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# **Elementary Quantum Mechanics**

# Drawbacks of Classical Mechanics

- ▶ Phenomenon associated with Large and small size objects
- ▶ The simultaneous determination of position and momentum of moving particle.
- ▶ Wave - particle duality
- ▶ Energy ?
- ▶ Black body radiation
- ▶ Variation of heat
- ▶ Photoelectric effect and line spectra



# Blackbody Radiation

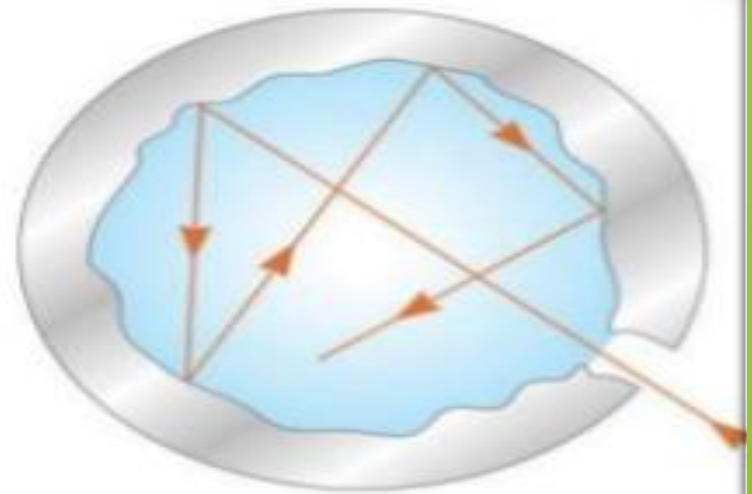
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- An object at any temperature is known to emit thermal radiation
  - Characteristics depend on the temperature and surface properties
  - The thermal radiation consists of a continuous distribution of wavelengths from all portions of the em spectrum

# Black Body Radiation

## Blackbody Approximation

- A good approximation of a black body is a small hole leading to the inside of a hollow object
- The hole acts as a perfect absorber
- The nature of the radiation leaving the cavity through the hole depends only on the temperature of the cavity

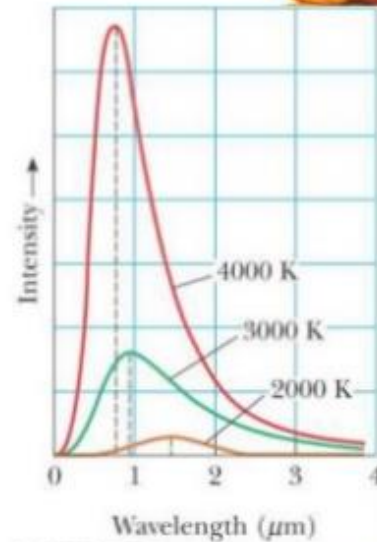


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# Black Body Radiation

## Intensity of Blackbody Radiation, Summary

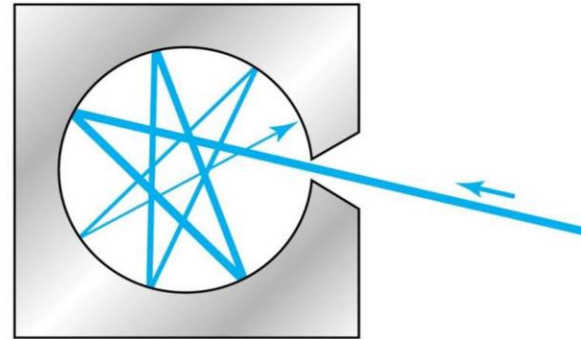
- The intensity increases with increasing temperature
- The amount of radiation emitted increases with increasing temperature
  - The area under the curve
- The peak wavelength decreases with increasing temperature



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# Blackbody Radiation

- When matter is heated, it emits radiation.
- A blackbody is a cavity in a material that only emits thermal radiation. Incoming radiation is absorbed in the cavity.

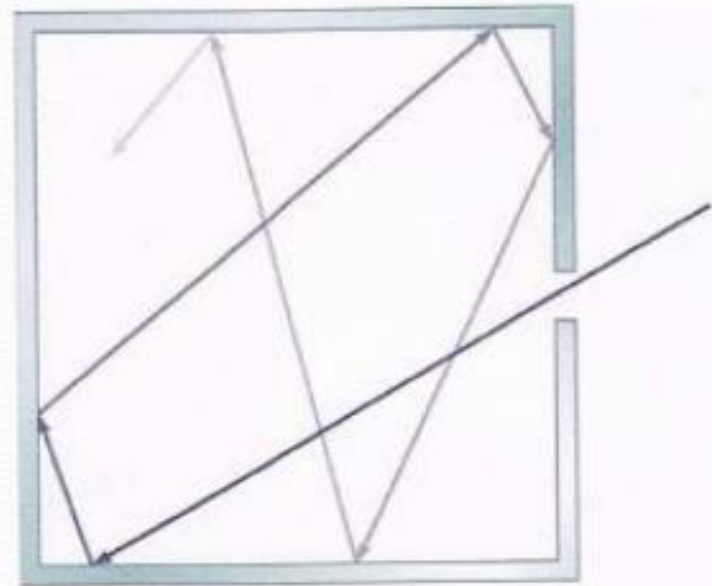


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- Blackbody radiation is theoretically interesting because the **radiation properties of the blackbody are independent of the particular material**. Physicists can study the properties of intensity versus wavelength at fixed temperatures.

# Blackbody Radiation & Planck's Hypothesis

- A blackbody is any object that absorbs all light incident upon it
- Shiny & reflective objects are poor blackbodies
- Recall: good absorbers and also good emitters
- Ideally we imagine a box with a small hole that very little light (EM radiation) can reflect back out



▲ **FIGURE 30-1 An ideal blackbody**  
In an ideal blackbody, incident light is completely absorbed. In the case shown here, the absorption occurs as the result of multiple reflections within a cavity. The blackbody, and the electromagnetic radiation it contains, are in thermal equilibrium at a temperature  $T$ .

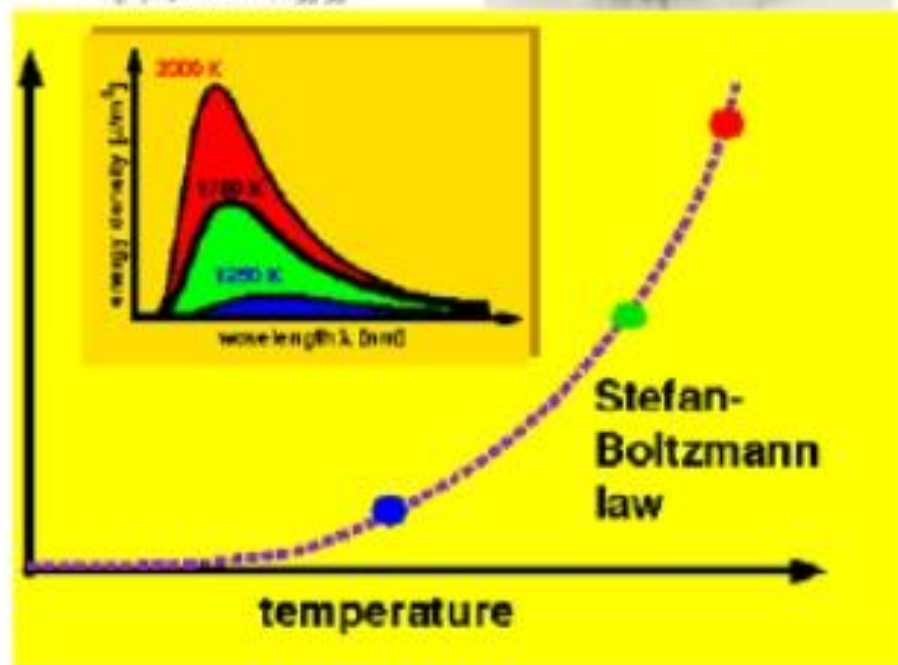
# Stephen Boltzmann Law

The *Stefan-Boltzmann Law* states that total spectral radiant exitance ( $M_b$ ) leaving a blackbody is proportional to the fourth power of its temperature ( $T$ ).

$$M_b = \sigma T^4$$



Fig. 4.1 Josef Stefan, 1835-93





# Stephen Boltzmann Law

The total spectral radiant flux exitance ( $M_b$ ) measured in watts  $m^2$  leaving a *blackbody* is proportional to the fourth power of its temperature ( $T$ ).

