3. QUANTUM MECHANICS

MILESTONE

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1. Introduction

- Quantum mechanics (QM) is a physical science dealing with the behavior of matter and energy on the scale of atoms and subatomic particles / waves.
- Quantum mechanics (QM) gives accurate prediction of the physical behavior of systems, including systems where Newtonian mechanics fails.
- Although foundations of QM started in early 1800s, its real beginnings date from the work of Max Planck in 1900 and Planks hypothesis serve as one of the fundamental equations in QM.

- Quantum mechanics plays important role in various engineering fields such as electrical engineering, material engineering, electronics engineering, transistor and semiconductor designing, nanomaterials, photonics, spintronics, quantum computing etc.
- Plank's theory of thermal radiation, Einstein explanation of photoelectric effect, Compton effect, emission and absorption of radiation by substance, black body radiation proves that electromagnetic radiation consist of discrete invisible packet of energy ($h\nu$) is known asphoton hence proves particle nature of radiation.
- On other hand, macroscopic optical phenomenon like interference, diffraction and polarization proved wave nature of electromagnetic radiation.
- From the second conclusion, we can say that EM radiation has dual nature. In certain situation proves wave nature and in other prove particle nature.
- These wave and particle are only modes of energy transmission from one place to other.
- A particle means an object having definite position in space and they are identifiable by their properties like mass, momentum, K.E., spin and electric charge.
- A wave means periodically repeated pattern in space which specified by wavelength, frequency, amplitude of disturbance, intensity.
- These two properties wave & particle of radiation can never be observed simultaneously.
- This new and overwhelming/ cover completely ability of electromagnetic radiation itself proves wave and particle nature and is now known as wave-particle dualism.

2. Wave-Particle Duality of Radiation and Matter

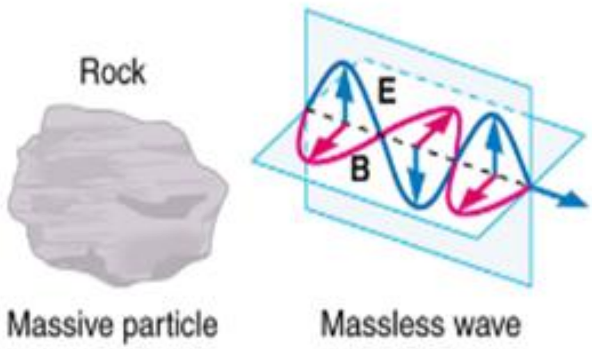


Figure On a classical scale (macroscopic), particles with mass behave as particles and not as waves. Particles without mass act as waves and not as particles.

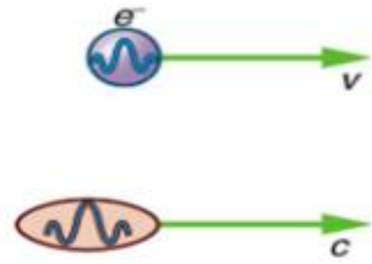


Figure On a quantum-mechanical scale (i.e., very small), particles with and without mass have wave properties. For example, both electrons and photons have wavelengths but also behave as particles.

- We know all object in our environment are composed of matter.
- Matter consists of a large number of Particles of atomic dimensions.
- The material particle in motion specified by mass (m), velocity (V), momentum (P=mv) and energy(E).
- Different phenomenon like photoelectric effect, black body radiation etc, have proved that Electromagnetic radiation has particle nature.
- Optical phenomenon like interference and diffraction have proved that Electromagnetic radiation has wave nature.
- We call this twofold nature the particle-wave duality, meaning that EM radiation has both particle and wave properties.
- The EM radiation we once thought to be a pure wave has particle properties, similarly, matter has both particle and wave properties.
- De-Broglie proposed that like radiation, matter should also exhibit wave nature.
- De Broglie took both relativity and quantum mechanics into account to develop the proposal that all particles have a wavelength.

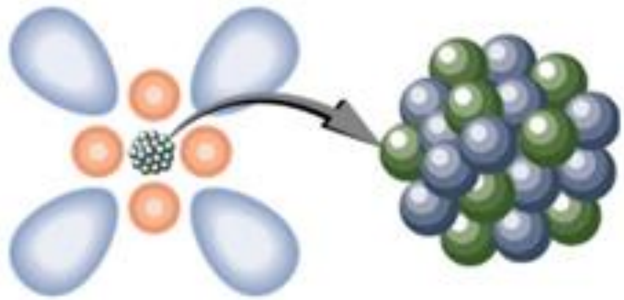
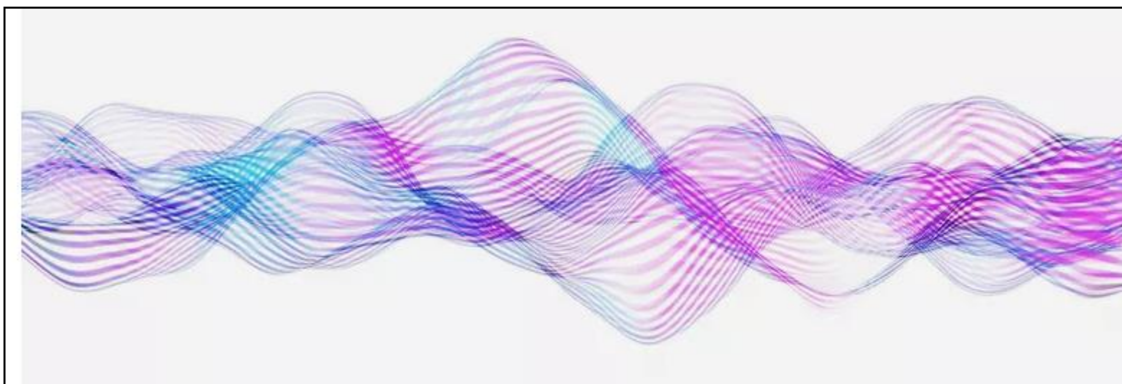


Figure Atoms and their substructure are familiar examples of objects that require quantum mechanics to be fully explained. Certain of their characteristics, such as the discrete electron shells, are classical physics explanations. In quantum mechanics we conceptualize discrete "electron clouds" around the nucleus.

3. De-Broglie's hypothesis

- In 1924, Louis de Broglie proposed a new speculative hypothesis that electrons and other particles of matter can behave like waves and wave-particle duality is not property of radiation but it is a universal characteristic of nature.



- According to him, although matter composed of particles and shows particle nature, but it can also exhibit a wave like property.
- According to De-Broglie's hypothesis "a moving particle always has a wave associated withit and motion of particles is guided by that wave in a similar manner as photon controlled by a wave.'
- The particle-wave duality refers to the fact that all particles—those with mass and

those without mass—have wave characteristics.

- For any photon,

$$\nu = \frac{E}{h}, \& \ \ \lambda = h/p.$$

From these equations, left hand side of these equation show wave aspect (frequency and wavelength) and R.H.S. shows particle nature (energy and momentum).

- Therefore, Plank's constant (h) acts as a bridge between particle and wave aspects.
- The de Broglie wavelength λ, associated with a particle and is related to its momentum, through the Planck's constant;

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

Where, m= mass of material particle and v- velocity

- The expression for wavelength can be derived using Planks -Einstein equations

$$E = h\nu \ \ - - - - - - - - -(2)$$

$$E = mc^2 - - - - - - - - -(3)$$

From above equation we have;

$$h\nu = mc^2$$

$$\therefore h\nu = mc \times c$$

$$\therefore h\nu = p \times \nu\lambda$$

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

De-Broglie wavelength in terms of K.E

We know

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

But $$E = \frac{mv^2}{2} = \frac{m^2v^2}{2m}$$

$$= \frac{p^2}{2m}$$

$$p^2 = 2mE$$

$$p = \sqrt{2mE}$$

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

This is De-Broglie wavelength (λ) in terms of kinetic energy (E)

De-Broglie wavelength in terms of Potential difference (P.D)

- To calculate the De-Broglie wavelength of electron, we know that for an electron kinetic energy is provided by electrical energy.

