Solid State Physics
PHY322

Chapter 1: Crystallography.
Chapter 2: Dielectric Properties of Materials.
Chapter 3: Magnetic Properties of Materials.
Chapter 4: Introduction to Quantum Mechanics.
Chapter 5: Energy-Band Theory.

Reference book: “Principles of Electronic Materials and Devices”, S. O. Kasap, 3rd Edition, McGraw-Hill,2005

PHY322 ILOs

ILO #	Description
1	Comprehend and understand several crystal structure of well-known solid-state materials.
2	Differentiate among different crystal bonds of solid states.
3	Know and understand the dielectric properties of solid states.
4	Know and understand the magnetic properties of solid states.
5	Comprehend the postulates of quantum mechanics.
6	Know how energy levels in solid states become bands used to differentiate among different categories of solid states..
7	Understand Schrodinger wave equation and use it to study solid states.

Lecture 1

http://eng.staff.alexu.edu.eg/~mbanna/

BannaElectronics https://www.youtube.com/channel/UCaKy_Y0LJaPieD4ve59LZEQ/playlist

Chapter 1: Crystallography

Why study Crystallography and crystal structures?

- Description of solids.
- Comparison with other similar materials and classifications.
- Correlation with physical properties, electric and magnetic.
- Stability of different alloys.

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Why Solid State?

- Most of the elements are solids at room temperature.
- Crystals are solid - but solids are not necessarily crystalline.

Crystals?

Regular repletion of building blocks (Basis).

↓	↓
Lattice	An atom
Bravais Lattice	A group of atoms

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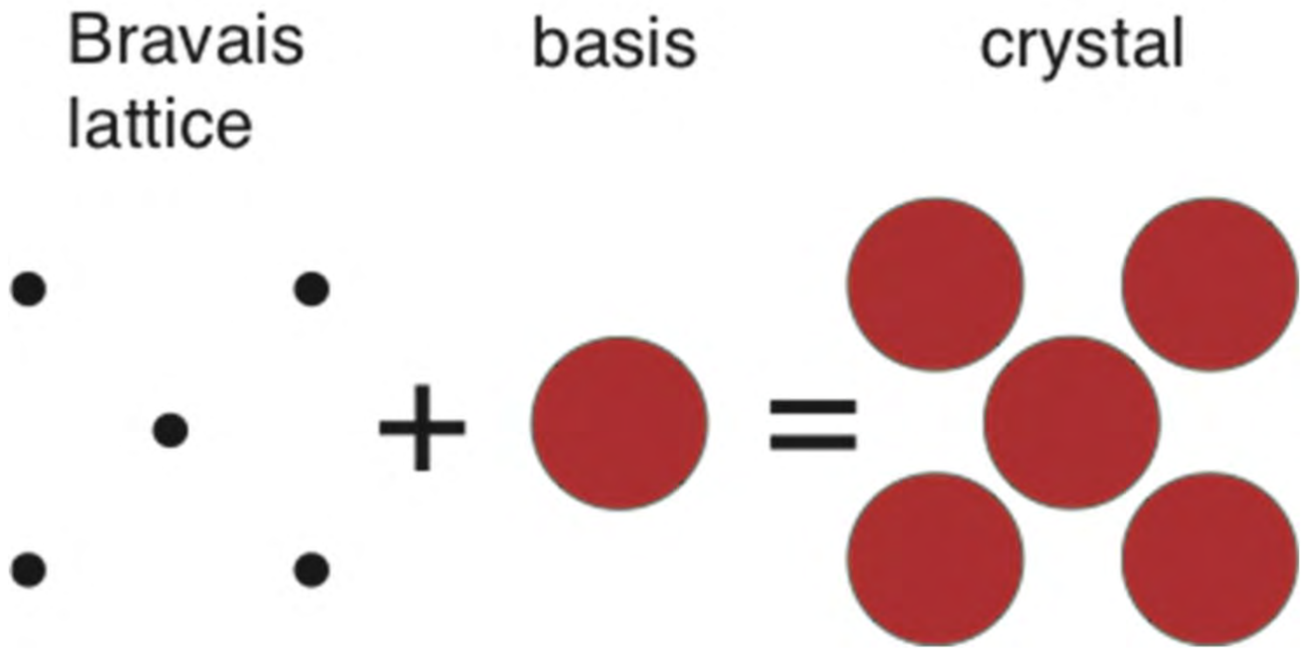
Examples:



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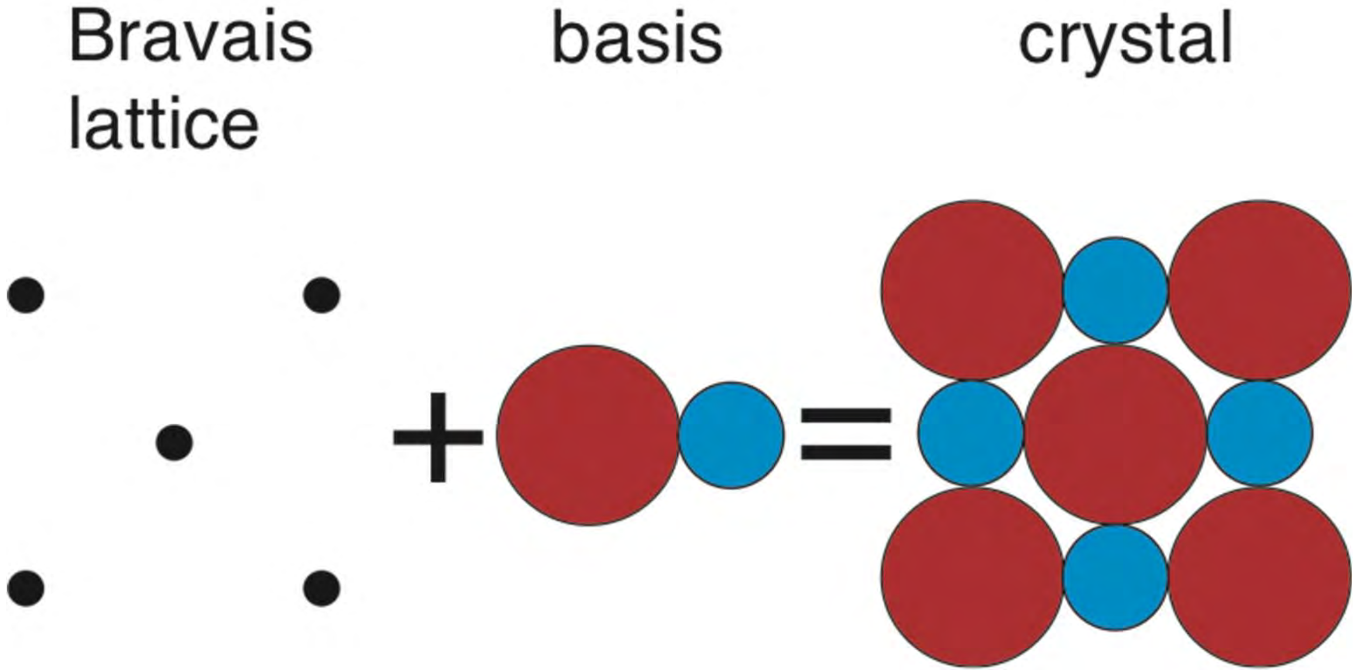

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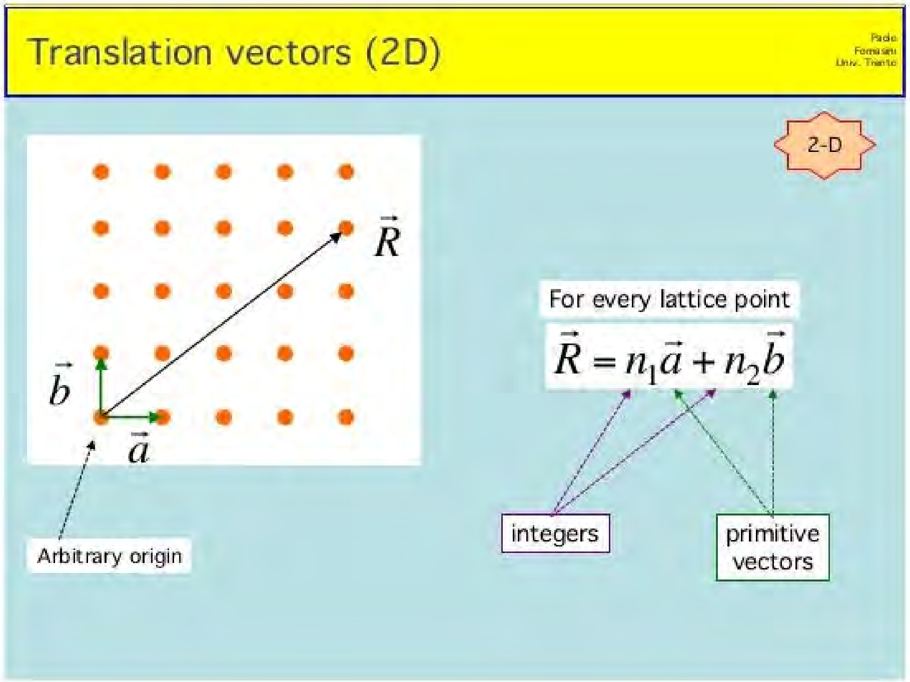
Lattice Translation Vector
Primitive



Translation vectors (2D)