The Stefan-Boltzmann law is expressed as:

$$M_b = \sigma T^4$$

where  $\sigma$  is the Stefan-Boltzmann constant equaling  $5.6697 \times 10^{-8} \text{ W m}^{-2} \text{ K}^{-4}$ , and  $T$  is temperature in degrees Kelvin. The total radiant exitance is the integration of all the area under the blackbody radiation curve.

The Sun produces more spectral radiant exitance ( $M_b$ ) at  $6,000 \text{ }^\circ\text{K}$  than the Earth at  $300 \text{ }^\circ\text{K}$ . As the temperature increases, the total amount of radiant energy measured in watts per  $m^2$  (the area under the curve) increases and the radiant energy peak shifts to shorter wavelengths.

## Stefan-Boltzmann Law

- The Stefan-Boltzmann law states that a blackbody radiates electromagnetic waves with a total energy flux  $E$  directly proportional to the fourth power of the Kelvin temperature  $T$  of the object:

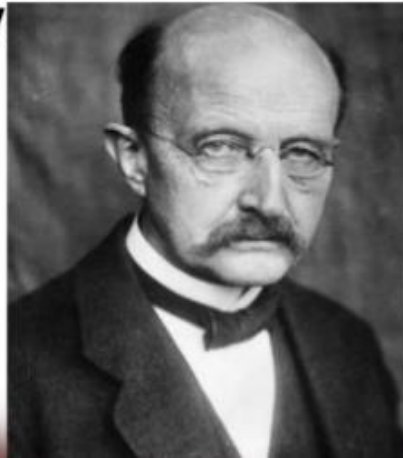
$$E = \sigma T^4$$

# The Planks Hypothesis (Quantum theory of radiation)

## Max Planck

Introduced the concept of “quantum of theory”

In 1918 he was awarded the Nobel Prize for the discovery of the quantized nature of energy



# The Planks Hypothesis (Quantum theory of radiation)

Plank observed the Rayleigh-jeans and wein's law and developed theory.

According to this theory

Radiant energy is emitted or absorbed discontinuously in the form of tiny bundles of energy known as quanta. This can be expressed by

$$E = h\nu$$

Where,

E = radiant energy of a unit (quantum)

h = Planck's constant =  $6.6262 \times 10^{-34}$

$\nu$  = frequency of radiation

$$E = N \cdot h \cdot \nu = \frac{N \cdot h \cdot c}{\lambda}$$

$$\rho(\lambda T) d\lambda = \frac{8\pi hc}{\lambda^5} \left( \frac{d\lambda}{e^{\frac{hc}{\lambda k_B T} - 1}} \right) |$$

# Max Planck theory

A body can emit or absorb energy only in whole number multiples of quantum number i.e  $1h\nu, 2h\nu, 3h\nu \dots \dots \dots, nh\nu$ . Energy in fraction of a quantum cannot be lost or absorbed. This is known as quantization of energy.

Based on this theory plank obtained the following expression for energy density of black body radiation

$$E\lambda = \frac{8\pi hc}{\lambda^5} \times \frac{1}{\exp\left(\frac{hc}{KT\lambda}\right) - 1}$$

Where,

$(h)$ = Planck's constant, the

$(c)$ = speed of light

$(k)$ = Boltzmann constant and

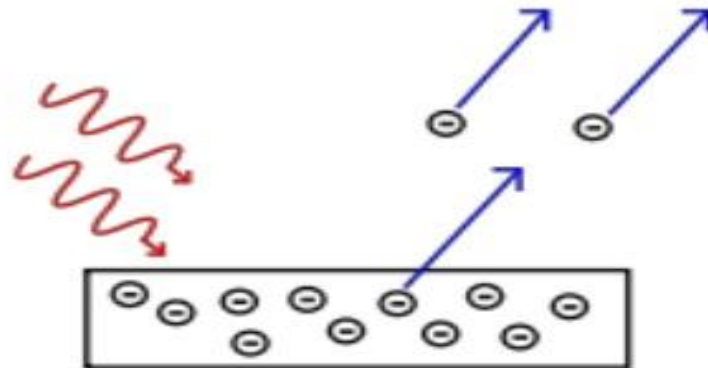
$(T)$ =absolute temperature

# Photoelectric Effect

The ejection of electrons from metals when exposed to light is called as “Photoelectric effect”

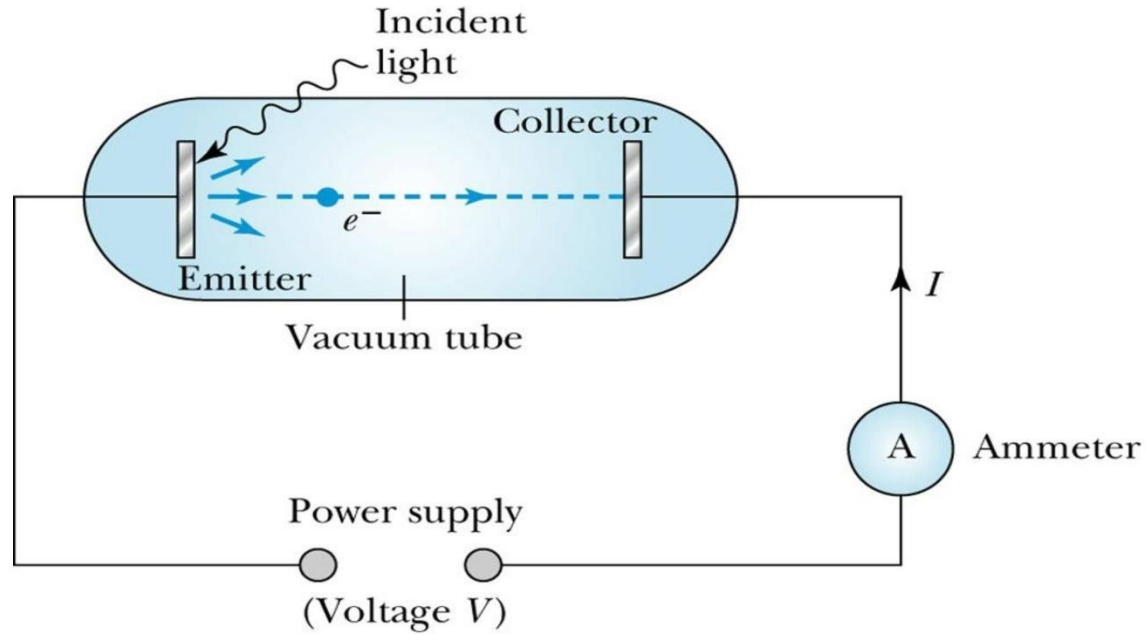
## Photoelectric Effect

- The photoelectric effect refers to the **emission**, or **ejection**, of **electrons** from the surface of, generally, a **metal** in response to incident light.



