QUANTUM MECHANICS

WAVE PROPERTIES OF PARTICLE

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Introduction

There are a few phenomenon which the classical mechanics failed to explain.

1. Stability of an atom
2. Spectral series of Hydrogen atom
3. Black body radiation

Max Planck in 1900 at a meeting of German Physical Society read his paper “On the theory of the Energy distribution law of the Normal Spectrum”. This was the start of the revolution of Physics i.e. the start of **Quantum Mechanics.**

Quantum Mechanics

It is a generalization of Classical Physics that includes classical laws as special cases.

Quantum Physics extends that range to the region of small dimensions.

Just as 'c' the velocity of light signifies universal constant, the Planck's constant characterizes Quantum Physics.

$$h = 6.65 \times 10^{-27}\, erg.\mathrm{sec}$$

$$h = 6.625 \times 10^{-34}\, Joule.\mathrm{sec}$$

Quantum Mechanics

It is able to explain

1. Photo electric effect
2. Black body radiation
3. Compton effect
4. Emission of line spectra

The most outstanding development in modern science was the conception of Quantum Mechanics in 1925. This new approach was highly successful in explaining about the behavior of atoms, molecules and nuclei.

WAVE-PARTICLE DUALITY OF LIGHT

In 1924 Einstein wrote:- " There are therefore now two theories of light, both indispensable, and … without any logical connection."

Evidence for wave-nature of light

- Diffraction and interference

Evidence for particle-nature of light

- Photoelectric effect
- Compton effect

- Light exhibits diffraction and interference phenomena that are *only* explicable in terms of wave properties
- Light is always detected as packets (photons); if we look, we never observe half a photon
- Number of photons proportional to energy density (i.e. to square of electromagnetic field strength)

De Broglie

MATTER WAVES

We have seen that light comes in discrete units (photons) with particle properties (energy and momentum) that are related to the wave-like properties of frequency and wavelength.

In 1923 Prince Louis de Broglie postulated that ordinary matter can have wave-like properties, with the wavelength λ related to momentum p in the same way as for light

de Broglie relation

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

de Broglie wavelength

Planck's constant

$$h = 6.63 \times 10^{-34}\,\mathrm{Js}$$

wavelength depends on momentum, not on the physical size of the particle

Prediction: We should see diffraction and interference of matter waves

De Broglie Waves

Not only the light but every materialistic particle such as electron, proton or even the heavier object exhibits wave-particle dual nature.

De-Broglie proposed that a moving particle, whatever its nature, has waves associated with it. These waves are called "**matter waves**".

Energy of a photon is

$$E = h\nu$$

For a particle, say photon of mass, m

$$E = mc^2$$

$$mc^2 = h\nu$$

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

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

Suppose a particle of mass, m is moving with velocity, v then the wavelength associated with it can be given by

$$\lambda = \frac{h}{mv} \quad \text{or} \quad \lambda = \frac{h}{p}$$

(i) If $v = 0 \Rightarrow \lambda = \infty$ means that waves are associated with **moving** material particles only.

(ii) De-Broglie wave does not depend on whether the moving particle is charged or uncharged. It means matter waves are not electromagnetic in nature.

Using de Broglie relation let's find the wavelength of a 10-6g particle moving with a speed 10-6m/s:

$$\boxed{\lambda = \frac{h}{p} = \frac{h}{mv} = \frac{6.63\times10^{-34}J\cdot s}{(10^{-9}kg)(10^{-6}m/s)} = 6.63\times10^{-19}m}$$

Since the wavelength found in this example is so small, much smaller than any possible apertures, diffraction or interference of such waves can not be observed.

The situation are different for low energy electrons and other microscopic particles.

Consider a particle with kinetic energy K. Its momentum is found from

$$\boxed{K = \frac{p^2}{2m} \quad or \quad p = \sqrt{2mK}}$$

Its wavelength is then

$$\boxed{\lambda = \frac{h}{p} = \frac{h}{\sqrt{2mK}}}$$

The de Broglie Wavelength

$$\boxed{\lambda = \frac{h}{p} = \frac{h}{\sqrt{2mK}}}$$

If we multiply the numerator and denominator by c we obtain:

$$\boxed{\lambda = \frac{hc}{\sqrt{2mc^2K}} = \frac{1240eV \cdot nm}{\sqrt{2(0.511 \times 10^6 eV)K}} = \frac{1.226}{\sqrt{K}} nm}$$

Where mc2=0.511MeV for electrons, and K in electron-volts.

The de Broglie Wavelength

We obtained the electron wavelength:

$$\boxed{\lambda = \left(\frac{1.226}{\sqrt{K}}\right) nm, \quad K \;\; in \;\; eV}$$

Similarly, for proton (mc2 = 938 MeV for protons)

$$\boxed{\lambda_p = \left(\frac{0.0286}{\sqrt{K}}\right) nm}$$

Estimate some de Broglie wavelengths

- Wavelength of electron with 50eV kinetic energy

$$\boxed{K = \frac{p^2}{2m_e} = \frac{h^2}{2m_e\lambda^2} \Rightarrow \lambda = \frac{h}{\sqrt{2m_e K}} = 1.7\times10^{-10}\,\mathrm{m}}$$

- Wavelength of Nitrogen molecule at room temp.

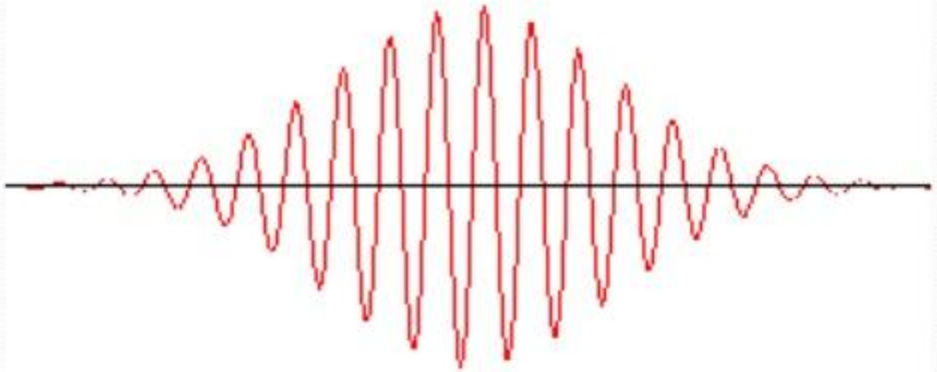
$$K = \frac{3kT}{2}, \quad \mathrm{Mass} = 28\mathrm{m_u}$$

$$\lambda = \frac{h}{\sqrt{3MkT}} = 2.8\times10^{-11}\,\mathrm{m}$$

- Wavelength of Rubidium(87) atom at 50nK

$$\boxed{\lambda = \frac{h}{\sqrt{3MkT}} = 1.2\times10^{-6}\,\mathrm{m}}$$

A "Wave Packet"



How do you construct a wave packet?

Wave function

The quantity with which Quantum Mechanics is concerned is the wave function of a body.

Wave function, ψ is a quantity associated with a moving particle. It is a complex quantity.

$|\Psi|^2$ is proportional to the probability of finding a particle at a particular point at a particular time. It is the probability density.

$$|\psi|^2 = \psi^* \psi$$

ψ is the probability amplitude.

Thus if $\psi = A + iB$ then $\psi^* = A - iB$

$$\Rightarrow |\psi|^2 = \psi^* \psi = A^2 - i^2 B^2 = A^2 + B^2$$

Normalization

$|\Psi|^2$ is the probability density.

The probability of finding the particle within an element of volume $d\tau$

$$|\psi|^2 \, d\tau$$

Since the particle is definitely be somewhere, so

$$\int_{-\infty}^{\infty} |\psi|^2 \, d\tau = 1 \qquad \therefore \text{ Normalization}$$

A wave function that obeys this equation is said to be normalized.

