

## Module 3

### INTRODUCTORY QUANTUM MECHANICS

(As per Revised Curriculum SVU R-2023)

- **Introduction**

Quantum mechanics emerged out of a process to reformulate our concepts and understanding of the nature. Most of our Engineering calculations including rocket science are still based on the traditional “classical physics” consisting of Newtonian mechanics, oscillations & wave motion, electromagnetism, heat & thermodynamics, optics etc. however, the quantum mechanical approach becomes essential as we probe further and further into the nature; particularly for studying the world of “very small”. When we deal with masses, dimensions and time scales at microscopic levels, we realise that things work quite differently than we thought otherwise. For example, the electrons, which were supposed to be particles obeying laws of mechanics show wave properties also, undergo interference and diffraction and the laws of mechanics cannot explain this strange behaviour. Here electron is taken just as an example but in practice, this wavelike behaviour is checked with many other microscopic objects. This wavelike behaviour plays miracles e.g. if a teacher is thought of made of waves, he/she can teach several classes simultaneously without requiring virtual classrooms! The wavelike behaviour also allows objects with low energy to “tunnel” through barriers e.g. if you toss a tennis ball against a wall, at some instances, you will find it has gone past as if the wall did not exist at those instances! Many such strange effects were beyond the scope of classical physics and that led to the development of quantum mechanics. Although the wave properties of matter are not observed at large scales, quantum mechanics essentially proposes that the wave nature exists at all scales and it is merely due to limits of measurements that they become non-verifiable. Inclusion of wave properties of matter adds further new features like uncertainties and statistical outcomes. Results are obtained in terms of “probability functions” and values of physical quantities are expressed as “most probable distribution” instead of an exact value. Quantum mechanics further proposes that at large scales, the results of classical physics match with that of quantum mechanics/physics. To drive the existing technology further, learning quantum mechanics is becoming demanding day by day. This is the main reason for keeping this introductory module on quantum mechanics for engineering students.

- **Background**

It would be relevant to discuss some of the important findings which led to reformulation of all of science. Some of them were as follows:

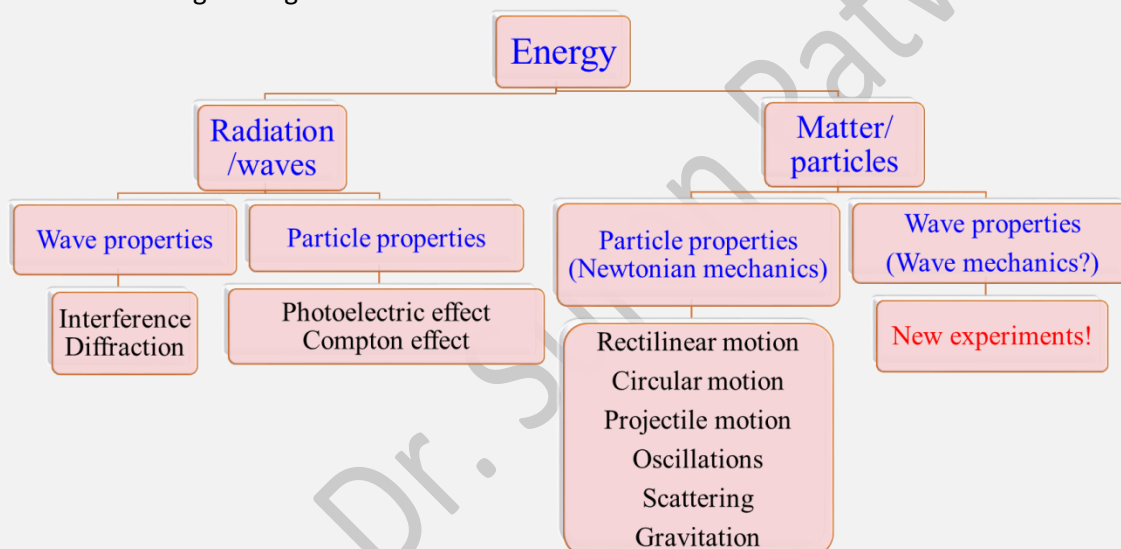
- 1) Blackbody radiation catastrophe: By and large, the Planck’s formula for blackbody radiation is considered as the birthplace of quantum physics. It used a novel concept of assuming every matter as made of small oscillating particles (oscillators) and that the energy emitted by their ensemble be in discrete manner rather than at any arbitrary value (continuous). The formula exactly matched with the experimental results at any wavelength and the discreteness of energy was established.
- 2) Specific heats of solids at low temperatures.
- 3) Constituents of matter, stability of atoms.
- 4) Origin of atomic and molecular spectra.
- 5) Fine structure and hyperfine structure splitting of spectral lines in magnetic field.
- 6) Wide range of conductivity of solids ( $10^{-14}$  S/m to  $10^8$  S/m).
- 7) Origin of magnetism, wide range of magnetisation ( $10^9$  A/m to  $10^{-6}$  A/m) and spontaneous magnetisation of ferromagnetic materials.
- 8) Cause of radioactivity.
- 9) Phenomenon of superconductivity.
- 10) Production of X-rays.
- 11) The photoelectric effect.

- 12) Zeeman effect.
- 13) Franck-Hertz Experiment.
- 14) Stern-Gerlach Experiment.

The events indicated above are essentially before de'Broglie put forward his hypothesis. Heisenberg (1925) and Schrödinger (1926) independently developed core theories of quantum mechanics. Later, Dirac (1928) contrived a general formalism and also included relativistic extensions to it. Since then there has been a continuous development in the quantum mechanics at atomic, nuclear and elementary particle scales but discussion on this development is beyond the scope of the syllabus.

- **de'Broglie's hypothesis**

Louis de'Broglie tried to sum up the experimental finding by his time into a set of logical arguments based on symmetry. Energy in the universe is manifested in two forms viz radiation and matter. By then, it was known that radiation shows both, particle properties and wave properties. de'broglie then argued that why can't matter, which is supposed to be made of particles and mostly governed by the laws of Newtonian mechanics, exhibit wave nature? Following chart can be useful to understand de'Broglie's arguments:



At that time, there was no experimental basis to his hypothesis but many took it seriously and soon wave nature of electrons, presumed as perfect particles was demonstrated by two independent experiments; one by Davison and Germer and the other by G P Thomson. Both these experiments were very similar to X-ray diffraction and based on diffraction of electrons by using crystals as three dimensional diffraction gratings.

