^2 + K.E}{E_0}$$

$$E = E_0 + K.E$$

$mc^2$  = rest energy of  $e^-$

$$E = \gamma mc^2 = \frac{mc^2}{\sqrt{1-v^2/c^2}}$$

Energy and momentum :  $E = pc$

Total Energy,  $E_0$  and momentum of the particle

$$E = \frac{mc^2}{\sqrt{1-v^2/c^2}} \quad E^2 = \frac{m^2 c^4}{\left(1-\frac{v^2}{c^2}\right)}$$

$$P = \frac{mv}{\sqrt{1-\frac{v^2}{c^2}}} \quad P^2 c^2 = \frac{m^2 v^2 c^2}{\left(1-\frac{v^2}{c^2}\right)}$$

$$E^2 = P^2 c^2 = \frac{m^2 c^2 (c^2 - v^2)}{\left(1-\frac{v^2}{c^2}\right)}$$

$$E^2 = \frac{m^2 c^2 (c^2 - v^2)}{1 - \frac{v^2}{c^2}} = \frac{m^2 c^2 (c^2 - v^2) \times c^2}{(c^2 - v^2)}$$

$$E^2 = m^2 c^4 + (mc^2)^2$$

T.E = (speed + mass energy)

$$E^2 - p^2 c^2 = m^2 c^4$$

mass-energy equivalence

$$\frac{h\nu}{c} + o = \frac{h\nu'}{c} \cos\phi + p \cos\theta$$

Initial momentum = final momentum

for perpendicular direction.

$$o = \frac{h\nu'}{c} \sin\phi - p \sin\theta$$

$\phi$  = angle between the incident and scattered photon.

$\theta$  = Between incident photon and recoil electron.

$$p \cos\theta = h\nu - h\nu' \cos\phi$$

$$p \sin\theta = h\nu' \sin\phi$$

$$P^2 c^2 = (h\nu)^2 - 2(h\nu)(h\nu') \cos\phi + (h\nu')^2 \quad \text{--- (1)}$$

$$E = k \cdot E + mc^2$$

$$E = \sqrt{m^2 c^4 + P^2 c^2} \quad k \cdot E = h\nu - h\nu'$$

$$P^2 c^2 = (h\nu)^2 - 2(h\nu)(h\nu') + (h\nu')^2 + 2mc^2(h\nu - h\nu')$$

Substituting (2) in (1),

$$(h\nu)^2 - 2(h\nu)(h\nu') + (h\nu')^2 + 2mc^2(h\nu - h\nu') \\ = (h\nu)^2 - 2(h\nu)(h\nu') \cos\phi + (h\nu')^2$$

$$2mc^2(h\nu - h\nu') = 2h\nu(h\nu')(1 - \cos\phi)$$

$$\text{Put } \frac{\nu}{c} = \frac{1}{\lambda}, \frac{\nu'}{c} = \frac{1}{\lambda'}$$

$$\frac{mc^2}{c} \left( \frac{h\nu}{c} - \frac{h\nu'}{c} \right) = \left( \frac{h\nu}{c} \right) \left( \frac{h\nu'}{c} \right) (1 - \cos\phi)$$

$$\frac{mc}{h} \left( \frac{1}{\lambda} - \frac{1}{\lambda'} \right) = \frac{1}{\lambda\lambda'} (1 - \cos\phi)$$

$$\frac{mc}{h} \left( \frac{\lambda' - \lambda}{\lambda\lambda'} \right) = \frac{1}{\lambda\lambda'} (1 - \cos\phi)$$

$$\boxed{(\lambda' - \lambda) = \frac{h}{mc} (1 - \cos\phi)}$$

- \* change in wavelength for a scattered photon
- \* change is independent of the wavelength of the incident photon

$$\Delta\lambda = \frac{h}{mc} (1 - \cos\phi) \text{ depends only on}$$

$\phi$  i.e angle of scattering.

$$\Delta\lambda = \lambda' - \lambda = \frac{h}{m_e c} (1 - \cos\phi)$$

$$\boxed{\lambda_c = \frac{h}{m_e c}}$$

## Compton Effect - Definition

The scattering of EM radiation such as  $\gamma$ -rays,  $\gamma$ -rays of wavelength  $\lambda$ , from certain low atomic no. material like paraffin or graphite into radiation of higher wavelength  $\lambda'$  is called as Compton Effect.

- The difference  $\lambda' - \lambda$  is independent of incident wavelength as well as nature of scatterer.
- It depends only on angle of scattering.

## Energy of Recoil-electrons

The energy transformed to the  $e^-$  by the incident photon is given as -

$$E = h\nu - h\nu' = h\nu \left(1 - \frac{\nu'}{\nu}\right)$$

$$\frac{E}{h\nu} = \left(1 - \frac{\nu'}{\nu}\right) = \frac{\lambda' - \lambda}{\lambda'}$$

we have

$$\frac{E}{h\nu} = \frac{\lambda_c (1 - \cos \phi)}{\lambda + \lambda_c (1 - \cos \phi)}$$

$$\therefore \boxed{E = \frac{h\nu}{1 + \frac{moc^2}{h\nu (1 - \cos \phi)}}}$$

14/02/19

Problems :

1.  $\lambda = 400 \text{ nm}$

2.  $\theta = 180^\circ$

$E' = ?$

$$\Delta\lambda = \frac{h}{m_e c} (1 - \cos \theta)$$

$$\Delta\lambda = \lambda (1 - \cos \theta)$$

$$= 2\lambda e$$

$$\Delta\lambda = \frac{6.624 \times 10^{-34}}{9.1 \times 10^{-31} \times 3 \times 10^8} (1 - \cos 180^\circ)$$

$$= 0$$

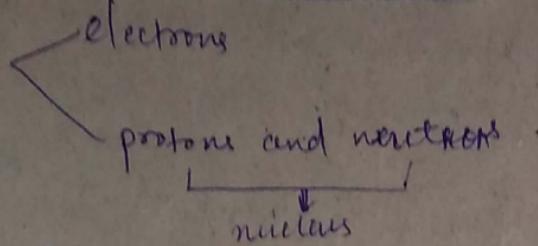
$$\Delta\lambda = 4.86 \text{ pm} = 0.00486 \text{ nm}$$

$$\lambda' = \lambda - \Delta\lambda$$

$$\lambda' = (400 - 0.00486) \text{ nm}$$

$$\lambda' =$$

# ATOMS

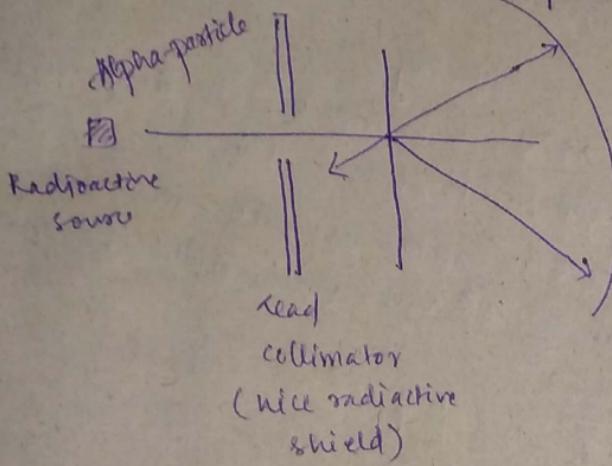


Thomson's Plum Pudding Model



J. J. Thomson

Rutherford's Gold foil experiment



- \* All the charges are conc. at the centre of the atom, and  $e^-$  are found to revolve around the nucleus.

27.02.19

$$N(\theta) = \frac{N_0 n t z^2 e^4}{(2\pi\epsilon_0)^2 r^2 k E^2 \sin^2(\theta/2)}$$

$N(\theta)$  → Number of  $\alpha$ -particles per unit area that reach the screen at a scattering angle  $\theta$ .

$N_i \rightarrow$  Total number of  $\alpha$ -particles that reaches the screen.

$n \rightarrow$  No. of atoms per unit volume in the foil.

$Z \rightarrow$  atomic number

$r_c \rightarrow$  distance of the screen from the foil.

$K.E \rightarrow$  K.E of the  $\alpha$ -particle

$t \rightarrow$  foil thickness

The nucleus also spins; but due to its huge high magnitude of mass, the spin is almost negligible. It has a non-zero spin-magnetic moment. But this magnetic moment scales with the mass.

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

$$F_e = \frac{1}{4\pi\epsilon_0} \frac{e^2}{r^2}$$

The condition for dynamically stable orbit is

$$F_c = F_e$$

$$\frac{mv^2}{r} = \frac{1}{4\pi\epsilon_0} \frac{e^2}{r^2}$$

$$v = \frac{e}{\sqrt{4\pi\epsilon_0 m r}}$$

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

$$= \frac{1}{2}mv^2 - \frac{e^2}{4\pi\epsilon_0 r}$$

When  $e^-$  and proton are infinitely far apart  
Substitute  $r$  in this eqn,

$$E = \frac{e^2}{8\pi\epsilon_0 r} - \frac{e^2}{4\pi\epsilon_0 r}$$

$$\boxed{E = -\frac{e^2}{8\pi\epsilon_0 r}}$$

\* Atomic spectra  $\rightarrow$  Absorption - Dark lines

$\searrow$  Emission - Bright lines

\* Missing of spectral lines is absorption.

### Spectral lines

Balmer (Visible region of H-atom spectrum),  $\frac{1}{\lambda} = R \left( \frac{1}{2^2} - \frac{1}{n^2} \right)$ ,  $n = 3, 4, 5$ .  
 $R$  - Rydberg constant  
 $= 1.097 \times 10^7 \text{ m}^{-1}$   
 $= 1.097 \text{ nm}^{-1}$

05/03/19

### Bohr's Model

1. To define the nature of orbit.

2.  $E = h\nu$ .

