20.7 G.P. THOMSONS'S EXPERIMENT

The de Broglie hypothesis was further confirmed in 1927 by the experiments conducted independently by G.P.Thomson in England and by Kikuchi in Japan.

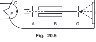

Fig. 20.5

Thomson's experimental arrangement is shown in Fig. 20.5. Electrons are produced from a heated filament F and accelerated through a high positive potential given to the anode A. The whole apparatus is kept highly evacuated. The electron beam passes through a fine hole in a metal block B and falls on a gold foil of thickness 0.1 μm. The electrons passing through the foil are received on a photographic plate P.

Metals are polycrystalline in which the grains are oriented completely at random. Therefore, some grains have always the right inclination θ towards the incident beam in order to produce a Bragg reflection. Owing to the random orientation, the reflections from a given set of lattice planes at the glancing angle occur in every azimuth about the incident beam. Consequently, the reflected beams form a cone of semi-vertical angles 2θ. Each set of lattice planes with its particular spacing d in the grain produces its own cone of diffracted rays. A concentric rings pattern is produced on the photographic plate when it intercepts the coaxial cones of diffracted rays.

The diffraction pattern produced by the electron beam was strikingly similar to the x-ray diffractions obtained from powder samples. Thus, the experiments of G.P. Thomson and Kikuchi provided irrefutable proof to the existence of de Broglie waves.

In 1937, C.J.Daavisson and G.P.Thomson were jointly awarded the Noble Prize in physics for their experimental discovery of electron diffraction.

In 1929, soon after the discovery of wave properties of electrons, the German physicist Otto Stern and his coworkers detected diffraction phenomena with neutral atomic and molecular beams.

20.8 VELOCITY OF DE BROGLIE WAVES

Any harmonic wave is characterized by a precise wavelength λ and constant amplitude. It is non-localized and has no beginning and end. It means that such a wave extends over a very large volume of space.

20.8.1 Phase Velocity

If we consider a harmonic wave, the wave has a single wavelength and a single frequency. The velocity of propagation of the wave is given by

$$\upsilon_p = \nu\lambda$$

Using, $\nu = \omega/2\pi$ and $\lambda = 2\pi/k$ into the above equation, we get

$$\upsilon_p = \frac{\omega}{2\pi}\cdot\frac{2\pi}{k} = \frac{\omega}{k} \tag{20.11}$$

υ_p is called the *phase velocity*. The velocity with which the plane of equal phase travels through a medium is known as the phase velocity. It thus represents the velocity of propagation of the wave front.

As $E = h\nu$ and $p = h/\lambda$, we get

$$\upsilon_p = \frac{E}{h}\cdot\frac{h}{p} = \frac{E}{p} \tag{20.12}$$

(*i*) When the atomic particle velocity is *non-relativistic*, the total energy $E = mc^2$ and momentum $p = m\upsilon$.

Therefore, the phase velocity of the de Broglie wave associated with the particle is

$$\upsilon_p = \frac{E}{p} = \frac{mc^2}{m\upsilon} = \frac{c^2}{\upsilon} \tag{20.13}$$

As $\upsilon < c$, the phase velocity of the de Broglie wave associated with the atomic particle is always greater than c.

(*ii*) When the atomic particle velocity is *relativistic*, the total energy $E = \sqrt{m_o^2c^4 + p^2c^2}$, where m_o is the rest mass of the particle.

Therefore, the phase velocity of the de Broglie wave associated with the particle is

$$\upsilon_p = \frac{E}{p} = \left[\frac{m_o^2c^4 + p^2c^2}{p^2}\right]^{1/2}$$

$$= c\left[\frac{m_o^2c^2}{p^2} + 1\right]^{1/2} = c\left[\frac{m_o^2c^2\lambda^2}{h^2} + 1\right]^{1/2} \tag{20.14}$$

As the term $\frac{m_o^2c^2\lambda^2}{h^2}$ is always a positive quantity, the phase velocity of the de Broglie wave associated with the atomic particle is always greater than c.

According to the theory of relativity, it is not possible that the velocity of the particle wave be greater than or equal to the velocity of light. Hence, a harmonic wave of wavelength λ cannot represent a moving atomic particle. Thus, ***de Broglie waves cannot be harmonic waves***.

20.9 WAVE PACKET – REPRESENTS A MICROPARTICLE

We have so far assumed that a particle may be represented by a monochromatic de Broglie wave. However, a wave spreads over a large region of space and cannot represent a highly localized particle. Schrödinger postulated that a **wave packet** rather than a single harmonic wave represents a particle. A wave packet consists of a group of harmonic waves. Each wave has slightly different wavelength. The superposition of a very large number of harmonic waves differing infinitesimally in frequency will produce a single wave packet (see Fig. 20.6 c). The waves interfere constructively over only a small region of space and cancel each other everywhere except in that small region. The position of the particle would then be approximately determined by the position of the wave packet.

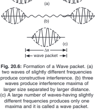

Fig. 20.6: Formation of a Wave packet. (a) two waves of slightly different frequencies produce constructive interference. (b) three waves produce interference maxima of larger size separated by larger distance. (c) A large number of waves-having slightly different frequencies produces only one maxima and it is called a wave packet.

The velocity with which the wave packet propagates is called the **group velocity** υ_g.

The individual waves forming the wave packet propagate at a velocity known as the **phase velocity** υ_p.

