Department of Physics
Online Courseware

Objective of the Physics-II Course: **Paper Code: PH (ECE) 401**

The **Physics-II Course** will

> ➢ provide exposure to the physics of electronic magnetic waves and its applications
>
> ➢ enable students to describe the physics of microscopic particles exhibiting wave nature
>
> ➢ provide exposure to the physics of materials that are applied in digital circuitry, storage devices.
>
> ➢ give an insight into the science & technology of next generation such as nanotechnology.
>
> ➢ form basics of new age scientific & technological fronts such as quantum computation and quantum circuits.

Pre-Requisites: 1st year Basic Physics knowledge

Delivery of the Course:

i) Preparation of Lecture plan by respective teacher(s).

ii) Preparation of session plan detailing the methodology, learners' activity, learning outcome (such as Skill, Competency etc).

ii) Preparation of delivery report by respective teacher(s) in the Institute specified book (Continuous Evaluation Diary)

Mode of Delivery of the course:

i) Chalk-talk method ii) Showing models (Demonstration)

iii) Analogy iii) Presentation

iv) Active learning: Cross-word puzzle

v) Active learning: Quiz/Brain storming

vi) Active learning: Role-play

vii) Active learning: Problem oriented guided inquiry learning (POGIL)

Course Evaluation: CIE (Continuous Internal Evaluation) and SEE (Semester End Examination) to constitute the major evaluations prescribed for the Course.

CIE (Continuous Internal Evaluation): To be conducted by the respective teacher and include mid-term/weekly/fortnightly class tests, surprise test, home work, problem solving, group discussion, quiz, problem oriented guided inquiry learning, mini-project & seminar throughout the Semester, with weightage for the different components being fixed at the institutional level. The teacher will discuss with students their performance, highlighting their strength and weakness.

SEE (Semester End Examination): To be conducted at the institutional level and cover the entire Course Syllabi; For this purpose, Syllabi to be modularized and SEE questions to be set from each module, with choice if any, to be confined to module concerned only. The questions to be comprehensive emphasizing analysis, synthesis, design, problems & numerical quantities.

Course Outcome of Advanced Physics Course (Theoretical: PH (IT) 301)

At the end of the course students' should have the

CO1: ability to apply the knowledge of ➢ **Operators in wave mechanisc** ➢ **Vector space & Heisenberg representation in developing knowledge of quantum bit** ➢ **Quantum bit and its representation as a two level system to design quantum logic gates** ➢ **Quantum gates in designing quantum circuits and teleportation** ➢ **Schrödinger equation in problems of junction diode, tunnel diode** ➢ **Magnetism and semiconductor physics in data storage** ➢ **Nano-range and various types of nanomaterials**	PO1
CO2: **Ability to analyze** ➢ **How use of superposition principle modifies the bits in quantum computation.** ➢ **How logical operation changes in quantum computation** ➢ **How to achieve quantum bit in practice** ➢ **Wide spread applications of electro-magnetic theoyr** ➢ **Physics of display devices** ➢ **Which type of magnetic materials to be used for data storage purpose** ➢ **Role of optoelectronic devices over usual semiconductor devices**	PO2
CO3: **ability to design and realize** ➢ **Quantum gates and quantum circuits** ➢ **High frequency oscillator from simple jn-diode like structure** ➢ **Storage devices using magnetic material, semiconductor devices.** ➢ **Modern display devices**	PO3
CO4: Ability to conduct experiments using ➢ **Band theory and electron transport in a semiconductor** ➢ **Intrinsic semiconductor under electric and magnetic field**	PO1, PO2, PO3, PO4,

	PO
➢ Temperature sensor, thermoelectric sensor	PO9
➢ Semiconductor Photovoltaic cell, Light emitting diodes, Light dependent resistor	PO10
➢ Cathode ray oscilloscope	
➢ Various types of magnetic materials	
CO5: Ability to communicate effectively, write reports and make effective presentation using available technology ➢ on topics allied to the subject particularly in areas of applications shared in student seminar	PO2 PO10
CO6: Ability to engage in independent self-study to formulate, design, enhance, demonstrate ➢ the N-Qubit Quantum gates and quantum ckts. ➢ Simple model to replicate Bell's inequality	PO2, PO3, PO4, PO9, PO10, PO12

CO-PO Mapping:

CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12
CO1	H											
CO2		H										
CO3			H									
CO4	H	M	L	L					M	M		
CO5		M								M		
CO6		M	M	L					M	M		H

CO-PEO Mapping: (Prepared based on the PEO of IT Dept.)

CO	PEO1	PEO2	PEO3	PEO4	PEO5
CO1	H	M	L		
CO2	H	M	L		
CO3	M	H	L		
CO4	M			M	M
CO5				M	M
CO6	L			M	M

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Module 1: Electricity and Magnetism (8L)

Module 1.01: Electrostatics

Gauss's law in integral form and conversion into differential form, Equation of continuity, Extend to Poisson's & Laplace's equation, Application to parallel plate, spherical and cylindrical capacitors (equivalent 1D problem). 3L

Module 1.02: Magnetostatics:

Lorentz force (concept in Hall effect-), force on a small current element placed in a magnetic field. Biot-Savart law-non existence of magnetic monopole, Ampere's circuital law, Magnetic vector and scalar potential. 3L

Module 1.03: Electro-magnetism & Electromagnetic theory

Faraday's law, Concept of displacement current, Maxwell's field equations with physical significance, wave equation in free space, transverse nature of electromagnetic wave.   2L

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Lesson plan for Electricity and Magnetism

Module No	Lecture No	Topic	Application	Reference Book
Module 1: Electricity and Magnetism	1	Gauss's law in integral form and conversion into differential form, Equation of continuity	Electric field determination for a symmetrical charge distribution Circuit theory Medical Acoustics Bubble chamber Traffic control MRI Magnetic tape	Electricity and Magnetism (In Si Units): Berkeley Physics Course - Vol.2, Edward M Purcell Introduction to Electrodynamics-Griffiths David J. The Feynman Lectures on Physics. *2 (2nd ed.)., Feynman, Richard P Addison-Wesley.* ISBN 978-0-8053-9065-0
	2	Extend to Poisson's & Laplace's equation, Application to parallel plate		
	3	Spherical and cylindrical capacitors (equivalent 1D problem)		
	4	Lorentz force (concept in Hall effect-), force on a small current element placed in a magnetic field		
	5	Biot-Savart law-non existence of magnetic monopole		
	6	Ampere's circuital law, Magnetic vector and scalar potential		
	7	Faraday's law, Concept of displacement current, Maxwell's field equations with physical significance		
	8	Wave equation in free space, transverse nature of electromagnetic wave		

Module 1: Electricity and Magnetism

1.1 Electrostatics

1.01.1 Gauss' Law

The net electric flux through any hypothetical closed surface is equal to $1/\varepsilon$ times the net electric charge within that closed surface.

The law can be expressed mathematically using vector calculus in integral form and differential form. Both are equivalent since they are related by the divergence theorem, also called Gauss' theorem.

Gauss' Law in Integral form

Gauss' law may be expressed as

$$\Phi_E = Q/\varepsilon_0$$

where Φ_E is the electric flux through a closed surface S enclosing any volume V, Q is the total charge enclosed within V, and ε_0 is the electric constant. The electric flux Φ_E is defined as a surface integral of the electric field:

$$\Phi_E = \oiint_S \mathbf{E \cdot dA}$$

where **E** is the electric field, d**A** is a vector representing an infinitesimal element of area of the surface.

Since the flux is defined as an integral of the electric field, this expression of Gauss' law is called the integral form.

Gauss' Law in Differential form

By the divergence theorem, Gauss' law can alternatively be written in the *differential form*:

$$\nabla \cdot \mathbf{E} = \rho/\varepsilon_0$$

where $\nabla \cdot \mathbf{E}$ is the divergence of the electric field, ε_0 is the electric constant, and ρ is the total electric charge density (charge per unit volume).

- The integral and differential forms are mathematically equivalent, by the divergence theorem.

Conversion of integral form to differential form:

The integral form of Gauss' law is:

$$\oiint_S \mathbf{E} \cdot \mathbf{dA} = Q / \varepsilon_0$$

for any closed surface S containing charge Q. By the divergence theorem, this equation is equivalent to:

$$\oiiint_V \nabla \cdot \mathbf{E} \, dV = Q/\varepsilon_0$$

for any volume V containing charge Q. By the relation between charge and charge density, this equation is equivalent to:

$$\int_V \nabla \cdot \mathbf{E} \, dV = \int \rho/E_0 \, dV$$

for any volume V. In order for this equation to be simultaneously true for every possible volume V, it is necessary (and sufficient) for the integrands to be equal everywhere. Therefore, this equation is equivalent to:

$$\nabla \cdot \mathbf{E} = \rho/\varepsilon_0$$

Thus the integral and differential forms are equivalent.

1.1.2 Equation of Continuity

A **continuity equation** in physics is an equation that describes the transport of some quantity. By the divergence theorem, a general continuity equation can also be written in a "differential form":

$$\nabla \cdot \mathbf{j} + \frac{\partial \rho}{\partial t} = \sigma$$

where

- ρ is the amount of the quantity q per unit volume,
- **j** is the flux of q,
- t is time,
- σ is the generation of q per unit volume per unit time. Terms that generate ($\sigma > 0$) or remove ($\sigma < 0$) q

In electromagnetic theory, the continuity equation is an empirical law expressing (local) charge conservation. Mathematically it is an automatic consequence of Maxwell's equations, although charge conservation is more fundamental than Maxwell's equations. It states that the divergence of the current density **j** (in amperes per square meter) is equal to the negative rate of change of the charge density ρ (in coulombs per cubic metre).

1.1.3   Poisson's & Laplace's Equation:

In mathematics, **Poisson's equation** is a partial differential equation of elliptic type with broad utility in mechanical engineering and theoretical physics. It arises, for instance, to describe the potential field caused by a given charge or mass density distribution; with the potential field known, one can then calculate gravitational or electrostatic field. It is a generalization of Laplace's equation, which is also frequently seen in physics.

Starting with Gauss's law for electricity (also one of Maxwell's equations) in differential form, one has

$$\nabla . \mathbf{D} = \rho$$

where, **D** = electric displacement field, and ρ = free charge volume density (describing charges brought from outside).

Assuming the medium is linear, isotropic, and homogeneous, we have the constitutive equation,

$$\mathbf{D} = \varepsilon \mathbf{E}$$

where ε = permittivity of the medium and **E** = electric field.

Substituting this into Gauss's law and assuming ε is spatially constant in the region of interest yields

$$\nabla \cdot \mathbf{E} = \rho / \varepsilon$$

where ρ is a total volume charge density. In the absence of a changing magnetic field, **B**, Faraday's law of induction gives

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial \mathbf{o}}$$

Since the curl of the electric field is zero, it is defined by a scalar electric potential field, φ as

$$\mathbf{E} = -\nabla \varphi$$

Substituting the potential gradient for the electric field, we get

$$\boxed{\nabla^2 \varphi = -\rho / \varepsilon}$$

which is **Poisson's equation** for electrostatics.

If ρ is 0, indicating zero volume charge density, but allowing point charges, line charge, and surface charge density to exist at singular locations as sources of the field, then

$$\Box^2 \varphi = 0$$

which is Laplace's equation. The operator $\Box^2$ is known as Laplacian of **φ.**

In Cartesian coordinates (x, y, z) Laplace's equation is

$$\Box^2 \varphi = \frac{\partial^2 \Box}{\partial x^2} + \frac{\partial^2 \Box}{\partial y^2} + \frac{\partial^2 \Box}{\partial z^2} = 0$$

In Spherical coordinates(r, θ, Ø) Laplace's equation is

$$\Box^2 \varphi = \frac{1}{r^2} \frac{o}{or}(r^2 \frac{o\emptyset}{or}) + \frac{1}{r^2 \sin 0} \frac{o}{\Box r}(\sin\Box \frac{\Box\emptyset}{\Box\Box}) + \frac{1}{r^2 \sin^2 \emptyset} \frac{o^2\emptyset}{o\emptyset^2} = 0$$

In Cylindrical coordinates (ρ, Ø, z) Laplace's equation is

$$\Box^2 V = \frac{1}{p} \frac{o}{o\emptyset}(r^2 \frac{oV}{or}) + \frac{1}{\Box^2} \frac{o^2V}{\partial \emptyset^2} + \frac{o^2 V}{\partial z^2} = 0$$

1.01.4 Application

Parallel plate capacitor:

Consider a parallel plate capacitor with a plate separation of d between the plates. The lower plate is grounded while the upper plate is maintained at a constant potential φ_0. Between the two plates there are no sources and hence Laplace's equation is valid in this region. Since the plates are assumed infinite in the x, y directions, the only variation is with respect to the z direction and we have,

$$\nabla^2 \varphi \equiv \frac{\partial^2 \varphi}{\partial z^2} = 0$$
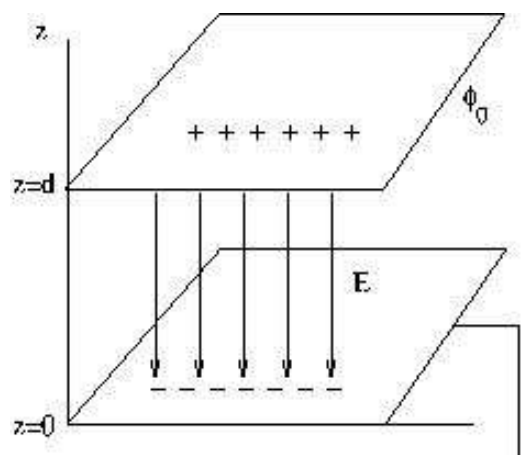
The solution of this equation is straightforward, and we get,

$$\varphi(z) = Az + B$$

where A and B are constants. Substituting the boundary conditions at z=0 and at z=d,

$$\varphi(z = 0) = 0 = B$$

$$\varphi(z = d) = \varphi_0 = Ad$$

which gives, $A = \overline{\frac{\varphi_0}{d}}$, $B = 0$
Substituting these, we get

$$\varphi(z) = \frac{\varphi_0}{d} z$$

The electric field in the region is given by $\vec{E} = -\nabla\varphi = -\hat{k}\,\frac{a\varphi}{az} = -\frac{\varphi_0}{d}\hat{k}$. This shows that the electric field

between the plates is constant and is directed from the upper plate toward the lower plate. If the upper plate is charged to a potential V_B and the potential of lower plate is V_A then

At z = 0, $\varphi = V_A$ and at z = d, $\varphi = V_B$
So, $V_A = B$ and $V_B = Ad + B$

Solving, $B = V_A$ and $A = -\frac{V_A\text{-}V_B}{d}$

Spherical capacitor:

$$\boxed{V = V_A - \frac{V_A\text{-}V_B}{d}}$$

Consider a spherical capacitor with the inner conductor having a radius a and the outer conductor a radius b.

The outer conductor is grounded and the inner conductor is maintained at a constant potential φ_0. Because of spherical symmetry, the potential can only depend on the radial distance r. The radial part of Laplace's equation, which is valid in the space between the conductors is given by
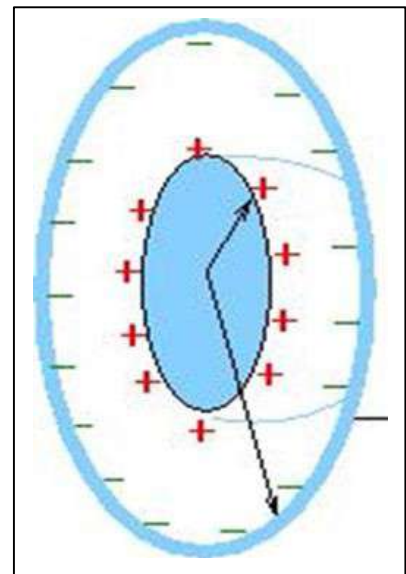
$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d\varphi}{dr}\right) = 0$$

This is a differential equation in a single variable, and the solution can be easily obtained as

$$\varphi(r) = -\frac{A}{r} + B$$

where AInserting the boundary conditions,

$$\varphi(r = b) = 0$$

Inserting the boundary conditions,

$$\varphi(r = b) = 0$$

gives $B = \frac{A}{b}$. The other boundary condition $\varphi(r = a) = \varphi_0$ gives

$$\varphi_0 = -\frac{A}{a} + \frac{A}{b}$$

Substituting these into the solution, we have,

$$A = -\frac{\varphi_0 ab}{b - a}$$

$$\varphi(r) = \frac{\varphi_0 ab}{b - a}\left(\frac{1}{r} - \frac{1}{b}\right)$$

As before, we find the charge density on the spheres by taking the normal component of the electric field. The electric field is given by,

$$\vec{E} = -\frac{d\varphi}{dr}\,\hat{r}$$

$$= \frac{\varphi_0 ab}{b - a}\frac{1}{r^2}\,\hat{r}$$

The charge density on the inner plate is given by

$$\sigma_{in} = \epsilon_0 \frac{\varphi_0 ab}{b - a}\frac{1}{a^2}$$

The total charge on the inner sphere is

$$Q = \frac{4\pi\epsilon_0\varphi_0 ab}{b - a}$$

It can be checked that the outer sphere has equal and opposite negative charge. The capacitance is given by
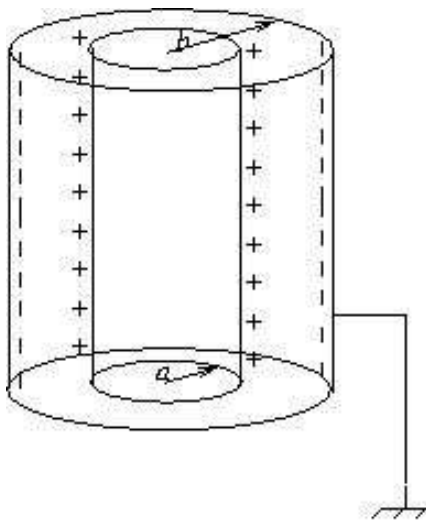
$$C = \frac{4\pi\epsilon_0 ab}{b - a}$$

The capacitance of a single spherical conductor is obtained by taking the outer sphere to infinity, i.e., $b \to \infty$, which gives the capacitance for a single conductor to be $4\pi\epsilon_0 a$. This result is not surprising because for a single conductor containing charge Q, the potential is $\varphi = \frac{Q}{4\pi\epsilon_0 a}$, so that the capacitance, which is given by $\frac{Q}{\varphi} = 4\pi\epsilon_0 a$.

Cylindrical capacitor:

Consider a coaxial cable of inner radius a and outer radius b. The outer conductor is grounded while the inner conductor is maintained at a constant potential φ_0. Taking the z axis of the cylindrical coordinate system along the axis of the cylinders, we can write down the Laplace's equation in the space between the cylinders as follows :

$$\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial\varphi}{\partial\rho}\right) + \frac{1}{\rho^2}\frac{\partial^2\varphi}{\partial\theta^2} + \frac{\partial^2\varphi}{\partial z^2} = 0$$

Here, ρ is the radial distance from the axis and θ is the polar angle. We assume the cylinders to be of infinite extend in the z direction. This implies that there is azimuthal symmetry and no variation with respect to z as well. The solution can only depend on the radial distance ρ.

Giving,

$$\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial\varphi}{\partial\rho}\right) = 0$$

The solution of the above equation is easy to obtain, and we get,

$$\varphi(\rho) = A\ln\rho + B$$

where A and B are two constants which must be determined from the boundary conditions.

$\varphi(\rho = b) = 0$, gives $A\ln b + B = 0$, so that $B = -A\ln b$. The boundary condition at $\rho = b$ gives $\varphi_0 = A\ln a - A\ln b$, so that

$$A = \frac{\varphi_0}{\ln\left(\frac{a}{b}\right)}$$

Substituting these in the expression for the potential, we get the potential in the region between the cylinders to be given by

$$\varphi(\rho) = \varphi_0\frac{\ln\left(\frac{\rho}{b}\right)}{\ln\left(\frac{a}{b}\right)}$$

The electric field in the region is given by the negative gradient of the potential which is simply the derivative with respect to ρ,

$$\vec{E} = -\nabla\varphi = -\rho\frac{\partial}{\partial\rho}\varphi(\rho)$$

$$= -\rho \, \frac{\varphi_0}{\ln(\frac{a}{b})} \, \frac{1}{\rho}$$

Since $\ln\left(\frac{a}{b}\right) < 0$, the direction of the electric field is outward from the inner conductor, which gets positively charged. The charge density of the inner conductor is given by

$$\sigma = \epsilon_0 E_n = +\varphi_0 \epsilon_0 \, a \, \ln(\frac{1}{\frac{b}{a}})$$

where we have taken care of the minus sign by inverting the argument of log.

Note that the expression for the charge density on the outer plate will not be identical because of the fact that the radii of the two cylinders are different. The total charge per unit length on the inner conductor is given by

$$Q = \varphi_0 \epsilon_0 \, \frac{2\pi a}{a \ln(\frac{b}{a})} = \frac{2\pi \varphi_0 \epsilon_0}{\ln(\frac{b}{a})}$$

The magnitude of the charge per unit length on the outer conductor can be seen to be the same. The capacitance per unit length is thus given by

$$C = \frac{2\pi\epsilon_0}{\ln(\frac{b}{a})}$$

1.2 MAGNETOSTATICS

1.2.1 Lorentz Force:

In physics (particularly in electromagnetism) the **Lorentz force** is the combination of electric and magnetic force on a point charge due to electromagnetic fields. A particle of charge q moving with velocity **v** in the presence of an electric field**E** and a magnetic field**B** experiences a force

$$\vec{F} = \mathbf{q} \, (\vec{E} + \vec{v} \times \vec{B})$$

A positively charged particle will be accelerated in the same linear orientation as the **E** field, but will curve perpendicularly to both the instantaneous velocity vector **v** and the **B** field according to the right-hand rule (in detail, if the fingers of the right hand are extended to point in the direction of **v** and are then curled to point in the direction of **B**, then the extended thumb will point in the direction of **F**).

The term q**E** is called the **electric force**, while the term q (**v** × **B**) is called the **magnetic force**. According to some definitions, the term "Lorentz force" refers specifically to the formula for the magnetic force, with the total electromagnetic force (including the electric force) given some other (nonstandard) name. This article

will not follow this nomenclature: In what follows, the term "Lorentz force" will refer only to the expression for the total force.

The magnetic force component of the Lorentz force manifests itself as the force that acts on a current-carrying wire in a magnetic field. In that context, it is also called the **Laplace force**.
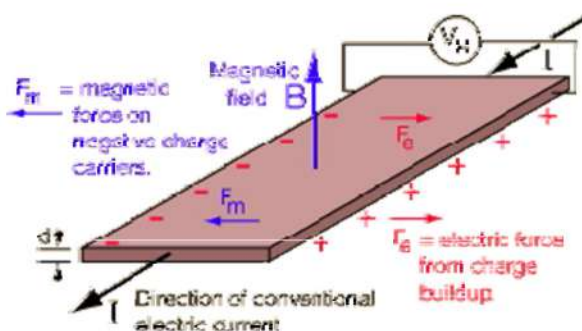
1.2.2 Hall Effect:

The **Hall effect** is the production of a voltage difference (the **Hall voltage**) across an electrical conductor, transverse to an electric current in the conductor and to an applied magnetic field perpendicular to the current. It was discovered by Edwin Hall in 1879.

The Hall coefficient is defined as the ratio of the induced electric field to the product of the current density and the applied magnetic field. It is a characteristic of the material from which the conductor is made, since its value depends on the type, number, and properties of the charge carriers that constitute the current.

If an electric current flows through a conductor in a magnetic field, the magnetic field exerts a transverse force on the moving charge carriers which tends to push them to one side of the conductor. This is most evident in a thin flat conductor as illustrated. A build up of charge at the sides of the conductors will balance this magnetic influence, producing a measurable voltage between the two sides of the conductor. The presence of this measurable transverse voltage is called the Hall effect.

Note that the direction of the current I in the diagram is that of conventional current, so that the motion of electrons is in the opposite direction. That further confuses all the "right-hand rule" manipulations you have to go through to get the direction of the forces.

The Hall voltage is given by

$$V_H = \frac{IB}{ned}$$

n = density of mobile charges
e = electron charge

The Hall effect can be used to measure magnetic fields with a Hall probe.

Hall Voltage for Positive Charge Carriers

The transverse voltage (Hall effect) measured in a Hall probe has its origin in the magnetic force on a moving charge carrier.

The magnetic force is $F_m = BeV_d$, where V_d is the drift velocity of the charge.

The current expressed in terms of the drift velocity is

$$I = n \, B \, eV_d$$

where n is the density of charge carriers. Then

$$F_m = \frac{eIB}{neA}$$

At equilibrium $F_e = F_m = \frac{e\,V_H}{W}$

And substituting gives $\qquad V_H = \dfrac{I\,B}{n\,e\,d}$

Hall Probe

The measurement of large magnetic fields on the order of a Tesla is often done by making use of the Hall effect. A thin film Hall probe is placed in the magnetic field and the transverse voltage (on the order of microvolts) is measured. Sometimes a thin copper film of thickness **d** on the order of 100 micrometers is used for a Hall probe.