Bohr's postulates : Hydrogen atom ( $Z = 1$ )

(i) Electron orbit - Privilileged orbits

(ii) Origin of spectral lines

# Nature of Privileged Quantum Orbits

$x \rightarrow$  displacement

't'  $\rightarrow$  time

$$x = A \sin 2\pi\gamma t \longrightarrow ①$$

$$= A \sin 2\pi\gamma t$$

$A$  = Amplitude of  $\gamma$ -frequency

$$K.E = \frac{1}{2} m \left( \frac{dx}{dt} \right)^2$$

$m \rightarrow$  mass

$\frac{dx}{dt} \rightarrow$  Linear velocity

$$\frac{dx}{dt} = 2\pi\gamma A \cos 2\pi\gamma t$$

$$\left( \frac{dx}{dt} \right)_{max} = 2\pi\gamma A$$

( Since the max value of  $\cos 2\pi\gamma t = 1$  )

$$\text{The total energy} = \frac{1}{2} m \left[ \left( \frac{dx}{dt} \right)_{max} \right]^2$$

$$= \frac{1}{2} m (2\pi\gamma A)^2$$

$$E = 2m\pi^2\gamma^2 A^2$$

Now,

$$nh\nu = 2m\pi^2\gamma^2 A^2$$

$$nh = 2m\pi^2\gamma^2 A^2 \longrightarrow ②$$

$$P_x = m \left( \frac{dx}{dt} \right) = m(2\pi\gamma A \cos 2\pi\gamma t)$$

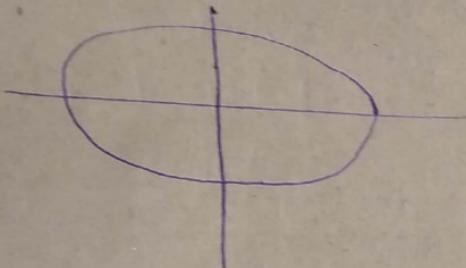
Put  $m \cdot 2\pi\gamma A = B$ ,  $P_x = B \cos 2\pi\gamma t$ .

$$\frac{P_x}{B} = \cos 2\pi\gamma t.$$

From (1),  $\frac{x}{A} = \sin 2\pi\gamma t$ .

Squaring and adding above eq's.

$$\frac{x^2}{A^2} + \frac{P_x^2}{B^2} = 1.$$



$dx \rightarrow$  width of an element at distance  $x$  from origin

let  $P_x \rightarrow$  ordinate corresponding to  $x$ .

$P_x dx \rightarrow$  phase integral.

$\oint P_x dx =$  area of the ellipse

$$= \bar{A} \times A \times B$$

$$= 2\pi^2 A^2 \gamma m$$

$$= nh$$

$\hbar \rightarrow$  Planck's constant

$$p_n \rightarrow p_\phi ; dx \rightarrow d\phi$$

$$\oint p_\phi \cdot d\phi = nh$$

$$p_\phi = Iw$$

$I \rightarrow$  Moment of inertia of an  $e^-$

$w \rightarrow$  angular velocity

### Limitations of Bohr's Model

- ① Higher 'Z'  $\rightarrow$  inadequate.
- ② splitting of spectral lines (in presence of electric & magnetic fields)
- ③ No. of spectral lines
- ④ Intensity of spectral lines.

### Bohr's Radius

$M, E \rightarrow$  Let be the mass and charge of the nucleus.

$m, e \rightarrow$  mass, charge of  $e^-$

$E = Ze ; Z \rightarrow$  atomic structure of element

$E = e \quad Z = 1$

$Ee/a^2 \rightarrow$  force of attraction between nucleus &  $e^-$ .

$\frac{mv^2}{a} \rightarrow$  centrifugal force.

$$\text{Now } \frac{Ee}{a^2} = \frac{mv^2}{a}$$

$$V = \frac{Ee}{am} \quad \text{--- (1)}$$

$$P_\phi = I\omega = n\left(\frac{h}{2\pi}\right)$$

$$I\omega = ma^2\omega = ma^2\left(\frac{V}{a}\right) = \frac{nh}{2\pi} = mav$$

$$V = \frac{nh}{2\pi ma} \quad \text{--- (2)}$$

Dividing (1) by (2),

$$\begin{aligned} V &= \frac{Ee}{am} = \frac{2\pi me}{nh} \\ &= \frac{2\pi Ee}{nh} \quad \text{--- (3)} \end{aligned}$$

$$a = \frac{nh}{2\pi m V} \quad \begin{matrix} \text{substitute value of } V \text{ in} \\ (2) \text{ from (3)} \end{matrix}$$

$$a = \frac{nh}{2\pi m} \times \frac{nh}{2\pi Ee} = \frac{n^2 h^2}{4\pi^2 Ee m}$$

$$a \propto n^2$$

$$\begin{aligned} n = 1 &\Rightarrow 0.53 \times 10^{-8} \text{ cm} \rightarrow 0.53 \times 10^{-10} \text{ m} \\ &= 53 \text{ pm Bohr's radius} \end{aligned}$$

13.03.19

### Bohr's Radius

$$a = \frac{n^2 h^2}{4\pi^2 E_0 m}$$

$$a \propto n^2 \quad n = 1, 2, 3, \dots$$

$$0.53 \times 10^{-8} \text{ cm} \quad (\text{Bohr's radius})$$

Orbital frequency,

$$f = \frac{4\pi^2 E_0 e^2 m}{n^3 h^3}$$

Orbital Energy;

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

$$K.E = \frac{1}{2} m v^2 = \frac{Ee}{2a}$$

$$P.E = -\frac{Ee}{a}$$

$$W = \frac{Ee}{2a} - \frac{Ee}{a}$$

$$= -\frac{Ee}{2a}$$

$$W = W_m = -\frac{Ee}{2} \cdot \frac{4\pi^2 E_0 m}{n^2 h^2}$$

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

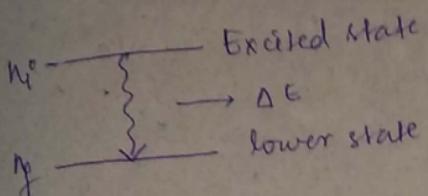
$W_m \rightarrow$  energy of  $e^-$  in the  $n$ th orbit.

## Atomic Spectra

Emission

Absorption

origin of spectral lines  
How/why they are spaced?



initial - final = photon energy

$$E_i^0 - E_f = h\nu$$

14.03.19

Q - Find the longest wavelength present in the Balmer series of hydrogen corresponding to the H<sub>a</sub> line

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

Quantum number  
of final state  
 $n = 2$

$$= R \left( \frac{1}{2^2} - \frac{1}{3^2} \right)$$

The longest  
wavelength in  
the series

$$= R \left( \frac{1}{4} - \frac{1}{9} \right)$$

correspond to  
small est  
energy diff.

$$= R \left( \frac{9-4}{36} \right)$$

the energy levels

$$\frac{1}{\lambda} = \frac{5}{36} R$$

Here  $n_i = 3$ .

$$\lambda = \frac{36}{5R}$$

$$= \frac{36}{5 \times 10^9 677} \text{ cm}$$

$$= 6.56 \times 10^{-5} \text{ cm} = 6.56 \times 10^{-7} \text{ m}$$

$$= 656 \text{ nm}$$

## Bohr's Correspondence Principle

The greater the quantum number, the closer quantum physics approaches classical physics.

$$v = \frac{e}{\sqrt{4\pi\epsilon_0 m r}} \quad , \quad r \rightarrow \text{radius of the orbit}$$

$$f = \frac{\text{electron speed}}{\text{orbital circumference}}$$

$$= \frac{v}{2\pi r} = \frac{e}{2\pi \sqrt{4\pi\epsilon_0 m r^3}}$$

$$\text{Also, } r_n = \frac{n^2 h^2 \epsilon_0}{\pi m_e^2} \quad \therefore f = \frac{me^4}{8\epsilon_0^2 h^3} \left( \frac{2}{n^3} \right)$$

$$= -\frac{E_1}{h} \left( \frac{2}{n^3} \right)$$

$$\gamma = -\frac{E_1}{h} \left( \frac{1}{n_f^2} - \frac{1}{n_i^2} \right)$$

$$\gamma = -\frac{E_1}{h} \left( \frac{1}{(n-p)^2} - \frac{1}{n^2} \right)$$

$$= -\frac{E_1}{h} \left[ \frac{2np - p^2}{n^2 (n-p)^2} \right]$$

$$2np - p^2 = 2np \quad [ \text{when } n > p ]$$

$$(n-p)^2 = n^2 \quad [ \text{when } n_i, n_f \gg 1 ]$$

$$\gamma = -\frac{E_1}{h} \left[ \frac{2p}{n^3} \right]$$

$$\text{when } n = 2, \text{ error} = 300\%.$$

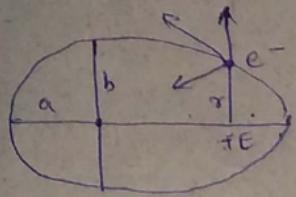
$$n = 10000, \text{ error} = 0.01\%.$$

20.03.19

## Sommerfeld model

problem with Bohr's model → couldn't explain fine structure.

## Elliptical orbits



electron moving in elliptical orbits.

$r$  = radius vector, the distance of the  $e^-$  from the nucleus + E

$\phi \rightarrow$  The angle which the nucleus radius vector makes with the major axis of the ellipse.

## Tangential Velocity ( $v$ )

One radial  $\rightarrow dr/dt$ .

Transverse at right angle to the radius

vector  $\rightarrow r \left( \frac{d\phi}{dt} \right)$

$P_r \rightarrow$  radial momentum  $\rightarrow m \left( \frac{dr}{dt} \right)$

$P_\phi \rightarrow$  angular or azimuthal  $\rightarrow m v^2 \left( \frac{d\phi}{dt} \right)$

$m \rightarrow$  mass of  $e^-$ .

$$\oint P_r \cdot dr = n_r \cdot h \quad \left. \right\} \quad \text{--- ①}$$

$$\oint P_\phi \cdot d\phi = n_\phi \cdot h$$

$n_r$  and  $n_\phi$  are the quantum number.

$$\therefore n = n_r + n_\phi \quad \text{--- (2)} \quad \begin{array}{l} n \rightarrow \text{total Quantum} \\ \text{number} \\ \text{and is identical} \\ \text{to Bohr} \end{array}$$

$$W = P \cdot E + \text{radial K.E.}$$

+ angular K.E.

$$W = -\frac{Ee}{r} + \frac{1}{2} m \left( \frac{dr}{dt} \right)^2 + \frac{1}{2} mr^2 \left( \frac{d\phi}{dt} \right)^2 \quad \text{--- (3)}$$

$$1 - e^2 = \frac{b^2}{a^2} = \frac{n_\phi^2}{(n_\phi + n_r)^2} \quad \text{--- (4)}$$

$e \rightarrow$  eccentricity of the ellipse whose semi-major and semi-minor axis are  $a, b$  respectively.

$$W = -\frac{2\pi^2 m E^2 e^2}{h^2} \left( \frac{1}{n_\phi + n_r} \right)^2$$

$$(1 - e^2)^{1/2} = b/a = \frac{n_\phi}{n_\phi + n_r} = \frac{n_\phi}{n}$$

$n_\phi \rightarrow$  cannot be zero.