20.9.1 Group Velocity

When a number of plane waves of slightly different wavelengths travel in the same direction, they form wave groups or wave packets. The velocity with which the wave group advances in the medium is known as the *group velocity* υ_g. Each component wave has its own phase velocity, $\upsilon_p = \nu\lambda$. The wave packet has amplitude that is large in a small region and very small outside it. The amplitude of the wave packet varies with x and t. Such a variation of amplitude is called the *modulation* of the wave. The velocity of propagation of the modulation is known as the *group velocity*, υ_g.

Here, we should note that *wave packets are only theoretical artifices to aid our visualization of various phenomena in the micro-world*.

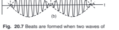

Fig. 20.7 Beats are formed when two waves of slightly different frequencies combine (a) the individual waves (b) the resultant wave.

Expression for the Group Velocity We derive now an expression for group velocity considering a group of waves consisting of two components of equal amplitude and slightly differing angular velocities ω_1 and ω_2.

Let the waves in Fig. 20.7 (a) be represented by the equations

$$y_1 = A\sin(\omega_1 t - k_1 x)$$

$$y_2 = A\sin(\omega_2 t - k_2 x)$$

The superposition of these two waves is given by

$$y_1 + y_2 = A\sin(\omega_1 t - k_1 x) + A\sin(\omega_2 t - k_2 x)$$

Using the trigonometric relation $\sin\alpha + \sin\beta = 2\sin\left(\frac{\alpha+\beta}{2}\right)\sin\left(\frac{\alpha-\beta}{2}\right)$, we write the above equation as

$$y_1 + y_2 = 2A\sin\left[\frac{(\omega_1+\omega_2)}{2}t - \frac{(k_1+k_2)}{2}x\right]\cos\left[\frac{(\omega_1-\omega_2)}{2}t - \frac{(k_1-k_2)}{2}x\right]$$

$$= 2A\sin(\omega t - kx)\cos\left(\frac{\Delta\omega t}{2} - \frac{\Delta kx}{2}\right) \quad (20.15)$$

where $\omega = (\omega_1 + \omega_2)/2$, $k = (k_1 + k_2)/2$, $\Delta\omega = \omega_1 - \omega_2$ and $\Delta k = k_1 - k_2$. Equ.(20.15) represents the resultant wave which is seen to have the following two parts.

(i) A wave of angular frequency ω and propagation constant k, moving with a velocity

$$\upsilon_p = \frac{\omega}{k} = \nu\lambda \text{ and}$$

(ii) A second wave of angular frequency $\Delta\omega/2$ and propagation constant $\Delta k/2$, moving with a velocity $\upsilon_g = \dfrac{\Delta\omega}{\Delta k}$.

When $\Delta\omega$ and Δk are very small, we can write the above equation as

$$\upsilon_g = \frac{d\omega}{dk} \quad (20.16)$$

or
$$\upsilon_g = \frac{2\pi\, d\nu}{2\pi\, d(1/\lambda)} = -\lambda^2 \frac{d\nu}{d\lambda}$$

20.9.2 Relation between Phase Velocity and Group Velocity

The velocity of the individual component wave of the wave packet is given by

$$\upsilon_p = \nu\lambda$$

Using, $\nu = \omega / 2\pi$ and $\lambda = 2\pi / k$ into the above equation, we get

$$\upsilon_p = \frac{\omega}{2\pi} \cdot \frac{2\pi}{k} = \frac{\omega}{k} \tag{20.17}$$

$$\therefore \quad \omega = k\upsilon_p$$

The group velocity is given by the relation (20.16) as

$$\upsilon_g = \frac{d\omega}{dk} = \frac{d}{dk}(k\upsilon_p) = \upsilon_p + k\frac{d\upsilon_p}{dk}$$

But
$$k = \frac{2\pi}{\lambda}.$$

Therefore,
$$dk = -\frac{2\pi}{\lambda^2} d\lambda$$

and
$$\frac{k}{dk} = -\frac{\lambda}{d\lambda}.$$

$$\therefore \quad \upsilon_g = \upsilon_p - \lambda \frac{d\upsilon_p}{d\lambda} \tag{20.18}$$

Group velocity will be the same as phase velocity if the entire constituent waves travel with the same velocity. It means that in a nondispersive medium, $\upsilon_g = \upsilon_p$. However, the waves of different wavelengths travel in a medium with different velocities. Therefore, the group velocity is in general less than the phase velocity.

20.9.3 The Velocity of a Particle Equals the Group Velocity of the Associated Matter Waves

A particle moving with a velocity υ is supposed to consist of a group of de Broglie waves. The group velocity of a wave packet is given by

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

which we can write as
$$\upsilon_g = \left(\frac{d\omega}{dE}\right)\left(\frac{dE}{dp}\right)\left(\frac{dp}{dk}\right) \tag{20.19}$$

As
$$E = h\nu = h \cdot \frac{\omega}{2\pi} = \frac{h}{2\pi} \cdot \omega = \hbar\omega, \quad \frac{d\omega}{dE} = \frac{1}{\hbar}$$

and
$$p = \frac{h}{\lambda} = h \cdot \frac{1}{\lambda} = h \cdot \frac{k}{2\pi} = \frac{h}{2\pi} \cdot k = \hbar k, \quad \frac{dp}{dk} = \hbar$$

$$\therefore \quad \upsilon_g = \left(\frac{d\omega}{dE}\right)\left(\frac{dE}{dp}\right)\left(\frac{dp}{dk}\right) = \frac{1}{\hbar}\left(\frac{dE}{dp}\right)\hbar = \left(\frac{dE}{dp}\right) \tag{20.20}$$

For a particle, $E = \frac{1}{2}m\upsilon^2 = \frac{1}{2}\frac{(m\upsilon)^2}{m} = \frac{p^2}{2m}$.

$$\therefore \qquad \upsilon_g = \frac{dE}{dp} = \frac{p}{m} = \upsilon. \tag{20.21}$$

Thus, the de Broglie wave group associated with an atomic particle travels with the same velocity as that of the particle itself.

