Wave Mechanics

(Quantum Mechanics)

Why Quantum Mechanics is Important ?

Classical Mechanics vs Quantum Mechanics

Classical Mechanics

- Macroscopic level
- Gravitational law, Newton's laws
- Electricity, magnetism and light: independent
- Position, mass, speed, force, energy
- Can not describe atomic behaviour
- Continuous energy level (ramp)
- Motion of object

Quantum Mechanics

- Microscopic level
- Electromagnetism: light
- Atomic behaviour
- Quantized or discrete energy levels (staircase)
- Motion of electron in atom

De Broglie's Hypothesis

- ❖ **Wave-Particle Duality**
- ❖ **De- Broglie Wavelength (Wavelength of matter waves)**
- ❖ **De- Broglie Wavelength by Analogy with Radiation**
- ❖ **De- Broglie Wavelength in terms of K.E. of Particle**
- ❖ **De- Broglie Wavelength for an Electron in terms of Potential Difference**

de Broglie Hypothesis:

It states that all matter has both particle and wave nature. The wave nature of particle is quantified by de Broglie wavelength.

Q.1. Show that De-Broglie wavelength of a charge particle is inversely proportional to the square root of the accelerating potential

Q.2. State De-Broglie hypothesis. Hence obtain the relation for the same in terms of energy

Q1. What is the De- Broglie wavelength of an electron when accelerated through a P.D. of 10000 volts?

Ans: 0.1227 A^0

Q2. **Compute the wavelength of the De- Broglie waves associated with a proton moving with 5 % of the velocity of light. Proton has 1836 times the mass of one electron.**

Ans: **2.64×10^{-14} m**

Q3. **De- Broglie wavelength of electrons in a monoenergetic beam is 7.2×10^{-11} meters. Calculate the momentum and energy in the beam in electron volts.**

Ans: **p = 0.9208 X 10-23 kg-m/sec**

E = 291 eV

Q4. **A beam of 10 kV electrons is passed through a thin metallic sheet whose interplanar spacing is 0.55 A^0. Calculate the angle of deviation of the first-order diffraction maximum.**

Ans: **6.40^0**

Q5. **An electron initially at rest is accelerated through a P.D. of 5000 V. Compute**

i) **The momentum**
ii) **De Broglie wavelength**
iii) **The wave number of the electron**

Ans: i) $p = 3.81 \times 10^{-23}$ **kg-m/s**

ii) $\lambda = 0.1735 \times 10^{-10}$ **m**

iii) **wavenumber** $= 5.7636 \times 10^{10}\ m^{-1}$

Phase Velocity and Group Velocity

➢ Phase velocity or Wave velocity

The phase velocity of a wave is the rate at which the particular phase of the wave propagates in space.

$$V_p = \frac{\omega}{k}$$

$y = A \sin(\omega t - kx)$ Equation of wave

❖ Show that the phase velocity is greater than the velocity of light

$$\mathrm{v}_p = \frac{c^2}{v}$$

- $mc^2 = h\nu$
- $\lambda = h/mv$
- $V_p = \nu\lambda$

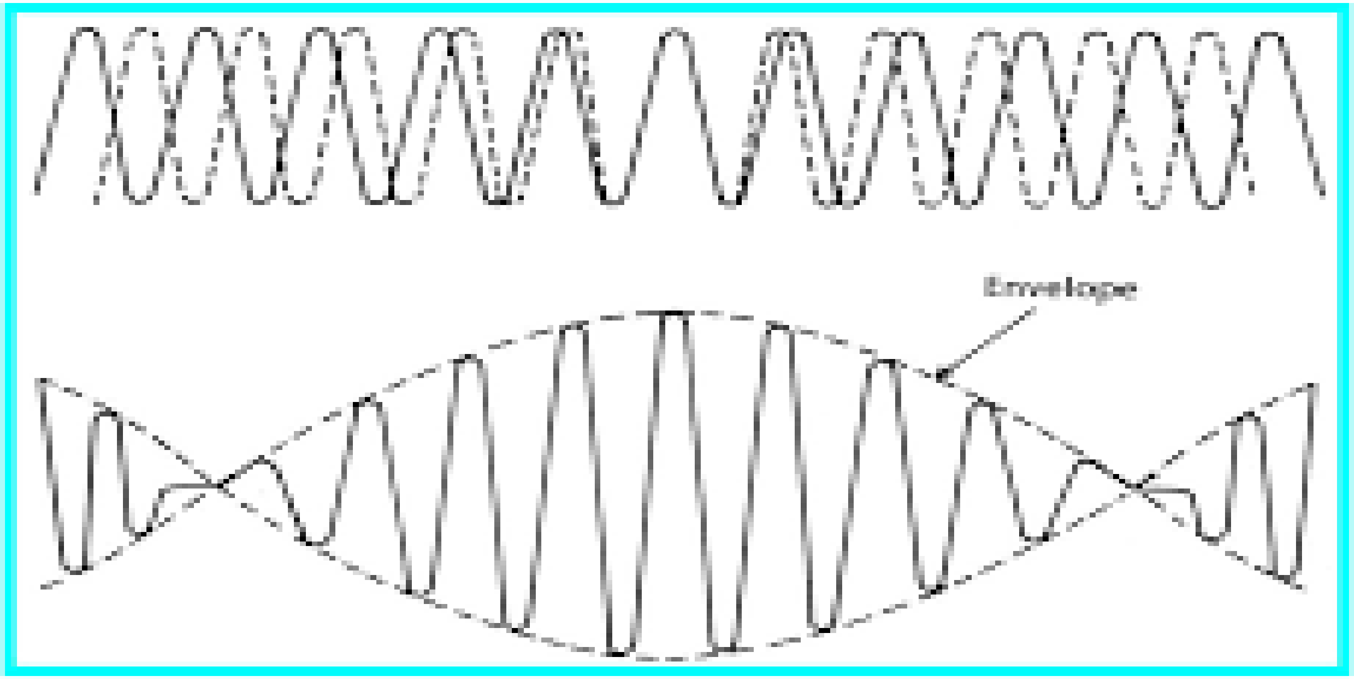
Group Velocity or Wave Group

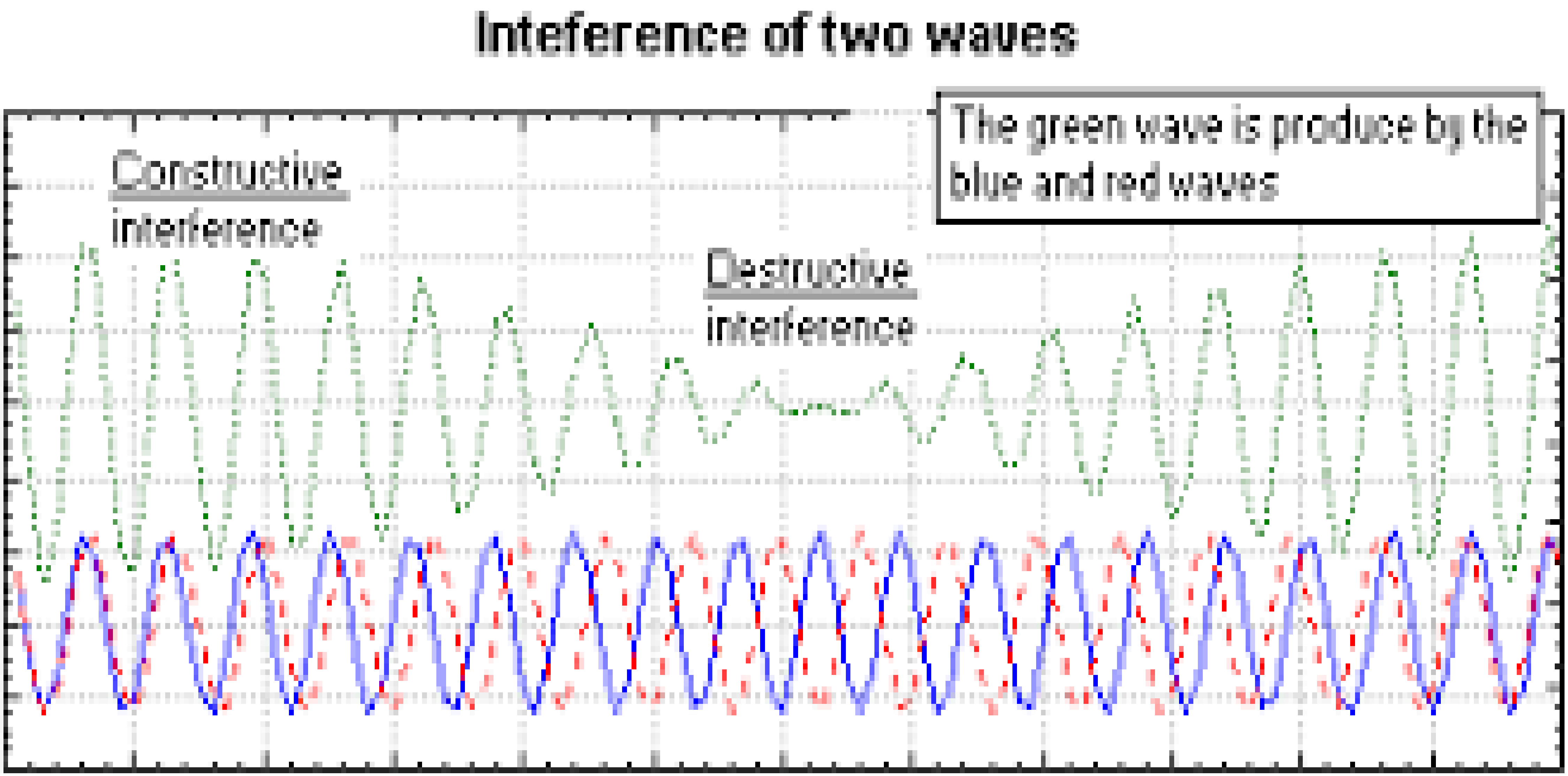
- The wave group can be obtained by superposition of many waves of different wavelengths and velocities.