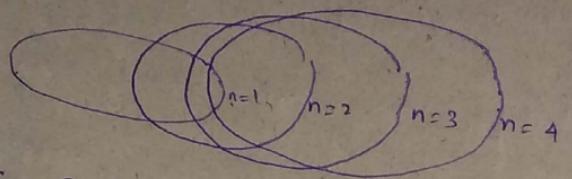
$n_\phi \rightarrow$  cannot be greater than  $n$ , since  $b$  is always less than  $a$ .

$n_\phi = n$ , the path becomes circular since

$$b=a, e=0.$$

For a given value of ' $n$ ',  ~~$n_\phi \rightarrow$~~  different ' $n$ ' values  
 There are possibilities of having ' $n$ ' elliptical orbits

$n=4$   
 four different ellipses are permitted.  
 $A_1, A_2, A_3, A_4 \dots$   
 $n, n_\phi$  and  $n_r$ .



$$\text{W} = -\frac{2\pi^2 m E^2 r^2}{h^2} \left( \frac{1}{n_\phi + n_r} \right)$$

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

Relativistic relation between mass and velocity.

\* mass of  $e^-$  from the set stationary rest frame of the nucleus.

Rosette shape - Precessing ellipse.

25/03/19

Sommerfeld's Model

$$n = n_r + n_\phi$$

- \* Splitting of spectral lines in the presence of external fields.
- \* Some transitions are permanent (selection rules).
- \* Precessing ellipse, in which,  $e^-$  have electrostatic force of attraction between  $e^-$  and nucleus
- \*  $e^-$  in an orbit is like revolving magnets.

- \* Magnetic moment which leads to splitting of spectral lines.
- \* Relativistic theory of Sommerfeld model helps to known splitting of lines.
- \* As  $V$  changes, mass also changes as it contributes to total energy (extra relativistic energy)

Proceeding ellipse  $\rightarrow$  doubly period.

- \* A revolving charge is itself a small magnet  
↳ non-zero magnetic moment.
- \* Double periodic besides original period of revolution, there is also the period of precessional motion.

'W'

$$W = -\frac{2\pi^2 m E^2 e^2}{h^2} \left[ \frac{1}{n^2} + \frac{4\pi^2 E^2 e^2}{c^2 h^2} \left( \frac{n}{n_\phi} - \frac{3}{4} \right) \frac{1}{n^4} + \dots \right].$$

$$= -\frac{2\pi^2 m e^4}{h^2} \cdot \frac{Z^4 d^2}{n^4} \left( \frac{n}{n_\phi} - \frac{3}{4} \right)$$

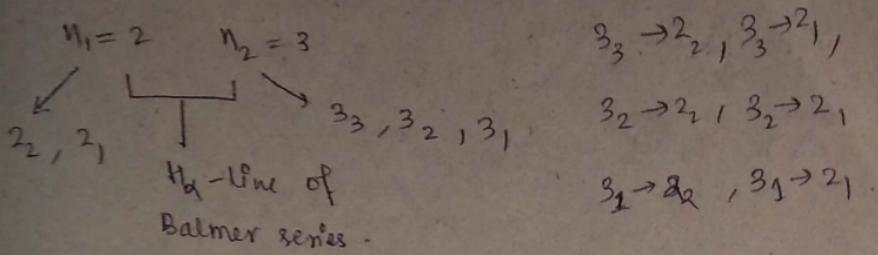
$$\begin{aligned} E &= Ze \\ d &= \frac{2\pi r e^2}{c h} \end{aligned}$$

'n'  $\rightarrow n\phi$  on account of  $\frac{n}{n_\phi}$ .

$n \rightarrow$  corr. to  $\phi$

$$\alpha^2, e, c, \dots, \alpha = 1.28 \times 10^{-3} \quad [\text{fine structure constant}]$$

## Application to the fine structure



Hydrogen doublet constant  $Z_2'$  and  $Z_1$

$$W_{n, n\varphi} = -R Z^2 c h \left\{ \frac{1}{n^2} + \frac{\alpha^2 Z^2}{n^4} \left( \frac{n}{n\varphi} - \frac{3}{4} \right) \right\}.$$

$W_{n, n\varphi} \rightarrow$  Energy corresponding to an orbit  
of total quantum number ( $n$ ) and ( $n\varphi$ ).

$$R = \frac{2\pi^2 me^4}{ch^3}$$

Energy for the ~~2, 2~~<sup>2, 2</sup> orbit.

$$W_{2, 2} = -R Z^2 c h \left\{ \frac{1}{Z^2} + \frac{\alpha^2 Z^2}{Z^4} \left( \frac{2}{2} - \frac{3}{4} \right) \right\}.$$

for 2<sub>1</sub> orbit.

$$W_{2, 1} = -e Z^2 c h \left\{ \frac{1}{Z^2} + \frac{\alpha^2 Z^2}{Z^4} \left\{ \left( \frac{2}{1} - \frac{3}{4} \right) \right\} \right\}.$$

$$W_{2, 2} - W_{2, 1} = R Z^2 c h \left\{ \frac{\alpha^2 Z^2}{Z^4} \left( \frac{2}{1} - \frac{3}{4} \right) - \left( \frac{2}{2} - \frac{3}{4} \right) \right\}.$$

$$= \frac{R Z^4 \alpha^2 c h}{Z^4}$$

$$\Delta W = W_{2,2} - W_{2,1} \quad z=1$$

$$\Delta \gamma = \frac{\Delta W}{h}$$

$$\Delta \bar{\gamma} = \frac{\Delta \gamma}{c} = \frac{\Delta W}{ch} = \frac{R\alpha^2}{T_b}$$

↓

$\frac{R\alpha^2}{T_b} \rightarrow$  hydrogen doublet constant  
denoted by 'd'.

$$R = 109700 \text{ cm}^{-1}$$

$$\alpha^2 = 5.3 \times 10^{-5}$$

$$d = 0.364 \text{ cm}^{-1} = \frac{R\alpha^2}{T_b}$$

$$\rightarrow W_{n,n_\Phi} = -\frac{RZ^2ch}{n^2} - \frac{RZ^2\alpha^2ch}{n^4} \left( \frac{n}{n_\Phi} - \frac{3}{4} \right)$$

↓  
uncorrected  
energy

↓  
Relatively corrections

$$(z=1) \Rightarrow W_{n,n_\Phi} = -W_n = \frac{R\alpha^2}{n^4} \left( \frac{n}{n_\Phi} - \frac{3}{4} \right)$$

uncorrected

26/03/19  
Distance between two lines

$$W_{n,n_\Phi} = -\bar{W}_n - \frac{R\alpha^2}{n^4} \left( \frac{n}{n_\Phi} - \frac{3}{4} \right)$$

$\bar{W}_n \rightarrow$  uncorrected energy level.

$$\left. \begin{array}{l} \bar{W}_{3,3} = -\bar{W}_3 - \frac{16d}{3^4} \left( \frac{3}{3} - \frac{3}{4} \right) = -\bar{W}_3 - \frac{4d}{81} \\ \bar{W}_{3,2} = -\bar{W}_3 - \frac{16d}{3^4} \left( \frac{3}{2} - \frac{3}{4} \right) = -\bar{W}_3 - \frac{12d}{81} \\ \bar{W}_{3,1} = -\bar{W}_3 - \frac{16d}{3^4} \left( \frac{3}{1} - \frac{3}{4} \right) = -\bar{W}_3 - \frac{36d}{81} \end{array} \right\}$$

$$\left. \begin{array}{l} \bar{W}_{2,2} = -\bar{W}_2 - d \left( \frac{2}{2} - \frac{3}{4} \right) = -\bar{W}_2 - \frac{d}{4} \\ \bar{W}_{2,1} = -\bar{W}_2 - d \left( \frac{2}{1} - \frac{3}{4} \right) = -\bar{W}_2 - \frac{5d}{4} \end{array} \right\}$$

$$\rightarrow \bar{W}_3 = \bar{W}_2$$

$$\rightarrow \bar{\gamma}_a, \bar{\gamma}_b, \bar{\gamma}_c, \bar{\gamma}_d, \bar{\gamma}_e, \bar{\gamma}_f$$

$$\rightarrow (3_3 \rightarrow 2_2) \quad \bar{\gamma}_a = \bar{\gamma} - \frac{4d}{81} + \frac{d}{4}$$

$$= \bar{\gamma} + \frac{65d}{324}$$

$$\rightarrow (3_3 \rightarrow 2_1) \quad \bar{\gamma}_b = \bar{\gamma} - \frac{4d}{81} + \frac{5d}{4}$$

$$= \bar{\gamma} + \frac{389d}{324}$$

$$(3_2 \rightarrow 2_1) \quad \bar{\gamma}_c = \bar{\gamma} - \frac{12d}{81} + \frac{d}{4}$$

$$= \bar{\gamma} + \frac{33d}{324}$$

$$(3_2 \rightarrow 2_1) \quad \bar{\gamma}_d = \bar{\gamma} - \frac{12d}{81} + \frac{5d}{4}$$

$$= \bar{\gamma} + \frac{357d}{324}$$

$$(3_1 \rightarrow 2_1) \quad \bar{\gamma}_e = \bar{\gamma} - \frac{36d}{81} + \frac{d}{4} = \bar{\gamma} - \frac{63d}{324}$$

relativistic  
correction levels  
to splitting if  
only single line.

$$(3_1 \rightarrow 2_1) \quad \bar{\gamma}_f = \bar{\gamma} - \frac{36d}{81} + \frac{5d}{4} = \bar{\gamma} + \frac{261d}{324}$$

$$\Delta n_q = \pm 1 \quad (3_2 \rightarrow 2_1), \quad (3_2 \rightarrow 2_2) d$$

$(3_1 \rightarrow 2_1) \rightarrow$  forbidden

$$\bar{\gamma}_a = \bar{\gamma} + \frac{65}{324} d.$$

$$\bar{\nu}_d = \bar{\nu} + \frac{357}{324} d.$$

$$\bar{\nu}_e = \bar{\nu} - \frac{63d}{324}$$

### Energy level Diagram

$$\bar{\nu}_a \text{ and } \bar{\nu}_d = \frac{292}{324} d$$

$$\bar{\nu}_a \text{ and } \bar{\nu}_e = \frac{128}{324} d$$

$$\bar{\nu}_d \text{ and } \bar{\nu}_e = \frac{420}{324} d.$$

$$Fe - (26) = Z$$

$$\text{Magnetic Moment} = 2.4$$

→ Partially filled d-shell  
 Transition metal called

bcz of

Drae form (fully relativistic)

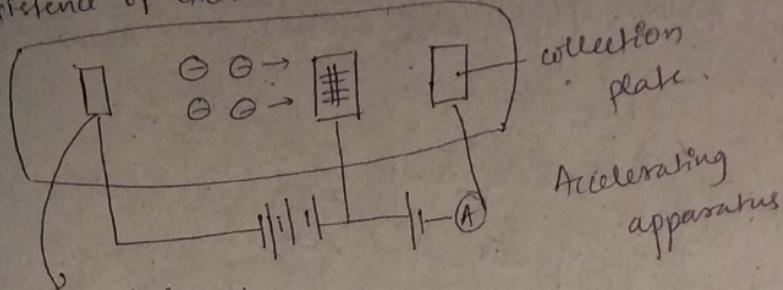
Bath Land 8

28.03.19

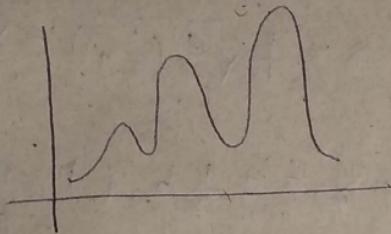
## Franck - Hertz Experiment

existence of excited in Hg atom

(1924)



Evaluated from here.



