What is quantum mechanics?

Classical reality $\longrightarrow$ physical reality $\longrightarrow$ treats particles and waves as separate component of reality.

The mechanics of particles and waves are traditionally independent disciplines, each with its own chain of experiment and hypothesis.

The essence of classical mechanics is given in Newton's law $\boxed{m\dfrac{d^2\vec{r}}{dt^2} = \vec{F}}$

(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 time can be calculated.)

The same law can be applied from the dust particles to massive astronomical bodies. The latter can be decomposed in large number of particles and Newton's laws can be applied to each part separately.

Till 19th century every thing will be well explained by Newton's law.

What is quantum mechanics? (cont)

The fundamental difference between Newtonian mechanics and quantum mechanics lies in what it is that they describe.

Newtonian mechanics is concerned with the motion of a particle under the influence of applied forces, Newtonian mechanics provides explanation for the behavior of moving bodies in the sense that the values it predicts for "**observable magnitudes**" (position, momentum, mass, velocities, etc.) agree with the experimental values.

However, *quantum mechanics*, consists of relationships between "observable magnitudes", but the uncertainty principle radically alters the definition of "observable magnitudes" in atomic scale.

What is quantum mechanics? (cont')

According to uncertainty principle, the position and momentum of a particle can not be accurately measured at the same time. But in Newtonian mechanics both are assumed to have definite, ascertainable values at every instant.

So a Newtonian mechanics is nothing but an approximate version of quantum mechanics.

Newtonian mechanics $\Longrightarrow$ *macroscopic world*

Quantum mechanics $\Longrightarrow$ *microscopic world*

Failure of classical mechanics and birth of quantum mechanics:

By the end of nineteenth century all the known laws of physics were easily understandable by the Newtonian mechanics, Maxwell's equations describing electricity and magnetism and on statistical mechanics describing the state of large collection of matter. However the observations of some experiments could not be explained on the basis of these known laws.

Some of the basic problems that led to the origin of quantum mechanics are as follows

1. Classical Physics predicted that heated objects emit instantly all their heat into EM waves. Maxwell's calculation showed that the radiation rate went to infinity as the EM wavelength went to zero,*"the ultraviolet catastrophe"*.

Failure of classical physics and birth of quantum mechanics:

2. Planck solved the problem by postulating that energy of EM wave is emitted in the form of quanta with energy E=hf, (f=frequency of the radiation). Observations of the *photoelectric effect* cannot be explained if we consider radiation to be wave like obeying classical electromagnetic theory. Einstein explained the photoelectric effect using planck's quantum hypothesis.

Failure of classical physics and birth of quantum mechanics:

4. After Rutherford suggested that positive charge in atoms was concentrated at the centre and negative electrons revolved around the nucleus, classical physics predicted that the electrons would radiate energy away and would spiral into the nucleus. This does not happen of course. Bohr's atomic model postulated an angular momentum quantization rule, $L=nh/2\pi$.

5. The scattering of light of electrons "***COMPTON SCATTERING***" showed that light behaves as a particle but changes wavelength in the scattering, providing evidence of the particle nature of light.

Quantum mechanics thus establishes the wave particle duality and explains all the above phenomenon. The approach is quite different from the classical physics. While the classical laws are deterministic quantum mechanics is probabilistic.

Uncertainty principle

The principle states that for a particle, of atomic magnitude, in motion, it is impossible to determine both the position and the momentum simultaneously with perfect accuracy.
Quantitatively the principle is represented by Heisenberg's uncertainty relation which is as follows:

The product of the uncertainty Δx (*or possible error*) in the x-coordinate of a particle, in motion, at some instant, and the uncertainty Δp_x in the x-componentof the momentum, at the same instant, is of the order of or greater than ħ (1.054 x 10^{-31} J sec)
i.e $\Delta x \, \Delta p_x \geq \hbar$

In three dimensions, $\Delta x \, \Delta p_x \geq \hbar$

$$\Delta y \, \Delta p_y \geq \hbar$$

$$\Delta z \, \Delta p_z \geq \hbar$$

Similarly $\Delta \mathcal{E}\, \Delta t \geq \hbar$

$\Delta \mathcal{L}\, \Delta \phi \geq \hbar$

Physical significance of Heisenberg's Uncertainty relation:

Physical significance of Heisenberg's Uncertainty relation

The uncertainty relation leads to the following conclusions:

(i) If the position coordinate x of a particle in motion is accurately determined at some instant, so that $\Delta x = 0$,then at same instant the uncertainty $\Delta p_x = 0$ in the determination of the momentum becomes infinite.