- The velocity associated with these wave group or wave packets is called group velocity

$$V_g = \frac{d\omega}{dK}$$

Group velocity




Inteference of two waves
The green wave is produce by the blue and red waves
Constructive interference
Destructive interference

$$y_1 = A \sin(\omega t - kx)$$

$$y_2 = A \sin[(\omega + d\omega)t - (k + dk)x]$$

$\sin A + \sin B = 2 \sin[(A+B)/2] \cos[(A-B)/2]$

$$Y = 2A \sin\left(\frac{2\omega + d\omega}{2}\, t - \frac{2k + dk}{2}\, x\right) \cos\left(\frac{d\omega}{2}\, t - \frac{dk}{2}\, x\right)$$

$$Y = 2A \sin(\omega t - kx) \cos\left(\frac{d\omega}{2}\, t - \frac{dk}{2}\, x\right)$$

- **Show that the group velocity is equal to particle velocity**

$$v_g = v$$

De-Broglie wave group associated with moving particle travels with the same velocity as the particle

Properties of Matter Waves/De Broglie waves

1. Matter particles: wave nature ($\lambda = h/mv$)
2. If m = constant, λ inversely proportional to v
3. If v = constant, λ inversely proportional to m
4. If v = 0, rest particle : do not have wave nature
5. $v_p = c^2/v$, phase velocity of matter waves > light velocity
6. Matter waves are not electromagnetic or mechanical in nature
7. **Particle:** localized in space and **Wave:** spread out – uncertainty in position of the particle
8. Wave and particle nature can not exhibited simultaneously
9. Probability waves

Heisenberg's Uncertainty Principle

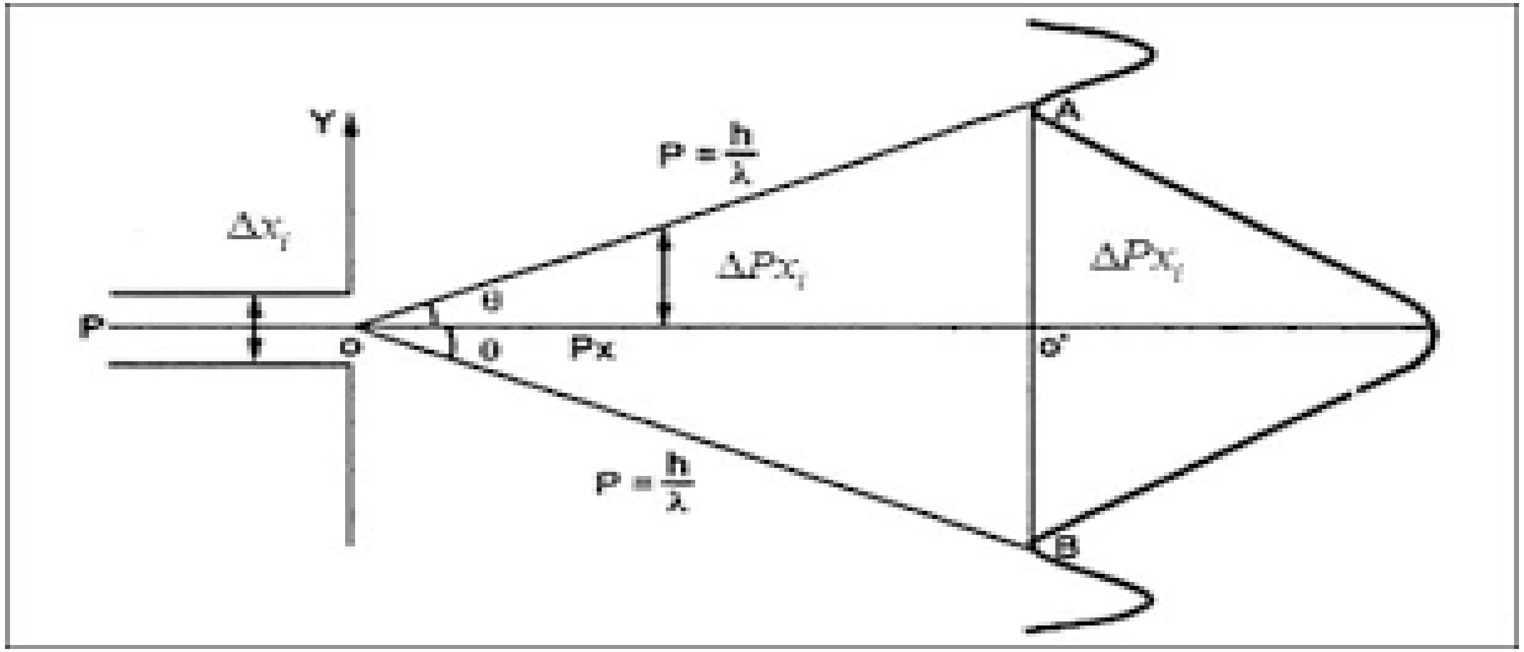
It is impossible to determine both the exact position and exact momentum of particle at the same time

- $\Delta x = \lambda$, for electron somewhere in wave group
- $\Delta p = h/ \lambda$, change in momentum after photon incident
- $\Delta x \times \Delta p = h$

Heisenberg's uncertainty principle for energy and time

$$\Delta E \times \Delta t > h$$

Illustration of uncertainty principle by single slit electron diffraction



- $a \sin\theta = n\lambda$
- $a = \Delta x$

Q. In order to locate the electron in an atom within a distance of $5X10^{-12}$ m using EM waves, the wavelength must be of the same order. Calculate the energy and momentum of the photon. What is the corresponding uncertainty in its momentum?

$$\Delta x = \lambda = 5X10^{-12}$$

P = 1.32 X 10-22 kg-m/s
E= 3.96 X 10-34 J
Δp = 1.32 X 10-22 kg-m/s

The uncertainty in the location of the particle is equal to its De Broglie wavelength. Show that the uncertainty in the velocity to a particle is equal to the velocity itself.

$$\Delta x = \lambda$$

$$\Delta x.\Delta p = h$$

$$\lambda.\Delta p = h$$

$$\Lambda.m\,\Delta v = h$$

$$m\,\Delta v = h/\lambda$$

$$m\,\Delta v = h\,mv/h$$

$$\Delta v = v$$

A bullet of mass 25 gm is moving with a speed of 400 m/s. The speed is measured accurate upto 0.02 %. Calculate the certainty with which the position of the bullet can be located.

$\Delta x \times \Delta p = h$

$\Delta v = 400 \times 0.02\% = 0.08$ m/s

$\Delta x = h/ m \Delta v = 3.315 \times 10^{-31}$ m

Compute the minimum uncertainty in the location of a 2 gm mass moving with a speed of 1.5 m/s and the minimum uncertainty in the location of an electron moving with speed of 0.5×10^{8} m/s, given that the uncertainty in the momentum is 10^{-3}p for both

$\Delta x = 2.21 \times 10^{-28}$ m for 2 gm mass

$\Delta x = 1.46 \times 10^{-8}$ m for electron

An electron is confined to a box of length $2A^0$. Calculate the minimum uncertainty in its velocity.

$$\Delta v = 3.64 \text{ X } 10^6 \text{ m/s}$$

Concept of wave function and its physical significance

- Wave function (Ψ): The quantity which describes the De Broglie wave
- It gives periodic variations of matter waves
- Ψ : positive, negative or complex
- Probability of finding the particle in space at time ‘t’: 0 and 1
- P = mod of Ψ square

Physical significance of wave function (Ψ)

- The probability of finding the particle in space (x, y, z) and time 't' is described by Ψ (x, y, z, t)
- dv = dx dydz
- P = (mod of Ψsquare) X dv : probability density
- $\int_{-\infty}^{\infty}$ (mod of Ψ square) X dv = 1
- Normalized wave function : Ψ must have to satisfy the normalized condition

i. Ψ must be single valued function; P can have only one value at given point and time

ii. Ψ must be finite at every point in space

iii. Ψ and its first order derivative ($d\Psi/dx$, $d\Psi/dy$, $d\Psi/dz$) must be continuous everywhere

Schrodinger's Wave Equation

- Wave function: to describe the behaviour of particle under the influence of potential
- Schrodinger : De-Broglie hypothesis to develop the equations

i. Schrodinger’s time independent wave equation

ii. Schrodinger’s time dependent wave equation

Applications of Schrodinger's time independent wave equation

- Schrodinger's wave equation: behaviour of particle in given space and time
- To find the energy and wave function of the system under given boundary conditions
- Electron bound to nucleus: potential of nucleus
- Proton and neutron bound to nucleus: potential due to nuclear force
- Consider potential function: understand particle behaviour

Applications of Schrodinger’s time independent wave equation

1. Particle in rigid box (infinite potential well)

2. Particle in non-rigid box (finite potential well)

3. Tunneling effect

Particle in rigid box (infinite potential well)

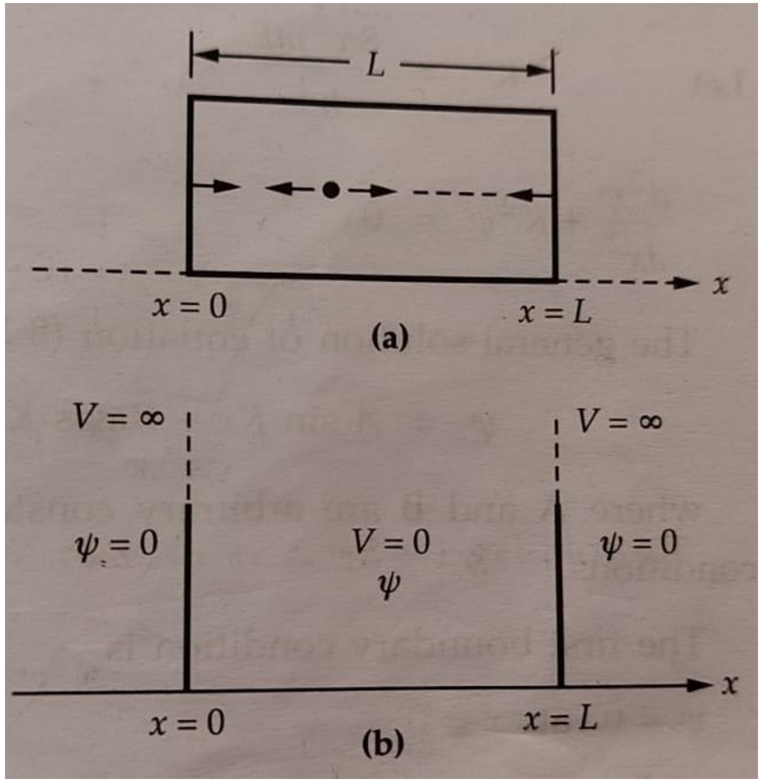
- Particle free to move in a small space surrounded by impenetrable barriers

- Differences between classical and quantum systems

- Classical system: particle can move at any speed within the box and it is no more likely to be found at one position than another

- Quantum system: particle may only occupy certain positive energy levels.