∴Kinetic energy = Electrical energy

$$\frac{mv^2}{2} = eV$$

$$\frac{m^2v^2}{2m} = eV$$

$$\frac{p^2}{2m} = \text{eV}$$

$$p^2 = 2meV$$

$$p = \sqrt{2meV}$$

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2meV}}$$

$\lambda = \frac{12.26}{\sqrt{V}} A^0$ For Electron only

Where,

$$h = 6.63 \times 10^{-34} J.S.$$

$$m_e = 9.1 \times 10^{-31} Kg$$

$$e = 1.6 \times 10^{-19} C.$$

4. Concept of group velocity and phase velocity

https://in.pinterest.com/pin/354940014355556566/

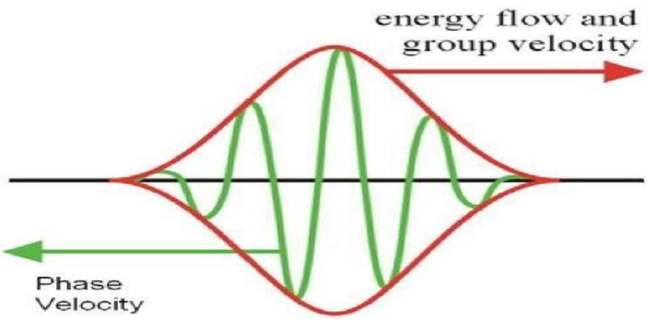
http://cs.westminstercollege.edu/~ccline/courses/phys301/GroupPhaseVelocity/vpvg.html

Phase velocity

- The velocity with which wave propagates is phase velocity (Vp).
- The phase velocity of a wave is the rate at which the wave propagates in some medium.
- The phase velocity also known as wave velocity of monochromatic wave is the velocity with which definite phase (i.e. crest, trough etc) of wave propagates in medium.

Group velocity

- Wave group is a series of individual waves of different wavelength, when interfere with each other results in variation in amplitude and the velocity with which hump i.e. wave group travels is called group velocity (Vg).



Group Velocity

- Consider formation of wave group by superposition of two waves of same amplitude A but slightly different angular frequencies (ω) and propagation constants (k).
- Let two waves be expressed as,

  $y1 = Asin\ (\omega t - kx)$

  $y2 = Asin\ [(\omega + d\omega)t - (k + dk)x]$
- The resultant displacement Y at any time t and position x is given by,'

$$Y = y1 + y2$$

$$Y = A\ sin\ (\omega t - kx) + Asin\ [(w + d\omega)t - (k + dk)x]$$

We know, $SinC + SinD = 2Sin\ [(C + D)/2]xCos[(C - D)/2$

$$Y = 2ACos\left\{\left[\left(\frac{d\omega}{2}\right)t\right] - \left[\left(\frac{dk}{2}\right)x\right]\right\}x$$

$$Sin\{[(2\omega + d\omega)/2)t] - [(2k + dk/2)x]\}$$

- But dω& dk are very small as compared to ω& k respectively.
- But $2\omega + d\omega\ \approx 2\omega$

$$2k + dk\ \approx 2k$$

$$Y = 2ACos\left\{\left[\left(\frac{d\omega}{2}\right)t\right] - \left[\left(\frac{dk}{2}\right)x\right]\right\}x\ Sin(\omega t - kx)$$

- This equation shows wave of angular frequency (ω) and propagation constant (k).
- The amplitude varies as per cosine term with angular frequency (d ω /2)

andPropagation constant (dk/2).

- The effect of this amplitude variation is to produce successive wave groups.
- The wave velocity or phase velocity is,

$Vp \ = \nu\lambda \ = \ 2\pi\nu/(2\pi/\lambda) = \ \omega/k$ --------------- Phase velocity

And group velocity is given by,

$$Vg \ = \ d\omega/dk$$

Relation between phase velocity and group velocity

- We know,

$$Vp \ = \frac{\omega}{k} ----------- (1)$$

$$Vg = \frac{d\omega}{dk} ------------(2)$$

$Diff. eqn$ (1) $w.r.t.k$

$$dVp/dk = (1/k)[(d\omega/dk) - (\omega/k)]$$

$$k\left(\frac{dVp}{dk}\right) = \left[\left(\frac{dw}{dk}\right) - \left(\frac{\omega}{k}\right)\right]$$

$$k(dVp/dk) \ = \ Vg - Vp$$

$Vg = Vp + k(dVp/dk)$----------------- (3)

$$Or$$

$Vg = Vp - \ \lambda(dVp/d\lambda)$ ------------------- (4)

Equation (3) and (4) shows relationship between phase velocity and group velocity.

Relation between phase velocity and group velocity for De-Broglie's wave

We know,

$\omega = \ 2\pi\nu$

$$= 2\pi E/h$$

$$= \frac{2\pi mc^2}{h}$$

$$\omega = \frac{2\pi m_0 c^2}{h\sqrt{1-\frac{v^2}{c^2}}} \text{ --------------- (1)}$$

$$K = \frac{2\pi}{\lambda}$$

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

$$= \frac{2\pi mv}{h}$$

$$K = \frac{2\pi m_0 v}{h\sqrt{1-\frac{v^2}{c^2}}} \text{ ---------------- (2)}$$

Divide equation (1) by (2)

$$\frac{\omega}{k} = \frac{2\pi m_0 c^2}{h\sqrt{1-\frac{v^2}{c^2}}} \times \frac{h\sqrt{1-\frac{v^2}{c^2}}}{2\pi m_0 v}$$

$$\boldsymbol{Vp = \frac{\omega}{k} = \frac{c^2}{v}} \text{ --------------------- (3)}$$

$$v_g = \frac{d\omega}{dk} = \frac{d\omega/dv}{dk/dv}$$

$$\frac{d\omega}{dv} = \frac{2\pi m_0\, v}{h}\left(1-\frac{v^2}{c^2}\right)^{\frac{-3}{2}} \text{---------------(4)}$$

$$\frac{dk}{dv} = \frac{2\pi m_0}{h}\left(1-\frac{v^2}{c^2}\right)^{-\frac{3}{2}} \text{-------------- (5)}$$

Divide (4) by (5)

$$v_g = \frac{d\omega}{dk} = \frac{d\omega/dv}{dk/dv} = v$$

$$Vg = v$$

$$Vp = \frac{c^2}{v} = \frac{c^2}{v_g}$$

$$v_p \times v_g = c^2$$

- This is relation between phase velocity and group velocity.

5. Heisenberg Uncertainty Principle

- In 1927, Heisenberg proposed a very interesting principle, which directly explains difficulty produced due to dual nature of matter, known as uncertainty principle.
- In classical mechanics, a moving particle at any instant has fixed position in space and a definite momentum.
- In wave mechanics particle is described in terms of wavelength.
- After de Broglie proposed the wave nature of matter, many physicists, including Schrödinger and Heisenberg, explored the consequences. The idea quickly emerged that, because of its wave character, a particle's trajectory and destination cannot be precisely predicted for each particle individually.
- A particle is always localized in space and hence a wave packet or wave group represents moving particle. The particle lies somewhere in wave packet and probability of finding particle at given point is proportional to wave amplitude at that point.

- Therefore, although particle lies within, wave packet moving with group velocity, it is impossible to determine exact position and exact velocity at any particular moment.
- There is always certain uncertainty in experimental measurement of position and momentum of particle of small size like an electron in motion.
- There is a certain *probability* of finding the particle at a given location, and the overall pattern is called a probability distribution.

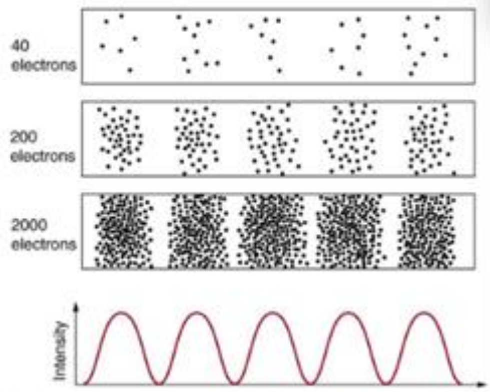


Figure The building up of the diffraction pattern of electrons scattered from a crystal surface. Each electron arrives at a definite location, which cannot be precisely predicted. The overall distribution shown at the bottom can be predicted as the diffraction of waves having the de Broglie wavelength of the electrons.

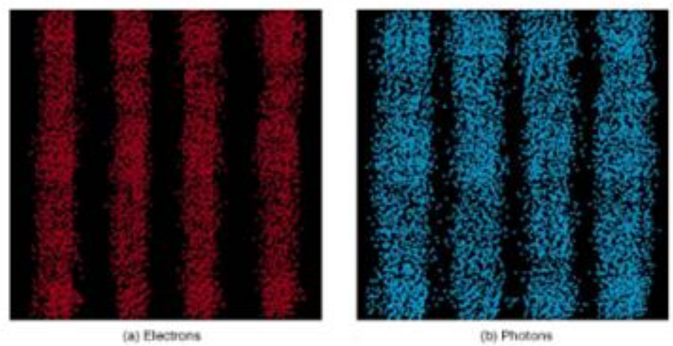


Figure Double-slit interference for electrons (a) and photons (b) is identical for equal wavelengths and equal slit separations. Both patterns are probability distributions in the sense that they are built up by individual particles traversing the apparatus, the paths of which are not individually predictable.