Paolo
Fornasini
Univ. Trento

2-D

For every lattice point

$$\vec{R} = n_1\vec{a} + n_2\vec{b}$$

integers

primitive vectors

Arbitrary origin

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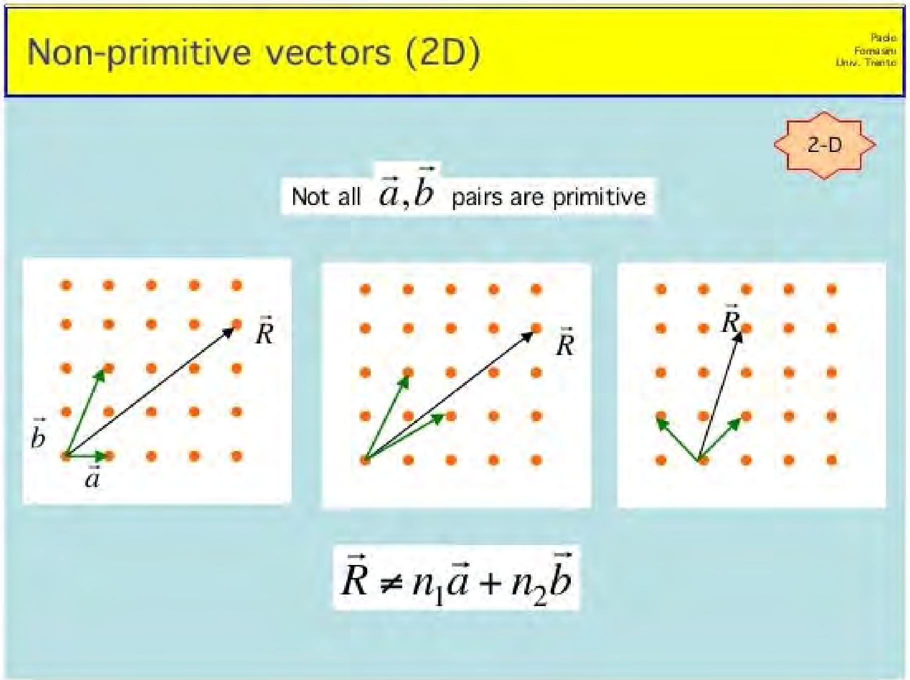
Lattice Translation Vector
Nonprimitive



Non-primitive vectors (2D)

2-D

Not all $\vec{a},\vec{b}$ pairs are primitive

$$\vec{R} \neq n_1\vec{a} + n_2\vec{b}$$

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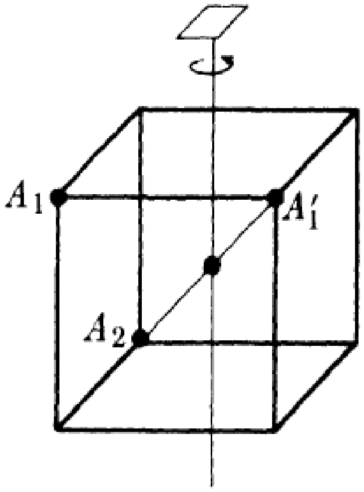
Symmetry Operations: Carry the lattice into itself.

- Rotation

  An axis around which the lattice is rotated without any change.



(d)

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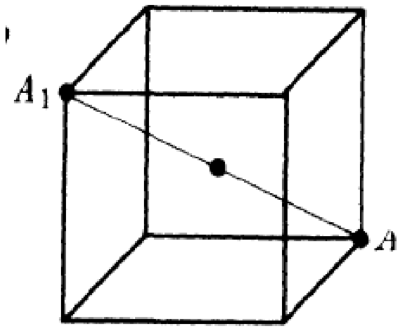
- Inversion

A lattice point pointed to by a translation vector R keeps the lattice unchanged if R is replaced by -R



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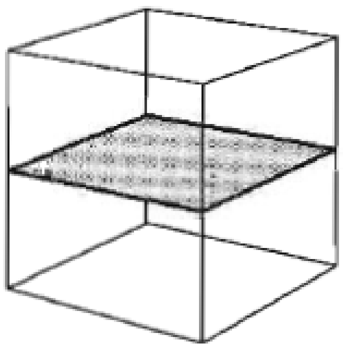
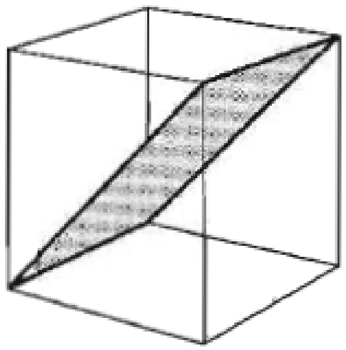
- Reflection

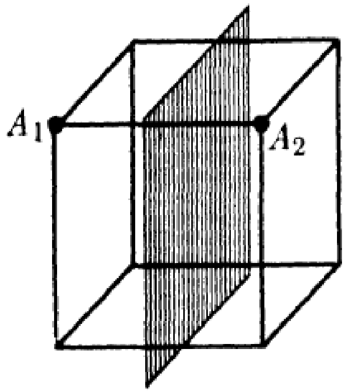
There exist a plane lattice which divides the lattice into two identical parts



(a)



(b)



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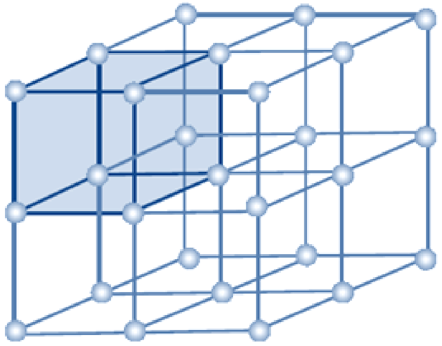
Primitive Lattice Cell

- Minimum volume.
- One lattice point.

Volume $V_c = |(a \times b).c|$



Representation of unit cell in cristal lattice

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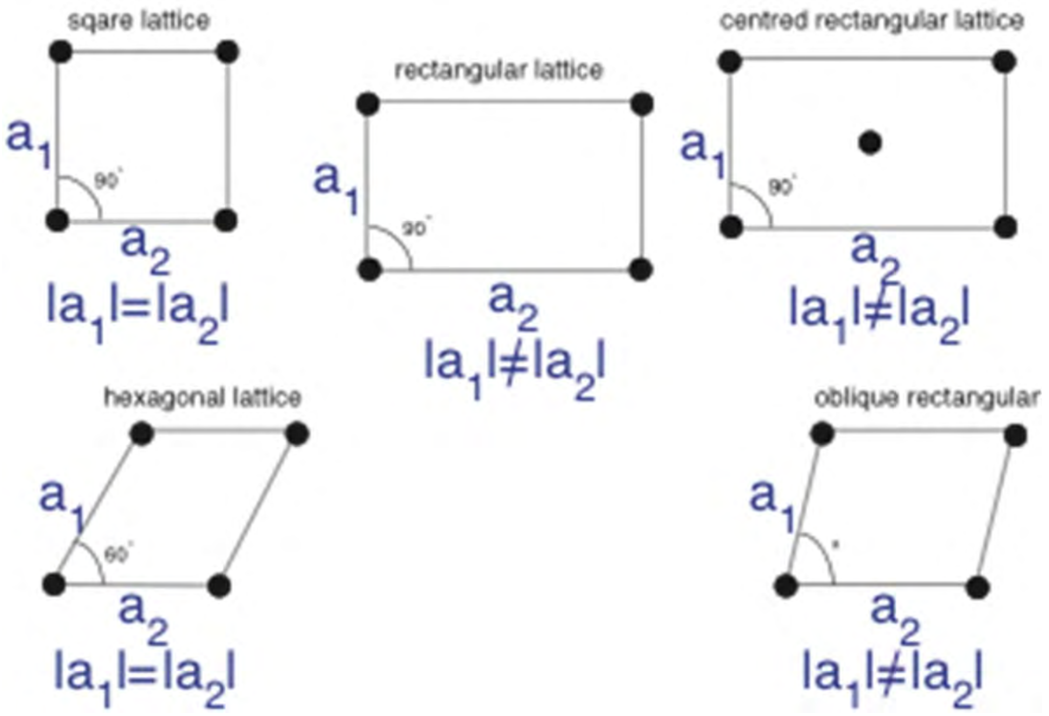
Two-dimensional lattice types