- It can never have zero energy, meaning that the particle can never "sit still



Energy Eigen values

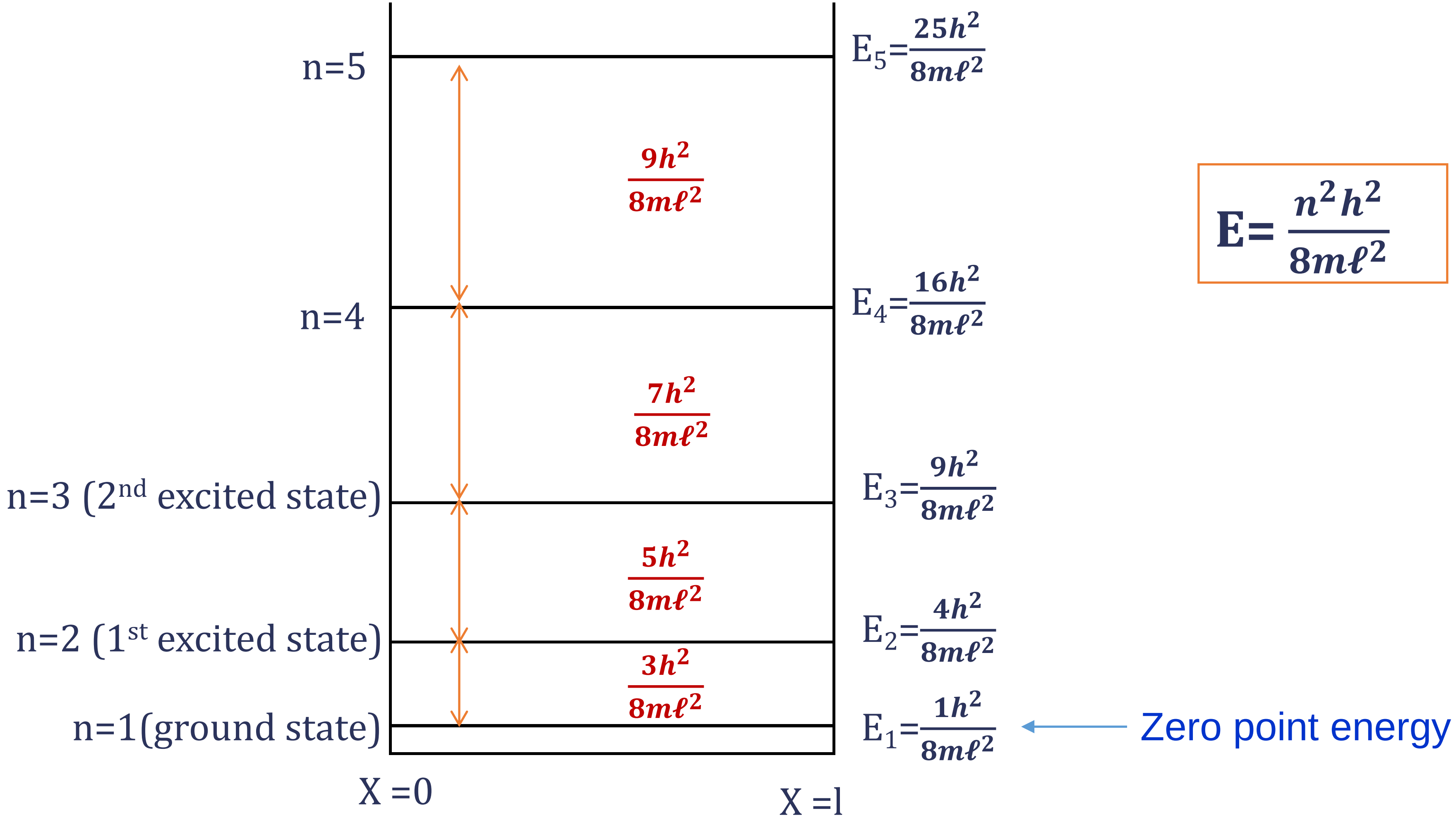
$$E = \frac{n^2\, h^2}{8mL^2}$$

Normalized wave function of the particle

$$\Psi_n = \sqrt{\frac{2}{L}}\sin\frac{n\pi x}{L}$$

Spacing between successive states becomes ***progressively larger*** as ‘*n*’ increases

The energy spacing between successive states

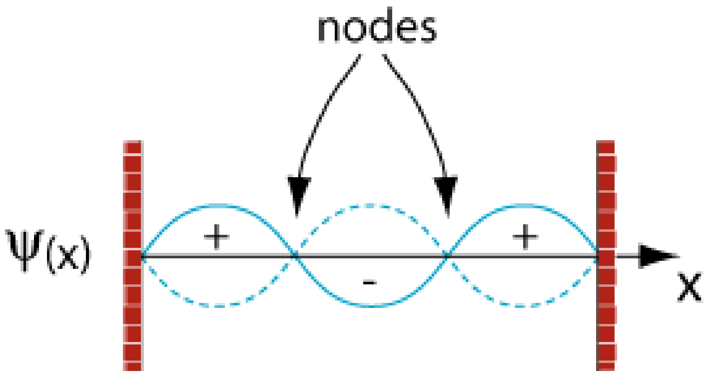


$$\boxed{E=\frac{n^2h^2}{8m\ell^2}}$$

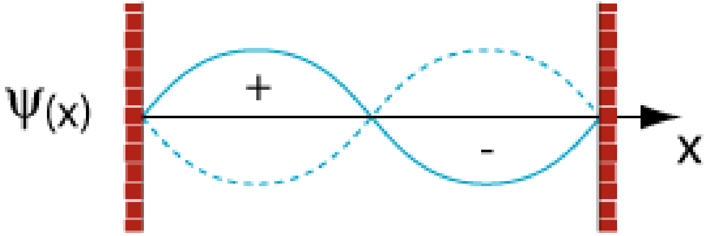
Graph of Wave Functions

The wave function $\psi(x)$ is sinusoidal . The number of nodes increases by 1 for each successive state.

No. of nodes = (n-1)

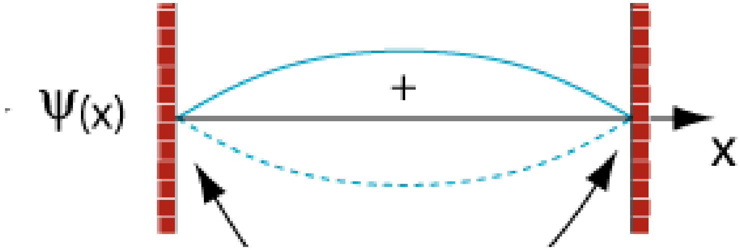


$\Psi_3 = A \sin\left(\frac{3\pi x}{l}\right)$ **2 nodes**



$\Psi_2 = A \sin\left(\frac{2\pi x}{l}\right)$ **1 node**

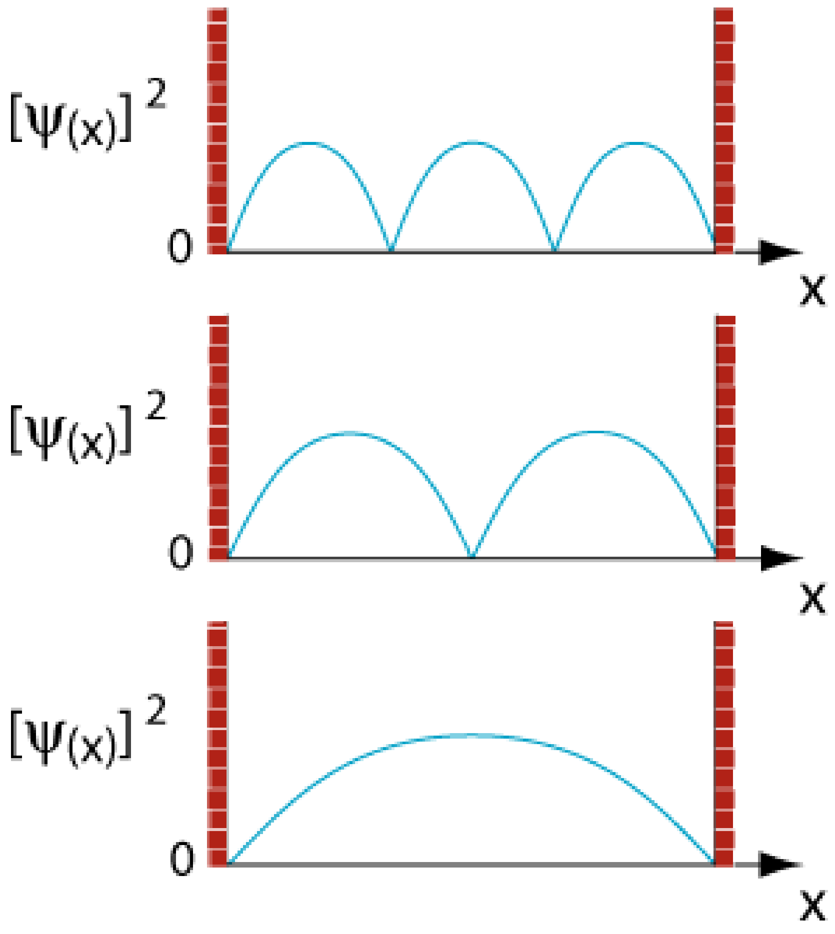
$\boldsymbol{\Psi = A \sin\left(\frac{n\pi x}{l}\right)}$



$\Psi_1 = A \sin\left(\frac{\pi x}{l}\right)$ **0 node**

Graph of Probability density $|\psi(x)|^2$

Maxima = n



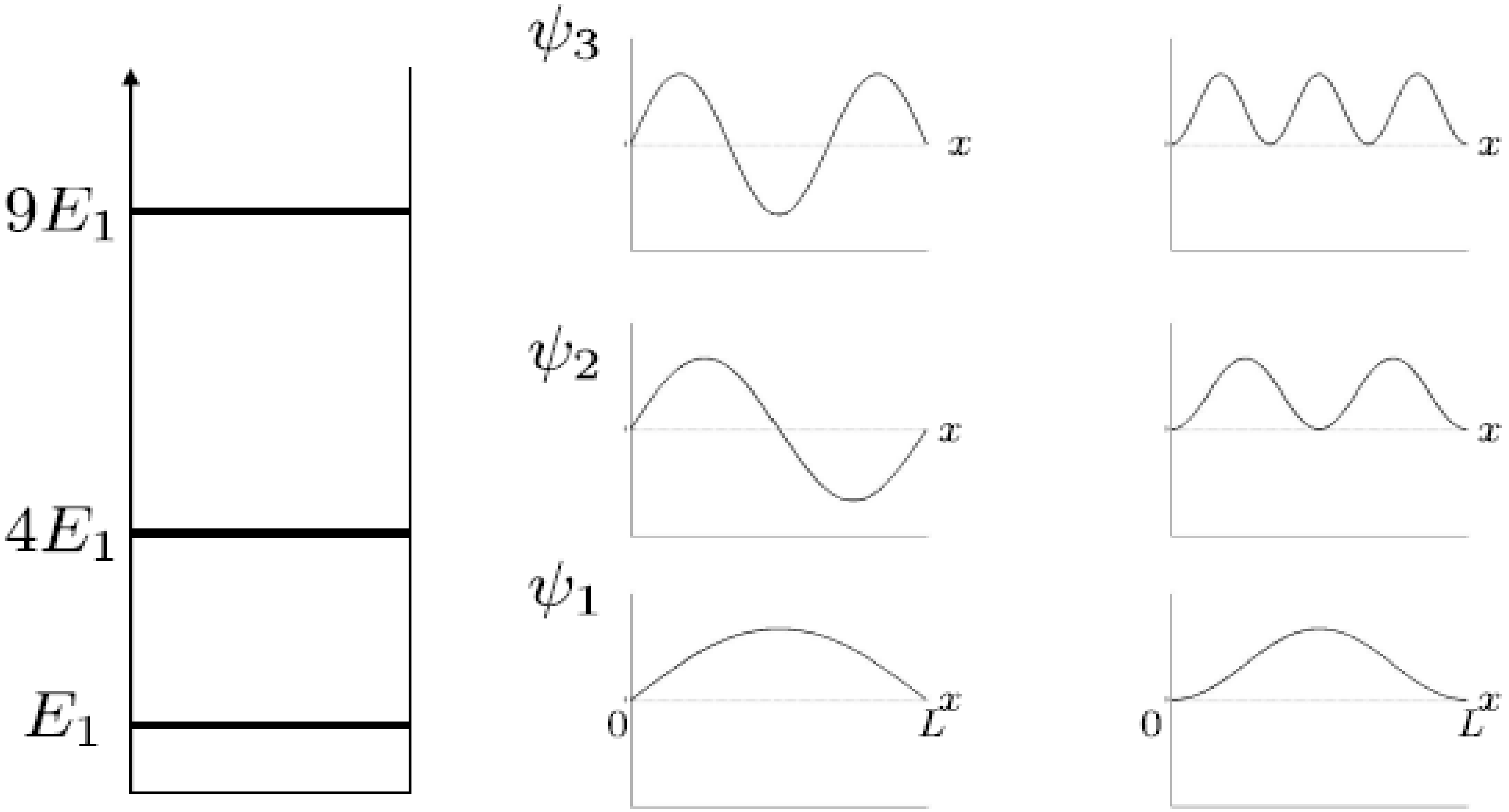
Maxima=3

Maxima=2

Maxima=1

Graphical representation of Wave Functions and Probability

EIGENENERGIES for 1-D BOX | EIGENSTATES for 1-D BOX | PROBABILITY DENSITIES



Quantum System	**Classical System**
Energy discretisation	continuous
E = 0: not possible	E = 0
P : different at different positions	Same everywhere
P : depends on n and hence energy state	P : independent on E
P = 0 at walls of potential well	P = maximum at walls

Q.1. Compute energy difference between the ground state and first excited state for an electron in a 1-D rigid box.

$$E_n = n^2h^2/8mL^2$$

$$\mathbf{E_2 - E_1 = 113.21\ eV}$$

Calculate the first four energy levels of an electron trapped in a rigid box having width 1.0 A^0 .
Also calculate the first four energy levels of a marble of mass 10 gm trapped in a rigid box of width 1.0 m.
Compare and interpret the results.

$$E_n = n^2h^2/8mL^2$$

Electron

$E_1 = 37.74$ eV

$E_2 = 150.96$ eV

$E_3 = 339.66$ eV

$E_4 = 603.84$ eV

marble

$E_1 = 5.5 \times 10^{-66}$ J

$E_2 = 22 \times 10^{-66}$ J

$E_3 = 50 \times 10^{-66}$ J

$E_4 = 88 \times 10^{-66}$ J

Q.2. Compute the lowest three permitted energy levels of an electron in an infinite potential well of width 1 A^0

$$E_n = n^2h^2/8mL^2$$

E1 = 38 eV

E2 = 152 eV

E3 = 342 eV

Q. 3. **Lowest energy of an electron trapped in potential well is 38 eV. Calculate the width of the well.**

$$L = 1A^0$$

Q.4. Calculate the energy and momentum of an electron confined in a rigid box of width 2A^0 for lowest energy state.

