Unit 3: Quantum Mechanics

Syllabus

- De-Broglie hypothesis
- Concept of phase velocity and group velocity (qualitative)
- Heisenberg Uncertainty Principle
- Wave-function and its physical significance
- Schrodinger's equations: time independent and time dependent
- Application of Schrodinger's time independent wave equation - Particle enclosed in infinitely deep potential well (Particle in Rigid Box)
- Particle in Finite potential well (Particle in Non Rigid box) (qualitative)
- Tunneling effect, Tunneling effect examples (principle only): Alpha Decay, Scanning Tunneling Microscope, Tunnel diode
- Introduction to quantum computing

Prerequisite: Basics of wave particle duality from 11th and 12th standard

3.1 Wave particle duality of radiation

- In classical mechanics, wave and particle are shows different properties and are given separate treatment.
- A matter particle is identified by the properties such as mass, momentum, kinetic energy, spin, electric charge, etc.
- A wave is identified by properties such as wavelength, frequency, amplitude, intensity, energy, etc.
- Electromagnetic radiations (e.g. light) show optical phenomenon such as interference, diffraction and polarization. These phenomenons require that electromagnetic radiations must have wave nature.
- However, phenomenon such as photoelectric effect, Compton Effect, emission and absorption of radiation by matter, black body radiations require that electromagnetic radiations must have particle nature.
- Thus the electromagnetic radiations have dual characteristics.
- Although particle and wave properties of radiation cannot be observed simultaneously, it is not possible to separate the particle and wave nature of electromagnetic radiations.

3.2 Wave particle duality of matter / De Broglie's hypothesis of matter waves

de Broglie hypothesis

Louis de Broglie extended the wave-particle duality of light to the material particles. If a light wave can show wave-particle duality in some conditions, then particles such as electrons should also act as waves at some times. This is known as de Broglie hypothesis.

Thus, according to de Broglie hypothesis, a moving particle always has a wave associated with it and the motion of that particle is guided by the associated wave. The waves associated with particle are known as matter waves or de Broglie waves.

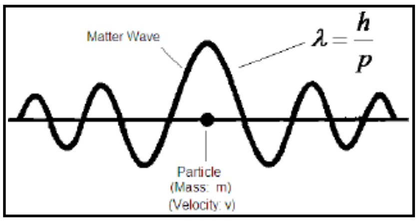
If a particle of mass ***m*** is moving with velocity ***v***, the wavelength λ of matter waves associated with a particle is inversely proportional to the momentum and is given by $\lambda = \frac{h}{p}$

As a photon travels with velocity ***c***, its momentum can be expressed as

$$p = \frac{E}{c} = \frac{h\nu}{c} = \frac{h}{\lambda}$$

Thus, wavelength of the photon is $\lambda = \frac{h}{p}$ (1)

de Broglie proposed that equation (1) is a universal and is applicable to photons and material particles also.



A particle of mass ***m*** moving with velocity v, has momentum $p = mv$. Thus the wavelength of de Broglie wave associated with it can be written as

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

The waves associated with a moving particle are called matter waves or de Broglie waves.

3.3 de Broglie wavelength of a particle in terms of its kinetic energy

Consider a particle of mass *m* moving with velocity *v*. Its momentum is *p=mv* and the de Broglie wavelength of matter waves associated with it is given by

$$\lambda = \frac{h}{p} = \frac{h}{mv} \quad \text{--- (1)}$$

The kinetic energy of the particle is given by $E = \frac{1}{2}mv^2$

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

As *p=mv* $E = \frac{p^2}{2m}$

Or $p^2 = 2mE$ or $p = \sqrt{2mE}$ --- (2)

Putting the value of *p* in the equation of matter wave,

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2mE}} \quad \text{--- (3)}$$

The above equation gives de Broglie wavelength of a particle of mass *m* and kinetic energy *E*. This equation is true for any particle irrespective of its charge or mass.

3.4 de Broglie wavelength of an electron/proton accelerated by Potential difference

If a charged particle such as electron or proton of rest mass m_0 is accelerated by a potential difference of ***V*** volts, the kinetic energy gained by it is given by

$KE = eV$ (where e is elementary charge)

$$\frac{1}{2}m_0v^2 = eV \quad \text{--- (1)}$$

$$\frac{1}{2m_0}m_0^2v^2 = eV$$

$$m_0^2v^2 = 2m_0eV$$

$$m_0v = \sqrt{2m_0eV} \quad \text{--- (2)}$$

Thus, the de Broglie wavelength associated charged particle is given by

$$\lambda = \frac{h}{p} = \frac{h}{m_0v} \quad \text{--- (3)}$$

From equations (2) and (3) $\lambda = \frac{h}{\sqrt{2m_0eV}}$ -- (4)

Where, $h = 6.63 \times 10^{-34}\,Js$ and $e = 1.6 \times 10^{-19}\,C$

For an electron

As rest Mass of electron, $m_{0e} = 9.1 \times 10^{-31}\,kg$, from equation (4)

$$\lambda = \frac{12.26}{V}\text{Å}$$

For a proton

Rest mass of proton, $m_{0p} = 1.673 \times 10^{-27}\,kg$, from equation (4)

$$\lambda = \frac{0.286}{V}\text{Å}$$

3.5 Properties of matter waves

According to de-Broglie hypothesis, for a particle mass ***m*** moving with velocity ***v***, the wavelength of matter wave associated with it is given by $\lambda = \frac{h}{p} = \frac{h}{mv}$, where ***h*** is Plank's constant. The properties of matter waves can be summarized as below:

(i) Wavelength is inversely proportional to the velocity of particle

The wavelength of matter waves is inversely proportional to the velocity of the particle i.e. $\lambda \propto \frac{1}{v}$. Thus, when a particle is at rest, its velocity is zero and $\lambda \rightarrow \infty$. Smaller is the value of ***v*** longer is the wavelength of the matter waves associated with it. It means that matter waves are detectable only for moving particles.

(ii) Wavelength is inversely proportional to the mass of particle

The wavelength of matter waves is inversely proportional to the mass of the particle i.e. $\lambda \propto \frac{1}{m}$. Lighter is the particle, smaller is the value of ***m*** and hence longer is the wavelength of the matter waves associated with it. Therefore, wave behavior of micro-particles will be significant whereas waves associated with macro-bodies can never be detected.

(iii) Matter waves are related with probability of finding the particle

If a photon is considered as a particle then corresponding electromagnetic wave is de Broglie wave for that photon. Similarly, atomic particles are associated with matter waves, which do not have similarity to any known waves such as electromagnetic or sound waves. de Broglie waves are associated with locating the probability of particle and hence also known as probability waves.

(iv) Matter waves are not electromagnetic waves

Any types of waves are produced by oscillations of certain quantity. When a charged particle oscillates, it produces electromagnetic waves. Matter waves are produced by the motion of the particles and do not depend on the charge of the particle. Therefore, matter waves are not electromagnetic waves.

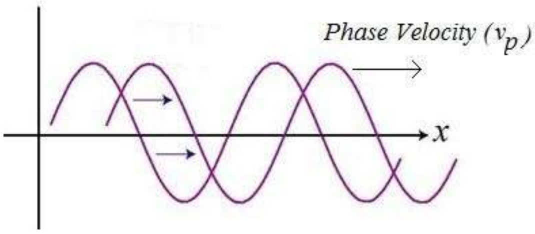
(v) Matter waves are not mechanical waves

Mechanical waves, such as sound waves, are produced by the vibrations of particles of the medium though which they travel. A particle can always travel in the vacuum and hence matter waves are associated with it even in vacuum. As matter waves do not require any medium for propagation, they are not mechanical waves.

3.6 Phase velocity and group velocity

Phase velocity (or wave velocity)

The phase velocity of a wave is the rate at which the phase of the wave propagates in space. Phase velocity of a single wave is the velocity with which a definite phase point (of either crest or trough) of the wave propagates in the medium.



The concept of phase velocity is meaningless

The phase velocity is given by, $v_p = \frac{\omega}{k}$

Where, $\omega = 2\pi\upsilon$ is angular frequency and $k = \frac{2\pi}{\lambda}$ is propagation constant.