1.2.3 Force on a small current element placed in a magnetic field

A conductor has free electrons which can move in the presence of a field. Since a magnetic field exerts a force $q\,(\vec{v} \times \vec{B})$ on a charge moving with a velocity $\vec{v}$, it also exerts a force on a conductor carrying a current. Consider a conducting wire carrying a current I. The current density at any point in the wire is given by

$$\vec{J} = \mathbf{n\,e\,\vec{v}}$$

where

n is the number density of electrons having a charge each and $\vec{v}$ is the average drift velocity at thatpoint. Consider a section of length dl of the wire. If A is the cross sectional area A of the section orientedperpendicular to the direction of $\vec{J}$, the force on the electrons in this section is
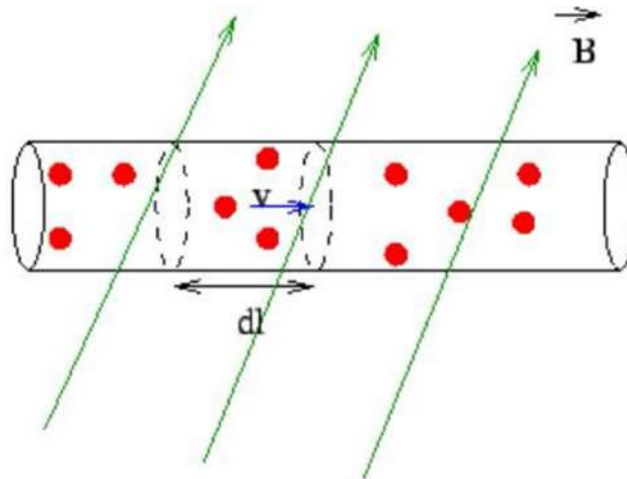
$$\mathbf{d\vec{F} = dq\,(\vec{v} \times \vec{B})}$$

where dq is the amount of charge in the section

Thus the force on the conductor in this section is

$$dq = n \, e \, A \, dl$$

Thus the force on the conductor in this section is

$$\vec{dF} = n\,e\,A\,\mathbf{dl}\,\vec{v}\,x\,\vec{B}$$

If $\vec{dl}$ represents a vector whose magnitude is the length of the segment and whose direction is along the direction of $\vec{v}$, we may rewrite the above as

$$
\begin{aligned}
dF &= neAv\vec{dl} \times \vec{B} \\
&= JA\vec{dl} \times \vec{B} \\
&= I\vec{dl} \times \vec{B}
\end{aligned}
$$

The net force on the conductor is given by summing over all the length elements. If $\hat{u}_l$ denotes a unit vect in the direction of the current, then $\vec{F} = I \int \hat{u}_l \times \vec{B} dl$

1.2.4 Biot Savart Law:

- The magnitude of the magnetic field **dB** at a distance **r** from a current element **dl** carrying current I is found to be proportional to I ,to the length dl and inversely proportional to the square of the distance |**r**|
- The direction of the magnetic Field is perpendicular to the line element **dl** as well as radius **r**
- Mathematically, Field **dB** is written as

$$dB = \left(\frac{\mu_0}{4\pi}\right)I\frac{dl \times r}{r^2}$$
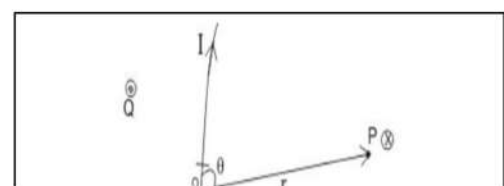
Here ($\mu_0/4\pi$) is the proportionality constant such that $\mu_0/4\pi = 10^{-7}$ Tesla Meter/Ampere(Tm/A).

So, the total magnetic flux is

$$\mathbf{B(r)} = \frac{\mu_0}{4\pi} \int_C \frac{Id\mathbf{l} \times \mathbf{r'}}{|\mathbf{r'}|^3}$$

Otherwise,

$$\mathbf{B(r)} = \frac{\mu_0}{4\pi} \int_C \frac{Id\mathbf{l} \times \hat{\mathbf{r}}'}{|\mathbf{r'}|^2}$$

Gauss's law for magnetism:

In physics, Gauss's law for magnetism is one of the four Maxwell's equations that underlie classical electrodynamics. It states that the magnetic fieldB has divergence equal to zero, or in other words, that it is a solenoidal vector field. **It is equivalent to the statement that magnetic monopoles do not exist.**

Gauss's law for magnetism can be written in two forms, a differential form and an integral form.

The differential form for Gauss's law for magnetism is:

$$\nabla \cdot \mathbf{B} = 0$$

where $\nabla \cdot$ denotes divergence, and **B** is the magnetic field.

The integral form of Gauss's law for magnetism states:

$$\oiint_S \mathbf{B} \cdot d\mathbf{A} = 0$$

where S is any closed surface (see image right), and $d\mathbf{A}$ is a vector, whose magnitude is the area of an infinitesimal piece of the surface S, and whose direction is the outward-pointing surface normal (see surface integral for more details).

The left-hand side of this equation is called the net flux of the magnetic field out of the surface, and Gauss's law for magnetism states that it is always zero.

The integral and differential forms of Gauss's law for magnetism are mathematically equivalent, due to the divergence theorem. That said, one or the other might be more convenient to use in a particular computation.

The law in this form states that for each volume element in space, there is exactly the same number of "magnetic field lines" entering and exiting the volume. No total "magnetic charge" can build up in any point in space. For example, the south pole of the magnet is exactly as strong as the north pole, and free-floating south poles without accompanying north poles (magnetic monopoles) are not allowed. In contrast, this is not true for other fields such as electric fields or gravitational fields, where total electric charge or mass can build up in a volume of space.

Non-existence of magnetic monopole:

Since $\oiint_S \mathbf{B} \cdot d\mathbf{A} = 0$, i.e., the lines of force are closed loops which leads to the fact that magnetic monopole does not exist. Magnetic lines of induction are continuous and join back on themselves, we can consider magnetic lines of induction to form a closed surface A in a magnetic field entering into the surface is equal to the number of lines of induction leaving the surface. This means **$\nabla \cdot \mathbf{B} = 0$ which indicates that a free isolated magnetic pole does not exist. So, magnetic poles always exist in pair.**

Ampere's Circuital Law:

The line integral of the magnetic field around some closed loop is equal to the μ_0 times the algebraic sum of

the currents which pass through the loop. $\oint \vec{B} \cdot d\vec{r} = \mu_0 I$

Ampère's circuital law is to magnetostatics (the study of the magnetic fields generated by steady currents) what Gauss' law is to electrostatics (the study of the electric fields generated by stationary charges). Like Gauss' law, Ampère's circuital law is particularly useful in situations which possess a high degree of symmetry.

The **differential form** of Ampere's circuital law: $\vec{\nabla} \times \vec{B} = \mu_0 \vec{J}$

Magnetic Vector Potential:

We have define a vector quantity $\vec{A}$ whose curl is equal to the magnetic field $\vec{B}$ i.e., :

$\vec{B} = \vec{\nabla} \times \vec{A}$, $\vec{A}$ is **Magnetic Vector Potential**

Also we know, $\qquad\qquad\qquad\qquad \vec{\nabla} \times \vec{B} = \mu_0 \vec{J}$

Or, $\qquad\qquad\qquad\qquad\qquad \vec{\nabla} \times \vec{\nabla} \times \vec{A} = \mu_0 \vec{J}$

Or, $\qquad\qquad\qquad\qquad\qquad \Box^2 \vec{A} = \Box_0 \vec{J} \rightarrow\rightarrow$ Poission's Equation in Vector Potential

In current free region $\vec{J} = 0 \Box^2 \vec{A} = \mathbf{0} \rightarrow\rightarrow$ Laplace's Equation in Vector Potential

Magnetic Scalar Potential:

In region of space in absence of currents, the current density $\vec{J} = 0$

$\vec{\nabla} \times \vec{B} = 0$

$\vec{B}$ is derivable from the gradient of a potential

$\vec{B} = -\Box\Box_m$

Φ_m is called **Magnetic Scalar Potential**

The presence of a magnetic moment m creates a magnetic field B which is the gradient of some scalar field.

We know $\vec{\nabla} \cdot \vec{B} = 0$

Or, by definition, The divergence of the gradient of the scalar field is also zero

i.e., $\qquad\qquad\qquad -\vec{\nabla} \cdot \nabla \Phi_m = 0$

or, $\qquad\qquad\qquad \Box^2 \Box_m = \mathbf{0} \rightarrow\rightarrow$ Laplace's Equation in Scalar Potential

Module 1.03: Electro-magnetism &Electromagnetic theory

1.3.1 Faraday's law

The induced electromotive force in any closed circuit is equal to the negative of the time rate of change of the magnetic flux enclosed by the circuit

Mathematically, $\varepsilon = -\dfrac{\partial \phi}{\partial t}$

Integral form of Faraday's law: $\oint \vec{E}.\vec{dl} = -\dfrac{d}{dt} \oiint \vec{B}.\vec{ds}$

Differential form of Faraday's law: $\vec{\nabla} x \vec{E} = -\dfrac{\partial \vec{B}}{\partial t}$

1.3.2 Concept of displacement current

Differential form of Ampere's circuital law: $\vec{\nabla} \mathbf{X} \ \vec{B} = \mu_0 \vec{J}$

Taking divergence on both sides, $\vec{\nabla} . \vec{J} = 0$

But Equation of continuity says $\vec{\nabla} . \vec{J} + \dfrac{\partial \rho}{\partial t} = 0$

Thus, $\vec{\nabla} . \vec{J} = 0$ is only true in a steady-state (*i.e.*, when $\dfrac{\partial}{\partial t} = 0$)

In the time-dependent situation $\left(\dfrac{\partial \rho}{\partial t} \text{ is not equal to zero} \right)$, a transient current flows in the wire as the capacitor charges up, or charges down, and so a transient magnetic field is generated. Thus, the line integral of the magnetic field around C is (transiently) non-zero.

So, let us consider a new quantity $\vec{J}_\mathbf{D}$ such that modified Ampere's circuital law can be written as

$$\vec{\nabla} \mathbf{X} \ \vec{B} = \mu_0 (\vec{J} + \vec{J}_\mathbf{D})$$

It can be proved that $\vec{J}_\mathbf{D} = \dfrac{\partial \vec{D}}{\partial t} = \varepsilon \dfrac{\partial \vec{E}}{\partial t}$

Modified Ampere's circuital law: $\vec{\nabla} \mathbf{X} \ \vec{B} = \mu_0 (\vec{J} + \vec{J}_\mathbf{D})$

Or, $\qquad \vec{\nabla} \mathbf{X} \ \vec{B} = \mu_0 \left(\vec{J} + \dfrac{\partial \vec{D}}{\partial t} \right)$

Or, $\qquad \vec{\nabla} \mathbf{X} \ \vec{B} = \mu_0 \left(\vec{J} + \varepsilon \dfrac{\partial \vec{E}}{\partial t} \right)$

1.3.3 Maxwell's field equations with physical significance

Maxwell's field equations

1. $\nabla \cdot \mathbf{E} = \square / \square_0 \square$ Gauss's law

2. $\nabla \cdot \mathbf{B} = \mathbf{0} \square$ Gauss's law in magnetostatics

3. $\nabla x E = - \dfrac{iJ\vec{B}}{iJt} \square$ Faraday's law

4. $\nabla \mathbf{x} B = \square_0 (J + \square_{iJt}) \rightarrow$ Modified Ampere's circuital law

Physical significance of Maxwell's 1st equation

According to this total electric flux through any closed surface is $1/\varepsilon_0$ times the total chargeenclosed by the closed surfaces, representing Gauss's law of electrostatics, As this does not depend on time, it is a steady state equation. Here for positive ρ, divergence of electric field ispositive and for negative ρdivergence is negative. It indicates that $\rho$is scalar quantity.

Physical significance of Maxwell's 2nd equation

It represents Gauss law of magnetostatic as $\nabla.\mathbf{B} = 0$ resulting that isolated magnetic poles or magnetic monopoles cannot exist as they appear only in pairs an d there is no source or sinkfor magnetic lines of forces. It is also independent of time i.e. steady state equation.

Physical significance of Maxwell's 3rd equation

It shows that with time varying magnetic flux, electric field is produced in accordance withFaraday is law of electromagnetic induction. This is a time dependent equation.

Physical significance of Maxwell's 4th equation

This is a time dependent equation which represents the modified differential form ofAmpere's circital law according to which magnetic field is produced due to combined effect ofconduction current density and displacement current density.

1.3.4 Wave equation in free space

Free space is defined as $\Box = \mathbf{0}$, $\Box = \mathbf{0}$, $\quad \vec{D} = \Box_0 \vec{E}, \quad \vec{B} = \Box_0 \vec{H}$

The wave equations are: $\quad \Box^2 \mathbf{E} = \Box_0 \Box_0 \ i\mathrm{J}^2 \mathbf{E}/i\mathrm{J}t^2 = 1/c^2 \ i\mathrm{J}^2 \mathbf{E}/i\mathrm{J}t^2$

And $\quad\quad\quad\quad\quad \Box^2 \mathbf{B} = \Box_0 \Box_0 \ i\mathrm{J}^2 \mathbf{B}/i\mathrm{J}t^2 = 1/c^2 \ i\mathrm{J}^2 \mathbf{B}/i\mathrm{J}t^2$

Solution $\quad\quad\quad\quad \vec{B} = \vec{B}_0 \, \mathbf{exp[i(} \vec{k}.\vec{r} - \Box \mathbf{t)}$

And $\quad\quad\quad\quad\quad \vec{E} = \vec{E}_0 \, \mathbf{exp[i(} \vec{k}.\vec{r} - \Box \mathbf{t)}$

1.3.5 Transverse nature of electromagnetic wave
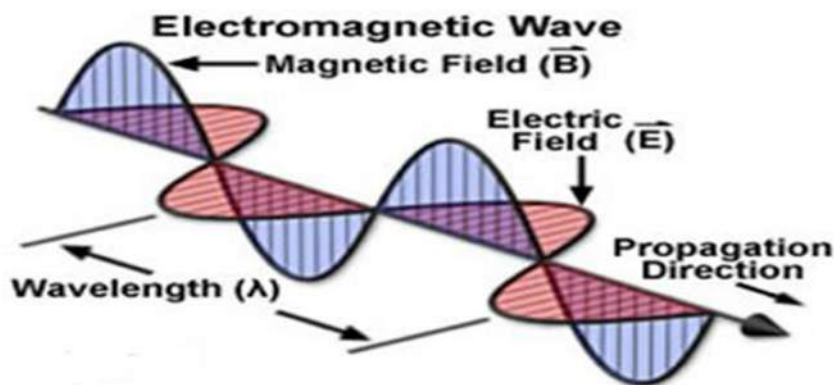
It can be proved that Magnetic field ($\vec{B}$), Electric field ($\vec{E}$) and propagation vector ($\vec{k}$) are mutually perpendicular.

Reference:
1. Electricity Magnetism-Basudev Ghosh (Books and Allied Pub)

1. Electricity Magnetism-Fewkes and Yardwood (Oxford University Press)

Potential Text Book:

1. Principles of Engineering Physics Vol 1 and Vol 2

Md. N. Khan and S. Panigrahi (Cambridge University Press)

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Physics-II (Gr-B)
Code: PH 301 [For CSE and IT]

Module 2: Quantum Mechanics-II, Quantum Computation and Communication (12L)

2.01: Quantum Mechanics-II
Formulation of quantum mechanics and Basic postulates- superposition principle, orthogonality of wave function, expectation value; operator correspondence, Commutator. Measurements in Quantum Mechanics-Eigen value, Eigen function, Schrödinger's equation as energy eigen value equation.   4L

Application of Schrödinger equation – Particle in an infinite square well potential (1-D and 3-D box); Discussion on degenerate levels), 1D finite barrier problem and concept of quantum tunnelling (solve only $E<V_0$).   3L

2.02: Quantum Computation and Communication
The idea of n- dimensional vector space, use of 'bra-ket' notation, matrix representation of bra & kets; basis, Hilbert space; Pauli matrices.   2L

Idea of qubit and examples of single qubit logic gates- Classical bits, qubit as a two level system; Bloch vector, Pauli gate, Hadamard gate, Phase shift gate, Quantum circuits related to Quantum gates.   3L

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Lecture Plan: Quantum Mechanics-II, Quantum Computation and Communication

Module No	Lecture No	Topic	Application	Reference Book
2	1	Introductory Lecture, Short recap of the topics of Quantum physics studied in 1st year and their connection to the 2nd year Quantum Mechanics part.	Recap	1. Introduction to Quantum Mechanics-S. N. Ghoshal (Calcutta Book House) 2. Quantum Mechanics-Bagde Singh (S. Chand Publishers)
2	2	Re-discussion on the basic parameter of Quantum Mechanics. Wave function, Concept of probability amplitude & probability density. Normalization condition & Probability interpretation.	Mathematical formulation of Q. Mech.	
2	3	Operators in Quantum Mechanics, need of introducing concepts of operators. Operator algebra, Commutator bracket, Commutation relation.	Measurement of physical parameters in Q. Mech	
2	4	Physical significance of various commutation relations, examples of commutation relations of few known operators.	Heisenberg's uncertainty relations and its applications	
2	5	Operator correspondence, Eigen value of any operator, Expectation value of any operator.	Extracting information from wave function Measurement of	
2	6	Formulation and basic postulates of Qunatum Mechanics. Time dependent Schrödinger equation. Time independent Schrödinger equation from the time dependent version.	Axioms of Q.Mech	
2	7	Time independent Schrödinger equation as the energy eigen value equation.	Avenue of getting wave function (state of a system)	
2	8	Applications of Schrödinger equation, particle in 1D potential well.	Somefeld's free electron theory	
2	9	Particle in 3D box. Degeneracy and degenerate states.	Applications to formation of energy bands	
2	10	Finite barrier problem-example of junction diode	Connecting the problem with electron crossing voltage barrier	
2	11	Solving the problem for E<V0, quantum tunneling and applictions	Tunnel diode	
2	12	Vector space. Properties of vector space. Inner product, outer product	Foundation of Q. Computations	1. Advanced Quantum Mechanics-J. J. Sakurai (TMH) 2. Quantum Computation and Quantum Information(10th Anniversary Edition)-Nielsen & Chuang (Cambridge University Press)
2	13	Basis vector and Hilbert space	Foundation of Q. Computations	
2	14	Qubit, realization of Qubit. Concept of electron spin. Pauli spin matrices	Pauli Gates	
2	15	Quantum logic gates and logic operation	Quantum gates	
2	16	Quantum gates and circuits. Difference between classical and quantum gates	Logic design of Quantum computers.	

Text Book: Principles of Engineering Physics Vol 1 and Vol 2; by Md. N. Khan and S. Panigrahi, Pub: Cambridge Univ. press

2.1 1: Quantum Mechanics-II

'Truth is stranger than fiction, but it is because fiction is obliged to stick to possibilities; truth isn't.' - Mark Twain

2.1.1   Formulation of Quantum Mechanics and Basic postulates:

Every physical theory is formulated in terms of mathematical objects. It is thus necessary to establish a set of rules to map physical concepts and objects into mathematical objects that we use to represent them. Sometimes this mapping is evident, as in classical mechanics, while for other theories, such as quantum mechanics, the mathematical objects are not intuitive. In the same way as classical mechanics is founded on Newton's laws or electrodynamics on the Maxwell-Boltzmann equations, quantum mechanics is also based on some fundamental laws, which are called the postulates or axioms of quantum mechanics.

We want in particular to develop a mathematical model for the dynamics of closed quantum systems (a closed system any system that is isolated, thus not exchanging any input or output and not interacting with any other system. An open system instead interacts e.g., with an external environment): therefore we are interested in defining

states – observables – measurements – evolution.

Some subtleties will arise since we are trying to define measurement in a closed system, when the measuring person is instead outside the system itself. A more complete picture, that can explain some of the confusion arising from the measurement process, is possible, but we will not study it in this course. We are interested in giving a description of physical phenomena and in particular in how they emerge during an experiment.

Experiments – A physical experiment can be divided into two steps: preparation and measurement.

In classical mechanics (CM): - the first step determines the possible outcomes of the experiment, - while the measurement retrieves the value of the outcome.

In quantum mechanics (QM) the situation is slightly different:

- the first step (preparation) determines the probabilities of the various possible outcomes,

- the second step (measurement) retrieve the value of a particular outcome, in a statistic manner.

This separation of the experiment in two steps is reflected into the two types of operators that we find in QM.

- The first step corresponds to the concept of a state of the system,

- while the second step corresponds to observables.

In CM the state of a system is described by a set of properties. For example, if we consider a ball, we can define its state by giving its position, momentum, energy, angular momentum (if for example the ball is spinning), its temperature etc. We can then perform a measurement on this ball, for example measuring its position. This will give us one value for one possible observable (the position). We can express this process in mathematical terms. The state of the system is defined by a set of values: {rr, r L, T, . . . p, E, }. r All of these values (and there might be of course more that I haven't written down) are needed to fully describe the state of the ball. Performing a measurement of the position, will retrieve the values $\{r_x, r_y, r_z\} = r$ (the same values that describe the state).

If we now consider a nucleus, we can as well give a description of its state. In quantum mechanics, a complete description of the state of a quantum object (or system) is given mathematically by the state vector $|\psi)$ (or wavefunction $\psi(r)$). The situation is however different than in classical mechanics.

The state vector is no longer a collection of values for different properties of the system. The state gives instead a complete description of the set of probabilities for all the physical properties (or observables). All the information is contained in the state, irrespectively on how I got the state, of its previous history

Quantum physicists are interested in all kinds of physical systems (photons, conduction electrons in metals and semiconductors, atoms, etc.). State of these rather diverse systems are represented by the same type of functions ➔ STATE FUNCTIONS.

All of these considerations are made more formal in the axioms of quantum mechanics that also indicate the mathematical formalism to be used.

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i) The properties of a quantum system are completely defined by specification of its state vector |ψ) (or wavefunction ψ(r)). The state vector is an element of a complex Hilbert space H called the space of states.

ii) If |ψ) [or wavefunction ψ(r))] is the vector representing the state of a system and if |φ) [or wavefunction φ(r))] represents another physical state, there exists a probability p(|ψ), |φ)) of finding |ψ) in state |φ), which is given by the squared modulus of the inner product on H: p(|ψ), |φ)) = |(ψ|φ)|2 (Born Rule).

iii) With every physical property A (energy, position, momentum, angular momentum, ...) there exists an associated linear, Hermitian operator A (usually called observable), which acts in the space of states H. The eigenvalues of the operator are the possible values of the physical properties.[^. i.e. for an eigenfunction of A, ψ, A ψ = a ψ.]. Where 'a' is the eigen value of the operator A.

iv) If A is an observable with eigenvalues an and eigenvectors |n) [such that the eigenvalue equation is A |n) = a_n |n)], given a system in the state |ψ), the probability of obtaining an as the outcome of the measurement of A is p(an) = |(n|ψ)|2. After the measurement the system is left in the state projected on the subspace of the eigenvalue an (Wave function collapse).

(v) For a system in a state described by a normalized wave function, the average or expectation value of the observable corresponding to A is given by:

$$\langle A \rangle = \int \Psi^* \hat{A} \Psi \, d\tau$$

Expectation value in general:
Expectation value in general:

$$\langle a \rangle = \frac{\displaystyle\int_{-\infty}^{\infty} \Psi^*(x)\hat{A}\Psi(x)\,dx}{\displaystyle\int_{-\infty}^{\infty} \Psi^*(x)\Psi(x)\,dx}$$

$$= \int_{-\infty}^{\infty} \Psi^*(x)\hat{A}\Psi(x)\,dx \quad (\text{if normalized})$$

The fourth postulates states what will be measured when large number of identical systems are interrogated one time. Only after large number of measurements will it converge to <a>.

In QM, the act of the measurement causes the system to "collapse" into a single eigenstate and in the absence of an external perturbation it will remain in that eigenstate.

vi) The evolution of a closed system is unitary (reversible). The evolution is given by the time-dependent Schrödinger equation,

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

2.1.2 : Illustrations of postulate 1:

❖ Every physically-realizable state of the system is described in quantum mechanics by a state function ψ that contains all accessible physical information about the system in that state.

– **Physically realizable states** ➜ states that can be studied in laboratory
– **Accesible information** ➜ the information we can extract from the wavefunction
– **State function** ➜ function of position, momentum, energy that is spatially localized.

❖ If ψ_1 and ψ_2 represent two physically-realizable states of the system, then the linear

combination $\quad \psi = c_1\psi_1 + c_2\psi_2$

where c_1 and c_2 are arbitrary complex constants, represents a third physically realizable state of the system. Above relation is known as superposition principle and is applied in the study of quantum computation.

2.1.3   : Illustrations of postulate 2:

According to the second postulate of quantum mechanics, the integrated probability density can be interpreted as a probability that in a position measurement at time t, we will find the particle anywhere in space.

Therefore, the normalization condition for the wavefunction is:

$$\int P dV = \int |\psi(x, y, z)|^2 dV = \int \psi^*(x, y, z)\psi(x, y, z)dV = 1$$

Limitations on the wavefunction:

 – Only normalizable functions can represent a quantum state and these are called physically admissible functions.
 – State function must be continuous and single valued function.
 – State function must be a smoothly-varying function (continuous derivative). All first-order derivatives of the wave function must be continuous. Following the same reasoning as in condition 3, a discontinuous first derivative would imply an infinite second derivative, and since the energy of the system is found using the second derivative, a discontinuous first derivative would imply an infinite energy, which again is not physically realistic.
 – The wave function must be square-integrable. In other words, the integral of $|\Psi|^2$ over all space must be finite.