# Photoelectric Effect

## Experimental Setup



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# The Photoelectric Effect

- In 1887 Hertz noticed, in the course of his investigations, that a negatively charged electroscope could be discharged by shining ultraviolet light on it.
- In 1899, Thomson showed that the emitted charges were electrons.
- The emission of electrons from a substance due to light striking its surface came to be called the **photoelectric effect**.
- The emitted electrons are often called *photoelectrons* to indicate their origin, but they are identical in every respect to all other electrons.



# Photo electric effect

UV light

On the basis of quantum theory Einstein gave an expression for the photo electric effect

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

where

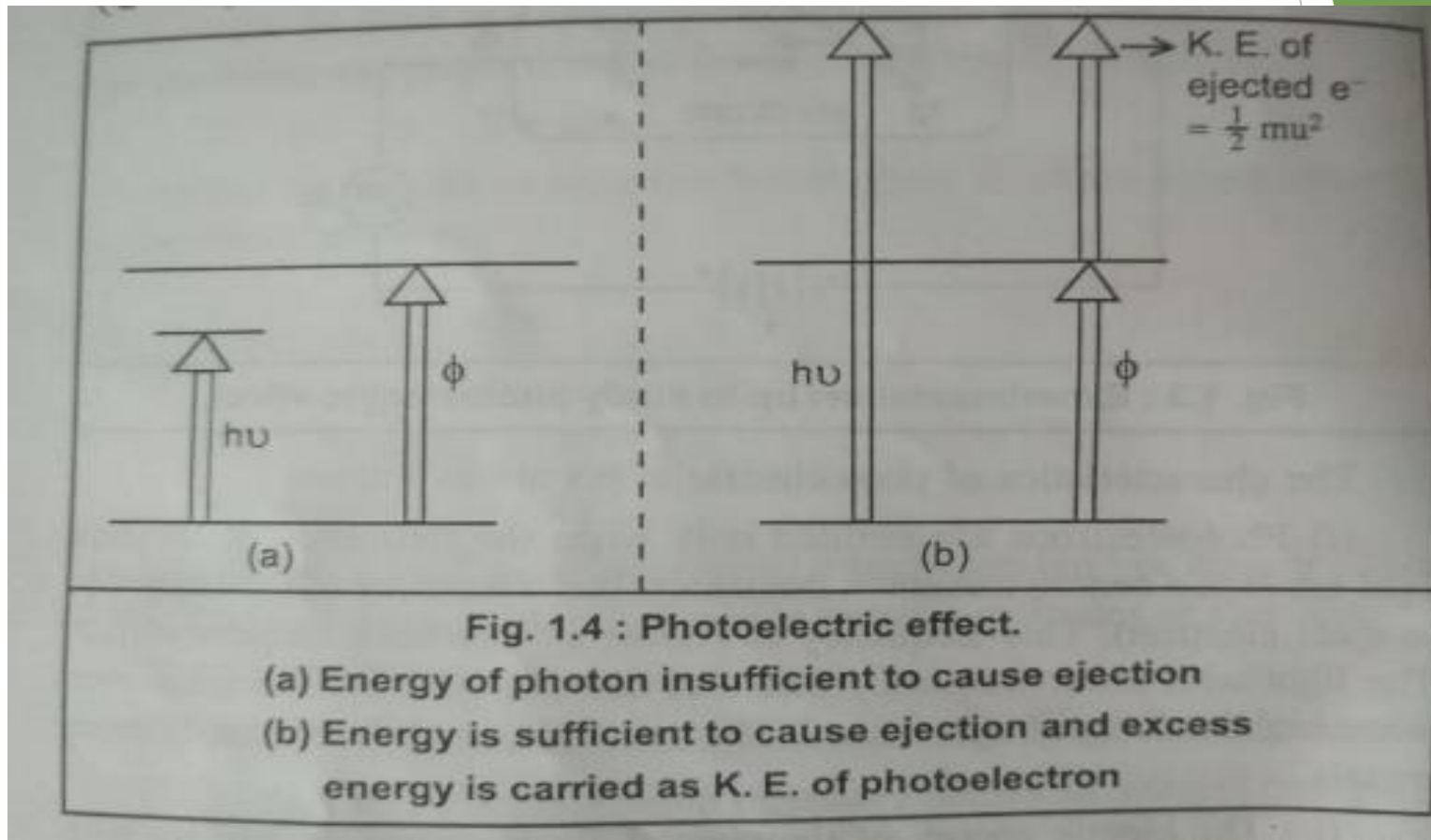
**CLEAN METAL SURFACE**

❖  $\Phi$  is threshold energy of the metal

❖  $\frac{1}{2}mv^2$  is kinetic energy



# Photoelectric Effect



# Photoelectric Effect

$$h\nu = \varphi + \frac{1}{2} mu^2$$

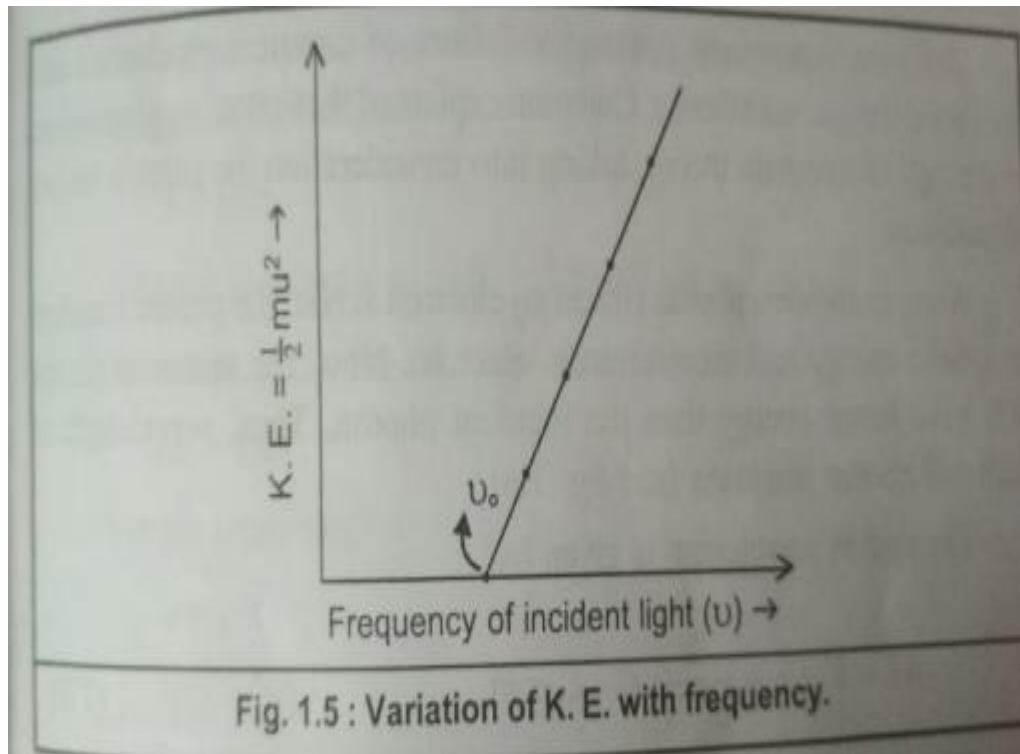
$$\varphi = h\nu_0$$

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

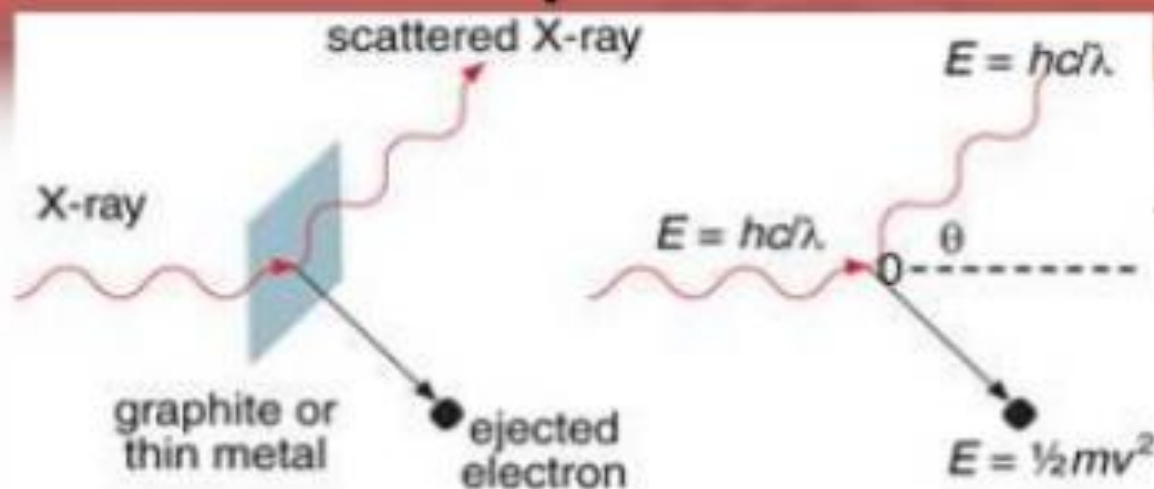
$$\frac{1}{2} mu^2 = h\nu - h\nu_0$$

$$\frac{1}{2} mu^2 = h(\nu - \nu_0)$$

# Photoelectric Effect



# Compton effect



Arthur Compton found that. "If monochromatic X-rays are allowed to fall on carbon or some other lighter elements, the scattered X-rays have wavelength larger than the incident rays. In other words, the scattered X-rays have low frequency than the incident rays. This causes decrease in the energy of incident ray.

$$\begin{aligned}\lambda' - \lambda &= \frac{h}{m_e c} (1 - \cos \theta) \\ &= \lambda_c (1 - \cos \theta) \geq 0\end{aligned}$$

# De Broglie Hypothesis

- The non-particle behavior of matter was first proposed in 1923, by **Louis de Broglie**, a French physicist.
- In his PhD thesis, he proposed that particles also have wave-like properties.
- Although he did not have the ability to test this hypothesis at the time, he derived an equation to prove it using Einstein's famous mass-energy relation and the Planck equation.

# De Broglie Hypothesis

## **De Broglie Hypothesis:**

In quantum mechanics, any object can behave both like wave-particle duality at the sub-microscopic level.

## **Wave-particle Duality:**

An object can act as both wave and particle at a same time. This phenomenon is called wave-particle duality.

So, the object would have energy packets, momentum (can be passed to another object), wave length, frequency and amplitude etc.

By using photo-electric effect and Compton effect we can easily describe about the wave particle duality



# De Broglie Hypothesis

$$E = hv \quad \text{-----1}$$

$$E = mc^2 \quad \text{-----2}$$

From Equation 1 and 2 we get,

$$hv = mc^2$$

we have,

$$v = c/\lambda$$

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

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