Only five 2D lattices



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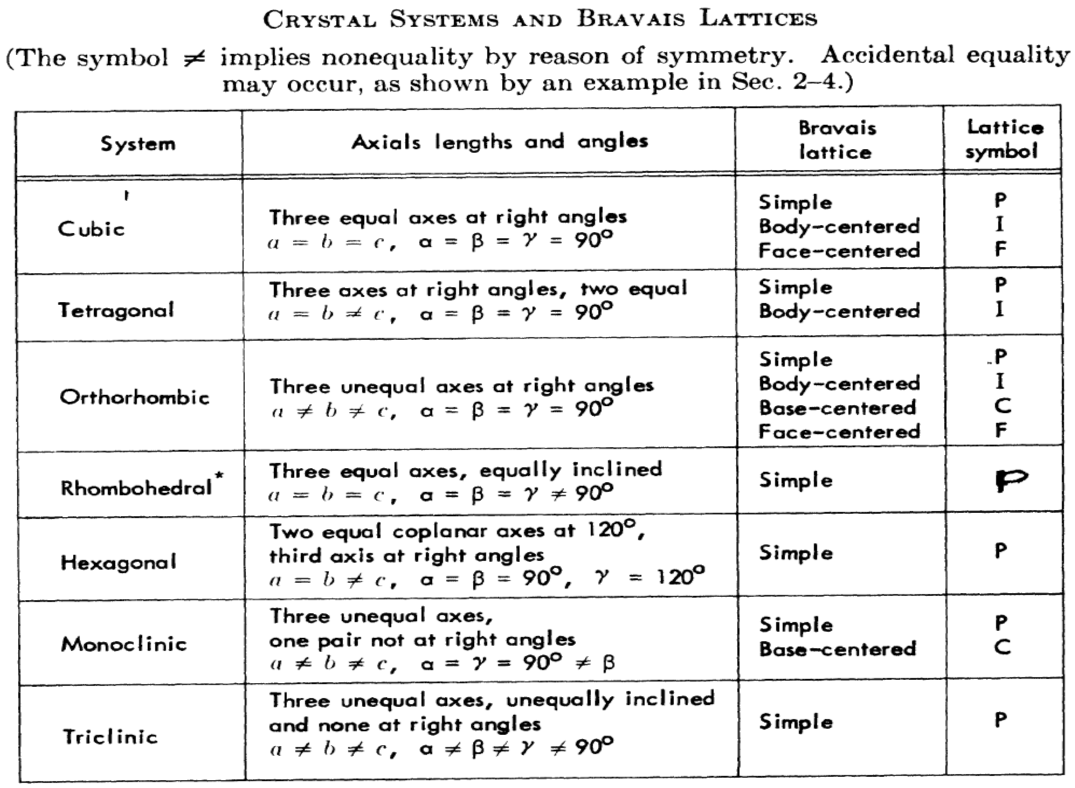
Three-dimensional lattice types

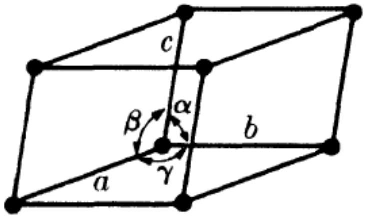
Only 14 3D lattices



CRYSTAL SYSTEMS AND BRAVAIS LATTICES

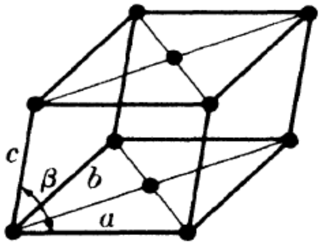
(The symbol $\neq$ implies nonequality by reason of symmetry. Accidental equality may occur, as shown by an example in Sec. 2–4.)

System	Axials lengths and angles	Bravais lattice	Lattice symbol
Cubic	Three equal axes at right angles $a = b = c, \quad \alpha = \beta = \gamma = 90°$	Simple Body-centered Face-centered	P I F
Tetragonal	Three axes at right angles, two equal $a = b \neq c, \quad \alpha = \beta = \gamma = 90°$	Simple Body-centered	P I
Orthorhombic	Three unequal axes at right angles $a \neq b \neq c, \quad \alpha = \beta = \gamma = 90°$	Simple Body-centered Base-centered Face-centered	P I C F
Rhombohedral*	Three equal axes, equally inclined $a = b = c, \quad \alpha = \beta = \gamma \neq 90°$	Simple	P
Hexagonal	Two equal coplanar axes at 120°, third axis at right angles $a = b \neq c, \quad \alpha = \beta = 90°, \quad \gamma = 120°$	Simple	P
Monoclinic	Three unequal axes, one pair not at right angles $a \neq b \neq c, \quad \alpha = \gamma = 90° \neq \beta$	Simple Base-centered	P C
Triclinic	Three unequal axes, unequally inclined and none at right angles $a \neq b \neq c, \quad \alpha \neq \beta \neq \gamma \neq 90°$	Simple	P



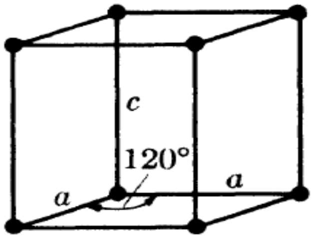
TRICLINIC (*P*)

$a \neq b \neq c, \quad \alpha \neq \beta \neq \gamma \neq 90^\circ$



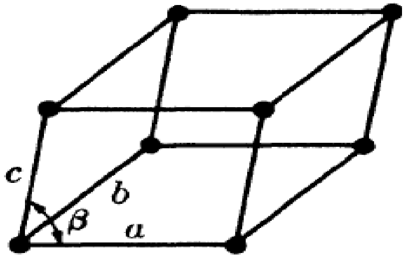
BASE-CENTERED
MONOCLINIC (*C*)

$a \neq b \neq c, \quad \alpha = \gamma = 90^\circ \neq \beta$

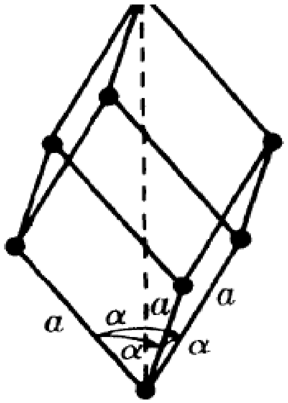


HEXAGONAL
(*P*)

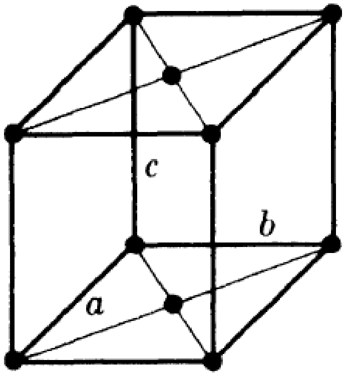
$a = b \neq c, \quad \alpha = \beta = 90^\circ, \quad \gamma = 120^\circ$



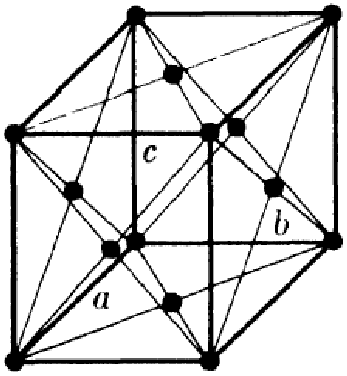
SIMPLE
MONOCLINIC (*P*)



RHOMBOHEDRAL
(*R*)

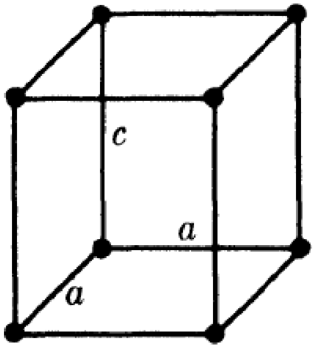


BASE-CENTERED
ORTHORHOMBIC
(*C*)

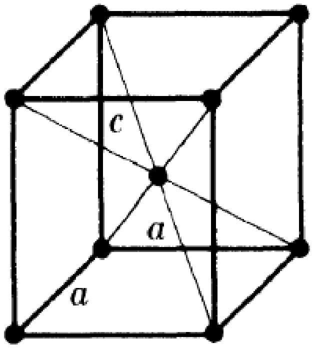


FACE-CENTERED
ORTHORHOMBIC
(*F*)

$$a \neq b \neq c, \quad \alpha = \beta = \gamma = 90^\circ$$

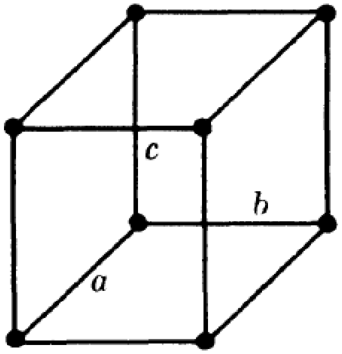


SIMPLE
TETRAGONAL
(*P*)

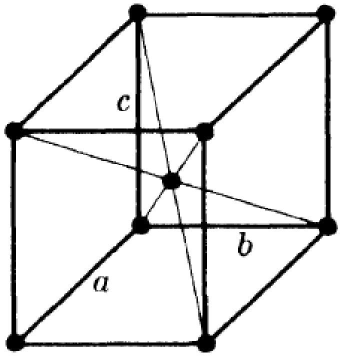


BODY-CENTERED
TETRAGONAL
(*I*)

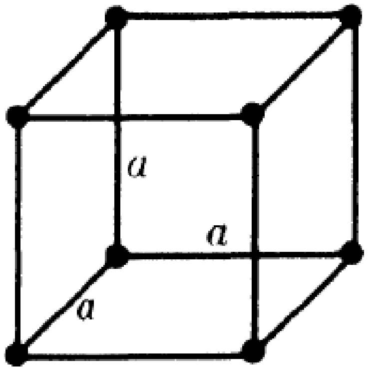
$$a = b \neq c, \quad \alpha = \beta = \gamma = 90^\circ$$



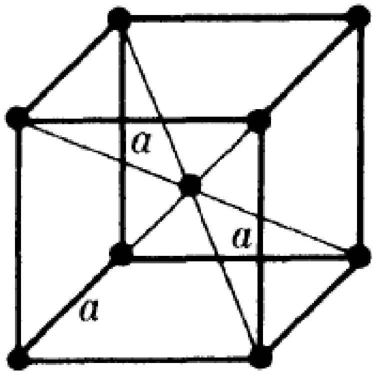
SIMPLE
ORTHORHOMBIC
(*P*)