E1 = 1.509 X 10-18 J or 9.44 eV

P1 = 1.66 X 10 -24 kg-m/sec

Q.5. What accelerating potential would be required for a proton with zero velocity to acquire a velocity corresponding to De Broglie wavelength of 10^{-10} m? ($m_p = 1.67 \times 10^{-27}$ kg)

$$V = h^2 / 2me\lambda^2$$

$$V = 8.2 \times 10^{-2} \text{ volts}$$

Q.6. Calculate the minimum uncertainty in the velocity of an electron confined to a box of length 10 A^0

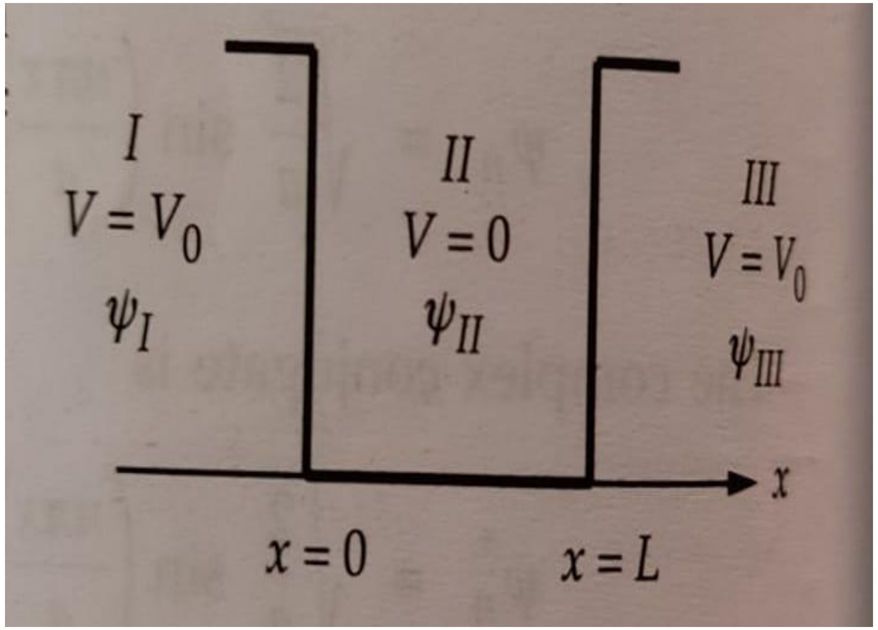
$$\Delta x \times \Delta p = h$$

$$\Delta x \times m(\Delta v) = h$$

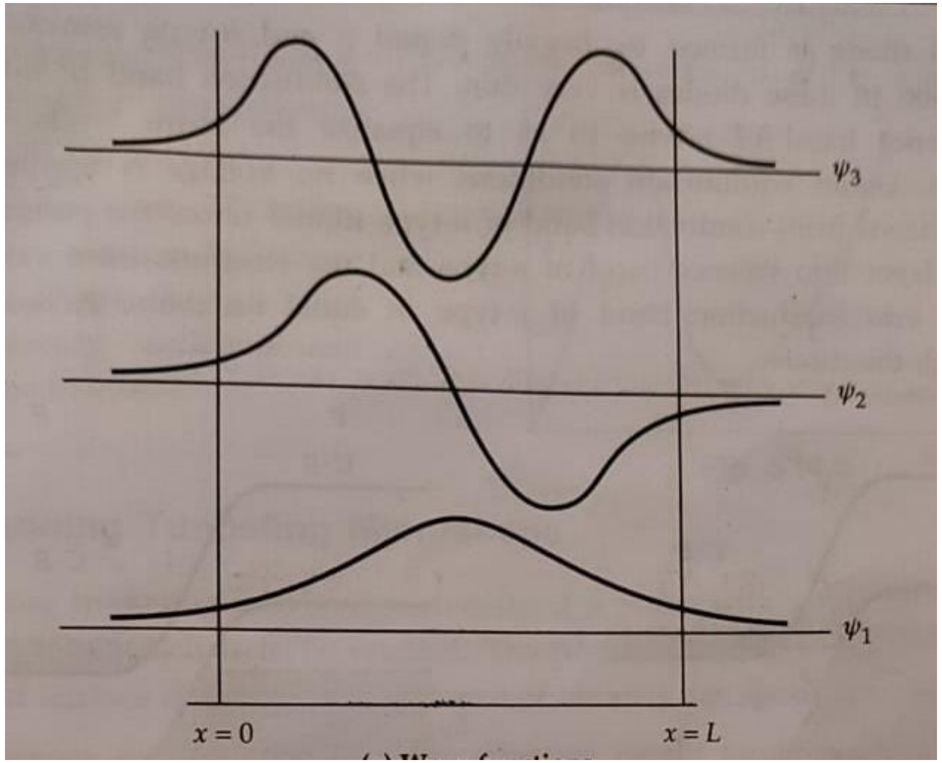
Particle in non-rigid box (finite potential well)

- Particle can penetrate through barrier
- Case I : Energy of particle is less than energy required to overcome the barrier ($E < V_0$)

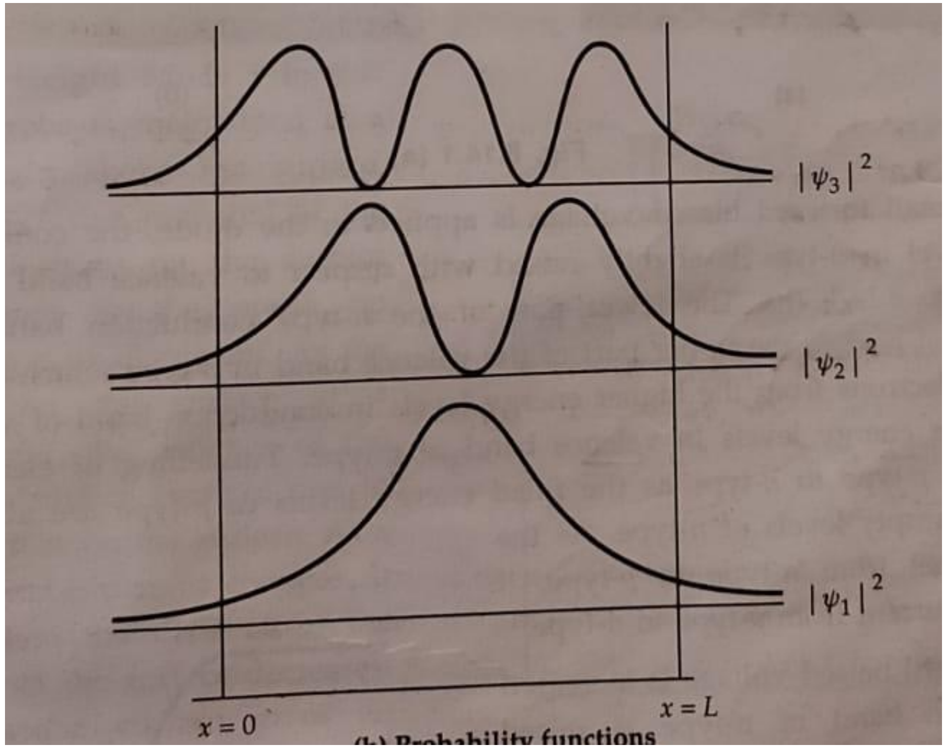
- **Region II:** wave function is same as rigid box
- **Rigid box:** wave function = 0 at walls (x = 0 and L)
- **Non-rigid box:** wave function ≠ 0 at walls
- At x < 0 (-∞), wave function decreases exponentially
- At x > L (∞), wave function decreases exponentially
- Probability of finding the particle outside the box



Particle in non-rigid box (finite potential well)



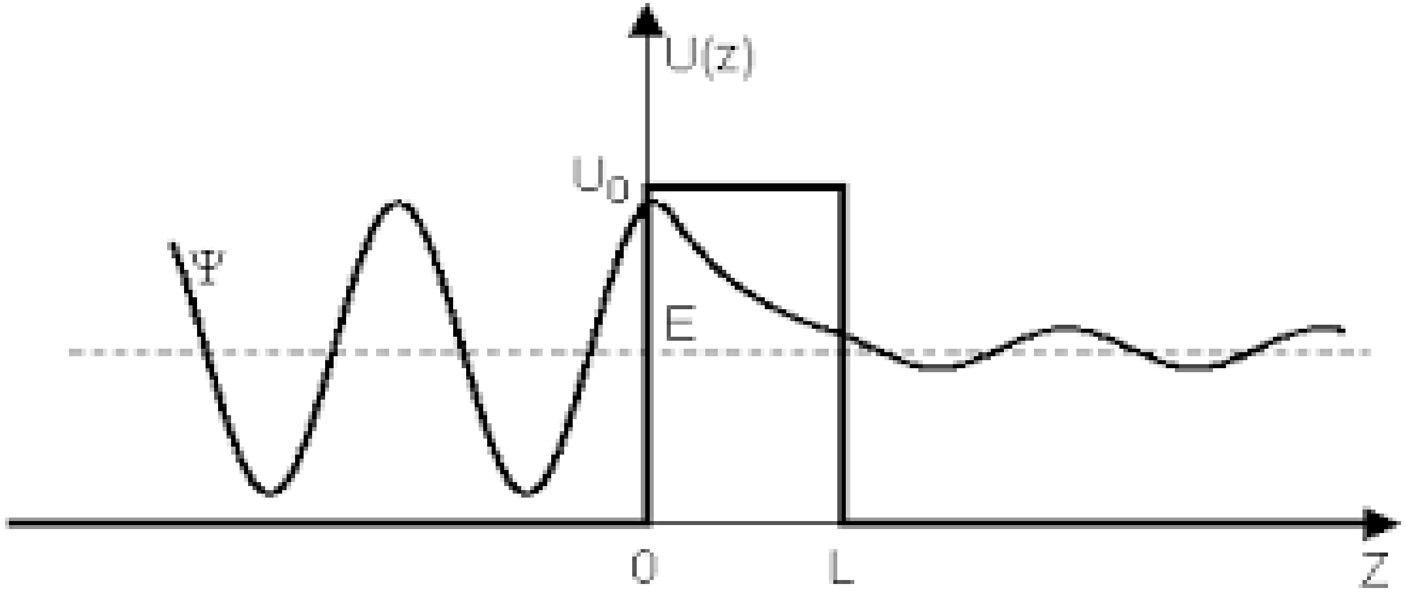
Wave functions



Probability functions

3. Tunnelling effect

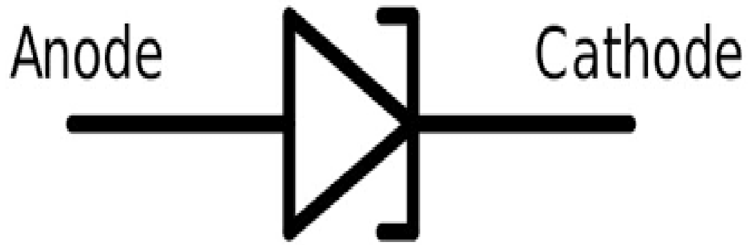
❖ Though the energy of particle is less than potential of barrier ($E<V_0$), it can tunnel or penetrate through the barrier. It is called tunnelling or quantum tunnelling.