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

$$p = \text{mass} \times \text{velocity} = mc$$

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

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

-----de Broglie Equation

# The Heisenberg's Uncertainty Principle

- ▶ Statement
- ▶ “It is impossible to determine simultaneously the position and momentum of the electron with any desired accuracy”

$$\Delta x \cdot \Delta p \geq h$$

$$\Delta x \cdot \Delta p \geq h / 4\pi$$

# Operators

- ▶ An operator is a mathematical instruction or procedure to be carried out on a function.
- ▶ Operand
- ▶ An operator  $A$  is written as  $(A)$
- ▶ Example:
- ▶  $(A) = \log$  and  $f(x) = 1$ , then
- ▶  $(A).f(x) = \log 1 = 0$ .

^

^

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# Operators

## ► Algebra of operators

(i) Addition and subtraction of operators:-

►  $(A + B) f(x) = A f(x) + B f(x)$        $\wedge$

►  $(A - B) f(x) = A f(x) - B f(x)$        $\wedge$

(ii) Multiplication of operators :

►  $A . B f(x)$  implies that  $B f(x) = F'$

$$A F' = F''$$

$$\wedge \quad \wedge$$
$$A . B f(x) = F''$$

$\wedge$

$\wedge \quad \wedge$

# Operators

▶ **(iii) Linear operators**

▶  $A[ f(x) + g(x) ] = A f(x) + A g(x)$        $\wedge$

▶  $A[ C \cdot f(x) ] = C \cdot A f(x)$   
 $\wedge$

# Hamiltonian operator

- ▶ The operator corresponding to total energy of a system, is called as Hamiltonian operator (H).

$$H = T + V \quad \text{-----1}$$

$$\hat{H} = \hat{T} + \hat{V} \quad \text{-----2}$$

As per Classical Theorv.

$$T = \frac{1}{2} m u^2 = \frac{p^2}{2m} \quad \text{--- -- -- -- --} \quad (p = m u) \text{-----3}$$

$$H = \frac{1}{2m} (p_x^2 + p_y^2 + p_z^2) + v(x, y, z) \text{-----4}$$

Corresponding Hamiltonian operator is,

$$\hat{H} = \frac{1}{2m} (p_x^2 + p_y^2 + p_z^2) + v(x, y, z) \text{-----5}$$



# Hamiltonian operator

The momentum Operator is given as,

$$p_x = \frac{h}{2\pi i} \cdot \frac{\delta}{\delta x}$$

$$p_y = \frac{h}{2\pi i} \cdot \frac{\delta}{\delta y}$$

$$p_z = \frac{h}{2\pi i} \cdot \frac{\delta}{\delta z} \text{ ----- } \mathbf{6}$$

Thus,

$$p_x = \frac{h}{2\pi i} \cdot \frac{\delta}{\delta x}$$

$$p_x^2 = \left[ \frac{h}{2\pi i} \cdot \frac{\delta}{\delta x} \right] \cdot \left[ \frac{h}{2\pi i} \cdot \frac{\delta}{\delta x} \right]$$

$$\therefore p_x^2 = \frac{-h^2}{4\pi^2} \cdot \frac{\delta^2}{\delta x^2} \text{ ----- (where, } i^2 = -1)$$

# Hamiltonian operator

Similarly,

$$\therefore p_y^2 = \frac{-h^2}{4\pi^2} \cdot \frac{\delta^2}{\delta y^2} \text{ and } \therefore p_z^2 = \frac{-h^2}{4\pi^2} \cdot \frac{\delta^2}{\delta z^2} \text{-----7}$$

$$H = \frac{-h^2}{8\pi^2 m} \left( \frac{\delta^2}{\delta x^2} + \frac{\delta^2}{\delta y^2} + \frac{\delta^2}{\delta z^2} \right) + v(x, y, z) \text{-----8}$$

$$H = \frac{-h^2}{8\pi^2 m} (\nabla^2) + v(x, y, z) \text{-----9}$$

$$\nabla^2 = \left[ \frac{\delta^2}{\delta x^2} + \frac{\delta^2}{\delta y^2} + \frac{\delta^2}{\delta z^2} \right] \text{-----Laplacian operator}$$