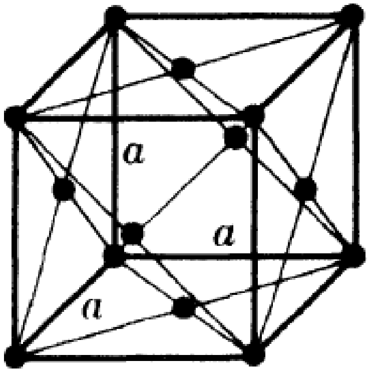
BODY-CENTERED
ORTHORHOMBIC
(*I*)



SIMPLE
CUBIC (*P*)



BODY-CENTERED
CUBIC (*I*)



FACE-CENTERED
CUBIC (*F*)

Conventional Cubic Lattices: a=b=c=a

Simple Cubic SC: It is the same as the primitive cell

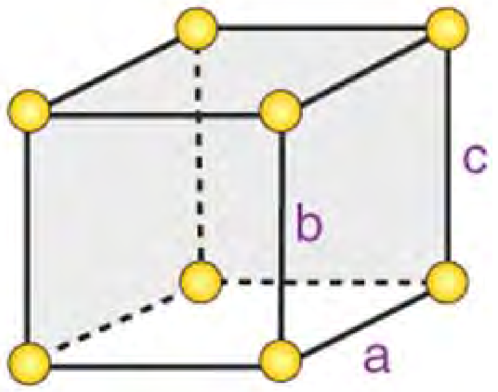
Nearest neighbors = 6 atoms at a distance a.

Lattice points $= 8 \times \frac{1}{8} = 1$ point

$$\bar{a} = a\,\hat{x}$$
$$\bar{b} = a\,\hat{y}$$
$$\bar{c} = a\,\hat{z}$$

Packing density (filling factor)

$$2r = a$$
$$r = \frac{a}{2}$$
$$\frac{\frac{4}{3}\pi r^3 .1}{a^3} = \frac{\pi}{6} = 52\%$$



Simple cubic

Lecture 1

Conventional Cubic Lattices: a=b=c=a

Body-Centered Cubic Lattice BCC: It is not the same as the primitive cell

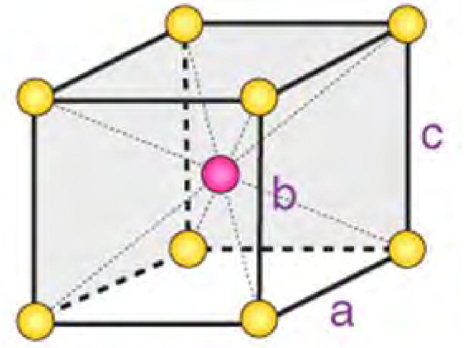
Nearest neighbors = 8 atoms at a distance $\frac{\sqrt{3}}{2}a$.

Lattice points $= 8 \times \frac{1}{8} + 1 = 2$ points

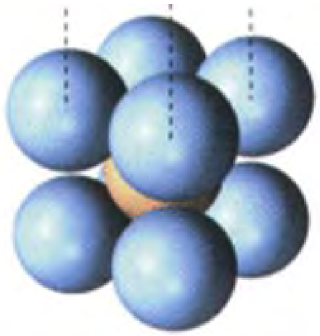
$$\bar{a} = \frac{a}{2}(\hat{x} + \hat{y} - \hat{z})$$
$$\bar{b} = \frac{a}{2}(-\hat{x} + \hat{y} + \hat{z})$$
$$\bar{c} = \frac{a}{2}(\hat{x} - \hat{y} + \hat{z})$$

Packing density (filling factor)

$$4r = \sqrt{3}\ a$$
$$r = \frac{\sqrt{3}\ a}{4}$$
$$\frac{\frac{4}{3}\pi r^3 . 2}{a^3} = \frac{\sqrt{3}\pi}{8} = 68\%$$



Body-centred Cubic Unit Cell (BCC)



Lecture 1

Conventional Cubic Lattices: a=b=c=a

Face-Centered Cubic Lattice FCC: It is not the same as the primitive cell

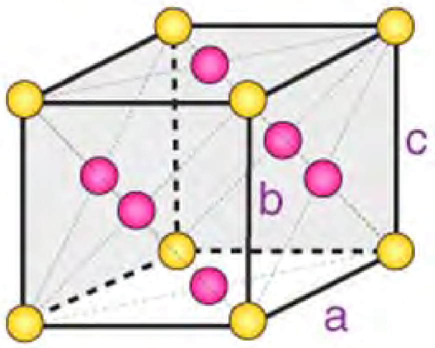
Nearest neighbors = 12 atoms at a distance $a/\sqrt{2}$.

Lattice points $= 8 \times \frac{1}{8} + 6 \times \frac{1}{2} = 4$ points

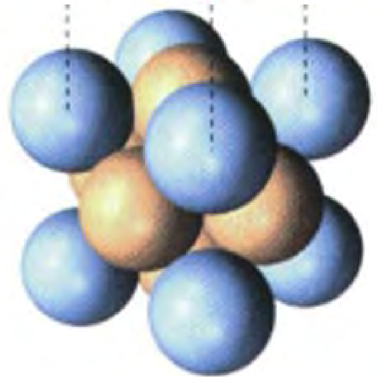
$$\bar{a} = \frac{a}{2}(\hat{x} + \hat{y})$$
$$\bar{b} = \frac{a}{2}(\hat{y} + \hat{z})$$
$$\bar{c} = \frac{a}{2}(\hat{x} + \hat{z})$$

Packing density (filling factor)

$$4r = \sqrt{2}\ a$$
$$r = \frac{\sqrt{2}\ a}{4}$$
$$\frac{\frac{4}{3}\pi r^3 . 4}{a^3} = \frac{\pi}{3\sqrt{2}} = 74\%$$



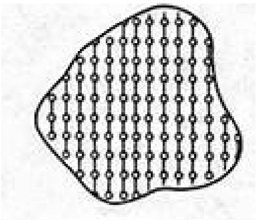
Face-centred Cubic Unit Cell (FCC)



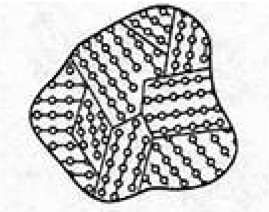
Lecture 2

Solids are classified according to:

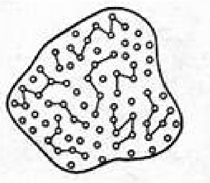
- Crystal Structures:
  - Single crystal where the unit cell occurs throughout the volume of the solid.



  - Polycrystal where regular structure occurs only in portions of the solids (grains or crystallites separated by grain boundaries).

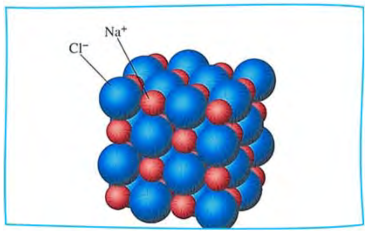


  - Amorphous where crystallites become unit cells and no regular structure exists.

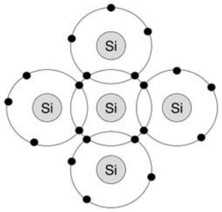


Lecture 2

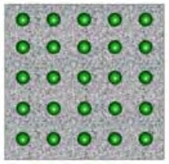
- ❖ Binding bonds:
  - ☐ Ionic Crystals, bonds highly depend on the freedom of valence electrons



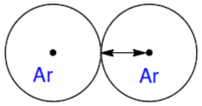
  - ☐ Covalent Crystals, bonds highly depend on the freedom of valence electrons



  - ☐ Metallic Crystals, bonds highly depend on the freedom of valence electrons

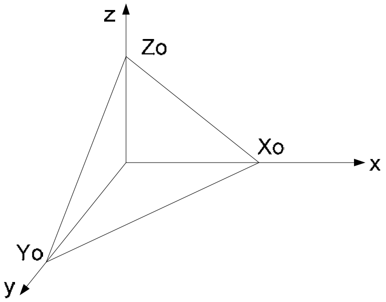


  - ☐ Van Dar Waals Crystals, valence electrons are tightly bound to the nuclei



Lecture 2

Lattice System for crystal planes



Planes are usually determined by noncolinear three points in the plane.

Equation of the plane: $\frac{x}{X_o} + \frac{y}{Y_o} + \frac{z}{Z_o} = 1$

In crystallography, planes are represented by three integer numbers h, k, and l related to the intersections with x-, y-, and z- axes X_o , Y_o , and Z_o .

Steps to get h, k, and l:

1. Get the intersections X_o , Y_o , and Z_o .
2. Form the reciprocals $\frac{1}{X_o}, \frac{1}{Y_o}, and \frac{1}{Z_o}$.
3. Multiply by a common factor to get the smallest integers h, k and l.

Lecture 2

Miller indices:

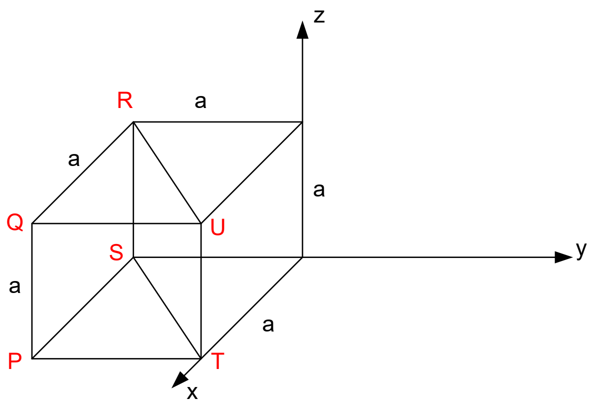
(hkl) : a plane or a set of parallel.