Properties of wave function

1. It must be finite everywhere.
   If ψ is infinite for a particular point, it mean an infinite large probability of finding the particles at that point. This would violates the uncertainty principle.

2. It must be single valued.
   If ψ has more than one value at any point, it mean more than one value of probability of finding the particle at that point which is obviously ridiculous.

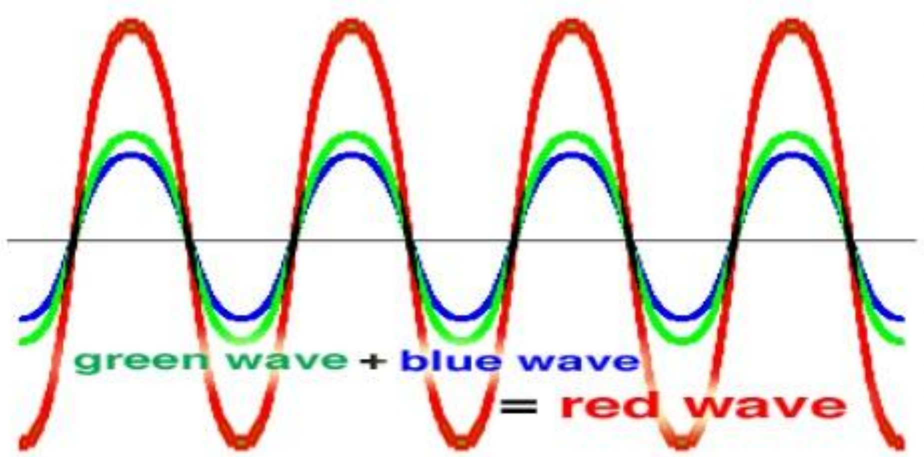
3. It must be continuous and have a continuous first derivative everywhere.

   $$\frac{\partial \psi}{\partial x}, \frac{\partial \psi}{\partial y}, \frac{\partial \psi}{\partial z} \quad \text{must be continuous}$$

4. It must be normalizable.

What happens when you add up waves?

The Superposition principle



Waves of same frequency

Wave Velocity or Phase Velocity

When a monochromatic wave travels through a medium, its velocity of advancement in the medium is called the wave velocity or phase velocity (V_p).

$$V_p = \frac{\omega}{k}$$

where $\omega = 2\pi\nu$ is the angular frequency

and $k = \dfrac{2\pi}{\lambda}$ is the wave number.

$$y = A\cos 2\pi\upsilon t \ldots\ldots\ldots$$

$$\text{ie,. } y = A\cos 2\pi\upsilon\left(t - \frac{x}{v_p}\right) \ldots\ldots\ldots$$

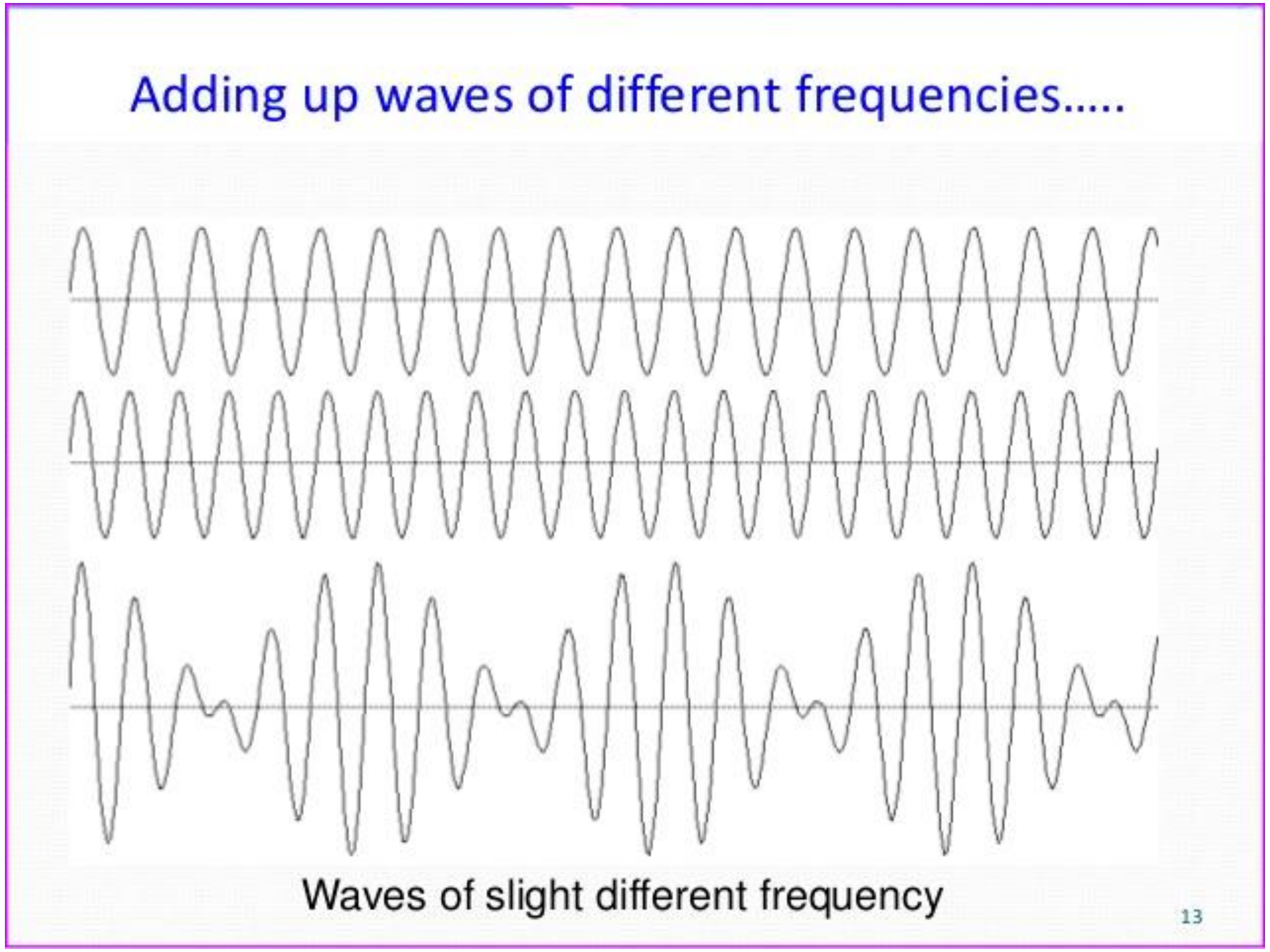
$$y = A\cos 2\pi\left(\upsilon t - \frac{\upsilon x}{v_p}\right)$$

$$\text{But } \frac{\upsilon}{v_p} = \frac{1}{\lambda}$$

$$\therefore\ y = A\cos 2\pi\left(\upsilon t - \frac{x}{\lambda}\right)$$

$$k = \frac{2\pi}{\lambda} = \frac{\omega}{v_p}.$$

GROUP VELOCITY



$$y_1 = A \cos (\omega t - kx)$$

$$y_2 = A \cos [(\omega + \Delta\omega)t - (k + \Delta k)x]$$

The resultant displacement y at any time t and any position x is the sum of y_1 and y_2

$$\therefore \quad y = y_1 + y_2$$

$$= A \cos (\omega t - kx) + A \cos [(\omega + \Delta\omega)t - (k + \Delta k)x]$$

$$= 2A \cos \frac{1}{2} [(2\omega + \Delta\omega)t - (2k + \Delta k)x] \cos \frac{1}{2} (\Delta\omega t - \Delta k x)$$

Since $\Delta\omega$ and Δk are small compared with ω and k respectively, we have

$$2\omega + \Delta\omega = 2\omega$$

$2k + \Delta k = 2k$ and so beats

$$y = 2A\cos(\omega t - kx)\cos\left(\frac{\Delta\omega}{2}t - \frac{\Delta k}{2}x\right) \qquad \text{......... (9)}$$

Equation (9) represents a wave of angular frequency ω and wave number k that has super imposed upon it a modulation of angular frequency $\frac{1}{2}\Delta\omega$ and of wave number $\frac{1}{2}\Delta k$. The effect of the modulation is to produce successive wave groups as in fig.2.2.

