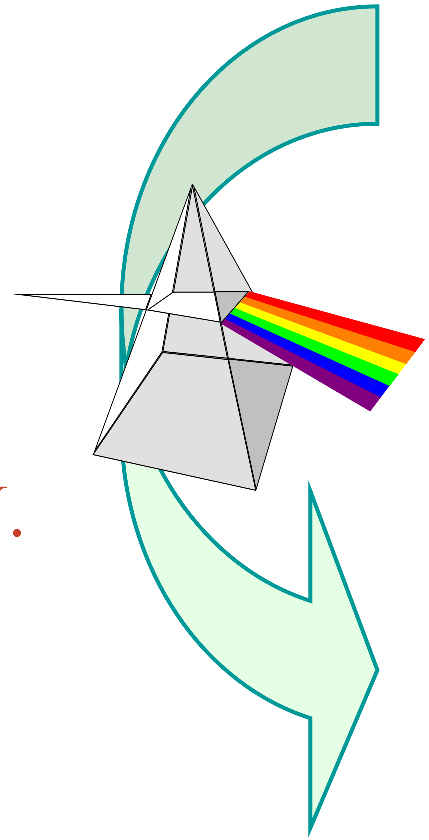
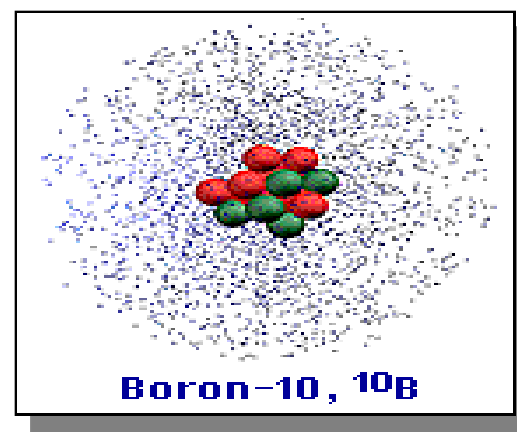
B.Sc. II year Physical Chemistry

Atomic Structure and Wave Mechanics:





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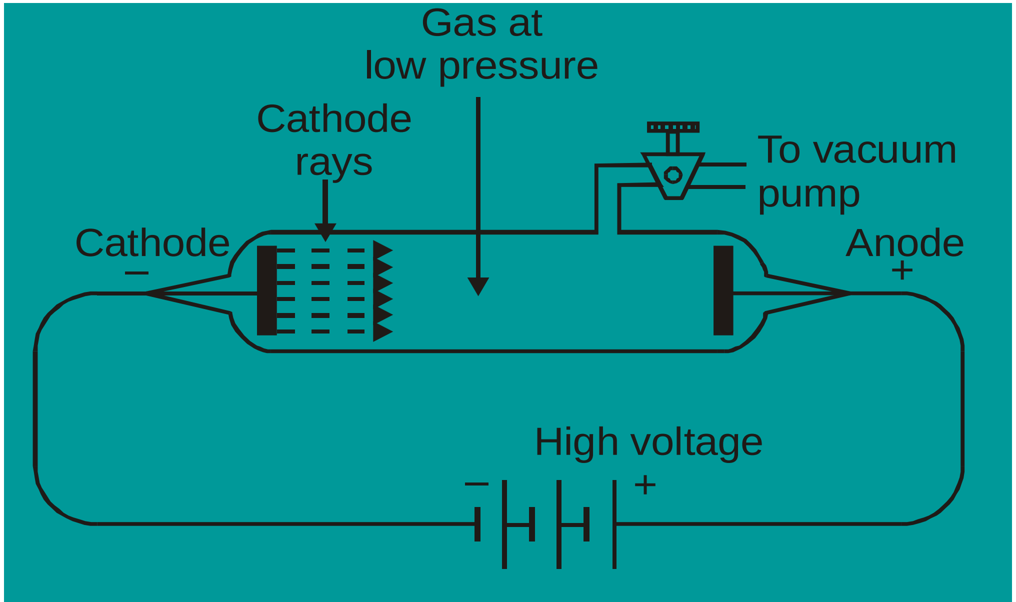
Dalton’s Theory – Atom Is Fundamental Particle

- All matter is composed of small particles called as atom.
- All atoms of a given element are identical.
- Atom can not be divisible and indestructible as it is a hard sphere.