- We know, Newtonian mechanics is applicable to motion of microscopic particles. There are two situations,

i) Infinitely small wave packet

ii) Wide wave packet

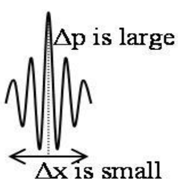
Narrow wave packet

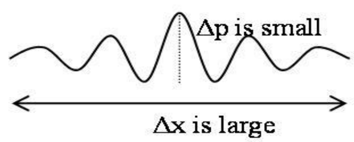
- In case of Narrow Wave packet amplitude is large over small region of space and is negligible elsewhere.
- Due to this small region of space we can determine position of particle, Hence, position of Particle can be fixed with minimum error or uncertainty.

- But at the sametime wavelength (λ) and hence momentum (p=h/λ) cannot be measured accurately and hence is uncertain.

Wide wave packet

- If wave packet is sufficiently wide then wavelength (λ) and hence momentum (p) can be determined very easily with more accuracy.
- But we cannot find the position of particle.
- Therefore, by using Narrow Wave packet and Wide wave packet, shows certainty about momentum involve complete uncertainty about position and vice-versa.
- Hence, we never determine simultaneously both momentum and position of a moving particle.





Narrow Wave Packet **Wide Wave Packet**

- We never calculate particular position at particular instant and has particular velocity atthat Instant. Therefore, they only give us limits within which position and momentum can be determined i.e. they only give probability.
- Heisenberg was 1st to realize this effect and then he expressed them mathematically by means of relation known as uncertainty principle.'
- The principle gives that "It is impossible to determine accurately and simultaneously the values of both position and momentum of physical variables which describe behavior of atomic system."
- There is always uncertainty between position and momentum. Therefore, particle is expressed by writing $(x + \Delta x)$ and $P_X + \Delta P_X$respectively.
- Therefore, uncertainty principle also states that "in any simultaneous determination

of position and momentum of a particle of atomic size, the product of uncertainties in position and in momentum is greater than or equal to planks constant h.

- Therefore, product $\Delta x. \Delta P_X \geq h$
- More precisely, uncertainty principle is expressed by relation,

$\Delta x. \Delta P_X \geq \hbar$-------------($\hbar = h/2$)

Uncertainty Principle Applied to Energy (E) and Time (t)

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

Differentiate above equation

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

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

As, p = mv

$$\Delta p = m\Delta v$$

$$\Delta E = v\Delta p$$

As,

$$v = \frac{\Delta X}{\Delta t}$$

$$\Delta E = \frac{\Delta X}{\Delta t}\Delta p$$

$$\Delta E\Delta t = \Delta X.\Delta p$$

According to uncertainty principle,

$$\Delta X.\Delta p \geq h$$

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

6. Concept of Wave Function and Probability Interpretation

https://en.wikipedia.org/wiki/Wave_function

- Wave function= $\psi(\bar{r},t)$ is nothing but a variable quantity which mathematically describes the wave characteristics of moving particle.
- The wave variable associated with matter waves is called wave function ψ and mathematically it represents motion of particles.
- The value of the wave function of a particle at a given point of space and time (x,y,z,t) is related to the likelihood of finding the particle that point (x, y, z) at given time (t).
- For sound waves pressure is wave variable which varies with space and time and they can exist only within a material medium.
- Wave function, $\psi=\psi(\bar{r},t)$ is analogous to pressure (P) in sound waves and electric field ($\bar{E}$) in electromagnetic waves.
- The wave function may be positive, negative or it may be a complex ($\psi= A + iB$) quantity and complex quantities does not have any direct significance.
- However, Max Born in 1926 suggested that the quantity probability density.

  $|\psi^2|=\psi^*\psi = (A+iB).(A-iB) =A^2+B^2$

  is always real and positive. So it has physical significance.
- The quantity $P=|\psi(\bar{r}, t)^2|/dV$ gives probability of finding moving particle at given point at given time. The term $|\psi(\bar{r}, t)^2|$ is also called as probability density and $\psi(\bar{r},t)$ as probability amplitude.

Physical significance of ψψ* and ψ²

- In 1926, Max Born gave a physical interpretation of wave function ψ.
- The wave function Ψ itself has no physical significance.

- According to Max Born, ψ^2 represents the probability density i.e. it represents probability per unit volume, it shows some particles found which described by wave function (ψ) at particular time, at particular point (x, y, z) in volume.
- If wave function is complex, its probability density given by product $\psi\psi^*$.
- When value of Ψ^2 is large, probability of finding particle there is strong and for small value, probability of finding particle is less.
- If $\Psi^2 = 0$, means absence of particle at that point at time t.
- The wave function ψ described as particle considered as being spread out in space, but it does not mean that particle is also spread out.
- The Ψ^2represents probability density, so probability of finding particle within a volume element dv = dx dydz will be given by, P = Ψ^2 dv.
- The total probability of finding particle somewhere in space at all time is unity, Hence, should satisfy condition

  $\int_{-\infty}^{+\infty} \Psi^2 dv = 1$

  $\iiint_{-\infty}^{+\infty} \Psi^2 \, dx \, dy \, dz = 1$ -------------- (1)

- The wave function that satisfies by equation (1) is called a normalized wave function. It
- If wave function is to represent a moving material particle, it should satisfy following condition gives normalization condition.

  a) ψ should be a normalized wave function.

  b) ψ should be a single valued function of space and time.

  c) ψ should be finite.

  d) ψ and its derivatives $\frac{\partial \Psi}{\partial x}, \frac{\partial \Psi}{\partial y}, \frac{\partial \Psi}{\partial z}$ must be continuous everywhere in the region.

- A wave function which satisfies all above condition called as a well-behaved function.

7. Schrodinger's Equation

- Erwin Schrodinger in 1926 developed wave equations that represent matter waves mathematically which are associated with a moving particle.
- These are linear partial differential equation helpful in understanding the nature of matter waves in quantum-mechanical systems.
- Schrodinger's equation defines the wave properties of sub atomic particles and also predicts particle- like behavior. These equations are basically wave equations predicting the probability of events or outcome which can be applied in various fields.
- The Schrodinger's equation is used to find the allowed energy levels of quantum mechanical systems.
- The associated wave-function gives the probability of finding the particle at a certain position.
- The solution to this equation is a wave that describes the quantum aspects of a system.
- The electronic structure of atoms and molecules can be well explained using Schrodinger equation.
- The shape of orbitals and their orientations can be described.

Schrdinger's time independent wave equation

STEP 1

- The general differential equation for a wave function 'Ψ', travelling with velocity 'u' in three dimensions is,

$\frac{\partial^2 \Psi}{\partial t^2} = u^2 \,[\frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} + \frac{\partial^2 \Psi}{\partial z^2}\,]$

$\frac{\partial^2 \Psi}{\partial t^2} = u^2 \nabla^2 \Psi$ ------------------------------ (1)

Where, $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$ = Laplacian operator.

STEP 2

- The general solution of equation is of the form,

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

Where, $\Psi_0(x,y,z)$ is the amplitude of wave at point (x,y,z).

- The above equation can also be written as,

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

STEP 3

- Differentiating equation (2) partially with respect to t twice,

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

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

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

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

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

STEP 4

Substitute in equation (1)

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

$\nabla^2\Psi + \frac{\omega^2}{u^2}\Psi = 0$ ---------------------- (3)

$$\omega = 2\pi\nu = 2\pi\frac{u}{\lambda}$$

$$\frac{\omega}{u} = \frac{2\pi}{\lambda}$$

$$\frac{\omega^2}{u^2} = \frac{4\pi^2}{\lambda^2}$$

From De-Broglie hypothesis for matter waves

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

$\lambda^2 = \frac{h^2}{p^2}$ ------------------ (4)

STEP 5

- The total energy (E) of particle is a sum of Kinetic energy (1/2 mV^2) and potential energy (V).