The phase velocity $v_p = \frac{\omega}{k}$

The velocity v_g of the wave groups is the group velocity $v_g = \frac{\Delta\omega}{\Delta k}$

When ω and k have continuous spreads, the group velocity is given by $v_g = \frac{d\omega}{dk}$

Group Velocity

In practice, we came across pulses rather than monochromatic waves. A pulse consists of a number of waves differing slightly from one another in frequency.

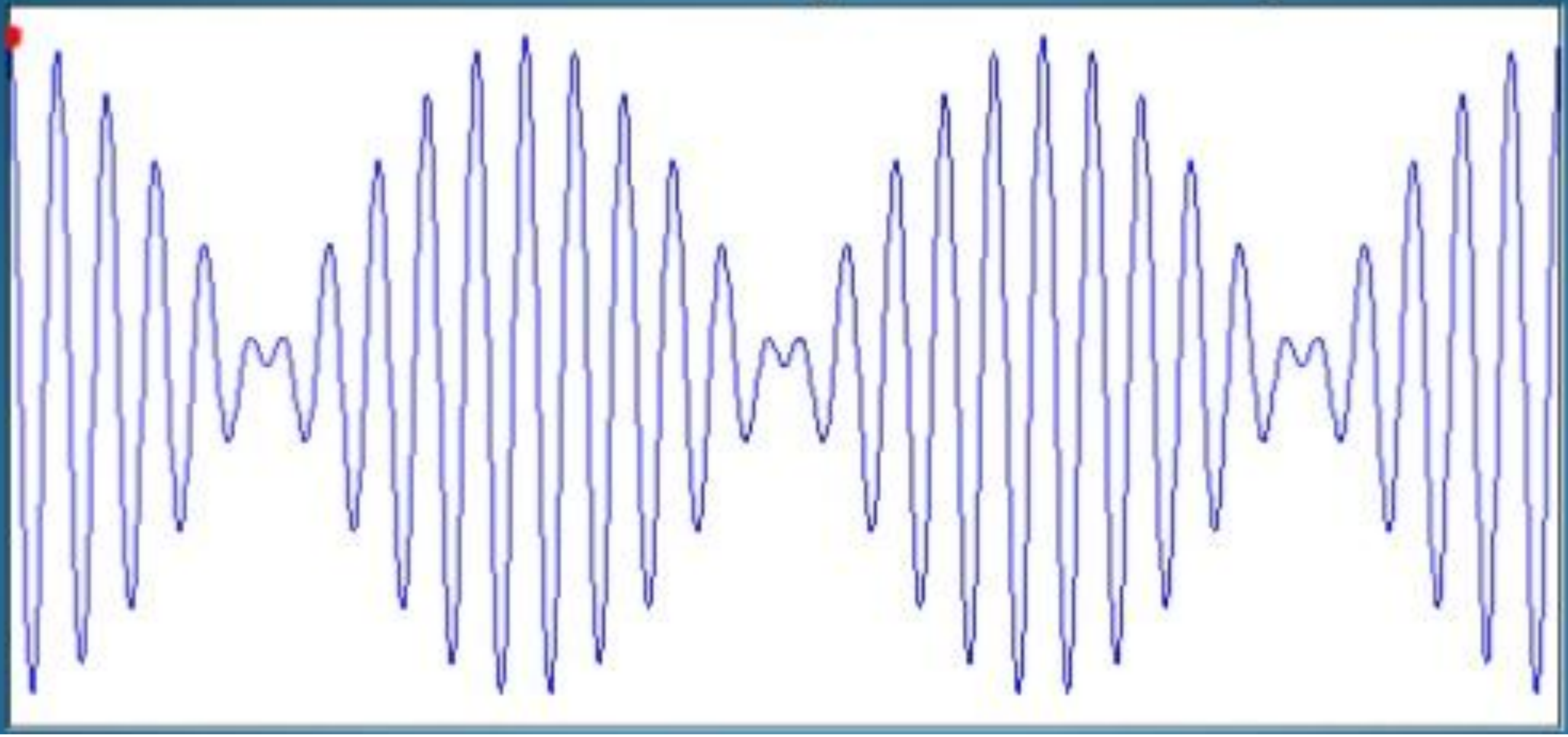
The observed velocity is, however, the velocity with which the maximum amplitude of the group advances in a medium.

So, the group velocity is the velocity with which the energy in the group is transmitted (V_g).

The individual waves travel "inside" the group with their phase velocities.

$$V_g = \frac{d\omega}{dk}$$

The Group Velocity



Phase Velocity of De-Broglie's waves

According to De-Broglie's hypothesis of matter waves

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

wave number $$k = \frac{2\pi}{\lambda} = \frac{2\pi mv}{h} \qquad \text{(i)}$$

If a particle has energy E, then corresponding wave will have frequency

$$\nu = \frac{E}{h}$$

then angular frequency will be $$\omega = 2\pi\nu = \frac{2\pi E}{h}$$

$$\omega = \frac{2\pi mc^2}{h} \qquad \text{(ii)}$$

Dividing (ii) by (i)

$$\frac{\omega}{k} = \frac{2\pi mc^2}{h} \times \frac{h}{2\pi mv}$$

$$V_p = \frac{c^2}{v}$$

But v is always < c (velocity of light)

(i) Velocity of De-Broglie's waves $V_p > c$ (not acceptable)

(ii) De-Broglie's waves (V_p) will move faster than the particle velocity (v) and hence the waves would left the particle behind.

Consider a particle of mass "m" moving with a velocity v

λ be the de wavelength

$$V_p = \nu\lambda$$

De-Broglie wavelength $\lambda = h/mv$

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

$$h\nu = mc^2$$

$$\nu = mc^2/h$$

$$V_p = (mc^2/h)\ (h/mv)$$

$$= c^2/v$$

Group Velocity of De-Broglie's waves

The discrepancy is resolved by postulating that **a moving particle is associated with a "wave packet" or "wave group", rather than a single wave-train.**

A wave group having wavelength λ is composed of a number of component waves with slightly different wavelengths in the neighborhood of λ.

Suppose a particle of rest mass m_o moving with velocity v then associated matter wave will have

$$\omega = \frac{2\pi mc^2}{h} \quad \text{and} \quad k = \frac{2\pi mv}{h} \quad \text{where} \quad m = \frac{m_o}{\sqrt{1 - v^2/c^2}}$$

$$\omega = \frac{2\pi m_o c^2}{h\sqrt{1 - v^2/c^2}} \quad \text{and} \qquad k = \frac{2\pi m_o v}{h\sqrt{1 - v^2/c^2}}$$

On differentiating w.r.t. velocity, v

$$\frac{d\omega}{dv} = \frac{2\pi m_o v}{h\left(1 - v^2/c^2\right)^{3/2}} \qquad \text{(i)}$$

$$\frac{dk}{dv} = \frac{2\pi m_o}{h\left(1 - v^2/c^2\right)^{3/2}} \qquad \text{(ii)}$$