Schrodinger  $\psi = A \sin \frac{2\pi x}{\lambda}$  -----1 on

First Differentiation:

$$\frac{\delta\psi}{\delta x} = A \cdot \frac{2\pi}{\lambda} \cos \frac{2\pi x}{\lambda}$$
 -----2

Second Differentiation:

$$\frac{\delta^2\psi}{\delta x^2} = -A \cdot \frac{4\pi^2}{\lambda^2} \sin \frac{2\pi x}{\lambda}$$
 -----3

From equation 1, we get,

$$\frac{\delta^2\psi}{\delta x^2} = -A \cdot \frac{4\pi^2}{\lambda^2} \psi$$
 -----4

The Kinetic energy is given as,

$$\text{K.E.} = \frac{1}{2} m u^2 = \frac{1}{2} \frac{m^2 u^2}{m}$$
 -----5

# Schrodinger wave equation

Thus,

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

$$\lambda = h^2 / m^2 u^2$$

$$\therefore m^2 u^2 = \frac{h^2}{\lambda^2} \text{ -----6}$$

Substituting equation 6 in 5 we get,

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

From equation 4 we get,

$$\lambda^2 = - \frac{4\pi^2 \psi}{\frac{\delta^2 \psi}{\delta x^2}} \text{ -----8}$$

Substituting equation 8 in equation 7 we get,

$$\text{K.E.} = - \frac{1}{2} \frac{h^2}{4\pi^2 m\psi} \frac{\delta^2 \psi}{\delta x^2}$$

$$\text{K.E.} = - \frac{h^2}{8\pi^2 m\psi} \frac{\delta^2 \psi}{\delta x^2} \text{ -----9}$$

Now, the total energy of particle is given as,

$$\text{E} = \text{K.E.} + \text{P.E.}$$

$$\text{K.E.} = \text{E} - \text{P.E.}$$

$$\text{K.E.} = \text{E} - V \text{ -----10}$$

Substituting equation 9 in 10 we get,

$$- \frac{h^2}{8\pi^2 m\psi} \frac{\delta^2 \psi}{\delta x^2} = E - V$$

$$\frac{\delta^2 \psi}{\delta x^2} = -(E - V) \frac{8\pi^2 m\psi}{h^2}$$

$$\frac{\delta^2 \psi}{\delta x^2} + \frac{8\pi^2 m}{h^2} (E - V)\psi = 0 \text{ -----11}$$

# Schrodinger wave equation

Equation 11 is time independent Schrödinger wave equation in one direction.

For an electron moving along three co ordinate axis, the Schrodinger wave equation can be written as,

$$\frac{\delta^2 \psi}{\delta x^2} + \frac{\delta^2 \psi}{\delta y^2} + \frac{\delta^2 \psi}{\delta z^2} + \frac{8\pi^2 m}{h^2} (E - V)\psi = 0 \text{ -----12}$$

Or

$$\nabla^2 \psi + \frac{8\pi^2 m}{h^2} (E - V)\psi = 0 \text{ -----13}$$

Where,

$$\nabla^2 = \left[ \frac{\delta^2}{\delta x^2} + \frac{\delta^2}{\delta y^2} + \frac{\delta^2}{\delta z^2} \right] \text{-----Laplacian operator}$$

# Physical Interpretation of $\psi$ and $\psi^2$

$\psi$  = Wave function = Amplitude of the wave

$\psi^2$  = The probability of finding an electron at any point -----(Born)

$\psi^2$  is real.

$$\psi^2 = \psi \cdot \psi^* \text{ -----}$$

$\psi$  is Complex and  $\psi^*$  is complex conjugate.

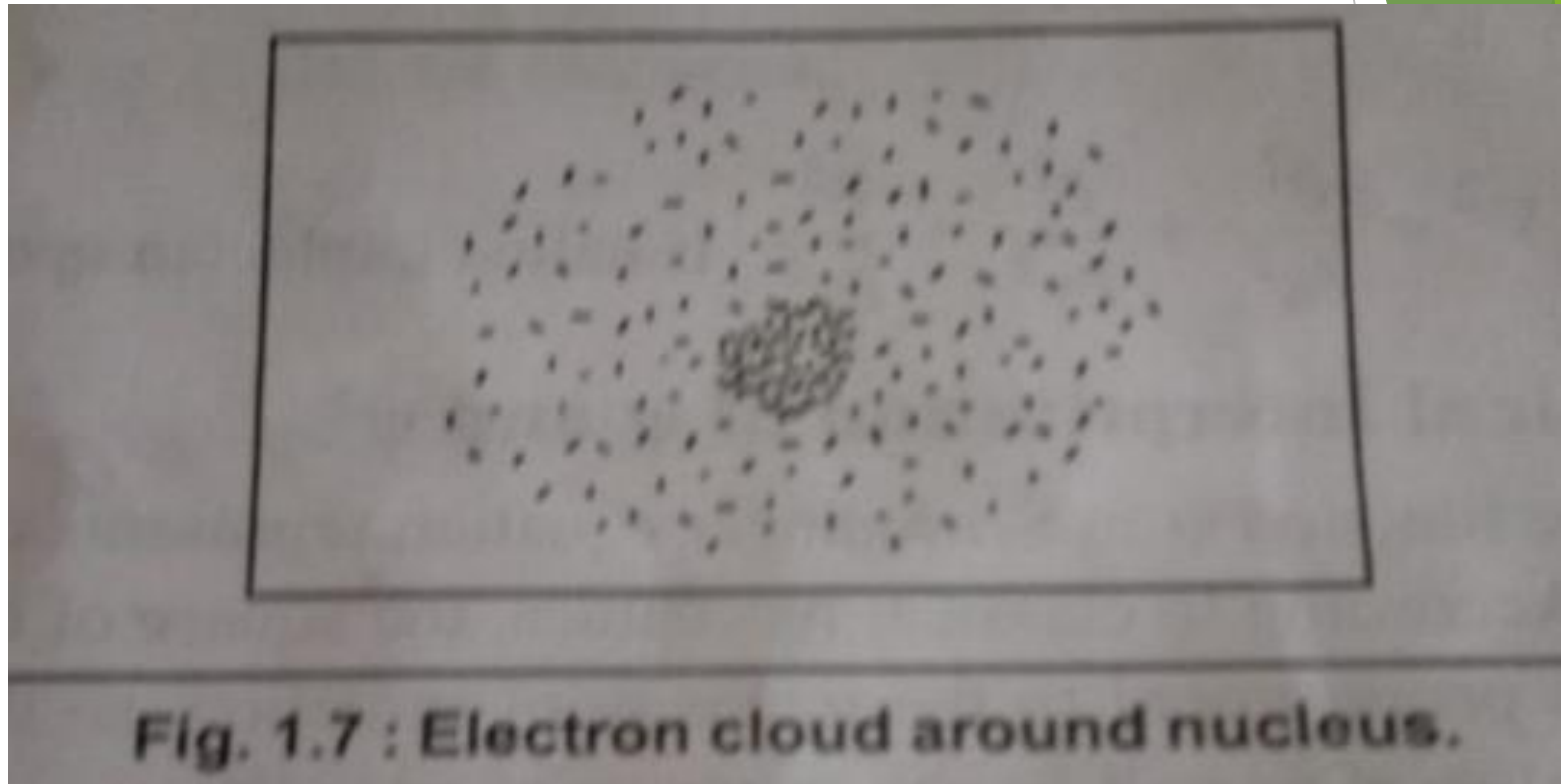
ex. if  $\psi = a + ib$ , then  $\psi^* = a - ib$ .