 Acceptable or Not ?? (little task to do)
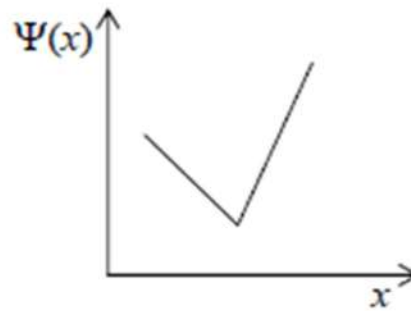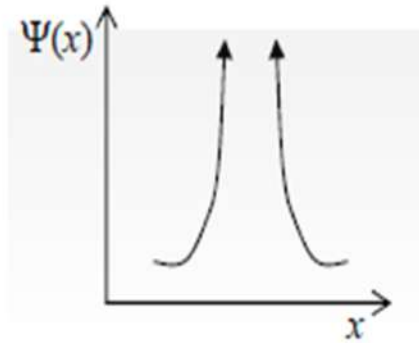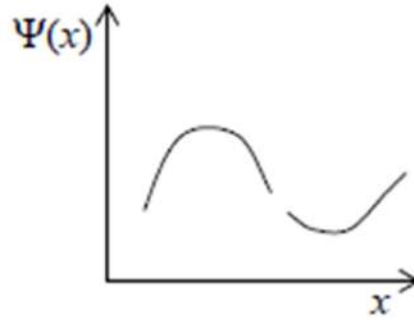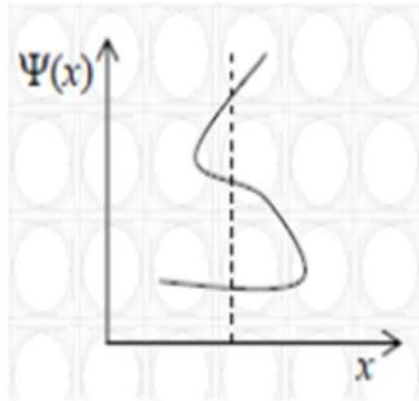
Acceptable or Not ?? (little task to do)

(i) $e^{-x} (0, \infty)$

(ii) $e^{-x} (-\infty, \infty)$

(iii) $\dfrac{\sin x}{x}$

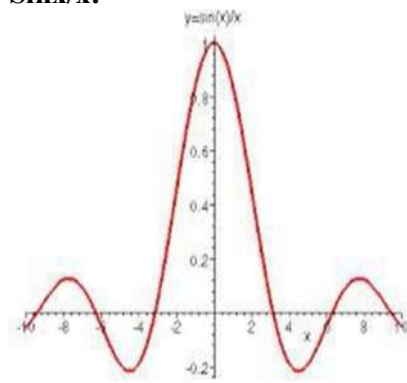(iv) $\sin^{-1} x$

Acceptable or not acceptable (few more examples) ??

Exp(x):

$y = e^{-x}$ $y = e^{x}$

Sinx/x:

y=sin(x)/x

Sin⁻¹x

y = arcsin(x)
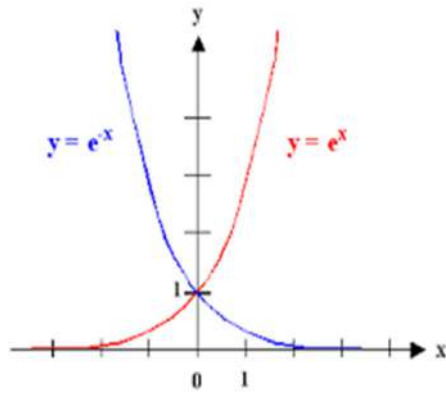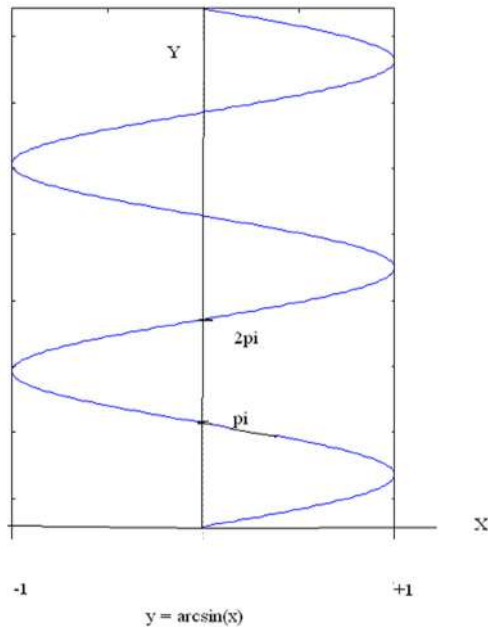
2.1.4   Illustrations of postulate 3:

To every physical property, observable in classical mechanics, there corresponds a <u>linear, Hermitian operator</u> in quantum mechanics.

Operator: A rule that transforms a given function into another function

A little task to do:

Example. Apply the following operators on the given functions:

- **(a) Operator d/dx and function x^2.**
- **(b) Operator d^2/dx^2 and function $4x^2$.**
- **(c) Operator $(\partial/\partial y)x$ and function xy^2.**
- **(d) Operator $-i\hbar d/dx$ and function $\exp(-ikx)$.**
- **(e) Operator $-\hbar^2 d^2/dx^2$ and function $\exp(-ikx)$.**

Hermitian Operator: Hermitian operators have two properties that forms the basis of quantum mechanics

  (i)   **Eigen value of a Hermitian operator are real.**

 (ii)   **Eigenfunctions of Hermitian operators are orthogonal to each other or can be made orthogonal by taking linear combinations of them.**

A Hermitian operator Â satisfies :

$$\int f^* \hat{A} g \, dx = \int g (\hat{A} f)^* \, dx \; ; \text{if } f \text{ and } g \text{ are well behaved}$$

A little task to do:

Check following are Hermitian operator or not ??

$$(i) \frac{\partial}{\partial x} \quad (ii) -i\hbar \frac{\partial}{\partial x} \quad (iii) \frac{\partial^2}{\partial x^2} \quad (iv) \, x$$

Linear Operator:

   • **A linear operator has the following properties**

$$\hat{A}(f_1 + f_2) = \hat{A} f_1 + \hat{A} f_2$$

$$\hat{A}(cf) = c \hat{A} f$$

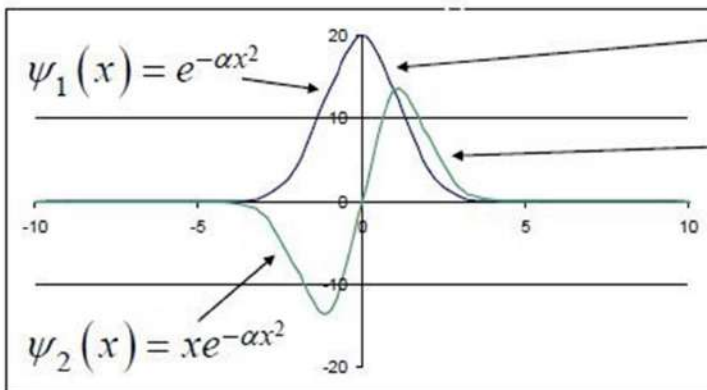**Examples of linear operators:**

Derivative

integrals

log

square root

Normalized wave function: $N^2 \int \square^* \square \, dx = 1$

Orthogonal wave functions:

$$\int \psi_m^* \, \psi_n \, d\tau = 0$$

$\psi_1(x) = e^{-\alpha x^2}$

$\psi_2(x) = xe^{-\alpha x^2}$

Even function: $f(x) = f(-x)$

Odd function: $f(x) = -f(-x)$

Integral of the product of an even and odd function over all space = 0!

Orthonormal set wave functions:

$$\int_{-\infty}^{\infty} \square_m^* \square_n \, dx = \square_{mn} = 1, \quad \text{if } m = n$$

$$= 0, \quad \text{if } m \neq n$$

Correspondence principle 1913 (Niels Henrik David Bohr Danish):

For every physical quantity one can define an operator. The definition uses formulae from classical physics replacing quantities involved by the corresponding operators

Quantum Mechanical Position and Momentum Operators

   1. Operator for position in the x-direction is just multiplication by x: $\hat{x}\psi = x\psi$

2. Operator for linear momentum in the x-direction: $\hat{\mathbf{p}}_{\mathbf{X}} = \left(\dfrac{\hbar}{i}\right)\dfrac{d}{dx}$

$$\square \ \hat{\mathbf{p}}_{\mathbf{X}}\psi = p_X\psi$$

$$\frac{\hbar}{i}\cdot\frac{d\psi}{dx} = p_X\psi$$

(solve first order differential equation $\square\square$, p_x).

3. Constructing Kinetic and Potential Energy QM Operators

      1. Write down classical expression in terms of position and momentum.

      2. Introduce QM operators for position and momentum.

Examples

1.   **Kinetic Energy Operator in 1-D:** $\hat{\mathbf{T}}_{\mathbf{X}}$

$$\hat{\mathbf{T}}_{\mathbf{X}} = \frac{\hat{\mathbf{p}}_X{}^2}{2m} = -\frac{\hbar^2}{2m}\left(\frac{d^2}{dx^2}\right)$$

2. KE Operator in 3-D: $\hat{\mathbf{T}}$

$$\hat{\mathbf{T}} = \frac{\hat{\mathbf{p}}^2}{2m} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) = -\frac{\hbar^2}{2m}\nabla^2$$

3. Potential Energy Operator $\hat{\mathbf{V}}$ (a function of position)

$\therefore$ PE operator corresponds to multiplication by V(x), V(x,y,z) etc.

Overall list of Quantum Mechanical Operators:

Observable	Classical Symbol	Quantum Operator	Operation
position	$\mathbf{r}$	$\hat{r}$	multiply by $\mathbf{r}$
momentum	$\mathbf{p}$	$\hat{p}$	$-ih(\hat{i}\frac{\partial}{\partial x} + \hat{j}\frac{\partial}{\partial y} + \hat{k}\frac{\partial}{\partial z})$
kinetic energy	T	$\hat{T}$	$\frac{-\hbar^2}{2m}(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2})$
potential energy	$V(\mathbf{r})$	$\hat{V}(\mathbf{r})$	multiply by $V(\mathbf{r})$
total energy	E	$\mathcal{H}$	$\frac{-\hbar^2}{2m}(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}) + V(\mathbf{r})$
angular momentum	l_x	$\hat{l}_x$	$-ih(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y})$
	l_y	$\hat{l}_y$	$-ih(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z})$
	l_z	$\hat{l}_z$	$-ih(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x})$

2.1.5 : Concept of Measurement

❖ **In any measurement of the observable associated with the operator , the only values that will ever be observed are the eigenvalues 'a' which satisfy the eigenvalue equation:**

For, An operator O is "the recipe to transform Y into Y' "

We write: O Y = Y'

If O Y = nY (n is a number, meaning that O does not modify Y, just a scaling factor), we say that Y is an eigenfunction of O and n is the eigenvalue.

❖ **This is the postulate that the values of dynamical variables are quantized in quantum mechanics.**

Eigen Function and Eigen value:

$\hat{A} f(x) = k f(x); \text{f(x) is eigenfunction of } \hat{A} \text{ with eigen value k}$

Idea of Eigenvalue equation

(Operator)(function) = (constant factor)*(same function)

Example: e^{ikx} is an eigenfunction of a operator $\hat{P}_x = -ih\dfrac{\partial}{\partial x}$

f(x) = e^{ikx}

$$-i\hbar\,\frac{\partial}{\partial x}\exp(ikx) = (i\hbar)(ik)\exp(ikx)$$

$$pf(x) = \hbar k f(x)$$

Thus e^{ikx} is an eigenfunction of momentum operator.

Commutation relation and its Significance:

Consider any two operators, the eigenvalues of two commuting operators can be computed by using the common set of eigenfunctions.

$$[A,B] = AB - BA; if$$
$$= 0, \text{A \& B commute with each other}$$
$$and\,if$$
$$\neq 0, \text{A \& B do not commute with each other}$$

Physical significance:

If the two operators commute, then it is possible to measure the simultaneously the precise value of both the physical quantities for which the operators stand for.

Small task to do: Find commutator of the operators x and p_x. Is it expected to be a non-zero or zero quantity?

Hint: Heisenberg Uncertainty Principle

2.1.6   : Illustrations of postulate 5:

Expectation value in general:

$$\langle a \rangle = \frac{\int\limits_{-\infty}^{\infty} \Psi^*(x)\,\hat{A}\Psi(x)\,dx}{\int\limits_{-\infty}^{\infty} \Psi^*(x)\,\Psi(x)\,dx}$$

$$= \int\limits_{-\infty}^{\infty} \Psi^*(x)\,\hat{A}\Psi(x)\,dx \quad \text{(if normalized)}$$

The fourth postulates states what will be measured when large number of identical systems are interrogated one time. Only after large number of measurements will it converge to <a>.

In QM, the act of the measurement causes the system to "collapse" into a single eigenstate and in the absence of an external perturbation it will remain in that eigenstate.

2.1.7 : Illustrations of postulate 6:

Schrödinger Representation – Schrödinger Equation

- The central equation in Quantum Mechanics.
- Observable = total energy of system.
-

Schrödinger Equation:

$\hat{H}\psi = E\psi$ $\qquad\qquad$ $\hat{H}$ *is* Hamiltonian Operator

where E $\qquad$ Total Energy; and $E = T + V$.

- **Schrödinger Equation** can be set up for any physical system.
- The form of $\hat{H}$ depends on the system.
- Solve **Schrödinger Equation** $\Rightarrow \psi$ and corresponding E.

2.1.8 : Getting the Time Independent Schrödinger Equation

$\Psi(x, y, z, t)$ **wavefunction**

$$i\hbar \frac{\partial}{\partial t} \Psi(x, y, z, t) = \underline{H}(x, y, z, t) \Psi(x, y, z, t)$$

If the energy is independent of time

Try solution

$$\Psi(x, y, z, t) = \psi(x, y, z) F(t) ;$$

product of spatial function and time function

Then

$$i\hbar \frac{\partial}{\partial t} \psi(x, y, z) F(t) = \underline{H}(x, y, z) \psi(x, y, z) F(t)$$

$$i\hbar \psi(x, y, z) \frac{\partial}{\partial t} F(t) = F(t) \underline{H}(x, y, z) \psi(x, y, z)$$

divide through by

$$\psi \cdot F$$

$$\frac{i\hbar \dfrac{dF(t)}{dt}}{F(t)} = \frac{H(x, y, z) \psi(x, y, z)}{\psi(x, y, z)}$$

depends only on t   **depends only on x, y, z**

Can only be true for any x, y, z, t if both sides equal a constant. Changing t on the left doesn't change the value on the right. Changing x, y, z on right doesn't change value on left

$$i\hbar \frac{\frac{dF}{dt}}{F} \square E \square \frac{H\square}{\square}$$

Both sides equal a constant, *E*.

$$\underline{H}(x,y,z)\square(x,y,z) \square \quad E \square(x,y,z)$$

2.1.9 Application of Schrödinger equation –

1. Particle Moving in 1-D Infinite Potential Well

$$\hat{\mathbf{H}}\psi = \hat{\mathbf{T}}\psi + \hat{\mathbf{V}}\psi = E\psi$$

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi}{\partial x^2}\right) + V(x)\psi = E\psi$$

- The form of V(x) depends on the physical situation:
  - Free particle   V(x) = 0 for all x.
  - Harmonic oscillator   V(x) = ½*k*x^2

2.1.10 : . Particle in a 1-D infinite potential well:

System
- – Particle of mass m in 1-D box of length L.
- – Position x = 0→L.
- – Particle cannot escape from box as PE V(x)= ∞ for x = 0, L (walls).
- – PE inside box: V(x)= 0 for 0< x < L.
- – V = 0 inside box).
- –
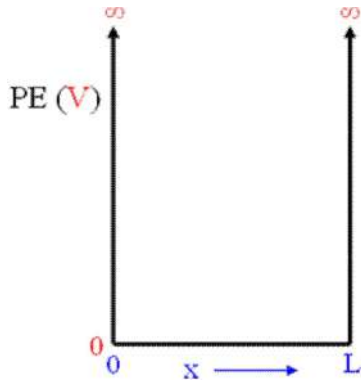
1-D Schrödinger Eqn. as V = 0 inside box).

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi}{\partial x^2}\right) = E\psi$$

- This is a second order differential equation – with general solutions of the form:
- $\psi = A \sin kx + B \cos kx$
- Where $k^2 = \frac{2mE}{\hbar^2}$

i.e

$$\frac{\hbar^2 k_n^2}{2m} = E_n$$

Between the kinetic energy Eigen value En and the wave number k_n (and the momentum p_n = ik_n).
For a free particle there is no restriction on the possible energies,
En can be any positive number.

The solution to the eigenvalue problem is then the eigenfunction
- □ = **A sin knx + B cos knx**

We see that there are two independent functions for each eigen value E_n. Also there are two distinct momentum Eigen values $\pm k_n$ for each energy Eigen value, which correspond to two different directions of propagation of the wave

$$\phi \equiv \psi \quad \left[\text{phi is equivalent to si}\right]$$

Check the boundary conditions

$$\phi(0) = 0 = B$$
$$\phi(a) = 0 = A\sin(ka)$$

Hence we have the trivial solution (no particle) unless

$$ka = n\pi \qquad (\text{n is an integer})$$
$$\sqrt{\frac{2mE}{\hbar^2}} a = n\pi$$
$$\Rightarrow E_n = \left(\frac{n\pi}{a}\right)^2 \frac{\hbar^2}{2m}$$

Hence E developed an index and energy quantization came out. Note that k also has an index:

$$k_n = \frac{n\pi}{a} \qquad \text{The wave-number is also quantized}$$

$$\phi_n(x) = A\sin\left(\frac{n\pi x}{a}\right)$$

Note the energy levels rise rapidly they go as n^2. Note we were dealing with a homogeneous differ hence isn't fixed yet. This can be done using the normalization condition:

$$\int_{-\infty}^{\infty} |\phi_n|^2 dx = \int_0^a A^2 \sin^2\left(\frac{n\pi x}{a}\right) dx$$
$$A^2 \frac{a}{2} = 1$$

Hence

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

Notice that the normalization constant is independent of the particular quantum number n. Therefore

$$\phi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right), \qquad E_n = \frac{n^2\hbar^2\pi^2}{2ma^2}$$
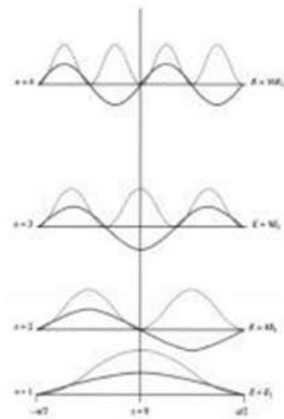
Since the energy increases with decreasing **a** it means that quantum mechanics opposes this motion.
This can be thought of as a quantum mechanical pressure on the outside of the box.

Note that **n** can equal any integer **n = 1, 2, ...** (Infinity many bound states)

Note the dimensions of **φ are 1/ √L**

And the dimensions of the **P (the probability density) is 1/L.** The energy levels

The Wavefunctions of the Square Well and Their Corresponding Probability Densities

as well as the corresponding wavefunctions are shown in figure 1.

Typically there are as many quantum numbers as dimensions of the problem.

In any problem as h → 0 we recover classical physics. E

quivalently we can recover classical physics as E → ∞.

In our problem as E becomes large we should recover the classical distribution. The classical distribution is given by

$$P(x) = \begin{cases} 1/a & 0 < x < a \\ 0 & x \le 0, x \ge a \end{cases}$$

In the limit of large E, we have a highly oscillating function from 0 to 2/a. For any experiment that tries to measure how likely it is we will get to any finite region it will be 1/a.

2.1.11 :. Particle in a 3-D box

We consider a particle in a box with lengths a, b, and c which is centered with one corner at the origin. The potential is then given by

$$V(x, y, z) = \begin{cases} & 0 < x < a \\ & 0 < y < b \\ & 0 < z < c \\ \infty & \text{elsewhere} \end{cases}$$

We know that the particle outside the box must be zero. Within the box the potential is zero and the Schrödinger equation is given as

$$-\frac{\hbar^2}{2m}\nabla^2\psi(x, y, z) = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\frac{\partial^2}{\partial z^2}\right)\psi(x, y, z) = E\psi(x, y, z)$$

To solve this equation we assume that the wave function can be written as

Lets differentiate this function twice with respect to x, y, z

$$\frac{\partial^2\psi(x, y, z)}{\partial x^2} = f''(x)g(y)h(z)$$

$$\frac{\partial^2\psi(x, y, z)}{\partial y^2} = f(x)g''(y)h(z)$$

Substituting this back into the Schrödinger equation gives

$$-\frac{\hbar^2}{2m}f''(x)g(y)h(z) - \frac{\hbar^2}{2m}f(x)g''(y)h(z) - \frac{\hbar^2}{2m}f(x)g(y)h''(z) - Ef(x)g(y)h(z) = 0$$

Dividing by the wave function we get,

$$-\frac{\hbar^2 f''(x)}{2mf(x)} - \frac{\hbar^2 g''(y)}{2mg(y)} - \frac{\hbar^2 h''(z)}{2mh(z)} - E = 0$$

$$-\frac{\hbar^2 f''(x)}{2mf(x)} = E_x = \frac{\hbar^2 g''(y)}{2mg(y)} + \frac{\hbar^2 h''(z)}{2mh(z)} + E$$

Since the the two sides of the equations depend only different variables they can only be true if Ex is a constant. Thus, we get with a similar argument for y and z

$$E_x = -\frac{\hbar^2 f''(x)}{2mf(x)}$$

$$E_y = -\frac{\hbar^2 g''(y)}{2mg(y)}$$

$$E_z = -\frac{\hbar^2 h''(z)}{2mh(z)}$$

The total energy is then given by

$$E = E_x + E_y + E_z$$

We have managed to use separation of variable to transform the 3D partial differential equation into three 1D differential equations given by

$$\frac{d^2 f(x)}{dx^2} + \frac{2m}{\hbar^2} E_x f(x) = 0$$

$$\frac{d^2 g(y)}{dy^2} + \frac{2m}{\hbar^2} E_y g(y) = 0$$

$$\frac{d^2 h(z)}{dz^2} + \frac{2m}{\hbar^2} E_z h(z) = 0$$

We know the solution to these equations of the 1D box, and the wave function in the x direction is

$$f(x) = \left(\frac{2}{a}\right)^{1/2} \sin\left(\frac{n_x \pi x}{a}\right)$$

and the energy

$$E_x = \frac{n_x^2 h^2}{8ma^2}, \quad n_x = 1, 2, 3, \cdots$$

Similar the solutions in the y direction is,

$$g(y) = \left(\frac{2}{b}\right)^{1/2} \sin\left(\frac{n_y \pi y}{y}\right)$$

$$E_y = \frac{n_y^2 h^2}{8mb^2}, \quad n_y = 1, 2, 3, \cdots$$

and z direction

$$h(z) = \left(\frac{2}{c}\right)^{1/2} \sin\left(\frac{n_z \pi z}{c}\right)$$

$$E_z = \frac{n_z^2 h^2}{8mz^2}, \quad n_z = 1, 2, 3, \cdots$$

Thus the solution to the Schrodinger equation for the particle in a 3D box is by an energy

$$E = \frac{h^2}{8m}\left(\frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} \frac{n_z^2}{c^2}\right)$$

and a wave function

$$\psi(x, y, z) = \left(\frac{8}{abc}\right)^{1/2} \sin\left(\frac{n_x \pi x}{a}\right) \sin\left(\frac{n_y \pi y}{b}\right) \sin\left(\frac{n_z \pi z}{c}\right)$$

We also know that the wave function is normalized

$$\int_{-\infty}^{\infty} |\psi(x, y, z)|^2 d\tau = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} |\psi(x, y, z)|^2 dx\,dy\,dz$$

$$= \int_0^a |f(x)|^2 dx \int_0^b |g(y)|^2 dy \int_0^c |h(z)|^2 dz = 1$$

Now let's consider a cube, i.e. a = b = c. The energy of a particle in cubic box becomes

$$E = \frac{h^2}{8m}\left(\frac{n_x^2}{a^2} + \frac{n_y^2}{a^2} + \frac{n_z^2}{a^2}\right) = \frac{h^2}{8ma^2}(n_x^2 + n_y^2 + n_z^2)$$

Ask for a volunteer to calculate the energy of quantum state (211), (121), (112).
This shows that the energy is the same for these three states due to symmetry,
we call this that the energy is degenerate. The degree of degeneracy is
the number of states with the same energy.

## 2.1.12 :.1D finite barrier problem and concept of quantum tunneling (E<V₀)

■ Consider a particle of energy E approaching a potential barrier of height V_0 and the
potential everywhere else is zero.

■ We will first consider the case when the energy is greater than the potential barrier.

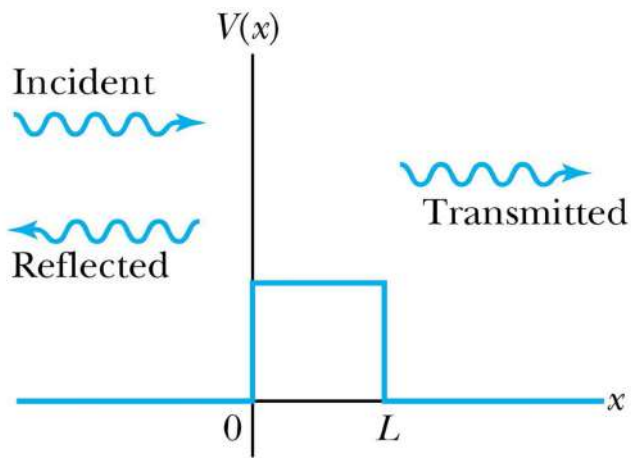$$k_{\mathrm{I}} = k_{\mathrm{III}} = \frac{\sqrt{2mE}}{\hbar}$$

■ In regions I and III the wave numbers are:
In the barrier region we have

$$k_{\mathrm{II}} = \frac{\sqrt{2m(E - V_0)}}{\hbar} \qquad \text{where } V = V_0$$
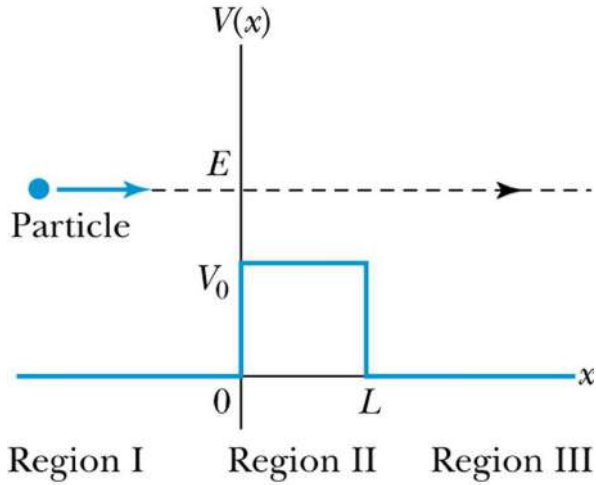
Reflection and Transmission

- The wave function will consist of an incident wave, a reflected wave, and a transmitted wave.
- The potentials and the Schrödinger wave equation for the three regions are as follows:

Region I $(x < 0)$ $V = 0$ $\dfrac{d^2\psi_1}{dx^2} + \dfrac{2m}{\hbar^2}E\psi_1 = 0$

Region II $(0 < x < L)$ $V = V_0$ $\dfrac{d^2\psi_{\mathrm{II}}}{dx^2} + \dfrac{2m}{\hbar^2}(E - V_0)\psi_{\mathrm{II}} = 0$

Region III $(x > L)$ $V = 0$ $\dfrac{d^2\psi_{\mathrm{III}}}{dx^2} + \dfrac{2m}{\hbar^2}E\psi_{\mathrm{III}} = 0$

■ The corresponding solutions are:

Region I $(x < 0)$ $\psi_{\mathrm{I}} = Ae^{ik_{\mathrm{I}}x} + Be^{-ik_{\mathrm{I}}x}$

Region II $(0 < x < L)$ $\psi_{\mathrm{II}} = Ce^{ik_{\mathrm{II}}x} + De^{-ik_{\mathrm{II}}x}$

Region III $(x > L)$ $\psi_{\mathrm{III}} = Fe^{ik_{\mathrm{I}}x} + Ge^{-ik_{\mathrm{I}}x}$

■ As the wave moves from left to right, we can simplify the wave functions to:

Incident wave $\psi_{\mathrm{I}}(\text{incident}) = Ae^{ik_{\mathrm{I}}x}$

Reflected wave $\psi_{\mathrm{I}}(\text{reflected}) = Be^{-ik_{\mathrm{I}}x}$

Transmitted wave $\psi_{\mathrm{III}}(\text{transmitted}) = Fe^{ik_{\mathrm{I}}x}$

Probability of Reflection and Transmission:

■ The probability of the particles being reflected R or transmitted T is:

$$R = \frac{|\psi_I(\text{reflected})|^2}{|\psi_I(\text{incident})|^2} = \frac{B*B}{A*A}$$

$$T = \frac{|\psi_{III}(\text{transmitted})|^2}{|\psi_I(\text{incident})|^2} = \frac{F*F}{A*A}$$

- The maximum kinetic energy of the photoelectrons depends on the value of the light frequency f and not on the intensity.