Prior to this, it was already established that particle aspect of radiation called as “photons” are governed by two important equations:

$$E = h\nu = \frac{hc}{\lambda} \text{ Also, } E = mc^2 = (mc)c = pc \Rightarrow \frac{hc}{\lambda} = pc \text{ or } \lambda = \frac{h}{p}$$

De Broglie extended this equation to all material particles having mass “m” and moving with speed “v”, so the matter has an associated wave whose wavelength can be estimated as

$$\lambda = \frac{h}{mv}; (v < c \text{ always}) \quad (1)$$

This relation is called de'Broglie equation.

Note that this equation connects two physical quantities which are usually not used together because the momentum is a typical particle parameter while the wavelength is a typical wave parameter. The notions of a particle and a wave as we learn describe them as opposite to each other. By “particle” we imagine a localized, concise entity and which can be obtained in a discrete fashion while by a “wave” we try to imagine a distributed entity continuous all over. For example,

the ocean wave hits the shore simultaneously all over but a marble can hit only at a particular point at a time.

For a particle moving with velocity  $v$ , its kinetic energy can be expressed as  $K = \frac{p^2}{2m}$ . Hence the de'Broglie wavelength can be written as

$$\lambda = \frac{h}{\sqrt{2mK}} \quad (2)$$

For a charged particle of charge " $q$ " accelerated through a potential difference of " $V$ ",  $qV$  = Potential energy gained = Kinetic energy of motion. Hence the de'Broglie wavelength can be written as

$$\lambda = \frac{h}{\sqrt{2mqV}} \quad (3)$$

- **Experimental verification of de'Broglie's hypothesis - The Davison-Germer Experiment**

An important demonstration of diffraction of electrons was given by Davison and Germer and independently by G P Thomson in 1927. These experiments confirmed de'Broglie's hypothesis and consequently, the wave nature of material particles. The demonstration is considered to be one of the important experiments in the development of quantum mechanics.

Later, experiments were performed by using beams of other particle such as protons, neutrons and alpha particles, which also agreed perfectly with the theoretical predictions. Similar experiments were done using heavier atoms, ions and even molecules such as buckyballs (C-60) to prove that wave nature is not restricted only to elementary particles but it applied virtually to all of matter. Thus, wave nature of matter is now well-established. The Davison-Germer experiment stood as the pioneering experiment in the confirmation of quantum mechanics.

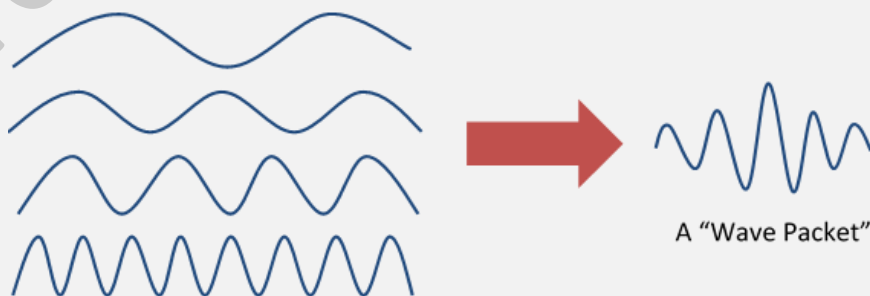
- **Phase velocity (wave velocity), wave packet and group velocity:**

The waves associated with all material particles moving with certain speed are called as "matter waves" but exactly what kind of waves are these? Let's find the velocity with which a wave associated with a particle moves. Traditionally, the rate at which the plane containing waves having the same phase (viz. the wave front) advances in a certain direction is called the phase velocity. It is the same as the wave velocity in ordinary sense in a wave motion. Thus,

$$v_{\text{phase}} = \frac{\omega}{k}; \text{ Where } \omega = 2\pi\nu \text{ and } k = \frac{2\pi}{\lambda}$$

$$\therefore v_{\text{phase}} = v\lambda = \frac{E}{h} \times \frac{h}{p} = \frac{E}{p} = \frac{mc^2}{mv} = \frac{c^2}{v} > c! \text{ as } v < c \text{ always. Here, "v" is particle velocity in the traditional sense.}$$

Estimation above gives an unusual and absurd result that the wave associated with particle moves with an extraordinary velocity leaving the particle far behind. Since this is impossible, it is concluded that particle cannot be associated with a single wave in ordinary sense. Next, it is proposed that a number of waves of different frequencies are associated with the particle.



The reason for this proposal is that a large number of waves can be added and it results in a repetitive pattern called as the "wave packet". This wave packet essentially carries the energy associated with the system (a particle; in this case). The collection of these waves is called as the wave group and the speed at which this entire group moves is different than velocities of individual

waves. It is not just the average velocity but it gives the rate at which frequency varies as a function of the wave vector “k” within the group. In mathematical terms,

Group velocity  $V_g = \frac{d\omega}{dk}$ . Let's estimate what is this group velocity.

Let  $V_g = \frac{d\omega}{dk} = \frac{d\omega/dv}{dk/dv}$ ; Where, “v” is the particle velocity in traditional sense.

We know that  $\omega = 2\pi\nu \therefore \omega = \frac{2\pi E}{h} = \frac{2\pi mc^2}{h} = \frac{2\pi m_0 c^2}{h\sqrt{1-v^2/c^2}}$ ; By using Planck's formula, Mass-energy

equivalence and relativistic expression for mass.

$$\therefore \frac{d\omega}{dv} = \frac{2\pi m_0 v}{h(1-v^2/c^2)^{3/2}}.$$

Also,  $k = \frac{2\pi}{\lambda} \therefore k = \frac{2\pi p}{h} = \frac{2\pi mv}{h} = \frac{2\pi m_0 v}{h\sqrt{1-v^2/c^2}}$ ; By using de'Broglie equation, definition of momentum

and relativistic expression for mass.

$$\therefore \frac{dk}{dv} = \frac{2\pi m_0}{h(1-v^2/c^2)^{3/2}}.$$

$$\therefore \frac{d\omega}{dk} = \frac{d\omega/dv}{dk/dv} = \frac{\frac{2\pi m_0 v}{h(1-v^2/c^2)^{3/2}}}{\frac{2\pi m_0}{h(1-v^2/c^2)^{3/2}}} = v \text{ i. e. } v_{\text{particle}}.$$

Thus the velocity with which the group moves in the form the new concept of a wave packet is the same as particle velocity in the traditional concept. So it is inferred that a particle can be represented by a wave packet.