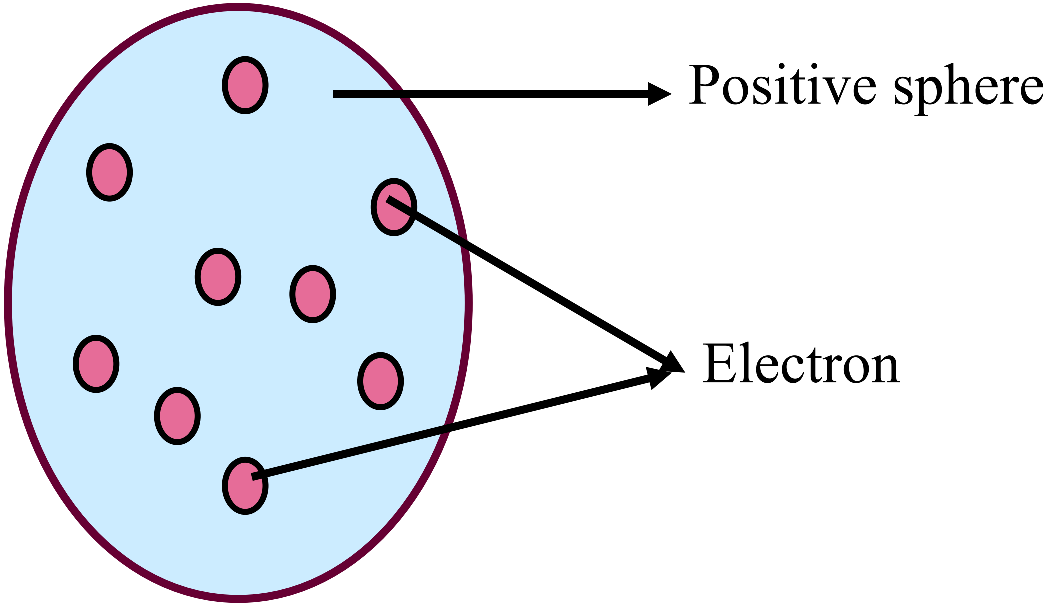
J.J. Thomson's Electron discovery (Cathode rays)