{hkl} : planes equivalent by symmetry {100} → (100) , (010), and (001).

[hkl] : direction, perpendicular to plane (hkl) in cubic lattices.

<hkl> : set of equivalent direction.

In cubic crystals the direction [hkl] is perpendicular to plane (hkl).



Examples: the plane RSTU

$$\frac{x}{a} - \frac{y}{a} + \frac{z}{\infty} = 1$$

1. Intersections : a, -a, and ∞.
2. Reciprocals : $\frac{1}{a}, \frac{-1}{a}$, and $\frac{1}{\infty}$
3. hkl are $1\bar{1}0$, so the plane is $(1\bar{1}0)$

Lecture 2

Plane QPTU

1. Intersections: a, ∞, ∞.
2. Reciprocals: $\frac{1}{a}, \frac{1}{\infty}, \frac{1}{\infty}$
3. hkl (100)

Usefulness of Miller Indices

- In Si, growing a crystal in <111> direction produces a stable crystal $(Si)_{111\ \text{separation}} = 3.1\ \dot{A}$.
- Al diffuses in Si faster in <100> direction than in <111> direction, a short circuit may occur.
- Si tears faster in <100> than in <111>.
- (100) is preferable for MOS devices.
- (100) Si has a relatively low packing density.
- (111) Si wafer gives the best mechanical properties.

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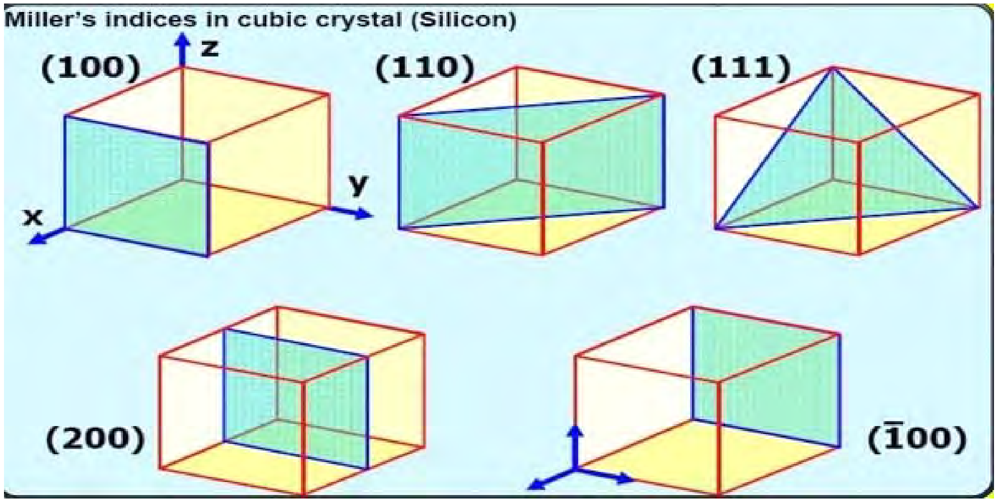
Examples

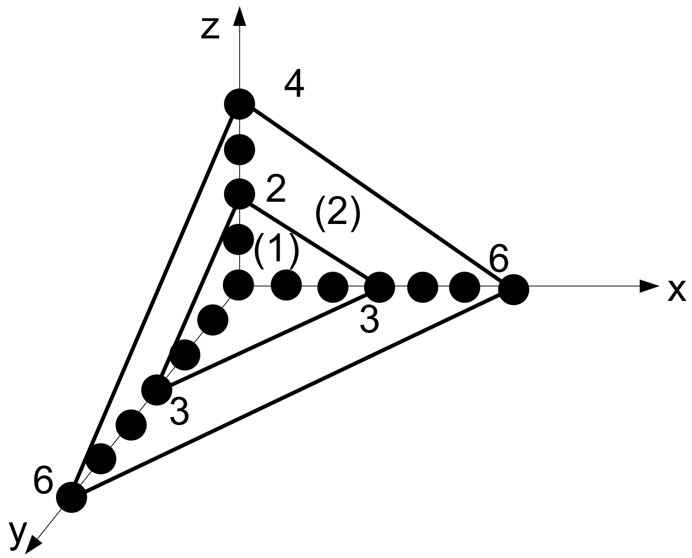


Parallel planes have the same Miller indices

Plane (1) is parallel to plane (2)

Plane (1): ratios $\frac{1}{3}, \frac{1}{3}, \frac{1}{2}$
(hkl) = (223)

Plane (2): ratios $\frac{1}{6}, \frac{1}{6}, \frac{1}{4}$
(hkl) = (223)



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Distance between parallel planes:

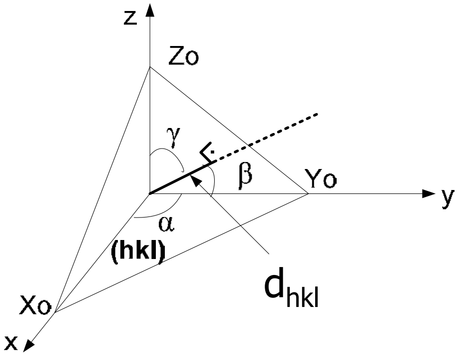
$\alpha, \beta, and\ \gamma$ are angles the normal d_{hkl} makes with the axes x-, y- and z-.

$$d_{hkl} = X_o \cos\alpha$$
$$= Y_o \cos\beta$$
$$= Z_o \cos\gamma$$

But $cos^2\alpha + cos^2\beta + cos^2\gamma = 1$

$$d_{hkl}^2\left[\left(\frac{1}{X_o}\right)^2 + \left(\frac{1}{Y_o}\right)^2 + \left(\frac{1}{Z_o}\right)^2\right] = 1$$

$$d_{hkl} = \frac{1}{\sqrt{\left(\frac{1}{X_o}\right)^2 + \left(\frac{1}{Y_o}\right)^2 + \left(\frac{1}{Z_o}\right)^2}}$$



Lecture 2

$$X_o = n_1 a, \quad Y_o = n_2 b, \quad and\ Z_o = n_3 c$$

$$h = \frac{n}{n_1}, \quad k = \frac{n}{n_2} \quad and \quad l = \frac{n}{n_3}$$

$\frac{1}{X_o} = \frac{h}{na}$, $\frac{1}{Y_o} = \frac{k}{nb}$, and $\frac{1}{Z_o} = \frac{l}{nc}$

Therefore, $d_{hkl} = \frac{n}{\sqrt{(\frac{h}{a})^2 + (\frac{k}{b})^2 + (\frac{l}{c})^2}}$

In cubic lattices, a = b = c = a,

Then, $d_{hkl} = \frac{na}{\sqrt{h^2+k^2+l^2}}$

Lecture 2

Example: Find the distance between the parallel planes (100) of a cubic lattice whose lattice constant is a.

Intersections: $1\ \infty\ \infty \quad hence\ \ n = 1$

$\therefore\ d_{hkl} = a$

For planes (111)

Intersections: $1\ 1\ 1 \quad hence\ \ n = 1$

$\therefore\ d_{hkl} = \frac{a}{\sqrt{3}}$

Lecture 2

Reciprocal Lattice: It is mathematical concept to explain physical phenomena.
The diffraction pattern of a crystal is a map of the reciprocal lattice

Real Lattice: The microscopic image of a crystal is a map of the real crystal structure.

The corresponding translation vectors of a reciprocal lattice whose primitive translation vectors $\overline{a}$, $\overline{b}$ and $\overline{c}$ are:

$\overline{a}^* = \frac{2\pi}{V}(\overline{b} \times \overline{c})$, so $\overline{a}^*$ $is\ perpendicular\ to\ \overline{b}\ and\ \overline{c}$

$\overline{b}^* = \frac{2\pi}{V}(\overline{c} \times \overline{a})$, so $\overline{b}^*$ $is\ perpendicular\ to\ \overline{c} \times \overline{a}$

$\overline{c}^* = \frac{2\pi}{V}\left(\overline{a} \times \overline{b}\right)$, so $\overline{c}^*$ $is\ perpendicular\ to\ \overline{a}\ and\ \overline{b}$

Lecture 2

Reciprocal lattice translation vectors satisfy the following relations:

$$\overline{a}^* \cdot \vec{a} = \frac{2\pi\overline{a}\cdot(\overline{b}\times\overline{c})}{V} = 2\pi \qquad ,\overline{a}^* \cdot \vec{b} = 0 \text{ and } \overline{a}^* \cdot \vec{c} = 0$$

$$\overline{b}^* \cdot \vec{b} = 2\pi \qquad ,\overline{b}^* \cdot \vec{c} = 0 \text{ and } \overline{b}^* \cdot \vec{a} = 0$$

$$\overline{c}^* \cdot \vec{c} = 2\pi \qquad ,\overline{c}^* \cdot \vec{a} = 0 \text{ and } \overline{c}^* \cdot \vec{b} = 0$$