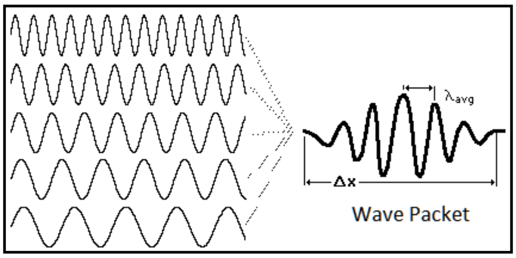
It can be shown that, phase velocity, $v_p = \frac{c^2}{v}$

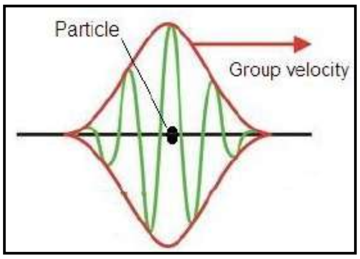
As per this equation, the phase velocity would always greater than velocity of the light. According to theory of relativity, the velocity of any particle ***v*** should always be less than velocity of the light ***c***. This result is thus unexpected and meaningless.

Group Velocity (or particle velocity)

The concept of phase velocity is meaningless as the velocity is always greater than velocity of light. Also it is assumed that de Broglie waves are monochromatic waves. As wave spreads over a large region of space, it cannot represent a highly localized particle. Schrodinger postulated that instead of single wave, a wave packet represents the particle. A wave packet consists of a group of harmonic waves. Each wave has slightly different wavelength. The superposition of very large number of harmonic waves will produce a **single wave packet**.

The velocity with which a wave packet propagates in the medium is called group velocity $\boldsymbol{v_g}$.





It can be shown that, group velocity $v_g = \frac{d\omega}{dk}$

The particle velocity is equal to its group velocity

The concept of phase velocity is meaningless as its phase velocity would be greater than particle velocity. However, it can be shown that group velocity of the particle is equal to the particle velocity

i.e. $v_g = \frac{d\omega}{dk} = \frac{p}{m} = v$

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

This "group velocity dispersion" is an important effect in the propagation of signals through optical fibers and in the design of high-power, short-pulse lasers.

3.7 Heisenberg's uncertainty principle

Heisenberg's uncertainty principle

It is not possible to know simultaneously and accurately both the position and the momentum of a micro-particle.

If, Δx – uncertainty in the position when momentum is measured accurately

Δp – uncertainty in the momentum when position is measure accurately

Then, according to Heisenberg's principle the product of uncertainties is of the order of Plank's constant.

Thus, $\Delta x \Delta p \geq h$ where $h = 6.63 \times 10^{-34}\, Js$ is Plank's costant

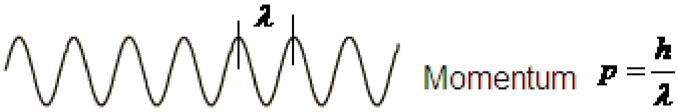
More accurately, $\Delta x \Delta p \geq \frac{\hbar}{2}$ or $\Delta x \Delta p \geq \frac{h}{4\pi}$

Heienberg's uncertainty principle arises from the wave properties of matter. Even with perfect instruments and technique, the uncertainty will always remain.

Explanation of Heisenberg's Uncertainty Principle

The wavelength of matter wave associated with a particle of mass *m* and having momentum *p* is given by $\lambda = \frac{h}{p} = \frac{h}{mv}$. A moving micro particle is associated with a wave packet. A wave packet spreads over a region of space. Although particle is located somewhere within the packet, it is difficult to locate the exact position of the micro particle at a given time.

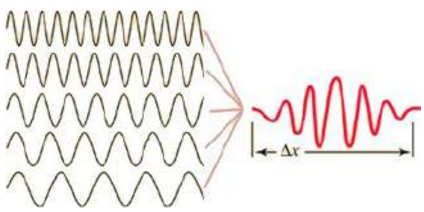
Broad wave packet



If a broad wave packet of de Broglie waves is associated with the particle, its wavelength λ and momentum $p = h/\lambda$ can be determined accurately. For matter waves, the amplitude indicates their most probable position within the wave packet. In broad wave packet, as amplitude is almost uniform everywhere, the probability of finding the particle will also be uniform. Hence the exact position of the particle cannot be located and it gives uncertainty in position of the particle.

Narrow wave packet

According to the concept of wave packet, a group of waves is associated with a moving matter particle. Superposition of these waves gives rise to a narrow wave packet. The waves interfere constructively over a small region and cancel each other everywhere else. The most probable position of the particle is thus determined by the amplitude of resultant wave in the wave packet.



However, in narrow wave packet, wavelength λ hence momentum $p = h/\lambda$ cannot be measured accurately. And thus, it introduces uncertainty in the momentum.

Heisenberg's principle applied to energy and time

The kinetic energy and time form a pair of canonically conjugate variables. The KE of the particle of mass *m* moving with velocity *v* is given by

$$E = \frac{1}{2} mv^2$$

Differentiating $\Delta E = \frac{1}{2} m 2v\Delta v$

$$\Delta E = v(m\Delta v)$$

Or $\Delta E = v(\Delta p)$

Or $\Delta E = \frac{\Delta x}{\Delta t}\Delta p$

Or $\Delta E\Delta t = \Delta x\Delta p$

According to Heisenberg's principle $\Delta x\Delta p \geq h$

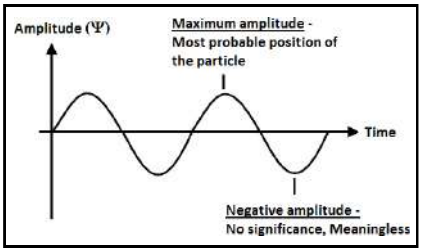
Thus $\Delta E\Delta t \geq h$

Thus, the product of uncertainties of energy and time is of the order of Plank's constant. Hence, it can be concluded that Heisenberg's uncertainty principle is also true for energy and time variables.

3.8 Physical significance of wave function ψ and |ψ|² [Born interpretation]

Interpretation of wave function ψ

Matter waves must be produced by vibration of some quantity. However, matter waves are neither electromagnetic waves nor they are sound waves. Thus, what quantity is vibrating to produce matter waves is not clear.



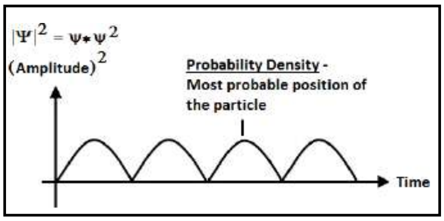
Schrodinger represented oscillations of the quantity by a mathematical function known as wave function ψ.

- ψ represents the wave as a function of position and time.
- Greater is the amplitude of wave function ψ, higher is the probability of finding the particle at that position and time. But as amplitude can be positive or negative. **The negative amplitude gives rise to negative probability which is meaningless**.
- Thus, due to negative probability, wave function ψ is a complex mathematical quantity. It has no direct physical significance and cannot therefore be measured experimentally.

Interpretation of $|\psi|^2$ [Born interpretation]

The wave function ψ is a complex quantity and cannot determine the position of the particle.

A probability interpretation of the wave function was given by Max Born. He suggested that the square of the magnitude of the wave function $|\psi|^2$ gives the probability of finding the particle in that region.



Probability, ***P*** of finding the particle in an infinitesimal volume $dV(= dx.dy.dz)$ is given by

$$P \propto |\psi(x,y,z)|^2 dV$$

$|\psi|^2$ is known as **probability density** and ψ is the **probability amplitude**.

Since the particle is certainly somewhere in the space, the probability P=1 and

$$\int_{-\infty}^{+\infty} |\psi|^2 dV = 1$$

The wave function ψ is in general a complex function. But the probability must be real. Therefore, ψ is multiplied by its complex conjugate ψ^*. Thus,

$$\int_{-\infty}^{+\infty} \psi\psi^2 dV = 1$$

Thus although ψ has no physical significance but $|\psi|^2$ gives the probability density of the particle i.e. probability of finding the atomic particle in a particular region.

Mathematical conditions wave function Ψ must obey

An acceptable wave function Ψ is a mathematical quantity that should obey some mathematical conditions as following.

(a) Ψ must be a finite function

The wave function Ψ must be finite everywhere. Even if, x or y or z → +∞ or +∞, the wave function should not tend to infinity. It must remain finite for all values of x, y and z. If ψ is infinite, it would imply an infinite large probability of finding the particle at that time. This would violet the uncertainty principle.

(b) Ψ must be a single valued function

Any physical quantity can have only one value at a point. Thus, at a given location and a time wave function Ψ can have only one value of probability. If it has more than one value at a point, it means that there is more than one value of probability of finding the at that point. It would imply that the particle would be found at multiple location at the same time which is not possible.

(c) Ψ must be a continuous function

The wave function ψ should be continuous across any boundary. Since ψ is related to a physical quantity, it cannot have a discontinuity at any point. Hence wave function Ψ and its space derivatives $\frac{\partial\Psi}{\partial x}, \frac{\partial\Psi}{\partial y}, \frac{\partial\Psi}{\partial z}$ should be continuous across any boundary. Since ψ is related to a real particle, it cannot have a discontinuity at any boundary where potential changes.