Dividing (i) by (ii)

$$\frac{d\omega}{dv}.\frac{dv}{dk}=\frac{2\pi m_o v}{2\pi m_o}$$

$$\frac{d\omega}{dk}=v=V_g$$

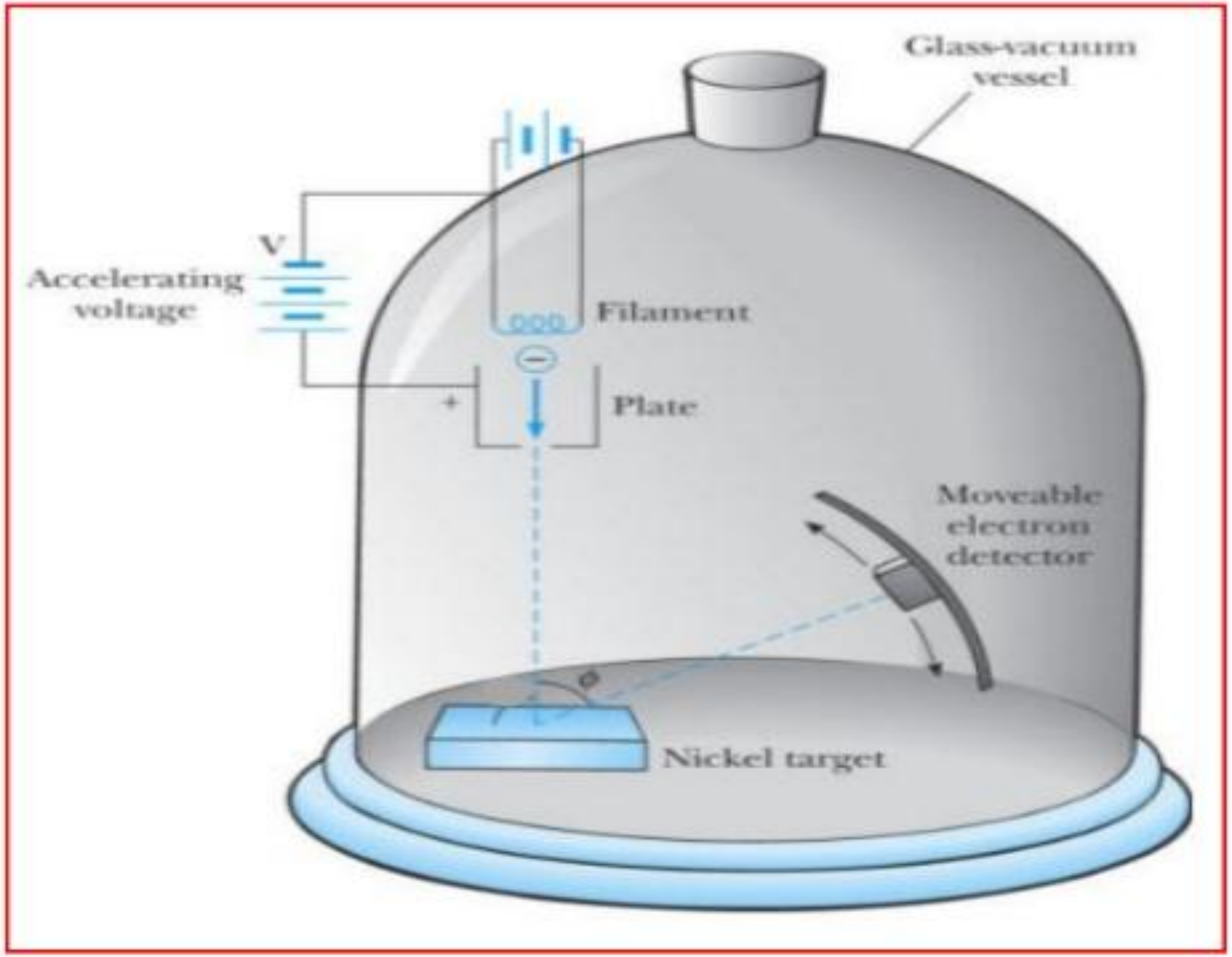
Wave group associated with a moving particle also moves with the velocity of the particle.

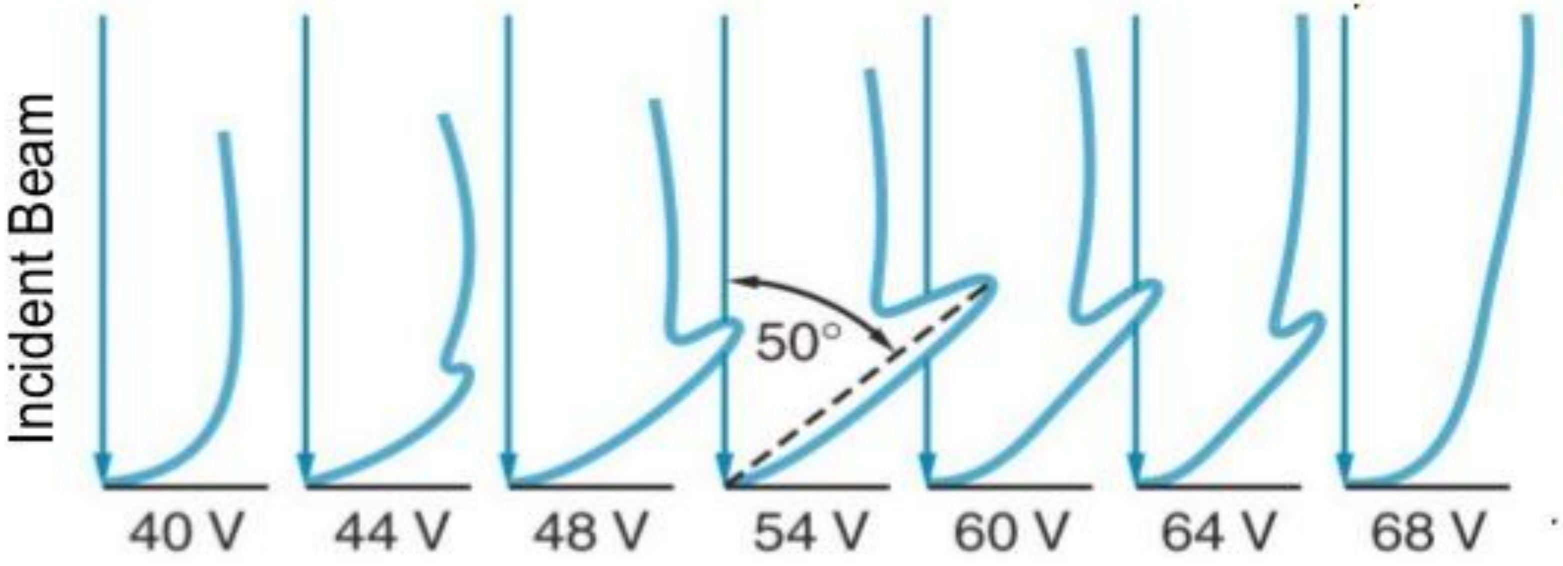
Moving particle $\equiv$ wave packet or wave group

Davisson & Germer experiment of electron diffraction

- If particles have a wave nature, then under appropriate conditions, they should exhibit diffraction
- Davisson & Germer measured the wavelength of electrons
- This provided experimental confirmation of the matter waves proposed by de Broglie

Davisson and Germer Experiment





Current vs accelerating voltage has a maximum (a bump or kink noticed in the graph), i.e. the highest number of electrons is scattered in a specific direction.