- **Matter waves and their properties**

Since all the material particles show wavelike properties such as interference or diffraction, we try to associate wave nature to matter in general. But it should be understood that it is an entirely different concept that our usual understanding of the waves and wave motion. In introductory section it was stated that quantum mechanical treatment of solving any problem is rather statistical in nature and it involves calculation of probability factors. For example, classically, the radius of first Bohr orbit in hydrogen atom is  $0.53 \text{ \AA}$  exactly but according to quantum mechanics, it is just the most probable value of the radius. When we attempt to measure the radius a number of times, many times we may obtain this value but occasionally we may get some other values also. Thus, any value is expressed with some distribution about the most probable value instead of an exact value. The exact value of a physical quantity is somehow a representation of pure particle picture used in classical mechanics while the probabilistic value with some spread (often taken as the uncertainty) is a kind of wave picture used in quantum mechanics. The wave nature of matter and the concept of wave packet are linked with this probabilistic interpretation. This connection was first proposed by Max Born. In quantum mechanics, this probabilistic nature is carried by an abstract mathematical quantity called as the “wave function”.

- **Properties of matter waves:**

- 1) Matter waves are associated with all moving particles.
- 2) Their wavelength is inversely proportional to momentum of the particle.
- 3) They are independent of charge of the particle.
- 4) They are neither mechanical nor electromagnetic kind of waves.
- 5) A particle cannot be represented by a single wave. Instead, it is associated with a large number of waves forming a wave packet.
- 6) The quantity that varies periodically with space and time is taken as the wave function.

7) Square of the wave function gives probability of locating the particle.

- Differences between electromagnetic waves and matter waves**

Electromagnetic waves	Matter waves
1) Electromagnetic waves are associated with photon, which has zero rest mass.	Matter waves are associated with all moving material particles having non-zero rest mass.
2) A single de'Broglie wave can be associated with the particle (photon).	A single de'Broglie wave cannot be associated with the material particle.
3) The quantities those vary periodically with space and time are the electric and magnetic fields.	The quantity that varies periodically with space and time is called the wave function.
4) Electric and magnetic fields are real physical quantities and can be measured experimentally.	The wave function is an abstract mathematical quantity and has no direct physical interpretation.
5) Square of field amplitude gives intensity of electromagnetic waves.	Square of wave function gives probability of locating the particle in a given interval.

- Wave packet, wave-particle duality and the uncertainty**

The concept of a wave packet is central and very important in quantum mechanics. The wave packet has finite extent and it is neither "localised" like an ideal particle nor spread all over from  $-\infty$  to  $+\infty$  like an ideal wave. This leads to an idea of wave-particle dualism. By wave-particle duality it means that matter as well as radiation cannot be assigned only wave nature or only particle nature but in principle, matter as well as radiation possesses dual nature. However, at a time only one nature is exhibited and never both simultaneously. This wave-particle duality can be explained by using the concept of a wave packet as follows:

- 1) In quantum mechanics, all material particles are represented by a wave packet of finite extent. Mathematically, the wave packet is formed by coupling a large number of waves by means of Fourier analysis.
- 2) Spread of the wave packet is linked with uncertainty in the exact location of the particle.
- 3) Classically, a particle has an exact location at a given time. Now if we try to have exact location of the particle, the wave packet should be restricted in its extent. But, in doing so, the wave nature becomes indeterminate. When the wave packet shrinks to a point giving exact particle picture, the wave nature collapses completely.
- 4) On the other hand, if we try to have a perfect wave picture, the wave packet should be extended further. But in doing so, the position of the particle and hence the particle nature itself becomes highly uncertain. When the wave packet extends to infinity giving exact wave picture, the particle nature collapses completely.

Since all the material particles show wavelike properties such as interference or diffraction effects, we try to associate wave nature to particle or matter in general.

- The uncertainty principle**

In 1927, with his matrix formulation of quantum mechanics, Heisenberg proposed the uncertainty principle. It puts forward the fundamental theoretical limit to the exact determination of physical quantities. It is particularly applicable to simultaneous measurement of certain pairs of dynamical variable. In classical physics also it was long known that certain pairs of physical quantities such as position-momentum are "non-commutative" (i.e.  $AB \neq BA$ ). Heisenberg showed that the product of uncertainties of such pairs is greater than or equal to the factor  $\frac{h}{4\pi}$ . In mathematical form,

$$\Delta x \Delta p_x \geq \frac{h}{4\pi}$$

It states that "It is impossible to exactly determine the position and momentum of an object simultaneously such that the product of their uncertainties is never better than the factor  $\frac{h}{4\pi}$ ."



- Other forms of uncertainty principle:

A. Energy-time uncertainty product:  $\Delta E \Delta t \geq \frac{h}{4\pi}$

B. Angular position-angular momentum uncertainty product:  $\Delta \theta \Delta L \geq \frac{h}{4\pi}$

Note that the uncertainty product of quantities measured in mutually independent directions is zero. For example,

