Chaudhary Mahadeo Prasad College

(A CONSTITUENT PG COLLEGE OF UNIVERSITY OF ALLAHABD)

E-Learning Module

Subject: Physics

(Study material for Under Graduate students)

B. Sc. III

Paper: First

Quantum Mechanics

NEED OF QUANTUM MECHANICS

(Wave Particle duality, de Broglie Hypothesis, Heisenberg Uncertainty Principle)

Prepared by

Dr. Rakesh Kumar

DEPARTMENT OF PHYSICS

Recommended Books

(i) Quantum Mechanics : L I Schiff

(ii) Quantum Mechanics: B K Agarwal

(iii) Introduction to Quantum Mechanics: D J Griffiths

(iv) Quantum Mechanics concept and Application: N Zettili

(v) Quantum Mechanics: R K Srivastava

(vi) Modern Quantum Mechanics : J J Sakurai

(vii) Quantum Mechanics: S L Kakani and H M Chandaliya

(viii) Quantum Mechanics: Richard L Liboff

(ix) Quantum Mechanics: E Merzbacher

Paper – I
QUANTUM MECHANICS SYLLABUS

- **Need of Quantum Mechanics, Schrodinger Equation and interpretation of wave function.**
- **Observables and Operators, Hermitian operator, Parity operator, Commutation relations, Eigen values and eigen functions, orthonormality and completeness, Dirac Delta function.**
- **Measurement in Quantum Mechanics, Non-Commutability, uncertainty, Expectation values,**
- **Ehrenfest's Theorem.**
- **Separation of variables in Time-Dependent Schrodinger Equation. Density of states, One dimensional Potential Barrier problems, Tunneling through square well potential.**
- **One – dimensional Harmonic Oscillator, Hermite Polynomials, Zero-point energy, Correspondence with Classical theory.**
- **Angular Momentum, Commutation Relations. Eigen Values and Eigen functions of L2 , LZ and ladder (L+, L_) operators.**
- **Spherically symmetric potentials, Complete solution of the Hydrogen – Atom Problem, Hydrogen**
- **Spectrum.**
- **Elementary concept of spin, Pauli Matrices and spin wave functions. Total angular momentum.**
- **Time-independent, non-degenerate, first – order Perturbation Theory, Spin – Orbit coupling.**
- **Ground and excited states of Helium atom and exchange degeneracy.**
- **Qualitative and Elementary Idea about Lamb Shift.**
- **Identical Particles, Symmetric and Antisymmetric wave functions, Pauli's Exclusion Principle.**

Inadequacy of Classical Mechanics & Origin of Quantum Mechanics

Before 1900 most of phenomenon could be explained on the basis of Classical Physics which is based on Newton's three laws of motion:- (i) Law of inertia (ii) Law of force and (iii) Law of action and reaction. The essence of classical mechanics is given in Newton's laws

$$m\frac{d^2\vec{r}}{dt^2} = F \quad .$$

For a given force if the initial position and the velocity of the particle is known all physical quantities such as position, momentum, angular momentum, energy etc. at all subsequent times can be calculated. Other formulations provide same information as obtained from Newton's Formulation.

Equations based on these laws are simplest and explained satisfactorily the motions of mechanical objects which are either directly observable or capable to observation with the help of simple instruments. Thus classical mechanics explained successfully the motion of celestial bodies and macroscopic as well as microscopic terrestrial bodies moving with no relativistic spread ($v << c$).

With the discovery of electron by J J Thomson (1897) exploration of atomic or microscopic systems were started. But it soon became clear that the classical concepts cannot be applied directly to the motion of electrons in an atom which are not observable with the help of instruments. Thus classical concepts do not hold in the region of atomic dimension.

Classical Mechanics does not explain the following:

(i) Spectral distribution of heat radiations from black bodies

(ii) Stability of atoms Specific heat at low temperature

(iii) Photoelectric effect

(iv) Compton scattering

(v) Optical line spectra

(vi) Specific heat of solids at low temperature

These are the failures of Classical mechanics. Failure of Classical mechanics led to the need of Quantum mechanics.

This inadequacy of classical mechanics led Max Planck in 1900 to introduce the new concept that the emission or observation of e. m. radiation takes as discrete quanta, each of which contain an amount of energy $E = h\upsilon$ where υ is the frequency of radiation, h is Planck's constant. This concept led to new mechanics which is known as *quantum mechanics*.

Planck was able to explain the black body spectrum in terms of the new quantum concepts. Einstein, 1905, used this concept to explain the photoelectric effect by assuming that energy of light quanta photon is transferred to a single electron within a metal. Thus a dual character of e. m. radiation that it behaves as waves as well as particle became established.