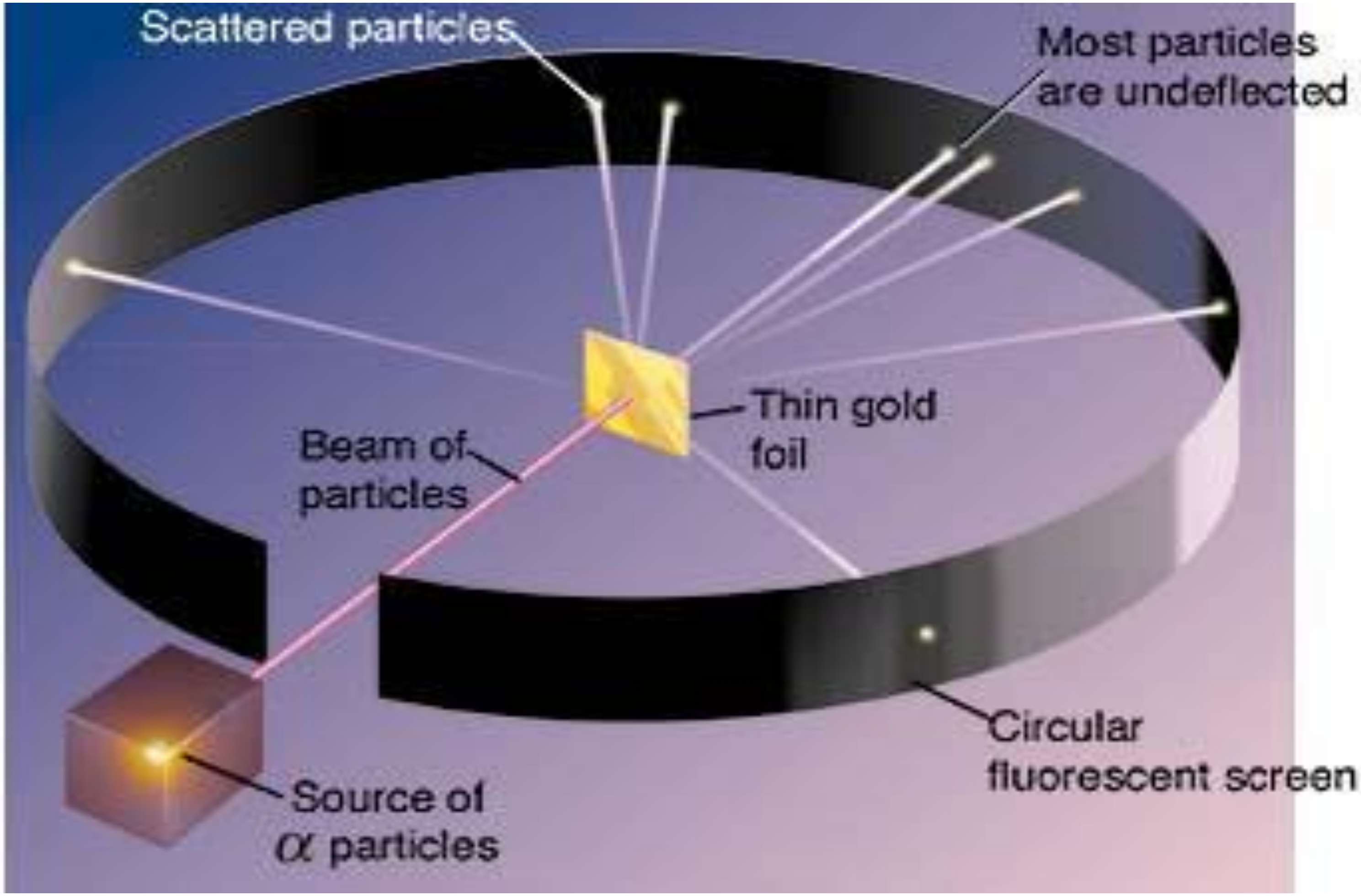
Discharge tube experiment-Production of cathode rays

Thomson’s Model of an Atom

- model of the atom had the positive charges spread uniformly throughout a sphere the size of the atom, with electrons embedded in the uniform background.