- Because the particles must be either reflected or transmitted we have: **$R + T = 1$.**

By applying the boundary conditions **$x \to \pm\infty$, $x = 0$, and $x = L$,** we arrive at the transmission probability
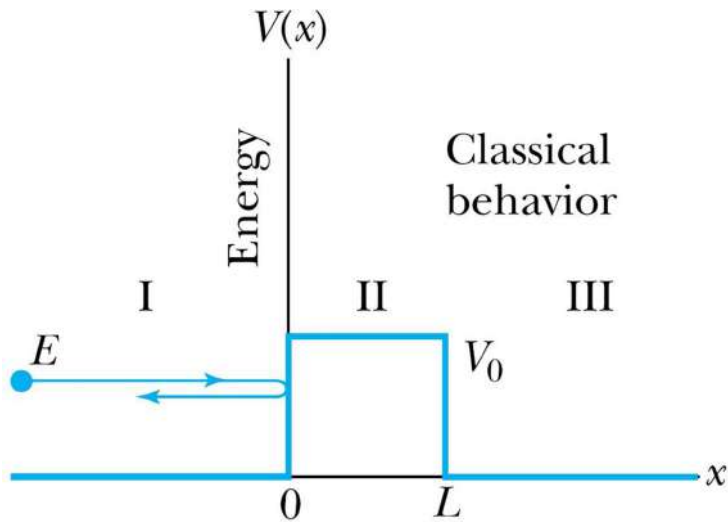
$$T = \left[1 + \frac{V_0{}^2 \sin^2(k_{II}L)}{4E(E-V_0)} \right]^{-1}$$

Notice that there is a situation in which the transmission probability is 1.

2.1.13 Tunneling:

- Now we consider the situation where classically the particle does not have enough energy to surmount the potential barrier, $E < V_0$.

- The quantum mechanical result, however, is one of the most remarkable features of modern physics, and there is ample experimental proof of its existence. There is a small, but finite, probability that the particle can penetrate the barrier and even emerge on the other side.

-

- The wave function in region II becomes

$$\psi_{II} = Ce^{\kappa x} + De^{-\kappa x} \quad \text{where} \quad \kappa = \frac{\sqrt{2m(V_0 - E)}}{\hbar}$$

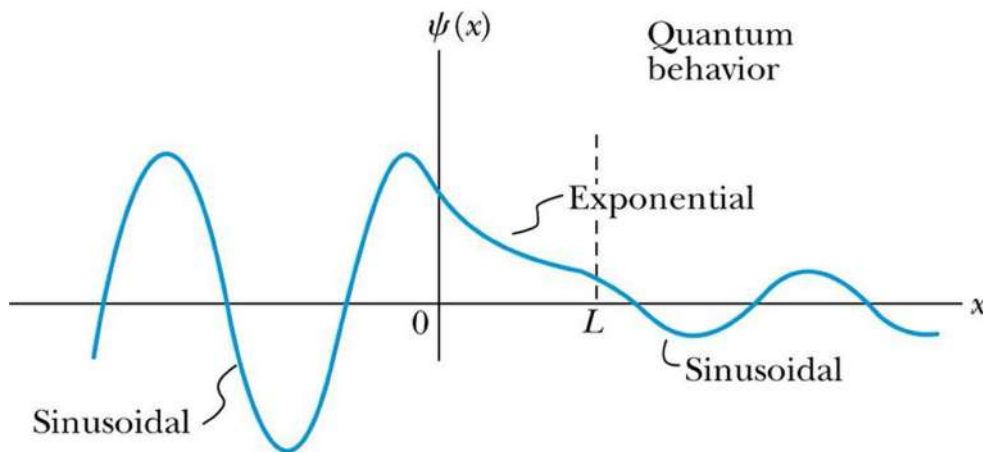- The transmission probability that describes the phenomenon of **tunneling** is

$$T = \left[1 + \frac{V_0^2 \sinh^2(\kappa L)}{4E(V_0 - E)}\right]^{-1}$$

Uncertainty Explanation:

■ Consider when $\kappa L \gg 1$ then the transmission probability becomes:

$$T = 16\frac{E}{V_0}\left(1 - \frac{E}{V_0}\right)e^{-2\kappa L}$$

■ This violation allowed by the uncertainty principle is equal to the negative kinetic energy required! The particle is allowed by quantum mechanics and the uncertainty principle to penetrate into a classically forbidden region. The minimum such kinetic energy is:

$$K_{min} = \frac{(\Delta p)^2}{2m} = \frac{\pi^2 \kappa^2}{2m} = V_0 - E$$

2.1.14 :. TUNNEL DIODE (Esaki Diode)

- It was introduced by Leo Esaki in 1958.

- Heavily-doped p-n junction
  - Impurity concentration is 1 part in 10^3 as compared to 1 part in 10^8 in p-n junction diode
- Width of the depletion layer is very small (about 100 A).
- It is generally made up of Ge and GaAs.
- It shows tunneling phenomenon.
- Circuit symbol of tunnel diode is :

Anode ▷|— Cathode

WHAT IS TUNNELING

- Classically, carrier must have energy at least equal to potential-barrier height to cross the junction .
- But according to Quantum mechanics there is finite probability that it can penetrate through the barrier for a thin width.
- This phenomenon is
  called tunneling and hence the Esaki Diodeis know asTunnel Diode.

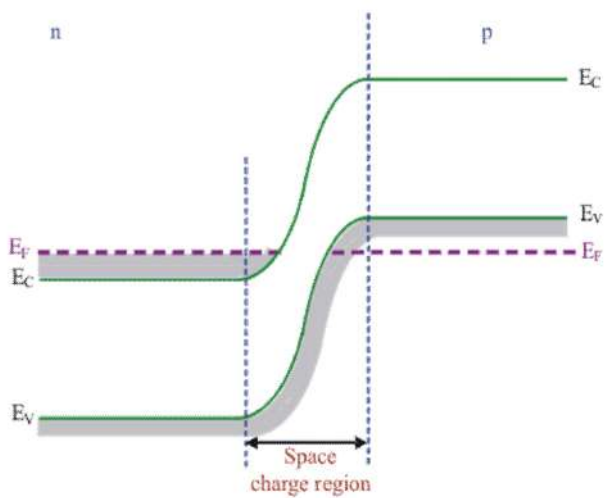Potential energy V(x) diagram with Space charge region labeled on x-axis
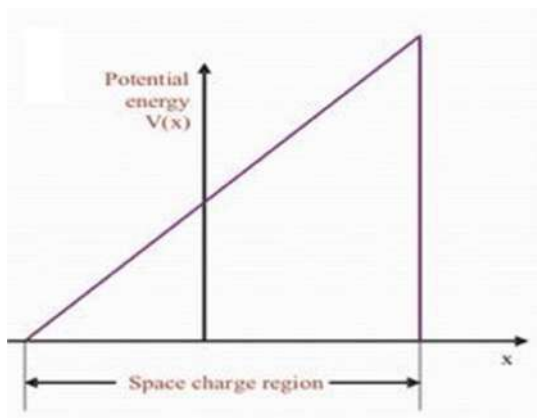
CHARACTERISTIC OF TUNNEL DIODE
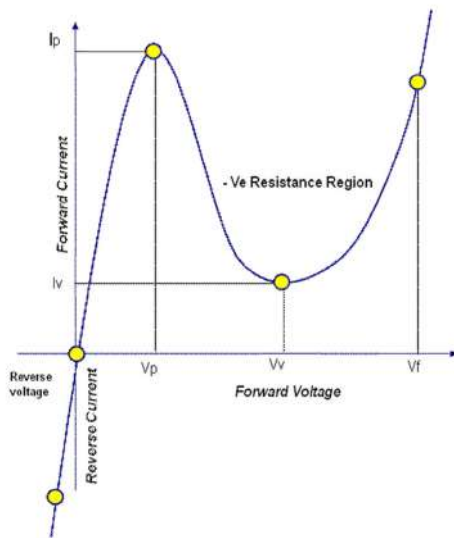
Ip:- Peak Current

Iv :- Valley Current

Vp:- **Peak** Voltage

Vv:- Valley Voltage

Vf:- Peak Forward
Voltage

ENERGY BAND DIAGRAM

Energy-band diagram of pn junction in thermal equilibrium in which both the n and p region are degenerately doped.
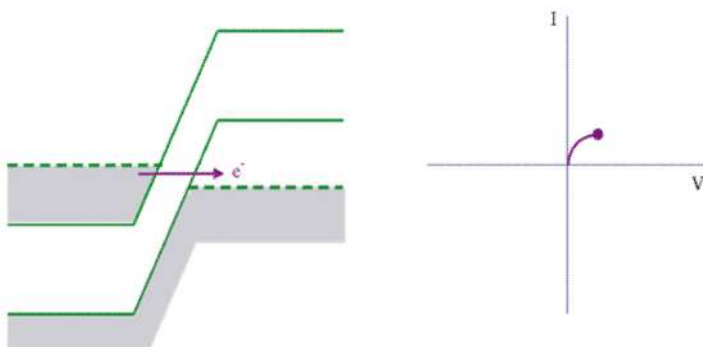
AT ZERO BIAS
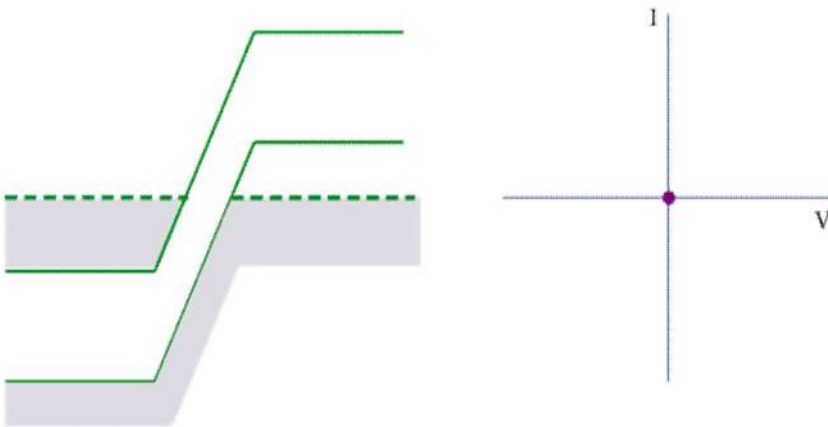
Simplified energy-band diagram and I-V characteristics of the tunnel diode at zero bias.

-Zero current on the I-V diagram;

-All energy states are filled below E_F on both sides of the junction;
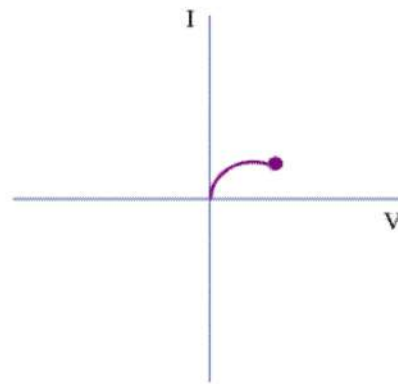
AT SMALL FORWARD VOLTAGE

Simplified energy-band diagram and I-V characteristics of the tunnel diode at a slight forward bias.

-Electrons in the conduction band of the n region are directly opposite to the empty states in the valence band of the p region.

-So a finite probability that some electrons tunnel directly into the empty states resulting in forward-bias tunneling current.

AT MAXIMUM TUNNELING CURENT
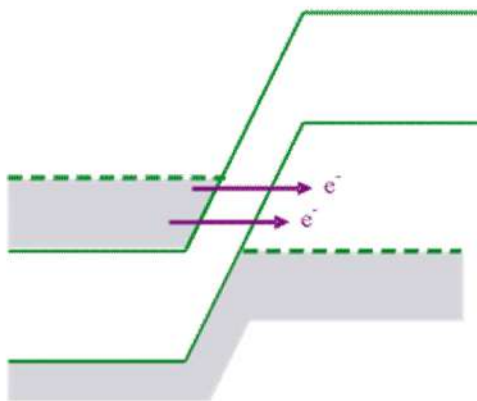
Simplified energy-band diagraam and I-V characteristics of the tunnel diode at a forward bias producing maximum tunneling current.

-The maximum number of electrons in the n region are opposite to the maximum number of empty states in the p region.

- Hence tunneling current is maximum.

AT DECREASING CURRENT REGION
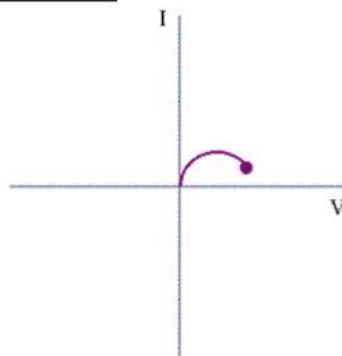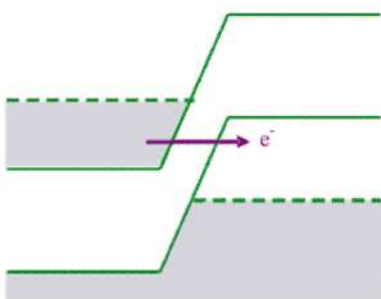
Simplified energy-band diagram and I-V characteristics of the tunnel diode at a higher forward bias producing less tunneling current

-The forward-bias voltage increases so the number of electrons on the n side, directly opposite empty states on the p side decreases.

- Hence the tunneling current decreases.

AT HIGHER FORWARD VOLTAGE
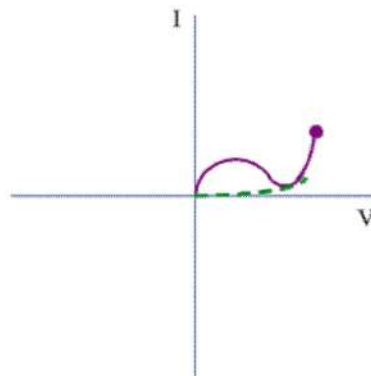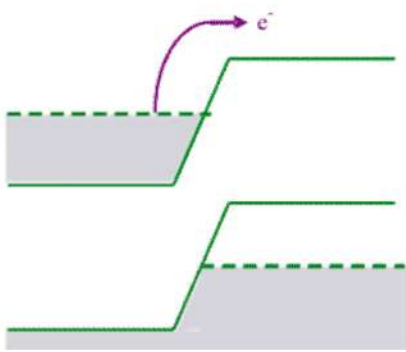
Simplified energy-band diagram and I-V characteristics of the tunnel diode at a forward bias for which the diffusion current dominates.

-No electrons on the n side are directly opposite to the empty states on the p side.

- The tunneling current is zero.

-The normal ideal diffusion current exists in the device.

AT REVERSE BIAS VOLTAGE
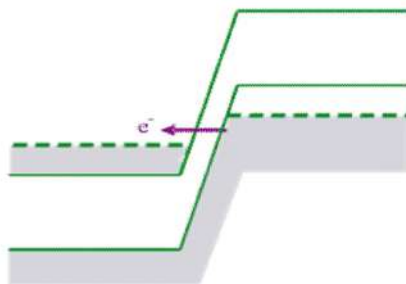
A simplified energy-band diagram of a tunnel diode with a reverse bias voltage
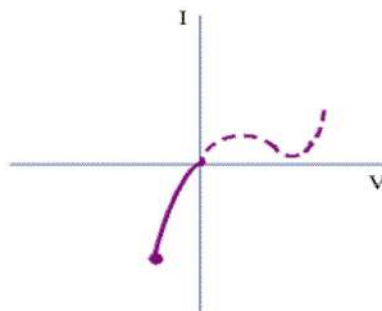
I-V characteristic of a tunnel diode with a reverse-bias voltage.

- Electrons in the valence band on the p side are directly opposite to empty states in the conduction band on the n side.

-Electrons tunnel directly from the p region into the n region.

- The reverse-bias current increases monotonically and rapidly with reverse-bias voltage.

TUNNEL DIODE EQUIVALENT CIRCUIT

- This is the equivalent circuit of tunnel diode when biased in negative resistance region.
- At higher frequencies the series R and L can be ignored.

- Hence equivalent circuit can be reduced to parallel combination of junction capacitance and negative resistance.
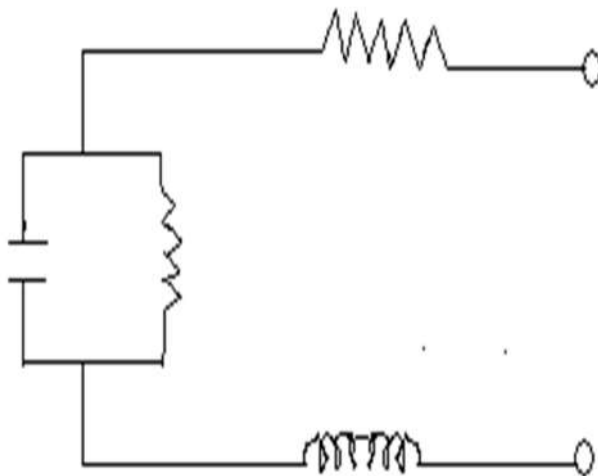
Optical analogy

If light passing through a glass prism reflects from an internal surface with an angle greater than the critical angle, total internal reflection occurs. However, the electromagnetic field is not exactly zero just outside the prism. If we bring another prism very close to the first one, experiments show that the electromagnetic wave (light) appears in the second prism The situation is analogous to the tunneling described here. This effect was observed by Newton and can be demonstrated with two prisms and a laser. The intensity of the second light beam decreases exponentially as the distance between the two prisms increases.

(a)

(b)
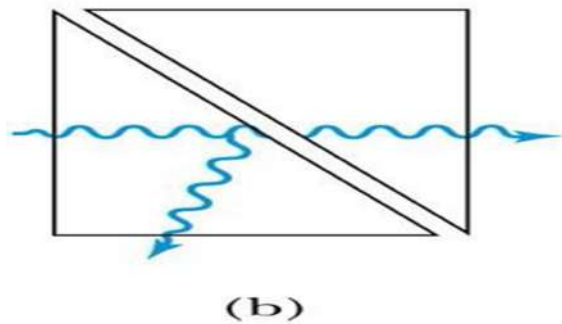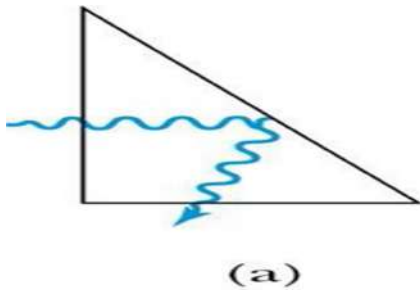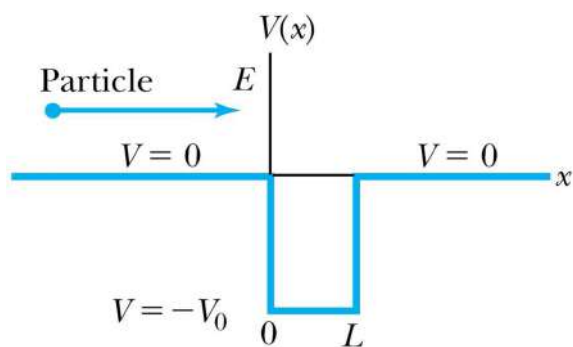
Potential Well:

- Consider a particle passing through a potential well region rather than through a potential barrier.
- Classically, the particle would speed up passing the well region, because $K = mv^2 / 2 = E + V_0$.

According to quantum mechanics, reflection and transmission may occur, but the wavelength inside the potential well is smaller than outside. When the width of the potential well is precisely equal to half-integral or integral units of the wavelength, the reflected waves may be out of phase or in phase with the original wave, and cancellations or resonances may occur. The reflection/cancellation effects can lead to almost pure transmission or pure reflection for certain wavelengths. For example, at the second boundary ($x = L$) for a wave passing to the right, the wave may reflect and be out of phase with the incident wave. The effect would be a cancellation inside the well.
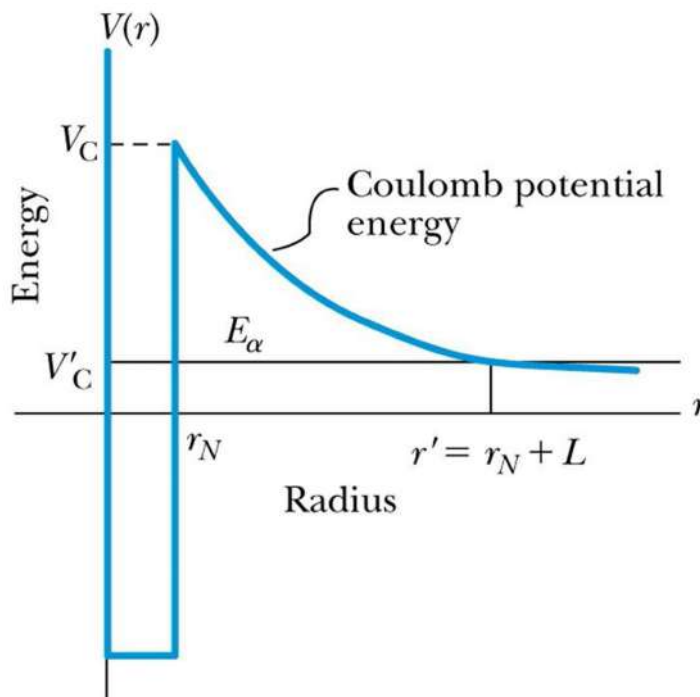
- The phenomenon of tunneling explains the alpha-particle decay of heavy, radioactive nuclei.
- Inside the nucleus, an alpha particle feels the strong, short-range attractive nuclear force as well as the repulsive Coulomb force.

- The nuclear force dominates inside the nuclear radius   where the potential is approximately a square well.
- The   Coulomb   force   dominates outside the nuclear radius.
- The   potential   barrier   at   the   nuclear radius   is   several   times   greater   than the energy of an alpha particle.

According to quantum mechanics, however, the alpha particle can "tunnel" through the barrier. Hence this is observed as radioactive decayAlpha-Particle Decay

2.2.1   Quantum Computation and Communication:

Why is a physicist teaching a course about information? In fact, the physics of information and computation has been a recognized discipline for at least several decades. This is natural. Information, after all, is something that is encoded in the state of a physical system; a computation is something that can be carried out on an actual physically realizable device. So the study of information and computation should be linked to the study of the underlying physical processes. Certainly, from an engineering perspective, mastery of principles of physics and materials science is needed to develop state-of-the art computing hardware. (Carver Mead calls his Caltech research group, dedicated to advancing the art of chip design, the "Physics of Computation" (Physcmp) group)

(Originally used by Neil Gershenfeld in a quantum computing paper published in Scientific America)

2.2.2   Definition of Vector:
It is set of elements satisfying certain properties e.g. ($|\psi>$, $|\varphi>$, $|\chi>$, $|\xi>$, $|\theta>$).

Number of elements is equal to the dimensionality of the vector space.

Each element can be represented as a column Matrix.

$|\psi>$ is called ket-vector.

$|\psi\rangle$ - vector, "ket" i.e.

$$\begin{bmatrix} c_1 \\ c_2 \\ \dots \\ c_n \end{bmatrix}$$

$\langle \psi |$ -bra vector which is adjoin of $|\psi\rangle$. Bra vector is an element of dual space of initial vector space and is represented as

$$\langle \psi | = (c_1^*, c_2^*, c_3^*, \dots, c_n^*)$$

Idea about taking adjoint of vectors,
A^* - complex conjugate of matrix A.

$$\text{if } A = \begin{bmatrix} 1 & 6i \\ 3i & 2+4i \end{bmatrix} \text{ then } A^* = \begin{bmatrix} 1 & -6i \\ -3i & 2-4i \end{bmatrix}$$

A^T - transpose of matrix A.

$$\text{if } A = \begin{bmatrix} 1 & 6i \\ 3i & 2+4i \end{bmatrix} \text{ then } A^T = \begin{bmatrix} 1 & 3i \\ 6i & 2+4i \end{bmatrix}$$

$A^\dagger$ - Hermitian conjugate (adjoint) of matrix A.
Note $A^\dagger = (A^T)^*$

$$\text{if } A = \begin{bmatrix} 1 & 6i \\ 3i & 2+4i \end{bmatrix} \text{ then } A^\dagger = \begin{bmatrix} 1 & -3i \\ -6i & 2-4i \end{bmatrix}$$

Concept of Field: A set of scalars (a, b, c, d, e, f….n).