Planck's hypothesis explained the spectral distribution of black body, photoelectric effect, Compton Effect etc. called old quantum theory. The new theory of quantum mechanics is based on two principles: Heisenberg Uncertainty Principle and Bohr's correspondence Principle. This type of mechanics is called matrix mechanics. Schrodinger developed quantum mechanics called wave mechanics. It could not explain complex atomic systems like Brehmstrlung, Cherenkov radiation etc. Further Klien Gordon and Dirac introduce new concepts based on relativistic theory called relativistic quantum mechanics.

Classical Mechanics vs Quantum Mechanics

Classical Mechanics	Quantum Mechanics
Applied to Macroscopic bodies	Applied to Microscopic bodies
Continuous e.g. Motion of snake	Discrete e.g. Motion of Frog; quantum jump
Like Integration	Like Differentiation

Black Body Radiation

The spectrum of radiation is continuous with a maximum at a wavelength, which is characteristic of the temperature of the body, decreases with an increase in temperature as shown in Fig.1. The Rayleigh-Jeans law agrees with the experimental result at low frequencies or high wavelengths but predicts a monotonic increase of energy density with an increase in frequency, leading to an ultraviolet catastrophe. The Wien law agrees with experiments only at high frequencies. Thus two laws only give two sides of the experimental curve.

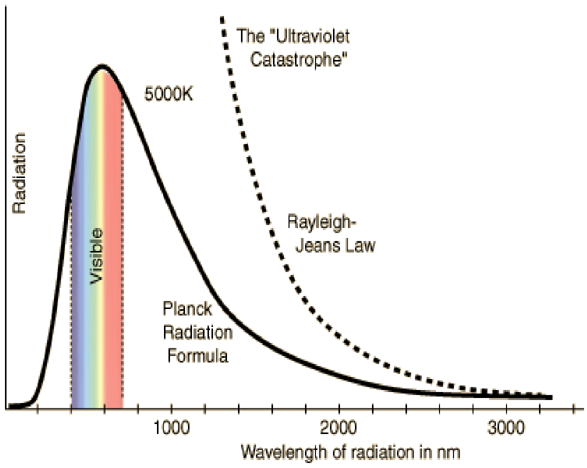


Fig.1

- Classical physics would predict that even relatively cool objects should radiate in the UV and visible regions. In fact, classical physics predicts that there would be no darkness!. The average energy per "mode" or "quantum" is the energy of the quantum times the probability that it will be occupied

Planck's Concept

$$\langle E \rangle = \frac{h\nu}{e^{h\nu/kT} - 1}$$

Planck won the Nobel Prize in Physics in 1918. **The recognition that energy changes in discreet quanta at the atomic level marked the beginning of quantum mechanics**.

Einstein Photoelectric effect

Einstein (1905) successfully resolved this paradox by employing Planck's idea of quantization of energy and proposed that the incident light consisted of individual quanta, called photons that interacted with the electrons in the metal like discrete particles, rather than as continuous waves emits photoelectrons,

$$h\nu = KE + W$$

Where ν is frequency of radiation, K.E. is kinetic energy of emitted electron, W is work potential (function) of the metal

$$W = h\nu_0 \ (\nu_0 \text{ is threshold frequency})$$

$$KE = h\nu - h\nu_0$$

$$KE = h(\nu - \nu_0)$$

Though most commonly observed phenomena with light like interference, diffraction, polarization etc. can be explained by waves. But the photoelectric effect suggested a **particle nature for light**.

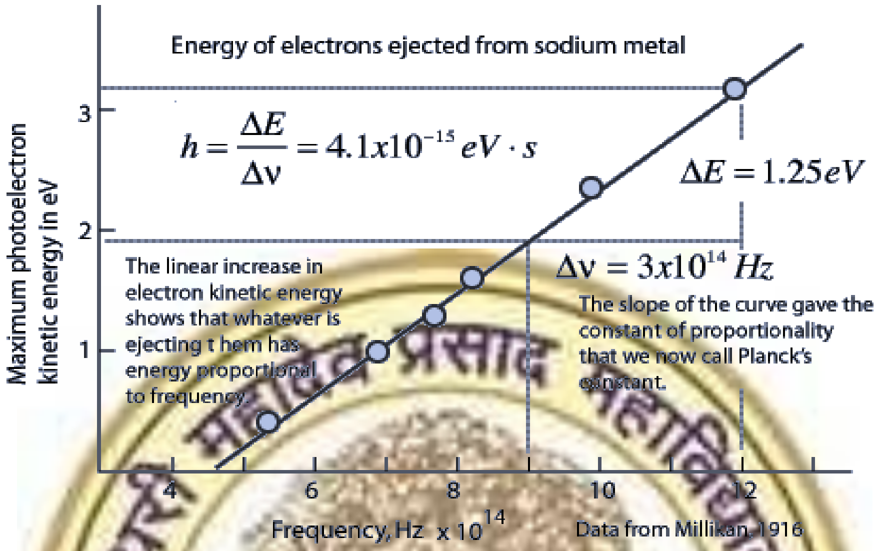


Fig.2

Wave Particle Duality

- In certain events light shows a wave like character while in others it shows particle like (Principle of complimentarity).
- Wave theory of light successfully explain the interference, diffraction, polarization etc. but this theory does not explain the phenomena like photoelectric effect, Compton effect, Zeeman effect etc. These phenomena are explained on the basis of Planck's quantum theory. Thus light confirms the dual nature.
- Most commonly observed phenomena with light like interference, diffraction, polarization etc. can be explained by waves. But the photoelectric effect and the Compton scattering suggested a particle nature for light. Then electrons were found to exhibit dual natures (particle and wave).