Rutherford experiment

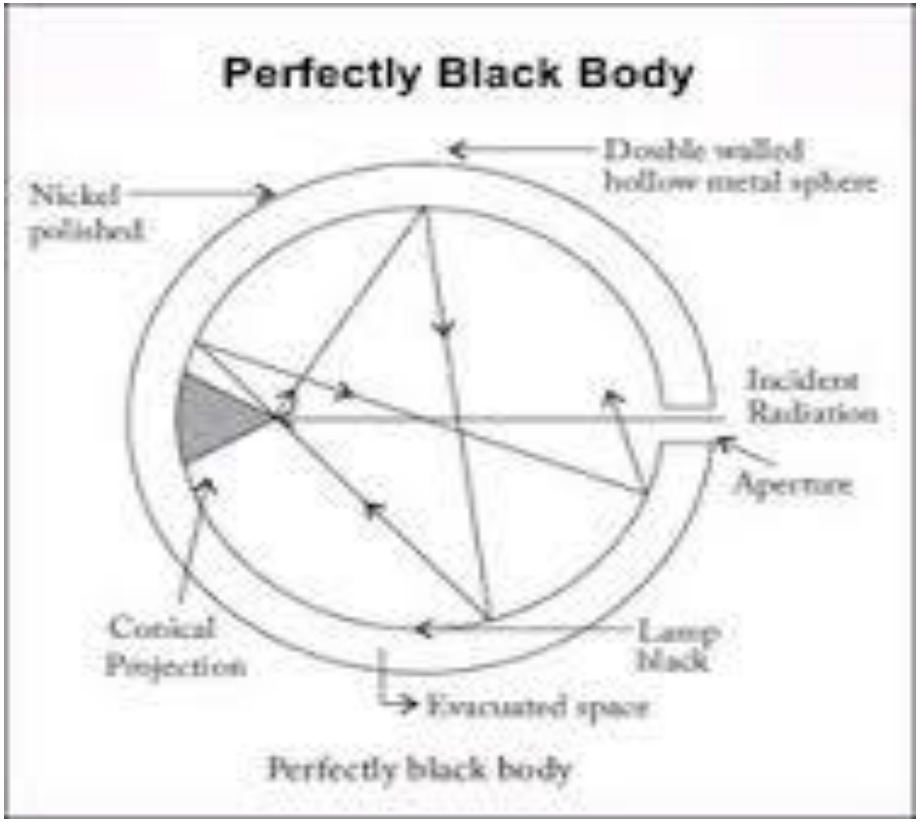


Rutherford’s Experiment - Results

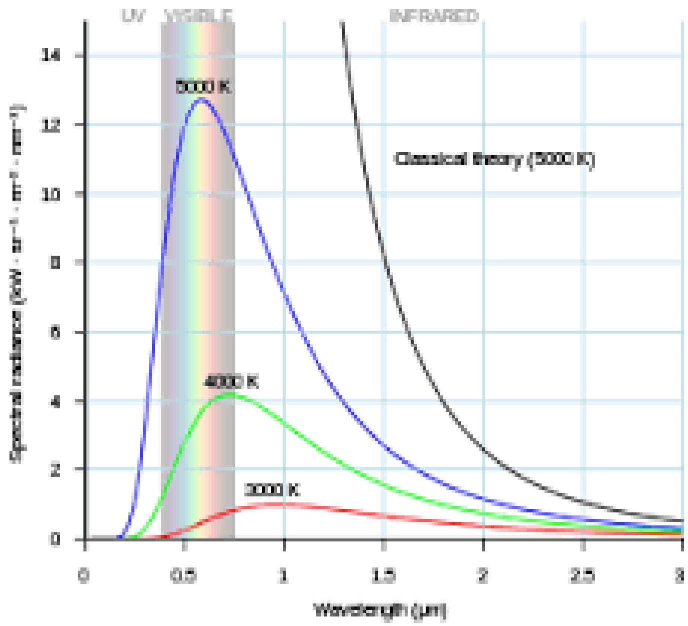
- A beam of α particles aimed at thin gold foil.
- Most of the particles passed through the gold foil.
- Most of the space is empty
- A few came back
- Presence of concentrated mass at the centre
- Others deflected at various angles
- Repulsion between two +ve ly charged particles
- According to him Negatively charged electrons revolve around the nucleus like planets around sun.

Blackbody radiation

- A blackbody is both a perfect absorber and perfect emitter of radiation. As its name suggests, it might be black.



1. The energy emitted depends on the wavelength and temperature.
2. For each temperature, there is wavelength at which there is maximum efficiency of energy.
3. As temperature increases, the position of maximum shifts towards lower wavelength



The Photoelectric Effect

- When a beam of light of sufficiently high frequency is allowed to strike on a metal surface, electrons are ejected from the metal surface the process is called the **photoelectric effect.**
- The emitted electrons are called photoelectrons.