$$\Delta x \Delta p_y = \Delta y \Delta p_x = 0.$$

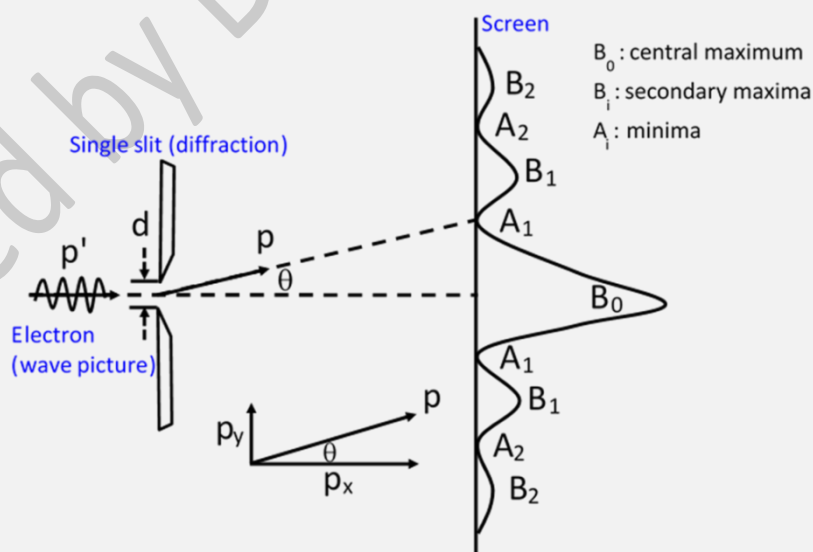
At first glance, the uncertainty principle may appear to be a negation since it puts forward the fundamental limit on exact measurements. It also leads to a misunderstanding that quantum mechanical approach does not yield exact value of any dynamical variable and hence it is incomplete. But it should be understood that the limitation comes due to the process of measurement itself. The fact is that the uncertainty principle is not just applicable at microscopic levels but virtually to *all* kinds of measurements; macroscopic as well as microscopic. At macroscopic levels, the uncertainties in the measurements are so small that we are usually unable to detect them and the results appear to be exact. But at the microscopic levels, the uncertainties become significant as compared to the actual values and the uncertainty principle becomes necessary. Uncertainty principle is not restricted just to put fundamental limit on measurements but it proved to be far more applicable to clarify a number of theoretical gaps as well as experimental findings.

- Proof-of-concept derivation for uncertainty principle**

Uncertainty principle first appeared through the matrix algebra developed by Heisenberg for quantum mechanics and its actual derivation is beyond the scope of this syllabus. Hence, one of the qualitative ways to arrive at the uncertainty principle is given here.

#### A. Single slit diffraction of electrons – the wave picture:

Here, we consider that electron is wave of wavelength  $\lambda$  be incident on a narrow slit of width  $d$ . Let  $p'$  be the corresponding initial momentum of electron as per de Broglie equation. The single narrow slit has the same effect as it would have on a monochromatic beam of light.



As an electron passes through the slit, its position becomes uncertain by an amount say  $\Delta y$ . Since it can pass anywhere from the slit, we can take  $\Delta y \approx d$ . Further, the electron gains y-component of momentum as it can reach anywhere on the screen on either sides of central maximum  $B_0$ . Let  $p$  be the momentum of electron after passing through the slit. The y-component of momentum is given

by  $p_y = p \sin \theta$ . For convenience, let the electron reach at point  $A_1$  on the screen. As this point corresponds to first minimum in the diffraction pattern, it is given by an equation  $\sin \theta = \frac{\lambda}{d}$ , where  $\theta$  is angle of diffraction.

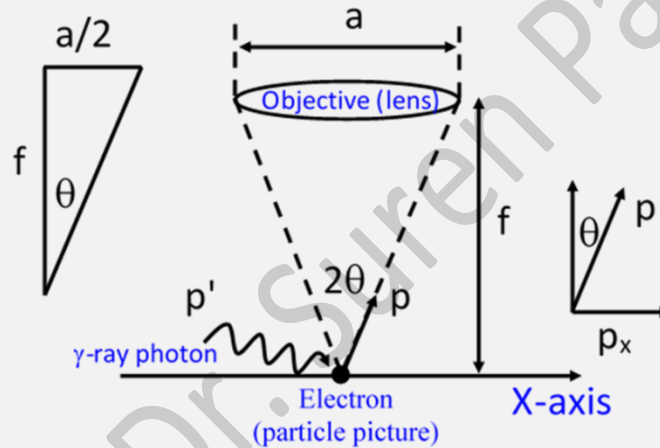
Now, letting the uncertainty in the y-component of momentum to be at the most equal to the y-component of momentum itself,

$\Delta p_y \approx p_y \approx p \sin \theta \approx \frac{h}{\lambda} \frac{\lambda}{d} \approx \frac{h}{\Delta y}$ ; By using de'Broglie's equation, expression for the first minimum in the diffraction pattern and the substitution  $\Delta y \approx d$ .

Thus,  $\Delta y \Delta p_y \approx h$ , as required.

### B. Seeing an electron with a gamma-ray microscope – the particle picture:

Here, we consider an electron as a perfect particle. For convenience, we assume that it is almost at rest and we try to locate its position by bouncing off a  $\gamma$ -ray photons from it. This  $\gamma$ -ray is a suitable choice, as one needs a beam having wavelength smaller than the object in order to resolve it. Only  $\gamma$ -rays have wavelength lesser than the de'Broglie wavelength of an electron. We imagine at least a single photon having momentum  $p'$  strikes the electron and it is scattered as per the Compton scattering mechanism.



The incident photon imparts some momentum on the electron. The microscope is held in a direction so as to collect the scattered photon which carries the “information” of position of the electron. The formation of “image” by the photon (i.e. position of the electron) is limited by the inherent diffraction effect. The position of the electron (i.e. the “image”) has a spread equal to the width of the central maximum, which is given by

$$\Delta x \approx \frac{\lambda f}{a} \quad \text{----- (1)}$$

Where  $f$  is the focal length of the lens and  $a$  is aperture size. Both are microscope parameters. This value represents uncertainty in the position of the electron.

Next, let the momentum imparted on the electron along the X-direction be approximately equal to the X-component of the momentum of scattered photon, which is scattered within an angle  $2\theta$  towards the microscope. From the diagram, this is  $p_x = p \sin \theta$ . Taking uncertainty in the momentum of the electron  $\Delta p$  to be at the most equal to  $p_x$ , we can write,  $\Delta p \approx p \sin \theta \approx \frac{h}{\lambda} \sin \theta$ .

From the diagram, for very small apertures,  $a \ll f$  and  $\sin \theta = \frac{a/2}{\sqrt{(a/2)^2 + f^2}} \approx \frac{a}{2f}$ . Therefore,

$$\Delta p \approx \frac{ha}{2\lambda f} \quad \text{----- (2)}$$

$$\text{From (1) and (2), } \Delta x \Delta p \approx \frac{\lambda f}{a} \times \frac{ha}{2\lambda f}$$

Thus,  $\Delta x \Delta p \approx h/2$ , as required.