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

$$= \frac{m^2v^2}{2m} + V$$

$$\therefore E = \frac{p^2}{2m} + V$$

$$\therefore p^2 = 2m(E - V)$$

- Substitute in equation (4)

$$\lambda^2 = \frac{h^2}{2m(E-V)}$$

$$\frac{\omega^2}{u^2} = 4\pi^2 \times \frac{2m(E-V)}{h^2}$$

$$\frac{\omega^2}{u^2} = \frac{8\pi^2 m(E-V)}{h^2}$$

Substitute in equation (3)

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

- The quantity $\frac{h}{2\pi}$ appears very frequently in quantum mechanics and hence is substituted as ђ. So ђ$^2 = \frac{h^2}{4\pi}$

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

This is Schrodinger's time independent wave equation.

Schrdinger'stimedependent wave equation

STEP 1

- The general differential equation for a wave function 'Ψ', travelling with velocity 'u' in three dimensions is,

$$\frac{\partial^2\Psi}{\partial t^2} = u^2\,[\frac{\partial^2\Psi}{\partial x^2} + \frac{\partial^2\Psi}{\partial y^2} + \frac{\partial^2\Psi}{\partial z^2}]$$

$$\frac{\partial^2\Psi}{\partial t^2} = u^2\nabla^2\Psi \quad \text{------------------------------ (1)}$$

Where, $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$ = Laplacian operator.

STEP 2

- The general solution of equation is of the form,

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

Where, $\Psi_0(x,y,z)$ is the amplitude of wave at point (x,y,z).

The above equation can also be written as,

$$\Psi\,(r,t) = \Psi_0\,(r)\,e^{-i\omega t} \text{ --------------------- } (2)$$

STEP 3

- Differentiating equation (2) partially with respect to t,

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

$$\frac{\partial\Psi}{\partial t} = -i\omega\Psi \text{ ----------------------- } (3)$$

As $\omega = 2\pi\nu$ and $E = h\nu$

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

$$\frac{\partial\Psi}{\partial t} = \frac{-i2\pi E}{h}\,\Psi$$

$$E\Psi = \frac{-h}{i2\pi}\frac{\partial\Psi}{\partial t}$$

$$E\Psi = \frac{ih}{2\pi}\frac{\partial\Psi}{\partial t} \text{ -------------------- } (4)$$

STEP 4

- Schrodinger’s time independent equation is,

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

Multiply by $\frac{-h^2}{8\pi^2\, m}$

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

$$\therefore\ \frac{-h^2}{8\pi^2\, m}\nabla^2\Psi + V\Psi = E\Psi$$

$$\therefore\ \frac{-h^2}{8\pi^2\, m}\nabla^2\Psi + V\Psi = \frac{i\hbar}{2\pi}\frac{\partial\Psi}{\partial t},$$

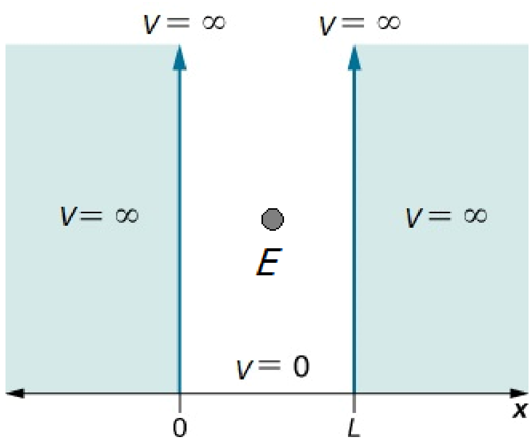
Where, E $=\frac{i\hbar}{2\pi}\frac{\partial}{\partial t}$ = Energy operator

This is Schrodinger's time dependent wave equation.

8. Applications of Schrodinger's Time Independent Wave Equation

- The Schrodinger equation is used to find the allowed energy levels of quantum mechanical system.
- The wave function associated with motion of atomic/molecular systems gives the probability of finding the particle at a certain position.
- The Schrodinger equation can be used to describe the behavior of a particle in a field of force.
- We will now apply Schrodinger's wave equation in several examples using various potential functions.
- These examples will demonstrate the techniques used in the solution of Schrodinger's differential equation and the results of these examples will provide an indication of the electron behavior under these various potentials

8a. Particle in a rigid box (infinite potential well)



- If a quantum 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 escape out from the well. In quantum mechanics, it is called as bound state.
- Consider a quantum particle of mass 'm' restricted to move along x axis between x=0 and x=L with velocity,' v' inside infinite rigid one-dimensional box of length L as shown in figure.
- The potential can be taken as V(x) = 0inside and since it cannot escape so potential outside the box is taken as V (x) = ∞.
- Schrodinger time independent wave equation can be applied in order to estimate various energy states of particles.
- For such cases equation can be as following.

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

But inside the box, V(x) = 0

$$\therefore \frac{\partial^2 \Psi}{\partial x^2} + \frac{2mE}{\hbar^2} \Psi = 0$$

$$\therefore \frac{\partial^2 \Psi}{\partial x^2} + k^2 \Psi = 0 \text{ , ------------ (1)}$$

Where $k^2 = \frac{2mE}{\hbar^2}$

- This is second order linear differential equation.
- By solving equation (1), general solution for wave function can be written as.

Ψ(x) = Asin(kx) + BCos(kx) ----------------(2)

Where A and B are arbitrary constants can be determined by the boundary conditions.

- Applying first boundary conditions, i.e. Ψ(x)=0 at x=0 we get

0 = 0 + B

B = 0

Put B = 0 in equation (2)

∴Ψ(x) = Asin(kx)

- Applying second boundary conditions i.e. Ψ(x)=0 at x=L we get

Asin(kL) =0

∴sinKL=0=nπ, ……………Where, n=1,2,3-----

(n=o is not possible because if n=o, then KL becomes zero which is not possible.)

∴KL= nπ

$$\therefore K = \frac{n\pi}{L}$$

$$\therefore K^2 = \frac{n^2\pi^2}{L^2}$$

$$\therefore \frac{2mE}{\hbar^2} = \frac{n^2\pi^2}{L^2}$$

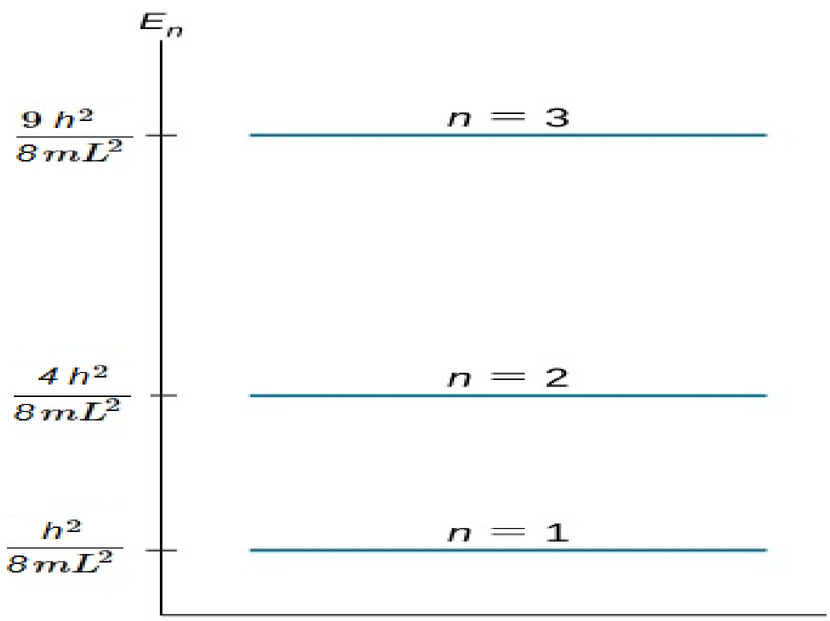
$$\therefore E_n = \frac{n^2\pi^2}{L^2} \times \frac{\hbar^2}{2m}$$

$$\therefore But\ \hbar = \frac{h}{2\pi}$$

$$\therefore E_n = \frac{n^2\pi^2}{2mL^2} \times \frac{h^2}{4\pi^2}$$

$$\therefore E_n = \frac{n^2h^2}{8mL^2}$$

- This relation shows that energy En of quantum particle is not continuous but discrete as shown in figure.
- Energy En is directly proportional to n^2 and inversely proportional to mass of particle and square of length of box.



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

- Classically-A particle enclosed in a rigid box can have any value of energyfrom0to∞.Minimumenergymaybezero.
- Quantum mechanically-Only certain values that are integral multiple of $h/2\pi$.
- Minimum energy is not zero but have minimum energy.

Normalization of wave function

- For the particle in a rigid box with infinite walls, the probability of finding it within the box must be equal to one.