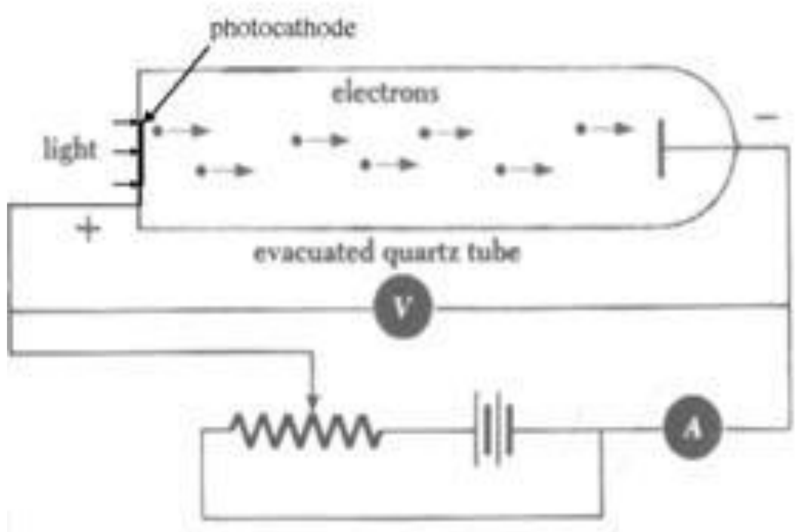
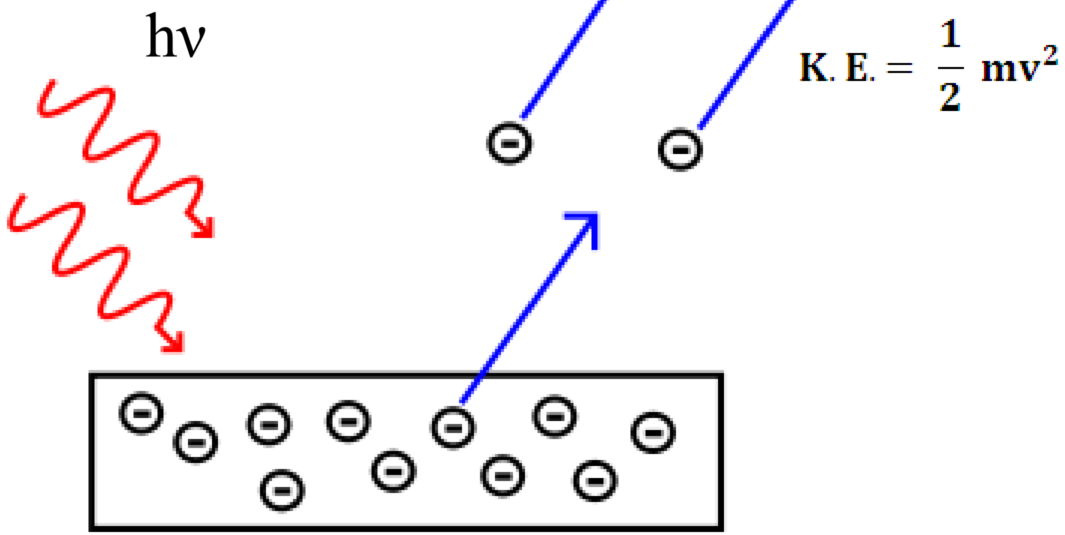


FIGURE 1 Experimental observation of the photoelectric effect.