$$\psi\psi^* = a^2 + b^2$$

$\psi^2$  = Probability density

= Region where the probability of finding an electron is high

# Physical Interpretation of $\psi$ and $\psi^2$



# Properties or Characterization of Wave function

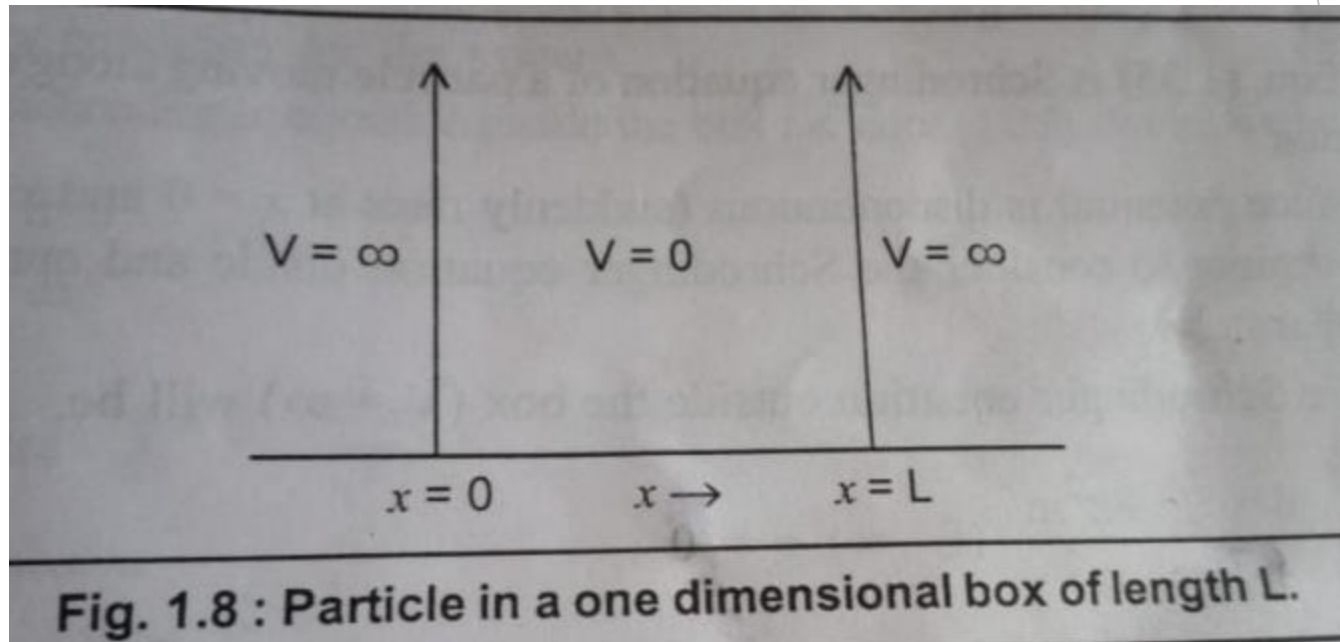
1) Single valued

2) Finite

3) The total probability must be unity  $\int \psi \psi^* dv = 1$

4) Continuous

# Particle in One Dimension Box



# Part 1 Dimension Box

$$H\psi = E\psi \quad \text{-----1}$$

H is the Hamiltonian Operator.

$$H = -\frac{h^2}{8\pi^2 m} \frac{d^2}{dx^2} + v$$
$$-\frac{h^2}{8\pi^2 m} \frac{d^2\psi}{dx^2} + v\psi = E\psi$$

$$-\frac{h^2}{8\pi^2 m} \frac{d^2\psi}{dx^2} + v\psi - E\psi = 0$$

$$\frac{h^2}{8\pi^2 m} \frac{d^2\psi}{dx^2} + (E - V)\psi = 0 \quad (\text{changing signs})$$

Multiplying throughout by  $\frac{8\pi^2 m}{h^2}$ , we get,

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

Equation 2 is Schrödinger wave equation of a particle moving along a single direction.



P Potential is discontinuous, it is convenient to the consider outside and inside the box separately.

The Schrödinger equation outside the box ( $V=\infty$ ) will be,

$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2 m}{h^2} (E - \infty) \psi = 0 \text{ -----3}$$

Multiplying throughout by  $\frac{h^2}{8\pi^2 m}$ , we get,

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

$$\frac{h^2}{8\pi^2 m} \frac{d^2\psi}{dx^2} + E\psi - \infty\psi = 0$$

On rearrangement,

$$\therefore \frac{h^2}{8\pi^2 m} \frac{d^2\psi}{dx^2} - \infty\psi = -E\psi$$

$$\therefore \frac{h^2}{8\pi^2 m} \frac{d^2\psi}{dx^2} + \infty\psi = E\psi \text{ -----4}$$

**P** The Schrödinger wave equation inside the box i.e.  $0 \leq x \leq L$  ( where  $V=0$ ) will be,

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

$$\therefore \frac{d^2\psi}{dx^2} + \frac{8\pi^2 m}{h^2} E\psi = 0 \text{ -----5}$$

$$-\frac{h^2}{8\pi^2 m} \frac{d^2\psi}{dx^2} = E\psi \text{ -----6}$$

$\psi$  must be zero

*Schrodinger equation inside the box can be written as,*

$$\frac{d^2\psi}{dx^2} + K^2 \psi = 0 \text{ -----7}$$

Where,  $K^2 = \frac{8\pi^2 m}{h^2} E \text{ -----8}$

$$E = \frac{K^2 h^2}{8\pi^2 m} \text{ -----9}$$

**Pa** The general solution to equation 7 is,

$$\psi = A \sin Kx + B \cos Kx \text{-----9}$$

a) At  $x = 0$ ,  $\psi = 0$ , therefore from eqn. 9

$$0 = A \sin ( K.0) + B \cos (K.0)$$

$$0 = 0 + B$$

$$\therefore B = 0$$

$$\psi = A \sin Kx \quad \text{for all values of } x \quad \text{-----10}$$

b) at  $x = L$ ,  $\psi = 0$ . therefore from eqn. 10

$$0 = A \sin KL \quad \text{-----11}$$

(i)  $A = 0$  and (ii)  $KL = n\pi$  where  $n = 1, 2, 3, \dots$

If both  $A$  and  $B = 0$ ,

$\psi = 0$  at all values of  $x$  which makes little sense.