de Broglie Hypothesis

In 1924, de Broglie suggested that "All material particles in motion possess a wave character", such wave are called Matter waves or de Broglie waves.

de Broglie Wavelength: According to Planck's hypothesis, $E = h\nu$ and also according to Einstein theory $E = mc^2$

from the above two equations, we get

$$h\nu = mc^2$$

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

This gives de Broglie wavelength $$p = mc = \frac{h}{\lambda} \text{ or } \lambda = \frac{h}{p}$$

where p is momentum of photon.

If a particle of mass m moving with velocity v its de Broglie wavelength is

$$\lambda = \frac{h}{m\,v}\ \mathring{A}$$

de Broglie wavelength for different charged particle

- If a charge particle q is accelerated through a potential difference V, then its kinetic energy be qV. If this charge particle of mass m moving with velocity υ after applying potential difference V the its kinetic energy also be $\frac{1}{2}m\upsilon^2$
- Both must be equal

$$\frac{1}{2}m\,\upsilon^2 = qV$$

$$\upsilon = \sqrt{\frac{2qV}{m}}$$

- de Broglie Wavelength $$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2mqV}}$$

which is required de Broglie wavelength for any charge particle q.

(i) For electron:

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2\,m\,q\,V}}$$

$$\lambda = \frac{h}{\sqrt{2\,m_e\,e\,V}} = \sqrt{\frac{150}{V}}\ \mathring{A}$$

(ii) For Proton:

$$\lambda = \frac{h}{\sqrt{2\ m_p\,p\,V}} = \frac{0.286}{\sqrt{V}}\ \mathring{A}$$

(iii) For α particle:

$$\lambda = \frac{0.101}{\sqrt{V}}\ \mathring{A}$$

de Broglie wavelength for uncharged(neutron) particle

- Kinetic energy of uncharged particle at room temperature T is $\frac{3}{2}k_BT$, where k_B is Boltzmann constant.
- Also Kinetic energy of uncharged particle moving with velocity υ is $\frac{1}{2}m\upsilon^2$

• Both must be equal

$$\frac{3}{2}k_BT = \frac{1}{2}m\upsilon^2$$

$$\upsilon = \sqrt{\frac{3k_BT}{m}}$$

• de Broglie Wavelength

$$\lambda = \frac{h}{\sqrt{3mk_BT}}\ \mathring{A}$$

• If a particle having energy E and momentum p then its Kinetic energy $E = \frac{p^2}{2m}$, it gives de Broglie wavelength

$$\lambda = \frac{h}{\sqrt{2mE}}\ \mathring{A}$$

Does de Broglie relation apply to all particles (Microscopic as well as Microscopic?)

Consider a pitched baseball of mass m = 0.15 kg is moving with velocity υ = 40 m/s then its de Broglie wavelength

$$\lambda = \frac{h}{mv} = \frac{6.626\times10^{-34}}{0.15kg\times40m/s} = 1.1\times0^{-36}\ m$$

which is much smaller than the atomic diameter 10^{-10} m as well as nuclear diameter 10^{-14} m. When an electron accelerated through potential 100 volts and its velocity $\upsilon = 5.9\times10^6$ m/s then its de Broglie wavelength

$$\lambda = \frac{h}{mv} = \frac{6.626\times10^{-34}}{9.31\times10^{31}kg\times5.9\times10^6m/s} = 1.2\times0^{-10}m = 0.12\ nm$$

This is on the order of atomic dimensions and is much shorter than the shortest visible light wavelength of 400 nm.

• The de Broglie wavelength λ for macroscopic particles are negligibly small and cannot observe our daily life.

• This effect is extremely important for microscopic particles, like electrons.