(d) Ψ must be a normalizable function

If at all the particle exists, it must be found somewhere in given region. Inside a wave packet the particle can be found in the region of coordinates (x, y, z), and hence probability density is represented by

$$|\psi(x,y,z)|^2 dxdydz = \text{Probability density}$$

As particle must be found inside the wave packet, the normalization condition implies that the sum of the probabilities over all values of x, y, z must be unity i.e.

$$\int_{-\infty}^{+\infty} |\psi|^2 dxdydz = 1$$

Normalization condition: Whenever the wave functions are normalized, $|\psi|^2 \mathrm{dV}$ equals the probability that a particle will be found in an elemental volume dV. Thus,

Probability, $P = |\psi\, x, y, z\,|^2 dV$

A wave function should always be normalizable as it would give us a definite probability of finding the particle in given space or volume.

A wave function that satisfies all above mathematical conditions is known as a well behaved wave function.

3.9 The need and significance of Schrodinger's equation

- Schrödinger developed wave equations for the matter waves that are associated with a moving particle. They are basically a linear partial differential equation developed to understand the nature of matter waves in a quantum-mechanical system.
- Schrödinger's equation defines the wave properties of sub atomic particles and also predicts particle-like behavior. They predict the future behavior of a dynamic system.
- Schrödinger's equations are basically wave equations predicting the probability of events or outcome.
- Schrödinger's equations predict atomic spectrum of hydrogen, energy levels of Plank's oscillator, non-radiation of electrons in atom, shift in energy levels in a strong electric field, etc.

3.10 Schrödinger's time independent equation *fundamental equation]

Consider a particle of mass ***m*** moving with velocity ***v***. *T*he wavelength of the de Broglie matter waves associated with it is given by

$$\lambda = \frac{h}{p} = \frac{h}{mv} \qquad \text{--- (1)}$$

(a) Differential equation for wave motion

Let a wave function ψ is associated with matter waves. The wave function ψ depend on position coordinates *x*, *y*, *z* and time coordinate *t*.

Differential equation for matter wave motion with wave function ψ and velocity ***v*** can be written as

$$\frac{\partial^2 \Psi}{\partial t^2} = v^2 \left(\frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} + \frac{\partial^2 \Psi}{\partial z^2} \right) \qquad \text{--- (2)}$$

OR

$$\frac{\partial^2 \psi}{\partial t^2} = v^2 \nabla^2 \psi \qquad \text{--- (3)}$$

Where $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$ is known as Lapace Operator

(b) **Differentiation of Wave function ψ**

The wave function ψ can be expressed as a function of space and time as

$$\Psi(x, y, z, t) = \Psi_0 (x, y, z)\, e^{-i\omega t}$$

Or simply

$$\Psi = \Psi_0 e^{-i\omega t} \qquad \text{--- (4)}$$

Differentiating

$$\frac{\partial \Psi}{\partial t} = \Psi_0 e^{-i\omega t} (-i\omega)$$

Differentiating again

$$\frac{\partial^2 \Psi}{\partial t^2} = \Psi_0 e^{-i\omega t} (-i\omega)^2$$

Or

$$\frac{\partial^2 \Psi}{\partial t^2} = -\omega^2 \Psi_0 e^{-i\omega t}$$

Putting $\Psi = \Psi_0 e^{-i\omega t}$

$$\frac{\partial^2 \Psi}{\partial t^2} = -\omega^2 \Psi \qquad \text{--- (5)}$$

(c) **Differential equation for wave function ψ**

Equating (3) and (5)

$$v^2 \nabla^2 \Psi = -\omega^2 \Psi$$

Dividing by v^2

$$\nabla^2 \Psi = -\frac{\omega^2}{v^2} \Psi$$

$$\nabla^2 \Psi + \frac{\omega^2}{v^2} \Psi = 0$$

As $v = \nu\lambda$, and $\omega = 2\pi\nu$ $\qquad \nabla^2 \Psi + \left(\frac{2\pi\nu}{\nu\lambda}\right)^2 \Psi = 0$

$$\nabla^2 \Psi + \frac{4\pi^2 \nu^2}{\nu^2 \lambda^2} \Psi = 0$$

Or $$\nabla^2 \Psi + \frac{4\pi^2}{\lambda^2} \Psi = 0$$

Putting $\lambda = \frac{h}{mv}$ $$\nabla^2 \Psi + \frac{4\pi^2}{\left(\frac{h}{mv}\right)^2} \Psi = 0 \qquad \text{--- (6)}$$

Thus, $$\nabla^2 \Psi + \frac{4\pi^2 m^2 v^2}{h^2} \Psi = 0 \qquad \text{--- (6)}$$

(d)* Total energy of the particle *E

Now, the total energy of particle *E*, is the sum of kinetic energy and potential energy. Thus,

$$E = KE + PE$$

$$E = \frac{1}{2} mv^2 + V,$$ Where, V represents Potential Energy

$$2E = mv^2 + 2V$$

$$mv^2 = 2(E - V)$$

Multiply by *m* $\qquad m^2 v^2 = 2m\,(E - V)$ --(7)

(e) Schrodinger's time independent equation

Putting the value of total energy E from equation (7) into equation (6)

$$\nabla^2 \Psi + \frac{4\pi^2 2m\,(E-V)}{h^2} \Psi = 0$$

Or $$\nabla^2 \Psi + \frac{8\pi^2 m\,(E-V)}{h^2} \Psi = 0$$

Or $$\nabla^2 \Psi + \frac{2m \cdot 4\pi^2 (E-V)}{h^2} \Psi = 0$$

Or $$\nabla^2 \Psi + \frac{2m\,(E-V)}{(h/2\pi)^2} \Psi = 0$$

Now $\hbar = \frac{h}{2\pi}$ is known as reduced Plank's constant. Thus,

$$\nabla^2 \Psi + \frac{2m}{\hbar^2} (E - V)\, \Psi = 0 \qquad \text{--- (8)}$$

This equation is known as Schrödinger's time independent equation. The wave function ψ and Laplace's operator $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$ depends on space coordinates *x*, *y* and *z* and does not depend on time.

3.11 Schrödinger's time dependent equation

Let a wave function ψ is associated with matter waves. The wave function ψ depend on position coordinates *x*, *y*, *z* and time coordinate *t*.

(a) Wave function Ψ in terms of space and time

We can express ψ as a product of two quantities: time dependent and time independent as

$$\Psi\ x, y, z, t = \Psi_0\ x, y, z\ e^{-i\omega t}$$

The term $\psi_0(x, y, z)$ depends on space and the term $e^{-i\omega t}$ depends on time.

This equation can conveniently be written as $\quad \Psi = \Psi_0 e^{-i\omega t}$ --- (1)

(b) Energy eigen operator from Schrödinger's time independent equation

$$\nabla^2\Psi + \frac{2m}{\hbar^2}E - V\ \Psi = 0$$

Or $$\nabla^2\Psi + \frac{2m}{\hbar^2}\ E\Psi - V\Psi\ = 0$$ --- (2)

Or $$\nabla^2\Psi = -\frac{2m}{\hbar^2}(E\Psi - V\Psi)$$

Multiplying by $-\frac{\hbar^2}{2m}$ $$-\frac{\hbar^2}{2m}\nabla^2\Psi = E\Psi - V\Psi$$

Thus, $$-\frac{\hbar^2}{2m}\nabla^2\Psi + V\Psi = E\Psi$$ --- (3)

Where, $E\Psi$ is known as energy eignen operator

(c) Energy eigen operator

Differentiating equation (2) with respect to time,

$$\frac{\partial\Psi}{\partial t} = -i\omega\Psi_0\ e^{-i\omega t}$$

$$\frac{\partial\Psi}{\partial t} = -i\omega\Psi$$

Now $\quad E = h\nu$

As $\quad \omega = 2\pi\nu \quad \nu = \frac{\omega}{2\pi}$

Thus, $\quad E = h\frac{\omega}{2\pi}$

And hence, $$\omega = \frac{2\pi}{h}E = \frac{E}{h/2\pi} = \frac{E}{\hbar}$$ --- (4)

Put value of ω into (3) $$\frac{\partial\Psi}{\partial t} = -i\frac{E}{\hbar}\Psi$$

Or $$E\Psi = -\frac{\hbar}{i}\frac{\partial\Psi}{\partial t}$$

Or $$E\Psi = \frac{i^2}{i}\hbar\frac{\partial\Psi}{\partial t} = i\,\hbar\frac{\partial\Psi}{\partial t}$$ --- (5)

(c) Schrödinger's time dependent equation

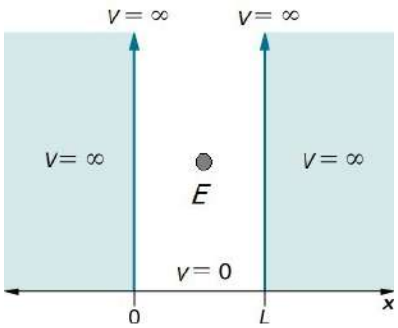
$$-\frac{\hbar^2}{2m}\nabla^2\Psi + V\Psi = i\hbar\frac{\partial\Psi}{\partial t}$$ --- (6)

This equation is known as Schrödinger's time dependent equation. The wave function ψ depends on space coordinates ***x***, ***y*** and ***z*** and also depend on time variable ***t***.