20.9.4 Relation Between the Group Velocity and Particle Velocity (in a Non-dispersive Medium)

A particle moving with a velocity υ is supposed to consist of a group of de Broglie waves. For an atomic particle of rest mass m_o moving with a velocity υ, the total energy and momentum are given by

$$E = mc^2 = \frac{m_o c^2}{\sqrt{1-\upsilon^2/c^2}} \text{ and } p = m\upsilon = \frac{m_o\upsilon}{\sqrt{1-\upsilon^2/c^2}} \text{ respectively.}$$

The frequency of the associated de Broglie wave is

$$\nu = \frac{E}{h} = \frac{m_o c^2}{h\sqrt{1-\upsilon^2/c^2}} \text{ and } \omega = 2\pi\nu = \frac{2\pi\, m_o c^2}{h\sqrt{1-\upsilon^2/c^2}}.$$

Therefore,

$$d\omega = \frac{2\pi m_o}{h\left(1-\upsilon^2/c^2\right)^{3/2}}\upsilon\cdot d\upsilon. \tag{20.22}$$

The wavelength of the de Broglie wave is

$$\lambda = \frac{h}{p} = \frac{h\left(1-\upsilon^2/c^2\right)^{1/2}}{m_o\upsilon} \text{ and } k = \frac{2\pi}{\lambda} = \frac{2\pi\, m_o\upsilon}{h\left(1-\upsilon^2/c^2\right)^{1/2}}$$

$$\therefore \qquad dk = \frac{2\pi m_o}{h}\left[\left(1-\upsilon^2/c^2\right)^{-1/2} d\upsilon + \upsilon\cdot\frac{\upsilon}{c^2}\left(1-\upsilon^2/c^2\right)^{-3/2} d\upsilon\right]$$

or

$$dk = \frac{2\pi m_o d\upsilon}{h\left(1-\upsilon^2/c^2\right)^{3/2}} \tag{20.23}$$

Dividing eq. (20.22) by (20.23), we get

$$\upsilon_g = \frac{d\omega}{dk} = \upsilon \tag{20.24}$$

Thus, the de Broglie wave group associated with an atomic particle travels with the same velocity as that of the particle itself in a non-dispersive medium.

20.10 APPLICATIONS OF DE BROGLIE WAVES

We discuss here some of the applications of de Broglie waves.

1. Possible energy states of a microparticle trapped in a box

Let us consider a microparticle trapped in a one-dimensional box of length L. According to de Broglie hypothesis, the particle is associated with a wave having a wavelength λ. The particle cannot move beyond the walls of the box. Hence, the amplitude of the de Broglie wave drops to zero at the walls. It implies that the de Broglie wave of the particle forms a standing wave pattern with nodes at the walls. The formation of standing wave pattern requires that the distance L must be an integral multiple of half-wavelength. Thus,

Example 20.2. *An enclosure filled with helium is heated to 400K. A beam of He-atoms emerges out of the enclosure. Calculate the de Broglie wavelength corresponding to He atoms. Mass of He atom is 6.7×10⁻²⁷kg.*

Solution. De Broglie wavelength $\lambda = \dfrac{h}{\sqrt{2mkT}}$

$$= \frac{6.63\times10^{-34}\,Js}{\sqrt{2\times6.7\times10^{-27}\,kg\times1.376\times10^{-21}\,J/\deg\times400}}$$

$= \mathbf{0.769}$ **Å**

Example 20.3: *Find the de Broglie wavelength of*

(*i*) *an electron accelerated through a potential difference of 182 volts, and*

(*ii*) *a 1 kg object moving with a speed 1 m/s. Comparing the results explain why the wave nature of matter is not more apparent in daily observations.*

Solution:

(*i*) $$\lambda_e = \frac{h}{\sqrt{2emV}} = \frac{6.626\times10^{-34}\,J.s}{\sqrt{2\left(1.602\times10^{-19}\,C\right)\left(9.11\times10^{-31}\,kg\right)182V}}$$

$$= \frac{6.626\times10^{-34}\,J.s.}{7.29\times10^{-24}\,kg.m/s} = 0.91\times10^{-10}\frac{kg.m^2/s}{kg.m/s} = 9.1\times10^{-11}\,m = \mathbf{0.91\,Å}$$

(*ii*) $$\lambda_m = \frac{h}{M\upsilon} = \frac{6.626\times10^{-34}\,J.s}{1kg\times1m/s} = 6.6\times10^{-34}\frac{kg.m^2/s}{kg.m/s} = \mathbf{6.6\times10^{-34}\,m}.$$

It is seen from the above that the wavelength of the accelerated electron is about 10^5 times larger then its own size ($\approx10^{-15}$ m) and is therefore significant. On the other hand, the wavelength associated with the macroscopic object is negligibly small and is thus not apparent in its interactions with other objects.