Quantization of angular momentum

Bohr makes assumption that the orbital angular momentum of the electron is quantized. Since v is perpendicular to r, the orbital angular momentum is just given by L = mvr. Bohr suggested that this is quantized, so that:

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

Bohr's suggestion that orbital angular momentum of electrons is quantized is equivalent to the requirement that an integer number of de Broglie wavelengths must fit into the electron orbit as shown in Fig.3:

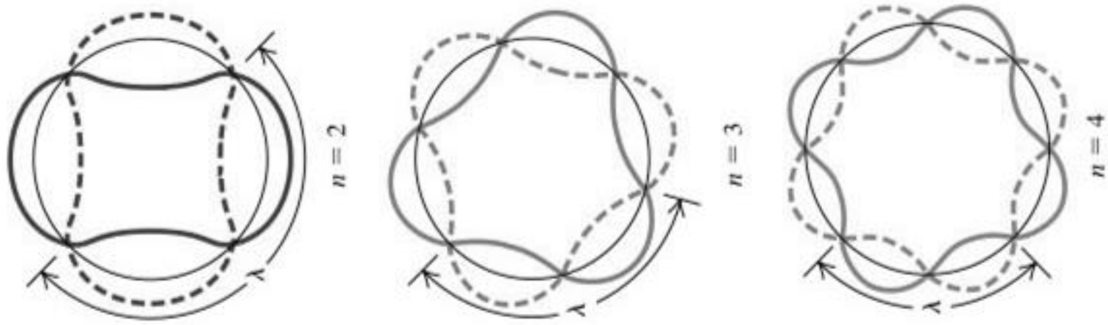


Fig.3

Electron standing waves and the Bohr Model

$n\lambda = 2\pi r_n$ (according to Bohr asumption)

$\Rightarrow$ $n\dfrac{h}{m_e v} = 2\pi r_n$ (de Broglie wavelength $\lambda = \dfrac{h}{m_e v}$)

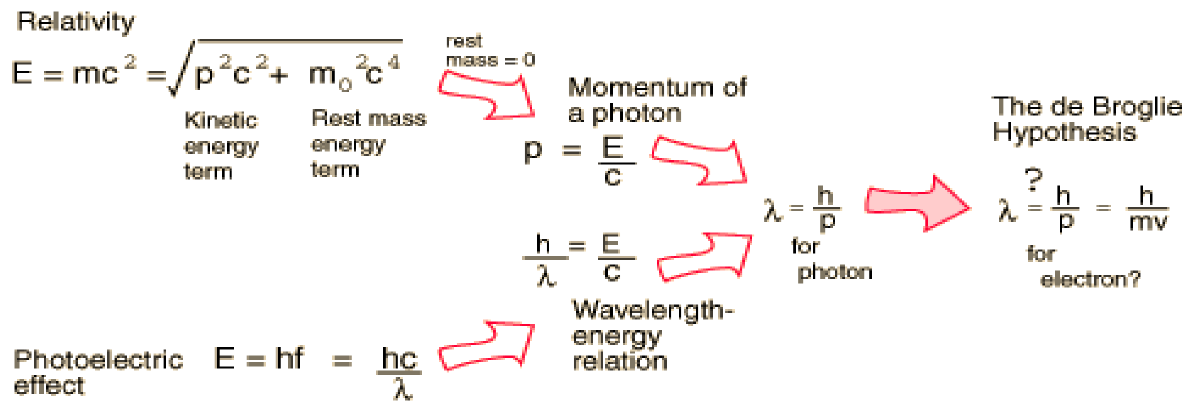
Since angular momentum of an electron $L_n = m_e v\, r_n$

$\Rightarrow$ $n\dfrac{h}{m_e v} = \dfrac{2\pi L_n}{m_e v}$

$\Rightarrow$ $L_n = \dfrac{nh}{2\pi} = n\hbar$

Wave Nature of Electron

Louis de Broglie had been impacted by relativity and the photoelectric effect, both of which had been introduced in his lifetime. The photoelectric effect pointed to the particle properties of light, which had been considered to be a wave phenomenon. He wondered if electrons and other "particles" might exhibit wave properties. The application of these two new ideas to light pointed to an interesting possibility:



Confirmation of the de Broglie hypothesis came in the Davisson- Germer experiment which showed interference/diffraction patterns – in agreement with de Broglie wavelength – for the scattering of electrons on nickel crystals.

Davisson Germer Experiment

Davisson and Germer proved the wave nature of electrons and verified the de Broglie equation. de Broglie argued the dual nature of matter back in 1924, but it was only later that Davisson and Germer experiment verified the results. The results established the first experimental proof of quantum mechanics. In this experiment, we will study the scattering of electrons by a Ni crystal.

The experimental arrangement (shown in Fig.4) of the Davisson Germer experiment is discussed below:

- An electron gun comprising a tungsten filament was coated with barium oxide and heated through a voltage power supply.
- While applying suitable potential difference from a high voltage power supply, the electron gun emits electrons which were again accelerated to a particular velocity.
- In a cylinder perforated with fine holes along its axis, these emitted electrons were made to pass through it, thus producing a fine collimated beam.
- The beam produced from the cylinder is again made to fall on the surface of a nickel crystal. Due to this, the electrons scatter in various directions.
- The beam of electrons produced has a certain amount of intensity which is measured by the electron detector and after it is connected to a sensitive galvanometer (to record the current), it is then moved on a circular scale.
- By moving the detector on the circular scale at different positions that is changing the θ (angle between the incident and the scattered electron beams), the intensity of the scattered electron beam is measured for different values of angle of scattering.