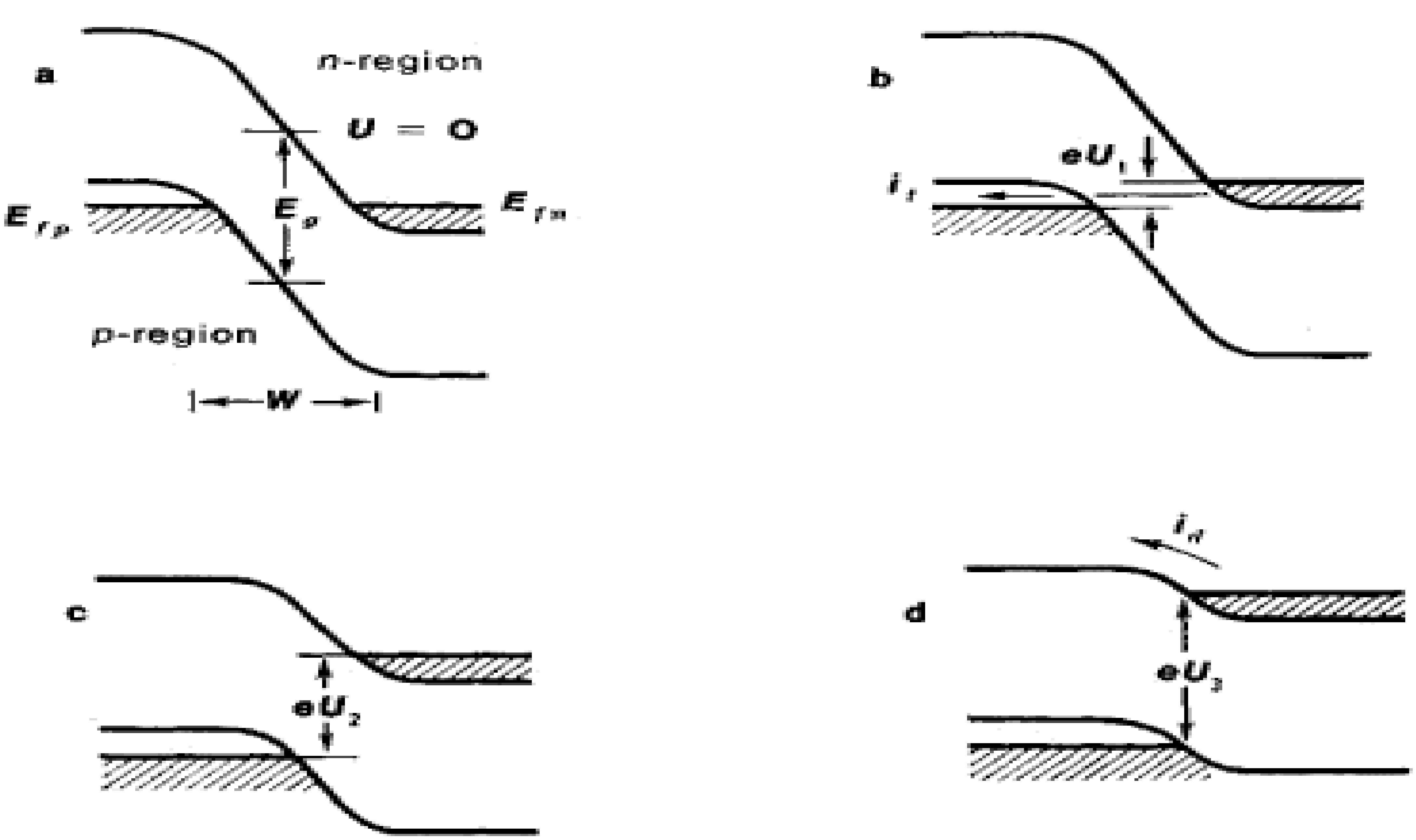


Tunnel Diode

- It is highly doped semiconductor device and mainly used for low voltage high frequency switching applications.

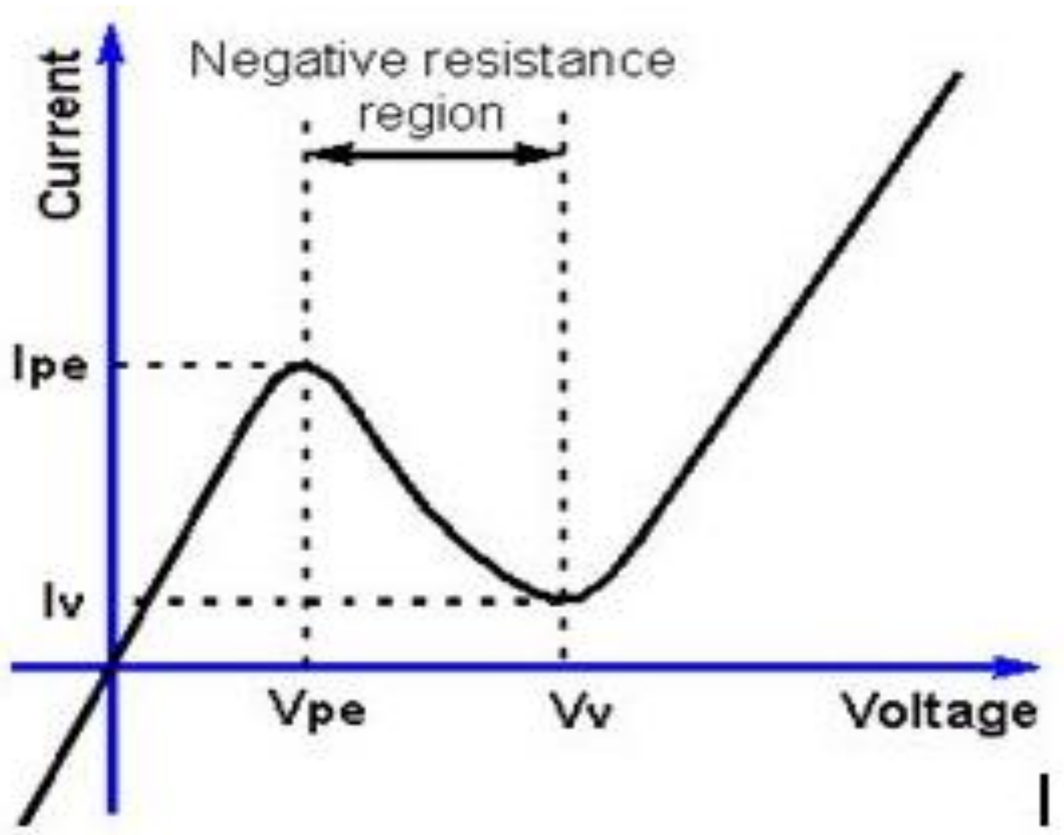
- Current flow: electrons tunnelling through potential barrier developed by depletion layer