## Magnetic moment of hydrogen atom

Original principle quantum number  $n = n_r + n_\phi$   
not adequate.

## Spin Quantum number

In irrespective of shape of orbitals, the  $e^-$  experiences a spin,  $e^- \rightarrow$  like magnets  $\rightarrow$  so spin contribut<sup>n</sup> also there.

$$||S|| = \sqrt{3(s+1)} \ h$$

$S \rightarrow$  quantised spin vector.

$||S|| \rightarrow$  norm of spin vector.

$s \rightarrow$  spin quantum number associated with spin angular momentum.

$h \rightarrow$  Planck's constant.

## Electron Spin

$n \rightarrow$  principle quantum no. (shell no.)

$l \rightarrow$  orbital  $n=1, 1s$

$m_l \rightarrow$  orbital ang. momentum  $n=2, 2s, 2p$

$l \rightarrow n^2$

$l \rightarrow 0 \text{ to } n-1$

$s = \frac{1}{2}$ , special for  $e^-$

$\uparrow$   
 $RO_2$

$$s = \frac{1}{2} \sqrt{\frac{1}{2}(\frac{1}{2}+1)} = \frac{\sqrt{3}}{2} \frac{1}{2}$$

(Molecular solid)

(p-band or orbital magnetism)  $s_z = \pm \frac{1}{2} \frac{1}{2}$  (thus H-atom  
2 lines)

$$\mu_s = -\frac{e}{2m} g_s \quad e \rightarrow \text{charge}, m \rightarrow \text{mass}$$

$g \rightarrow \text{Lande } g \text{ factor}$

ESR  $\rightarrow$  Electron Spin

$$\mu_z = \pm \frac{1}{2} g \mu_B$$

Resonance

$\mu_B \rightarrow$  Bohr Magneton.

## Angular Momentum (Classical)

$$L = r \times p$$

$I \rightarrow$  Moment of Inertia

$$L = Iw$$

$w \rightarrow$  angular velocity.

## Angular Momentum (Quantum Mechanics)

$$L = r \times p$$

$r \rightarrow$  Quantum position operator.

$\phi \rightarrow$  Quantum momentum

operator.

$L \rightarrow$  Orbital Momentum Operator

$J \rightarrow$  Total angular momentum

$$J = L + S$$

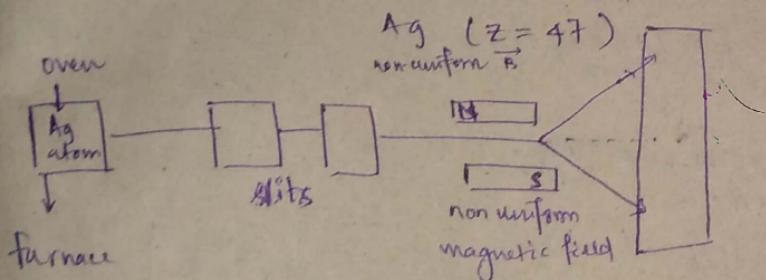
$$\hat{p}_x = -i\hbar \frac{\partial}{\partial x}$$

Spatial quantization of  $\vec{p} = i\hbar \vec{\nabla}$

an  $e^-$  → spin-spin & contributor → also orbital contribution.

02.04.19

### STERN - GERLACH EXPERIMENT (1920)

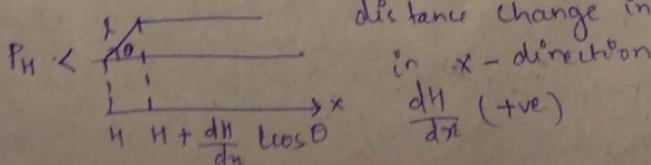


It is not uniform magnetic field.

Silver atom has one unpaired  $e^-$  in its outermost shell  
for other atoms like H, Cu, Na, K, Ag ( $e^-$  rotation  
corresponding to direction of  $B$ ).

+ $\frac{1}{2}$  or - $\frac{1}{2}$   $e^-$  spin (spatial quantization)  
If it was uniform  $B$ , it will get deflected

Expressions for the amt. of deflection w.r.t to distance change in deflection



P → Pole strength

l → length

M → Magnetic moment

Field strength H →  $H + \left(\frac{dH}{dn}\right) l \cos\theta$

$$PH + P \left\{ H + \left(\frac{dH}{dn}\right) l \cos\theta \right\}.$$

Extra force is acting on it; the force coming out is not same as the original force PH.

$$P \left( \frac{dH}{dn} l \cos\theta \right) \rightarrow F_x$$

$$F_x = Pl \cdot \left( \frac{dH}{dn} \right) \cos\theta$$

$$= M \cos\theta \cdot \frac{dH}{dn}$$

where  $Pl = M$ .

Each  $e^-$  coming out is like tiny magnet, corresponding to strength of  $N_{2S}$ , it gets

turned / velocity → v, 'm', 'L', time 't'

$$\text{acceleration, } ax = \frac{F_x}{m}$$

$$Dn = \frac{1}{2} ax t^2 = \frac{1}{2} \left( \frac{F_x}{m} \right) \left( \frac{L}{v} \right)^2$$

$$\rightarrow t = \frac{LN}{v}$$

$$Dn = \frac{1}{2} \cdot \frac{\cos\theta}{m} \cdot \frac{dH}{dn} \left( \frac{L}{v} \right)^2$$

$$Dn = \frac{1}{2} \cdot \frac{M}{m} \cdot \frac{dH}{dn} \left( \frac{L}{v} \right)^2$$

Dn is  $m, \frac{dH}{dn}$

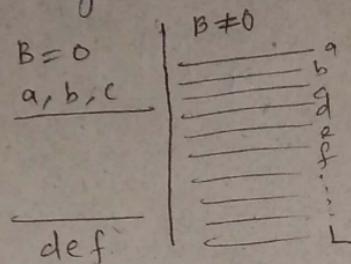
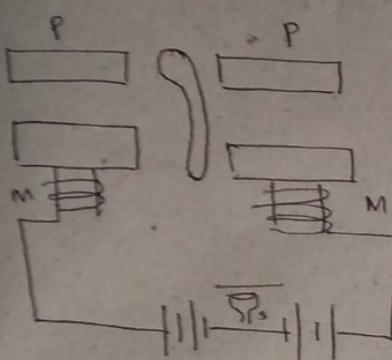
L, v are known

Sanjay  
2022

If  $\frac{H}{dn} = 0$ , then  $Dn = 0$ ,  $Dn \propto \frac{dH}{dn}$

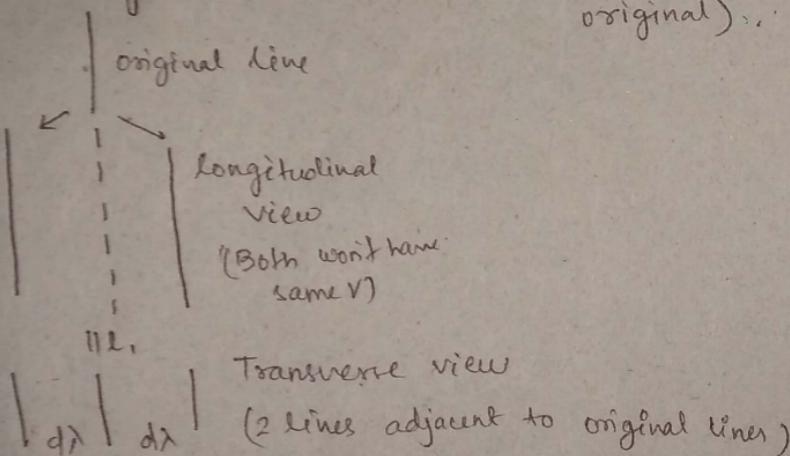
### Zeeman effect

splitting of spectral lines in several components  
in the presence of a static magnetic field.



It is reversible  
(After \_\_\_\_\_,  
every thing go back to  
original).

### Electromagnetic



$d\lambda \rightarrow$  difference in wavelength.

Zeeman shift  $\rightarrow d\lambda$  (splitting of energy  
levels)

4/04/19 — Taken by PHD Student

$$T = 600K$$

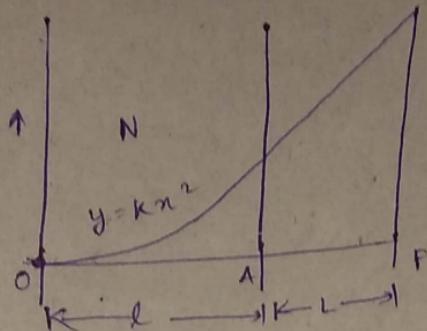
$$l = 0.6m$$

$$L = 1m$$

$$\frac{\partial B}{\partial y} = 20 \text{ T m}^{-1}$$

$$\frac{1}{2}mv^2 = 2kT$$

$$\mu_B = 1.$$



N.

5/4/19

- Simple harmonic motion,  $e^-$  coming have a vibration towards mean position, if it is like SHM.
- The frequency of  $e^-$  radiates some energy.
- MOKE - Polarise the motion of the  $e^-$  like Fe, Co, try to make  $e^-$  polarise w.r.t  $B$ .
- External B, Additional torque acting on the  $e^-$ , energy on the  $e^-$  is attained.
- Theoretical Analysis - spin property; orbital motion -  $B$ , additional  $B$  dominate this  $B$ .  
Paschen brackett effect - It will try to clustering original one.
- Total Hamiltonian  
 $H = H_0 + V_m$ .  
 $H_0 \rightarrow$  Unperturbed Hamiltonian.  
 $V_m \rightarrow$  Perturbation due to  $B$ .  
(Magnetic Component).  
 $V_m = -\vec{M} \cdot \vec{B}$   
Total energy will be altered if we freeze to give one perturbation to the system.