3.12 Particle enclosed in a rigid box [infinite potential well]

If a particle is in a potential well and the total energy of the particle is less than the height of the potential well, it is considered as trapped inside the well. In classical mechanics this particle can vibrate back and forth due to collision with walls but cannot leave the well. In quantum mechanics, it is called as bound state.

Consider a particle is enclosed in a potential well of rigid box having infinite potential. Inside the box motion of particle is restricted between *x*=0 and *x*=*L*. Assuming the collision of the particle with walls as elastic, total energy of the particle *E* remains constant.



The potential energy of the particle is infinite outside the box and it can be considered as zero inside the box.
Thus, the boundary conditions for potential energy are:

$$V\ x = \infty \text{ for } x \leq 0 \text{ and } x \geq L$$

$$V\ x = 0 \text{ for } 0 < x < L$$

The wave function ψ is associated with the particle. As particle cannot leave the box, its probability outside the box is zero. Thus, boundary conditions for wave function are:

$$\psi\ x = 0 \text{ for } x \leq 0$$

And $$\psi\ x = 0 \text{ for } x \geq L$$

To find out the wave function of the particle inside the box, we have to apply Schrödinger's time independent equation.

Step-I: Setting up Schrödinger's equation

Schrödinger's time independent equation is $$\nabla^2 \Psi + \frac{2m}{\hbar^2} E - V\ \Psi = 0 \quad \text{...(1)}$$

Now $$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

As particle is moving in one-dimension along X-axis, y and z coordinates are zero

Thus, ***y***=0, ***z***=0, and Laplace's operator is $$\nabla^2 = \frac{\partial^2}{\partial x^2}$$

Equation (1) thus reduces to $$\frac{\partial^2 \Psi}{\partial x^2} + \frac{2m}{\hbar^2} E - V\ \Psi = 0$$

Inside the box, potential energy of particle *V*=0 $$\frac{\partial^2 \Psi}{\partial x^2} + \frac{2m}{\hbar^2} E \Psi = 0 \quad \text{... (2)}$$

Let $$\frac{2mE}{\hbar^2} = k^2 \quad \text{... (3)}$$

Thus equation (2) reduces to $$\frac{\partial^2 \Psi}{\partial x^2} + k^2 \Psi = 0 \quad \text{... (4)}$$

Step-II: General solution of Schrödinger's equation

Equation (4) is a second order differential equation. Its general solution can be written as

$$\Psi x = A \sin kx + B \cos kx \quad \text{--- (5)}$$

Where *A* and *B* are constants

At x=0, the particle would be present on the boundary and its energy would be infinite i.e. equal to the energy of the potential well. Hence it cannot be present at x=0, and thus its wave function ψ =0 at x=0. By applying boundary condition $\psi x = 0$ for $x \leq 0$, we get

$0 = A \sin kx + B \cos kx$

And $0 = A \sin(k \times 0) + B \cos(k \times 0)$

As $A \sin(k \times 0) = 0$, and $B \cos(k \times 0) = 1$ $B = 0$

Putting *B*=0 in equation (5), $\Psi\ x\ = A \sin kx$ --- (6)

At x=L, the particle would be present on the boundary and its energy would be infinite i.e. equal to the energy of the potential well. Hence it cannot be present at x=L, and thus its wave function ψ =0 at x=L. By applying boundary condition $\psi x = 0$ for $x \geq L$, we get

$\Psi x = 0$ at $x = L$

Putting this in equation (6) $0 = A \sin kL$

But *A*≠0 since Ψ will become zero. Thus $\sin kL = 0$

Above equation implies $kL = n\pi$, where n is integer and *n*≠0

This equation is known as **quantization condition**.

In the equation, $kL = n\pi$, *n*≠0 as it may lead to either

(a) *L*=0. As *L* is the width box the box, *L* cannot be zero

(b) *k*=0. As *k* depends on total energy E of the system, *k* cannot be zero.

3.12 A – Energy of particle

Thus, quantization conidian is $kL = n\pi,$ where $n = 1,2,3,..$ but $n \neq 0$

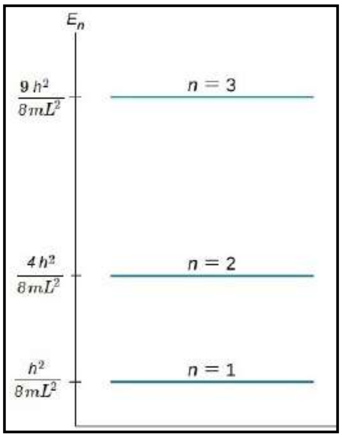
Thus, $k = \frac{n\pi}{L}$

Squaring both sides $k^2 = \frac{n^2\pi^2}{L^2}$

From equation (3) $k^2 = \frac{2mE}{\hbar^2}$

Equating above equations, $\frac{2mE}{\hbar^2} = \frac{n^2\pi^2}{L^2}$

Or $E = \frac{n^2\pi^2\hbar^2}{2mL^2}$



As n is an integer, energy varies as per the values of n. Thus, above equation can be written as $E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}$

As $\hbar = \frac{h}{2\pi}$ $E_n = \frac{n^2\pi^2(\frac{h}{2\pi})^2}{2mL^2} = \frac{n^2h^2}{8mL^2}$

Thus, energy $E_n = \frac{n^2h^2}{8mL^2}$, where n is integer but $n \neq 0$

As ***n*** is integer, from above it is clear that the particle inside an infinite potential well can have only certain discrete values of energies. However, the minimum value of energy can never be zero as ***n* ≠ 0**. These values of energies are known as **energy eigen values**.

Comparison of results in classical and quantum mechanics – Energy of Particle

Sr.	Particular	Classical Mechanics	Quantum Mechanics
1	Energy of particle	A particle enclosed in a rigid box can have any value of energy from 0 to ∞	Only certain discrete values of energy that are integral multiples of $\frac{h^2}{8mL^2}$ are permitted
2	Minimum value of energy	Minimum energy of the particle can be zero.	Minimum energy of the particle cannot be zero.

3.12 B – Wave function of the particle

From equation (6), the wave function ψ of the particle inside the rigid box is given by

$$\Psi(x) = A \sin kx$$

Thus, quantization condition is $kL = n\pi$, where n is integer but $n \neq 0$

As $k = \frac{n\pi}{L}$, $\Psi(x) = A \sin\frac{n\pi x}{L}$

Thus for each energy value E_n, there is a wave function ψ_n which is known as eigen function.

The particle can be found at any location inside the box. It means its probability of finding inside the box is one. Thus, the wave function ψ_n should satisfy normalization condition i.e. the probability that the particle can be found in the region between x=0 and x=L is one.