- Therefore, condition for normalization is written as;

$$\int_0^L \Psi^* \Psi dx = 1$$

$\Psi(x) = Asin\frac{n\pi x}{L}$- ------------------------------(3)

$$-\int_0^L Asin\frac{n\pi x}{L} Asin\frac{n\pi x}{L} dx = 1$$

$$A^2 \int_0^L sin^2 \frac{n\pi x}{L} dx = 1$$

$$\frac{A^2}{2} \int_0^L \left(1 - cos\frac{2n\pi x}{L}\right) dx = 1$$

$$\frac{A^2}{2} \int_0^L \left(1dx) - \frac{1}{2} \int_0^L (cos\frac{2n\pi x}{L} dx\right)] = 1$$

$$[A^2 \times \frac{L}{2} - 0] = 1$$

$$A^2 \times \frac{L}{2} = 1$$

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

Substituting value of A in Equation (3) wave function becomes.

$$\Psi(x) = \sqrt{\frac{2}{L}} sin\frac{n\pi x}{L}-$$

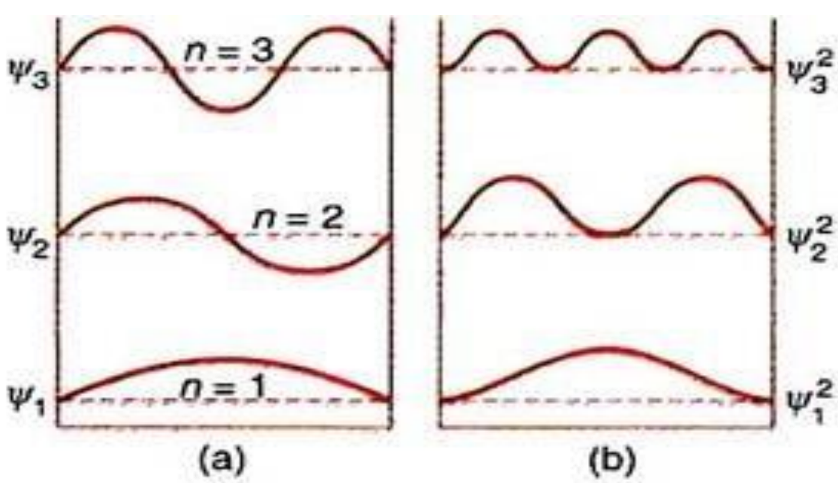
- The above equation represents the wave function of the particle enclosed in rigid box of length L.
- As ψ gives negative probability, probability density i.e. $|\psi|^2$ determines the

position of the particle inside the box.

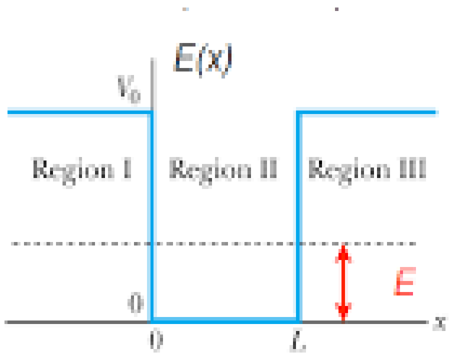
- The wave function ψ and probability density $|\psi|^2$ of the particle can be plotted.
- The locations where probability densities show peaks are the most probable position of the particle.
- Normalized wave functions ψ_1, ψ_2, ψ_3 shown in figure and probability density for first three wave functions $\boldsymbol{\Psi_1^2}, \boldsymbol{\Psi_2^2}, \boldsymbol{\Psi_3^2}$ are shown in figure.

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 $L = 3L/4$.



8b. Particle in non-rigid box (Finite potential well)



$$V(x) = \begin{cases} V_0 & x \leq 0 & \text{region I} \\ 0 & 0 < x < L & \text{region II} \\ V_0 & x \geq L & \text{region III} \end{cases}$$

- In real life situations potential energies are never infinite but there exist barriers of finite height.
- Consider a particle of mass 'm' traveling along x axis between $x = 0$ and $x = L$ is trapped inside a well of potential V_0 see figure.
- In case of non-rigid box, it is divided into three regions, Region I ($x \leq 0$), region II $0 < x < L$ and third region is at the right side of box where $X \geq L$.
- Consider the energy of particle $E < V_0$. Classically, the particle strikes the walls of the well. It is reflected and cannot enter regions II and III.
- Apply Schrodinger's time-independent wave equation for three regions.

$$For\ Region\ I, \quad \nabla^2\Psi_1(x) + \frac{2m(E - V_{0)}}{\hbar^2}\Psi_1(x) = 0 \quad , \quad x \leq 0$$

$$For\ Region\ II, \quad \nabla^2\Psi_2(x) + \frac{2mE}{\hbar^2}\Psi_2(x) = 0 \quad , \quad 0 < x < L$$

$$For\ Region\ III, \quad \nabla^2\Psi_3(x) + \frac{2m(E - V_{0)}}{\hbar^2}\Psi_3(x) = 0 \quad , \quad X \geq L$$

- The solution of differential equation in region II is very similar to particle in rigid box, so itsequation and solution is given below.

$$\frac{\partial^2\Psi_2(x)}{\partial x^2}+\frac{2mE\Psi_2(x)}{\hbar^2}=0$$

$$\frac{\partial^2\Psi_2(x)}{\partial x^2}+k^2\Psi_2(x)=0\quad ,$$

But $k^2=\frac{2mE}{\hbar^2}$

$$\psi_2(x)=Ce^{ikx}+De^{-ikx}$$

- But, for region I and region III are different. Although classically particle cannot escape from region I (($\therefore E<V_0$) there is small probability that quantum particle can be found in region I or III.
- For this one can solve differential equation by taking

$k'^2=-\frac{2m(E-V_0)}{\hbar^2}$ Equations and wave functions for region II and III are,

For Region I, $\frac{\partial^2\Psi_1(x)}{\partial x^2}-k'^2\Psi_1(x)=0$

Therefore, $\psi_1(x)=Ae^{k'x}+Be^{-k'x}$

For Region III, $\frac{\partial^2\Psi_3(x)}{\partial x^2}-k^2\Psi_3(x)=0$

Therefore, $\Psi_3(x)=Ee^{K'x}+Fe^{-k'x}$

- Applying boundary Conditions at $x=0$ and $x=L$ as following values of arbitrary constants A,B,C,D,E and F can be found.

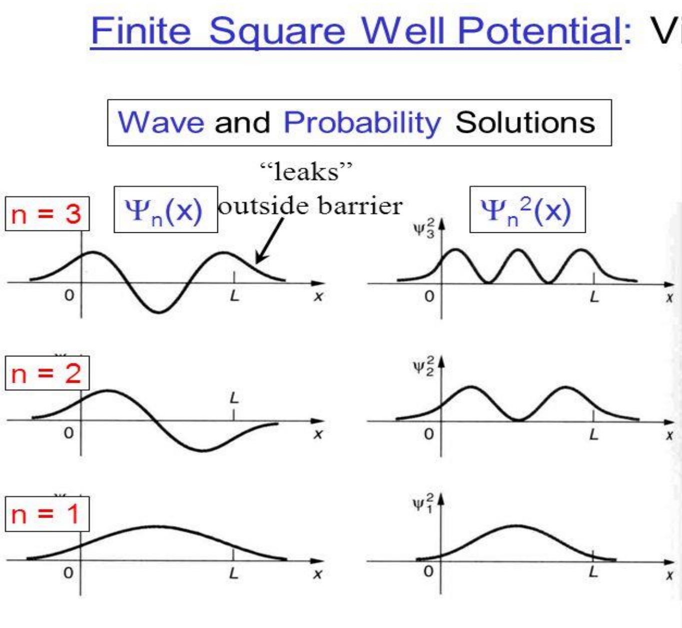
$$\psi_{1(x=0)}=\psi_{2(x=0)}$$

$$\psi_{2(x=L)}=\psi_{3(x=L)}$$

$$(\frac{\partial \Psi 1}{\partial x})_{x=0} = (\frac{\partial \Psi 2}{\partial x})_{x=0}$$

$$(\frac{\partial \Psi 2}{\partial x})_{x=L} = (\frac{\partial \Psi 3}{\partial x})_{x=L}$$

- Solving above equations values of A, B, C, D, E and F can be obtained. Constants D in region I and E in region III should be zero in order to satisfy the conditions $\psi_1 = 0|_{x \to -\infty}$ and $\psi_3 = 0|_{x \to +\infty}$.