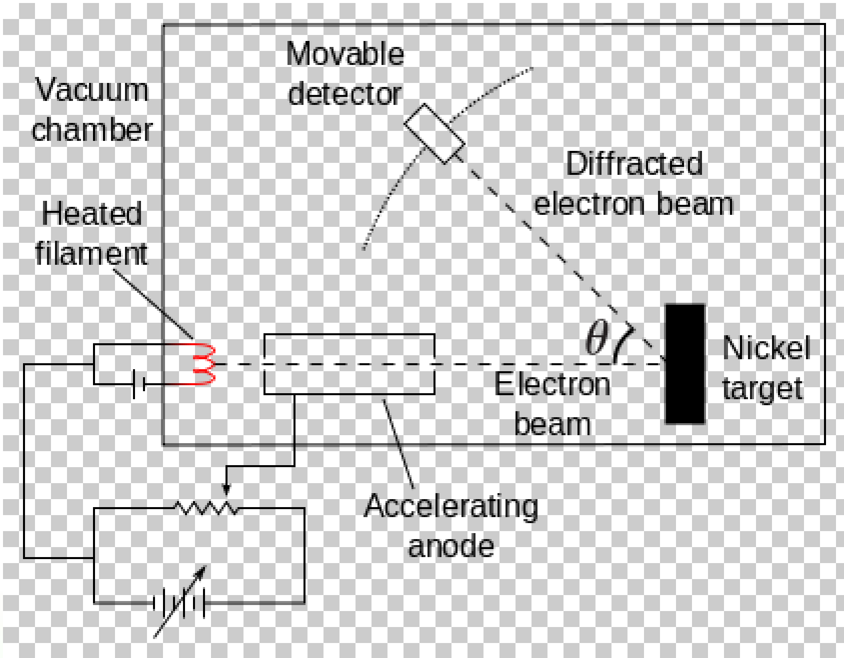


Fig.4

Observations of Davisson Germer experiment:

From the above experiment we can derive the following observations:

- We obtained the variation of the intensity (I) of the scattered electrons by changing the angle of scattering, θ.
- By changing the accelerating potential difference, the accelerated voltage was varied from 44V to 60 V.
- With the intensity (I) of the scattered electron for an accelerating voltage of 54V at a scattering angle θ = 50°, we could see a strong peak in the intensity (Fig.5).

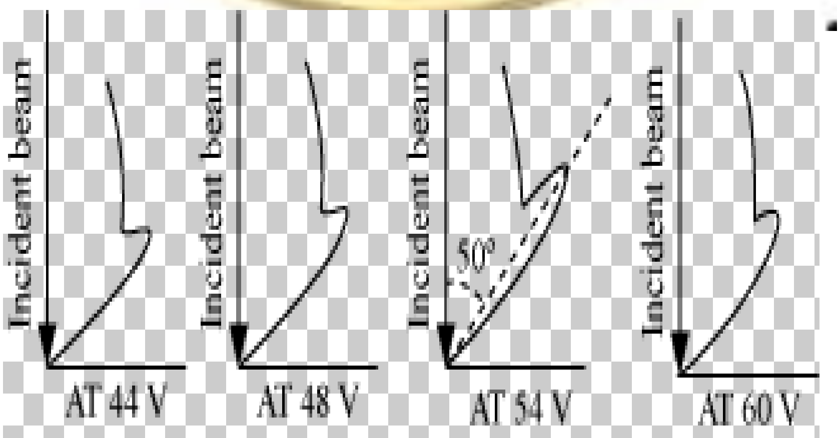


Fig.5

- This peak was the result of constructive interference of the electrons scattered from different layers of the regularly spaced atoms of the crystals.

With the help of electron diffraction $2d \sin\theta = n\lambda$;

For $d = 2.15$ and $\theta = 50^{o}$; the wavelength of matter waves was calculated to be 0.165 nm.

Co-relating Davisson Germer experiment and de Broglie relation: According to de Broglie,

For $V = 54$ volt; $\lambda = 0.167$nm

Thus, Davisson Germer experiment confirms the wave nature of electrons and the de Broglie relation.

Problems:

1. A particle of rest mass m_0 has kinetic energy K. Show that its de Broglie wavelength is given by $\lambda = \dfrac{hc}{\sqrt{K(K+2m_0c^2)}}$.
2. Show that the de Broglie wavelength for a material particle of rest mass m_0 and charge q accelerated from rest trough potential difference V volts relativistically is given by, $\lambda = \dfrac{h}{\sqrt{2m_0qV(1+\frac{qV}{2m_0c^2})}}$.
3. Calculate the de Broglie wavelength corresponding to the most probable velocity of thermal neutrons at 300K. Given mass of neutron $m = 1.676\times10^{-27}$kg.
4. A proton and an electron have equal K. E. compare their de Broglie Wavelength.
5. Calculate the de Broglie wavelength of a particle having energy 10MeV.