Thus, $$\int_{x=0}^{x=L} \Psi_n^2 \, dx = 1$$

As $\Psi(x) = A \sin kx$ $$\int_{x=0}^{x=L} A^2 \sin^2\left(\frac{n\pi x}{L}\right) dx = 1$$

$$A^2 \int_{x=0}^{x=L} \sin^2\left(\frac{n\pi x}{L}\right) dx = 1$$

Using, $\sin^2\theta = \frac{1}{2}(1 - \cos 2\theta)$

$$\frac{A^2}{2}\int_{x=0}^{x=L}\left(1 - \cos\frac{2n\pi x}{L}\right) dx = 1$$

Or $$\frac{A^2}{2}\int_{x=0}^{x=L}\left(dx - \cos\frac{2n\pi x}{L} dx\right) = 1$$

Or $$\frac{A^2}{2}\left(\int_{x=0}^{x=L} dx - \int_{x=0}^{x=L}\cos\frac{2n\pi x}{L} dx\right) = 1$$

Or $$\frac{A^2}{2}\left[x - \frac{L}{2\pi n}\sin\frac{2\pi n x}{L}\right]_0^L = 1$$

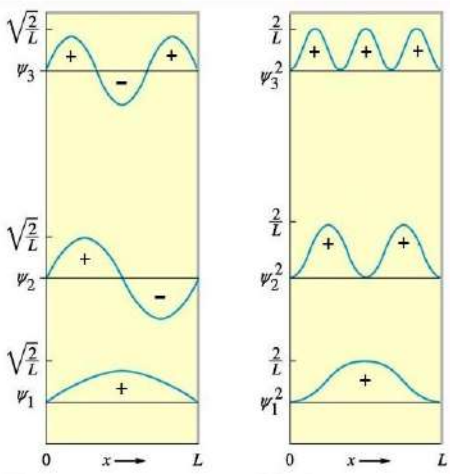
Or $$\frac{A^2}{2}\left[\left(L - \frac{L}{2\pi n}\sin\frac{2\pi n L}{L}\right) - \left(0 - \frac{L}{2\pi n}\sin\frac{2\pi n 0}{L}\right)\right] = 1$$

As $\sin 2\pi n = 1, \sin 0 = 0$ $$\frac{A^2}{2}L = 1$$

Or $$A = \sqrt{\frac{2}{L}}$$

Putting value of A in equation (9) $$\Psi_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)$$

The above equation represents the wave function ψ of the particle enclosed in rigid box of length L. As ψ gives negative probability, probability density i.e. $|\psi|^2$ determines the position of the particle inside the box. The wave function ψ and probability density $|\psi|^2$ of the particle ψ can be plotted as below. The locations where probability densities show peaks are the most probable position of the particle.

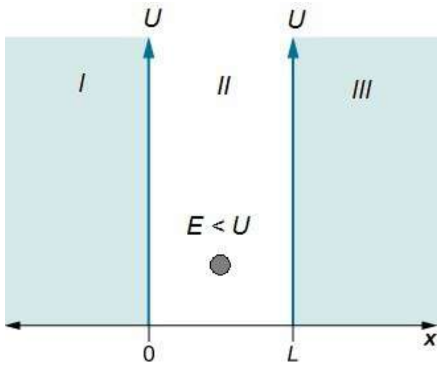


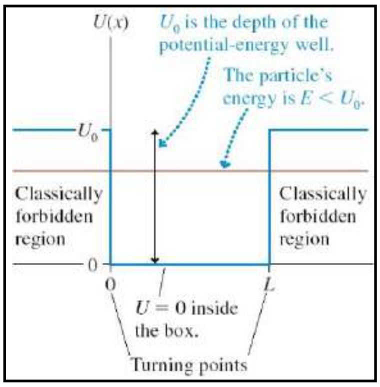
Comparison of results in classical and quantum mechanics – Position of particle

- According to classical mechanics, a particle with any energy can be present at any location inside the box. Quantum mechanically, probability of the particle being present in the box is different according to its quantum number ***n***.
- For example, at *n*=1, $|\psi_1|^2$ i.e. the probability of finding the particle is maximum at L/2
- Similarly, at *n*=2, $|\psi_2|^2$ i.e. probability of finding the particle is maximum at L/4 and L=3L/4

3.13 Particle enclosed in a non-rigid box [Finite potential well]

In real situations potential energies are never infinite and potential barriers of finite height exist. Consider a particle is enclosed in a potential well of energy *U* width *L.* Consider the energy of particle *E* less than *U*. Classically, the particle strikes the walls of the well. It is reflected and cannot enter regions I and III.

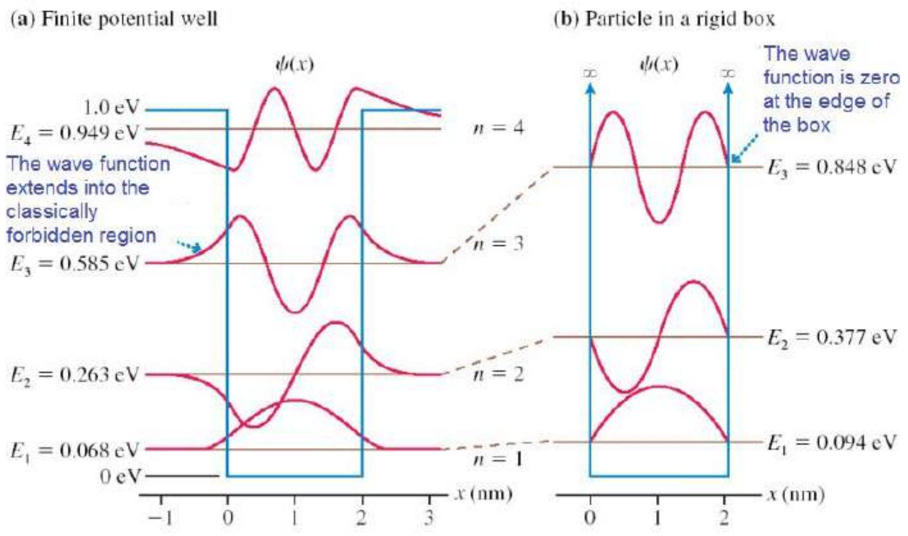




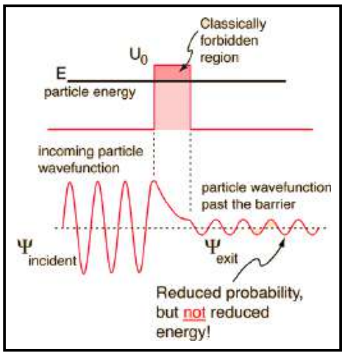
In quantum mechanics, the particle strikes the walls, but now it has a certain non-zero probability of entering into regions I and III even though *E<U*.

Following conclusions can be drawn by solving Schrodinger's equation for non-rigid box of finite potential well.

1. The wave functions are similar to those of infinite well. However, at the boundary wave function is not zero and it also extends a little outside the box. It means probability of particle penetrating through the wall is not zero.
2. Even though the particle energy *E* is less than the potential energy *U*, there is a definite probability that the particle is found outside the box.



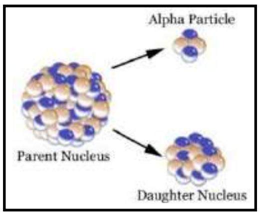
3.14 Tunneling Effect



Consider a particle of energy *E* trying to pass through a barrier of potential energy *U*. When energy of particle $E < U_0$ classically it cannot pass through the potential energy barrier. It is called as forbidden region.

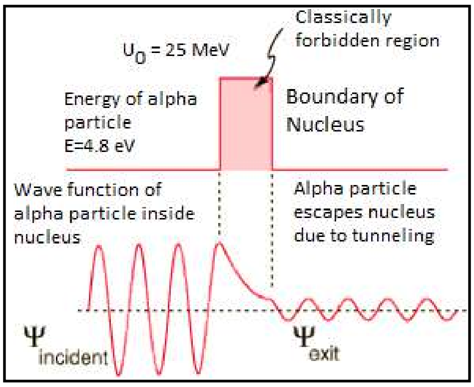
However, quantum mechanically, de Broglie waves are associated with particle. The wave function of particles (and hence the particles itself) has a very small but non-zero probability that it can ***tunnel*** through the barrier. This effect is called as **quantum mechanical tunneling**.

3.14 (a) Alpha Decay



An alpha particle (α particle) consists of two protons and two neutrons bound together ($_2He^4$). Alpha decay is a type of radioactive decay in which an atomic nucleus emits an alpha particle.

Binding energy of α-particle
An α-particle is bounded inside the nucleus, with energy around 25 MeV which is its potential barrier. Thus classically α-particle requires a minimum energy of 25 MeV to escape from the nucleus.



Energy of emitted α-particle
A free α-particle has energy of only around 4.8 MeV. Thus, it is impossible for α-particle to escape from nucleus that has potential barrier of 25 MeV.

Tunneling of α-particle
Quantum mechanically, de Broglie waves are associated with α-particles. The wave function of α-particles (and hence α-particles themselves) has a very small but definite value so that it can "tunnel" through the barrier of binding energy of nucleus and free itself.

The probability of escape of alpha particle is very small i.e. 1 in 10^{38} i.e. alpha particle has to strike potential well of nucleus 10^{38} or more times before it emerges, but it would definitely escape from the nucleus.

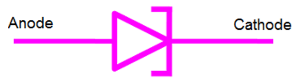
3.14 (b) Tunnel Diode

Doping and potential barrier in normal PN junction diode

In normal PN junction diodes, doping levels are of the order 1 dopant atom in 10^8 atoms of intrinsic semiconductor. Electron cannot move from N region to P region as depletion region acts as a potential barrier. When an external potential difference greater than potential barrier is applied, electrons get sufficient energy to cross the potential barrier and conduction starts.