The bump becomes most prominent for 54 V at $\varphi \sim 50°$

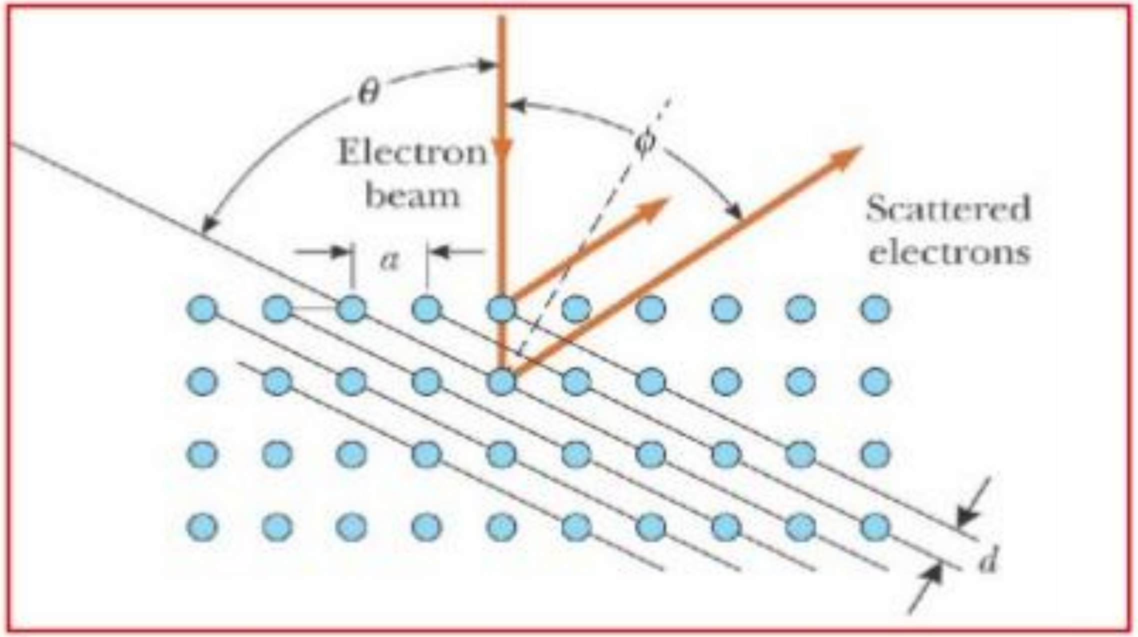
According to de Broglie, the wavelength associated with an electron accelerated through V volts is

$$\lambda = \frac{12.28}{\sqrt{V}} \overset{o}{A}$$

Hence the wavelength for 54 V electron

$$\lambda = \frac{12.28}{\sqrt{54}} = 1.67 \overset{o}{A}$$

From X-ray analysis we know that the nickel crystal acts as a plane diffraction grating with grating space d = 0.91 Å



Here the diffraction angle, $\varphi \sim 50°$

The angle of incidence relative to the family of Bragg's plane

$$\theta = \left(\frac{180^o - 50^o}{2} \right) = 65^o$$

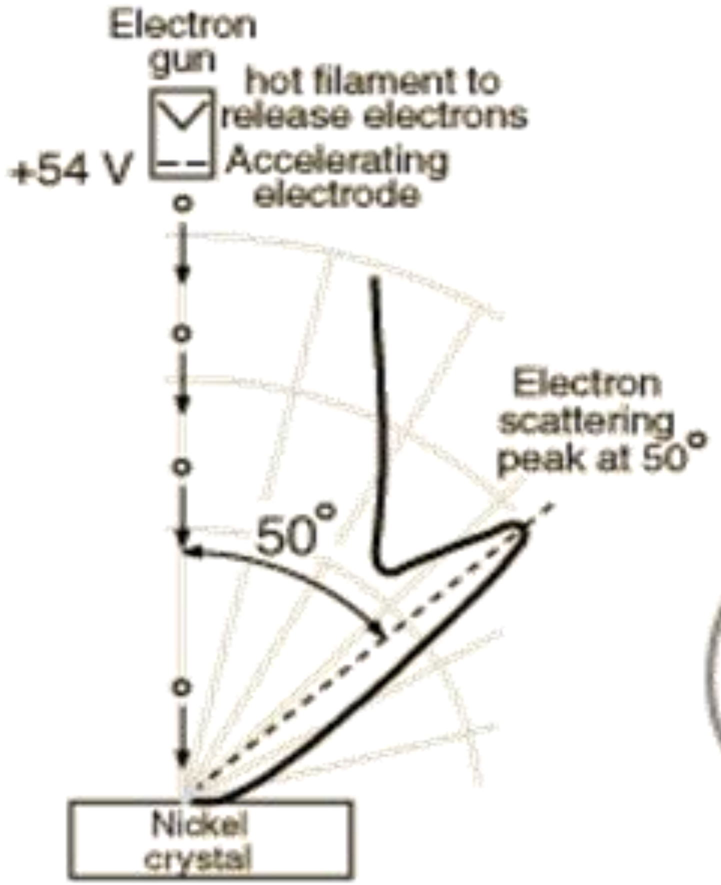
From the Bragg's equation

$$\lambda = 2d \sin\theta$$

$$\lambda = 2 \times (0.91\,\overset{o}{A}) \times \sin 65^{o} = 1.65\,\overset{o}{A}$$

which is equivalent to the λ calculated by de-Broglie's hypothesis.

It confirms the wavelike nature of electrons



Theory

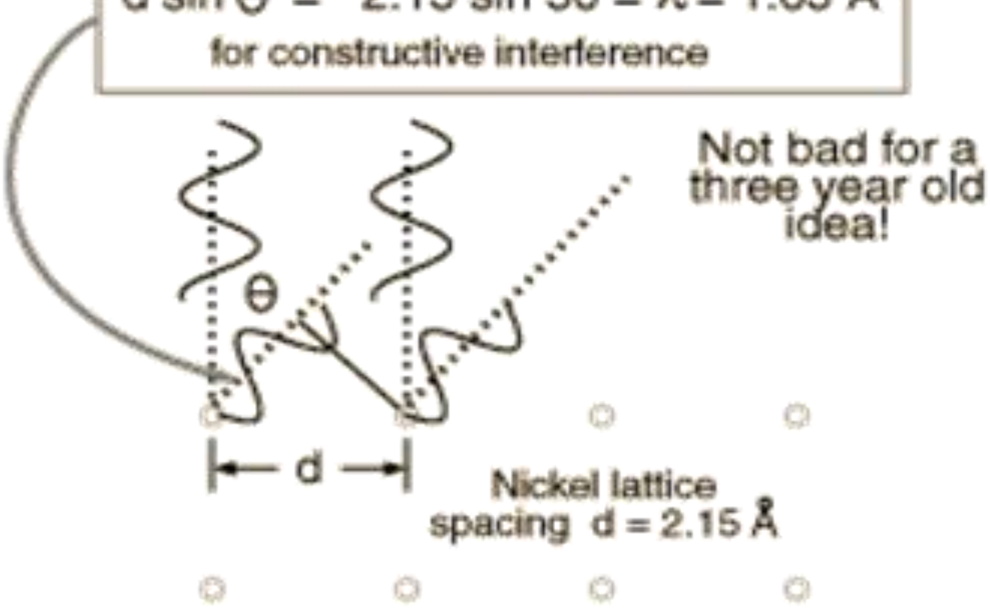
$$\lambda = \frac{h}{mv} = 1.67\ \text{Å for 54 V}$$

Experiment

Pathlength difference

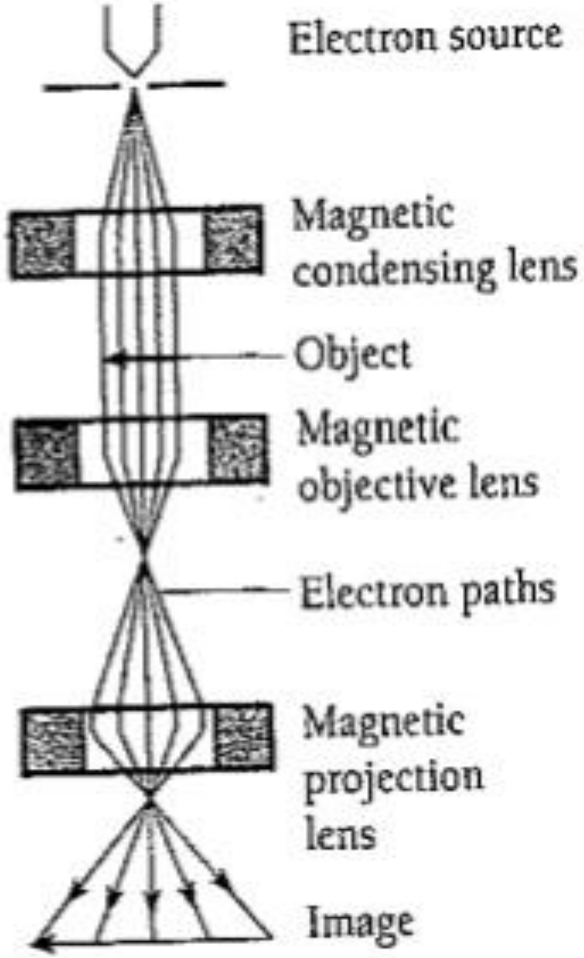
$$d \sin\theta = 2.15 \sin 50^\circ = \lambda = 1.65\ \text{Å}$$

for constructive interference



1924	1927	1929
de Broglie's hypothesis	Davisson-Germer experiment	Nobel Prize for de Broglie