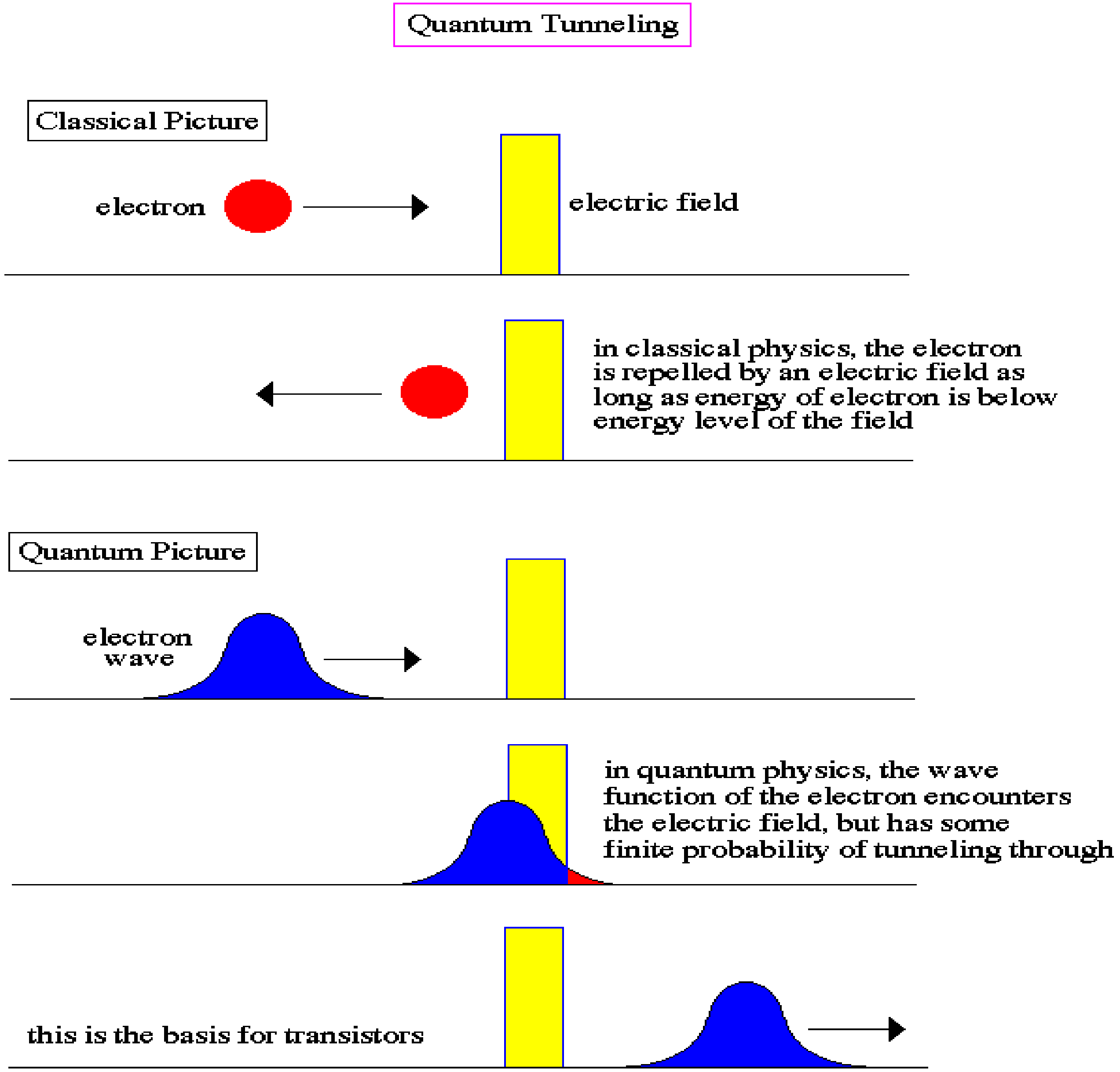




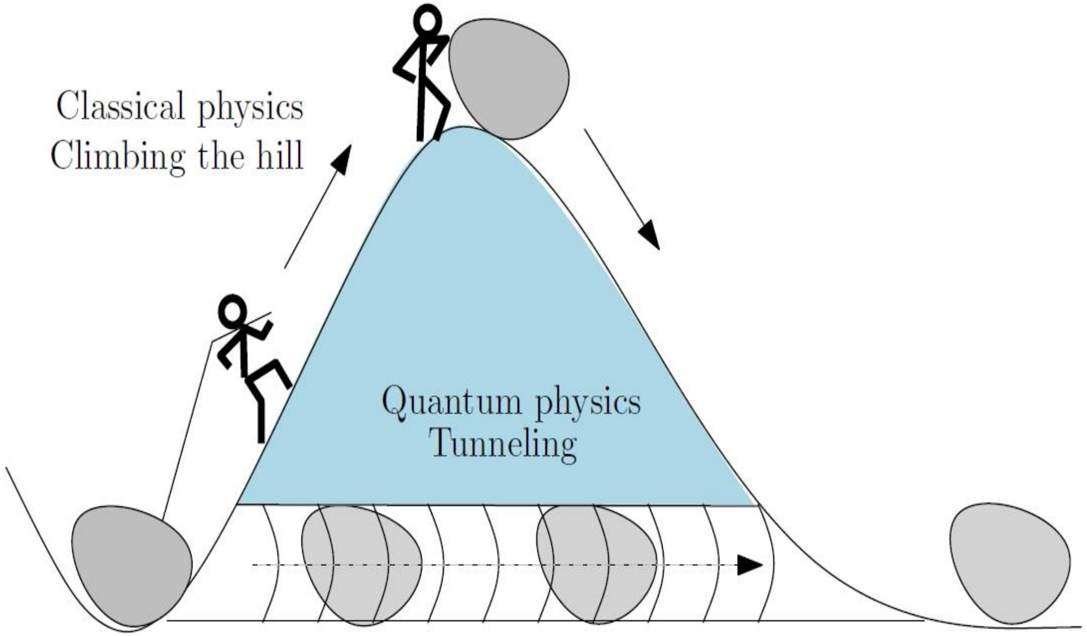
a
n-region
U = O
E_fp
E_g
E_fn
p-region
W
b
eU_1
i_t
c
eU_2
d
i_d
eU_3

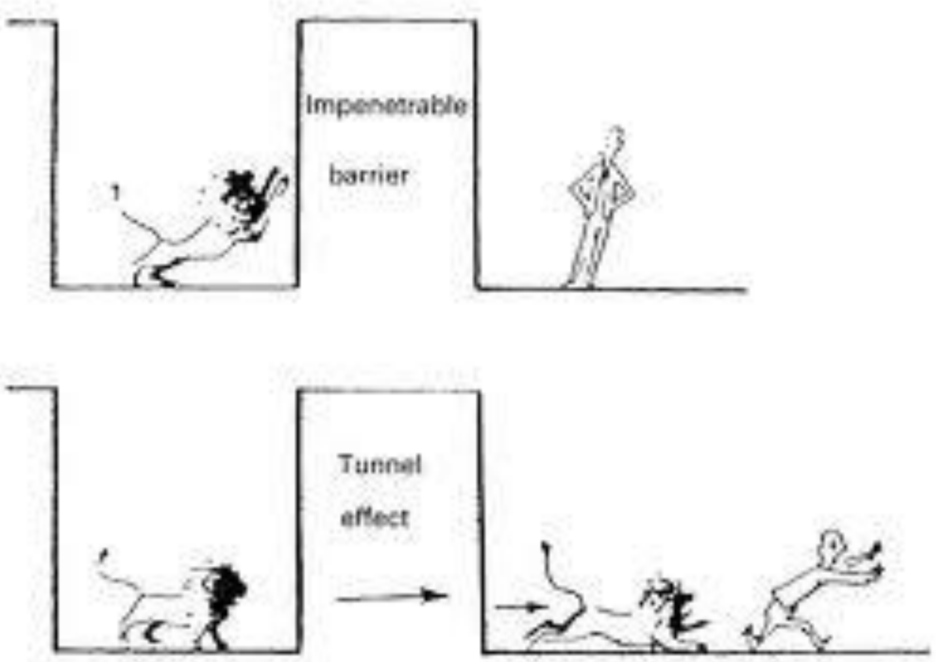
I-V characteristics of tunnel diode




Quantum Tunneling
Classical Picture
electron
electric field
in classical physics, the electron is repelled by an electric field as long as energy of electron is below energy level of the field
Quantum Picture
electron wave
in quantum physics, the wave function of the electron encounters the electric field, but has some finite probability of tunneling through
this is the basis for transistors

Tunneling Effect



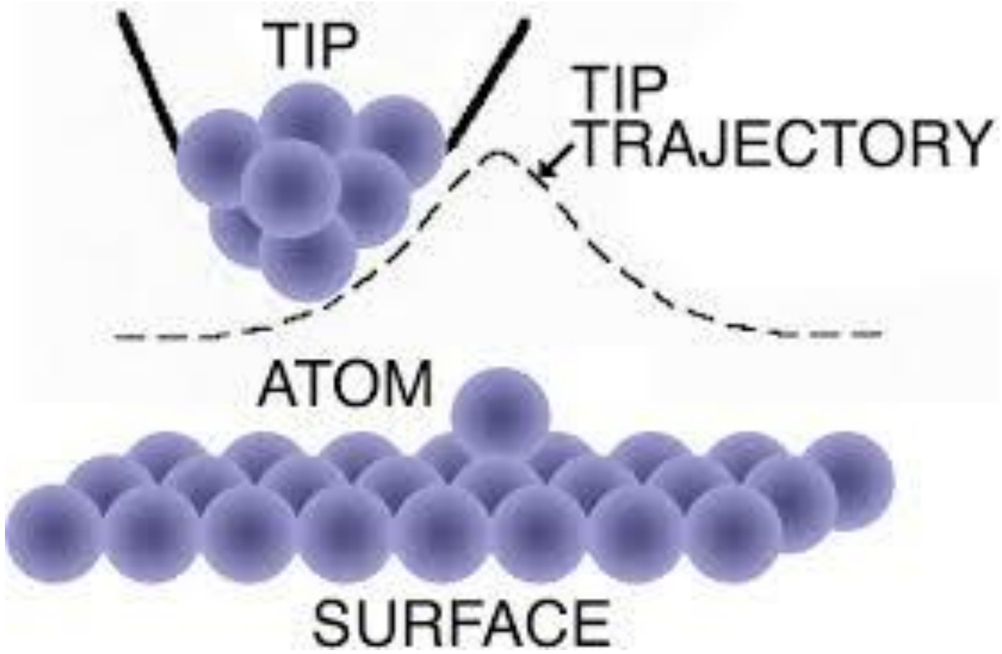


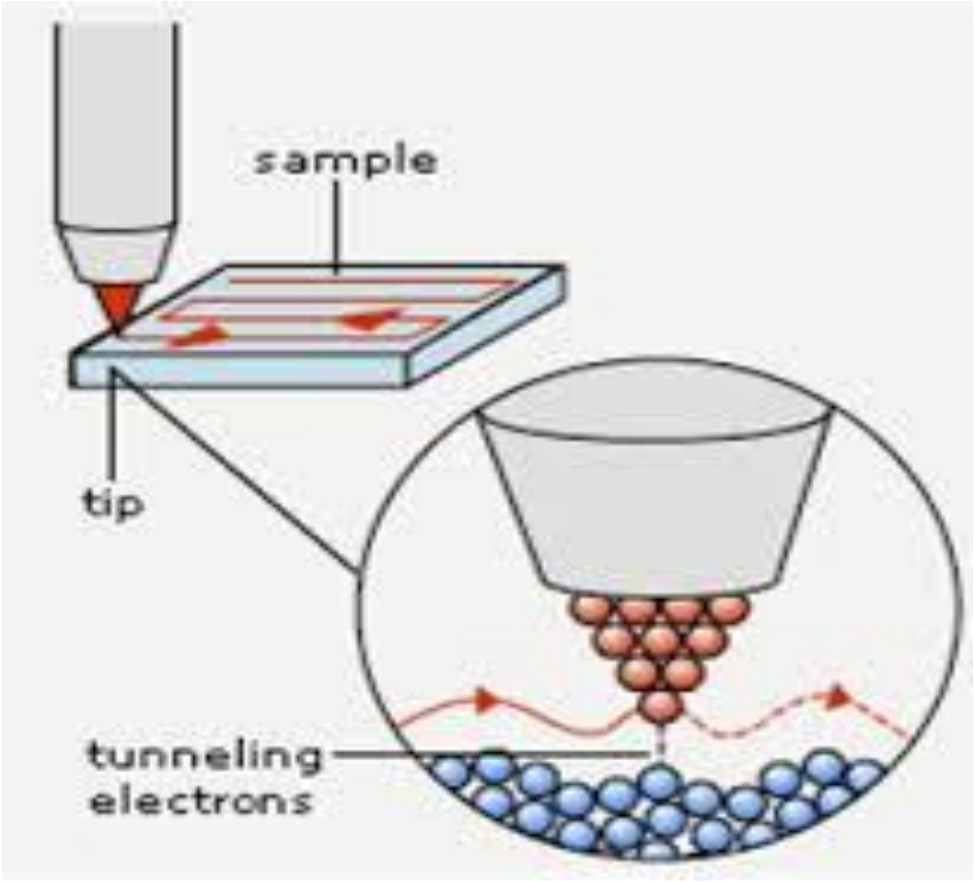
Applications of Tunnel Diode

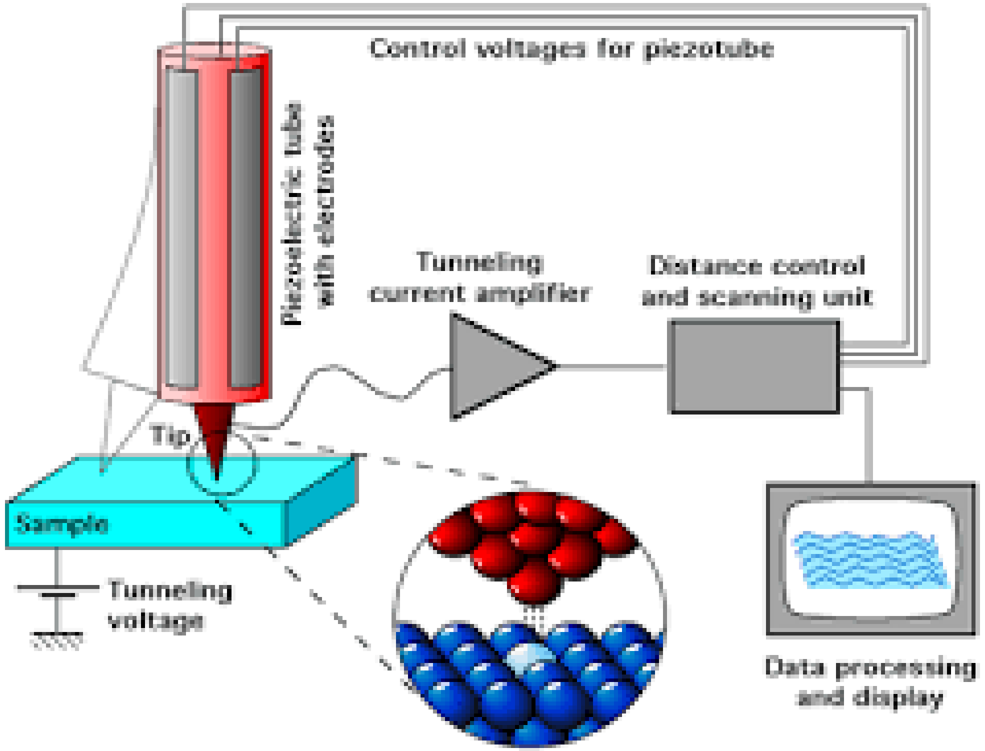
1. Used in microwave frequency range
2. Oscillator Circuits
3. Microwave generators and amplifiers
4. Satellite communication equipment