20.11 HEISENBERG UNCERTAINTY PRINCIPLE

The wave nature of atomic particles leads to some inevitable consequences. Classically, the state of a particle can be defined by specifying its position and momentum at any given time *t*. If a body is moving along *x*-direction with a velocity υ, its position is given by $x = \upsilon\, t$ and its momentum by $p = m\upsilon$. From this,

$$x = \frac{p}{m}t \tag{20.28}$$

At each instant, the position and momentum can be measured to a very high accuracy. When an atomic particle is conceptualized as a de Broglie wave packet such a precision becomes restricted.

Schrödinger postulated that a moving microparticle is equivalent to a wave packet. A wave packet spreads over a region of space. Therefore, it is difficult to locate the exact position of the microparticle. Although the particle is somewhere within the wave packet, it is impossible to know where exactly the particle is at a given instant. If the linear spread of the wave packet is Δx, the particle would be located somewhere within the region Δx. The probability of finding the particle is a maximum at the centre of the wave packet and falls off to zero at its ends. Therefore, there is an **uncertainty** Δx in the position of the particle. As a result, the momentum of the particle at that instant cannot be determined precisely. It means that the location and momentum of a microparticle cannot be **simultaneously** determined with certainty. Any attempt to determine these variables will lead to uncertainties in each of the variables.

In 1927 Heisenberg showed that the product of uncertainty Δx in the x-coordinate of a quantum particle and the uncertainty Δp_x in the x-component of the momentum would always be of the order of Planck's constant h. Thus,

$$\Delta x \cdot \Delta p_x \approx h$$

or more precisely

$$\Delta x \cdot \Delta p_x \geq \frac{\hbar}{2} \qquad (20.29)$$

This is known as Heisenberg's uncertainty principle for position and momentum, which may be stated as follows:

"*It is not possible to know simultaneously and with exactness both the position and the momentum of a microparticle*".

The Uncertainty Principle implies a built-in, unavoidable *limit to the accuracy with which we can make measurements*. Classically, it is thought that the precision of any measurement was limited only by the accuracy of the instruments the experimenter used. Heisenberg showed that whatever may be the accuracy of the instruments used, quantum mechanics limits the precision when two properties are measured at the same time. These are *not just any* two properties but pairs of measurable quantities whose product has dimensions of energy × time. Such quantities are called *conjugate quantities* in quantum mechanics, and have a special relation to each other. Position–linear momentum, energy-time, time-frequency and angular momentum-angular displacement are conjugate pairs of variables.

The uncertainty principle asserts that it is physically impossible to know simultaneously the exact position ($\Delta x = 0$) and exact momentum ($\Delta p_x = 0$) of a micro-particle. According to it, the more precisely we know the position of the particle, the less precise is our information about its momentum. To localize a wave packet, we have to add more wavelengths to form the wave packet. More wavelengths mean larger $\Delta\lambda$ and more uncertainty in momentum (note that $\Delta p \propto \Delta\lambda$). Conversely, in order to have more precise value of momentum, the wave packet should contain less number of waves. Less number of waves produces a longer wave packet. Thus, the momentum of a particle cannot be precisely specified without our loss of knowledge of the position of the particle at that time. Similarly, a particle cannot be precisely localized in a particular direction without our loss of knowledge of momentum in that particular direction. We can at best specify that certain momentum of the particle is more probable than the other or that the particle is more likely to be here than there. We cannot use classical notions like coordinates and momentum to describe the motion of quantum particles. Thus, the uncertainty principle implies that we can never define the path of an atomic particle with the absolute precision indicated in classical mechanics. Therefore, concepts such as velocity, position, and acceleration are of limited use in quantum world.

Relations similar to (20.29) hold good for other components of position and linear momentum. Thus,

$$\Delta y \cdot \Delta p_y \geq \frac{\hbar}{2} \qquad (20.29a)$$

$$\Delta z \cdot \Delta p_z \geq \frac{\hbar}{2} \qquad (20.29b)$$

20.11.1 Energy - Momentum Uncertainty

The uncertainty relation for the simultaneous measurement of energy E and time t is expressed as

$$\Delta E \cdot \Delta t \geq \frac{\hbar}{2} \tag{20.30}$$

The physical significance of the energy-time uncertainty relation is different from that of the position –momentum uncertainty. If ΔE is the maximum uncertainty in the determination of the energy of a particle, then the minimum time interval for which the particle remains in that state is given by

$$\Delta t = \frac{\hbar / 2}{\Delta E}$$

And, if a particle remains in a particular energy state for a maximum time Δt, then the minimum uncertainty in the particle energy is given by

$$\Delta E = \frac{\hbar / 2}{\Delta t}$$

Derivation: We can obtain the result (20.30) as follows. Let us consider a microparticle of mass m moving with a velocity υ. Its kinetic energy will be

$$E = \frac{1}{2} m\upsilon^2$$

If the uncertainty in the energy is ΔE, then $\Delta E = \Delta\left[\frac{1}{2} m\upsilon^2\right] = m\upsilon\ \Delta\upsilon = \upsilon\ \Delta p$

As the velocity $\upsilon = \frac{\Delta x}{\Delta t}$, the uncertainty in energy may be written as $\Delta E = \frac{\Delta x}{\Delta t} \Delta p$

Thus, $\Delta E \cdot \Delta t = \Delta x \cdot \Delta p$

But $\Delta x \cdot \Delta p \geq \frac{\hbar}{2}$

Therefore, $\Delta E \cdot \Delta t \geq \frac{\hbar}{2}$

The above relations are to be supplemented by the following uncertainty relation

$$\Delta M_x \cdot \Delta \varphi_x \geq \frac{\hbar}{2} \tag{20.31}$$

where ΔM_x is the uncertainty in the projection of the angular momentum on the x-axis and $\Delta \Phi_x$ is the uncertainty in the angular coordinates of the microparticle.