$$K = n\pi/L$$

# Particle in One Dimension Box

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

$$E = \frac{K^2}{8mL^2}$$

$$E = \frac{K^2 h^2}{8m\pi^2} = \frac{n^2 \pi^2}{L^2} \times \frac{h^2}{8\pi^2 m}$$

$$E = \frac{n^2 h^2}{8mL^2}$$

Where  $n=1, 2, 3, \dots$

Where  $n=1, 2, 3, \dots$

$$E = \frac{h^2}{8mL^2}$$

# SCHRÖDINGER EQUATION FOR HYDROGEN MOLECULE

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

$$V = -\frac{Ze^2}{4\pi\epsilon_0 r}$$

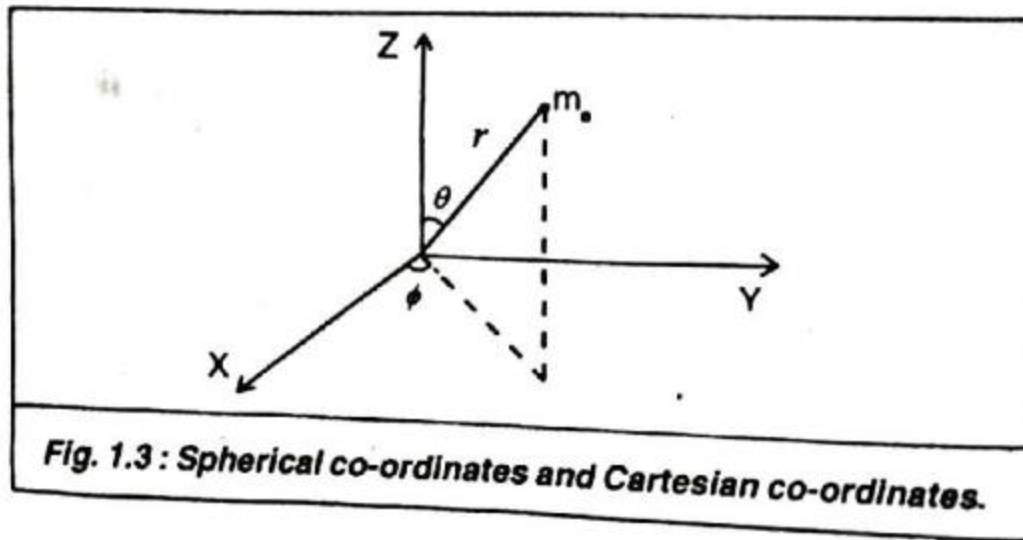
Here, for hydrogen atom  $Z = 1$ ,

$$\therefore V = -\frac{1 \times e^2}{4\pi\epsilon_0 r}$$

Where,  $\epsilon_0$  is permittivity of the vacuum,  $r$  is the distance between two particles (here for hydrogen atom it is distance between electron and atomic nucleus).

# SCHRÖDINGER EQUATION FOR HYDROGEN MOLECULE

$$\frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} + \frac{\partial^2 \Psi}{\partial z^2} + \frac{8\pi^2 m}{h^2} \left( E + \frac{e^2}{4\pi\epsilon_0 r} \right) \Psi = 0$$



$$x = r \sin \theta \cos \phi$$

$$y = r \sin \theta \sin \phi$$

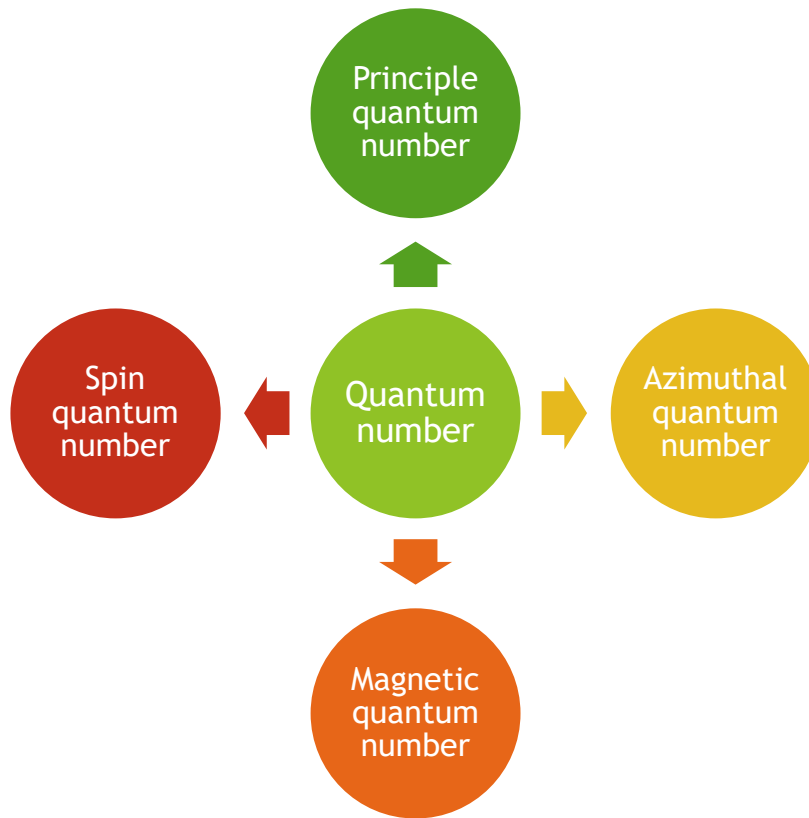
$$\text{and } z = r \cos \theta$$

# SCHRÖDINGER EQUATION FOR HYDROGEN MOLECULE

$$\frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial \Psi}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial \Psi}{\partial \theta} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial^2 \Psi}{\partial \phi^2} + \frac{8\pi^2 \mu}{h^2} \left( E + \frac{e^2}{4\pi\epsilon_0 r} \right) \Psi = 0$$

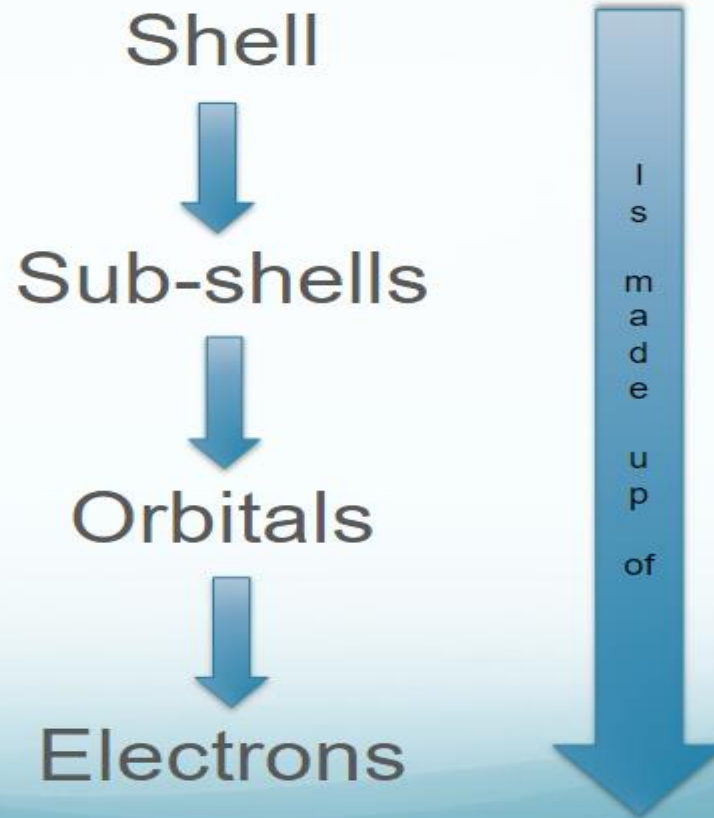
$$\mu = \frac{m_e \times m_{nucleus}}{m_e + m_{nucleus}}$$

# Quantum number





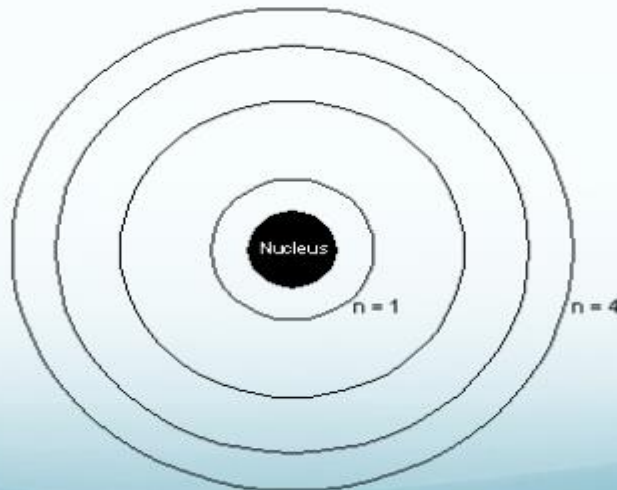
# Quantum number



# Quantum number

## The Principal Quantum Number ( $n$ )

- The larger the value of ' $n$ ' the further the shell is from the nucleus.
- As the value of ' $n$ ' increases the energy gap between successive shells decreases.