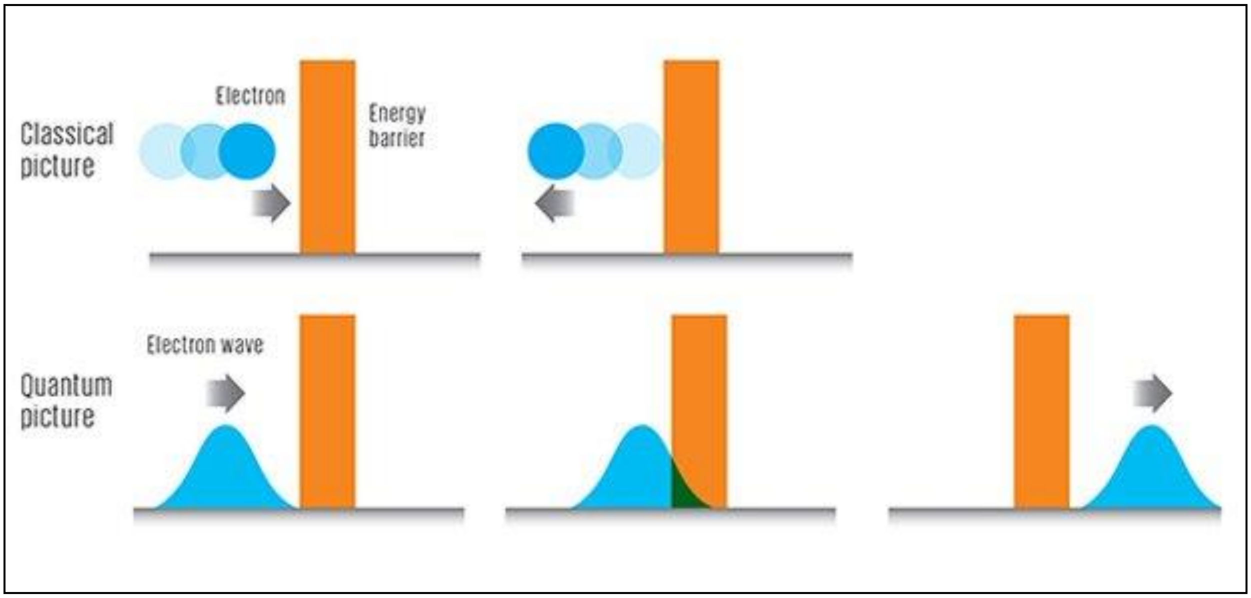


Following conclusions can be drawn by solving Schrdinger's equation for non-rigid box of finite potential well.

- The wave functions are similar to those of infinite well. However, atthe boundary wave function is not zero and it also extends a little outside the box on either side.
- It means probability of particle penetrating through the wall is not zero but there is small chance to find the particle at left and right sides of the box.

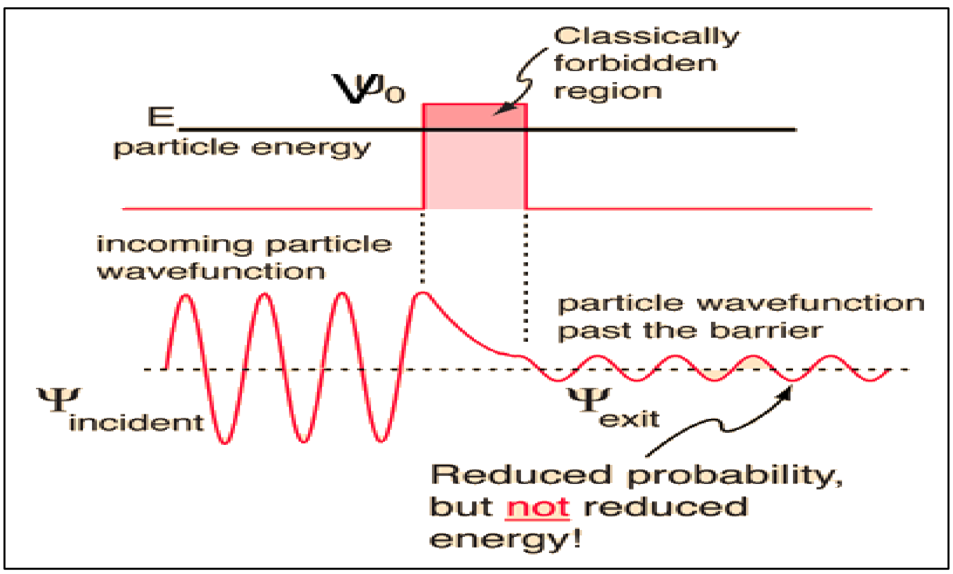
- Even though the particle energy E is less than the potential energy V_0, there is a definite probability that the particle is found outside the box.

9. Tunneling Effect



- According to classical ideas particle with energy less than potential barrier ($E < V_0$) striking to wall of potential barrier it cannot leak through it.
- However, quantum mechanics principle is different than classical one and particle possess a wave like behavior which enables it to leak through barrier.
- This type of penetration of particles is known as tunneling effect.
- Tunneling effect plays an essential role in several physical phenomena, such as the nuclear fusion that occurs as main source of energy inside stars like the Sun.
- It has important applications in the tunnel diode, quantum computing(QC), and in the scanning tunneling microscope(STM).
- The effect was predicted in the early 20th century, and its acceptance as a general physical phenomenon came midcentury.
- Nature of wave function for particle showing wave-like behavior if passed through step potential is shown in figure.

- Figure shows that where it is not possible to penetrate the particle in classical case.
- But as per quantum mechanics particle strikes from left side (Region I) of potential barrier where it has some amplitude at this wall part of wave function reflected and part is transmitted to region II with slightly reduced amplitude and at another boundary it again suffers reflection and transmission and it can penetrate through the barrier with finite probability.
- Although its amplitude is quit less interestingly its energy is same.
- Thus, where region is classically forbidden for micro-particles quantum particle can tunnel through barrier.



Tunneling Of Wave Function through Barrier

Alpha decay

- An alpha α particle consists of two protons and two neutrons bound together. (${}_2He^4$).

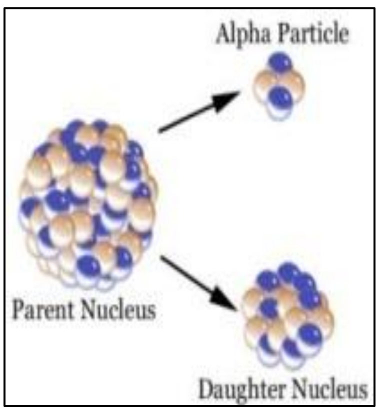
- Alpha decay is a type of radioactive decay where an atomic nucleus emits an alpha particle.

Binding energy of α-particle

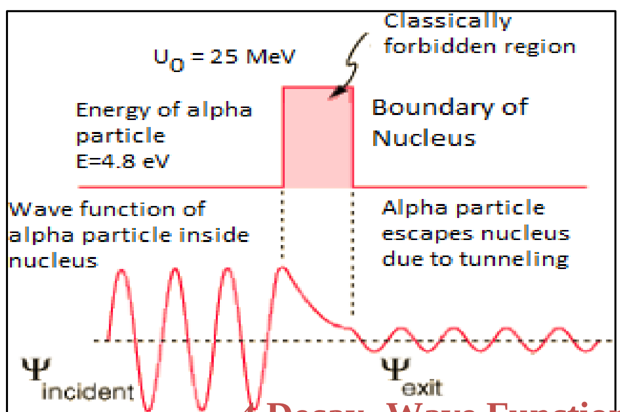
- An α -particle is bounded inside the nucleus with energy around $25MeV$ which is its potential barrier.
- Thus, classically α-particle requires a minimum energy of $25MeV$ to escape from the nucleus.

Energy of emitted α-particle

- A free α-particle has energy of only around 4.8MeV.



Alpha Decay



A Decay- Wave Functions

- Thus, it is impossible for α-particle to escape from nucleus that has potential barrier of $25MeV$.

Tunneling of α-particle

- Quantum mechanically, de Broglie waves are associated with α particle.

- The wave function of α particles (and hence- particles themselves) has a very small but definite value so that it can" tunnel" through the barrier of binding energy of nucleus and make free itself.