Heisenberg Uncertainty Principle

This principle is the direct consequence of the dual nature of light/matter. According to classical mechanics a moving particle has a definite momentum (velocity) and a definite position in space and it is possible to determine both its position and momentum (velocity).

In Quantum mechanics a particle is described by a wave. A wave packet is formed by adding many waves of different amplitudes and with the wave numbers spanning a range of Δk (or equivalently, $\Delta\lambda$). A particle is represented by a wave packet. Experiment confirmed that particles are wave in nature at the quantum scale h (matter wave) we now have to describe particles in term of waves (relevant only at the quantum scale). Since a real particle is localised in space (not extending over an infinite extent in space), the wave representation of a particle has to be in the form of wave packet (Fig.6).

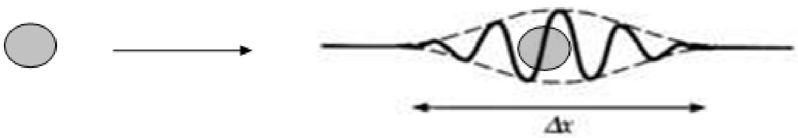


Fig.6

Due to its nature, a wave packet must obey the uncertainty relationships for classical waves (which are derived mathematically with some approximations)

$$\Delta\lambda\Delta x \geq \lambda^2 \equiv \Delta k\Delta x \geq 2\pi \qquad \text{and} \qquad \Delta t\Delta\nu \geq 1$$

However a more rigorous mathematical treatment (without the approximation) gives the exact relations

$$\Delta\lambda\Delta x \geq \frac{\lambda^2}{4\pi} \equiv \Delta k\Delta x \geq 1/2 \qquad \Delta\nu\Delta t \geq \frac{1}{4\pi}.$$

To describe a particle with wave packet that is localised over a small region Δx requires a large range of wave number; that is, Δk is large. Conversely, a small range of wave number cannot produce a wave packet localised within a small distance (Fig.7).

- A narrow wave packet (small Δx) corresponds to a large spread of wavelengths (large Δk).
- A wide wave packet (large Δk) corresponds to a small spread of wavelengths (small Δk).

Fig.7

- Matter wave representing a particle must also obey similar wave uncertainty relation. For matter waves, for which their momentum and wavelength are related by $p = h/\lambda$, the uncertainty relationship of the classical wave $\Delta\lambda\Delta x \geq \frac{\lambda^2}{4\pi} \equiv \Delta k\Delta x \geq 1/2$ is translated into $\Delta p_x \Delta x \geq \frac{\hbar}{2}$ where $\hbar = h/2\pi$

Time-energy uncertainty

- Just as $\Delta p_x \Delta x \geq \frac{\hbar}{2}$ implies position-momentum uncertainty relation, the classical wave uncertainty relation $\Delta \nu \Delta t \geq \frac{1}{4\pi}$ also implies a corresponding relation between time and energy $\Delta E \Delta t \geq \frac{\hbar}{2}$
- This uncertainty relation can be easily obtained:

$$h\Delta \nu \Delta t \geq \frac{h}{4\pi} = \frac{\hbar}{2};$$

$$\because E = h\nu, \Delta E = h\Delta \nu \Rightarrow \Delta E \Delta t = h\Delta \nu \Delta t = \frac{\hbar}{2}$$

Thus, Heisenberg uncertainty relation $\Delta p_x \Delta x \geq \frac{\hbar}{2}$ and $\Delta E \Delta t \geq \frac{\hbar}{2}$ shows that the product of the uncertainty in momentum (energy) and in position (time) is at least as large as Planck's constant.

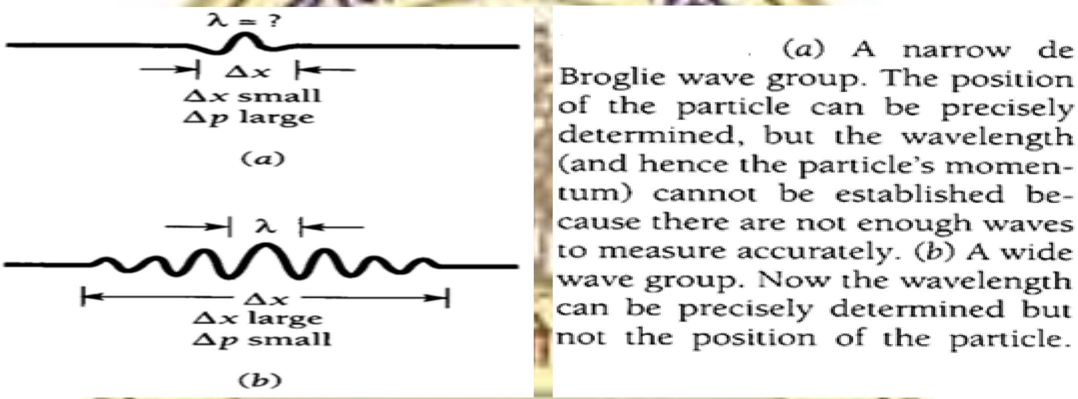


Fig.8

What $\Delta p_x \Delta x \geq \frac{\hbar}{2}$ **means** (Fig.8, 9):