By analogy with (20.28a) and (20.28b), we may write down relations for other projections of momentum and angular momentum as follows:

$$\Delta M_x \cdot \Delta\varphi_y \geq \hbar/2 \text{ and } \Delta M_z \cdot \Delta\varphi_z \geq \hbar/2 \tag{20.31a}$$

In general if q and p denote two canonically conjugate variables, the uncertainty relation is given by

$$\Delta q \cdot \Delta p \geq \hbar/2 \tag{20.32}$$

The above relations do not mean that the uncertainty principle creates certain obstacles to the understanding of the atomic phenomena; it only reflects certain peculiarities of the objective properties of a quantum particle.

20.12 ELEMENTARY PROOF OF UNCERTAINTY PRINCIPLE USING DE BROGLIE WAVE CONCEPT

A wave packet produced by a superposition of large number of harmonic waves is shown in Fig. 20.10. Since a wave packet is not an infinite harmonic wave, it has a range of wave numbers Δk instead of one definite wave number. Δk is thus the uncertainty in wave number. Further, the position of the particle cannot be given with certainty. It will lie somewhere between the two consecutive nodes (see Fig. 20.7b and Fig. 20.10). Thus, the uncertainty in the position of the particle is equal to the distance between two consecutive nodes. Referring to equ. (20.15), the condition for formation of a node is

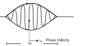

Fig. 20.10

$$\cos\left(\frac{\Delta\omega t}{2} - \frac{\Delta k x}{2}\right) = 0$$

i.e.,
$$\frac{\Delta\omega}{2}t - \frac{\Delta k}{2}x = \frac{\pi}{2}, \frac{3\pi}{2}, \frac{5\pi}{2}, \ldots, (2n+1)\frac{\pi}{2}$$

Thus, if x_1 and x_2 are the positions of two consecutive nodes, then

$$\frac{\Delta\omega}{2}t - \frac{\Delta k}{2}x_1 = (2n+1)\frac{\pi}{2}$$

and
$$\frac{\Delta\omega}{2}t - \frac{\Delta k}{2}x_2 = (2n+3)\frac{\pi}{2}$$

Subtracting the above upper equation from the lower one, we find that

$$\frac{\Delta k}{2}(x_2 - x_1) = \pi \quad \text{or} \quad \frac{\Delta k}{2}\Delta x = \pi$$

where $\Delta x = (x_2 - x_1)$ is the uncertainty in the position of the particle. Thus,

$$\Delta x = \frac{2\pi}{\Delta k}.$$

Since
$$k = \frac{2\pi}{\lambda} = \frac{2\pi p}{h},$$

$$\Delta k = \frac{2\pi}{h}\Delta p$$

Therefore,
$$\Delta x = \frac{2\pi}{\Delta k} = \frac{2\pi h}{2\pi\,\Delta p} = \frac{h}{\Delta p}$$

or
$$\Delta x \cdot \Delta p = h$$

When we consider a group consisting of very large number of harmonic waves of continuously varying frequencies, the product of the uncertainties comes to

$$\Delta x \cdot \Delta p \geq \frac{1}{2}\hbar$$

20.13 IMPLICATION OF UNCERTAINTY PRINCIPLE

The uncertainty principle expresses a fundamental limitation in nature that also limits the precision of our measurements. According to classical mechanics the position and momentum of a macro-particle can be determined exactly. But the uncertainty principle asserts that it is physically impossible to know simultaneously the exact position ($\Delta x = 0$) and exact momentum ($\Delta p_x = 0$) of a microparticle. According to it, the more precisely we know the posistion of the particle, the less precise is our information about its momentum. Thus, the momentum of a particle cannot be precisely specified without our loss of knowledge of the position of the particle at that time. Similarly, a particle cannot be precisely localized in a particular direction without our loss of knowledge of momentum in that particular direction. We can at best specify that certain momentum of the particle is more probable than the other or that the particle is more likely to be here than there. It means that our classical notions like coordinates and momentum derived from ordinary macroscopic experiences are inadequate to describe the atomic world. The uncertainty principle points out that in the microscopic world,

(1) the dynamical variables of a particle are combined in sets of *simultaneously determined* quantities which are known as *complete sets* of quantities;
(2) the coordinate and momentum components of a particle etc are **pairs of concepts** which are interrelated and fall in different complete sets of quantities. They cannot be defined simultaneously in a precise way.

Thus, the uncertainty principle implies that we can never define the path of an atomic particle with the absolute precision indicated in classical mechanics. Therefore, concepts such as velocity, position, and acceleration are of limited use in quantum world. To describe the quantum particle the concept of *energy* becomes important since it is related to the *state* of the system rather than to its path.