Define the reciprocal lattice operator as:

$$\overline{G} = n_1\overline{a}^* + n_2\overline{b}^* + n_3\overline{c}^*$$

$\overline{a}, \overline{b}$, and $\overline{c}$ are real crystals primitive vectors and lead to the same set of reciprocal lattice points:

$$\overline{G} = h\overline{a}^* + k\overline{b}^* + l\overline{c}^*$$

Lecture 2

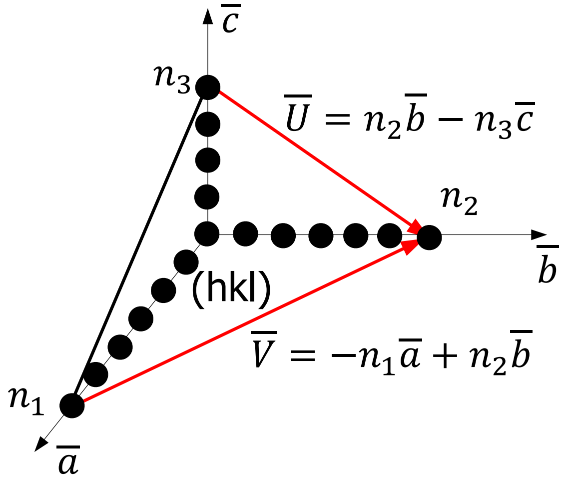
Theorem: Every reciprocal lattice vector (operator) $\overline{G_{hkl}}$ is normal to a crystal lattice plane:

Need to prove that $\overline{G_{hkl}}$ is perpendicular to the plane (hkl)

If $\overline{G_{hkl}}$ is perpendicular to both $\overline{U}$ and $\overline{V}$

$$\overline{G_{hkl}}.\ \overline{U} = (h\overline{a}^* + k\overline{b}^* + l\overline{c}^*).(n_2\overline{b} - n_3\overline{c})$$
$$= 2\pi(n_2k - n_3l)$$

$$\overline{G_{hkl}}.\ \overline{V} = (h\overline{a}^* + k\overline{b}^* + l\overline{c}^*).(-n_1\overline{a} + n_2\overline{b})$$
$$= 2\pi(-n_1h + n_2k)$$



From Miller indices $h = \frac{n}{n_1}$, $k = \frac{n}{n_2}$, and $l = \frac{n}{n_3}$

So, $n = hn_1 = kn_2 = ln_3$

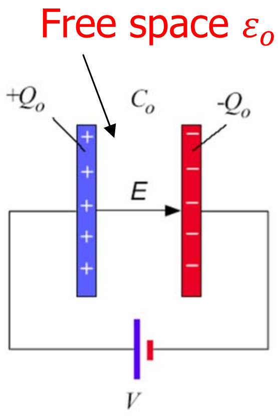
Hence, $\overline{G_{hkl}}.\ \overline{U} = 0$ and $\overline{G_{hkl}}.\ \overline{V} = 0$ *and* $\overline{G_{hkl}}.$ is perpendicular to the plane (hkl)

Lecture 3

Chapter 2: Dielectric Properties of Solids

- Dielectric materials do not ideally conduct electrical charges, so that an applied field does not cause a flow of charge but instead relative displacement of opposite charges and hence polarization of the medium.
- Thus, energy can be stored in the material by the polarization of the molecules.

- One use of dielectric is to increase the capacitance or charge storage ability of a capacitor.



2.1 Capacitors:

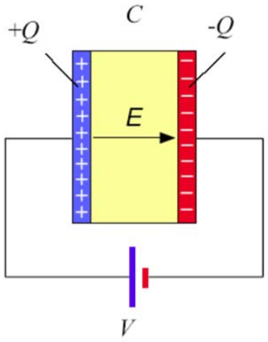
- Consider a parallel plate capacitor with free space between the plates.
- The capacitor is charged to a voltage V with Q_o charges by connecting it to a battery of voltage V.

Lecture 3

- The ability of the capacitor to store an electric charge per unit volt is measured by **capacitance**

$$C_o = \frac{Q_o}{V}\ F$$

- A dielectric slab is inserted between the plates and V is kept constant.



- More charges are stored on the plates denoted by Q.

$$Q > Q_o$$

- As a result, the capacitance is increased

$$C = \frac{Q}{V} \quad > \ C_o$$

2.2 Relative Permittivity (ϵ_r)

- It is the fractional increase in the capacitance of a capacitor when the insulation between the plates is changed from a vacuum to a dielectric material.

$$\epsilon_r = \frac{C}{C_o} = \frac{Q}{Q_o}$$

Lecture 3

- It is a macroscopic quantity which depends on the manner in which the atoms are assembled to form a crystal.

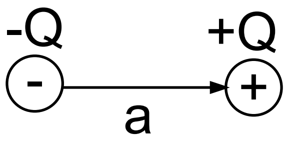
Absolute permittivity (in vacuum)

$$\varepsilon_o = 8.85 \times 10^{-12}\ F/m$$

Material permittivity: $\epsilon = \epsilon_o \epsilon_r$

2.3 Polarization

Electric Dipole: A pair of equal and oppositely charged bodies separated by a small distance.



Dipole moment: measures the polarity of a system of charges. It is a vector points from –ve to +ve charge.

$$\bar{p} = Q\bar{a}$$

Lecture 3

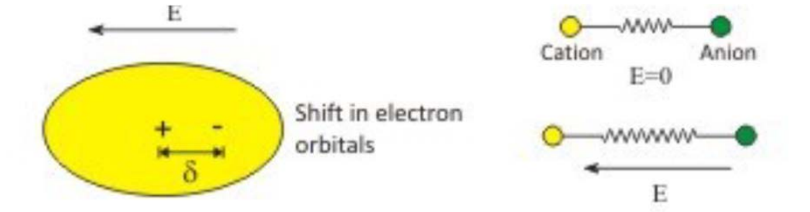
- If the positive charge coincides with the negative charge, this means that $\bar{p}$ = 0.

2.4 Sources of Electric Moments

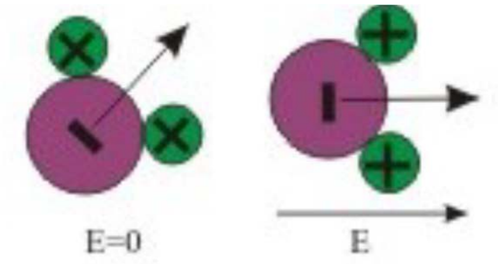
a-Electronic Polarization: occurs in all insulators.

b- **Ionic Polarization**: occurs in all ionic solids.

c- **Orientation Polarization:** occurs in all polar gases, liquids and solids , materials which have permanent dipoles.



(a) Electronic Polarizaton in an atom (b) Ionic Polarization

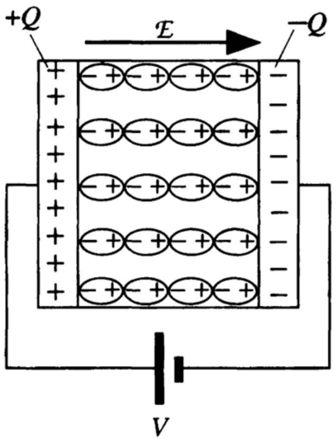


(c) Orientation Polarization

Lecture 3

2.5 Polarization Vector

- When a dielectric is placed in an electric field E, the particles of the medium become polarized due to the slightly shift of their positive and negative charges caused by the applied field E



- The induced dipole moments $\overline{p}_j$ associated with every particle point towards the direction of the field $\overline{E}$. The total dipole moment is:

$$\overline{p}_{tot} = \sum_j \overline{p}_j = n\overline{p}_{av}$$

n : Number of dipoles in the medium.

$\overline{p}_{av}$: Average dipole moment per atom in the direction of $\overline{E}$.

- Inside the polarization medium, there is no net charge within the bulk as the positive charges cancel the negative ones.

Lecture 3

- Bound polarization charges appear on the opposite surfaces due to the polarization of the medium particles denoted by Q_p.

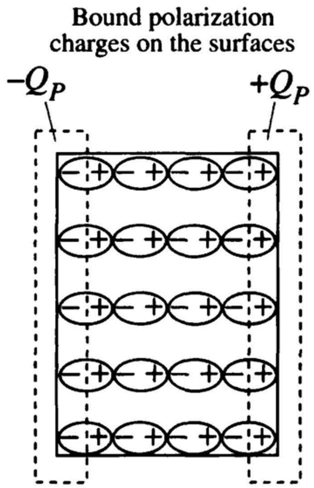
- Thus, the total dipole moment is $p_{tot} = Q_p d$

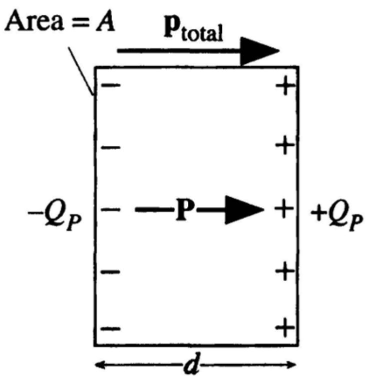
- The total dipole moment per unit volume named as **polarization vector is**

$$\overline{p} = \frac{p_{tot}}{Vol} = N\overline{p}_{av}$$

N : Number of dipoles per unit volume.

Vol : Volume of material.