- **Implications of the uncertainty principle**

The uncertainty principle could answer many unsolved questions in different branches of physics such as nuclear, atomic and molecular, solid state, spectroscopy, astrophysics and cosmology. Creation of very short-lived elementary particles, wave-particle duality, non-existence of electrons in the nucleus, zero-point energy possessed by atoms in solids at absolute zero, finite width of spectral lines, limits of measurements of frequencies of radiations, beta-decay (emission of an electron by the nucleus), sharing of electrons in covalent bonds, exact energy value of the ground state and many other effects can be satisfactorily explained with the help of the uncertainty principle. We take a look at some common implications of the uncertainty principle.

**A. non-existence of electrons in the nucleus:**

The maximum kinetic energies possessed by electrons during beta decay are about 100 keV. Let an electron be a part of the nucleus. The average nuclear dimensions are about  $10^{-15}$  m. Taking  $\Delta x \approx 10^{-15}$  m,  $\Delta p \approx 0.527 \times 10^{-19}$  kg-m/s. Assuming the momentum possessed by such electron to be at least equal to uncertainty in it,  $p \approx 0.527 \times 10^{-19}$  kg-m/s. This electron is indeed a relativistic electron as  $v \rightarrow c$ . Using the expression of kinetic energy,  $K = \sqrt{m_0^2 c^4 + p^2 c^2} - m_0 c^2$ . Here,  $(m_0 c^2)^2 \ll (pc)^2$ . Therefore,  $K \approx pc = 1.581 \times 10^{-11}$  J  $\approx 98$  MeV! Electrons never have so large energy and it contradicts the experimental results. Hence the initial argument is wrong and it can be concluded that electrons cannot be constituents of the nucleus.

**B. Minimum energy possessed by an electron in the atom:**

Here, the average atomic dimensions are about  $10^{-10}$  m and an electron is a part of the atom. Taking  $\Delta x \approx 10^{-10}$  m,  $\Delta p \approx 0.527 \times 10^{-24}$  kg-m/s. Assuming the momentum possessed by such electron to be at least equal to uncertainty in it,  $p \approx 0.527 \times 10^{-24}$  kg-m/s. This electron is not a relativistic electron as  $v \ll c$  for this electron. Using the normal expression for kinetic energy,  $K = \frac{p^2}{2m}$ ,  $K = 1.526 \times 10^{-19}$  J =  $0.96 \approx 1$  eV. It suggests that the minimum energy possessed by any electron in any atom cannot be less than 1 eV. Indeed, for the ground state electron in a hydrogen atom, the electron energy is 13.6 eV, which is well-above this limit.

**C. Finite width of spectral lines**

Wavelengths (or frequencies) of radiation emitted from any monochromatic source are never sharp at a particular value but always have some "spread", which is usually referred as "line width". This is true even for a laser source. In spectroscopy, for many years, it was a wonder but finally, the explanation was provided by the uncertainty principle. The average lifetime of an excited state is typically  $10^{-8}$  sec. When an electron makes a downward jump from such state, it introduces an uncertainty in the exact time interval for de-excitation. Taking maximum uncertainty in the measurement of time to be the lifetime of the excited state,  $\Delta E \approx \frac{h}{4\pi \Delta t}$ .

$$\therefore \Delta \nu = \frac{\Delta E}{h} \approx \frac{1}{4\pi \Delta t} \approx 7.96 \times 10^6 \text{ Hz} = 7.96 \text{ MHz.}$$

This is the theoretical line width of any spectral line emitted from a perfect monochromatic source. The important point is that it is *non-zero*.

**D. Virtual particle/vacuum fluctuations**

An interesting consequence of uncertainty principle comes in the form of spontaneous generation of virtual particles, which take energy from vacuum within the limits of energy-time uncertainty at short time and range. These virtual particles play a crucial role in high-energy particle physics.

**E. Zero-point energy**

In quantum electrodynamics, zero-point energy is the lowest possible energy level or ground state in a quantized electromagnetic field. This is also a consequence of the uncertainty principle



- **Wave Mechanics**

Material particles follow laws of Newtonian mechanics. These laws and equations are based on classical concept of “perfect particles”. But at the beginning of 20<sup>th</sup> century, many experimentalists showed that material particles had effects which were typically regarded for many years as “wave properties” (for example, diffraction of electrons). There was no explanation to these newly demonstrated wave properties of matter in the framework of classical Newtonian mechanics. Hence, there was a need of mechanics, which could incorporate the wave nature of matter. This was developed independently by Werner Heisenberg and Erwin Schrödinger. Heisenberg’s formulation contains matrix algebra while that of Schrödinger’s is based on wave equations. Schrödinger’s approach is called as the wave mechanics.

For this work, quantum mechanics introduced new physical properties and concepts. For example, the wave packet was introduced to explain wave nature shown by material particles and later it was supported by a foundation theory. A general practice in quantum mechanics in the early stage was to assign certain properties to microscopic objects, to form some models, to predict some effects and to link them with some observable/measurable macroscopic parameter. Further, this model should be consistent for any other kind of such experimentations. For example, all elementary particles like electrons and protons have been assigned an additional property called the spin and it is modelled that atoms possess magnetic moments due to intrinsic spins as well as orbital motion of electrons. Now, although we can’t see how an electron is, whether it actually “spins” and “revolves” and in what sense it interacts with a magnetic field, we can verify effect of the spin and orbital magnetic moments due to a collection of large number atoms in terms of magnetisation possessed by certain ferromagnetic materials. The amount of magnetisation can be measured experimentally and it becomes the “observed/measured macroscopic parameter” in this case. Later of course, the concept of spin was supported by a foundation theory developed by Dirac based on relativistic quantum mechanics.

- **The Wave function  $\psi(x, t)$**

A wave is said to be doubly periodic phenomenon meaning, in any kind of a wave, we can associate at least one physical quantity which is a periodic function of space (position) and time. For example, in electromagnetic waves, they are the electric and magnetic fields while in sound waves, it is the acoustic pressure that varies and gives rise to a compression or a rarefaction. In matter waves, this job has been assigned to the wave function. The only difference is that unlike electric/magnetic fields or pressure, which are real, physical quantities, the wave function is an abstract mathematical term and it can be a complex quantity to have a more general approach. However, the square of the wave function i.e.  $\psi^*\psi$  or  $|\psi|^2$  is called as the “probability” of finding the particle and this is a real number between 0 and 1 (or 0% and 100%). Thus, the matter waves or wave associated with material particles are somewhat related to the probabilistic outcome for any kind of measurement performed on the particle. Therefore, sometimes, matter waves are called as “waves of probability”.