2.2.3 Properties of the vector space:

i) Elements would follow additive property (Addition of two elements produces element same vector space).
ii) Elements would follow associative property in addition and scalar multiplication.
iii) Inner product of vectors produces a scalar.
Inner product of two vectors $|\psi\rangle$ and $|\varphi\rangle$ is,

$|\psi\rangle * |\varphi\rangle$ = Cannot be multiplied between vectors of same space rather from left it would be bra-vector and from right it would be ket vector; so that final inner product is bra-ket and is represented as

$<\psi \mid \varphi>$. Resultant is a scalar number, not a vector.

$$\text{Example: } |\varphi\rangle = \begin{bmatrix} 2 \\ 6i \end{bmatrix}, |\psi\rangle = \begin{bmatrix} 3 \\ 4 \end{bmatrix}$$

$$\langle\varphi|\psi\rangle = [2, -6i]\begin{bmatrix} 3 \\ 4 \end{bmatrix} = 6 - 24i$$

iv) Outer product of two vectors: It is taken between two vector of same space. Final element is a tensor.

$|\varphi\rangle \otimes |\psi\rangle$ - tensor product of $|\varphi\rangle$ and $|\psi\rangle$.
Also written as $|\varphi\rangle|\psi\rangle$

$$\text{Example: } |\varphi\rangle|\psi\rangle = \begin{bmatrix} 2 \\ 6i \end{bmatrix} \otimes \begin{bmatrix} 3 \\ 4 \end{bmatrix} = \begin{bmatrix} 2 \times 3 \\ 2 \times 4 \\ 6i \times 3 \\ 6i \times 4 \end{bmatrix} = \begin{bmatrix} 6 \\ 8 \\ 18i \\ 24i \end{bmatrix}$$

$\| \ |\psi\rangle \ \|$ - norm of vector $|\psi\rangle$
$\| \ |\psi\rangle \ \| = \sqrt{\langle\psi|\psi\rangle}$
Important for normalization of $|\psi\rangle$ i.e. $|\psi\rangle / \| \ |\psi\rangle \ \|$

$\langle\varphi|A|\psi\rangle$ - inner product of $|\varphi\rangle$ and $A|\psi\rangle$.
or inner product of $A^\dagger|\varphi\rangle$ and $|\psi\rangle$

2.2.4   Hermitian matrix: $A = A^t$

2.2.5   Unitarian matrix: $A A^t = I$

2.2.6   Basis Vector: Any arbitrary vector in a vector space can be expressed as linear combination of elements of that vector space. E.g

$|\psi\rangle = a_1| \varphi_1> + a_2| \varphi_2> + a_3| \varphi_3> + a_4| \varphi_4> + \ldots\ldots + a_n| \varphi_n> +$

$$= \sum_{i=1}^{n} a_i |\square_i>$$

Then $|\square_i>$ are called basis vectors and a_i as the coefficient of linear expansion.

2.2.7   Hilbert space: n dimensional linear vector space with complex coefficient is known as Hilbert space. A point in that space represents quantum mechanical state of an object.
Therefore, our quantum mechanical state vector |ψ> is represented by a point in Hilbert space.

Quibit: A vector in 2D Hilbert space with basis vectors, $|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $|1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$.
Therefore,

$$|\square\rangle = \square|0\rangle + \square|1\rangle$$ will represent a Qubit.

Probability, of being in the $|0\rangle$ state is $|\square|^2$ and $|1\rangle$ sate is $|\square|^2$ with total probability being
$$|\square|^2 + |\square|^2 = 1$$

Above equation is the equation of a circle and can be represented as (in 2D)

$|1\rangle$

$\alpha|0\rangle + \beta|1\rangle$

$|0\rangle$

"Normalization"

$$|\alpha|^2 + |\beta|^2 = 1$$

$|0\rangle$ and $|1\rangle$ are the
computational basis states
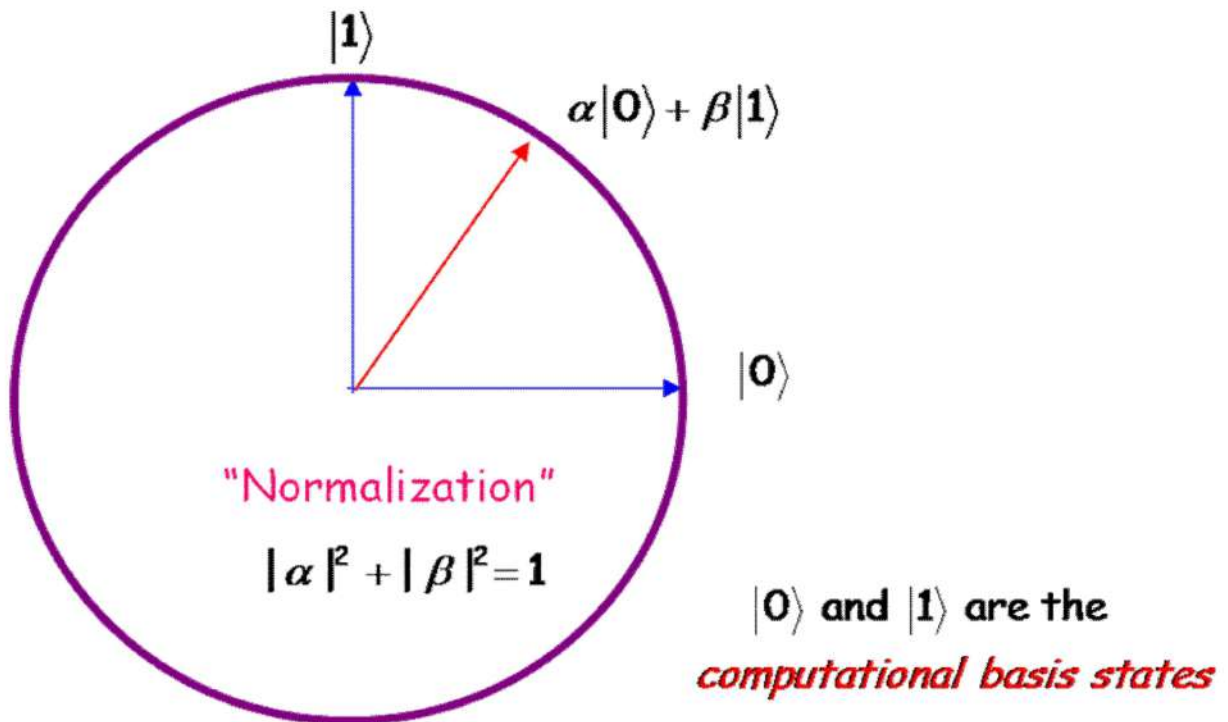
2.2.7 **In 3D the representation is Bloch-Sphere representation:**

$|+\rangle = |0\rangle$

$|-\rangle = |1\rangle$
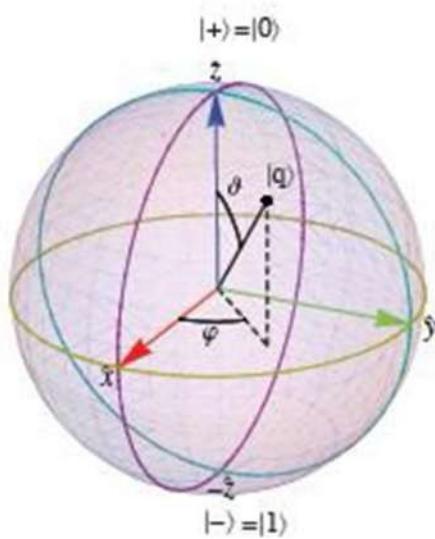
$$|q\rangle = \cos\left(\frac{\theta}{2}\right)|0\rangle + \sin\left(\frac{\theta}{2}\right)e^{i\varphi}|1\rangle.$$

It is important to note that While a **bit** can either have value 0 or 1, a **qubit** is a linear superposition of both a |*0*> and |*1*> value. In addition, a qubit can be **en- tangled** with other qubits, which is the real

reason for the surprising computational power of a quantum computer.

2.2.8   Realizing quantum bit (Qubit in practice):

Physical system that can represent a Qubit should be a Quanutm mechanical state so that principle of superposition could be applied and any superposed state also represent a Qubit. Potential system with these possibilities include,

i) electron spin states

ii) polarization states of light

iii) a two-level atom/system (ground state and excited state of an atom) and many more.

We will focus on electron spin states:

Electron spin is connected with the magnetic property of an electron and is described as magnetic sate of electron. Electron has two magnetic states referred as spin up and spin down states. We can represent,

Spin up sate (indicated as |↑>) many represented by basis vector |0>

Spin down sate (indicated as |↓>) many represented by basis vector |1>.

Linear combination $\left|\square\right\rangle = \square\left|0\right\rangle + \square\left|1\right\rangle$ representing a Qubit will be a intermediate magnetic state.

$$P(O) = P(1) = \frac{1}{2}$$
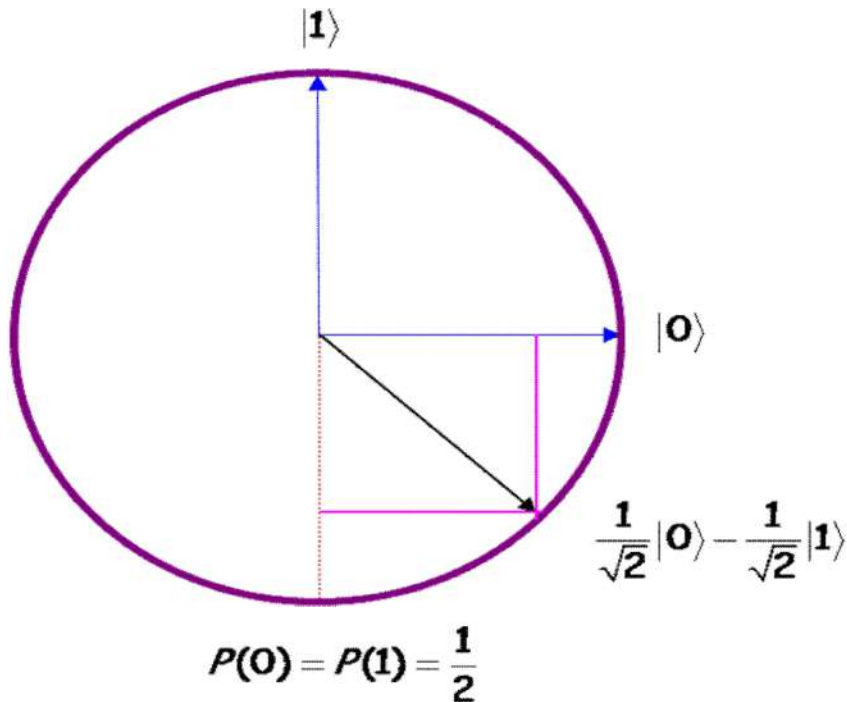
According to Quantum Mechanics, a quantum mechanical state could be modified by the action of suitable operator action. Obviously, in order to modulate spin states we need its corresponding operator. It is also according to Quantum mechanics, in order to attain measurable information the quantum mechanical state need to be an eigenfunciton of that operator.

Likewise Quantum states, operators could also be represented in terms of matrices.

In general, The process of extracting information from a set of qubits is called **measurement**. A measurement is represented by a hermitian matrix

$$A = \sum_i \Box_i \left| \Box_i \right\rangle \left\langle \Box_i \right|$$

The result of the measurement will be one of the eigenvalues $\Box_i$ of A, and the state of the

measured system will after the measurement be exactly in the state $\left| \Box_i \right\rangle$ described by the

corresponding eigenvector. Measurement changes the state of the system and cannot provide a snapshot of the entire state.

2.2.9   Spin as operator of Qubit:

The spin states of electron are eigen function of operator related to 3 Pauli spin operator and is expressed by three Pauli matrices,

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Operation of these spin matrices on individual Qubit would act as quantum logic operation and result in related Quantum Logic gates,

Basic 3 logic gates are call Pauli gates, related logic operations are as follows,

Pauli gates

X gate (AKA σ_x or σ_1)
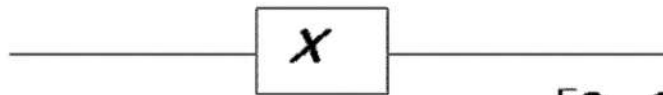
$$X|0\rangle = |1\rangle; \quad X|1\rangle = |0\rangle; \quad X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

Y gate (AKA σ_y or σ_2)
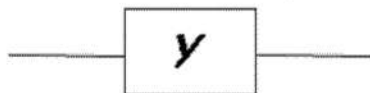
$$Y|0\rangle = i|1\rangle; \quad Y|1\rangle = -i|0\rangle; \quad Y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$$

Z gate (AKA σ_z or σ_3)
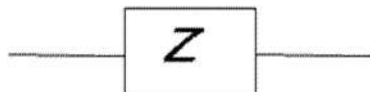
$$Z|0\rangle = |0\rangle; \quad Z|1\rangle = -|1\rangle; \quad Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

Notation: $\sigma_0 \equiv I$

2.2.10 : Pauli-X gate (= NOT gate)

The Pauli-X gate acts on a single qubit. It is the quantum equivalent of a NOT gate (with respect to the standard basis which privileges the Z-direction) . It equates to a rotation of the Bloch

sphere around the X-axis by π radians. It maps |0> to |1> and |1> to |0> . Due to this nature, it is sometimes called bit-flip.

Related Quantum Circuit is represented as,

2.2.11 : Pauli-Y gate

The Pauli-Y gate acts on a single qubit. It equates to a rotation around the Y-axis of the Bloch sphere by π radians. It maps |0> to i1> and|1> to -i|0> . It is represented by the Pauli Y matrix:

2.2.12 : Pauli-Z gate

he Pauli-Z gate acts on a single qubit. It equates to a rotation around the Z-axis of the Bloch sphere by π radians. Thus, it is a special case of a phase shift gate (next) with θ=π. It leaves the basis state|0> unchanged and maps |1> to -|1> . Due to this nature, it is sometimes called phase-flip.

2.2.13 : Hadamard gate

It is notable that in all three Pauli gates, we achieved mainly single qubit state due to logic operations. A simple Quantum logic operation that creates a mixed state is Hadamard gate.

$$H|0\rangle = \frac{|0\rangle + |1\rangle}{\sqrt{2}}; \quad H|1\rangle = \frac{|0\rangle - |1\rangle}{\sqrt{2}}; \quad H = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

The Hadamard operation implies a measurement will have equal probabilities to become 1 or 0.

Related Quantum Circuit is represented as,

2.2.14 : Phase shift gates

This is a family of single-qubit gates that leave the basis state |0> unchanged and map |1> to $e^{i\square}$ |1 >. The probability of measuring a |0> or |1> is unchanged after applying this gate, however it modifies the phase of the quantum state. This is equivalent to tracing a horizontal circle (a line of latitude) on the Bloch sphere by $\square$ radians.

$$R_\square = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\square} \end{pmatrix}$$

where $\square$ is the *phase shift*. Some common examples are the $\dfrac{\square}{8}$ gate where $\square = \dfrac{\square}{4}$, the phase gate where $\square = \dfrac{\square}{2}$ and Pauli Z-gate where $\square = \square$. Rotation of $\dfrac{\square}{2}$ refers to root NOT operation.

2.2.15 : Controlled NOT gates:

Two Qubit Quantum gate. Controlled gates act on 2 or more qubits, where one or more qubits act as a control for some operation. For example, the controlled NOT gate (or CNOT) acts on 2 qubits, and performs the NOT operation on the second qubit only when the first qubit is |1>, and otherwise leaves it unchanged.
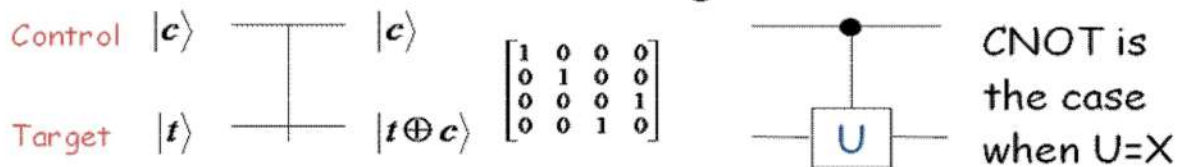
Related Quantum Circuit is represented as,

2.02.16: Classical bit vs quantum bit:

Classical bit	quantum bit
Binary numbers	Quantum Mechanical state
Available only in two states 0 and 1	Basis vectors and their superposed states
Realized as voltages states.	Realized as quantum mechanical state of an object. E.g. electron spin
Related circuits are digital logic circuits, which are essentially voltage values	Related circuits are quantum gates, which are essentially rotation of spin state by spin

	operators.

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Module 3: Statistical Mechanics (6L)

Module 3.01: Basics of Statistical Mechanics:
Concept of energy levels and energy states. Microstates, Macrostates and thermodynamic probability, MB, BE, FD, statistics (Qualitative discussions)- physical significance, conception of bosons, fermions, classical limits of quantum statistics, Fermi distribution at zero & non-zero temperature, Concept of Fermi level. 4L

Module 3.02: Applications of Statistical Mechanics:
Fermi level in metals, total energy at absolute zero and total number of particles. Fermi level for intrinsic and extrinsic semiconductors (pictorial representations on temperature dependence and doping concentration viz. p type, n-type).   2L

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Lesson plan: Statistical Mechanics

Module No	Lecture No	Topic	Application	Reference Book
2.01	1	Inadequacy of Newtonian mechanics, Concept of energy levels and energy states. Microstates, macrostates and thermodynamic probability	Knowing about MB statistics it is possible to know about energy states of occupied gas molecules.	Fundamental of Statistical Mechanics: B Laud Introduction to statistical mechanics : .Pathria Fundamental of Statistical and Thermal Physics: .F. Reif
2.01	2	Qualitative discussion of MB, BE statistics, and their physical significance	Knowing BE statistics it is possible to know 4th state of matter BE Condensed state	Fundamental of Statistical Mechanics: B Laud Introduction to statistical mechanics : .Pathria Fundamental of Statistical and Thermal Physics: .F. Reif
2.01	3	Qualitative discussion of FD statistics, physical significance, conception of bosons, fermions, classical limit of quantum statistics.	Quantum Tunne Knowing FD statistics it is possible to know Fermi temperature and Degeneracy pressure and existence of stars .	Fundamental of Statistical Mechanics: B Laud Introduction to statistical mechanics : .Pathria Fundamental of Statistical and Thermal Physics: .F. Reif
2.01	4	Fermi distribution at zero & non-zero temperature, Concept of Fermi level.	In Band theory, Concept of metal, insulator and semiconductor.	Fundamental of Statistical Mechanics: B Laud Introduction to statistical mechanics : .Pathria Fundamental of Statistical and Thermal Physics: .F. Reif
2.02	1	Qualitative study: Fermi level in metals, total energy at absolute zero and total number of particles.	Detail idea about metal and its applications.	1.Fundamental of Statistical Mechanics: B Laud 2.Introduction to statistical mechanics : .Pathria 3. Fundamental of Statistical and Thermal Physics: .F. Reif
2.02	2	Fermi level for intrinsic and extrinsic semiconductors (pictorial representations on temperature dependence and doping concentration viz. p type, n-type).	Detail idea about intrinsic and extrinsic semiconductors and their applications in different fields.	Fundamental of Statistical Mechanics: B Laud Introduction to statistical mechanics : .Pathria 3.Fundamental of Statistical and Thermal Physics: .F. Reif

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Module 3: Statistical Mechanics (3L)

Module 3.1: Basics of Statistical Mechanics:-

3.01.1: Concept of energy levels and energy states:-

<u>**Concept of energy levels and energy states:-**</u>

Consider a H_2 atom, which has the simplest atomic configuration with a single electron revolving round the nucleus. The total energy of such an electron is given by

$-\dfrac{m e^4}{8 \varepsilon_0 h^2 n^2}$, where m and e are mass and charge of the electron respectively, ε_0 is the permittivity of free-space, h is the Planck's constant and n is known as principal quantum number. Thus the total energy for such an electron solely depends on n. We know that for a given value of n, we get other three quantum three quantum numbers whose values depend on n in the following manner:

l (orbital quantum number) = 0,1,2,3,……..,(n-1)

m_l (magnetic orbital quantum number) = -l,(-l+1),(-l+2),….,-2,-1,0,1,2,…..,(l-1),l m_s (magnetic spin quantum number) = $-\dfrac{1}{2} , +\dfrac{1}{2}$ (for each value of m_l)

All n, l, m_l integers or zero.

A specific energy level corresponds to a specific value of n. For different integral values of n, we get different discrete energy levels. On the other hand, each discrete set of the four quantum numbers, i.e. $\{n,l,m_l,m_s\}$, designates each energy state. Let's have an example to make these concepts clear.

Consider n = 2 energy level. For n = 2, l = 0,1.

For l = 0, m_l = 0 and m_s = $-\dfrac{1}{2} , +\dfrac{1}{2}$

For l = 1, m_l = -1,0,+1 and m_s = $-\dfrac{1}{2} , +\dfrac{1}{2}$ for each value of m_l.

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n-value	l-value	m_l- value	m_s- value	energy states	no.of energy states
2	0	0	$-\frac{1}{2}, \frac{1}{2}$	$\{2,0,0,-\frac{1}{2}\}$ $\{2,0,0,+\frac{1}{2}\}$	2
2	1	-1	$-\frac{1}{2}, \frac{1}{2}$	$\{2,1,-1,-\frac{1}{2}\}$ $\{2,1,-1,\frac{1}{2}\}$	6
		0	$-\frac{1}{2}, \frac{1}{2}$	$\{2,1,0,-\frac{1}{2}\}$ $\{2,1,0,\frac{1}{2}\}$	
		+1	$-\frac{1}{2}, \frac{1}{2}$	$\{2,1,+1,-\frac{1}{2}\}$ $\{2,1,+1,\frac{1}{2}\}$	

Thus for n = 2 energy level, we get eight distinct energy states. But all these eight energy states have the same value of the total energy because, the total energy, as already stated, depends only on the principal quantum number. Such type of distinct energy states having the same total energy are known as *degenerate states* and it is said that the energy level n = 2 is *8-fold degenerate*. Similarly we can show that n = 3 energy level is 18-fold degenerate. Note that this type of degenerate states is direct consequence of the symmetry of the respective system.

3.1.2 Microstates:-

In statistical mechanics, a microstate is a specific microscopic configuration of a thermodynamic system that the system may occupy with a certain probability in the course of its thermal fluctuations
Since a gas consists of large number of particles, the state of a gas can also be characterized in terms of the states of the constituent particles. The state of the particles can be specified by ascertaining their positions (Coordinates q_i) and velocities and momentum p_i . Thus state of the gas thus described in terms of the properties of constituent particles is called the **Microscopic state**

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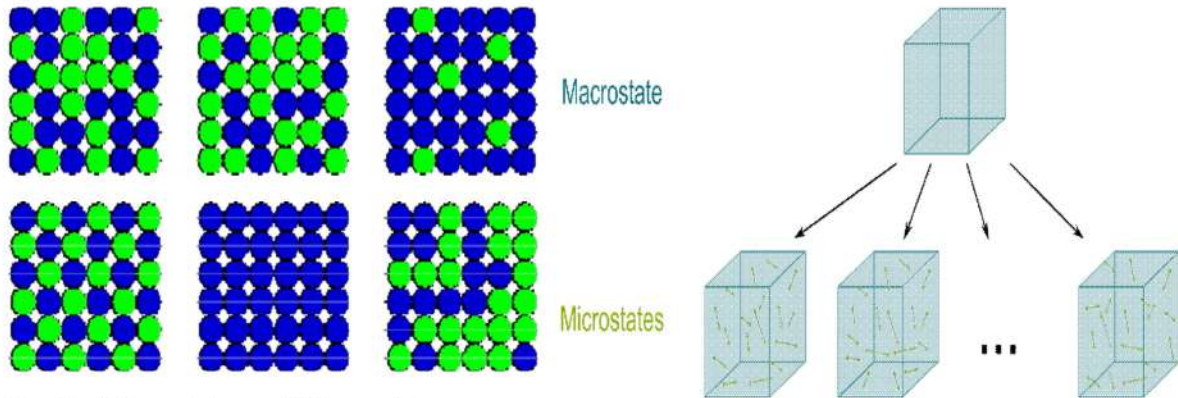
Fig-2.a Microstates and Macrostates

3.1.3 Macrostates:-

Macrostate: the state of a macro system specified by its macroscopic parameters. Two systems with the same values of macroscopic parameters are thermodynamically indistinguishable. A macrostate tells us nothing about a state of an individual particle.
For a given set of constraints (conservation laws), a system can be in many macrostates. Macrostate refers to the state of the system as a whole. The quantities like pressure, volume and temperature are macroscopic. They do not give the position   momentum values of constituent particles.

3.1.4 Thermodynamic probability:-

The total number of possible microstates of a system corresponding to given macrostate is called thermodynamic probability

For n particles the number of microstates for its (n_1,n-n_1) macrostate is

$$W_{n1,n-n1} = \frac{n!}{n1!(n-n1!)}$$

3.1.5 Phase Space:-

To describe both the position and the state of the motion of the particle, it is require to set up a six dimensional space in which a point has six co-ordinates x, y, z (three position co-ordinates) and p_x, p_y, p_z (three momentum co-ordinates) along six mutually perpendicular axes in space. This combined position and momentum space is called phase spacel.

3.1.6 <u>Formalisms in Statistical Mechanics</u>

The various methods of statistical mechanics are applied to discuss some average or most probable properties of large assemblies of electrons, atoms, molecules etc. Before the advent of quantum mechanics, Maxwell, Boltzmann, gibbs etc, applied statistical methods with the help of classical physics. These methods are collectively known as Classical Statistics or Maxwell-Boltzmann (MB) Statistics. These statistics were proved to be

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successful in explaining pressure, temperature etc. of gaseous systems. But these couldn't explain some experimental results like the energy distribution in case of black-body radiation, specific heat at low temperature etc. For explaining such phenomena Satyen Bose, Albert Einstein, Enrico Fermi, Paul A. Dirac had made use of some new statics with the help of newly discovered quantum theories. The new statistics are known as Quantum Statistics and can be divided into following two categories:-
(i)   Bose-Einstein (BE)
statistics (ii)Fermi-Dirac (FD)
statistics
        We'll discuss the various interesting features of these three (MB,BE,FD) statistics one by one in the following subsections.