(ii) if the momentum p_x of a particle is accurately determined at some instant, so that $\Delta p_x = 0$, then at same instant, the uncertainty Δx in the determination of the position coordinate becomes infinite. Thus if an experiment is designed to measure x or p_x accurately, the other quantity will become completely uncertain. We can measure both the quantities by means of an experiment, but only within certain limits of accuracy specified by the uncertainty relation.

Physical significance of Heisenberg's Uncertainty relation

(iii) For a particle of mass m moving with velocity v the product of the uncertainty Δx and the uncertainty Δv in the velocity is given by

$$\Delta x . \Delta v \geq \hbar/m$$

For a heavy metal $\hbar/m$ is very small and therefore, the product $\Delta x . \Delta v$ will be very small. For such particles both the position x and the velocity can be determined accurately.

Physical significance of Heisenberg's Uncertainty relation

(iv) For very heavy bodies, $\hbar/m = 0$, the uncertainties vanish and all quantities can be determined with perfect accuracy.

This is the limiting case of classical mechanics. Thus classical mechanics is true for heavy bodies and uncertainties are a characteristics of quantum mechanics, which is applicable to light particle, such as electrons , neutrons, protons etc.

Non-existence of Free Electrons in the Nucleus : An application of the Uncertainty Principle

We know that :

(i) The maximum possible kinetic energy of an electron emitted by radio-active nuclei is about 4 MeV.

(ii) the rest mass of electron, m_0 = 9.11 x E (-31) kg

(iii) the diameter of the nucleus is = 2 x E (-14) m

If the electron exists in the nucleus, it can be anywhere within the diameter of the nucleus. Therefore, the maximum uncertainty Δx in the position of the electron is the same as the diameter of the nucleus,

i.e $\Delta x =$ 2 x E (-14) m

Non-existence of Free Electrons in the Nucleus : An application of the Uncertainty Principle

We also know that

$\Delta x \, \Delta p_x \geq \hbar$

The uncertainty in the momentum p_x is $\Delta p_x \geq \hbar / \Delta x$

Therefore, the minimum uncertainty in the momentum is given by $\Delta p_x = \hbar / \Delta x$

$= (1.054 \times 10^{-31}) / (2 \times E(-14))$

$= 5.278 \times E(-21)$ kg.m/s

It means that if the electron exists in the nucleus, its minimum momentum must be

$p_{min} = 5.278 \times E(-21)$ kg.m/s

Non-existence of Free Electrons in the Nucleus : An application of the Uncertainty Principle

Again, according to the theory of relativity,

$E^2 = p^2c^2 + m_0^2c^4$

$E_{min}^2 = p_{min}^2c^2 + m_0^2c^4$

$= 2.5 \times E(-24) + 6.72 \times E(-27)\ J^2$

$E_{min} = 1.58 \times E\ (-12)\ J$ [2^{nd} term is neglected]

$= 9.\ 875\ MeV$ [1 eV = 1.6x E(-19) J]

If a free electron exists in the nucleus it must have a minimum energy of about ~10 MeV.

The maximum kinetic energy which a beta particle, emitted from radioactive nuclei, can have is 4 MeV. Therefore, free electrons can not present within nuclei.

Wave function

A mathematical function, similar to a wave, associated with the quantum properties of a particle. *The square of the wave function at any point equals the probability of finding the particle there.*

In classical waves, there is always something that is ‘waving’. Thus in water waves the water surface moves up and down, in sound waves the air pressure oscillates and in electromagnetic waves the electric and magnetic fields vary.