-ve sign is due to fact that the perturbation will alter the energy.

$\vec{M}$  → Magnetic moment of the atom.  
Nucleus also has the spin due to its mass.

$$\vec{M} = -\mu_B \vec{J}/\hbar, \quad \mu_B \rightarrow \text{Bohr Magneton}$$

$\vec{J} \rightarrow \text{Total electronic ang. momentum}$

$$\vec{\mu} = -\mu_B (g_L \vec{L} + g_S \vec{S})$$

↓  
orbital component      spin component

$g \rightarrow g\text{-factor } \vec{L} \text{ & } \vec{S}$

$g_L \rightarrow \text{normally, } g_S \rightarrow \text{normally.}$

### LS-Coupling

$$J = L + S$$

$$j_J = \langle \frac{1}{2} (g_L \vec{L}_i + g_S \vec{S}_i) \rangle$$

$\vec{L} \rightarrow \text{Total orbital moment.}$

$$= \langle \frac{1}{2} (g_L \vec{L} + g_S \vec{S}) \rangle$$

$\vec{S} \rightarrow \text{Total spin momentum}$

### DEBYE'S EXPLANATION

(Normal Zeeman effect)

$$\text{spin (neglect)} ; P_L = \frac{k \cdot h}{2\pi} \quad \text{--- (1)}$$

$$M_L = \frac{k \cdot e h}{4\pi m_e} = \frac{e}{2m_e} \cdot P_L \quad \text{--- (2)}$$

e<sup>-</sup> have effects of external B, makes its direction towards its direction when e<sup>-</sup> was moving L to its ~~not~~ orbital motion.

~~100%~~  
e, dE → Field

## Larmor Precession

$e^-$  moving in a particular orbit.

$\rightarrow m$  .  
 $\downarrow$  /  $e$   
mass charge

$\rightarrow V$  and  $\vec{\omega}$   $\rightarrow$  Linear and Angular Velocity.

$$F = \frac{mv^2}{r} = m\omega^2 r \quad \text{--- (1)}$$

'H'  $\rightarrow$  Intensity of B,

$\rightarrow$  Force acting on  $e^-$  is HeV.

Depends upon motion of  $e^-$ . whether it is  
anticlockwise or clockwise.

H is in incorrect or outward direction.

Let  $\delta\omega$ ,

$$F - HeV = m(\omega + \delta\omega)^2 r \quad \text{--- (2)}$$

Since  $F = mw^2 r$  and  $V = rw\omega$

$$mw^2 r - HeV = mw^2 r + 2m\omega\delta\omega r$$

$$\delta\omega = \frac{-He}{2m} \quad \begin{matrix} \text{(neglecting terms} \\ \text{involving } \delta\omega^2 \end{matrix}$$

(-ve sign indicates the ~~back~~ larmor precession  
to the ~~reversing~~ of motion of the  $e^-$ ).

$$n \rightarrow \text{revolutions per sec}, n = \frac{\omega}{2\pi}$$

$\alpha \rightarrow$  area of the circle.

$\parallel \rightarrow$  current

L.P.V.

$$\Delta E = Q \cdot P_L$$

$$\Delta E_L = E_h - E_0$$

~~\*~~  $Q = \frac{eH}{2\pi c}$   $\leftarrow$  Larmour precession

$P_L \rightarrow$  ang. momentum

$$M = I^\alpha$$

~~\*~~  $n_i a \rightarrow$  magnetic moment of e

$$= - \frac{4\pi}{H^2 n^2}$$

$$= e \left( \frac{3}{2} \right)$$

$$= e \cdot a \left( \frac{3\pi}{2} \right)$$

$$= ea g_n$$

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## Schrodinger Equations

Plane wave described by  $\Psi(\vec{r}, t) = A e^{i(\vec{k} \cdot \vec{r} - \omega t)}$

$A$  = Amplitude

$$\lambda = \frac{2\pi}{k}, \quad \vec{k} = \text{Phase velocity } \frac{\omega}{k}$$

If we assume the propagation is along  $x$ -axis

$$\vec{k} = k \hat{x}$$

$$\Psi(x, t) = A e^{i(kx - \omega t)}$$

$$P = \hbar k \quad \text{and} \quad E = \hbar \omega.$$

$$\Psi(x, t) = A \exp \left[ \frac{i}{\hbar} (P_x - Et) \right]$$

$$\frac{d\Psi}{dt} = A \exp \left[ \frac{i}{\hbar} (P_x - Et) \right] \left( -\frac{iE}{\hbar} \right)$$

Multiply by  $i$ ,

$$i\hbar \frac{d\Psi}{dt} = E\Psi(x, t)$$

$$\frac{d\Psi}{dx} = A \exp \left[ \frac{i}{\hbar} (P_x - Et) \right] \left( \frac{iP}{\hbar} \right)$$

Again multiply by  $i$ ,

$$-i\hbar \frac{\partial \Psi}{\partial x} = P\Psi(x, t)$$

$$-i\hbar \frac{\partial \Psi}{\partial x} = P\Psi(x, t) = \frac{\partial \Psi}{\partial x} = -\frac{P}{i\hbar} \Psi(x, t)$$

$$-i\hbar \frac{\partial^2 \Psi}{\partial x^2} = P \frac{\partial \Psi(x, t)}{\partial x}$$

$$i\hbar \cdot \frac{\partial^2 \Psi}{\partial x^2} = p \left( \frac{-p}{i\hbar} \right) \Psi(x, t)$$

$$\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} = -p^2 \Psi(x, t)$$

$$\frac{-\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} = \frac{p^2}{2m} \Psi(x, t)$$

$$E = \frac{p^2}{2m}$$

$$\boxed{i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2}}$$

One-dimensional time-dependent Schrödinger eqn.

$$R \rightarrow i\hbar \frac{\partial}{\partial t} \text{ and } P \rightarrow -i\hbar \frac{\partial}{\partial x}$$

$$E\Psi = \frac{p^2}{2m} \Psi(x, t)$$

$$\Psi(x, t) = A \exp \left[ \frac{i}{\hbar} (p_n - Et) \right]$$

$$\Psi(\vec{r}, t) = A \exp \left[ \frac{i}{\hbar} (\vec{p} \cdot \vec{r} - Et) \right]$$

$$= A \exp \left[ \frac{i}{\hbar} (p_x \cdot x + p_y y + p_z z) - Et \right]$$

$$i\hbar \frac{d\Psi}{dt} = E\Psi$$

$$-i\hbar \frac{\partial \Psi}{\partial x} = p_x \Psi$$

$$\frac{-\hbar^2}{2m} \frac{d^2 \Psi}{dx^2} = \frac{p_x^2 \Psi}{2m}$$

$$E = \frac{p^2}{2m} = \frac{1}{2m} (p_x^2 + p_y^2 + p_z^2)$$

$$i\hbar \frac{d\Psi}{dt} = E\Psi = \frac{\mathbf{p}^2}{2m} = \frac{1}{2m} (\mathbf{p}_x^2 + \mathbf{p}_y^2 + \mathbf{p}_z^2)$$

$$i\hbar \frac{d\Psi}{dt} = -\frac{\hbar^2}{2m} \left[ \frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} + \frac{\partial^2 \Psi}{\partial z^2} \right]$$

$$i\hbar \frac{d\Psi}{dt} = -\frac{\hbar^2}{2m} \nabla^2 \Psi. \quad [3D \text{ Schrodinger eqn for a free particle}]$$

$$E \rightarrow i\hbar \frac{\partial}{\partial t}$$

$$\mathbf{p} \rightarrow -i\hbar \nabla \quad E\Psi = \frac{1}{2m} (\mathbf{p}_x^2 + \mathbf{p}_y^2 + \mathbf{p}_z^2) \Psi$$

$$\mathbf{p}_x \rightarrow i\hbar \frac{\partial}{\partial x} \quad E\Psi = \frac{\mathbf{p}^2}{2m} \Psi$$

$$\mathbf{p}_y \rightarrow i\hbar \frac{\partial}{\partial y}$$

$$\mathbf{p}_z \rightarrow i\hbar \frac{\partial}{\partial z}$$

$$\mathbf{V}(\vec{r}, t) \rightarrow \mathbf{P} \cdot \mathbf{E}$$

$$E = \frac{\mathbf{p}^2}{2m} + V(r, t)$$

$$i\hbar \frac{\partial \Psi}{\partial t} = \left[ \frac{\mathbf{p}^2}{2m} + V(r, t) \right] \Psi.$$

$$= \left[ -\frac{\hbar^2}{2m} \nabla^2 \Psi + V\Psi \right]$$

$$i\hbar \frac{\partial \Psi}{\partial t} = H\Psi$$

$$H = \frac{\mathbf{p}^2}{2m} + V$$

Hamiltonian.

$$-\frac{\hbar^2}{2m} \nabla^2 + V \rightarrow \text{Operator}$$

$$i\hbar \frac{d\psi}{dt} = H\psi = \left[ -\frac{\hbar^2}{2m} \nabla^2 + V(r) \right] \psi$$

↓  
1-Dimensional time dependent Schrödinger  
Eq<sup>n</sup>.

Experiment → charge density distribution  
function → Maximum entropy method

$$f(r) = \langle \langle \langle \psi(r) \rangle \rangle \rangle$$

Physical Interpretation of  $\psi$

$$i\hbar \frac{\partial \psi}{\partial t} = H\psi$$

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi + V\psi \quad \text{--- (1)}$$

The complex conjugate,

$$-i\hbar \frac{\partial \psi^*}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi^* + V\psi^* \quad \text{--- (2)}$$

$V(\vec{r}, t)$  is assumed to be real.