Einstein’s explanation of Photoelectric Effect

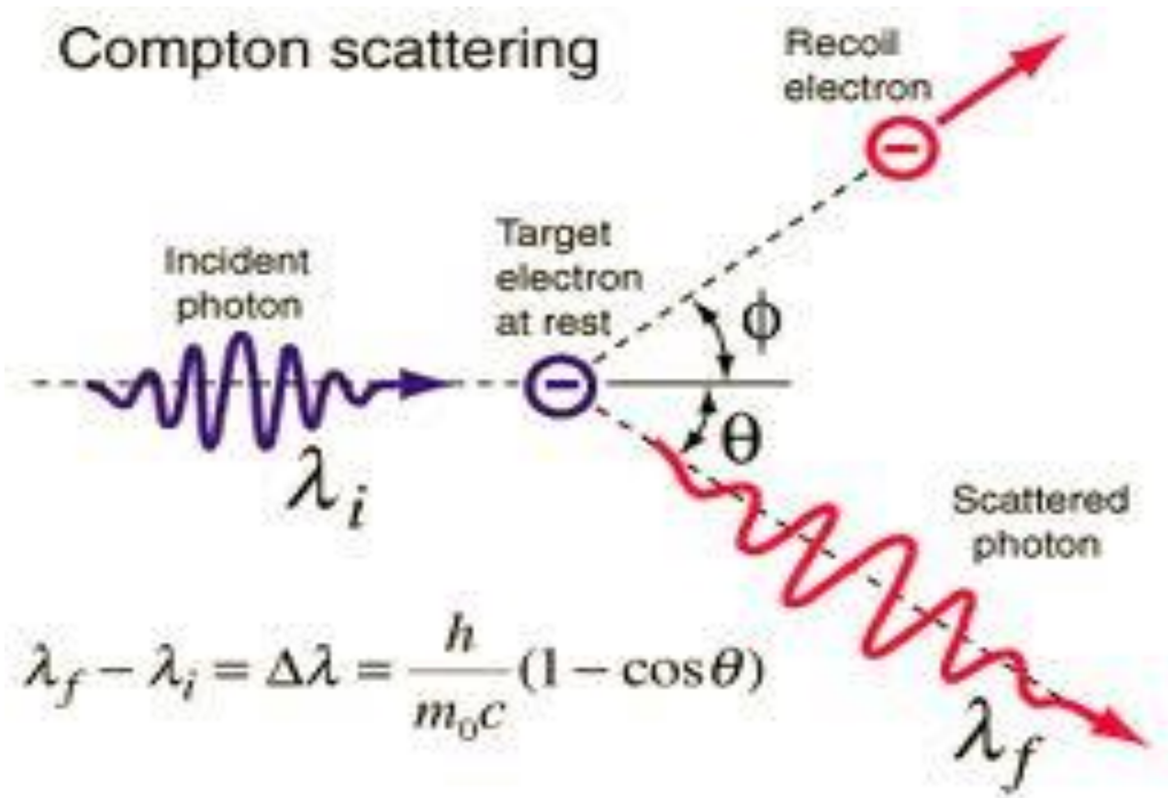
- A photon of incident light transmits its energy hν to an electron on the metal surface, which escapes with kinetic energy $K.E. = \frac{1}{2} mv^2$
- A more intense light delivers a larger number of light quanta.
- In order to release the electron from metal surface, minimum energy is required will be the threshold frequency. The light having frequency less than threshold frequency can not be eject the electron.



The Compton Effect

- High-energy X-ray photons strikes a graphite surface, electrons ejected and x-ray scattered with an angle and have higher wavelength.
- Compton won the Nobel Prize in 1927 for his work
- Compton shift is given by

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



de Broglie Equation

- According to Planck Light has both wave & particle properties
- de Broglie (1924) proposed that all moving objects have wave and particle properties.

According to Planck, $E = h\nu$ $E = h\frac{c}{\lambda}$

According to Einstein,

$$E = mc^2$$

$$mc^2 = \frac{hc}{\lambda}$$

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

L. de Broglie
(1892-1987)

Since mc is the momentum of a photon, we replace this with the momentum of a particle

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

This suggests that particles have wave-like characteristics

λ for particles is called the de Broglie wavelength

Uncertainty Principle

- Problem of defining nature of electrons in atoms solved by W. Heisenberg.
- According to him, it is impossible to determine simultaneously both the position and momentum (= m•v) of an electron accurately.

W. Heisenberg
1901-1976

$$\delta x . \delta p = \frac{h}{4\pi}$$

At best we can describe the position and velocity of an electron by a PROBABILITY DISTRIBUTION, which is given by Ψ^2