- **Conditions on the wave function**

The wave function should satisfy following requirements:

- 1) It must be finite, single valued and continuous (and hence differentiable) everywhere.
- 2) Its derivatives ( $\frac{\partial \psi}{\partial x}$ ,  $\frac{\partial \psi}{\partial t}$  etc.) must also be finite, single valued and continuous.
- 3) It must be “normalised” meaning as  $x \rightarrow \pm\infty$ ,  $\psi(x, t) \rightarrow 0$ .
- 4) It must have at least one physically acceptable solution.
- 5) It must obey the principle of superposition of waves i.e. if  $\psi_1$  and  $\psi_2$  are solutions of the wave equation then  $A\psi_1 + B\psi_2$  is also a solution.

- **Schrödinger's time dependent wave equation (STDE)**

With the wave function being complex and representing periodicity in space and time, there are many forms of the wave function one can think of. The most obvious form as it involves periodic functions (through Euler's relation) is  $\psi(x, t) = Ae^{i(kx - \omega t)}$ ; Where, A is amplitude.

Let us develop Schrödinger's equation from this expression of wave function. Taking partial derivatives with respect of space (x) and time (t),

$$\frac{\partial \psi}{\partial t} = Ae^{i(kx - \omega t)} \times (-i\omega) = -i\omega\psi = -i(2\pi\nu)\psi = -i\left(\frac{2\pi E}{h}\right)\psi = -\frac{iE}{h}\psi.$$

$$\therefore i\hbar \frac{\partial \psi}{\partial t} = E\psi. \quad (1)$$

Similarly,

$$\frac{\partial \psi}{\partial x} = Ae^{i(kx - \omega t)} \times (ik) = ik\psi = i\left(\frac{2\pi}{\lambda}\right)\psi = i\left(\frac{2\pi p}{h}\right)\psi = \frac{ip}{h}\psi$$

$$\therefore \frac{\partial^2 \psi}{\partial x^2} = -\frac{p^2}{\hbar^2}\psi. \text{ Multiplying both sides by } -\frac{\hbar^2}{2m},$$

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} = \frac{p^2}{2m}\psi = K\psi. \quad (2)$$

Equations (1) and (2) are called "eigenvalue equations". From both the equations we can identify an operator which operates on the wave function  $\psi$  and yields a parameter (physical quantity) multiplied by  $\psi$  again. For example, in equation (1), the term " $i\hbar \frac{\partial}{\partial t}$ " is called the "energy operator" as it operates on the wave function to give total energy "E". This can be expressed as  $E_{op}(\psi) = E\psi$ . Similarly, let  $V(x)$  be a potential energy operator such that  $V(x)\psi(x, t) = V\psi$ . (3)

Note that potential energy is considered as a function of only position, which is true for most of the dynamical systems in mechanics. (For example, the gravitational potential)

As the second equation yields kinetic energy, we can couple equations (1), (2) and (3) to get a very familiar equation in mechanics that is T. E. = K. E. + P. E. Thus,

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V(x)\psi(x, t) \quad (\text{STDE})$$

Equation above is known as *Schrödinger's time dependent wave equation*. It is the central equation of wave mechanics just as the Newton's second law is to classical mechanics.

- **Reduction to time-independent form (STIE)**

In many applications, it is sufficient to use the wave function which is the function of position alone. The applications include central force field problems (formation of the periodic table and all of chemistry!), harmonic oscillator (all types of SHM), potential well (traps such as electron in a quantum dot), potential barrier (tunnel effect), potential step (reflection and refraction), periodic potential (metals, semiconductors and insulators).

The simplified version is obtained by using method of separation of variables. Let us express the wave function as

$$\psi(x, t) = \varphi(x).f(t)$$

$$\therefore i\hbar \varphi(x) \frac{\partial f}{\partial t} = -\frac{\hbar^2}{2m} f(t) \frac{\partial^2 \varphi}{\partial x^2} + V(x)\varphi(x)f(t)$$

Dividing everywhere by  $\varphi(x).f(t)$ ,

$$i\hbar \frac{1}{f} \frac{\partial f}{\partial t} = -\frac{\hbar^2}{2m} \frac{1}{\varphi} \frac{\partial^2 \varphi}{\partial x^2} + V(x).$$

The LHS is a function of only time whereas the RHS is a function of only position. Equating both sides to a common separation constant say “s”,

$$i\hbar \frac{1}{f} \frac{\partial f}{\partial t} = s.$$

Integrating,  $f(t) = e^{-ist/\hbar}$ . Comparing this form with the time-factor part of the original expression of the wave function viz.  $e^{-i\omega t}$ , we get  $s = \hbar\omega = \hbar\nu = E$ .

Thus the separation constant is nothing but the total energy “E”. Using this result for the RHS,

$$-\frac{\hbar^2}{2m} \frac{1}{\phi} \frac{\partial^2 \phi}{\partial x^2} + V(x) = E.$$

Multiplying everywhere by  $\phi(x)$  and using complete derivative instead of partial since the reduced wave function  $\phi(x)$  is a function of position alone,

$$-\frac{\hbar^2}{2m} \frac{d^2 \phi}{dx^2} + V(x)\phi(x) = E\phi(x) \quad (\text{STIE})$$

Equation above is known as *Schrödinger's time independent wave equation*. Many microscopic systems are studied by using this equation. In fact, the whole of periodic table with the electron configurations, shells, orbitals, stationary orbits, selection rules, l-s/j-j coupling, bonding-antibonding, the numbers  $n/l/m_l/m_s$  and the entire *chemistry* of elements is in fact, derived from solution of this Schrödinger's equation in the electrostatic central force field problem having spherical symmetry.