Multiplying (1) by  $\psi^*$ ;

$$i\hbar \psi^* \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \psi^* \nabla^2 \psi + V\psi^* \psi \quad \text{--- (3)}$$

$$-i\hbar \psi \frac{\partial \psi^*}{\partial t} = -\frac{\hbar^2}{2m} \psi \nabla^2 \psi^* + V\psi \psi^* \quad \text{--- (4)}$$

$$i\hbar \left[ \Psi^* \frac{\partial \Psi}{\partial t} + \Psi \frac{\partial \Psi^*}{\partial t} \right] = -\frac{\hbar^2}{2m} \left[ \Psi^* \nabla^2 \Psi - \Psi \nabla^2 \Psi^* \right]$$

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \quad \text{--- (5)}$$

$$(\Psi^* \Psi) + \left[ \frac{\partial J_x}{\partial x} + \frac{\partial J_y}{\partial y} + \frac{\partial J_z}{\partial z} \right] = 0 \quad \text{--- (6)}$$

$$J_x = \frac{i\hbar}{2m} \left[ \Psi \frac{\partial \Psi^*}{\partial x} - \Psi^* \frac{\partial \Psi}{\partial x} \right]$$

$$J_y =$$

$$J_z =$$

$$J = \frac{i\hbar}{2m} (\Psi \nabla \Psi^* - \Psi^* \nabla \Psi)$$

$$\frac{\partial \Psi}{\partial t} + \nabla \cdot J = 0 \quad \text{--- (7)}$$

$$\Psi = \Psi^* \Psi$$

$$\iiint |\Psi|^2 dz = 1 \quad (\text{How?})$$

9/4/19

## Physical Interpretation of wave function

$$\Psi(\vec{r}, t) ; \Psi^*(\vec{r}, t)$$

$$P(\vec{r}, t) = \Psi^*(\vec{r}, t) \Psi(\vec{r}, t) = |\Psi(\vec{r}, t)|^2 \quad \text{--- (1)}$$

$|\Psi(\vec{r}, t)|^2 \rightarrow$  Probability of finding a system  
at time 't' in vol  $d\vec{z}$ .

$$\int_{-\infty}^{+\infty} |\Psi(\vec{r}, t)|^2 d\vec{z} = 1 \quad \text{--- (2)}$$

$$\left| N \right|^2 \int_{-\infty}^{+\infty} |\Psi(\vec{r}, t)|^2 d\vec{z} = 1 \quad \text{--- (3)}$$

$N \rightarrow$  Normalisation constant.

## Probability Current Density

$$\Psi(\vec{r}, t) = \sqrt{V} \int \Psi^* \Psi d\vec{z}$$

$$i\hbar \frac{\partial \Psi(\vec{r}, t)}{\partial t} = \left[ -\frac{\hbar^2}{2m} \nabla^2 + V(\vec{r}) \right] \Psi \quad \text{--- (1)}$$

$$i\hbar \frac{\partial \Psi^*(\vec{r}, t)}{\partial t} = \left[ -\frac{\hbar^2}{2m} \nabla^2 + V(\vec{r}) \right] \Psi^* \quad \text{--- (1)}$$

Here  $V \rightarrow$  Potential which is real.

Multiplying ① by  $\psi^*$  and ② by  $\psi$  from left and subtracting from other,

$$i\hbar \left( \psi^* \frac{\partial \psi}{\partial t} + \psi \frac{\partial \psi^*}{\partial t} \right) = \frac{-\hbar^2}{2m} \left[ \psi^* \nabla^2 \psi - \psi \nabla^2 \psi^* \right]$$

$$\therefore \frac{\partial}{\partial t} (\psi^* \psi) = -\frac{i\hbar}{2m} \left[ \nabla \cdot (\psi^* \nabla \psi - \psi \nabla \psi^*) \right] \quad \text{--- (11.1)}$$

Integrating we get,

$$\begin{aligned} \frac{\partial}{\partial t} \int_{-\infty}^{\infty} \psi^* \psi dz &= \frac{i\hbar}{2m} \int_{-\infty}^{\infty} \nabla \cdot (\psi^* \nabla \psi - \psi \nabla \psi^*) dz \\ &= \frac{i\hbar}{2m} \left[ \psi^* \nabla \psi - \psi \nabla \psi^* \right]_{-\infty}^{\infty} \quad \text{--- (3)} \end{aligned}$$

$\psi d\psi^* \rightarrow 0$  [when we have a localised wave packet]

$$z \rightarrow \pm \infty$$

$$\frac{\partial}{\partial t} \int_{-\infty}^{\infty} \psi^* \psi dz = 0 \text{ or, } \int_{-\infty}^{\infty} \psi^* \psi dz = \text{constant in time}$$

Normalisation integral is constant in time

$J(\vec{r}, t) \rightarrow$  Probability current density

$$j(\vec{r}, t) = \frac{i\hbar}{2m} (\psi \nabla \psi^* - \psi^* \nabla \psi)$$

Subtract the above in (11.1),

$$\frac{\partial P(\vec{r}, t)}{\partial t} + \nabla \cdot \vec{J}(\vec{r}, t) = 0$$

$\Rightarrow$  Equation of continuity for probability.

Expectation Value

Large number of measurement on  $\vec{r}$ .

$\Psi(\vec{r}, t)$

$$\langle r \rangle = |\Psi(\vec{r}, t)|^2$$

$$\langle r \rangle = \int r \Psi^* \Psi d\tau = \int \Psi^* r \Psi d\tau$$

$$\langle f(r) \rangle = \int \Psi^*(\vec{r}, t) f(\vec{r}) \Psi(\vec{r}, t) d\tau$$

Left multiply by time dependent Schrödinger equation.

$$i\hbar \frac{\partial \Psi(\vec{r}, t)}{\partial t} = \left[ -\frac{\hbar^2}{2m} \nabla^2 + V(\vec{r}, t) \right] \Psi(\vec{r}, t)$$

Multiplying by  $\Psi^*$  and integrating from  $-\infty$  to  $\infty$

$$\int_{-\infty}^{\infty} \Psi^* \left( i\hbar \frac{\partial \Psi}{\partial t} \right) d\tau = \int_{-\infty}^{\infty} \Psi^* \left( -\frac{\hbar^2}{2m} \nabla^2 \right) \Psi d\tau + \int_{-\infty}^{\infty} \Psi^* V(\vec{r}, t) \Psi d\tau$$

$$\langle i\hbar \frac{\partial}{\partial t} \rangle = \left\langle -\frac{\hbar^2}{2m} \nabla^2 \right\rangle + \langle V \rangle$$

$$\langle i \rangle = \left\langle P^2 / 2m \right\rangle + \langle V \rangle$$

$$\langle A \rangle = \int \psi^* \Lambda_{op} \psi dz$$

If the wave function is not normalised

$$\langle A \rangle = \frac{\int \psi^* \Lambda_{op} \psi dz}{\int \psi^* \psi dz}$$

10.4.19

Time - Independent Schrodinger Equation

Time dependent S.E -

$$i\hbar \frac{\partial \Psi(r, t)}{\partial t} = \left[ -\frac{\hbar^2}{2m} \nabla^2 + V(r, t) \right] \Psi(r, t)$$

$$\Psi(r, t) = \psi(r) \text{ and } \psi(t)$$

$$\Psi(r, t) = \psi(r) \phi(t)$$

Dividing by  $\psi(r) \phi(t)$

$$i\hbar \left( \frac{1}{\phi(t)} \right) \frac{\partial \phi(t)}{\partial t} = \frac{1}{\psi(r)} \left[ -\frac{\hbar^2}{2m} \nabla^2 + V(r) \right] \psi(r)$$

$$\frac{1}{\phi(t)} \frac{\partial \phi(t)}{\partial t} = -\frac{iE}{\hbar}$$

$$\left[ -\frac{\hbar^2}{2m} \nabla^2 + V(r) \right] \psi(r) = E \psi(r)$$

$$\frac{\partial \phi(t)}{\phi(t)} = -\frac{iE}{\hbar} t$$

$$\Rightarrow \int \frac{\partial \phi(t)}{\phi(t)} = \frac{iE}{\hbar} \int dt$$

$$\phi(t) = c \exp\left(\frac{-iEt}{\hbar}\right)$$

$c$ -constant

$$\Psi(r, t) = \psi(r) \exp\left(\frac{-iEt}{\hbar}\right)$$

$$\Psi(r, t) = \psi(r) \phi(t)$$

w.r.t to  $t$  and multiply by  $i\hbar$ ,

$$i\hbar \frac{\partial [\Psi(r, t)]}{\partial t} = E \Psi(r, t)$$

Multiply both sides by  $\Psi^*$  from left and  
integrate over the space coordinate,

$$\int_{-\infty}^{\infty} \Psi^* \left( i\hbar \frac{\partial}{\partial t} \right) \Psi(r, t) = E. \text{ as } \int_{-\infty}^{+\infty} \Psi^* \Psi = 1$$

$$\left[ -\frac{\hbar^2}{2m} \nabla^2 + V(r) \right] \Psi(r) = E \Psi(r)$$

↓  
Hamiltonian Operator

Stationary states:

$$\left[ -\frac{\hbar^2}{2m} \nabla^2 + V(r) \right] \Psi(r) = E \Psi(r)$$

$$\Psi_n(r, t) = \Psi_n(r) \exp\left(\frac{-iEn t}{\hbar}\right)$$

$$\Psi_n(r, t) = \Psi_n(r, 0) \exp\left(-\frac{iE_n t}{\hbar}\right)$$

$$P(r, t) = |\Psi_n(r, t)|^2 = |\Psi_n(r, 0)|^2$$

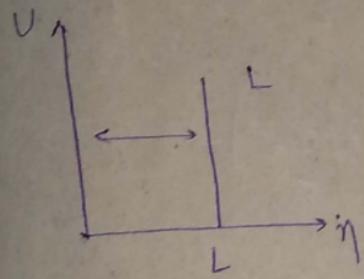
↓  
Constant in time

## Particle in a box

One dimensional energy eigenvalue problem

$U(\Psi) \rightarrow \text{zero outside}$

$U=0$  for  $0 < r < L$ ,  $U=\infty$  for  $r < 0$  or  $r > L$ .