Tunnel diode

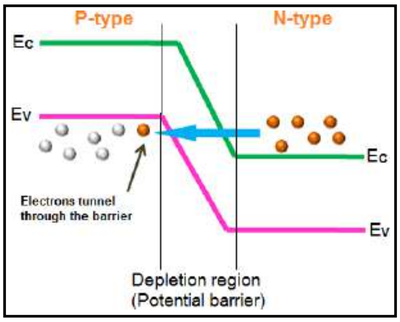
Tunnel diode (or Esaki diode) was invented by Leo Esaki and received Nobel Prize in Physics for the same. It is a PN junction device which exhibits negative resistance. It means when potential difference across tunnel diode is increased, current through it decreased. Tunnel diode is capable of making very fast operations and hence it is useful in microwave frequency region



Tunnel diode symbol

Principle of Tunnel diode

In tunnel diode P and N regions are heavily doped of the order of 1 dopant atom per n 10^3 atoms of intrinsic semiconductor. The width of depletion layer is very narrow which is of the order of 10^{-8} m.



When a very small potential difference is applied across the PN junction, there is a direct flow of electrons across the junctions even when electrons do not have sufficient energy to cross the potential barrier of depletion region.

Quantum mechanically, de Broglie waves are associated with the electrons. The wave function of electrons (and hence electrons themselves) has a very small but definite value so that it can "tunnel" across the depletion region or potential barrier.

Advantages of tunnel diodes

Advantages of tunnel diode are - very fast switching, long life, high-speed operation, low noise, low power consumption

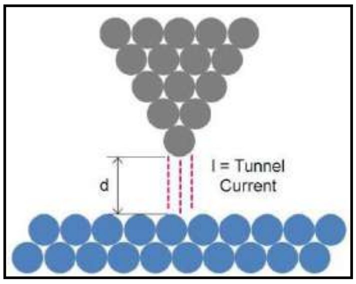
Applications of tunnel diodes

Tunnel diodes are used as logic memory storage devices, relaxation oscillator circuits, ultra high-speed switch, FM receivers, etc.

3.14 (c) Scanning Tunneling Microscope

Scanning Tunneling Microscope (STM) is a non-optical microscope that is used for observing surfaces of materials atom by atom. Gerd Binnig and Heinrich Rohrer developed the first working STM in 1981 at IBM Zurich Research Laboratories in Switzerland for which they were awarded the Nobel Prize in physics in 1986.

Principle of STM



In the STM, sharp tip of a tungsten needle is positioned a few angstroms away from the sample surface. A small voltage is applied between the tip of the probe and the sample surface. Classically, electrons are not permitted to leave the surface of the solid and enter into the regions of space.

Quantum mechanically, de Broglie waves are associated with the electrons. The wave function of electrons (and hence electrons themselves) has a very small but definite value so that it can "tunnel" across the gap between the tip and the sample.

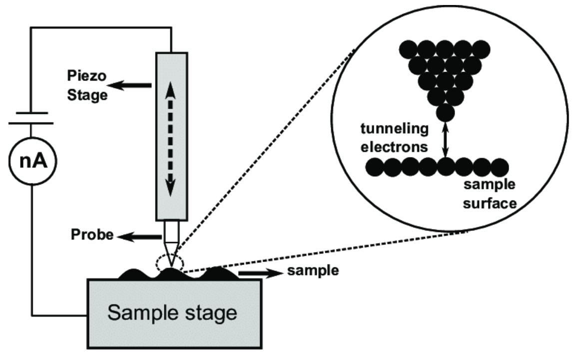
The probability of tunneling electrons decreases exponentially as the distance of the tip from the surface increases. The probe is scanned over the surface of solid. Due to the variation in surface geometry of atoms, the tunneling current changes. When distance between atoms on the surface and tip is minimum, current through tip is maximum. Current is less at other locations. By processing information of position of the probe versus tunneling current, a topographical image of the surface can be created.

Construction of STM

Basically STM include scanning tip, piezoelectric controlled scanner, distance control and scanning unit, vibration isolation system, and computer.

Scanning tip

- The STM has a metal needle that scans a sample horizontally. The needle is so sharp that it has just a single atom on its tip.
- The distance between the tip and the surface is generally in the range of 0.5 to 1.0 nm, i.e. 2 to 4 atomic diameters.
- A small potential difference typically a few milliVolts (mV) to a few Volts (V) is applied to the sample and the STM tip.



Working

Tunnel current

Tip of STM scans the sample surface. The electrons "tunnel" from tip to the sample. This creates a tunneling current of the order of few picoAmperes (pA) to a few nanoAmperes (nA). This current is amplified and given to data processing unit.

Sensitivity of STM

As the tip of the STM moves over the sample surface, its distance continuously changes due to curvature of atoms. Thus, the output current also changes. Approximately, for a distance of an atomic diameter, the current changes by a factor of 1000 times. Thus, STM is very sensitive.

Processing the data

The computer records the tunneling current at each location over the surface and produces a 3D map of the sample surface. The periodic arrangement of atoms is visualized after processing of the data.

Applications of STM

1. STM is used to study the arrangement of individual atoms on the solid surfaces.
2. STM can be used for examining characteristics of material surface including roughness, surface defects and molecular size.

3. The STM can be operated from temperatures ranging from 4 K (- 269 °C) to 973 K. Thus various properties of the solids can be studied at lower and higher temperatures.
4. The strong electric field between tip and sample has been utilized to remove atoms from the sample surface and drop or deposit the removed atoms at other location. Thus STM can manipulate atoms and plays very important role in nanotechnology.

3.15 Introduction to Quantum Computing

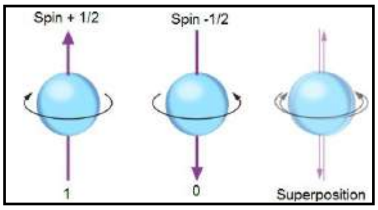
Principle and limitation of classical computing

Classical computing relies on principles of Boolean algebra and logic gates. Data is processed in binary system that is, either 0 (off / false) or 1 (on / true) that are called as bits. The transistors and capacitors in CPU can only be in one state at any point either in 0 or 1. For more processing power, we need small dimensional transistors in large density on chip of the processor. Thus, we need to reach very smaller dimension of materials in the range of few nanometers. At this nano scale, a threshold is reached and quantum mechanical effects such tunneling, uncertainty principle comes becomes dominant. Hence, there is limit to the size of transistors at nano level and also on its processing power.

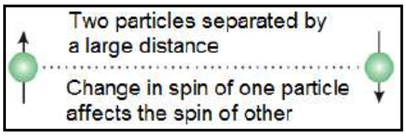
Principle of quantum computing

Quantum computing applies the properties of quantum physics to process information. A number of elemental particles such as electrons or photons can be used for storing the information. Either the charge of particles or polarization acts as a representation of 0 and/or 1. Each of these particles is known as a quantum bit, or qubit. A qubit is a unit of quantum information. Quantum computer uses mainly two principles of quantum mechanics superposition and entanglement.

(a) **Superposition:** A qubit can hold both values (0 and 1) at the same time which known as a superposition state. Thus, at one time the number of computations possible in a quantum computer is 2^n, where n is the number of qubits used. For example, a quantum computer consisting of 500 qubits has a potential to perform 2^{500} calculations in a single step.



(b) **Entanglement:** Entanglement is correlation between particles acting as q-bits such as photons, electrons. By knowing the spin state of one entangled particle (up or down) we can know the spin of its correlated particle. Quantum entanglement allows qubits separated by distances to interact with each other instantaneously. When multiple qubits act coherently, they can process multiple operations simultaneously. Thus, large information is processed within a fraction of the time.



Speed of Quantum Computer

A classical computer has processing speed of few gigahertzes. Thus about 10^9 operations are possible per second. In quantum computing the processing speed is measured in teraflops. Thus about 10^{12} operations can be performed per second. In 2015, Google and NASA reported that then developed 1097-qubit D-Wave quantum computers would be almost 100 million times faster than a regular computer chip. It is estimated that quantum computer would process the information within few seconds that classical computer would take 10,000 years to solve.

Potential Applications of Quantum Computing

Currently, quantum computers are in the stage of development. Based on estimation, it is predicted that quantum computers has tremendous potential to deal with many challenges that are almost impossible to handle by the existing classical computers.

Artificial intelligence: Artificial intelligence requires analysis of data from images, videos and text. This data is available in vast quantity. For analyzing and processing this huge data, traditional computers would require thousands years. Quantum computers would be able to process this data in few seconds.

Drug Design: For many of the drugs, it requires trial and error methods to understand how they will react. These methods are very expensive, complex and require much processing time. Using quantum computers the process can be simulated more effectively.