Electron Microscope: Instrumental Application of Matter Waves



Resolving power of any optical instrument is proportional to the wavelength of whatever (radiation or particle) is used to illuminate the sample.

An optical microscope uses visible light and gives 500x magnification/200 nm resolution.

Fast electron in electron microscope, however, have much shorter wavelength than those of visible light and hence a resolution of ~0.1 nm/magnification 1,000,000x can be achieved in an Electron Microscope.

An electron microscope consists of an electron gun, electrostatic and magneto static lenses and fluorescent screen

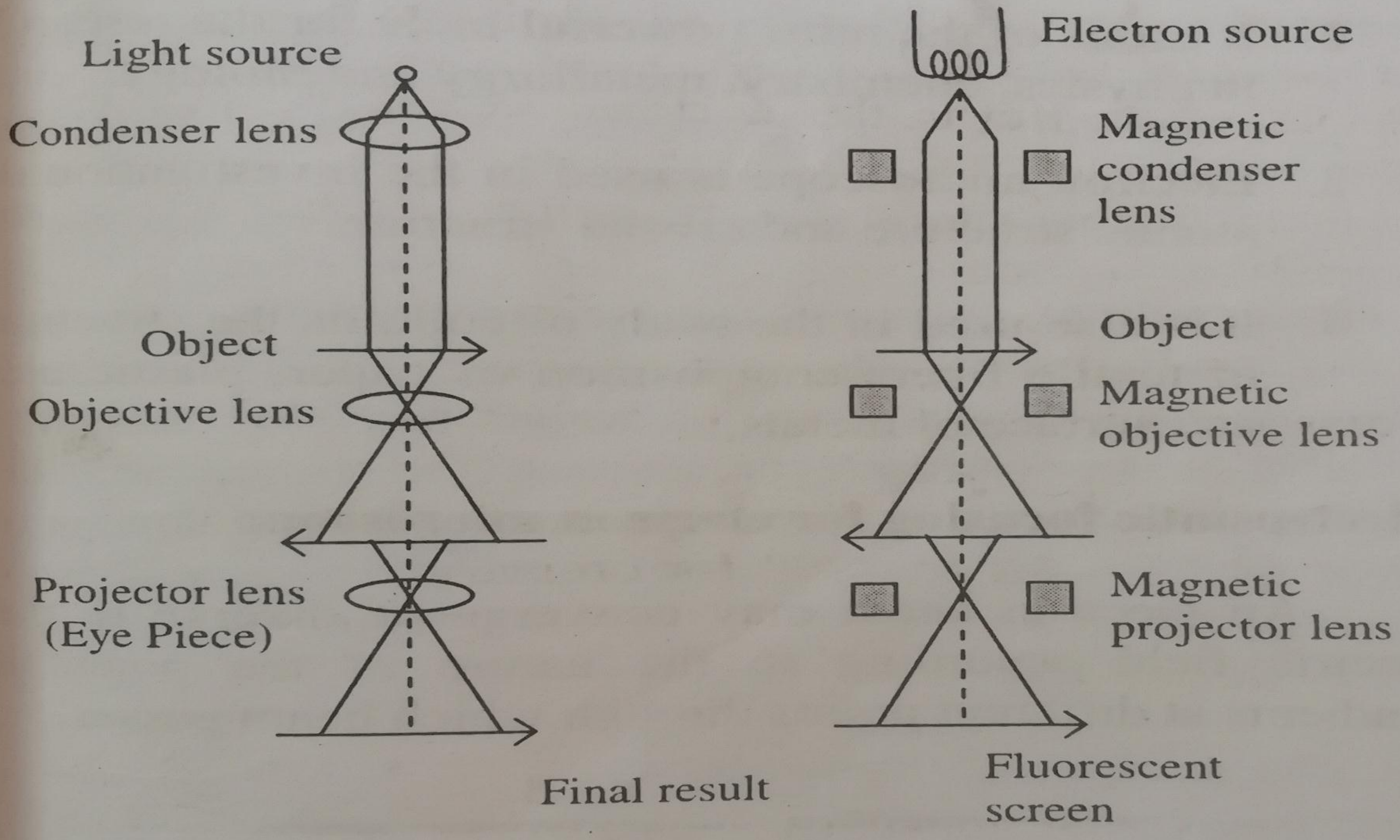

Light source
Condenser lens
Object
Objective lens
Projector lens
(Eye Piece)
Final result
Electron source
Magnetic
condenser
lens
Object
Magnetic
objective lens
Magnetic
projector lens
Fluorescent
screen

Fig. 2.5

Uses

1. Due to high magnification and great resolving power electron microscopes are used in the study of bacteria and viruses.

2. It is one of the most powerful tools for the research in physics, chemistry, metallurgy and biology.

3. Electron microscope is used in the investigation of atomic structure and crystal structure.

4. It is also used in the study of colloids the structure of textile fibers composition of paper, plastic etc. and surface of metals.