- It sets the intrinsic lowest possible limits on the uncertainties in knowing the values of p_x and x, no matter how good an experiments is made
- ***It is impossible to specify simultaneously and with infinite precision the linear momentum and the corresponding position of a particle***
- It is impossible for the product $\Delta x \Delta p_x$ to be less than $h/4\pi$

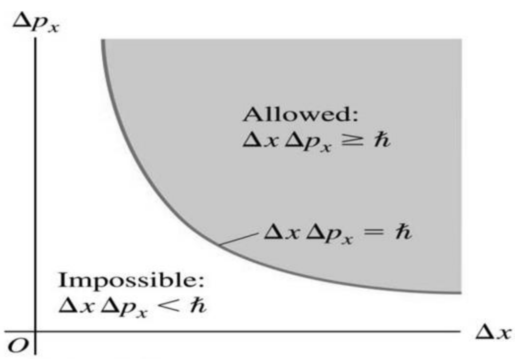


Fig.9

What $\Delta E \Delta t \geq \frac{\hbar}{2}$ **means** (Fig.10):

- Uncertainty principle for energy.
- The energy of a system also has inherent uncertainty, Δ*E*
- Δ*E is* dependent on the *time interval* Δ*t* during which the system remains in the given states.
- If a system is known to exist in a state of energy *E* over a limited period Δ*t*, then this energy is uncertain by at least an amount *h*/(4πΔ*t*). This corresponds to the 'spread' in energy of that state

- Therefore, the energy of an object or system can be measured with infinite precision (Δ*E*=0) only if the object of system exists for an infinite time (Δ*t*→∞)

- A system that remains in a metastable state for a very long time (large Δ*t*) can have a very well-defined energy (small Δ*E*), but if remain in a state for only a short time (small Δ*t*), the uncertainty in energy must be correspondingly greater (large Δ*E*).

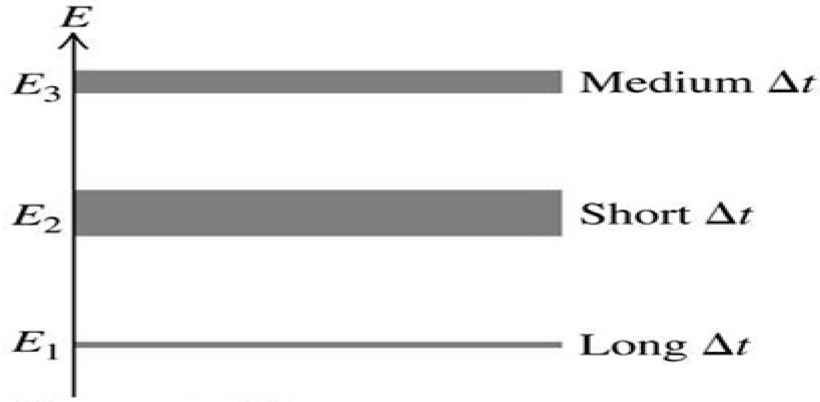


Fig.10

Note:

- **The Uncertainty relation is universal and holds for all the canonically conjugate physical quantities like position-momentum, energy-time, angular momentum-angle etc. whose product has dimensions of action.**
- **According to Heisenberg Principle, "*It is impossible to measure the position (time) of a particle along a particular direction and also its momentum (energy) in the same direction with unlimited accuracy*".**

Validity of Heisenberg Uncertainty Principle using gamma ray microscope

The absolute limit to the accuracy Δx with which position can be determined by the microscope is given by resolving power of the microscope

$$\Delta x = \frac{\lambda}{2\sin\theta} \quad (1)$$

Where Δx represents the distance between two points which resolved by Microscope and θ is the angular aperture of the microscope. **To minimize this uncertainty we must use gamma rays**, **smaller the wavelength smaller the uncertainty.**

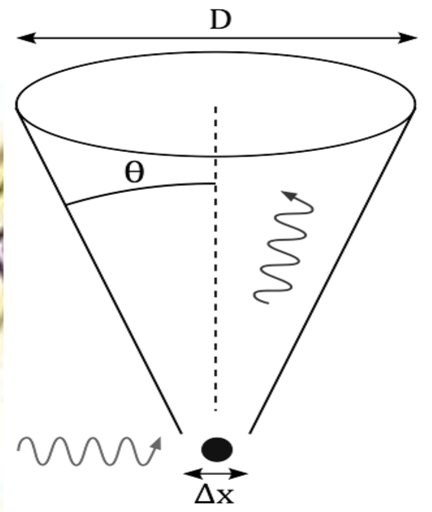


Fig.11

- One of the incident photon strikes the electron it scatters into the microscope. The scattered photon can travel anywhere in the cone of illumination of the objective. This involves Compton Effect.