A sq. potential well  
with infinitely high barriers  
at each end.

$$\frac{d^2\Psi}{dx^2} + \frac{2m}{\hbar^2} E \Psi = 0 \quad \text{when } V=0$$

$$\Psi = A \sin \frac{\sqrt{2mE}}{\hbar} n + B \cos \frac{\sqrt{2mE}}{\hbar} n, \quad A, B \text{ constant}$$

$\Psi < 0$  for  $n=0$  and  $n=L$

Since  $\cos 0 = 1$ , hence  $B = 0$ .

$$\frac{\sqrt{2mE}}{\hbar} = n\pi, \quad n = 1, 2, 3, \dots \quad (3)$$

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2m L^2}, \quad n = 1, 2, 3, \dots$$

$$\Psi_n = \frac{A \sin \sqrt{2mE_n} n}{\hbar} x$$

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

$\Rightarrow \int_0^L |\Psi_n|^2 dx = \int_0^L |\Psi_n|^2 dn$

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

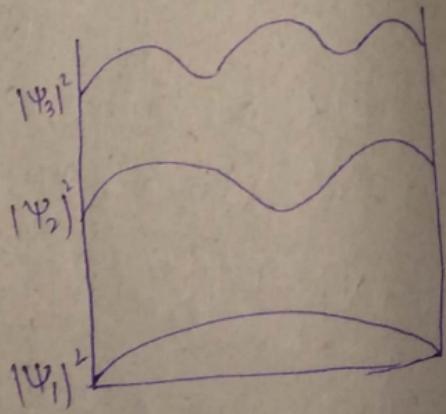
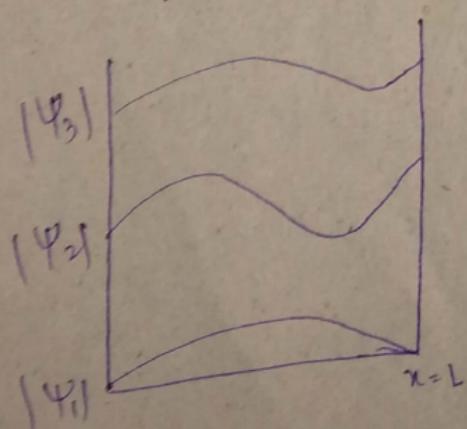
$$= \frac{A^2}{2} \left[ \int_0^L dx \int_0^L \cos \left( \frac{2\pi n x}{L} \right) \right]$$

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

$$= \frac{LA^2}{2}$$

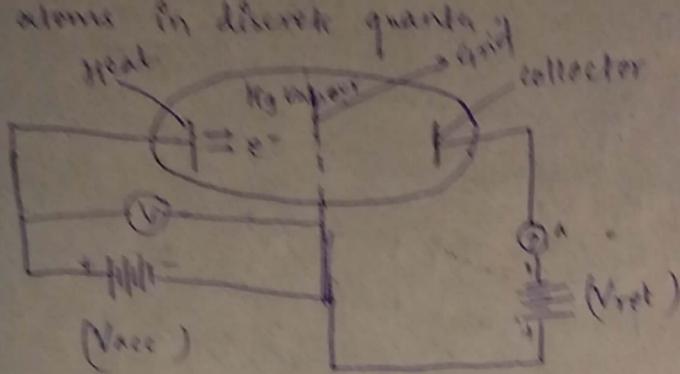
then,  $\int |\Psi_n|^2 dx = 1$

$$A = \sqrt{\frac{2}{L}}, \Psi_n = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}, n = 1, 2, \dots$$

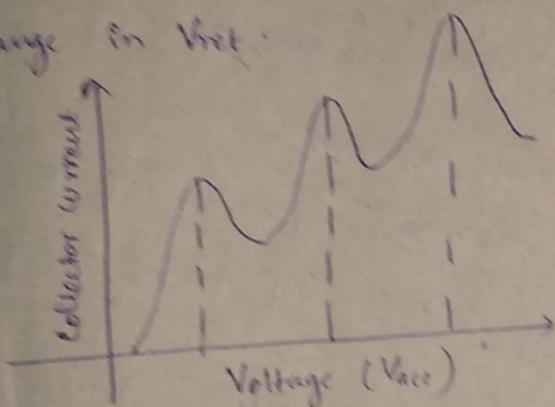


## FRANK - HERTZ EXP.

It demonstrates that mechanical energy is absorbed by atoms in discrete quanta.



The energy of  $e^-$  passing through Hg vapours and reaching the collector can be determined from variation of collector current with change in  $V_{ret}$ .



- The  $e^-$  travel under influence of  $V_{acc}$  betw<sup>n</sup> heater and grid and  $V_{ret}$  under ~~heat~~ betw<sup>n</sup> grid and collector.
- $e^-$  gain energy when they move in electric field existing betw<sup>n</sup> heater and grid, on their way the  $e^-$  collide with Hg vapors and can lose energy in collision.

\* When total energy  $\leq 4.9$  Volts, there was no energy loss, hence a rise in collector current.

→ When  $V_{AC}$  was increased above 4.9 volts, inelastic collision occurred near the grid in which  $e^-$  gave up their K.E. to Hg vapour atoms; hence they were unable to traverse the  $V_{CE}$  and collector current falls.

→ Again  $V_{AC}$  was increased to critical energy of 4.9 eV; after attaining critical energy and losing it through collisions,  $e^-$  picked up new energy and collector current rose again.

→ This process was repeated.

These results show that Hg atoms absorb mechanical energy in quanta of 4.9 eV energy.

→ The expt was repeated in diff condition of radiation and materials.

It demonstrated the emission or absorption of radiation is not continuous, but takes place in units of quanta of energy.

## Wave - Particle Duality

### Wave Nature

→ Interference, diffraction,  
Polarizn, reflection,  
refraction.

### Particle Nature

→ BB radiation,  
photoelectric effect,  
Compton effect.

## Schrodinger Wave Equation

$$\frac{i\hbar d\psi(x,t)}{dt} = -\frac{\hbar^2}{2m} \nabla^2 \psi(x,t) + V\psi(x,t)$$

Time ↓  
dependent one-dimensional  
eqn.

$\int_0^t \dots dt$  ??

for in  
an  
y's  
points

$$\frac{\partial^2 \Phi}{\partial x^2} + \frac{2m}{\hbar^2} (E - V) \Phi = 0$$

→ 1-D time  
independent  
eqn.

where  $\Phi = A \exp \left[ -\frac{i}{\hbar} (Et - px) \right]$

## Selection Rules

The general condition necessary for an atom in an excited state to radiate is that the integral  $\int_{-\infty}^{+\infty} \psi_n^* \psi_m dx$  should be non-zero.

Since the intensity of radiation is proportional to it.

Transitions between any two states  $n_1$  and  $n_2$  for which this integral is finite

are called allowed transitions, while those for which it is zero is called forbidden transitions.

- In case of H-atoms, 3 quantum no. are needed to specify the initial and final states involved in radiative transition.

→ If principle, orbital and magnetic QN of initial state are  $n_1, l_1, m_{l1}$  and final state are  $n_2, l_2, m_{l2}$ ; so condition for an allowed transition is -

$$\int_{-\infty}^{\infty} u \Psi_{n_1, l_1, m_{l1}}^* \Psi_{n_2, l_2, m_{l2}} du \neq 0$$

In evaluating the integral, it was found that the transitions for which orbital quantum number  $l$  changes by  $\pm 1$  and  $m_l$  either does not change or change by  $\pm 1$ , are the allowed transition, i.e. conditions are

$$\boxed{\Delta l = \pm 1, \Delta m_l = \pm 1}$$

The change in total QN  $n$  is not restricted.

### Electron Spin

$$S = \sqrt{s(s+1)} \hbar$$

S → Spin Ang. Momentum  
S → spin & N.

$$S = \sqrt{\frac{3}{2}} \hbar$$

$$s = \pm \frac{1}{2}$$

The space quantisation of e<sup>-</sup> spin is described by ~~as~~ spin magnetic QN m<sub>s</sub> as the orbital ang. momentum vector can have (2l+1) orientations in a magnetic field, from +l to -l, through zero, the spin ang. momentum vector can have 2s+1 = 2 orientation specified by m<sub>s</sub> = ± 1/2.

- The component S<sub>z</sub> of the spin ang. momentum of an e<sup>-</sup> along a magnetic field in the z-direction is determined by the spin magnetic QN, so that

$$S_z = m_s \hbar = \pm \frac{1}{2} \hbar$$

## ATOMIC STRUCTURE

### Thomson's Model

#### first model

- Two facts  $e^-$  are essential part of atom  
atom as a whole is electrically neutral.
- The charges were uniformly distributed in a sphere of atomic dimensions, while the  $e^-$  were arranged inside the positive sphere in a way that the force of attraction towards the centre of the sphere exactly balance their mutual repulsion.
- He could account for single line in the spectrum of hydrogen.

### RUTHERFORD'S MODEL

- gold-foil experiment
  - Bombarded  $\alpha$ -particles ( ${}_{2}^{4}\text{He}$  nucleus) on a thin gold foil and observed scattered  $\alpha$ -particles on ZnS screen.
  - The scattering of  $\alpha$ -particles (positively charged) is caused by coulomb repulsive forces between these particles and the charges of atom in scattering target.

#### OBSERVATIONS:

- \* Atom is composed of tiny nucleus containing all the positive charge with nearly all the mass of the atom concentrated in it;  $e^-$  are arranged some distance away from it.

- \*  $\alpha$ - particles which interacted with the nuclei suffered deflection through large angles.
- \* Due to large empty spaces present in the atom, most of the particles went through foil undeflected or suffered very small deflections.

$$N_0 = \frac{Q \cdot n \cdot t \cdot (Ze)^2 \cdot e^2}{r^2 m^2 V_0^2 \sin^2(\theta/2)}$$

$N_0$  - No. of  $\alpha$ -particle scattered through  $\theta$  striking per unit area of the screen at a distance  $r$  from the scatterer.

$Q$  - total no. of  $\alpha$ -particle that reach the screen.

$n$  - no. of atoms per unit vol in foil.

$t$  - foil thickness.

$(Ze)$  - Nuclear charge

$mV_0^2$  = K.E of  $\alpha$ -particle

- \* Limitations of Rutherford's model:
- \* Stability of nuclear atom.

Rutherford assumed that  $e^-$  should revolve round the nucleus at such a speed that the mechanical centrifugal force would just balance the net excess of electrostatic attraction and as a result stability could be established.

electromagnetic theory was not in accordance to an accelerating electric charge radiate energy in the form of EM radiation. This energy can only come from the atomic system and hence it will loose energy continuously. As a result, the  $e^-$  will approach the nucleus by a spiral path, giving out a radiation of constantly increasing freq. and finally fall into nucleus; thus orbital motion of  $e^-$  destroys the stability of the atom.

## BOHR'S ATOMIC MODEL.

Bohr developed the theory of atomic structure on the basis of two postulates:

- (1) The  $e^-$  can revolve only in certain circular orbits satisfying quantum conditions; these orbits were termed as stationary states and hence stable orbits in which  $e^-$  could revolve without radiating energy as demanded EM theory.
- (2) When an  $e^-$  jumps from one permitted orbit to the other, it emits energy in the form of EM radiation.

for a linear harmonic oscillator, the displacement  $x$  and momentum  $p$ , are related through the eqn of ellipse and the phase integral has value equal to integral multiple of  $\hbar$ .

$$\oint p_n dx = nh$$

If linear mom is replaced by ang. mom,  
 $L = Iw$

$$\oint L \cdot d\theta = nh$$

If  $\omega = \text{constant}$ , then  $L$  becomes constant

$$L \oint d\theta = L \cdot 2\pi$$

$$L \cdot 2\pi = nh$$

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

Important Note : Hence,  $e^-$  were allowed to revolve in circular orbits for which the ang. momentum is integral multiple of  $h/2\pi$ .