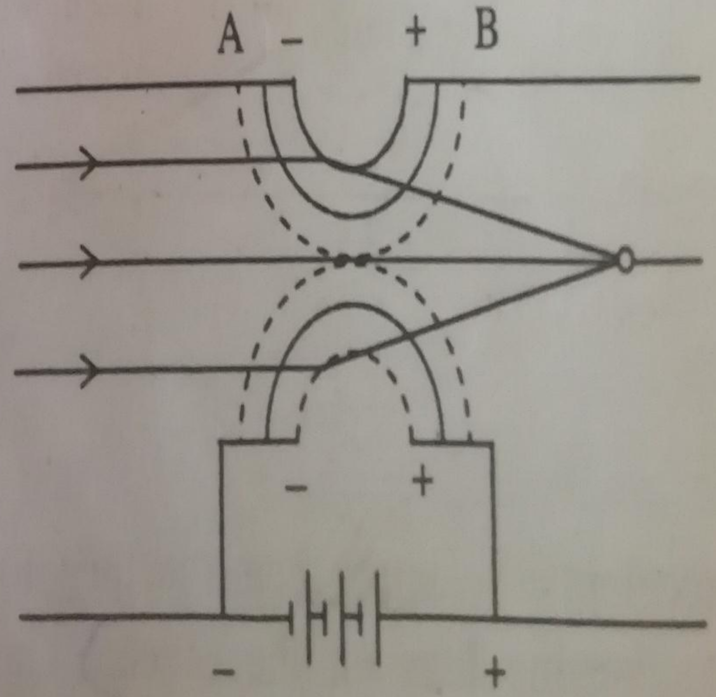


Fig. 2.6

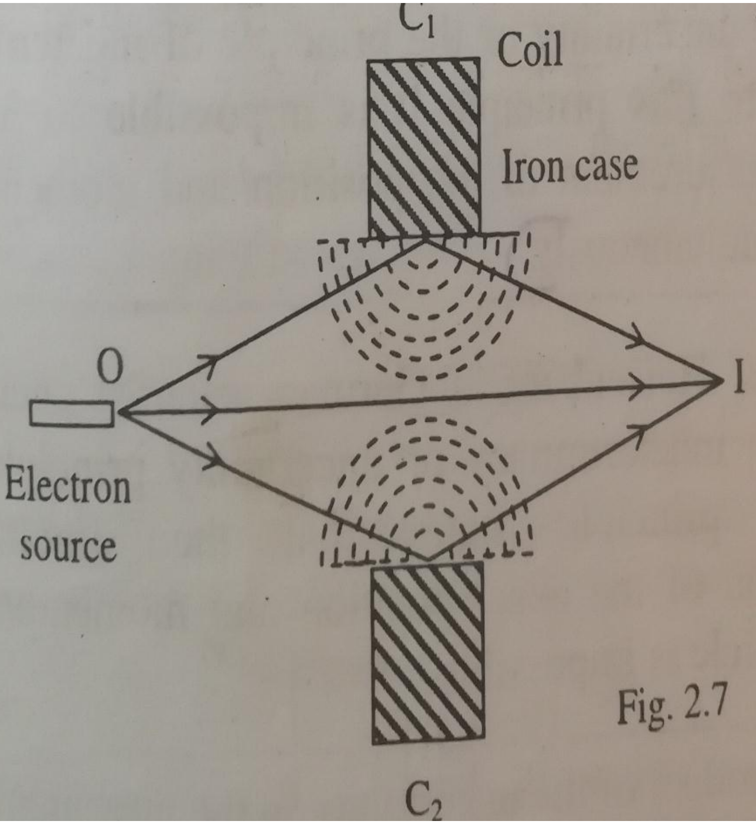


Fig. 2.7

The Heisenberg Uncertainty Principle

- Whenever a measurement is made there is always some uncertainty
- Quantum mechanics limits the accuracy of certain measurements because of wave – particle duality and the resulting interaction between the target and the detecting instrument

The Heisenberg Uncertainty Principle

The **Heisenberg uncertainty principle** states that it is impossible to know both the momentum and the position of a particle at the same time.

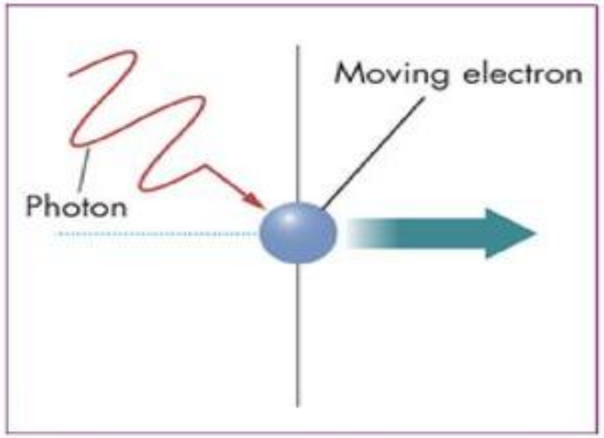
- This limitation is critical when dealing with small particles such as electrons.
- But it does not matter for ordinary-sized objects such as cars or airplanes.

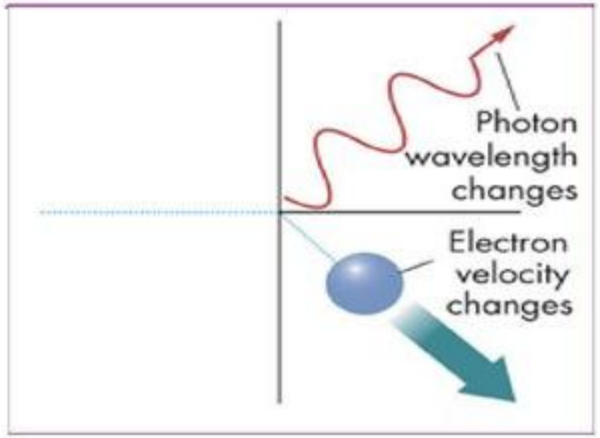
The Heisenberg Uncertainty Principle

- To locate an electron, you might strike it with a photon.
- The electron has such a small mass that striking it with a photon affects its motion in a way that cannot be predicted accurately.
- The very act of measuring the position of the electron changes its momentum, making its momentum uncertain.

The Heisenberg Uncertainty Principle

Before collision: A photon strikes an electron during an attempt to observe the electron's position.