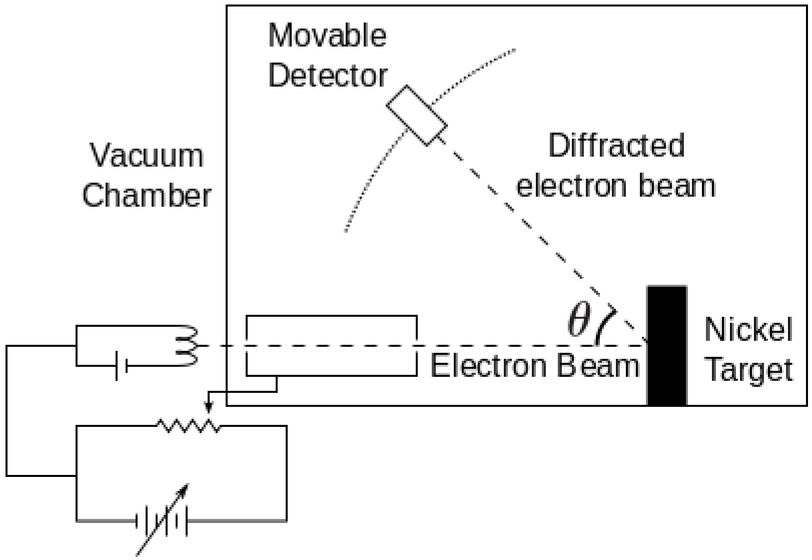
Davisson-Germer Experiment

- The first experimental proof of the wave nature of electron was demonstrated in 1927 by two American physicists C.J Davison and L.H. Germer.
- In Davisson and Germer experiment electrons from a heated filament were accelerated by a voltage and allowed to strike the surface of nickel metal.
- They found that the impact of electrons shows diffraction effects when incident on a crystal surface which is similar to X-ray diffraction pattern.
- Since X-ray posses wave nature, the experiment gave direct evidence for wave nature of electron.
- Wavelength calculated by using formula at 54 V which is lies in the range of X-rays.

$$\lambda = \frac{h}{(2mev)^{\frac{1}{2}}}$$

$$\lambda = 1.67 \times 10^{-10}\ m$$

$$\lambda = 1.67 A^{\circ}$$



Schrodinger wave equation

- In order to provide the meaning to the probability of finding an electron at a given point around the nucleus, Schrodinger derived an equation known as Schrodinger's wave equation.
- The equation is based on the idea of treating electron as standing wave around the nucleus.
- The equation of standing wave is, $\Psi = A \sin \frac{2\pi x}{\lambda}$ Ψ = wave function
- differentiating wave equation twice we get,

$$\frac{d\Psi}{dx} = \frac{2\pi}{\lambda} A\cos \frac{2\pi x}{\lambda} \qquad \frac{d^2\Psi}{dx^2} = -\frac{4\pi^2}{\lambda^2} A\sin \frac{2\pi x}{\lambda} \qquad \frac{d^2\Psi}{dx^2} = -\frac{4\pi^2}{\lambda^2}\Psi$$

- the total energy of system is, E = K.E + P.E, $E = \frac{1}{2}mv^2 + V$

$$\frac{1}{2}mv^2 = E - V \qquad \frac{m^2v^2}{2m} = E - V$$

- from de-Broglie's equation we have, $\lambda = \frac{h}{mv}$ $mv = \frac{h}{\lambda}$ $m^2v^2 = \frac{h^2}{\lambda^2}$

$$\frac{h^2}{2m\lambda^2} = E - V \qquad \frac{1}{\lambda^2} = \frac{2m(E - V)}{h^2}$$

$$\frac{d^2\Psi}{dx^2} = -4\pi^2 \frac{2m(E-V)}{h^2}\Psi \qquad \frac{d^2\Psi}{dx^2} = -\frac{8\pi^2 m(E-V)}{h^2}\Psi$$

$$\frac{d^2\Psi}{dx^2} + \frac{8\pi^2 m(E-V)}{h^2}\Psi = 0$$

- This equation is known as Schrodinger's wave equation for a particle in one direction.
- The equation for a particle moving in x, y and z direction is given by

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

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

Where,

$$\nabla^2 = \frac{d^2}{dx^2} + \frac{d^2}{dy^2} + \frac{d^2}{dz^2}$$

$\nabla^2 =$ Laplacian operator

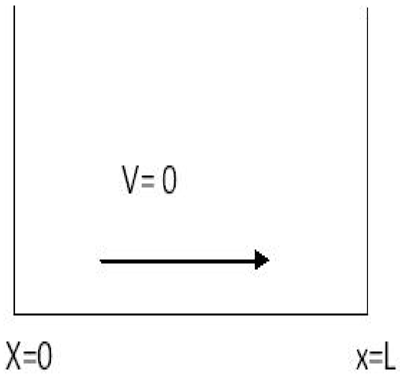
This equation is known as Schrodinger's wave equation in Laplacian operator form.

Application of Schrodinger's wave equation to a particle in one dimensional box

- The equation for the energy of the particle in one dimensional box is,

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

where n = 1, 2, 3, -----------



Thank You…