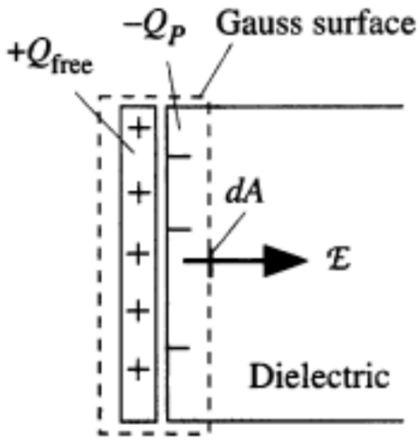
- For rectangular slab with volume Vol = $A\ d$, the magnitude of $\overline{P}$ can be simply represented in terms of its surface polarization charge density as

$$P = \frac{Q_p}{A} \quad C/m^2$$

Lecture 3

- Notice that for a general case the magnitude P is the component of the vector $\mathbf{P}$ normal to the surface of the polarized medium.
- Let the applied voltage V and hence the field E be fixed after the insertion of dielectric. Thus, the stored free-surface charges Q on the capacitor plates are increased by an amount Q_p :

$$Q = Q_o + Q_p$$



- From **Gauss's Law:** $\oint \boldsymbol{\epsilon_o E_{norm} dA} = \boldsymbol{Q_{tot}}$
- Before the dielectric is inserted between the parallel-plate capacitor

$$Q_0 = \epsilon_o EA$$

- Since $Q = \epsilon_r Q_o$, then $\epsilon_r \epsilon_o EA = \epsilon_o EA + Q_p$
- Dividing by the surface area A,

$$\therefore\ \epsilon_o \epsilon_r E = \epsilon_o E + P = D$$

- Thus P and E can be related by

$$P = \epsilon_o(\epsilon_r - 1)E = \epsilon_o \chi_e E$$

where χ_e is defined as the electric susceptibility

Lecture 3

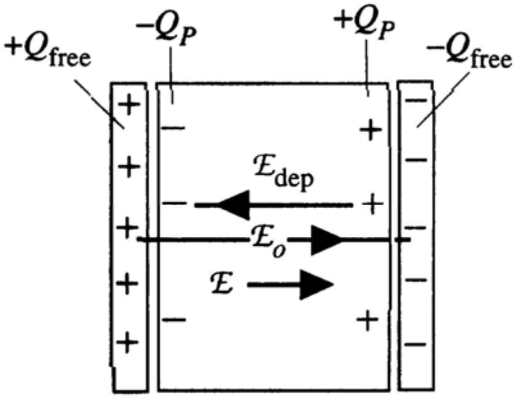
- In free space,

$$\epsilon_r = 1\,,\quad \chi_e = 0,\quad P = 0,\qquad and\ D = \epsilon_o E$$

2.6 Depolarization Field

- We can view the field E as arising from two electric fields: that due to the free charges E_o, and that due to the polarization charges, denoted as E_{dep}. These two fields are indicated in the Figure. E_o is called the applied field as it is due to the free charges that have been put on the plates.

- Although E_o polarizes the molecules of the medium, E_{dep}, being in the opposite direction, tries to depolarize the medium. It is called the depolarizing field



$$\therefore E = E_o - E_{dep} = \frac{E_o}{\epsilon_r}$$

$$E_{dep} = E_o - E$$

$$E_{dep} = E\left(\frac{E_o}{E} - 1\right) = E(\epsilon_r - 1)$$

Lecture 3

- ❖ The polarization P is related to the field E by:

$$P = \epsilon_o(\epsilon_r - 1)E$$

- ❖ Thus, the depolarization field E_{dep} is given by:

$$E_{dep} = \frac{P}{\epsilon_o}$$

2.7 Polarization Mechanisms

- ❖ It is the mechanism in which atoms and molecules respond to an electric field.
- ❖ For low electric field, the relation between the induced average dipole moment $\overline{p}_{av}$ and the field $\overline{E}$ that acts to produce it is given by:

$$\overline{P} = N\overline{p}_{av} = \epsilon_o(\epsilon_r - 1)\overline{E}$$

- ❖ Define the ability of an atom or molecule to become polarized in the presence of electric field by the **polarizability** (α). Then we get $\overline{p}_{av} = \alpha\overline{E}$

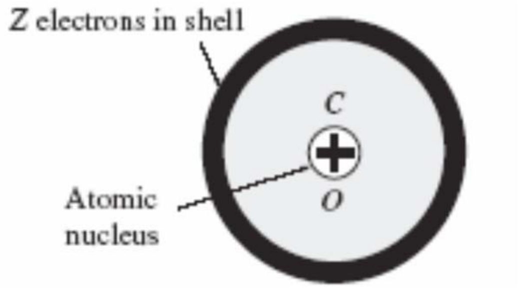
Lecture 3

- Therefore, the relation between macroscopic ϵ_r and microscopic α properties can be expressed as :

$$\epsilon_r = 1 + N\alpha/\varepsilon_o$$

2.8 Electronic Polarization

- Recall that an atom consists of nucleus with positive charge and surrounded by electrons with negative charge.
- In the absence of field E, the centers of positive and negative charges coincide, i.e. no polarization.



Lecture 3

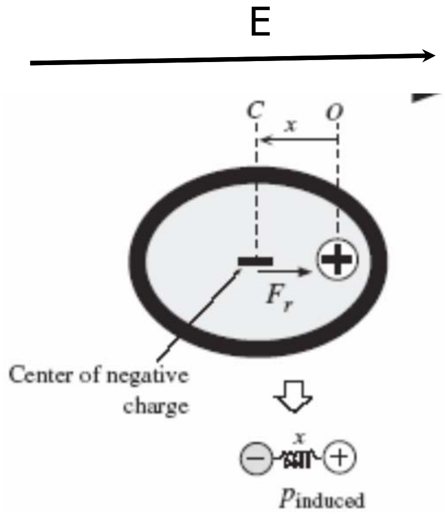
- When E is applied, the displacement of the center of negative charge from the electron cloud with respect to the positive charge in nucleus produces an electric dipole.
- Let α_e be electronic polarizability, then the average induced electronic dipole moment is:

$$\overline{p}_{av} = \alpha_e \overline{E}$$

- Therefore, the relation between the macroscopic ϵ_r and microscopic α properties can be expressed as :

$$\epsilon_r = 1 + \frac{N\alpha}{\epsilon_o}$$

- Since all materials consist of atoms, thus every atom has an electronic polarization. On other words, all insulators are capable of electronic polarization.



Lecture 3

- The applied field E tends to separate the e's from the nucleus. The nucleus can be considered as massive particle that remains fixed while the e' cloud is light that follows E. Let Z be the number of e's. The separation force (F_s) on electrons due to E is expressed as:

$$F_s = (Ze)E$$

- Restoration (attractive) force (F_r) between all the e's and the nucleus tends to return the charge cloud centroid to the nuclear position. Assume the electron cloud is bound to the nucleus by a kind of spring force. Given a separation distance x and a spring constant β_e, thus from Hooke's law:

$$F_r = \beta_e x$$

- Using a classical mechanical system, from Newton's 2nd law and by neglecting damping effect

$$Zm_e \frac{d^2x}{dt^2} = F_s - F_r$$

2.9 DC Electric Field

- For static dc electric field (E=E_o), the net force is zero at **equilibrium** where separation force is balance by restoration force (F_s=F_r).

Then, $(Ze)E_o = \beta_e x_o \qquad and \qquad \frac{d^2x}{dt^2} = 0$

Lecture 3

- The induced electronic dipole moment is then given by:

$$\therefore x_o = \frac{ZeE_o}{\beta_e}$$

$$p_e = (Ze)x_o = \frac{(Ze)^2}{\beta_e}E_o$$

$$and\ \alpha_e = \frac{p_e}{E_o} = \frac{(Ze)^2}{\beta_e}$$

- At the removal of E at t=0, velocity x'(0) = 0 and displacement x(0) = x_o. Solving the differential equation gives a harmonic oscillation

$$x(t) = x_o \cos(\omega_e t)$$

Where $\omega_e = \sqrt{\left(\frac{\beta_e}{Zm_e}\right)}$ is called a **resonance** or natural radial frequency.

- Substituting $\beta_e = Zm_e{\omega_e}^2$ in x_o and α_e, we get

$$x_o = \frac{(Ze)E_o}{(Zm_e){\omega_e}^2} \qquad \text{and} \qquad \alpha_e = \frac{(Ze)^2}{(Zm_e){\omega_e}^2}$$

Lecture 4

2.10 AC Electric Field

- Let E be sinusoidally varying with exponential representation $E = E_o e^{j\omega t}$. Then,

$$Zm_e \frac{d^2x}{dt^2} = F_s - F_r = ZeE \; - \; \beta_e x$$

$$\frac{d^2x}{dt^2} + \omega_e^2 x = (\frac{e}{m_e})E_o e^{j\omega t}$$

- Assume the solution be in the form $x = x_o e^{j\omega t}$, then by substituting in the equation we get,

$$-\omega^2 x_o + \omega_e^2 x_o = (\frac{e}{m_e})E_o$$

- Thus, the displacement amplitude x_o

$$x_o(\omega) = \frac{eE_o}{m_e} \; \frac{1}{\omega_e^2 - \omega^2}$$

- The ac electronic polarizability $\alpha_e(\omega) = \frac{p_e(\omega)}{E(\omega)}$.

$$\therefore \alpha_e(\omega) = \frac{(Ze)x_o}{E_o} = \frac{(Ze)^2}{Zm_e} \; \frac{1}{\omega_e^2 - \omega^2}$$

Lecture 4

- During the oscillation of the charges, they **lose** some of the energy **as heat**. As in classical mechanics, this loss can be represented as a friction force which is proportional to the velocity of the charged particle. Let γ_e be the damping constant per electrons' mass(Zm_e). The equation of motion (Newton's 2nd law) can be extended as

$$\frac{d^2x}{dt^2} + \gamma_e \frac{dx}{dt} + \omega_e^2 x = \left(\frac{e}{m_e}\right) E$$

- Note that the same equation would describe the damped motion of a ball attached to a spring in a rough surface and oscillates by an applied force.