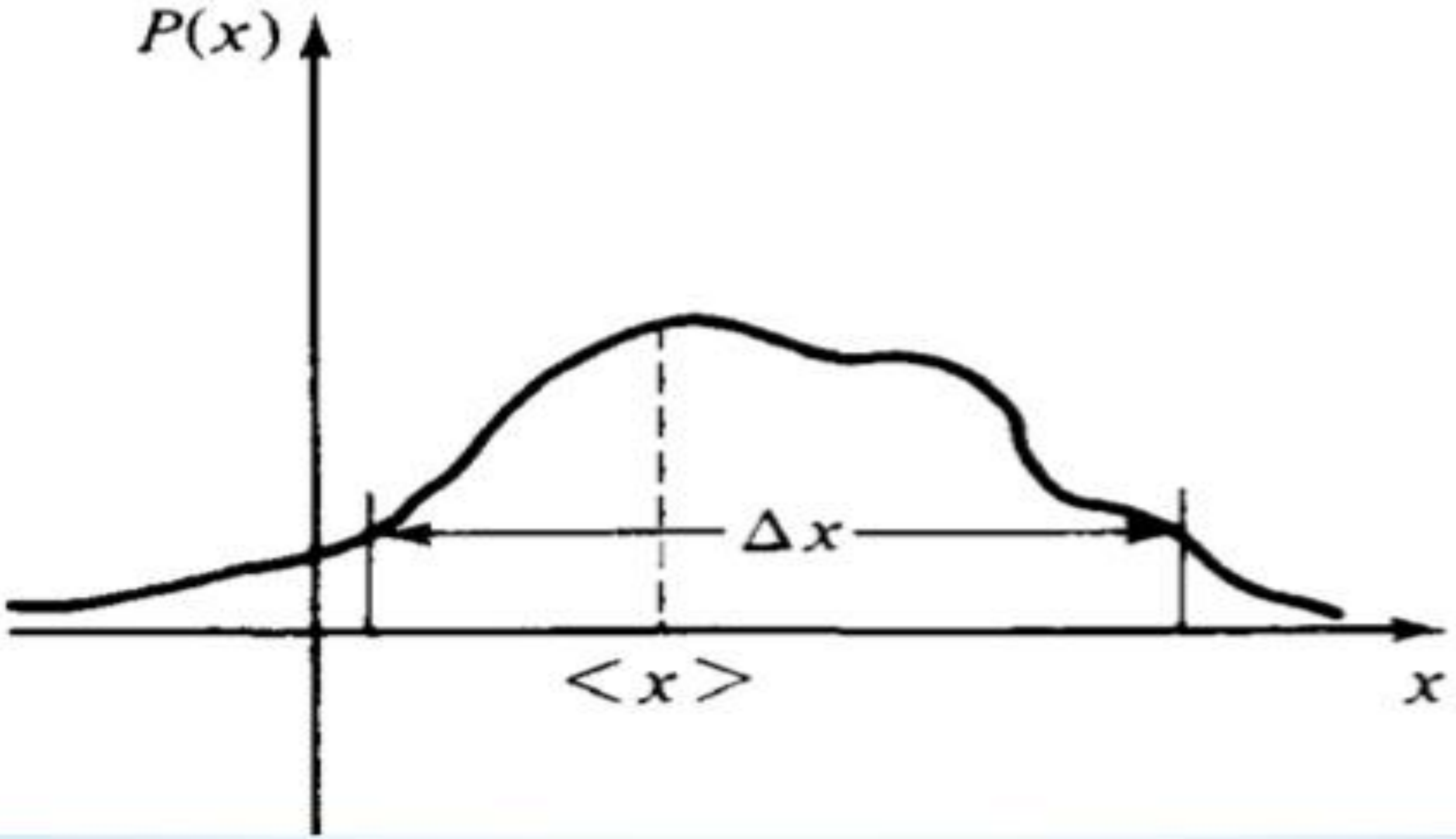




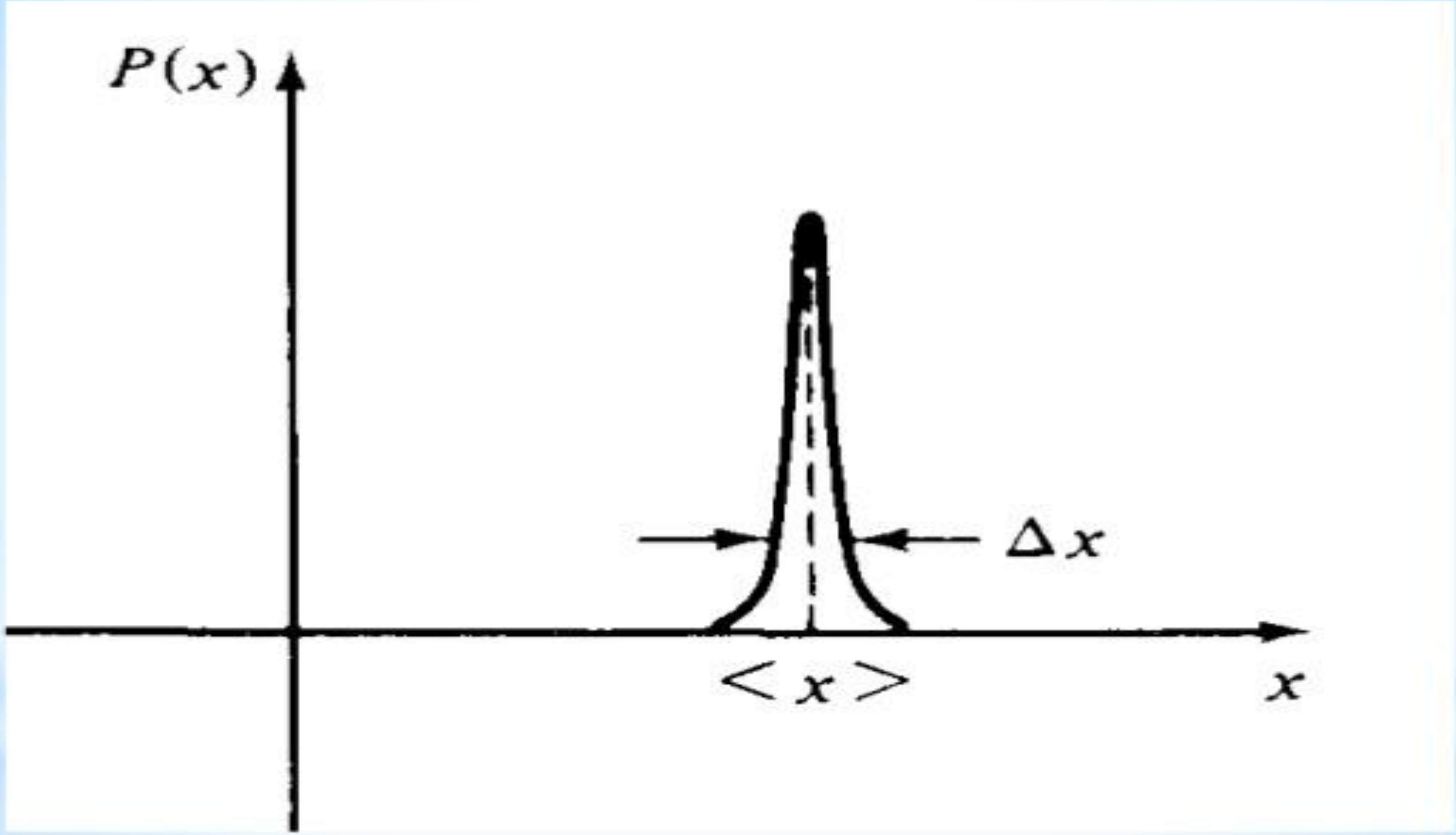
- **After collision:** The impact changes the electron's momentum, making it uncertain.

The Heisenberg Uncertainty Principle

- If we want accuracy in position, we must use short wavelength photons because the best resolution we can get is about the wavelength of the radiation used. Short wavelength radiation implies high frequency, high energy photons. When these collide with the electrons, they transfer more momentum to the target. If we use longer wavelength, i.e less energetic photons, we compromise resolution and position.



Large uncertainty in x**:** $(\Delta x)^2 = \langle x^2 \rangle - \langle x \rangle^2$



Small uncertainty in x.

Heisenberg Uncertainty Principle

It states that only one of the "position" or "momentum" can be measured accurately at a single moment within the instrumental limit.

or

It is impossible to measure both the position and momentum simultaneously with unlimited accuracy.

$\Delta x \rightarrow$ uncertainty in position

$\Delta p_x \rightarrow$ uncertainty in momentum

then $$\Delta x \Delta p_x \geq \frac{\hbar}{2} \qquad \therefore \hbar = \frac{h}{2\pi}$$

The product of Δx & Δp_x of an object is greater than or equal to $\frac{\hbar}{2}$

If Δx is measured accurately i.e. $\Delta x \to 0 \quad \Rightarrow \Delta p_x \to \infty$

The principle applies to all canonically conjugate pairs of quantities in which measurement of one quantity affects the capacity to measure the other.

Like, energy E and time t.

$$\Delta E \Delta t \geq \frac{\hbar}{2}$$

and angular momentum L and angular position θ

$$\Delta L \Delta \theta \geq \frac{\hbar}{2}$$

HEISENBERG UNCERTAINTY PRINCIPLE

$$\boxed{\begin{aligned}\Delta x \Delta p_x &\geq \hbar / 2 \\ \Delta y \Delta p_y &\geq \hbar / 2 \\ \Delta z \Delta p_z &\geq \hbar / 2\end{aligned}}$$

<u>HEISENBERG UNCERTAINTY PRINCIPLE</u>.

We cannot have simultaneous knowledge
of 'conjugate' variables such as position and momenta.

Note, however, $\boxed{\Delta x \Delta p_y \geq 0}$ etc

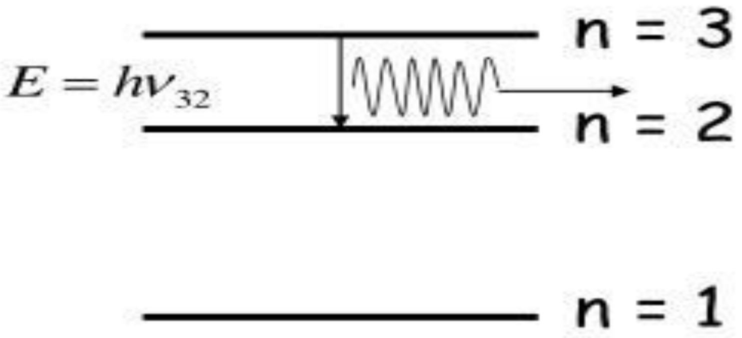
Arbitrary precision is possible in principle for
position in one direction and momentum in another

HEISENBERG UNCERTAINTY PRINCIPLE

There is also an energy-time uncertainty relation

$$\boxed{\Delta E \Delta t \geq \hbar / 2}$$

Transitions between energy levels of atoms are not perfectly sharp in frequency.



An electron in n = 3 will spontaneously decay to a lower level after a lifetime of order $\sim 10^{-8}\,\mathrm{s}$

There is a corresponding 'spread' in the emitted frequency