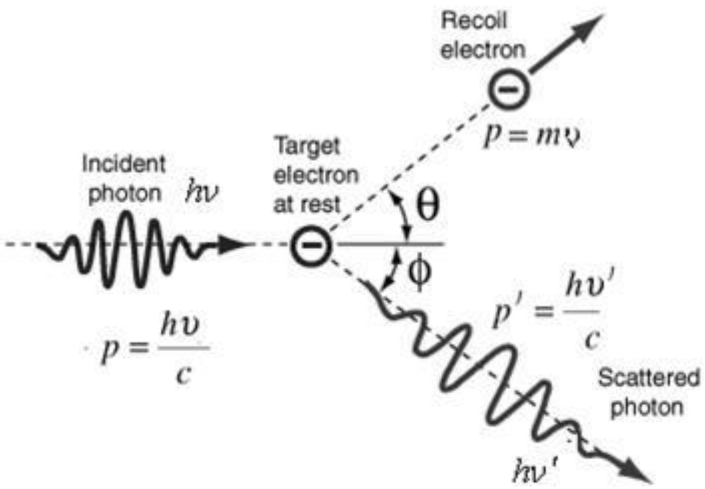


Fig.12

- Let a photon momentum $\frac{h\upsilon}{c}$ strikes an electron initially at rest, so that its initial momentum is zero. The striking photon transfers momentum mv to the electron and scatters into microscope.

- According to principle of conservation the momentum, along X-axis be

$$\frac{h\upsilon}{c}=\frac{h\upsilon'}{c}\cos\phi+mv\cos\theta$$

- The momentum along X axis transferred by the photon to an electron is given by

$$mv\cos\theta=\frac{h\upsilon}{c}-\frac{h\upsilon'}{c}\cos\phi$$
$$=\frac{h}{c}(\upsilon-\upsilon'\cos\phi)$$

- The limit of angle ϕ within the microscope are from $90^\circ-\theta$ to $90^\circ+\theta$ and so the spread in the x component of momentum will be given by

$$\frac{h}{c}(\upsilon-\upsilon'\cos(90^\circ-\theta)\le p_x\le\frac{h}{c}(\upsilon-\upsilon'\cos(90^\circ+\theta)$$

- Therefore the uncertainty in momentum is given by

$$\Delta p_x=\frac{h}{c}(\upsilon+\upsilon'\sin\theta)-\frac{h}{c}(\upsilon+\upsilon'\sin\theta) \qquad (2)$$
$$=2\frac{h}{c}\upsilon'\sin\theta=2\frac{h}{\lambda}\sin\theta$$

- Multiplying Eq.(1) and (2), we get

$$\Delta x\Delta p_x=h$$

- The momentum of the electron and the uncertainty in its position along X axis is of the order of Planck's constant h which is greater than $\frac{1}{2}\hbar$ in this case, we get

$$\Delta x\Delta p_x\ge\frac{1}{2}\hbar$$

Application of Heisenberg Uncertainty Principle

1. **The non-existence of the electron in the nucleus:**

Radius of nucleus of any atom $\cong 10^{-14}$m

If electron is confined with nucleus, the nucleus in its position must not be greater than $\cong 10^{-14}$m

Since

$$\Delta x\Delta p_x\ge\frac{1}{2}\hbar$$

$$\Delta p_x=\frac{1}{2\Delta x}\hbar=10^{-21}\ \text{Kg m/sec}$$

The momentum of the electron must be at least comparable with its magnitude

$$p_x=10^{-21}\ \text{Kg m/sec}$$

Thus K.E. of the electron of mass m is

$$T_x=\frac{(p_x)^2}{2m}=97\text{MeV}$$

If electron exists inside the nucleus then K.E. must be of the order of 97MeV, but experimental observations shows that no electron in the atom possesses energy greater than 4 MeV. This clearly shows that **electrons do not exist inside the nucleus.**

2. Spectral line has finite width:

Uncertainty relation for energy and time is

$$\Delta E \Delta t \geq \frac{1}{2}\hbar$$

According to Plancks hypothesis $E = h\upsilon$

Then uncertainty relation becomes

$$h\Delta\upsilon\Delta t \geq \frac{1}{2}\hbar$$

This gives $\Delta\upsilon \approx \frac{1}{4\pi\Delta t}$

If Life time of ordinary atom is $\cong 10^{-8}$ sec

$$\Delta\upsilon \approx 10^{7}\text{Hz}$$

It means **spectral line has finite width**.