# Quantum number

## The Angular Momentum Quantum Number ( $l$ )

- $l = 0, 1, 2, \dots, (n - 1)$   
e.g. when  $n = 2$ ,  $l = 0, 1$  and when  $n = 4$ ,  $l = 0, 1, 2, 3$
- When  $l = 0$  the subshell is an 's' subshell  
When  $l = 1$ , the subshell is a 'p' subshell  
When  $l = 2$ , the subshell is a 'd' subshell  
When  $l = 3$ , the subshell is an 'f' subshell
- Hence in the first shell where  $n = 1$ ,  $l = 0$  and so the first shell consists of only an s-subshell and in the third shell where  $n = 3$ ,  $l = 0, 1$  &  $2$  and so the third shell consists of an s, a p and a d-subshell.

# Quantum number

## The Magnetic Quantum Number ( $m_l$ )

- $m_l = -l$  to  $+l$

e.g. for an s-subshell,  $l = 0$  and so  $m_l = 0$

i.e. in an s-subshell, there is only one orbital as there is only one value for  $m_l$ .

e.g. for a p-subshell,  $l = 1$  and so  $m_l = -1, 0, +1$

i.e. in a p-subshell, there are three orbitals as there are three values for  $m_l$ .

# Quantum number

## Orbitals

- Although subshells have different energies (see the Aufbau Principle), orbitals within a sub-shell are degenerate i.e. they have equal energy e.g. all five orbitals within a d-subshell are degenerate.
- Each orbital can hold a maximum of two electrons hence, an s-subshell, made up of only one orbital, can hold a maximum of 2 electrons and a p-subshell made up of three orbitals can hold a maximum of 6 electrons. How many electrons can a d and f-subshell hold?

# Quantum number

Consider the quantum numbers of the two electrons in the 1s orbital:



For 1 electron

$$n = 1$$

$$l = 0$$

$$m_l = 0$$

$$m_s = +\frac{1}{2}$$

For the second electron

$$n = 1$$

$$l = 0$$

$$m_l = 0$$

$$m_s = -\frac{1}{2}$$

# Numerical Problems

1. An electron is accelerated by applying the potential the application difference of 1000 eV. What is the de Broglie wavelength associated with it?

**Solution:**

**Formula:**  $\lambda = \frac{h}{mv}$ ,

$$\lambda = \frac{6.626 \times 10^{-34} \text{ Js}}{9.1 \times 10^{-31} \text{ kg} \times 1000 \times 1.602 \times 10^{-19} \text{ J}}$$
$$= 4.54 \times 10^{-12} \text{ m}$$

# Numerical Problems

2. What is the wavelength of  $H^+$  ion (mass =  $1.7 \times 10^{-27} \text{ kg}$ ) moving with a velocity equal to  $\frac{1}{200^{\text{th}}}$  of light?

Solution:-

Formula :  $\lambda = \frac{h}{P} = \frac{h}{mv}$

Given:

$$m = 1.7 \times 10^{-27} \text{ kg}, \quad v = \frac{1}{200} \times c$$

Thus,

$$\lambda = \frac{6.626 \times 10^{-34} \text{ Js}}{1.7 \times 10^{-27} \times \frac{1}{200} \times 3 \times 10^8}$$

$$\lambda = 25.99 \times 10^{-14} \text{ m.}$$



# Numerical Problems

3. A photon of wavelength  $4500\text{\AA}$  strikes on the metal surface, the work function of metal being  $2.55\text{ eV}$ . Calculate (i) the energy of photon in eV, (ii) the kinetic energy of electron (iii) the velocity of photo electron ( $m = 9.109 \times 10^{-31}\text{ Kg}$ )

Solution:  $E = h\nu = \frac{hc}{\lambda}$ ,  $E = \phi + K.E.$

Given: -  $\phi = 2.55\text{ eV}$ ,  $m = 9.109 \times 10^{-31}\text{ Kg}$

$\lambda = 4500\text{\AA} = 4500 \times 10^{-10}\text{ m}.$

*Thus, (i) Energy of Photon:*

$$E = h\nu = \frac{hc}{\lambda} = \frac{6.26 \times 10^{-34}\text{ Js} \times 3 \times 10^8\text{ m/s}}{4500 \times 10^{-10}\text{ m}}$$

$$E = 4.417 \times 10^{-19}\text{ J}$$

Since,  $1\text{ eV} = 1.602 \times 10^{-19}\text{ J}$

$$E = 2.76\text{ eV}.$$

Ans: Energy of Photon:  $2.76\text{ eV}.$

# Numerical Problems

(ii) Kinetic energy of emitted photoelectron:

$$E = h\nu = \phi + K.E.$$

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

$$= 2.76 - 2.55$$

$$= .021\text{ev}$$

Ans: Kinetic energy of photoelectron = 0.21ev.

(iii) Velocity of photoelectron:

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

$$0.21\text{ev} = \frac{1}{2} 9.109 \times 10^{-31} \times u^2$$

$$u^2 = \frac{0.21 \times 1.602 \times 10^{-19}\text{J} \times 2}{9.109 \times 10^{-31}\text{kg}}$$

$$u^2 = 0.07387 \times 10^{12}$$

$$u = 2.72 \times 10^5 \text{ m/s}$$

Ans: Velocity of photoelectron =  $2.72 \times 10^5 \text{ m/s}$

# Numerical Problems

4. An electron is confined in one dimensional box of length  $12 \text{ \AA}$ . Calculate its ground state energy in electron volts (ev). ( $m = 9.109 \times 10^{-31} \text{ Kg}$ )

Solution:

Formula :-  $E = \frac{n^2 h^2}{8mL^2}$

Given :  $n = 1, L = 12 \text{ \AA} = 12 \times 10^{-10} \text{ m}$

$$E = \frac{(1) \times (6.626 \times 10^{-34} \text{ Js})^2}{8 \times 9.109 \times 10^{-31} \text{ Kg} \times (12 \times 10^{-10} \text{ m})^2}$$

$$E = \frac{4.390 \times 10^{-67}}{1.0493 \times 10^{-47}}$$

$$E = 4.1837 \times 10^{-20} \text{ J}$$

Since,  $1 \text{ ev} = 1.602 \times 10^{-19} \text{ J}$

$$E = \frac{4.1837 \times 10^{-20} \text{ J}}{1.602 \times 10^{-19} \text{ J}}$$

$$E = 2.611 \times 10^{-1} \text{ ev.} = 0.26 \text{ ev}$$

Ans: Ground state energy =  $0.26 \text{ ev}$ .