Financial Optimization: Currently classical computers are analyzing many financial tasks such as market analysis, estimated returns, risk assessment, financial transactions, etc. It requires complex algorithms and tremendous computational time. By utilizing quantum technology great improvements could be achieved in terms of time saving and more accuracy.

Development of new materials: In materials science to develop new materials or to increase efficiency of existing materials, it requires lot of simulating. Although classical computers deal with these simulations, they have limitations in terms of speed, accuracy and time. Quantum computers would be able to deal with these challenges more effectively.

Logistics and scheduling: In industry optimizations are used in logistics and scheduling. Few examples, to optimize route based on real time traffic analysis. At present classical computing is heavily used to optimize these tasks. Some of the processes are very complicated for classical computers to handle. Quantum computing would be able to perform these tasks provide a solution in terms of less time and more accuracy.

Cyber Security: Cyber security is one of the biggest challenges of today. Malware and viruses spread through internet within fraction of seconds. It is very difficult for classical computing to handle these threats. Various techniques can be developed to deal with cyber security threats using quantum machine learning approaches.

Dealing with encryption: Security encryption methods are heavily used in defense, financial sectors, banks, user data security, etc. Despite of heavy deployment of security measures using classical computing, these organizations are under constantly under threat of cyber attack. The complex encryptions such as 2048 bit RSA encryptions are extremely difficult to deal with existing computing technologies. It would take around 10^{15} years for classical computers to decode these algorithms. It has been demonstrated that quantum computing would deal with these tasks very easily.

Software testing, Fault Simulation: Very large software programs have billions of lines of codes. Using classical computers, it becomes difficult and expensive to verify the correctness of the codes. Quantum computers can deal with these tasks very efficiently.

Questions on: Quantum Mechanics

6 Marks

1. Derive Schrodinger's time independent wave equation. ***[Dec 19, 6m]***
2. What is significance of Schrodinger's equation? Derive Schrodinger's time dependent wave equation. ***[Dec 19, 6m]***
3. State and explain Heisenberg's uncertainty principle. Explain it by the concept of narrow and broad wave packet. ***[Dec 19, 4m]***
4. State and explain Heisenberg's uncertainty principle. Derive the expression in terms of energy and time.
5. Derive the equation for energy of a particle enclosed in one dimensional rigid box (infinite potential well).
6. Derive the equation of wave function of a particle enclosed in one dimensional rigid box (infinite potential well).
7. What is tunneling effect? Explain principle and working of scanning tunneling microscope (STM). State applications of STM.

4 Marks

1. State de Broglie hypothesis. Derive the equation of de Broglie wavelength by analogy with radiation.
2. State de Broglie hypothesis. Derive the equation of de Broglie wavelength of a particle in terms of its Kinetic Energy.
3. State de Broglie hypothesis. Derive the equation of de Broglie wavelength of an electron when it is accelerated by a potential difference V.
4. State de Broglie hypothesis. Derive the equation of de Broglie wavelength of a proton when it is accelerated by a potential difference V.
5. State de Broglie hypothesis and explain any three properties of matter waves. ***[Dec 19, 4m]***
6. Define phase velocity and group velocity. Explain why the concept of phase velocity is meaningless and that of group velocity is significant.
7. State and explain Heisenberg's uncertainty principle.
8. What is wave function ψ? Explain physical significance of $|\psi|^2$. ***[Dec 19, 4m]***
9. State and explain mathematical conditions that wave function ψ need to obey. What is well behaved wave function?
10. What is condition of normalization of wave function? Explain why a wave function should be normalized.
11. Explain quantum mechanical tunneling effect and its role in alpha decay.
12. Explain quantum mechanical tunneling effect. How this principle is applied in tunnel diode?
13. Explain tunneling effect. Explain this principle is applied in scanning tunneling microscope. ***[Dec 19, 4m]***
14. Explain in brief, principle of quantum computing. State the potential applications of quantum computers.

Numericals on: Quantum Mechanics

Formulae:

1. Momentum of particle with KE 'E' = $p = \sqrt{2mE}$
2. de-Broglie wavelength in terms of its kinetic energy: $\lambda = \frac{h}{\sqrt{2mE}}$
3. de-Broglie wavelength for a particle accelerated by Potential Difference V: $\lambda = \frac{h}{\sqrt{2meV}}$
4. Heisenberg's Uncertainty Principle: $\Delta x . \Delta p_x = h$
5. Energy of a particle enclosed in a rigid box: $E_n = \frac{n^2 h^2}{8 m L^2}$

<u>De Broglie wavelength in terms of Energy and Potential Difference</u>

Example: *Calculate de-Broglie wavelength for a proton moving with velocity of 1 percent of velocity of light.*

Solution: m_p = 1.673x10^{-27} kg, h=6.63x10^{-34} J.s,

Velocity of proton= 1% of velocity of light = $\frac{1}{100} \times 3 \times 10^8 = 3 \times 10^6$m/s

de-Broglie wavelength = $\lambda = \frac{h}{mv} = \frac{6.63\times10^{-34}}{1.673\times10^{-27}\times3\times10^6} = 1.32 \times 10^{-13}$ m

Example: *Calculate the de-Broglie wavelength of an electron of energy 1 keV.*

Solution: Energy of electron = E = 1 keV = 1.6x10^{-19}x10^3 eV J = 1.6x10^{-16} J

Mass of electron = 9.1x10^{-31} kg

de-Broglie wavelength = $\lambda = \frac{h}{\sqrt{2m_e E}} = \frac{6.63\times10^{-34}}{\sqrt{2\times9.1\times10^{-31}\times1.6\times10^{-16}}} = 3.88 \times 10^{-11} m = 0.338\ AU$

Example: *Calculate the de-Broglie wavelength of a 10 keV proton.*

Solution: Energy of proton = E = 10 keV = 10x1.6x10^{-19}x10^3 eV J = 1.6x10^{-15} J

Mass of proton = 1.673 x 10^{-27} kg

$$\lambda = \frac{h}{\sqrt{2m_p E}} = \frac{6.63 \times 10^{-34}}{\sqrt{2 \times 1.67 \times 10^{-27} \times 1.6 \times 10^{-15}}} = 2.862 \times 10^{-13}\ \mathrm{m} = 0.00286\ \mathrm{AU}$$

Example: *A neutron has a de Broglie wavelength of 0.1 A^0. Calculate its energy in eV in ground state.*

Solution: λ = 0.1 A^0 = 0.1 x 10^{-10} m, mass of neutron = 1.673x10^{-27} kg

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

$$E = \frac{h^2}{2 \times m \times \lambda^2} = \frac{(6.63 \times 10^{-34})^2}{2 \times 1.673 \times 10^{-27} \times (10^{-11})^2} = 1.310 \times 10^{-18} J = 8.18\ eV$$

Example: *What accelerating potential would be required for a proton with a zero initial velocity to acquire a velocity corresponding to its de-Broglie wavelength of 1 AU. [m_p=1.673x10^{-27} kg]*

Solution: De-Broglie wavelgth of proton = $\lambda_p = \frac{h}{\sqrt{2 m_p eV}}$

λ_p = 1 AU = 10^{-10} m, m_p = 1.673x10^{-27} kg

$(\lambda_p)^2 = \frac{h^2}{2 m_p eV}$

$$V = \frac{h^2}{2 m_p e (\lambda_p)^2} = \frac{(6.63 \times 10^{-34})^2}{2 \times 1.673 \times 10^{-27} \times 1.6 \times 10^{-19} \times (10^{-10})^2} = \frac{4.39 \times 10^{-67}}{5.33 \times 10^{-66}} = 0.082\ \mathrm{V}$$

Example: *Find energy associated with a photon of wavelength 1 Å and an electron of wavelength 1 Å.*

Solution:

For a photon, $E = h\nu = \frac{hc}{\lambda} = \frac{6.63\times10^{-34}\times3\times10^{8}}{1\times10^{-10}} = 1.986\times10^{-15}\,\mathrm{J} = \mathbf{12.39\ keV}$

For electron, $\lambda = \frac{h}{\sqrt{2\,m\,E}}$

$$E = \frac{h^2}{2m\lambda^2} = \frac{\left(6.63\times10^{-34}\right)^2}{2\times9.1\times10^{-31}\times\left(1\times10^{-10}\right)^2} = 2.409\times10^{-17}\,\mathrm{J} = \mathbf{150.41\ eV}$$

Example: *A proton and an alpha particle are accelerated by the same PD. Find the relation between their de-Broglie wavelengths.*

Solution: Mass of alpha particle = 4 x (mass of proton)