3.1.7 *Maxwell-Boltzmann (MB) Statistics:-*

The basic postulates of MB statistics are:-(i)The
 associated particles are distinguishable.
(ii)Each energy state can contain any number of particles. (iii)Total number of particles in the entire system is constant. (iv)Total energy of all the particles in the entire system is constant. (v)Particles are spinless.
Examples: gas molecules at high temperature and low pressure.

Maxwell-Boltzmann Distribution Law

Consider a system composed of N distinguishable, non-interacting particles. Let out of these N particles N_1, N_2,….., N_i particles are to be distributed in energy levels E_1,E_2,…..,E_i respectively and these energy levels have g_1,g_2,…..,g_i number of quantum states correspondingly. Since the total energy E and total number of particles N are constant for the system, we can write

$$\sum N_i E_i = Ei \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots (2a)$$
$$\sum N_i = Ni \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots (2b)$$

The number of ways in which the groups of particles N_1, N_2,….., N_i could be chosen from N particles is

$$W_1 = \frac{N!}{N_1! N_2! \dots\dots N_i!} = \frac{N!}{\prod\limits_{i}^{n} N_i!} \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots (2c)$$

Where $\prod$ denotes the product.

        Now, N_i particles can be distributed in g_i states in $(g_i)^{N_i}$ ways. Considering all the values of i, total number of arrangement would be

$$W_2 = \prod^{n} (g_i)^{N_i} \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots (2d)$$

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Therefore, the total number of ways W by which all the N particles could be distributed among the quantum states is

$$W = W_1 W_2 = \frac{N!}{\prod N_i!} \prod_i^n \left(g_i\right)^{N_i} \qquad \dots\dots\dots\dots\dots\dots\dots(2e)$$

Now calculating the ratio of $\frac{N_i}{g_i}$ we get

$$f(E_i) = \frac{N_i}{g_i} = \frac{1}{e^{\alpha+\beta E_i}} \qquad \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots (2f)$$

N_i and g_i are the no of particles and no of states respectively.

3.1.8 *Bose- Einstein (BE) Statistics:-*

The basic postulates of BE statistics are:-:
(i)The associated particles are identical and *indistinguishable*.
(ii)Each energy state can contain any number of particles.
(iii)   Total energy and total number of particles of the entire system is constant
(iv)   The particles have zero or integral spin,i.e. 0 , 1 ,5 ,50 etc, where is the unit of spin.

(v) The wave function of the system is symmetric under the positional exchange of any two particles.
Examples: photon, phonon, all mesons (□,□,□) etc., these are known as ***Bosons***.
[*Note*: ***Symmetric and Anti-symmetric wave function***
        *Suppose the allowed wave function for a n-particles system is ψ(1,2,3,.....,r,s,...n),
where the integers within the argument of ψ represent the coordinates of the n-particles
relative to some fixed origin. Now, if we interchange the positions of any two particles, say,
r and s, the resulting wave function becomes ψ(1,2,3,....s,r,.....n). The wave function ψ is
said to be symmetric when*
        *ψ(1,2,3,.....,r,s,...n)   =
ψ(1,2,3,....s,r,.....n) and anti-symmetric when*
        ψ(1,2,3,.....,r,s,...n) = - ψ(1,2,3,....s,r,.....n)]

Bose-Einstein Distribution Law:

        Let N_i number of identical, indistinguishable, non-interacting particles are to be distributed among g_i quantum states each having energy E_i. So, in the ith energy level, there are $(N_i + g_i)$ total objects. Keeping the first quantum state fixed, the remaining $(N_i + g_i -1)$ objects can permuted in $(N_i + g_i - 1)!$ possible ways. But since the particles and the quantum states are indistinguishable, we have to deduct $N_i!$ ways and $(g_i - 1)!$ ways from the all possible ways to get effective number of arrangements. Thus total number of possible ways of arrangement for the ith state is

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$$W_i = \frac{(N_i + g_i - 1)!}{N_i! \, g_i - 1 !} \quad \text{...(3a)}$$

Hence the total number of ways of the entire distribution of N particles in n number of energy levels of the system is

$$W = \prod_i^n \frac{(N_i + g_i - 1)!}{N_i! (g_i - 1)!} \quad \text{.......................................(3b)}$$

where $\prod$ denotes the product symbol.

Now calculating the ratio of $\frac{N_i}{g_i}$ is given by

$$f(Ei) = \frac{N_i}{g_i} = \frac{1}{e^{(\alpha + \beta E_i)} - 1} \quad \text{.............................(3c)}$$

Where N_i and g_i are no of particles and no of states respectively.

3.01.9. *Fermi-Dirac (FD) Statistics:-*

The basic postulates of FD statistics are:-
(i) Particles are identical and indistinguishable.
(ii) Total energy and total number of particles of the entire system is constant
(iii) Particles have half-integral spin, i.e $\frac{1}{2}, \frac{3}{2}, \frac{37}{2}, etc.$
(iv) Particles obey Pauli's exclusion principle, i.e. no two particles in a single system can have the same value for each of the four quantum numbers. In other words, a single energy state can contain at best a single particle with appropriate spin.
(v) The wave function of the system is anti-symmetric under the positional exchange of any two particles.
Examples: electron, proton, neutron, all hyperons ($\Lambda, \Sigma, \Xi, \Omega$) etc., these are known as **Fermions.**

Fermi-Dirac Distribution Law:

Consider a system of N indistinguishable, non-interacting particles obeying Pauli's exclusion principle. Let N_1, N_2, N_3, ...N_i,....N_n Particles in the system have energies E_1, E_2, E_3, ...,E_i,...E_n respectively and let g_i is the number of degenerate quantum states in the energy level E_i. According to Pauli's exclusion principle a single quantum state can be occupied by at best one particle. Since N_i particles are to be distributed among g_i degenerate states ($g_i \geq N_i$) having the same energy E_i, N_i states will be filled up and ($g_i - N_i$) states will remain vacant. Now g_i states can be arranged in $g_i!$ possible ways, . But since the particles and the quantum states are indistinguishable, we have to deduct $N_i!$ ways and ($g_i - N_i$)! ways from the all possible ways to get effective number of arrangements. Thus total number of possible ways of arrangement for the ith state is

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$$W_i = \frac{(g_i)!}{N_i!\,g_i - N_i\,!} \quad \text{..................................(4a)}$$

Hence the total number of ways for the entire distribution of N particles in n number of

energy levels of the system is

$$W = \prod_i^n \frac{(g_i)!}{N_i!(g_i-N_i)!} \quad \text{..(4b)}$$

where $\prod$ denotes the product symbol.

Now taking natural logarithm on both sides of eqn.(7.30) and applying Stirling approximation,

$$\ln W = \sum \left[\ln g_i - \ln N_i - \ln (g_i - N_i) \right]$$

Now calculating the ratio of $\frac{N_i}{g_i}$ is given by

$$f(E_i) = \frac{N_i}{g_i} = \frac{1}{e^{(\alpha + \beta E_i)} + 1} \quad \text{..(4c)}$$

Where N_i and g_i are no of particles and no of states respectively.

3.1.10 Physical significance:-

Maxwell–Boltzmann statistics may be used to derive the Maxwell–Boltzmann distribution (for an ideal gas of classical particles in a three-dimensional box). However, they apply to other situations as well. Maxwell–Boltzmann statistics can be used to extend that distribution to particles with a different energy–momentum relation, such as relativistic particles (Maxwell–Jüttner distribution). In addition, hypothetical situations can be considered, such as particles in a box with different numbers of dimensions (four-dimensional, two-dimensional, etc.).

Maxwell–Boltzmann statistics are often described as the statistics of "distinguishable" classical particles. In other words, the configuration of particle A in state 1 and particle B in state 2 is different from the case in which particle B is in state 1 and particle A is in state 2. This assumption leads to the proper (Boltzmann) statistics of particles in the energy states, but yields non-physical results for the entropy, as embodied in the Gibbs paradox.

In quantum statistics, Bose–Einstein statistics (or more colloquially B–E statistics) is one of two possible ways in which a collection of non-interacting indistinguishable particles may occupy a set of available discrete energy states, at thermodynamic equilibrium. The aggregation of particles in the same state, which is a characteristic of particles obeying Bose–Einstein statistics, accounts for the cohesive streaming of laser light and the frictionless creeping of superfluid helium. The theory of this behaviour was developed (1924–25) by Satyendra Nath Bose, who recognized that a collection of identical and indistinguishable particles can be distributed in this way. The idea was later adopted and extended by Albert Einstein in collaboration with Bose.

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The Bose–Einstein statistics apply only to those particles not limited to single occupancy of the same state—that is, particles that do not obey the Pauli exclusion principle restrictions. Such particles have integer values of spin and are named bosons, after the statistics that correctly describe their behaviour. There must also be no significant interaction between the particles.

In metal, the weakly attached conducting electrons are \free" to move in the lattice. The electrons interact with the electrostatic potential of the positive ions in the lattice. If we consider the periodicity of the potential, we will obtain the solution to the Schrodinger equation in the form of Bloch waves. The energy will form a band. For perfect stationary lattice, there is free propagation and infinite conductivity of electrons. However lattice imperfections, lattice vibrations (phonons) and the scattering by the other electrons leads to resistance in the lattice. In the free electron model, we apply Fermi-Dirac Statistics - electrons of spin 1/2 and $= 1/2$.

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3.1.11 Conception of boson & fermions :-

In quantum mechanics, a boson is a particle that follows Bose–Einstein statistics. Bosons make up one of the two classes of particles, the other being fermions. The name boson was coined by Paul Dirac to commemorate the contribution of the Indian physicist Satyendra Nath Bose in developing, with Einstein, Bose–Einstein statistics—which theorizes the characteristics of elementary particles Examples of bosons include fundamental particles such as photons, gluons, and W and Z bosons
An important characteristic of bosons is that their statistics do not restrict the number of them that occupy the same quantum state. This property is exemplified by helium-4 when it is cooled to become a super fluid.. Whereas the elementary particles that make up matter (i.e. leptons and quarks) are fermions, the elementary bosons are force carriers that function as the 'glue' holding matter together. This property holds for all particles with integer spin (s = 0, 1, 2,)etc.

In particle physics, a fermion (a name coined by Paul Dirac from the surname of Enrico Fermi) is any subatomic particle characterized by Fermi–Dirac statistics. These particles obey the Pauli exclusion principle. Fermions include all quarks and leptons, as well as any composite particle made of an odd number of these, such as all baryons and many atoms and nuclei.
A fermion can be an elementary particle, such as the electron, or it can be a composite particle, such as the proton. According to the spin-statistics theorem in any reasonable relativistic quantum field theory, particles with integer spin are bosons, while particles with half-integer spin are fermions.

3.01. 12 Classical limits of quantum statistics:-

The distribution functions for MB,BE and statistics are respectively given by

$$[f(E_i)]MB = \frac{N_i}{g_i} = \frac{1}{e^{\alpha+\beta E_i}}$$

$$[f(E_i)]BE = \frac{N_i}{g_i} = \frac{1}{e^{(\alpha+\beta E_i)}-1}$$

$$[f(E_i)]FD = \frac{N_i}{g_i} = \frac{1}{e^{(\alpha+\beta E_i)}+1}$$

in above all the three cases $\beta = KT$

Thus in general the distribution function for all the three statistics can be written as
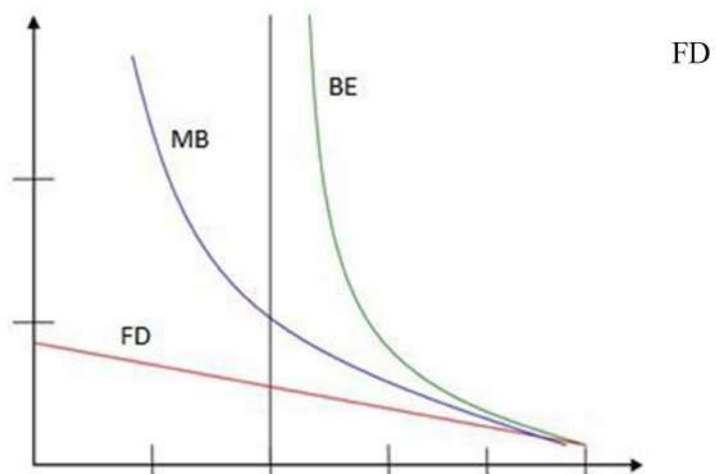
Fig.2b : Plot of distribution function $f(E_i)$ with $(\alpha+\beta E_i)$ for the *three statistics*

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$$[f(E_i)]FD = \frac{N_i}{g_i} = \frac{1}{e^{(\alpha + \beta E_i)} + \delta}$$

where, $\delta = 0$ for MB statistics $\delta = -1$ for BE statistics, $\delta = +1$ FD Statisiics.

It is obvious that the quantum statistics (BE and FD) would tend to the classical one (MB) only when $e^{e_i/kT} \gg 1$, then $\frac{N_i}{g_i} \ll 1$. Now the parameter α for both BE and FD statistics is inversely proportional to T. Thus if very high value of the temperature T corresponds to very low value of $\frac{N_i}{g_i}$ the quantum statistics reduces to the classical one.

Here $\frac{N_i}{g_i}$ is the number of particles per unit state and can be treated as the particle density. Hence under **high temperature** and **low particle density** *the quantum statistics tend to the classical one.*

MCQ for Statistical Mechanics:-

1. The number of macrostates for N particles in MB distribution are
   (a) N+1   (b) N - 1   (c) N   (d) N/2

2. The MB statistics is applicable for
   (a) distinguishable particle   (b) indistinguishable particle   (c) semi distinguishable particle
   (d) none of these

3. MB statistics
   (a) obeys Paulies exclusion principle
   (b) does not obeys Paulies exclusion principle
   (c) Hunds principle
   (d) None of these

4. In BE statistics each quantum state can accommodate
   (a) Only one particle (b) one or more particle (c) two particles (d) none of these

5. FD statistics is applicable for

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(a) Photon   (b) electron   (c) ideal gas   (d) X-rays

6. The Fermi Dirac distribution is expressed as

(a) $\dfrac{1}{e^{\alpha+\beta E_i}}$ (b) $\dfrac{1}{e^{(\alpha+\beta E_i)}-1}$ (c) $\dfrac{1}{e^{(\alpha+\beta E_i)}+1}$ (d) None of these

Problems in Statistical Mechanics:-

1. Find out the different macrostates and microstates of a system of three particles distributed in three cells assuming the particles to be (i) indistinguishable, (ii) distinguishable

2. Two particles are to be distributed in three cells. Find out the total number of possible ways both from formula and in tabular form if the particles follow (i) MB statistics (ii)BE statistics (iii) FD statistics.

3.A system has non-degenerate single-particle states with 0,1,2,3 energy units. Three particles are to be distributed in these states such that the total energy of the system is 3 units. Find the number of microstates if the particles obey

(i) MB statistics (ii) BE statistics (iii)FD statistics. Find the corresponding macrostates and microstates also.

4. Calculate the probability of finding an electron with energy 6eV in an electron gas at 10000C if the Fermi energy of the gas is 5eV.

5. If the probability of finding an electron of energy 6eV in an electron gas at 10000C is 0.01105 %, calculate the Fermi energy of the gas.
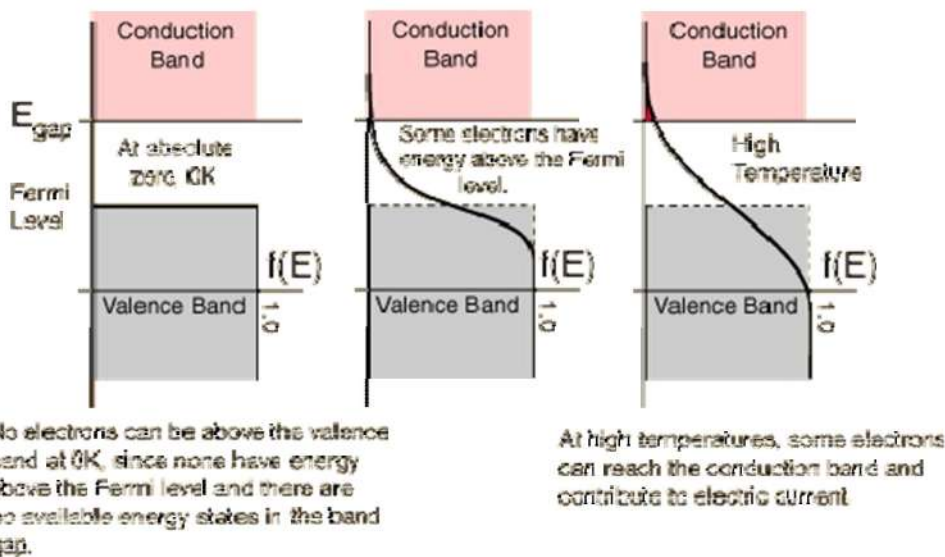
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3.2.1 : FERMI LEVEL

"Fermi level is the term used to describe the top of the collection of electron energy levels at absolute zero temperature. This concept comes from Fermi-Dirac statistics. Electrons are fermions and by the Pauli exclusion principle cannot exist in identical energy states. So at absolute zero they pack into the lowest available energy states and build up a "Fermi sea" of electron energy states. The Fermi level is the surface of that sea at absolute zero where no electrons will have enough energy to rise above the surface. The concept of the Fermi energy is crucially important for the understanding of the electrical and thermal properties of solids. Both ordinary electrical and thermal processes involve energies of a small fraction of an electron volt. But the Fermi energies of metals are of the order of electron volts. This implies that the vast majority of the electrons cannot receive energy from those processes because there are no available energy states for them to go to within a fraction of an electron volt of their present energy. Limited to a tiny depth of energy, these interactions are limited to ripples on the Fermi sea.

At higher temperatures a certain fraction, characterized by the Fermi function, will exist above the Fermi level. The Fermi level plays an important role in the band theory of solids. In doped semiconductors, p-type and n-type, the Fermi level is shifted by the impurities, illustrated by their band gaps. The Fermi level is referred to as the electron chemical potential in other contexts.

No electrons can be above the valence band at 0K, since none have energy above the Fermi level and there are no available energy states in the band gap.

At high temperatures, some electrons can reach the conduction band and contribute to electric current

3.2.2 : Fermi distribution at zero & non-zero temperature

The Fermi-Dirac distribution function is

$$\frac{N_i}{g_i} = \frac{1}{e^{(\alpha + \beta E_i)} + 1}$$

Now for the fermions in statistical equilibrium at absolute temperature T, it is found that

$$\alpha = -E_F/kT, \text{ and } \beta = 1/kT$$

Where, E_F is the *Fermi energy* of the system (i.e. the maximum energy at absolute zero) k is the Boltzmann constant = 1.38×10^{-23} Joule/Kelvin.

Here $\frac{N_i}{g_i}$ is known as *Occupation index*

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Thus the F-D distribution function reduces to

$$f(E_i) = \frac{1}{e^{(E_i - E_F)/kT} + 1}$$

Now, let us discuss two distinct cases.

Case – 1 (T= 0 K)

$f(E_i) = 1$, when $E_i < E_F$
$\quad\quad\quad = 0$, when $E_i > E_F$
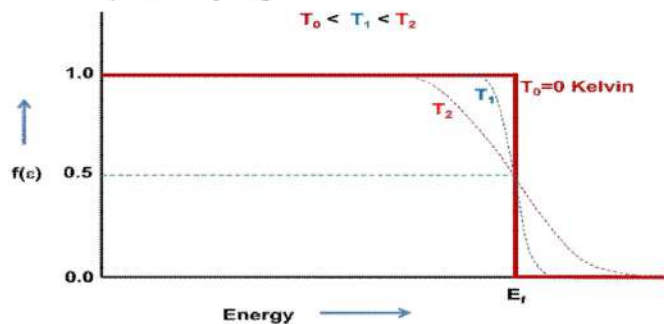
Plot of Fermi-Dirac distribution function as a function of E_i

Thus at T = 0K, $f(E_i)$ is a step function (See the Fig) which implies all the energy states upto $E_i = E_F$ are filled up and the states above E_F are empty.

Case – 2 (T> 0 K)

As the temperature increases beyond T= 0K, some of the electrons in the levels just below the Fermi level go to levels just above E_F resulting a gradual change in the occupation index $f(E_i)$. If $E_i = E_F$,

$$f(E_i) = \frac{1}{e^0 + 1} = \frac{1}{2}$$

i.e. at a finite temperature Fermi energy of a system is that energy for which 50% energy states are filled and 50% states are vacant.

3.2.3 : Qualitative study: Fermi level in metals

In a metal the conduction electrons are not bound to individual atoms. They are free to roam within the entire crystal. (This is what allows metals to conduct electricity.) However, the states the electrons can occupy are quantized. If we cool a metal down, the electrons would settle into the available lowest energy states. However, due to the Pauli exclusion principle, each allowed quantum state can only be occupied by one electron. Once the lowest energy state is filled, the next electron has to drop into the

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second lowest energy state, and so on. The last state that would be occupied (at zero temperature) is the Fermi level.

3.2.4 : *Fermi energy for electron gas in metals*

Metals are characterized by the presence of a good number of free electrons. These electrons move about at random within the metals. While moving the free electrons collide among themselves and also encounter with the fixed ion cores. Such behavior of the free electrons is similar to that of molecules of a gas. Thus metals can be treated as electron gas. Since the electrons have half-integral spin angular momenta, they obey
Pauli's exclusion principle and hence they follow F-D statistics.

Let us consider an electron gas consisting of N electrons occupying volume V. If N is very large, the spacing between two successive energy levels becomes very small making the energy levels almost continuous. Then if the energy of the electrons ranges between E to E+dE, the number of degenerate states g_i should be replaced by g(E)dE and the total number of electrons N_i in these states should be replaced by N(E)dE in the distribution function given by the following equation. Thus the total number of electrons in the electron gas having energy between E to E+dE can be as

$$N(E)dE = \frac{g(E)dE}{\exp\left(\frac{E_i - E_F}{kT}\right) + 1}$$

Since the electrons have *two* allowed values of spin quantum number ($m_S = \pm \frac{1}{2}$), the total number of their allowed states between energy for the energy range E to E+dE can be written as

$$g(E)dE = 2 \times \frac{1}{h^3}(4\pi V \sqrt{2E}\, m^{\frac{3}{2}})dE$$

Hence the density of states g(E) for a Fermionic gas is given by

$$g(E)dE = \frac{1}{h^3}(4\pi V \sqrt{E}\, 2m^{3/2})dE$$

which shows that g(E) depends only on E for a single type of fermionic gas kept in a fixed volume V.

It is obvious that at T = 0K, all the single-particle states upto energy E_F are filled up. Thus at T = 0K,

$$N(E)dE = \frac{g(E)dE}{e^{-\infty} + 1}$$

$$= g(E)dE \quad [e^{-\infty} = 0]$$

i.e., total number of electrons is equal to the total number of single-particle energy states, hence

$$N = \int_0^{E_F} N(E)dE$$

E_F

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$$= \int_0^{} g(E)dE$$

$$= \frac{4\pi V}{h^3}(2m)^{3/2}\int_0^{E_f} E^{1/2}\,dE$$

$$= \frac{4\pi V}{h^3}(2m)^{\frac{3}{2}}\frac{2}{3}(E_F)^{3/2}$$

$$= \frac{8\pi V}{3h^3}(2m)^{\frac{3}{2}}(E_F)^{3/2}$$

which is the expression for the *total number of electrons* in the metal at T = 0K. Therefore,

$$E_F=\left(\frac{3N}{8\pi V}\right)^{2/3}\frac{\hbar^2}{2m}$$

which is the expression for *Fermi energy* of the electrons in the metal.
If n = N/V denotes the concentration of the electrons in the metal, the Fermi energy of the electrons in the metal is

$$E_F=\left(\frac{3n}{8\pi}\right)^{2/3}\frac{h^2}{2m}$$

which shows the Fermi energy of the electrons depends solely on their *concentration*.

3.2.5 : *Total energy at absolute zero temperature:*

The total energy of electrons at absolute zero (T = 0K) is given by

$$E_0 = \int_0^{E_F} EN(E)dE$$
$$= \frac{4\pi V}{h^3}(2m)^{3/2}\int_0^{E_F} E^{1/2}.E\,dE$$
$$= \frac{4\pi V}{h^3}(2m)^{3/2}\int_0^{E_F} E^{3/2}\,dE$$
$$= \frac{4\pi V}{h^3}(2m)^{\frac{3}{2}}\frac{2}{5}[E_F]^{5/2}$$
$$= \frac{4\pi V}{h^3}(2m)^{\frac{3}{2}}\frac{2}{5}[E_F]^{3/2}E_F\frac{3}{3}$$
$$= \frac{8\pi V}{3h^3}(2m)^{\frac{3}{2}}\frac{3}{5}[E_F]^{3/2}E_F$$
$$= \frac{3}{5}NE_F$$

which shows *quantum effect* because, *classically the total energy of a system at absolute zero is nothing but zero*.
The average energy per electron at T = 0K can be written as

$$\langle E_0\rangle=\frac{E_0}{N} = \frac{3}{5}E_F$$

3.2.6 : Fermi Level in Intrinsic and Extrinsic Semiconductors

In an intrinsic semiconductor, n = p. If we use the band-symmetry approximation, which assumes that there are equal number of states in equal-sized energy bands at the edges of the conduction and valence

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bands, n = p implies that there is an equal chance of finding an electron at the conduction band edge as there is of finding a hole at the valence band edge:

$$f(E_C) = 1 - f(E_V)$$

The Fermi level E_F must be in the middle of the bandgap for an intrinsic semiconductor, as seen in Figure given below. In fact, this level is called the "intrinsic Fermi level" and shown by E_i:

$$E_i = E_C - E_g/2 = E_V + E_g/2$$

Where E_g is the bandgap energy.