20.14 UNCERTAINTY PRINCIPLE IS NOT SIGNIFICANT IN CASE OF MACRO-BODIES

The Heisenberg Principle is of no practical importance for heavy bodies where the de Broglie wavelength is negligibly small.

For example, let us take the case of a cricket ball in flight. The indeterminacy in the position of the ball is, say, 1 mm. We can determine the indeterminacy of velocity of the ball from uncertainty principle.

$$\Delta x \cdot \Delta p \approx h$$

$$\therefore \qquad \Delta x \cdot m\Delta \upsilon \approx h$$

$$\Delta \upsilon \approx \frac{h}{m\Delta x} = \frac{6.62\times 10^{-34} J.s}{0.5kg\times 10^{-3} m} \cong 10^{-30} m/s.$$

The above inaccuracy is negligible and not detectable. It implies that the uncertainties are of no importance in case of macro bodies; and the position and velocity of a macro body can be simultaneously determined with a high degree of accuracy. As a result, macroscopic body follows a well defined trajectory.

In contrast if we take the example of an electron orbiting in a hydrogen atom, the inaccuracy in its position is $\pm$ 1Å. The uncertainty in its speed is

$$\Delta \upsilon = \frac{h}{m\Delta x} = \frac{6.62\times 10^{-34} J.s}{9.11\times 10^{-31} kg\times 2\times 10^{-10} m} \approx 2\times 10^{5} m/s$$

which is of the same order as the velocity of the electron in the orbit. It means that it is not possible to determine the velocity and the position of a microparticle with certainty and as such we cannot talk of a specific trajectory. Instead we have to be content knowing only the probable values.

20.15 THOUGHT EXPERIMENTS

It is not possible to verify Heisenberg uncertainty principle in the laboratory. Therefore, we illustrate it with the help of two *thought experiments*.

1. Treating the electron as a wave

We assume that an electron has wave character. Suppose that we want to determine the y-coordinate of an electron moving along the x-axis. We place a slit of width 'd' perpendicular to the direction of motion of the electron (Fig. 20.11). The precision of the position of electron, Δy, in y-direction is limited by the size of the slit. That is, $\Delta y \approx d$.

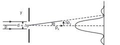

Fig. 20.11

If the slit is narrow enough, it causes a change in the motion of the electron after going through the slit and brings out the wave character of electron as evidenced from the diffraction pattern observed on the screen. The uncertainty in the electron momentum parallel to y-axis depends on the diffraction angle θ. According to the theory of diffraction at a single slit, the angle θ is given by

$$\sin\theta = \lambda/d \tag{20.33}$$

The uncertainty in the momentum of the electron parallel to y-axis is given by

$$\Delta p_y = p\sin\theta = \frac{h}{\lambda}\frac{\lambda}{d} = \frac{h}{d} \approx \frac{h}{\Delta y}$$

$$\therefore \qquad \Delta y\, \Delta p_y \approx h \tag{20.34}$$

If we wish to determine the exact position of the electron along the y-axis, we have to use a very narrow slit. However, a very narrow slit produces a wider diffraction pattern, which leads to a larger uncertainty in our knowledge of the Y-component of the momentum. Conversely, if we attempt to reduce the uncertainty in our knowledge of Y-component of momentum, the diffraction pattern should be very narrow. Therefore, we have to use a very wide slit, which in turn results in a large uncertainty in the y-coordinate of the electron. Thus, our efforts to simultaneously reduce the uncertainties Δy and Δp will get frustrated.

2. Treating the Electron as a Particle

We now consider that electron is a particle and attempt to measure its position. For the sake of convenience, we assume that the electron is at rest and use a microscope to locate it. We cannot use an optical microscope for this purpose. The act of observing an object requires that light from a source be reflected by the object and enter a recording instrument such as eye. An object reflects a wave when the size of the object is sufficiently larger than the wavelength of the wave. In the present case, if we use light waves, they would pass on without getting reflected by the electron, since the size of the electron

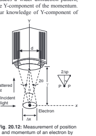

Fig. 20.12: Measurement of position and momentum of an electron by means of a γ-microscope.

is about 10^5 times smaller than the wavelength of light. Therefore, we use a γ-ray microscope to detect and locate an electron.

Let a free electron be directly beneath the center of the γ-ray microscope's lens. The circular lens forms a cone of angle 2α from the electron. The electron is illuminated from the left by γ-rays. The microscope can resolve objects to a size of Δx. Δx is given by the expression

$$\Delta x = \frac{\lambda}{2\sin\alpha} \qquad (20.35)$$

To be observed by the microscope, the γ-ray must be scattered into any angle within the cone of angle 2α. A γ-photon carries a very large momentum. When the γ-photon strikes the electron, part of the momentum and energy are transferred to the electron due to Compton scattering. Consequently, as the scattered photon enters the microscope, the electron has already moved away in a certain direction (Fig. 20.12). The total momentum p is related to the wavelength by the formula $p = \frac{h}{\lambda}$.