Scanning Tunnelling Microscope

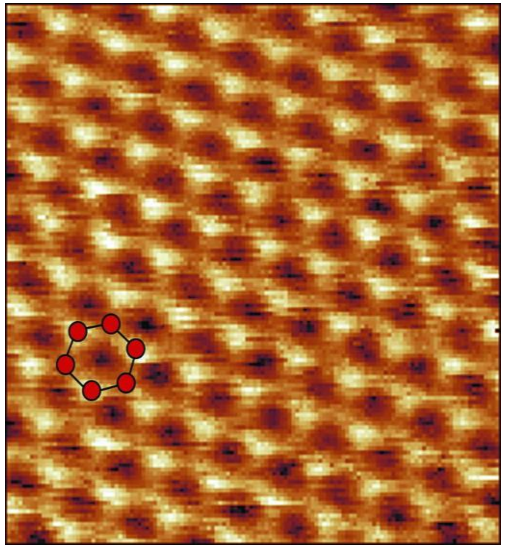
Electron microscope, used to create 3-D image of sample



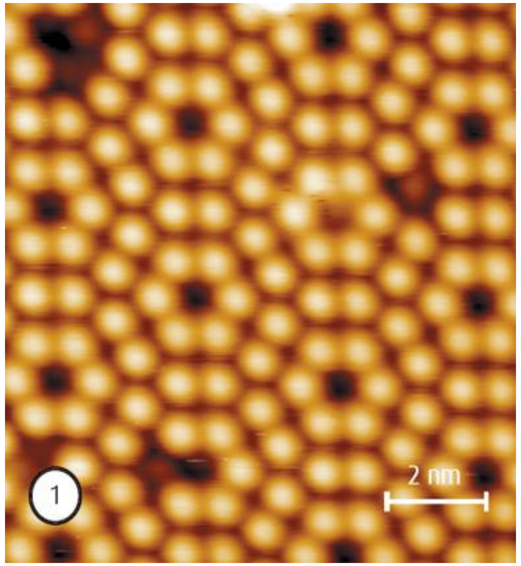




Graphite



Silicon



Commonly used Techniques in Materials Analysis

Microscopes - Optical microscope, confocal microscope, Scanning Electron Microscope (SEM), Transmission Electron Microscope (TEM), scanning Tunneling Microscope (STM), Atomic Force Microscope (AFM)

- **Useful to investigate morphology, size, structure and even composition depending upon the type of microscope**

Diffraction Techniques – X-ray Diffraction(XRD), Electron Diffraction, Neutron Diffraction, Small Angle X-ray scattering (SAXS)

- **Used in average particle size analysis as well as structural determination.**

Spectroscopies – UV-Vis-IR absorption (transmission and reflection modes), Fourier Transform Infra Red (FTIR), Atomic Absorption Spectroscopy (AAS), Electron Spin (or Paramagnetic) Resonance (ESR or EPR), Nuclear Magnetic Resonance (NMR), Raman Spectroscopy, various luminescence spectroscopies, Electron Spectroscopy for Chemical Analysis (ESCA) or X-ray Photoelectron Spectroscopy (XPS), Auger Electron Spectroscopy (AES)

- **useful for chemical state analysis (bonding or charge transfer amongst the atoms), electronic structure (energy gaps, impurity levels, band formation, transition probabilities etc.)**

Electric and magnetic measurements – two or four probe measurements, Magnetoresistivity, Vibrating Sample Magnetometer (VSM), Superconducting Quantum Interference Device (SQUID) etc.

Atomic Force Microscopy (AFM)

- The atomic force microscope (AFM) was developed to overcome a basic drawback with STM
- STM can only image conducting or semiconducting surfaces.
- The AFM has the advantage of imaging almost any type of surface, including polymers, ceramics, composites, glass, and biological samples.
- Based on interaction between tip and sample

Electron Microscope

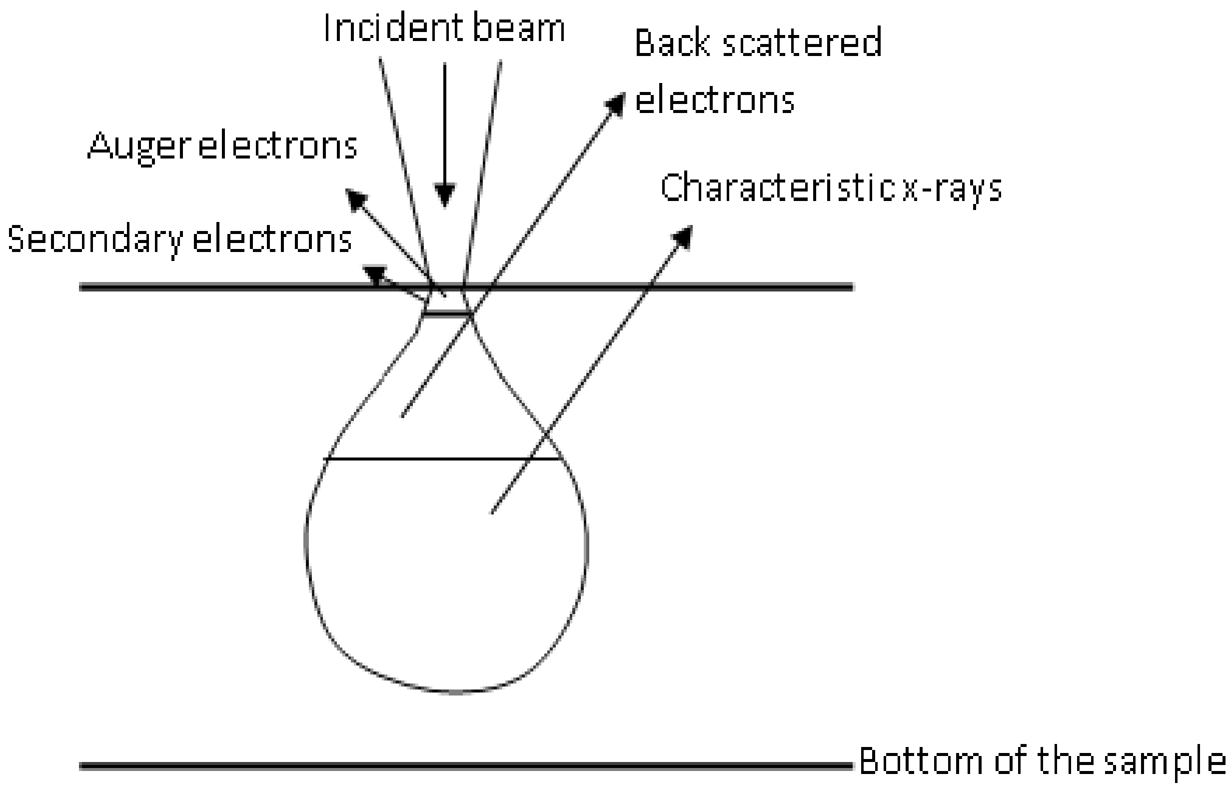
- **Optical microscopes** in general can resolve upto ~ 0.2 μm as visible light ranges from 400 – 700 nm

- Resolution is poor for microscopic particles

- **Electron microscopes** –

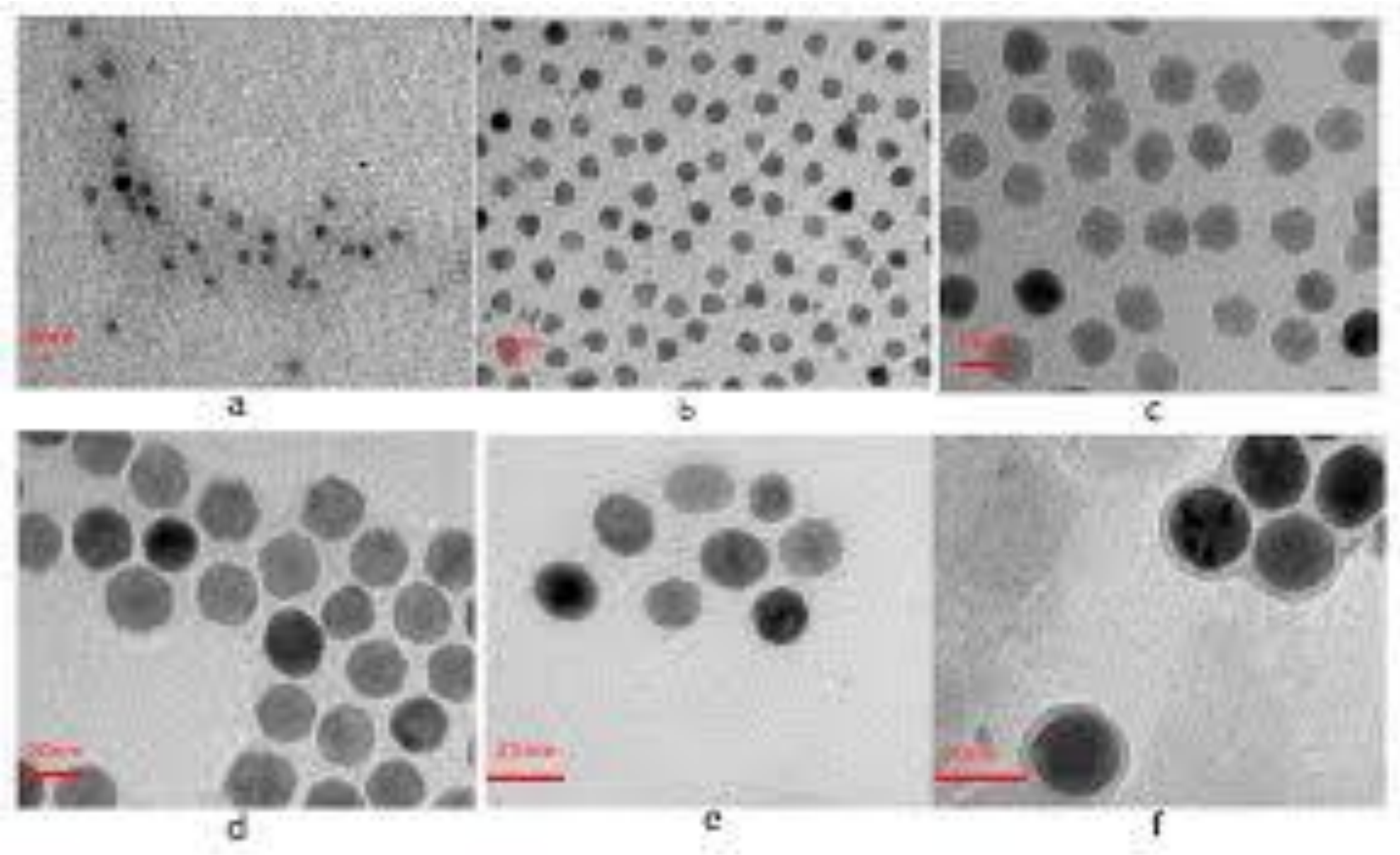
- electrons are used instead of radiations
- electrostatic or magnetic lenses are used instead of glass lenses
- electron waves can be used to image the objects – due to wave-particle duality
- wavelength can be tuned to a very small value, just by changing their energies: Resolution is better
- **Wavelength; de Broglie relation $\lambda = h/mv$**