For an n-type semiconductor, there are more electrons in the conduction band than there are holes in the valence band. This also implies that the probability of finding an electron near the conduction band edge is larger than the probability of finding a hole at the valence band edge. Therefore, the Fermi level is closer to the conduction band in an n-type semiconductor:
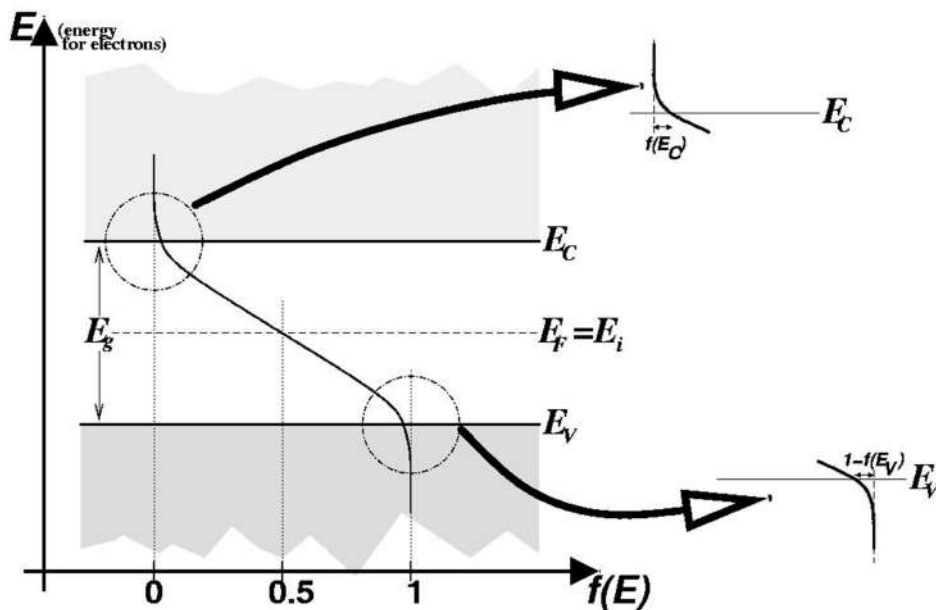
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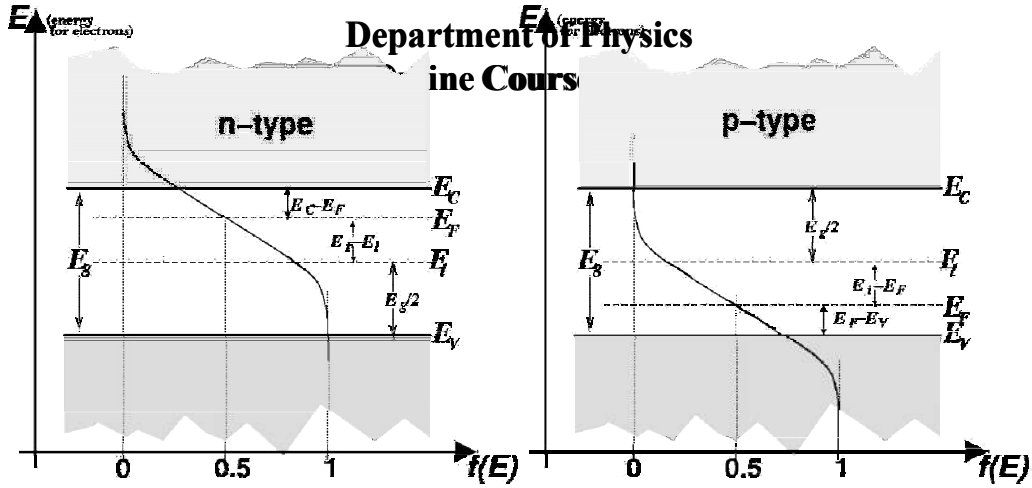
Figure :The extrinsic Fermi levels. The curvature of the Fermi-Dirac distribution function is exaggerated to emphasize the difference between f(E_C) and $1 − f(E_V)$ in the n-type and p-type materials.

Material type	Relationships
n-type	$E_F > E_i$ $E_C − E_F = \dfrac{E_g}{2} − (E_F − E_i)$
p-type	$E_F < E_i$ $E_F − E_V = \dfrac{E_g}{2} − (E_i − E_F)$

Table

For a p-type semiconductor, there are more holes in the valence band than there are electrons in the conduction band. This also implies that the probability of finding an electron near the conduction band edge is smaller than the probability of finding a hole at the valence band edge. Therefore, the Fermi level is closer to the valence band in an n-type semiconductor.

The following relationships summarize these last points:

$$n-\text{type}: f(E_C) > (1 - f(E_V)) \quad \Rightarrow \quad |E_C - E_F| < |E_F - E_V| \Rightarrow E_F > E_i$$

$$p-\text{type}: f(E_C) < (1 - f(E_V)) \quad \Rightarrow \quad |E_C - E_F| > |E_F - E_V| \Rightarrow E_F < E_i$$

Figure above shows the situation for extrinsic materials.

Finally, since the bandgap energy is a constant, with $E_g = E_C - E_V$, the relationship between E_g, E_i, E_C, E_V and E_F can be deduced also by looking at the above Figure. The Table shown summarizes these relationships.

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Module 4: Storage and display Devices (4L)

Different storage and display devices-Magnetic storage materials, Hard disc (examples related to computers compared with semiconductor storage viz. Pen drive), Optical storage-CD, DVD, Blu-ray Disc.

Operation and application of CRT, Liquid crystal display (LCD), LED, Plasma display, Thin film transistor display).   4L

Reference & Text: Storage devices & Applications

1 Introduction to solid state physics-Kittel (TMH)
2. Solid State Physics- Ali Omar (Pearson Eduction)
3. Solid state physics- S. O. Pillai
4. Solid State Physics-A. J. Dekker (Prentice-Hall India)
5. Materials Science-Raghavan

Lesson plan for Storage and display devices:

Module No	Lecture No	Topic	Application	Reference Book
4	1	To know about magnetic storage materials, Hard disc (examples related to computers compared with semiconductor storage viz. Pen drive)	Computer Storage Devices	1 Introduction to solid state physics-Kittel 2. Solid State Physics- Ali Omar 3. Solid state physics- S. O. Pillai 4. Solid State Physics-A. J. Dekker 5. Materials Science-Raghavan
4	2	Discussion on Pen drives, Optical storage devices - CD, DVD, Blu-ray Disc		
4	3	Qualitative discussion on operation and application of CRT, Plasma display	Display devices	
4	4	To know about Liquid crystal display (LCD), LEDs and Thin film transistor (TFT) display		

4.01: Any Computer system has two basic storage units.

1. Primary Storage or Main Memory

The main memory, also called random access memory (RAM) is the work area of the computer which stores program instructions or part of data for immediate needs. The storage capacity of RAM is limited. A typical modern computer can have a RAM size of upto 8GB. It is the volatile memory of the computer and when the power goes, the contents stored in RAM are lost.

2. Secondary Storage

The secondary storage devices are used to store programs and data on a permanent basis. Their storage capacity is much higher compared to main memory of the computer. Secondary Storage devices accept data or program instructions from the processor, retain them and then write them back to the processor as and when needed.

Now in secondary storage, there are several different ways of storing information in the computer. Out of them, the three main categories of storage devices are :
   a. Magnetic
   b. Semiconductor.
   c. Optical
The examples of secondary storage devices are Floppy disk, Hard Disk, Magnetic tapes, Pen drives or jump drives, Compact Disks (CD), DVDs, Blu-ray Disks etc.

   a. **4.02: Magnetic Storage Devices**

Computer systems need to store data in digital format. One of the most widely used types of digital data storage is magnetic storage where any type of data storage is done using magnetized medium. Most common magnetized media currently used in computer systems include floppy disks and hard disk drives though magnetic tape was initially used for the storage purpose. The basic approach to magnetic data storage, however, is very similar for the different types of media.

Magnetic Tape

Working of magnetic tape is based on analogue recording where remanant magnetisation of a given material depends on the magnitude of the applied field. The magnetic tape, in its blank form being initially demagnetised during recording runs at a constant speed. The writing head magnetises the tape with current proportional to the signal. A magnetisation distribution is achieved along the magnetic tape. Finally, the distribution of the magnetisation can be read out, reproducing the original signal. The magnetic tape is typically made by embedding magnetic particles in a plastic binder on polyester film tape. The commonly used magnetic particles are iron oxide particles or chromium oxide. Though they provide unlimited storage capacity they suffer from a very serious problem. Since the data stored in them is sequential in nature, retrieval of data takes a very long time. These are used for archival backup storage.

Instead of creating a magnetisation distribution in analog recording, digital recording only needs two stable magnetic states, on the hysteresis loop. Examples of digital recording are floppy disks and hard disk drives (HDDs).

Floppy Diskette

The floppy diskette is a direct access storage device although its capacity is much less than a hard disk. The diskette is made out of a flexible plastic material. This base is coated with an iron-oxide recording material. Data is recorded as tiny magnetic spots. The surface is divided into tracks and sectors, same as in a hard disk. The number of tracks on a diskette depends on the recording density. The size of each sector is fixed (512 bytes). Data is stored on both sides of the diskette. There is one head per surface in the floppy drive for reading/writing data on the diskette. The circular plastic disk is enclosed within a smoothly lined, protective square jacket to protect it from dust and scratches. The standard size available nowadays is: 3.5 inch.

Hard Disk & Hard Drive

The primary storage device for a personal computer is a hard drive which are specific kind of storage devices that can not be removed and are fixed inside the computer. That is why these are also called as fixed disks and store programs permanently. They are composed of platters that are typically 3½ inches in diameter with storage capacities ranging from 60 gigabytes to over 2 terabytes. The storage capacity of the disks that are used these days are having gigabytes of storage and these are faster in comparison to Floppy disks.

Here data is written to a hard drive using magnetism and is read by the computer as a combination of 1s or 0s, depending on whether or not there is a piece of data in a particular location. Data is read from the hard drive by means of a read-write head on a mechanical arm that scans the surface of the disk for the presence or absence of magnetism, or 1s and 0s.

Hard Disk & Drive

Magnetic storage is a form of non-volatile storage. This means that the data is not lost when the storage device is not powered. This is in contrast to volatile storage, which is typically used for the main memory of a computer system. Volatile storage requires a constant power supply - when a computer system is turned off, the data is lost.

For reliable storage of data, the recording material needs to resist self-demagnetisation, which occurs when the magnetic domains repel each other. Older hard disk drives used iron oxide as the magnetic material, but current disks use a cobalt-based alloy.

Advantage : Magnetic storage is widely used because it is relatively cheap in comparison with other storage technologies. Magnetic storage is read-write, which makes it possible to re-use the storage capacity over and over again by deleting older data. The storage capacity is also very large, making it attractive for storing very large amounts of data.

The major limitation of magnetic storage is that accessing the data is quite slow. As a result, most computer systems use magnetic storage for non-volatile storage of large amounts of data (typically in a form of a hard-disk drive) but a different type of storage for system memory, such as read-only memory (RAM), which is much smaller but can be accessed much faster.

4.3 : Semi conductor State Storage

Semi conductor storage devices, in the form of flash drives and USB drives, have become very popular these days as a way to transport data from one device to another. Due to this they are considered to be better than the other conventional storage devices like floppy disks or CD ROMs.They are also quieter during usage and require less energy. These devices store data in durable, erasable, lower-power chips or series of transistors using electrical current to represent the data. A 1 bit is represented by a transistor that accepts electrical current while a 0 bit is represented by one that does not.

Pen drive or commonly called as USB (Universal Serial Bus) flash drive is a popular data storage media having a storage capacity of 512 GB. This is a kind of **memory** card that can be plugged into

the computers USB port and they are considered to be the best because they are faster, smaller and have longer life span. It is known as Pen drive mainly because of its size. They come in a wide variety of shapes, but the most common is the rectangular and flat shape. This small external hard drive does not require any outside power source for its operation because they get the power from the computer they are plugged in.

Usually, a pen drive consists of a **flash memory** integrated with a USB interface. The great advantage of such a device is that they are rewritable and removable. Today, pen drive is supported by modern operating systems like Windows, Mac OS X, Linux etc. Pen drive or USB flash drive are supported with **USB standards** like USB 1.0 (12Mbps), USB 2.0 (480Mbps) and USB3.0 (4.8 Gbps).

Inside a Pen drive there are following parts.
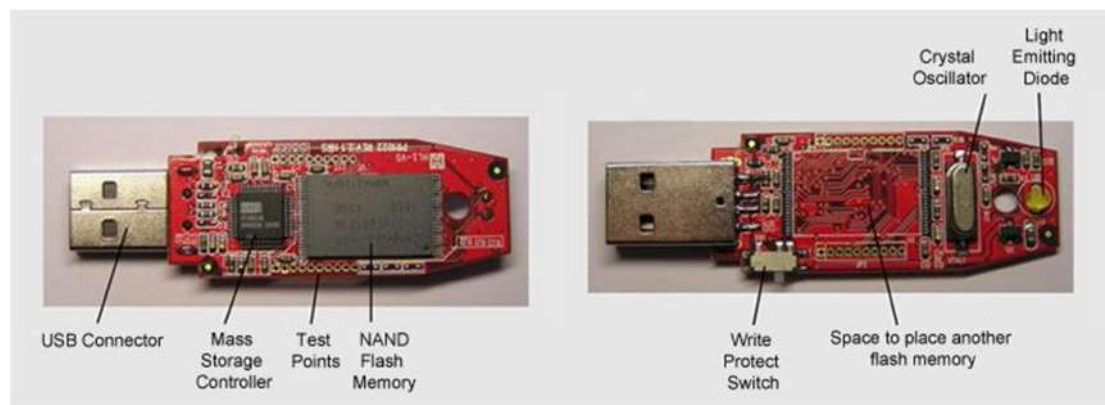
1. USB Connector: It acts as an interface between the NAND flash memory chip and the computer to which the pen drive is plugged. The pen drive utilize the power from computer via USB connector.

2. USB mass storage controller (or the controller chip): This chip helps to retrieve the information from the pen drive and it also helps in recording/reading the information on the NAND flash memory. It is basically a **microcontroller** with on-chip RAM and ROM.

3. Test points: They are electric pins used to stimulate and exercise the pen drive during assembly process.

4. NAND flash memory chip: Helps in the storage of files and all data. Also it allows the erasing the information so that we can delete files and put new files into the pen drive.

5. Crystal Oscillator: It is a piece of quartz crystal designed to vibrate at a very particular frequency.

6. LED: Used to indicate if the flash drive is working properly.

7. Write-protect switch: An optional component used to safeguard the information saved on the flash drive.

8. Space to put a second NAND flash memory chip: Additional slot to put another memory chip which can increase the storage capacity.

Applications

- Data Transport

Pen drive is commonly used to store and transport files like pictures, videos, any private documents etc.

- Security for the storage of Data, Application and Other software Files

The issue of data security and information security is very essential since the pen drive are used in many outside environments. For providing security, today many encryption systems are used.

- Computer Forensics and Law Enforcement

USB flash drive is used to carry the Computer Online Forensic Evidence Extractor (COFEE) application. COFEE is a set of applications designed to search and extract digital evidence on computers confiscated from suspects.

- Boot Operating Systems

Today most PC firmware helps in permitting booting from a USB drive which helps to provide the launch of an OS from a bootable pen drive.

- Operating system installation

Many operating systems can be installed from the pen drive. Some of the operating systems are Windows7, Windows 8, Linux, Mac OS etc.

- Backup

Today pen drives are used as a backup. By using the pen drive backup data is updated to the drive.

Conclusion

Pen drive or USB flash drive is a data storage device. As of the year 2013, pen drive with storage capacity of 1TB is available. Even though they have serious disadvantage of being affected by viruses very easily, its advantages make them to be used at a rapid pace with the increasing advancement in technology.

4.4 : Optical Storage

Rather than using magnetic media, optical storage uses microscopic light spots to represent the 1 bit and dark spots to represent the 0 bit. As opposed to hard drives, optical storage devices are a single platter, 4.7 inches in diameter and 0.5 inches thick. Variations in spots are detected by specialized lasers similar to how magnetic storage is read.

There are primarily three types of optical storage devices: CDs or compact discs, DVDs or digital video discs, and BDs or Blu-ray discs. They differ in the amount of data they can hold.

CDs can store about 700 megabytes of data and are most often used these days for distributing software. DVDs hold around 4.7 gigabytes of data used for movies while Blu-ray disks have five times the storage of DVDs and are used primarily for high-definition movies.

An optical storage device is written and read with a laser. It is strong and can handle temperature fluctuations much better than magnetic media. Because the floppy was so inexpensive at a time, it took several years before the optical drives became affordable to the general and small business consumer. It actually took until CD players became common in homes and cars for the playing of music for CDs to come down in price enough for more use by consumers.
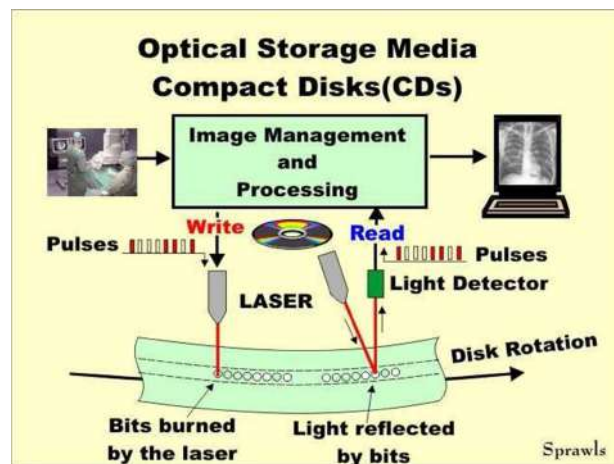
It was found that by using optical means, large data storing devices can be made which in turn gave rise to the optical discs. The very first application of this kind was the Compact Disc (CD) which was used in audio systems.

Sony and Philips developed the first generation of the CDs in the mid 1980s with the complete specifications for these devices. With the help of this kind of technology, the possibility of representing the analogue signal into digital signal was exploited to great level. The DVD appeared after the CD-ROM had become widespread in society.

The third generation optical disc was developed in 2000–2006, and was introduced as Blu-ray Disc. First movies on Blu-ray Discs were released in June 2006. Blu-ray eventually prevailed in a high definition optical disc format over a competing format, the HD DVD.

CD-ROM

Compact disk is read-only memory optical disks have a very large storage density and the access time is relatively low.

Digital Versatile Disc (DVD)

Digital Versatile Disk is in general optical discs with same overall dimension of CDs but much higher capacity. These can store at least 7 times more data than CD ROM.

Digital video discs began being issued for consumer-released movies. A single-sided DVD holds 4.7 gigabytes (GB) of data, so a normal, not overly-computerized two-hour movie will fit.

First-generation

Initially, optical discs were used to store music and computer software. The Laserdisc format stored analog video signals for the distribution of home video, but commercially lost to the VHS videocassette format, due mainly to its high cost and non-re-recordability; other first-generation disc formats were designed only to store digital data and were not initially capable of use as a digital video medium.

Most first-generation disc devices had an infrared laser reading head. The minimum size of the laser spot is proportional to the wavelength of the laser, so wavelength is a limiting factor upon the amount of information that can be stored in a given physical area on the disc. The infrared range is beyond the long-wavelength end of the visible light spectrum, so it supports less density than shorter-wavelength visible light. One example of high-density data storage capacity, achieved with an infrared laser, is 700 MB of net user data for a 12 cm compact disc.

Other factors that affect data storage density include: the existence of multiple layers of data on the disc, the method of rotation (Constant linear velocity (CLV), Constant angular velocity (CAV), or zoned-CAV), the composition of lands and pits, and how much margin is unused is at the center and the edge of the disc.

- Compact Disc (CD) and derivatives

4.05: Second-generation

Second-generation optical discs were for storing great amounts of data, including broadcast-quality digital video. Such discs usually are read with a visible-light laser (usually red); the shorter wavelength and greater numerical aperture allow a narrower light beam, permitting smaller pits and lands in the disc. In the DVD format, this allows 4.7 GB storage on a standard 12 cm, single-sided, single-layer disc; alternatively, smaller media, such as the DataPlay format, can have capacity comparable to that of the larger, standard compact 12 cm disc.

- DVD and derivative
-

Module 4.06: Third-generation

Third-generation optical discs are in development, meant for distributing high-definition video and support greater data storage capacities, accomplished with short-wavelength visible-light lasers and greater numerical apertures. Blu-ray Disc and HD DVD uses blue-violet lasers and focusing optics of greater aperture, for use with discs with smaller pits and lands, thereby greater data storage capacity per layer.

- Blu-ray Disc (up to 400 GB - experimental)

4.7 : Display Devices

Present day computer technology is going to see major advances in sophisticated 3-D modelling and image processing; Even graphics capabilities would be available to the average user at a reasonable cost. To make this, an ultra high resolution monitors will be required. There are different display systems like cathode ray tubes (CRTs), liquid crystal displays (LCDs), plasma displays and light emitting diodes (LEDs) available in the present technology, are discussed in order as given below.

1. **Cathode Ray Tube (CRT) : Principle of working**

The cathode ray tube was the workhorse of text and video display technology for several decades until being replaced by plasma, liquid crystal (LCD) and solid-state devices such as LEDs. It is a specialized vacuum tube in which images are produced when an electron beam strikes a phosphorescent surface. Most desktop computer displays the output in a standard composite video signal making use of **CRTs.** The working of CRT depends on movement of an electron beam which moves back and forth across the back of the screen.

A cathode ray tube consists of several basic components- the cathode, control grid, deflecting plates and screen. A simple CRT is shown below.

Cathode

The source of the electron beam is the electron gun located in the narrow, cylindrical neck at the extreme rear of a CRT which produces a stream of electrons through thermionic emission. Actually in an electron gun, a metal plate-the cathode , is heated by a small filament wire connected to a low voltage. The conduction electrons are free to move in the metal and as the metal is heated, some of them gain sufficient kinetic energy to escape from the metal surface. If the hot metal plate is in a vacuum, then the evaporated electrons are free to move which can be pulled away from the hot surface of the plate by putting a positive electrode (anode) nearby. The accelerating anode has a small

hole at its center and is maintained at a high potential, which is of positive polarity. The order of this voltage is 1 to 20 kV, relative to the cathode. This potential difference creates an electric field directed from right to left in the region between the accelerating anode and the cathode. Electrons pass through the hole in the anode travel with constant horizontal velocity from the anode to the fluorescent screen. The electrons strike the screen area and it glows brightly.

Now moving electron behaves like a tiny magnet, and it can interact with an external magnetic field and is deflected by the field which when reversed, the beam of electrons is deflected in the opposite direction.

The Control Grid

The control grid regulates the brightness of the spot on the screen. By controlling the number of electrons the focusing anode ensures that electrons leaving the cathode in slightly different directions are focused down to a narrow beam and all arrive at the same spot on the screen. The whole assembly of cathode, control grid, focusing anode, and accelerating electrode is called the electron gun.
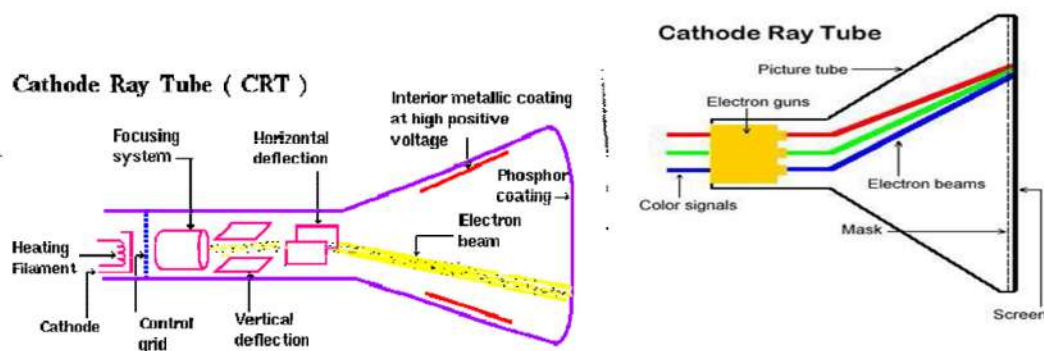
Deflecting Plates

Two pairs of deflecting plates allow the beam of electrons. An electric field between the first pair of plates deflects the electrons horizontally, and an electric field between the second pair deflects them vertically, the electrons travel in a straight line from the hole in the accelerating anode to the centre of the screen when no deflecting fields are present, where they produce a bright spot..

Screen

Usually, A CRT has a fluorescent screen to display the output signal whose operation is very simple. Screen is coated with special type of fluorescent material. Fluorescent material absorbs its energy and re-emits light in the form of photons when electron beam hits the screen. When it happens some of them bounces back which are called secondary electrons. They must be absorbed and returned back to

cathode, if it is not so they accumulate near screen and produce space charge or electrons cloud. To avoid this, aquadag coating which is a water-based colloidal graphite coating, .is applied on funnel part of CRT from inside.

Now a cathode ray tube consists of one or more electron guns along with internal electrostatic deflection plates and a phosphor target. CRT has three electron beams – one for each of Red, Green, and Blue. Thus CRT produces the three colour images which are primary colours. In every monitor device the entire front area of the tube is scanned repetitively and systematically in a fixed pattern called a raster. An image (raster) is displayed by scanning the electron beam across the screen. The phosphor's impacts begins to fade after a short time, the image needs to be refreshed continuously.

Advantages of CRT

The use of CRT technology has quickly declined since the introduction of LCDs but they are still unbeatable in certain ways. CRT monitors are widely used in a number of electrical devices such as computer screens, television sets, radar screens, and oscilloscopes used for scientific and medical purposes. Brightness, contrast ratio, high image quality, speed and resolution were the main high standard specifications that CRTs were satisfied.

But the display device in a CRT monitor is a cathode ray tube which is inherently bulky and power-thirsty. But in the last two decades there was a tremendous growth in small portable applications which required the necessary adjustment of the display technology to them. The large depth of the CRTs was the main disadvantage for preventing them to be used in these kinds of applications.