In the extreme case of diffraction of the gamma ray to the right edge of the lens, the total momentum in the x direction would be the sum of the electron's momentum p'_x in the X direction and the gamma ray's momentum in the x-direction:

$$p'_x + \left(\frac{h\sin\alpha}{\lambda'}\right) \qquad (20.36)$$

where λ′ is the wavelength of the deflected gamma ray. In the other extreme, the observed gamma ray recoils backward, just hitting the left edge of the lens. In this case, the total momentum in the X-direction is:

$$p''_x - \left(\frac{h\sin\alpha}{\lambda''}\right) \qquad (20.37)$$

The final X-momentum in each case must equal the initial X-momentum, since momentum is *conserved*. Therefore, the final X-momenta are equal to each other:

$$p'_x + \left(\frac{h\sin\alpha}{\lambda'}\right) = p''_x - \left(\frac{h\sin\alpha}{\lambda''}\right)$$

If α is small, then the wavelengths are approximately the same, $\lambda' \approx \lambda'' \approx \lambda$. And we have

$$p''_x - p'_x = \frac{2h\sin\alpha}{\lambda}$$

or

$$\Delta p_x = \frac{2h\sin\alpha}{\lambda} \qquad (20.38)$$

Using eq.(20.35) into the above equation, we obtain

$$\Delta p_x = \frac{h}{\Delta x}$$

$$\therefore \qquad \Delta x \cdot \Delta p_x = h$$

20.16 APPLICATIONS OF UNCERTAINTY PRINCIPLE

We deal here with three simple examples to illustrate the application of uncertainty principle.

(a) Bohr's Orbit and Energy

Let us consider the electron in a hydrogen atom. We cannot know at any instant the position of the electron in its orbit. It might be on the left or right of the nucleus, as sketched in

Fig. 20.13. The electron position has an uncertainty $\pm r$. We cannot know likewise whether the electron is moving upward or downward .The uncertainty in its velocity therefore $\pm\upsilon$. Taking $\Delta x = r \approx 0.5 \times 10^{-10}$ m, the uncertainty in the electron speed is

$$\Delta\upsilon = \frac{h}{2\pi m\Delta x}$$

$$= \frac{6.62\times10^{-34}\,J.s}{2\times3.124\times9.11\times10^{-31}\,kg\times0.5\times10^{-10}\,\mathrm{m}}$$

$$\cong 2 \times 10^6 \text{ m/s}$$

The velocity 'υ', of an electron in an atom is of the order of 1.0×10^6 m/s and is of the same order as the uncertainty $\Delta\upsilon$. Therefore, we conclude that the uncertainty in momentum is of the same order as the momentum. That is $\Delta p \approx p$. It means that sharp position and momentum do not exist simultaneously for the electron in an atom. Hence it is not possible to ascribe any specific trajectory to an electron in an atom. It can only be said that atomic electrons traverse the whole of the space about the nucleus, but however, they move most of the time at a distance corresponding to a permitted Bohr radius.

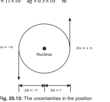

Fig. 20.13: The uncertainties in the position and velocity of electron in an atom.

Now let us calculate the energy of the Bohr's first orbit. The total energy of the electron in the first orbit is given by

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

$$= \left[\frac{1}{2}m\upsilon^2\right] - \frac{e^2}{4\pi\varepsilon_o r} = \left[\frac{p^2}{2m}\right] - \frac{e^2}{4\pi\varepsilon_o r} \tag{20.39}$$

where p is the momentum of the electron.

As $\Delta p \approx p$, we can write $p \approx \dfrac{h}{2\pi\Delta x} = \dfrac{h}{2\pi r}$. (20.40)

$$\therefore \quad E = \frac{h^2}{8\pi^2 mr^2} - \frac{e^2}{4\pi\varepsilon_o r} \tag{20.41}$$

But r is given by $r = \dfrac{\varepsilon_o h^2}{\pi\, me^2}$.

$$\therefore \quad E = -\frac{me^4}{8\varepsilon_o^2 h^2} \tag{20.42}$$

The above expression (20.42) is the same as that is given by Bohr theory.

(*b*) Particle in a Box:

Let us consider a particle confined to a box of length l. The uncertainty Δx in the position is l.

$$\Delta x \cdot \Delta p \cong \hbar$$

$$\therefore \quad \Delta p = \frac{h}{\Delta x} = \frac{\hbar}{l} \tag{20.43}$$

Energy is given by $$E = \frac{p^2}{2m} \approx \frac{(\Delta p)^2}{2m} = \frac{(\hbar/l)^2}{2m} = \frac{\hbar^2}{2ml^2} \qquad (20.44)$$

This result agrees with the result obtained from Schrödinger equation. Refer to **§ 20.95.**

(c) Electrons cannot be present in the nucleus:

The radiation emitted by radioactive nuclei consists of α, β and γ-rays, out of which β-rays are identified to be electrons. We apply uncertainty principle to find whether electrons are coming out of the nucleus. The radius of the nucleus is of the order of 10^{-14} m. Therefore, if electrons were to be in the nucleus, the maximum uncertainty Δx in the position of the electron is equal to the diameter of the nucleus. Thus,

$$\Delta x = 2 \times 10^{-14} \text{ m.}$$

The minimum uncertainty in its momentum is then given by

$$\Delta p = \frac{\hbar}{\Delta x} = \frac{1.04 \times 10^{-34} J.s}{2 \times 10^{-14} m} = 5.2 \times 10^{-21} \text{ kg-m/s.}$$

The minimum uncertainty in momentum can be taken as the momentum of the electron. Thus,

$$p = 5.2 \times 10^{-21} \text{ kg-m/s.}$$

The minimum energy of the electron in the nucleus is then given by

$$E_{min} = p_{min}\, c = (5.2 \times 10^{-21} \text{ kg-m/s})(3 \times 10^8 \text{ m/s}) = 1.56 \times 10^{-12} \text{ J} = 9.7 \text{ MeV.}$$

It implies that if an electron exists within the nucleus, it must have a minimum energy of about 10 MeV. But the experimental measurements showed that the maximum kinetic energies of β-particles were of the order of 4 MeV only. Hence electrons are not present in the nucleus. It is subsequently established that emission of β-particles occurs due to transformations in the nucleus. The transformation of a neutron into a proton produces an electron.