## (2) Radius of permitted orbits

For H-atom, the electrostatic force of attraction between  $e^-$  and proton provides the centripetal force required for revolution in the orbits.

$$\frac{1}{4\pi\epsilon_0} \frac{e^2}{r^2} = \frac{mv^2}{r}$$

## (1) Nature of stationary orbits

for a linear harmonic oscillator, the displacement  $\vec{r}$  and momentum  $\vec{p}$ , are related through the eqn of ellipse and the plane integral has value equal to integral multiple of  $\hbar$ .

$$\oint \vec{p} \cdot d\vec{r} = nh$$

If linear mom is replaced by ang. mom,

$$L = Iw$$

$$\oint L \cdot d\theta = nh$$

If  $w = \text{constant}$ , then  $L$  becomes constant

$$L \oint \vec{\phi} d\theta = L \cdot 2\pi$$

$$L \cdot 2\pi = nh$$

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

Important Note: Hence,  $e^-$  were allowed to revolve in circular orbits for which the ang. momentum is integral multiple of  $\hbar/2\pi$ .

## (2) Radius of permitted orbits

For H-atom, the electrostatic force of attraction between  $e^-$  and proton provides the centripetal force required for revolution in the orbits.

$$\frac{1}{4\pi\epsilon_0} \frac{e^2}{r^2} = \frac{mv^2}{r}$$

For H-atom,  $Q = e$   $[z=1]$

$$\frac{1}{4\pi\epsilon_0} \frac{e^2}{r^2} = \frac{mv^2}{r}$$

$$\frac{e^2}{4\pi\epsilon_0 mr} = v^2 \quad \text{--- (1)}$$

eq(1.1)

$$v^2 = \frac{e^2}{4\pi\epsilon_0 mr}$$

$$V = \frac{e}{\sqrt{4\pi\epsilon_0 mr}} = \frac{e}{\sqrt{mr}} \sqrt{\frac{1}{4\pi\epsilon_0}}$$

$$V = \frac{(1.6 \times 10^{-19})^2 (9 \times 10^9)^{1/2}}{(9.11 \times 10^{-31} \times 0.5 \times 10^{-10})^{1/2}}$$

$$V \approx 2.2 \times 10^6 \text{ m/s}$$

From Bohr's quantisation of ang. momentum,

$$L = n \frac{h}{2\pi}$$

$$\text{And } L = mv r$$

$$\frac{nh}{2\pi} = mv r$$

$$V = \frac{nh}{2\pi mr}$$

$$V^2 = \left( \frac{nh}{2\pi mr} \right)^2$$

$$V^2 = \left( \frac{nh}{mr} \right)^2 \quad \text{--- (2)}$$

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

from (1) and (2),

$$\frac{e^2}{4\pi\epsilon_0 m s} = \frac{n^2 h^2}{m^2 c^2}$$

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

$$r_n = n^2 a_0$$

$$a_0 = \frac{h^2 4\pi\epsilon_0}{m e^2}$$

$$= 0.53 \text{ Å}^\circ$$

$$r_n = \frac{n^2}{Z} a_0$$

$$r_n = 0.53 \frac{n^2}{Z} a_0$$

(3) Energy of  $e^-$  in permitted orbits

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

$$K.E = \frac{1}{2} m v^2 = \frac{1}{2} \gamma P \frac{Ze}{m s} \quad (\text{from 1.1})$$

$$K.E = \frac{1}{2} \gamma P \frac{Ze^2}{r}$$

$$P.E = -\frac{P Ze^2}{r}$$

$$E = \frac{1}{2} \gamma P \frac{Ze^2}{r} - \frac{P Ze^2}{r}$$

$$= \gamma P Ze^2 \left( \frac{1}{2r} - \frac{1}{r} \right)$$

$$E = -\frac{\gamma P Ze^2}{2r}$$

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$$E = -\frac{\beta \frac{ze^2}{42}}{\frac{\beta \cdot me^2}{n^2 h^2}}$$

$$= -\frac{\beta^2 e^4 z m \times 4\pi^2}{2\pi^2 h^2}$$

$$= -\frac{2\beta^2 e^4 m \pi^2 z}{n^2 h^2}$$

$$= -\frac{2\pi^2 \beta^2 m e^4 (z)}{n^2 h^2}$$

$$= -\frac{2\pi^2 m e^4 (z)}{16\pi^2 \epsilon_0^2 n^2 h^2}$$

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

-ve energy signifies another imp. concept of binding energy. It means that the  $e^-$  is bound to the nucleus by attractive forces so that energy must be supplied to the  $e^-$  in order to separate it completely from the nucleus. In this sense, the orbital energy is known as binding energy.

### ATOMIC SPECTRA

$$\frac{1}{\lambda} = R = R \left[ \frac{1}{\alpha^2} - \frac{1}{n^2} \right]$$

→ wave no.  
 $R \rightarrow 109677 \text{ cm}^{-1}$   
 (Rydberg constant)

Series :  $\bar{V} = R \left[ \frac{1}{1^2} - \frac{1}{n^2} \right] \quad n=2,3,$

R series :  $\bar{V} = R \left[ \frac{1}{2^2} - \frac{1}{n^2} \right]$

Paschen series :  $\bar{V} = R \left[ \frac{1}{3^2} - \frac{1}{n^2} \right]$

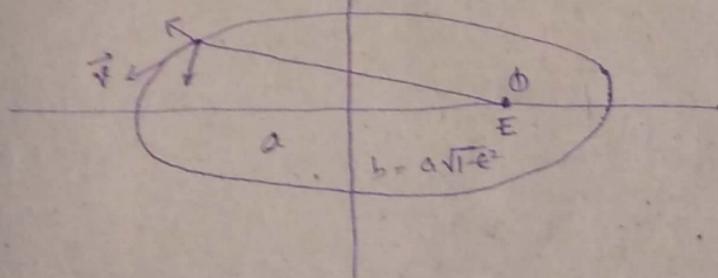
Balmer series ,  $\bar{V} = R \left[ \frac{1}{4^2} - \frac{1}{n^2} \right]$

Pfund series ,  $\bar{V} = R \left[ \frac{1}{5^2} - \frac{1}{n^2} \right]$ .

### BOHR'S CORRESPONDENCE PRINCIPLE

## SOMMERFIELD ATOMIC MODEL

- Bohr's structure couldn't explain the fine structure in the spectral lines of H-atom.
- Sommerfield came up with an argument that since  $e^-$  is moving under the influence of a massive nucleus, it might also rotate in the elliptical orbits as planets do.
- Therefore, the position of  $e^-$  at any instant can be fixed in terms of polar coordinates  $r$  and  $\phi$ , where  $r$  is the radius vector i.e. the distance of the  $e^-$  from the nucleus at one of the foci of ellipse and  $\phi$  is the vectorial angle i.e. the angle which the radius makes with the major axis of ellipse.



- Tangential Velocity  $v$  of  $e^-$  at instant can be resolved into two components; one radial i.e. along radius vector equal to  $(dr/dt)$  and other transverse i.e. at the right angle to the radius vector equal to  $r \left( \frac{d\phi}{dt} \right)$ .

Corresponding, radial momentum  $P_r = m \frac{dr}{dt}$   
 ang. or azimuthal momentum  $P_\phi = m r^2 \frac{d\phi}{dt}$

Phase integral of Quantum Theory might be applied to both of these momentum,

$$\oint P_r \cdot dr = n_r h$$

$$\oint P_\phi \cdot d\phi = n_\phi h$$

•  $n_r$  and  $n_\phi$  are related by equation

$$n = n_r + n_\phi$$

• Total Energy is given by,

$$E = P \cdot E + \text{Radial K.E} + \text{Angular K.E.}$$

$$= -\frac{Ee}{r} + \frac{1}{2} m \left( \frac{dr}{dt} \right)^2 + \frac{1}{2} m r^2 \left( \frac{d\phi}{dt} \right)^2$$

• Now,

$$1 - e^2 = \frac{b^2}{a^2} = \frac{n_\phi^2}{(n_\phi + n_r)^2}$$

$E \rightarrow$  Eccentricity  
of ellipse

$a \rightarrow$  semi-major axis  
 $b \rightarrow$  semi-minor axis

$$\boxed{\sqrt{(1-e^2)} = \frac{b}{a} = \frac{n_\phi}{n}}$$

$$E = -\frac{2\pi^2 m Z^2 e^4}{h^2} \left( \frac{1}{n_\phi + n_r} \right)^2$$

•  $n_\phi$  cannot be zero, since ellipse would then degenerate into a straight line passing through nucleus.

•  $n_\phi$  cannot be greater than  $n$ , since  $b$  is always less than  $a$ ,

• When  $n_p = n$ ; path is circular.  $b=a$ ,  $\theta=0$

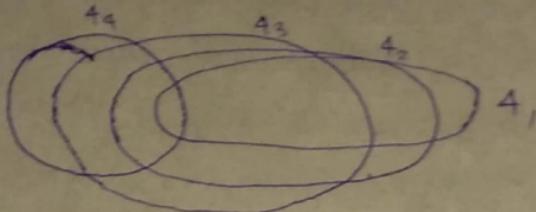
• Given value of  $n$ ,  $n_p$  can assume only  $n$  diff. values

↓  
n diff. elliptical orbits  
with diff. eccentricities

$$n = 4,$$

$$4_1, 4_2, 4_3, 4_4$$

$n = 4_4$  = circular orbital



Relativistic Variation of mass

## Zeeman effect

The splitting up of spectral lines in a strong magnetic field is referred to as Zeeman effect.

- In normal Zeeman effect, a single spectral line is split up into 3 spectral lines, when viewed in transverse direction to magnetic field and into 2 lines when viewed longitudinally.  
→ Normal ZE can be explained on the basis of magnetic quantum number ( $m_l$ ).
- In anomalous Zeeman effect, single line splits up into more than 2 lines.
- To account for fine structure as well as the anomalous Zeeman effect, S. Goudsmith and U. Uhlenbeck proposed that -  
"An  $e^-$  has an intrinsic ang. momentum commonly known as spin ang. momentum or simply spin. A magnetic field is associated with this ang. momentum."