Interaction of high energy electron with solid material



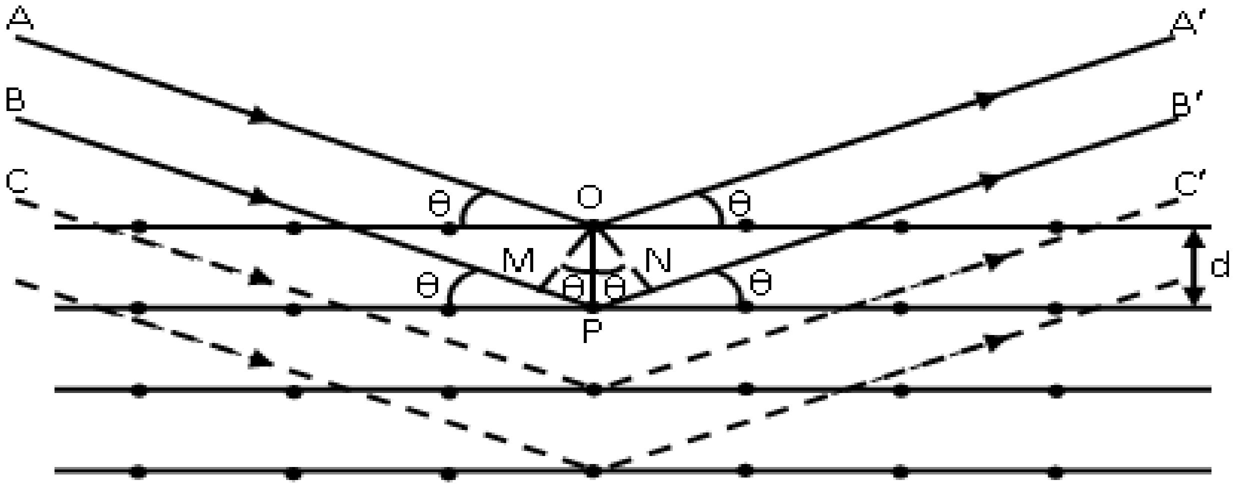
Scanning electron microscope, Transmission electron microscope (high resolution)

TEM images of sample



X ray diffractometer

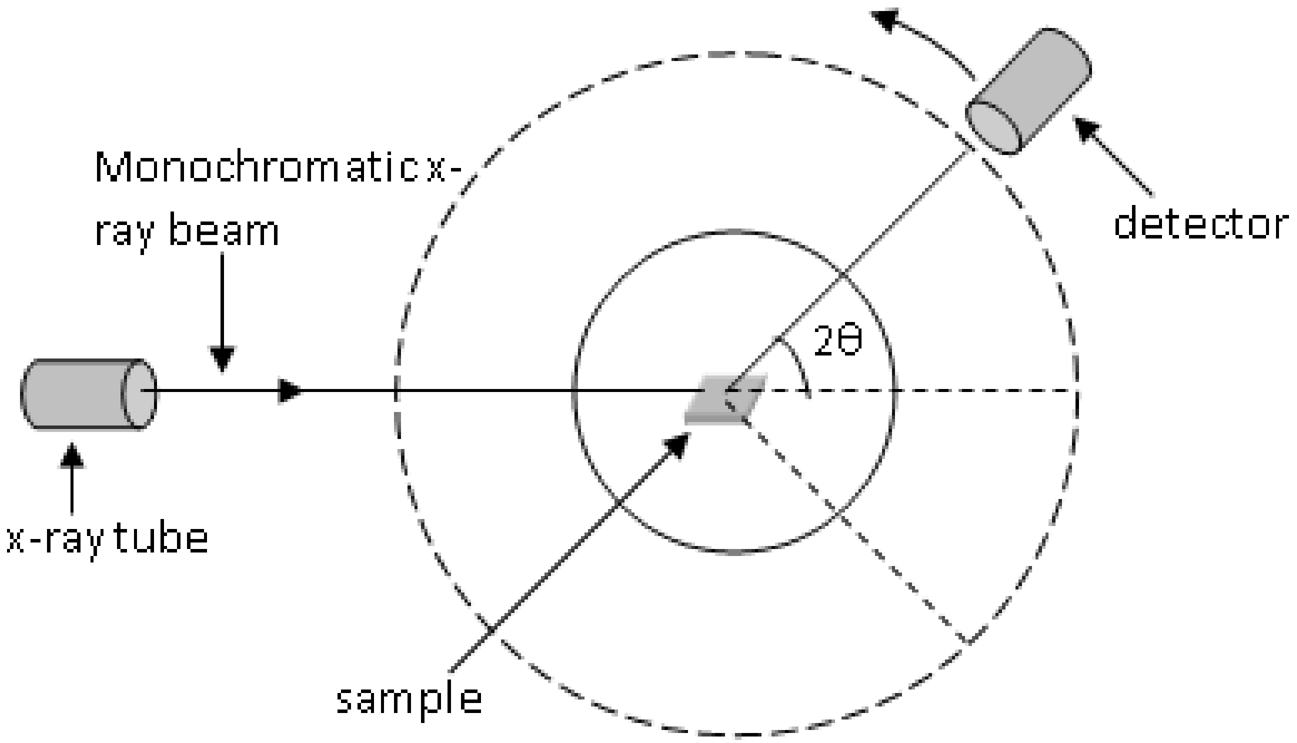
- To study crystal structure of bulk materials
- X-rays are scattered by electrons of atoms of solid material
- X-ray wavelength is comparable to distance between atoms (crystal planes); diffraction is possible



Bragg diffraction condition

$$n\lambda = 2d\sin\theta$$

Powder Diffractometer or Debye-Scherrer Diffractometer



Superconducting Quantum Interference Devices (SQUID)

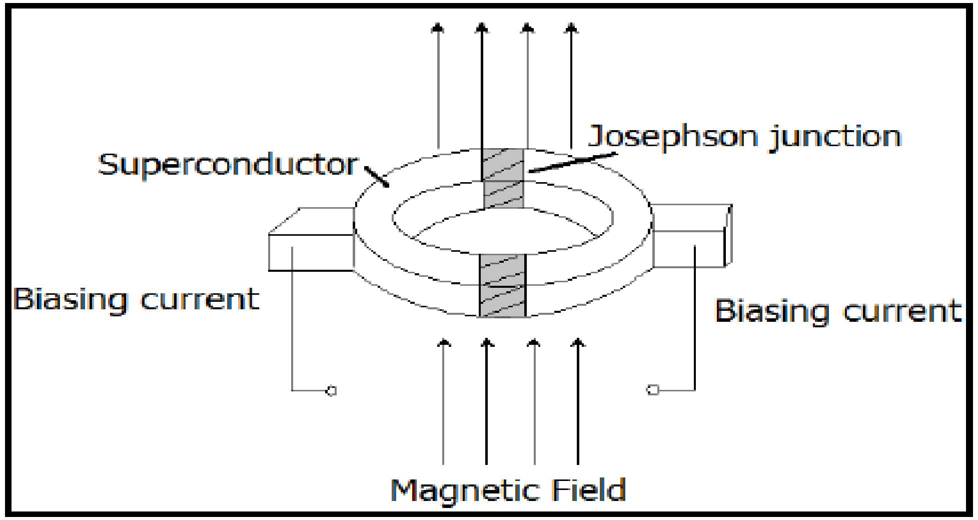
A SQUID (Superconducting Quantum Interference Device) is a very sensitive magnetometer used to measure extremely subtle (small) magnetic flux of the order of 10^{-18} Tesla. Their working is based on superconducting loops containing Josephson junctions.

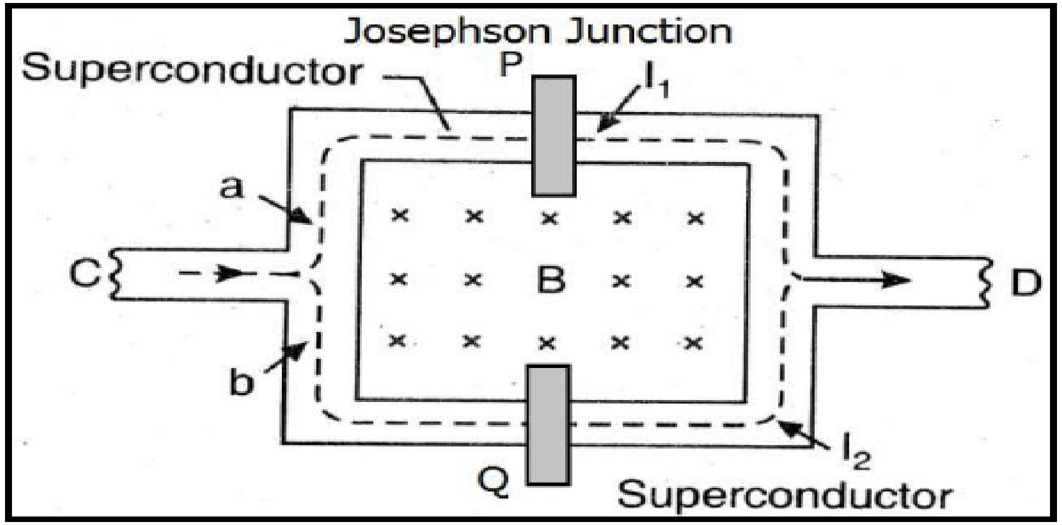
Construction of SQUID

There are two main types of SQUID: direct current (DC) and radio frequency (RF). A radio frequency (RF) SQUID is made up of one Josephson junction, which is mounted on a superconducting ring. A direct current (DC) SQUID consists of two Josephson junctions in parallel, which is more sensitive.

Construction

SQUIDs are usually fabricated from lead or pure niobium. The tunnel barrier is oxidized onto lead or niobium surface. The entire device is cooled to within a few degrees of absolute zero with liquid helium. A schematic of a two-junction dc SQUID is shown in figure. It consists of two Josephson junctions arranged in parallel.





Schrodinger’s cat

- After consultation with Einstein, Schrodinger proposed a thought experiment in which he highlighted the apparent inconsistencies between the so-called Copenhagen interpretation of Quantum Mechanics and the reality of macroscopic measurements.
- He proposed that a cat be placed in a sealed box. The release of a poison is then subject to the probabilistic decay of a radioactive isotope. If the isotope decays, the poison is released. If no decay occurs, the poison is not released.
- The result is that the cat is in a superposition of states between being dead, and being alive. This is very unintuitive.

Schrodinger’s Cat Experiment
Quantum Entanglement
Quantum Superposition

https://www.youtube.com/watch?v=67MG6_N0msg

https://www.ted.com/talks/josh_samani_what_can_schrodinger_s_cat_teach_us_about_quantum_mechanics?language=en

Quantum bits or qubits

https://www.youtube.com/watch?v=g_IaVepNDT4