Example 20.4: *Uncertainty in time of an excited atom is about 10^{-8}s. What are the uncertainties in energy and in frequency of the radiation?*

Solution: $$\Delta E\, \Delta t \approx \frac{h}{2\pi}$$

$$\therefore \quad \Delta E = \frac{1.054 \times 10^{-34} J.s}{10^{-8} s} = \frac{1.054 \times 10^{-26}}{1.602 \times 10^{-19}} eV = 6.58 \times 10^{-8} eV.$$

$$\Delta \nu = \frac{\Delta E}{h} = \frac{1.054 \times 10^{-26} J}{6.626 \times 10^{-34} J.s} = 15.9 \text{ MHz.}$$

Example 20.5. *An electron is confined to a potential well of width 10 nm. Calculate the minimum uncertainty in its velocity.*

Solution. $$\Delta x\, \Delta p \approx \frac{h}{2\pi} \quad \text{or } \Delta x\, \Delta p \approx \frac{h}{2\pi}$$

$$\therefore \quad \Delta \upsilon = \frac{h}{2\pi\, m \cdot \Delta x}$$

$$\therefore \quad \Delta \upsilon = \frac{6.63 \times 10^{-34} Js}{2 \times 3.143 \times 9.11 \times 10^{-31} kg \times 10 \times 10^{-9} m} = \mathbf{12.1\ km/s.}$$

Example 20.6: *If the kinetic energy of an electron known to be about 1 eV, must be measured to within 0.0001 eV, what accuracy can its position be measured simultaneously?*

Solution:
$$E = \frac{p^2}{2m} \qquad \therefore \quad \Delta E = \frac{2p\,\Delta p}{2m} \qquad \therefore \quad \Delta p = \frac{m}{p}\Delta E$$

$$\Delta x \Delta p = \frac{h}{2\pi}$$

$$\therefore \quad \Delta x = \frac{h}{2\pi \cdot \Delta p} = \frac{h}{2\pi} \cdot \frac{p}{m\Delta E} = \frac{h\sqrt{2mE}}{2\pi\, m\Delta E} = \frac{h}{\pi\,\Delta E}\sqrt{\frac{E}{2m}}$$

$$\therefore \quad \Delta x = \frac{6.63\times10^{-34} Js}{3.143\times0.0001\times1.602\times10^{-19} J} \cdot \sqrt{\frac{1.602\times10^{-19} J}{2\times9.11\times10^{-31} kg}}$$

$$= \mathbf{1.95\ \mu m.}$$

Example 20.7: *An electron and a 150 gm base ball are traveling at a velocity of 220 m/s, measured to an accuracy of 0.005 %. Calculate and compare uncertainty in position of each.*

Solution: The uncertainty in the velocity is $\Delta \upsilon = \upsilon \times 0.065\% = (220 \text{m/s}) \times \frac{0.065}{100} = 0.143$ m/s.

(*i*) The uncertainty in the position of electron is

$$\Delta x_e = \frac{\hbar}{2\,m\Delta\upsilon} = \frac{1.05\times10^{-34} J.s}{2\times9.11\times10^{-31} kg\times0.143\ \text{m/s}} = \mathbf{0.4\ mm}.$$

(*ii*) The uncertainty in the position of baseball is

$$\Delta x_B = \frac{\hbar}{2\,M\Delta\upsilon} = \frac{1.05\times10^{-34} J.s}{2\times0.15\ kg\times0.143\ \text{m/s}} = \mathbf{2.5\times10^{-33} m}.$$

20.17 WAVE FUNCTION AND PROBABILITY INTERPRETATION

Waves represent the propagation of a disturbance in a medium. We are familiar with light waves, sound waves, and water waves. These waves are characterized by some quantity that varies with position and time. Light waves consist of variations of electric and magnetic fields in space, and sound waves consist of pressure variations. We cannot specify in a similar way what is actually varying in de Broglie waves. Since microparticles exhibit wave properties, it is assumed that a quantity ψ represents a de Broglie wave. This quantity ψ is called a **wave function**. ψ describes the wave as a function of position and time. However, it has no direct physical significance, as it is not an *observable* quantity. In general, ψ is a complex-valued function. According to Heisenberg uncertainty principle, we can only know the probable value in a measurement. The probability cannot be negative. Hence ψ cannot be a measure of the presence of the particle at the location (x, y, z). But it is certain that it is in someway an index of the presence of the particle at around (x, y, z, t).

Probability Interpretation of Wave Function given by Max Born

A probability interpretation of the wave function was given by Max Born in 1926. He suggested that *the square of the magnitude of the wave function $|\psi|^2$ evaluated in a particular region represents the probability of finding the particle in that region*. In other words,