- Schrodinger equation v/s Newton's equation: A comparison**

Schrodinger's equation	Newton's equation (2 <sup>nd</sup> law of motion)
It is regarded as the central equation of (non-relativistic) quantum mechanics	It is regarded as the central equation of classical mechanics (i.e. non-quantum)
General (time-dependent) form is $i\hbar \frac{\partial \Psi}{\partial t} = \hat{H}\Psi$	General form is $\vec{F} = \frac{d\vec{p}}{dt}$
It describes both, wave and particle properties of matter	It describes only particle properties of matter
It obeys principle of linear superposition	It does not fit into the context of linear superposition
It is an energy equation	It is a force equation
It is a scalar equation	It is a vector equation
It applies to both, microscopic as well as macroscopic scales	It applies only at macroscopic scales
Newton's 2 <sup>nd</sup> law of motion can be derived from Schrodinger's equation	Schrodinger's equation cannot evolve from Newton's equations of motion

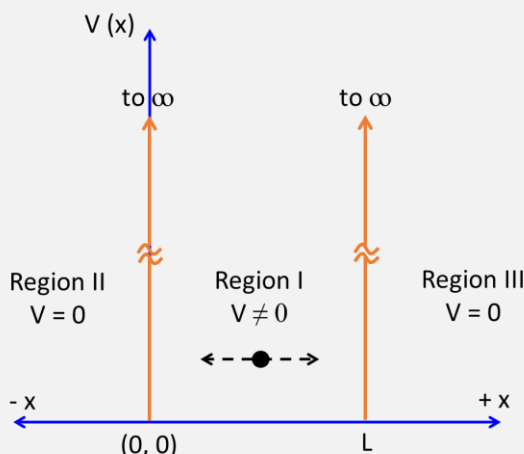
- Application to particle trapped in a 1-dimensional potential well (particle in a box problem)**

Here, we consider a classic example of a particle trapped in a one dimensional “potential well” of infinite height. It is of course, an idealistic example but it is the most simple and gives a quick start understanding of the solution of STIE. The potential function is described as follows:

$$V(x) = 0; \quad \text{for } 0 < x < L$$

$$= \infty; \quad \text{for } x \leq 0, \text{ and } x \geq L$$

Following is a sketch of the same:



- Wavefunction of particle in region II and III**

The particle cannot exist in region II and III since it needs to possess infinite energy to move into these regions, which is not possible (as potential shoots up to infinity at  $x = 0$  and  $x = L$ ). In Quantum mechanics, the wave function is related to the probability of locating the particle. Since particle cannot exist in both these regions, the probability is zero and the wavefunction  $\varphi(x) = 0$  identically for all values of  $x$  in region II and III i.e.  $x \leq 0$  and  $x \geq L$

- Wavefunction of particle in region I**

The Schrödinger's equation for region I can be written as

$$-\frac{\hbar^2}{2m} \frac{d^2\varphi}{dx^2} = E\varphi(x); \text{ As } V = 0.$$

$$\therefore \frac{d^2\varphi}{dx^2} = -\frac{2mE}{\hbar^2} \varphi = -k^2\varphi; \text{ Where, } k = \frac{\sqrt{2mE}}{\hbar} = \frac{2\pi}{\lambda}$$

The real part of the general solution of differential equation of the form  $\frac{d^2\varphi}{dx^2} + k^2\varphi = 0$  is  $\varphi(x) = A \sin kx + B \cos kx$ ; Where, A and B are constant to be evaluated.

Using boundary conditions for region I viz.  $\varphi(x) = 0$  at  $x = 0$ , we get  $B = 0$  (as  $\cos(0) = 1$ ). This implies that "A" cannot be zero as the wave function must have at least one non-zero solution. This requirement comes from the fact that the wave function is related with the probability of finding the particle in region I and if it is zero for any value of  $x$  between 0 and L, it means the particle does not exist in region I. This would contradict the statement of the problem itself as the particle is confined to region I.

Thus,  $\varphi(x) = A \sin kx$

Using the second boundary condition  $\varphi(x) = 0$  at  $x = L$ ,

$$0 = A \sin kL \Rightarrow k = \frac{n\pi}{L}; n = 1, 2, 3, \dots$$

The value  $n = 0$  is omitted as it would again mean that the wave function is zero for *any* value of  $x$  between 0 and L and thus, non-existence of particle in region I. This is absurd since the particle is constrained in region I with infinite boundaries. Thus, we get  $k$  or  $k_n = \frac{n\pi}{L}$ .

- Energy quantization**

As  $k = \pm \frac{n\pi}{L}$  as obtained from the boundary condition and earlier, we have substituted  $k$  for  $\frac{\sqrt{2mE}}{\hbar}$ , equating the two expressions, we get

$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2} = \frac{n^2h^2}{8mL^2}; n = 1, 2, 3, \dots$$

As  $n$  takes integer values, above equation implies an interesting result that energy possessed by the particle confined to a small region is “quantised” ( $E_n \propto n^2$ )

- **Momentum quantization**

According to de’ Broglie equation, momentum of the particle can be expressed as  $p = \frac{h}{\lambda}$ . Putting  $\hbar = \frac{h}{2\pi}$  and  $k = \frac{2\pi}{\lambda}$ , momentum can be expressed in terms of  $k$  as  $p = \hbar k$ . As above,  $k = \pm \frac{n\pi}{L}$ . Thus, the momentum can be expressed as

$$p = \pm \frac{nh}{2L}$$

It is seen that the momentum is also quantised. The  $\pm$  sign indicates two directions of the momentum (since it is a vector quantity). These are nothing but the positive and negative directions of the X-axis. As the potential well is one-dimensional, there are the only possible directions along which, the particle can move.

- **Wave function of the particle**

To find the exact wave function, the constant  $A$  needs to be evaluated. It is evaluated using the “normalization condition” given by

$$\int_0^L |\varphi(x)|^2 dx = 1.$$

Here,  $\varphi(x) = A \sin \frac{n\pi}{L}x$ . When integrated, It turns out that  $A = \sqrt{\frac{2}{L}}$ . Hence the complete wave function of the particle trapped in a one-dimensional infinite potential well is then

$$\varphi(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi}{L}x \text{ for the interval } 0 < x < L$$

- **Position of the particle**

Here, the particle exists only in region I ( $0 < x < L$ ). Inside these boundaries, position of the particle within any arbitrary interval say ( $x_1, x_2$ ) is obtained by using the probability factor  $P(x) \equiv |\varphi(x)|^2$ . Thus, in Quantum mechanics, we can at best get the probability of locating the particle in the given interval. This is evaluated as

$$P\{x \in [x_1, x_2]\} = \int_{x_1}^{x_2} |\varphi(x)|^2 dx = \int_{x_1}^{x_2} \frac{2}{L} \sin^2 \frac{n\pi}{L}x dx.$$

In practice, we get finite potential well instead of the infinite well discussed above. But the calculations used here apply to a good extent to microscopic problems. Many modern electronic devices (e.g. MOSFETs, laser diodes and LEDs) use these calculations for deciding the design criteria and material selection for these devices.