Flat Panel Displays seem to be the most attractive solution to this problem. The first successfully established flat panel technology was the **plasma displays**, which demonstrated to be of larger size and higher image quality compared to the CRT technology where plasma screens emit light by itself, rather than relying on a backlight.

4.8 : Plasma Display : Its working

Two plates of glass are taken between which millions of tiny cells containing gases like xenon and neon are filled. Electrodes are also placed inside the glass plates in such a way that they are positioned in front and behind each cell. The rear glass plate has with it the address electrodes in such a position that they sit behind the cells. The front glass plate has with it the transparent display electrodes, which are surrounded on all sides by a magnesium oxide layer and also a dielectric material. They are kept in front of the cell.
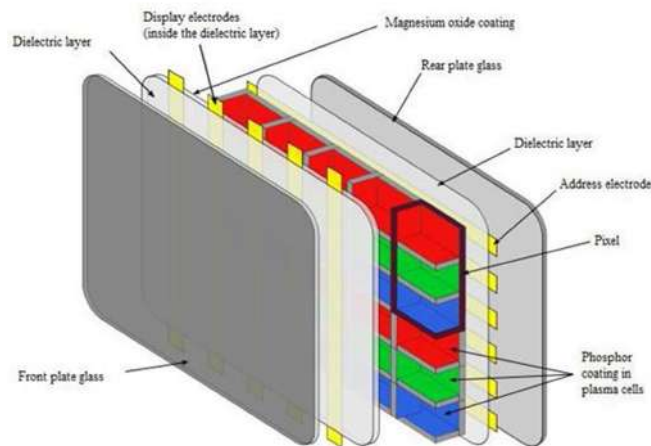
Working of Plasma Display

When a voltage is applied, the electrodes get charged and cause the ionization of the gas resulting in plasma. This also includes the collision between the ions and electrons resulting in the emission of photon light.

The state of ionization varies in accordance to colour plasma and monochrome plasma. For monochrome plasma panel a low voltage is applied between the electrodes – even after the ionizing voltage is removed. This type of panel has inherent memory and does not use phosphors. To obtain colour plasma, the back of each cell has to be coated with phosphor. The ultraviolet photons emitted by the plasma excite these phosphors to give off coloured light in the visible range. The operation of each cell is thus comparable to that of a fluorescent lamp. Every pixel is made up of three separate sub pixel cells, each with different coloured phosphors-the red, green and blue. These colours blend together to create the overall colour of the pixel.

Advantages of Plasma Display

▪ The slimmest of all displays

- Very high contrast ratios [1:2,000,000] and resolution
- Weighs less and less bulky than CTR's.
- Can be placed even on walls.
- High clarity and hence better colour reproduction.
- Has a life span of about 100,000 hours.

Disadvantages of Plasma Display

- Cost is much higher compared to other displays.
- Energy consumption is more.
- Produces glares due to reflection.
- These displays are not available in smaller sizes than 32 inches
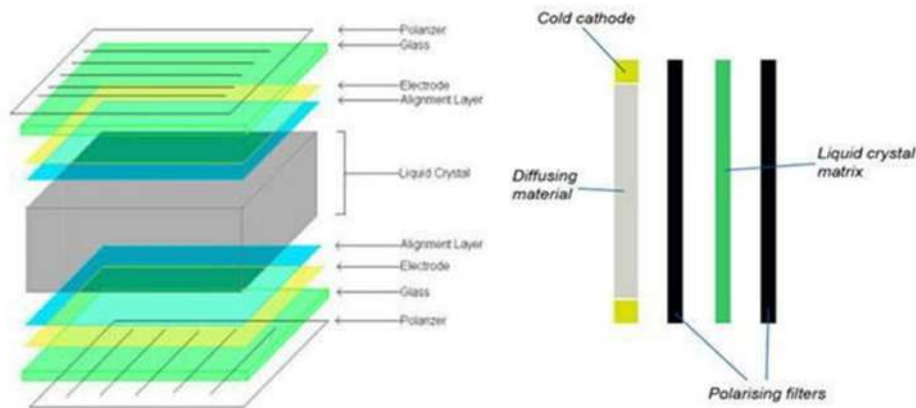- plasma display generate large amount of heat.

The first colour plasma display was introduced in the year 1992 by the Fujitsu company. This technology began to overrule the CRT revolution for the coming years. However, the problem with the integration of plasma displays in small portable applications still exists. Finally, the inroad of the thin-film transistors liquid crystal displays (TFT-LCD), in late 1990's, was a milestone in the displays industry and technology and the demand for Plasma TV became lesser. As the same configuration for a lesser price is available, the sale of Plasma TV became lesser.

4.9 : Liquid Crystal Display (LCD)

Liquid Crystal Display is one of the most popular display technologies currently. LCD monitors are lightweight, compact, occupy less space, consume low power and are available in a reasonable price. Currently there are two types of LCD technology in use – Active matrix LCD technology or TFT and Passive matrix technology. The TFT technology is more reliable with better image quality while the passive matrix technology has a slower response and gradually becoming outdated.

As the name indicates, liquid crystals are the key elements of the display screen. There is a display controller in the monitor which receives the display signals from the video adaptor in the motherboard. The display controller controls two things – the electric signals to the liquid crystals and the back light. Structure of an LCD is shown below.

Each pixel of an LCD typically consists of a layer of molecules aligned between two transparent electrodes, and two polarizing filters. Actually LCD configured to place a liquid crystal in the two parallel sheets of glass, behind which the Cold Cathode Fluorescent Lamp is designed as a backlight. The liquid crystals used in the LCD are Twisted Nemantic (TN), a

Polarizer
Glass
Electrode
Alignment Layer

Cold cathode

Liquid Crystal

Liquid crystal matrix

Diffusing material

Alignment Layer
Electrode
Glass
Polarizer

Polarising filters

 a type of liquid crystals that are twisted at 90° with the surface. In this state, crystals allow the light to pass through the polarizer but on applying a voltage, they get untwisted and block the light to passing through the polarizer. The display controller starts the backlight that passes through the first piece of the glass. At the same time the display controller also send the electrical currents to the liquid crystal molecules to align and allowing the varying level of light to pass through the second piece of glass, forming the desired picture on the screen. In colour monitors, each pixel is made of three liquid crystal cells fronted with red, green and blue filters. The light passing through the filtered screen forms the colour what are seen on the monitor. A wide range of colours are formed by varying the intensity of coloured pixels.

LCD Monitor

An active matrix liquid crystal display (AMLCD) is a type of flat panel display, currently the overwhelming choice of notebook computer manufacturers, due to light weight, very good image quality, wide colour gamut, and response time. The most common example of an active matrix display contains, besides the polarizing sheets and cells of liquid crystal, a matrix of thin-film transistors (TFTs) to make a TFT LCD.

Thin Film Transistor Liquid Crystal Display

At the beginning, when LCDs were used in calculators, watches and small sized displays, direct and passive matrix addressing were the applicable addressing methods. As the size, resolution and information content of the displays were increased, the number of the pixels array was, also, increased leading the existing addressing methods to become non-applicable. A solution to this problem was proposed as a switch TFT which was added at each pixel of the display matrix and in this way the pixels were controlled independently with the use of the external driving voltages. This addressing method is called Active Matrix and the displays that used this method are called Active Matrix Liquid Crystal Displays (AMLCDs) or TFTs.

TFT Display

The display device in a TFT monitor is a flat array of Thin Film Transistors which makes the TFT monitors much smaller in size and also less power consuming. Now a thin-film transistor is a special kind of field-effect transistor made by depositing thin films of an active semiconductor layer as well as the dielectric layer and metallic contacts over a supporting (but non-conducting) substrate. A common substrate is glass, because the primary application of TFTs is in liquid-crystal displays. This differs from the conventional transistor, where the semiconductor material typically is the substrate, such as a silicon wafer.

Manufacture

TFTs can be made using a wide variety of semiconductor materials. A common material is silicon. The characteristics of a silicon-based TFT depend on the silicon's crystalline state, the semiconductor layer can be either amorphous silicon, microcrystalline silicon, or it can be annealed into polysilicon. Other materials which have been used as semiconductors in TFTs include compound semiconductors such as cadmium selenide, or metal oxides such as zinc oxide or hafnium oxide.

Applications

TFT technology can be used to give one of the clearest pictures of any flat screen display and it uses much less electricity than older screens. TFT displays are very fragile because they are made as thin and light as possible but this means they need far less space. TFT-LCDs were rapidly grown and dominated the displays industry, especially in small portable applications. They can be used in an extremely wide range of our everyday life products, like mobile phone applications, ATMs, PDAs, navigation systems, notebook PCs and home applications, such as wide screen TVs. The most beneficial aspect of TFT technology is its use of a separate transistor for each pixel on the display. Because each transistor is small, the amount of charge needed to control it is also small. This allows for very fast re-drawing of the display.

4.10   : LED Display

LED display refers to the light emitting elements which is composed by the LEDs. LED , the light emitting diode array is directly used as pixels to emit red, green, and blue light, thereby forming coloured images, such as traffic lights, outdoor big screen.

Now a **light-emitting diode** (**LED**) is a semiconductor diode that emits incoherent narrow-spectrum of light when electrically biased in the forward direction of the p-n junction. This effect is a form of electroluminescence. An LED is usually a small area source. The colour of the emitted light depends on the composition and condition of the semi conducting material used, and can be infrared, visible, or near-ultraviolet. An LED can be used as a regular household light source.

In silicon or germanium diodes, the electrons and holes recombine by a non-radiative transition which produces no optical emission, because these are indirect band gap materials. The materials used for an LED have a direct band gap with energies corresponding to near-infrared, visible or near-ultraviolet light. LEDs are usually built on an n-type substrate, with an electrode attached to the p-type layer deposited on its surface.

So LED consists of a chip of semi conducting material impregnated or doped with impurities to create a p-n junction. When this p-n junction diode is forward biased, carriers are injected across the junction to establish excess carriers above their thermal equilibrium values. These excess carriers recombine and release e.m. energy. The wavelength of the light emitted, and therefore its colour, depends on the band gap energy of the materials forming the p-n junction.

In the case of GaAs, the energy appears in the form of infra red radiation. For the alloy semi conductor, GaAs-P, the energy appears is in the form of visible light. the p-n junction diode constructed with such semi conductors is called the light emitting diode (LED). Here we get optical energy from the biasing electrical energy. The electrons that are injected into the p side make a downward transition from conduction band to the valence band and recombine with holes , emitting

photon with energy $h\nu = E_g$, corresponding emission wavelength is so given by $\lambda = hc / E_g$, the symbols have their usual meaning.

Diodes built with GaAs-P are most commercially available because of lower cost and easy fabrication. These LEDs are used for in the manufacture of signals and displays. The infra red LED is a potential source for optical fibre communication.

The LED display should be precisely called as "LED-backlit LCD monitor", the principle of which is converting the traditional CCFL into LCD backlight source is into LED. So far, the advantages of LED backlit display is in the theoretical stage, the display is not as good as what the display market advocated . The main advantages are: energy saving, ultra-thin, light leakage control is better.

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Narula Institute of Technology (An Autonomous Institute)
Gurunanak Institute of Technology (An Autonomous Institute)
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Module 5: Physics of Nanomaterials (3L)

Reduction of dimensionality, properties of nanomaterials, Quantum wells (two dimensional), Quantum wires (one dimensional), Quantum dots (zero dimensional); Application of nanomaterials (CNT, grapheme, electronic, environment, medical).   3L

Department of Physics
Online Courseware

Lesson plan for Physics of Nanomaterials

Module No	Lecture No	Topic	Application	Reference Book
Module 5:Physics of Nanomaterials	1	Reduction of dimensionality, properties of nanomaterials, Quantum wells (two dimensional)	Bacterial sensors Bending of the wings of morphing aircraft Boron or gold doped nanotubes to trap oil spills, include smaller transistors Chemotherapy drugs Graphene sheets as electrodes in ultracapacitors nanotube-polymer nanocomposite uses to form a scaffold which speeds up replacement of broken bones	Nanostructure and Nanomaterials, B.K. Parthasarathy Introduction to Nanotechnology, B.K. Parthasarathy Essentials of Nanotechnology, RishabhAnand Nanomaterials Handbook (Advanced Materials and Technologies)- YuryGogotsi (Editor)
	2	Quantum wires (one dimensional), Quantum dots (zero dimensional); Quantum size effect and Quantum confinement		
	3	Carbon allotropes. Application of nanomaterials(CNT, grapheme, electronic, environment, medical).		

Module 5: Physics of Nanomaterials

5.1 Reduction of dimensionality

What is Nanomaterial?

Nanoscale: generally refers to the size scale of 1 –100 nm in at least one dimension.

$$1 \text{ nanometer (nm)} = 10^{-9} \text{ m}$$

Nanomaterials or the **Nanoparticles** are the set of particles or the substances where atleast one dimension is less than approximately 100nm.

Note:Richard Feynman is known as the father of nanotechnology.

What are Low-Dimensional Structures?

When one or more of the dimensions of a solid are reduced sufficiently, its physicochemical characteristics notably depart from those of the bulk solid. With reduction in size, novel electrical, mechanical, chemical, magnetic, and optical properties can be introduced. The resulting structure is then called a low-dimensional structure (or system). The confinement of particles, usually electrons or holes, to a low- dimensional structure leads to a dramatic change in their behaviour and to the manifestation of size effects that usually fall into the category of quantum-size effects. The low dimensional materials exhibit new physicochemical properties not shown by the corresponding large-scale structures of the same composition. Nanostructures constitute a bridge between molecules and bulk materials. Suitable control of the properties and responses of nanostructures can lead to new devices and technologies.

Classificationofthenanomaterials:

Classification of Low-dimensional Materials Hence classification of the nanostructured materials and systems essentially depends on the number of dimensions which lie within the nanometer range.

a)Low-dimensional structures are usually classified according to the number of reduced dimensions they have. More precisely, the dimensionality refers to the number of degrees of freedom in the particle momentum. Accordingly, depending on the dimensionality, the following classification is made:

Three-dimensional (3D) structure or bulk structure: No quantization of the particle motion occurs, i.e., the particle is free.

Two-dimensional (2D) structure or quantum well: Quantization of the particle motion occurs in one direction, while the particle is free to move in the other two directions.

Examples:discs;platelets;ultrathin films;super lattices; quantum wells; Film Graphene.

One-dimensional (1D) structure or quantum wire: Quantization occurs in two directions, leading to free movement along only one direction.

Examples: Nanorods;Nanofilaments;Nanotubes;quantum wires; nanowires.

Zero-dimensional (0D) structure or quantum dot (sometimes called "quantum box"): Quantization occurs in all three directions.

Examples: Nanoparticles;Nanograins;Nanoshells;Nanocapsulparticles;activatedcarbon; nanoporous silicon;quasi crystals.

Nanostructures	Typical nanoscale dimension
Thin films and quantum wells (two-dimensional structures)	1–1000 nm (thickness)
Quantum wires, nanowires, nanorods and nanopillars (one-dimensional structures)	1–100 nm (radius)
Nanotubes	1–100 nm (radius)
Quantum dots, nanodots (zero-dimensional structures)	1–10 nm (radius)
Porous nanomaterials, aerogels	1–50 nm (particle size, pore size)
Sculptured thin films	10–500 nm

- **N**anomaterials can be metals, ceramics, polymeric materials, or composite materials.

5.2 Properties of Nanomaterials

What has happened when reduced to the nanoscale?

Now lets list out the various properties of the Nanoparticles

Magnetic properties:

1. Magnetic nanoparticles are used in a range of applications like imaging, bioprocessing,refrigeration as well as high storage density magnetic memory media.
2. The large surface area to volume ratio results in a substantial proportion of atoms having different magnetic coupling with neighbouring atoms leading to differing magnetic properties.
3. Bulk gold and platinum are non magnetic but at the nano size they act as magnetic particles.Au nanoparticles become ferromagnetic when they are capped with the appropriate molecules such as thiol.
4. Giant magnetoresistance(GMR) is a phenomenon observed in nanoscale multilayers consisting of strong ferromagnet (Fe,Co,Ni)and a weaker magnetic or non magnetic buffer(Cr,Cu).It is usually employed in data storage and sensing.

<u>Optical properties</u>:

1. In small nano clusters the effect of reduced dimensionality on electronic structure has the most profound effect on the energies of highest occupied molecular orbital (HOMO) which is valence band and the lowest unoccupied molecular orbital(LUMO),essentially the conduction band.

2. The optical emission and adsorption occurs when the transition of the electrons occur between these two states.

3. Semiconductors and many metals show large changes in optical properties such as color, as a function of particle size.

4. Colloidal suspension of gold nano particles have a deep red color which becomes progressively more yellow as the particle size increases.

- Gold spheres of 10-20nm exhibit red color
- Gold spheres of 2-5nm exhibit yellow color.
- Gold spheres of >20nm exhibit purple color

Similarly,

- Silver particles of 40nm exhibit blue color
- Silver particles of 100nm exhibit yellow color
- Prism shaped Silver particles red color.

Other properties which may be affected by reduced dimensionality include photocatalysis, photoconductivity, photoemission and electroluminescence.

<u>Electronic properties:</u>

1. The changes which occur in electronic properties as the system length scale is reduced are related mainly to the increasing influence of the wave-like property of the electrons (quantum mechanical effects) and the scarcity of scattering centres.

2. As the size of the system becomes comparable with the de Broglie wavelength of the electrons, the discrete nature of the energy states becomes apparent once again, although a fully discrete energy spectrum is only observed in systems that are confined in all three dimensions.

3. In certain cases, conducting materials become insulators below a critical length scale, as the energy bands cease to overlap. Owing to their intrinsic wave-like nature, electrons can tunnel quantum mechanically between two closely adjacent nanostructures, and if a voltage is applied between two

nanostructures which aligns the discrete energy levels in the DOS, resonant tunnelling occurs, which abruptly increases the tunnelling current.

4. Conduction in highly confined structures, such as quantum dots, is very sensitive to the presence of other charge carriers and hence the charge state of the dot.

5. These Coulomb blockade effects result in conduction processes involving single electrons and as a result they require only a small amount of energy to operate a switch, transistor or memory element.

6. All these phenomena can be utilised to produce radically different types of components for electronic, optoelectronic and information processing applications, such as resonant tunnelling transistors and single-electron transistors.

Overall

Small size effect (Quantum size effect)Quantum Mechanics

--Contain very small number of atoms(molecules)

--Electromagnetic forces are dominant.

--Wave particle duality. The electrons exhibit wave behavior.

--Quantum confinement.

--Discrete energy levels

5.3 Introduction about Quantum Wells, Quantum Wiresand Quantum Dots

5.3.1 Quantum Wells

The most significant nanostructures required to design nanoelectronic devices are Quantum Wells, Quantum Wires and Quantum Dots. They are the basic building blocks of nanoelctronic devices.

Quantum wells are real-world implementation of the "particle in the box" problem; they act as potential wells for charge carriers and are typically experimentally realized by epitaxial growth of a sequence of ultrathin layers consisting of semiconducting materials of varying composition.A **quantum well** is a potential **well** with only discrete energy values. The classic model used to demonstrate a **quantum well** is to confine particles, which were originally free to move in three dimensions, to two dimensions, by forcing them to occupy a planar region.**quantum well** — flat thin layer of semiconductor material (typically between 1 and 10 nm thick) within which the potential energy of an electron is less than outside the layer, therefore the motion of the electron is limited in one dimension. The motion of the electron perpendicular to the quantum well plane is quantised, and its energy can take on only discrete values.

Two dissimilar semiconductors with different band gaps can be joined to form a heterojunction. The discontinuity in either the conduction or the valence band can be used to form a potential well. If a thin layer of a narrower-band gap material 'A' say, is sandwiched between two layers of a wider-band gap material 'B', then they form a double heterojunction. If layer 'A' is sufficiently thin for quantum properties to be exhibited, then such a band alignment is called a single quantum well. Additional semiconductor layers can be included in the heterostructure, for example a *stepped* or *asymmetric* quantum well can be formed by the inclusion of an alloy between materials A and B.

5.3.2 Quantum Wires

In condensed matter physics, a **quantum wire** is an electrically conductingwire in which quantum effects influence the transport properties. Usually such effects appear in the dimension of nanometers, so they are also referred to as nanowires.

If the diameter of a wire is sufficiently small, electrons will experience quantum confinement in the transverse direction. As a result, their transverse energy will be limited to a series of discrete values. One consequence of this quantization is that the classical formula for calculating the electrical resistance of a wire,

$$R = \rho l/A$$

is not valid for quantum wires (where ρ is the material's resistivity, l is the length, and A is the cross-sectional area of the wire).

Instead, an exact calculation of the transverse energies of the confined electrons has to be performed to calculate a wire's resistance. Following from the quantization of electron energy, the electrical conductance (the inverse of the resistance) is found to be quantized in multiples of $2e^2/h$, where e is the electron charge and h is the Planck constant. The factor of two arises from spin degeneracy.

The importance of the quantization is inversely proportional to the diameter of the nanowire for a given material. From material to material, it is dependent on the electronic properties, especially on the effective mass of the electrons. Physically, this means that it will depend on how conduction electrons interact with the atoms within a given material. In practice, semiconductors can show clear conductance quantization for large wire transverse dimensions (~100 nm) because the electronic modes due to confinement are spatially extended. As a result, their Fermi wavelengths are large and thus they have low energy separations. This means that they can only be resolved at cryogenic temperatures (within a few degrees of absolute zero) where the thermal energy is lower than the inter-mode energy separation.

For metals, quantization corresponding to the lowest energy states is only observed for atomic wires. Their corresponding wavelength being thus extremely small they have a very large energy separation which makes resistance quantization observable even at room temperature.

5.3.3 Quantum Dots:

Quantum dots (QD) are very small semiconductor particles, only several nanometres in size, so small that their optical and electronic properties differ from those of larger particles. They are a central theme in nanotechnology. Many types of quantum dot will emit light of specific frequencies if electricity or light is applied to them, and these frequencies can be precisely tuned by changing the dots' size, shape and material, giving rise to many applications.

In the language of materials science, nanoscale semiconductor materials tightly confine either electrons or electron holes. Quantum dots are also sometimes referred to as **artificial atoms**, a term that emphasizes that a quantum dot is a single object with bound, discrete electronic states, as is the case with naturally occurring atoms or molecules.

Quantum dots exhibit properties that are intermediate between those of bulk semiconductors and those of discrete molecules. Their optoelectronic properties change as a function of both size and shape. Larger QDs (radius of 5–6 nm, for example) emit longer wavelengths resulting in emission colors such as orange or red. Smaller QDs (radius of 2–3 nm, for example) emit shorter wavelengths resulting in colors like blue and green, although the specific colors and sizes vary depending on the exact composition of the QD.

Because of their highly tunable properties, QDs are of wide interest. Potential applications include transistors, solar cells, LEDs, diode lasers and second-harmonic generation, quantum computing, and medical imaging. Additionally, their small size allows for QDs to be suspended in solution which leads to possible uses in inkjet printing and spin-coating. These processing techniques result in less-expensive and less time consuming methods of semiconductor fabrication.

5.4 Application of nanomaterials:

- The tensile strength of high carbon steel is around 1.2 GPa but the tensile strength of carbon nanotubes (CNT) is 63 GPa. Also they are known to be one of the strongest materials having been produced by nanotechnology so far. **Graphene** is the world's strongest material, and so can be used to enhance the strength of other materials. ... Such **graphene**-enhanced composite materials can find **uses** in aerospace, building materials, mobile devices, and many other **applications**.

- CNT has been used for applications in energy storage, automotive parts, boat hulls, sporting goods, water filters, thin-film electronics, coatings, actuators and electromagnetic shields. CNT-related publications more than tripled in the prior decade, while rates of patent issuance also increased.Most output was of unorganized architecture. Organized CNT architectures such as "forests", yarns and regular sheets were produced in much smaller volumes.CNTs have even been proposed as the tether for a purported space elevator.

- A Carbon Nanotube is a tube-shaped material, made of carbon, having a diameter measuring on the nanometre scale. Carbon Nanotubes are formed from essentially the graphite sheet and the graphite layer appears somewhat like a rolled-up continuous unbroken hexagonal mesh and carbon molecules at the apexes of the hexagons. Nanotubes are members of the fullerene structural family.

Recently, several studies have highlighted the prospect of using carbon nanotubes as building blocks to fabricate three-dimensional macroscopic (>1mm in all three dimensions) all-carbon devices. There is a report that a novel radical initiated thermal crosslinking method to fabricated macroscopic, free-standing, porous, all-carbon scaffolds using single- and multi-walled carbon nanotubes as building blocks. These scaffolds possess macro-, micro-, and nano- structured pores and the porosity can be tailored for specific applications. These 3D all-carbon scaffolds/architectures may be used for the fabrication of the next generation of energy storage, supercapacitors, field emission transistors, high-performance catalysis, photovoltaics, and biomedical devices and implants.

- **Nanotechnology in Electronics**- Nanoelectronics refer to the use of **nanotechnology** on **electronic** components, especially transistors. Nanoelectronics often refer to transistor devices that are so small that inter-atomic interactions and quantum mechanical properties need to be studied extensively.

- Nanotechnology is being used in several applications to improve the environment. This includes cleaning up existing pollution, improving manufacturing methods to reduce the generation of new pollution, and making alternative energy sources more cost effective.

- Nanotechnological products, processes and applications are expected to contribute significantly to environmental and climate protection by saving raw materials, energy and water as well as by reducing greenhouse gases and hazardous wastes. Using nanomaterials therefore promises certain environmental benefits and sustainability effects. Note, however, that nanotechnology currently plays a rather subordinate role in environmental protection, whether it be in research or in practical applications. Environmental engineering companies themselves attach only limited importance to nanotechnology in their respective fields.

- Nanomedicine is the medical application of nanotechnology. Nanomedicine ranges from the medical applications of nanomaterials and biological devices, to nanoelectronic biosensors, and even possible future applications of molecular nanotechnology such as biological machines.

    Nanotechnology in medicine involves applications of nanoparticles currently under development, as well as longer range research that involves the use of manufactured nano-robots to make repairs at the cellular level (sometimes referred to as nanomedicine).