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

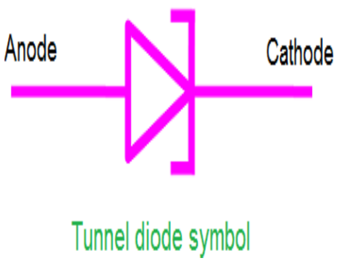
Tunnel diode

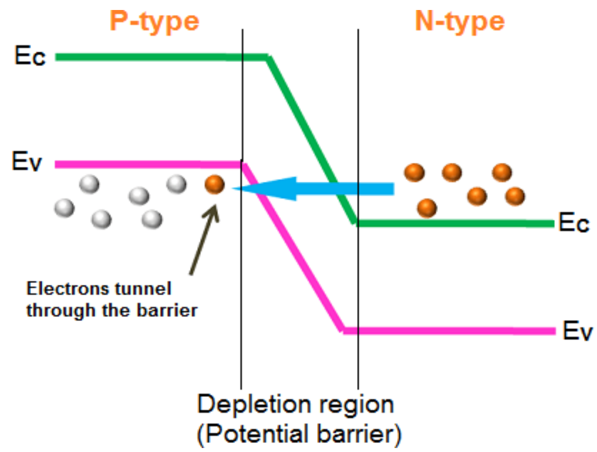
- Tunnel diode (or Esaki diode) was invented by Leo Esaki and received Nobel Prize in Physics for the same.
- It is a PN junction device which exhibits negative resistance.
- It means when potential difference across tunnel diode is increases, current through it decreases.
- Tunnel diode is capable of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

Principle of Tunnel diode

- In tunnel diode P and N regions are heavily doped of the order of 1 dopant in 10^3 atoms of intrinsic semiconductor. (For normal N and P - 1 dopant atom for 10^{28}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.





Tunnel Diode Symbol

Advantages and application tunnel diodes

- Very fast switching, long life, high-speed operation, low noise, low power consumption are few advantages of tunnel diode.
- Applications-Tunnel diodes are used as logic memory storage devices, relaxation oscillator circuits, ultra high- speed switch, FM receivers, etc.

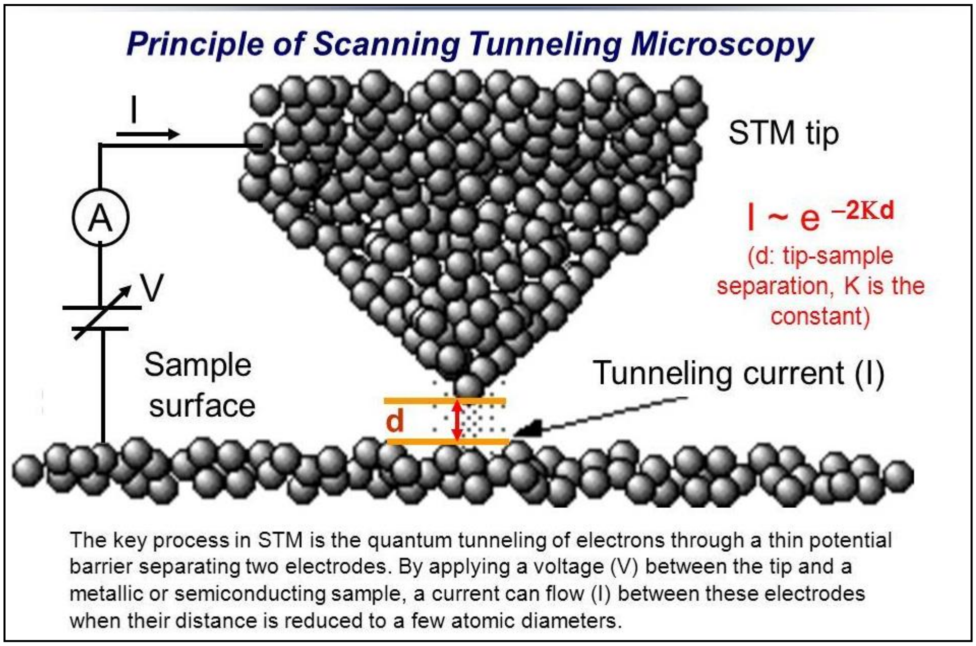
10.Scanning Tunneling Microscope(STM)

http://www.chembio.uoguelph.ca/educmat/chm729/STMpage/stmconc.htm

https://makeagif.com/gif/principle-behind-the-working-of-scanning-tunneling-microscope-stm-4tY1LW

- Scanning Tunneling Microscope (STM) is a non-optical microscope which is used for observing surfaces of materials atom by atom.

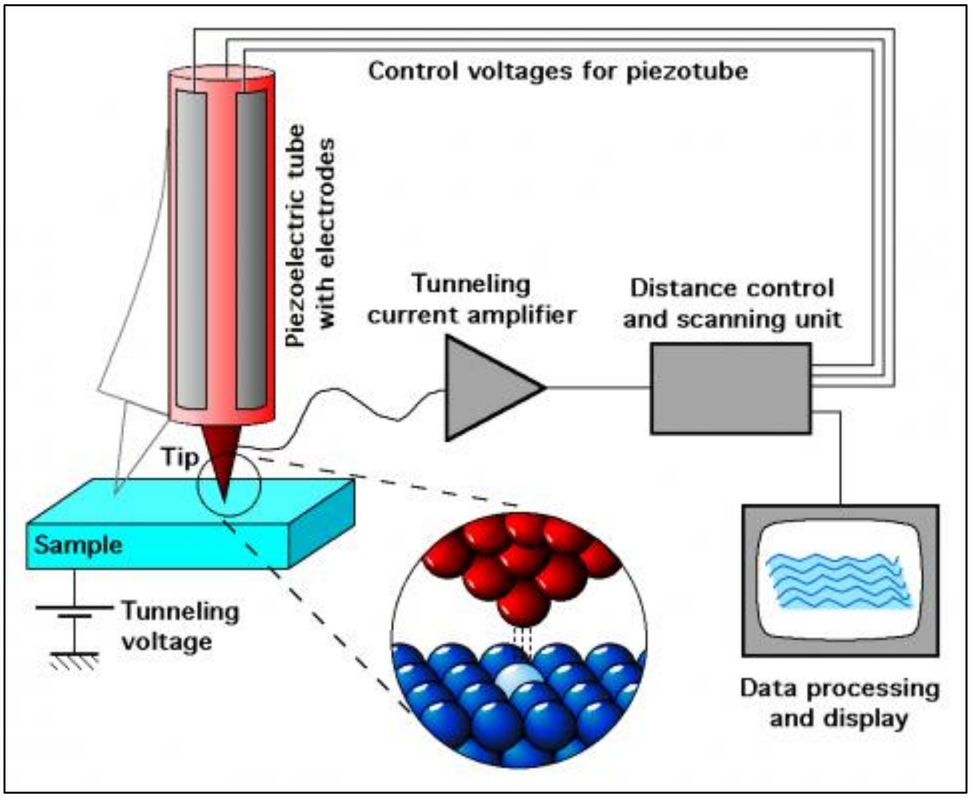
Principle of STM



- 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, at

graphical image of the surface can be created.

Construction of STM



- Basically, STM include scanning tip, piezoelectric controlled scanner, tunneling current amplifier, distance control and scanning unit, 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 mili-volts (*mV*) to a few Volts (*V*) is applied to the sample and the STM tip.
- **Working**
- Tip of STM scans the sample surface and electrons tunnel from tip to the sample.

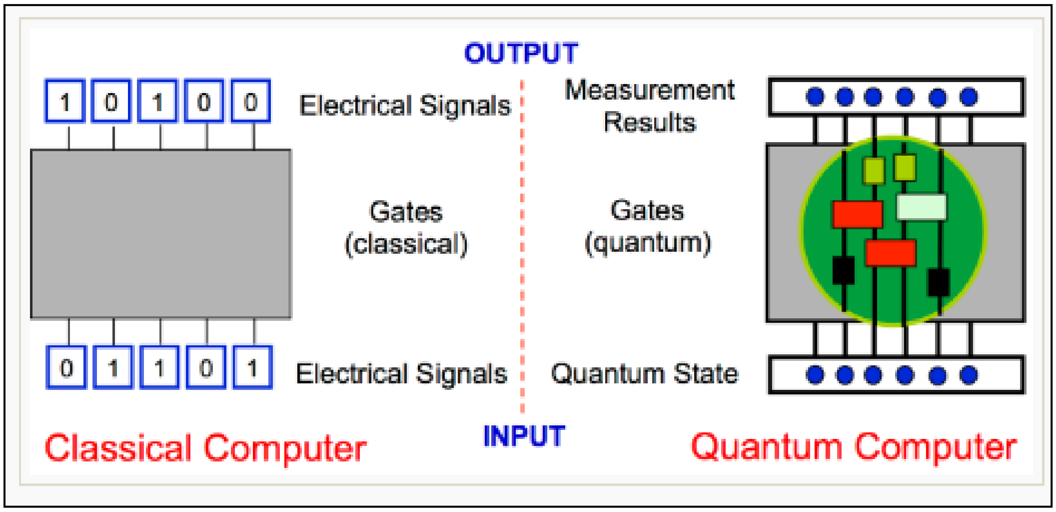
- This creates a tunneling current of the order of few pico amperes (pA) to a few nano amperes (nA).
- This current is amplified and given to data processing unit.
- As the tip of the STM moves over the sample surface, its distance continuously changes due to curvature of atoms.
- Thus, the output current 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

- STM is used to study the arrangement of individual atoms on the solid surfaces.
- STM can be used for examining characteristics of material surface including roughness, surface defects and molecular size.
- The STM can be operated from temperatures ranging from $4K$ to $973K$.
- Thus, various properties of the solids can be studied at lower and higher temperatures.
- The strong electric field between tip and sample has been utilized to remove atoms from the sample surface and drop or deposit there moved atoms at other location.
- Thus, STM can manipulate atoms and plays very important role in nanotechnology.