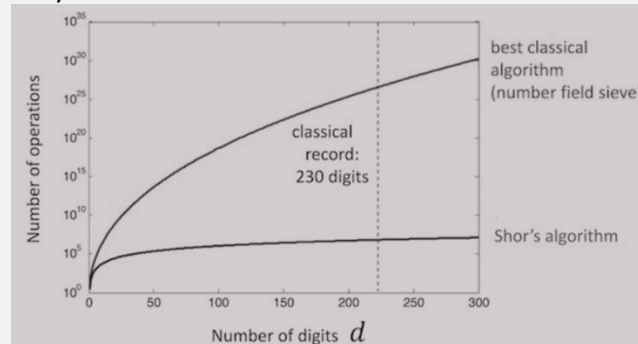
- **Quantum computing**

Richard Feynman, a Nobel Laureate once suggested that we could use quantum mechanical concepts for computer algorithms. Today, this field is called quantum computing. A “quantum computer” is that machine, which utilizes quantum mechanical effects such as the superposition or quantum entanglement to improve computational power.

- **Physics of information**

Today’s computers are essentially classical in a sense that the fundamental building block viz. the “bit” can be either “0” or “1” at a given time but never both (!) at the same time. In practice, it is realized by making tiny transistors in the IC “on” (saturated) or “off” (cut-off). No transistor can be both on and off at the same time! Imagine a computer which uses 2-bit “words” where the possible words are “00”, “01”, “10” and “11”. Today’s computer performs operation on these words one at a time but in a quantum computer, these words can exist at least in principle in a “superposed” state of all. An operation performed on this special state would virtually act on all the four words

simultaneously and this is a direct advantage in terms of the time required to perform a computation. It has been demonstrated by Peter Shor (1994) that to factorise a number having 400 digits by using today's computational methods would take time more than the age of known universe but by using quantum algorithm, it would merely take 3 years. Following graph depicts this advantage as worked out by IBM:



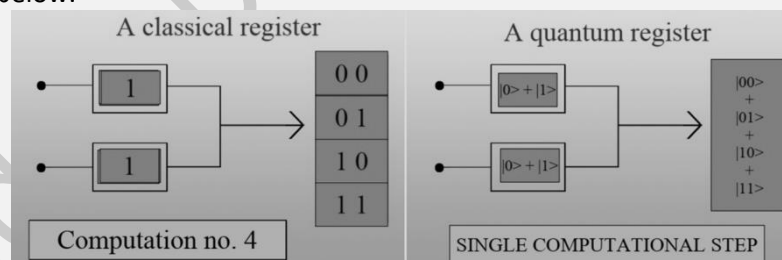
In an another algorithm put forward by Grover (1996), it was shown that time to search a specific entry in a database consisting of "N" entries would take " $\sqrt{N}$ " trials by using quantum algorithm whereas it normally takes "N/2" trials by using today's methods of database search. The advantage would be very clear for larger and larger values of N.

- Qubit and Dirac Notations**

A qubit is the basic unit in a quantum computer (the same way bit is to today's classical computers). However, the qubit can be represented by a multiple ways e.g. ground state (0) and excited state (1) of an ion, electron/nucleon spin state up (1) or down (0), photon left polarized (1) or right polarized (0) etc. accordingly, there is a variety of hardware. In quantum mechanics, these base states are represented by vectors in a  $2^n$  dimensional space where n is the size of the computer word. The qubit with two possible states (0 and 1) is represented as:

$$|\psi\rangle = a|0\rangle + b|1\rangle$$

A combination of such qubits in superposed state will also be in a superposed state. Under this advantage, an operation performed would work on all the possible outcomes simultaneously as shown in figure below.



For example, in a three-qubit system, there are total 8 outcomes possible so a quantum algorithm works on all these 8 possible outcomes unlike a classical computer, which works on one outcome at a time. Here, the notation  $|\ \rangle$  is called as "ket" vector and it is basically a column matrix. It is popularly called as Dirac's notation. The output is probabilistic and the probability amplitude in this example will be  $a^2 + b^2$  for a particular output.

- Quantum hardware**

There are a number of models proposed for realizing the potentials of quantum computing. The main objective is to hold the quantum superposition. Following are some of the models:

1. Quantum dot: a quantum dot consists of an electron trapped in a cage of atoms. Such electron possesses discrete energy levels. The ground state and excited state of this electron are regarded as logic 0 and 1 while a laser source is used as a gate (control).



2. Ion trap: it uses some ions such as Ca. The Ca atom/ion in its ground state and metastable state is interpreted as logic 0 and 1 respectively.
3. NMR: in this, qubits are represented by nuclear spin states using nuclei of certain elements. A magnetic field is used as gate.

- **Classical vs. Quantum computers**

Classical Computer	Quantum Computer
Uses semiconductor-based CMOS logic gates	May use atomic, electronic, nuclear or photonic properties
ON/OFF state of CMOS transistor determines logic 1/0	Logic 1/0 represented by spin up/down, ground state/excited state, right/left polarization etc.
Bit can be 1 or 0 at a specific time	Bit (qubit) can be both 1 and 0 at a specific time
Processor executes bit by bit operation	Processor operates on all bits simultaneously

- **Quantum computer – potentials and challenges**

In principle, computing machines based on quantum algorithms are far more superior to today's state of the art machines based on "classical" operations. The advantages are clear when the data sizes are huge. The major sectors which have been considered include cryptography, big data analysis, astronomical computations, weather models, finance and e-commerce. The main challenge in developing a quantum computer is "decoherence". In simple words, decoherence is the loss of state of superposition (quantum entanglement) of qubits. Such a state can be lost due to a measurement performed on the system. Another problem is to interpret the probabilistic outcome of any measurement. Here, the main challenge is to develop suitable error correcting codes for the output.

- Note: Additional notes on quantum computing involving qubit operations, quantum logic gates and quantum circuits are provided separately.

=====

END OF DOCUMENT