For proton, $\lambda_p = \frac{h}{\sqrt{2\,m_p E_p}}$

Energy of proton accelerated by PD "V",

E_p = (charge on proton) x PD

E_p = eV

For alpha particle, $\lambda_\alpha = \frac{h}{\sqrt{2\,m_\alpha E_\alpha}}$

Energy of alpha particle accelerated by PD "V",

E_α = (charge on alpha particle) x PD = 2 eV

Ratio: $\frac{\lambda_p}{\lambda_\alpha} = \sqrt{\frac{2\,m_\alpha E_\alpha}{2\,m_p E_p}} = \sqrt{\frac{m_\alpha\,(2eV)}{m_p\,(eV)}} = \sqrt{\frac{2\times m_\alpha}{m_p}} = \sqrt{\frac{2\times4\times m_p}{m_p}} = \sqrt{\frac{8}{1}} = 2.828$

Heisenberg Uncertainty Principle

Example: *If uncertainty in the position of a particle is equal to de Broglie wavelength, show that uncertainty in velocity is equal to the velocity of the particle assuming product of uncertainties as 'h'.* ***[Dec 19, 4m]***

Solution: Uncertainty in position Δx =λ

According to Uncertainty principle,

$$\Delta x.\Delta p_x = h \ \text{or}\ \ \Delta x.(m.\Delta v_x) = h$$

$$\therefore \Delta v_x = \frac{h}{m.\Delta x} = \frac{h}{m.\lambda}$$

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

$$\therefore \Delta v_x = \frac{h}{m\,\frac{h}{mv}} = \boldsymbol{v}$$

Example: *An electron is confined to a box of length 2AU. Calculate the minimum uncertainty in its velocity.*

Solution: According to Uncertainty principle,

$\Delta x.\Delta p_x = h$ or $\Delta x.(m.\Delta v_x)$

Thus, $\Delta v_x = \frac{h}{m\,\Delta x} = \frac{6.63\times10^{-34}}{9.1\times10^{-31}\times2\times10^{-10}} = 3.636\times10^{6} m/s$

Example: *An electron has a speed of 600 m/s with an accuracy of 0.005 %. Find the uncertainty in its position.*

Solution: v= 600 m/s, *Δ*v= 0.005% of v = 600 x (0.005/100) = 0.03 m/s

According to Uncertainty principle, $\Delta x.\Delta p = h$

$$\Delta x = \frac{h}{\Delta p} = \frac{h}{m\Delta v} = \frac{6.63\times10^{-34}}{9.1\times10^{-31}\times0.03} = 0.024\ \mathrm{m}$$

Example: *The position and momentum of 1 keV electron are simultaneously measured. If its position is located within 1A⁰, find the uncertainty in its momentum.*

Solution: According to Uncertainty principle, $\Delta x.\Delta p = h$

Uncertainty in position = Δx= $1A^0$

Uncertainty in momentum = $\Delta p = \frac{h}{\Delta x} = \frac{6.63\times10^{-34}}{1\times10^{-10}} = 6.63 \times 10^{-24}$ kg.m/s

Example: *An electron accelerated by a potential difference 1 kV. Its position and momentum are measured simultaneously. If its position is located within 1 AU, find the percentage of uncertainty in its momentum.*

Solution: V= 1 kV = 1000 V

$$\lambda = \frac{h}{2\,meV} = \frac{6.63\times10^{-34}}{2\times9.1\times10^{-31}\times1.6\times10^{-13}\times1000} = 0.387\times10^{-10}\,\text{m}$$

Momentum of electron = $p = \frac{h}{\lambda} = \frac{6.63\times10^{-34}}{0.387\times10^{-10}} = 1.17\times10^{-23}\,kg\,m/s$

$\Delta x.\Delta p_x = h$

$\Delta p_x = \frac{\text{h}}{\Delta\text{x}} = \frac{6.63\times10^{-34}}{1\times10^{-10}} = 0.664\times10^{-23}\,\text{m/s}$

Thus, change in momentum = $\frac{1.71-0.664}{1.71}\times 100 = 61\%$

Energy of particle trapped in infinite potential well

Example: *Lowest energy of an electron trapped in a potential well is 38 eV. Calculate the width of the potential well in A.U.* ***[Dec 19, 4m]***

Solution: E_1 = 38 eV = 38 x 1.6 x 10^{-19} Joules

The lowest energy of electron is then given by $\text{E}_1 = \frac{1^2.\text{h}^2}{8.\text{m}.\text{L}^2}$

where L is the width of the well.

$$\text{L}^2 = \frac{1^2.\text{h}^2}{8.\text{m}.\text{E}_1} = \frac{\text{n}^2\times 6.63\times10^{-34\,2}}{8\times9.1\times10^{-31}\times38\times1.6\times10^{-19}} = 9.895\times10^{-21}$$

Thus, $L = \sqrt{9.895\times10^{-21}} = 9.947\times10^{-11} = 0.9947\,AU \cong 1\,AU$

Example: *The lowest energy of an electron trapped in a rigid box is 4.19 eV. Find width of the box in AU.*

Solution: E_1 = 4.19 eV = 4.19 x 1.6 x 10^{-19} = 6.704x10^{-19} Joules

The lowest energy of electron is then given by $\text{E}_1 = \frac{1^2.\text{h}^2}{8.\text{m}.\text{L}^2}$

where L is the width of the well.

$$\text{L}^2 = \frac{1^2.\text{h}^2}{8.\text{m}.\text{E}_1} = \frac{\text{n}^2\times 6.63\times10^{-34\,2}}{8\times9.1\times10^{-31}\times6.704\times10^{-19}} = 8.974\times10^{-20}\ \text{m}$$

$$\text{or L} = 2.995\times10^{-10}\,m = 2.995\,AU \cong 3\,AU$$

Example: *Calculate the first eigen value of electron in eV trapped in a rigid box of length 1 AU*

Solution: Width of potential well = 1 A^0 =10^{-10} m, n=1

Formula: $\text{E}_\text{n} = \frac{\text{n}^2\,\text{h}^2}{8\text{m}\,\text{L}^2}$

$$\text{E}_1 = \frac{1\times 6.63\times10^{-34\,2}}{8\times9.1\times10^{-31}\times(10^{-10})^2} = 0.603\times10^{-17}\ \text{J} = 37.60\ \text{eV}$$

Example: *A neutron is trapped in infinite potential well of width 10⁻¹⁴ m. Calculate its first energy eigen value in eV.*

Solution:

m_n= 1.675x10^{-27} kg, h = 6.63x10^{-34} J.s, Width of potential well = 10^{-14} m, n=1

Formula: $\text{E}_\text{n} = \frac{\text{n}^2\,\text{h}^2}{8\text{m}\,\text{L}^2}$

$$E_1 = \frac{(1\times 6.63\times10^{-34})^2}{8\times1.675\times 10^{-27} \times (10^{-14})^2} = 3.276 \times 10^{-13}\ \text{J} = 2.045 \times 10^{6}\ \text{eV} = 2.045\ MeV$$

Example: *A neutron is trapped in infinite potential well of width 1A^0. Calculate the values of energy and momentum in its ground state. [m_n= 1.675x10^{-27} kg, h = 6.63x10^{-34} J.s]*

Solution: Width of potential well = 1 A^0 =10^{-10} m, n=1

Formula: $E_n = \frac{n^2 h^2}{8m L^2}$

$$E_1 = \frac{(1\times 6.63\times10^{-34})^2}{8\times1.675\times 10^{-27} \times(10^{-10})^2} = 3.276 \times 10^{-21}\ \text{J} = 0.02\ \text{eV}$$

Momentum = $p = \sqrt{2mE_1} = \sqrt{2 \times 1.675 \times 10^{-27} \times 3.276 \times 10^{-21}} = 3.312 \times 10^{-24} kg.m/s$

Example: *Calculate the energy difference between the ground state and first excited state of an electron in the rigid box of length 1 A^0. [Plank's constant = h = 6.63x10^{-34} Js, Mass of electron = m = 9.1 x 10^{-31} kg]*

Solution:

Length of the rigid box = 1A^0 = 10^{-10} m

Formula: Energy of the particle $E_n = \frac{n^2h^2}{8mL^2}$

For ground state, n=1 $E_1 = \frac{h^2}{8mL^2}$

For first excited state, n=2 $E_2 = \frac{4h^2}{8mL^2}$

The difference in two states = $E_2 - E_1 = (4-1)\frac{h^2}{8mL^2}$

$= (4-1)\frac{(6.63\times10^{-34})^2}{8\times9.1\times10^{-31}\times(10^{-10})^2}$

= $1.807 \times 10^{-17} J$

= 112.80 eV