11. Introduction to Quantum Computing

Principle and imitation of classical computing

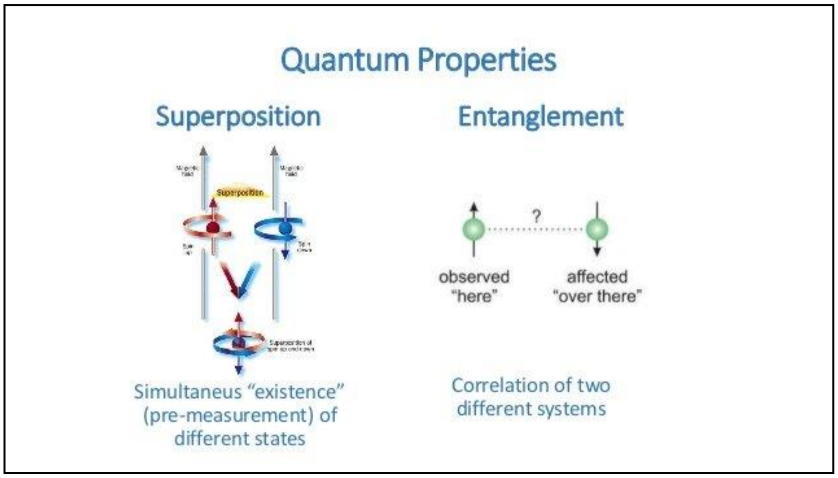


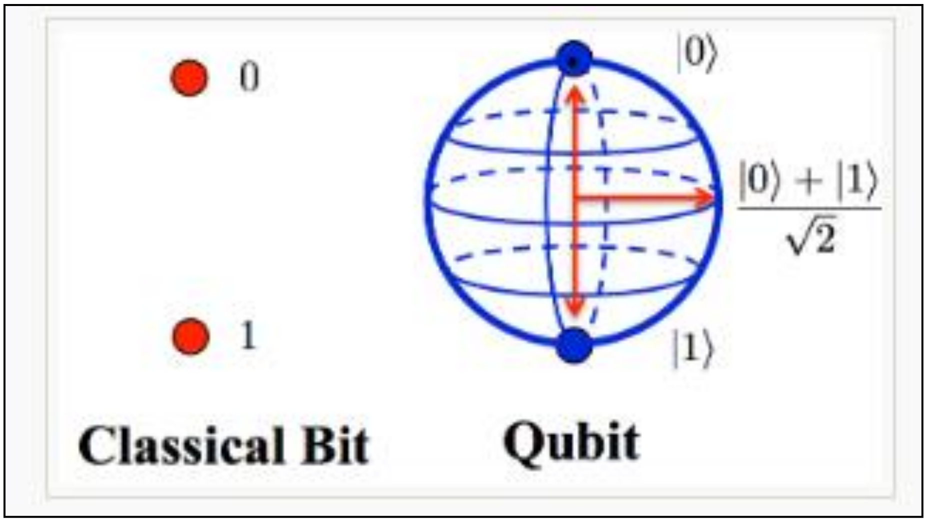
- Classicalcomputing works on principles of Boolean algebra and logic gates where computersmanipulate individual bits, which store information as binary 0 and 1 state.
- The transistors and capacitors in CPU can only be either in 0 (off) or 1(on) state.
- In order to raising processing power, dimensions of transistors need tobe reduced at the order of few nanometers to accommodate very large transistors on a chip.
- But, at such nano scale, a threshold is reached and quantum mechanical effects such tunneling, uncertainty principle 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.

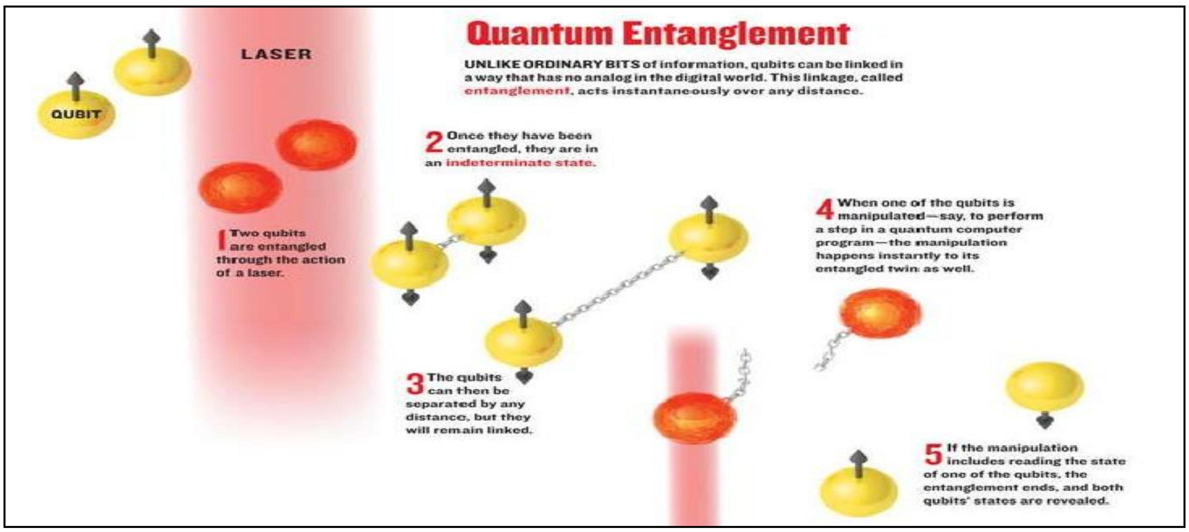
- A number of elemental particles such as electrons or photons can be used for storing the information.
- Either the charge of particles or polarization acts as a representation of 0 and/or 1.
- Each of these particles is known as a quantum bit, or qubit.
- A qubit is a unit of quantum information.
-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

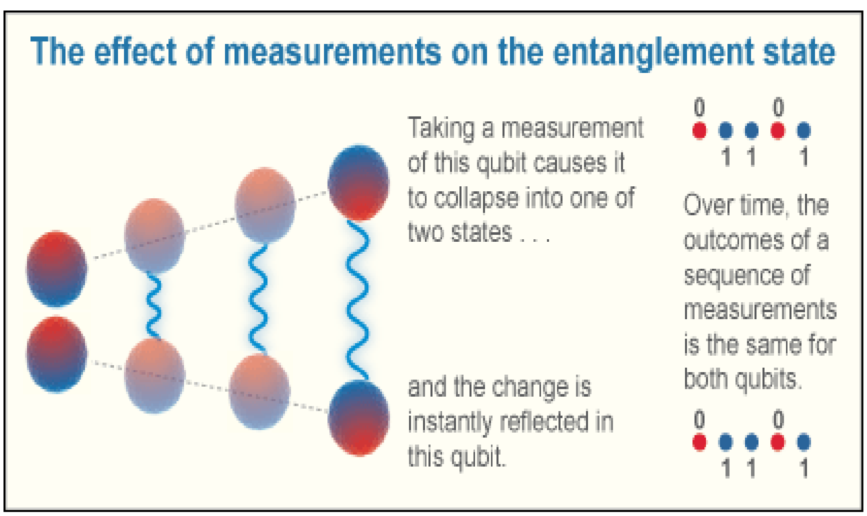




Superposition

- 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.
- **Entanglement**





- Entanglement is correlation between particles acting asqubits 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 giga-hertz.
- 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 have 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 requirethousands of 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 times having 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.