What is the equivalent quantity in the case of matter waves? The conventional answer to this question is that there is no physical quantity that corresponds to this.

We can calculate the wave using the ideas and equations of quantum physics and we can use our results to predict the values of quantities that can be measured experimentally, but we cannot directly observe the wave itself, so we need not define it physically and should not attempt to do so.

To emphasize this, we use the term ‘wave function’ rather than wave, which emphasizes the point that it is a mathematical function rather than a physical object. Another important technical difference between wave function and the classical waves is that the classical wave oscillates at the frequency of the wave, in the matter-wave case the wave function remains constant in time.

However, although not physical in itself, the wave function plays an essential role in the application of quantum physics to the understanding of real physical situations.
Firstly, if the electron is confined within a given region, the wave function forms standing waves, as a result, the wavelength and therefore the particle’s momentum takes on one of a set of discrete quantized values.

Secondly, if there is a wave associated with a particle, then there must be a function to represent it. This function is called wave function.

Wave function is defined as that quantity whose variations make up matter waves. It is represented by Greek symbol ψ (psi), ψ consists of real and imaginary parts. ***Significance*** of wave function are:

1. The wave function ψ contains measurable information about the particle.

2. $\Psi^*\Psi$ summed over all space = 1 (if the particle exists, the probability of finding it somewhere must be 1)

3. It is continuous

4. It allows energy calculations via Schrödinger equation

5. It establishes the probability distribution in three dimensions

6. For a free particle it is a sine wave.

7. The square of its absolute magnitude $|\psi^2|$ has significance when evaluated at a particular point and at a particular time $|\psi^2|$ gives the probability of finding the particle there at that time.

The Schrödinger Wave Equation

Wave function of a particle of fixed energy E could most naturally be written as a linear combination of wave function of the form $\psi(x,t) = Ae^{i(kx-\omega t)}$ (1)

representing a wave travelling in the positive x direction, and a corresponding wave travelling in the opposite direction, so giving rise to a standing wave, this being necessary in order to satisfy the boundary conditions. This intuitively corresponds to our classical motion of a particle bouncing back and forth between the walls of the potential well, which suggests that we adopt the wave function above as being the appropriate wave function for a *free* particle of momentum: $p = \hbar k$ and energy $E = \hbar\omega$.

With this in mind, we can then note that

$$\frac{\partial^2 \psi}{\partial x^2} = -k^2 \psi \qquad (2)$$

which can be written, using $E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$

or, $k^2 = \frac{2mE}{\hbar^2}$

From Eqn (2), $\frac{\partial^2 \psi}{\partial x^2} = -\frac{2mE}{\hbar^2}\psi$

Multiply both side by $\hbar^2$ and divide by 2m gives:

$-\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} = E\psi$ but $E = \frac{p^2}{2m}$

So, $-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} = \frac{p^2}{2m}\psi$ (3)

Similarly, $\frac{\partial\psi}{\partial t} = i\omega\psi$ (4)

Which can be written, using $E = \hbar\omega$;or, $\omega = \frac{E}{\hbar}$

using this in Eqn. (4) can be rewritten as:

$\frac{\partial\psi}{\partial t} = -i\frac{E}{\hbar}\psi$ multiply both side by $i\hbar$ gives,

$$i\hbar\frac{\partial\psi}{\partial t} = -i\frac{E}{\hbar}\psi.i\hbar = \hbar\omega\psi = E\psi \qquad (5)$$

We now generalize this to the situation in which there is both a kinetic energy and a potential energy present, then

$$E = \frac{p^2}{2m} + V(x) \quad \text{so that}$$

$$E\psi = \frac{p^2}{2m}\psi + V(x)\psi \qquad (6)$$

where ψ is now the wave function of a particle in the presence of a potential V(x). But if we assume that the results Eqns. (3) and (5) still apply in this case then we have

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\psi = i\hbar\frac{\partial\psi}{\partial t} \qquad (7)$$

Which is time dependent **Schrödinger Wave Equation**