- Assume the solution be in the form $x = x_o e^{j\omega t}$. By solving the equation, we get x, from which we obtain the polarizability in a complex form as

$$\alpha_e^*(\omega) = \frac{(Ze)^2}{Zm_e} \left(\frac{1}{\omega_e^2 - \omega^2 - j\omega\gamma_e}\right)$$

  - The polarizability α_e^* is a complex number. It can be written in the form of real α_e and imaginary α_e' or as magnitude $|\ \alpha_e|$ and phase φ_e , such that

$$\alpha_e^*(\omega) = \alpha_e(\omega) - j\alpha_e'(\omega) = |\alpha_e(\omega)| e^{j\varphi_e(\omega)}$$

Lecture 4

- Recall that $p_e = \alpha_e E$, thus φ_e is the phase of the polarization p_e with respect to E, such that

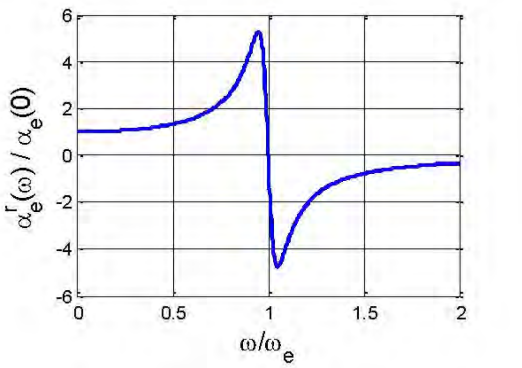
$$p_e = |\alpha_e(\omega)| E_o e^{j[\omega t + \varphi_e(\omega)]}$$

- The frequency dependence of the normalized polarizability $\frac{\alpha_e(\omega)}{\alpha_e(0)}$ versus $\frac{\omega}{\omega_e}$ for $\frac{\gamma_e}{\omega_e} = 0.1$ is shown in the figure for real and imaginary parts and for magnitude and phase components.

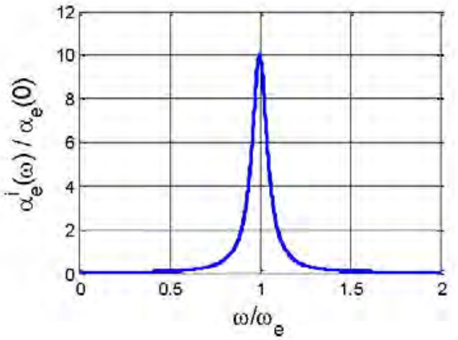
- For low frequencies $(\omega \ll \omega_e)$, α_e goes to DC value with real quantity and thus no phase shift.

$$\alpha_e(\omega) \rightarrow \frac{Ze^2}{m_e \omega_e^2} \ , \varphi(\omega) \rightarrow 0$$

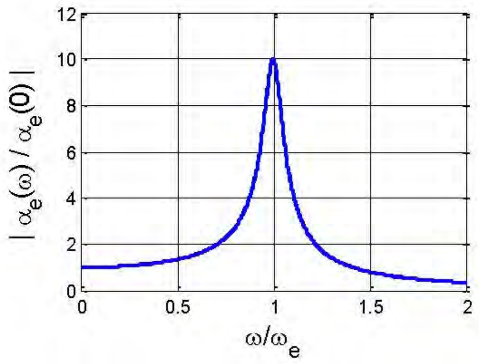
Lecture 4



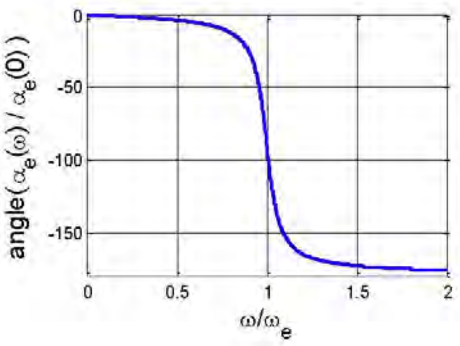
6
4
2
0
-2
-4
-6
0
0.5
1
1.5
2
$\alpha_e^r(\omega) / \alpha_e(0)$
ω/ω_e



12
10
8
6
4
2
0
0
0.5
1
1.5
2
$\alpha_e^i(\omega) / \alpha_e(0)$
ω/ω_e



12
10
8
6
4
2
0
0
0.5
1
1.5
2
$| \alpha_e(\omega) / \alpha_e(0) |$
ω/ω_e



0
-50
-100
-150
0
0.5
1
1.5
2
$\text{angle}(\alpha_e(\omega) / \alpha_e(0))$
ω/ω_e

Lecture 4

- For high frequencies $(\omega \gg \omega_e)$, the dipole can not follow the change of the field E, i.e.$x_o(\omega) \rightarrow 0$

$$\alpha_e(\omega) \rightarrow 0 \quad and \quad \varphi(\omega) \rightarrow -180^o$$

- At resonant frequency $(\omega = \omega_e)$, the polarization is maximum. This leads to a maximum energy transfer from the field to the dipole.

$$|\alpha_e(\omega)| \ \rightarrow \ \frac{Ze^2}{m_e \omega_e \gamma_e} \ , \varphi(\omega_e) \rightarrow -90^o$$

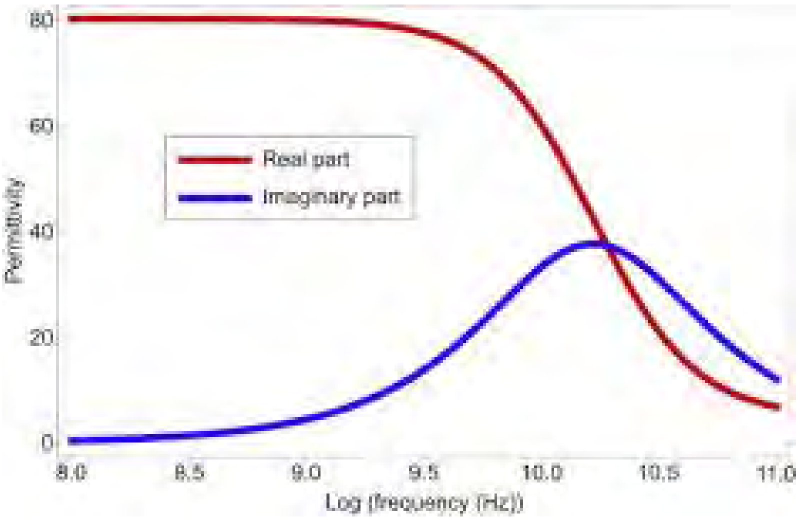
2.11 Complex permittivity

- Recall that the ac polarizability is a complex number $\alpha*(\omega) = \alpha(\omega) - j\ \alpha'(\omega)$. Then, the medium relative permittivity is also a complex number given by

$$\epsilon_r^* = 1 + \frac{N}{\epsilon_o}\alpha^*(\omega) = 1 + \frac{N}{\epsilon_o}\alpha(\omega) - j\frac{N}{\epsilon_o}\alpha'(\omega) = \epsilon_r(\omega) - j\epsilon_r'(\omega)$$

  - *Real part* (ϵ_r) determines the charge storage ability.
  - *Imaginary part* (ϵ_r') represents the energy lost in the dielectric medium due to polarization.

Lecture 4

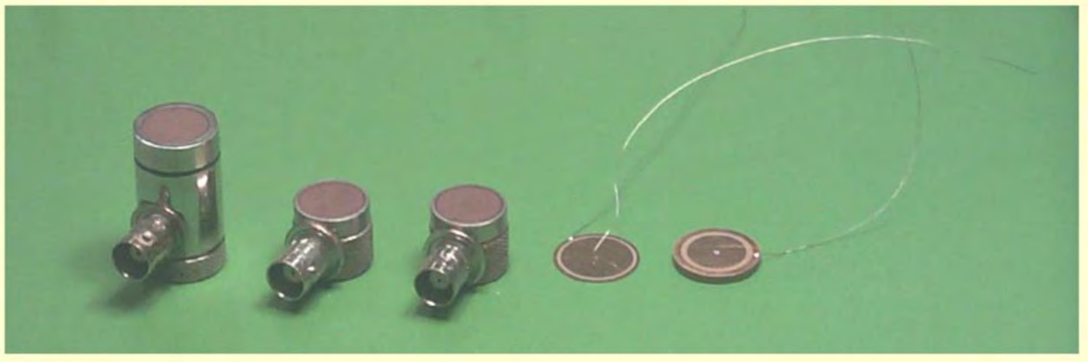

80
60
40
20
0
Permittivity
Real part
Imaginary part
8.0
8.5
9.0
9.5
10.0
10.5
11.0
Log (frequency (Hz))

Lecture 4

2.12 Piezoelectric Crystals

- They are special dielectric crystals which become electrically polarized when they are mechanically stressed.
- Conversely, they become strained when polarized (placed in an electric field)

- The most commonly piezoelectric materials are Quartz (SiO_2) and Barium titanate ($BaTiO_3$).



Lecture 4

2.12 Piezoelectric Effect

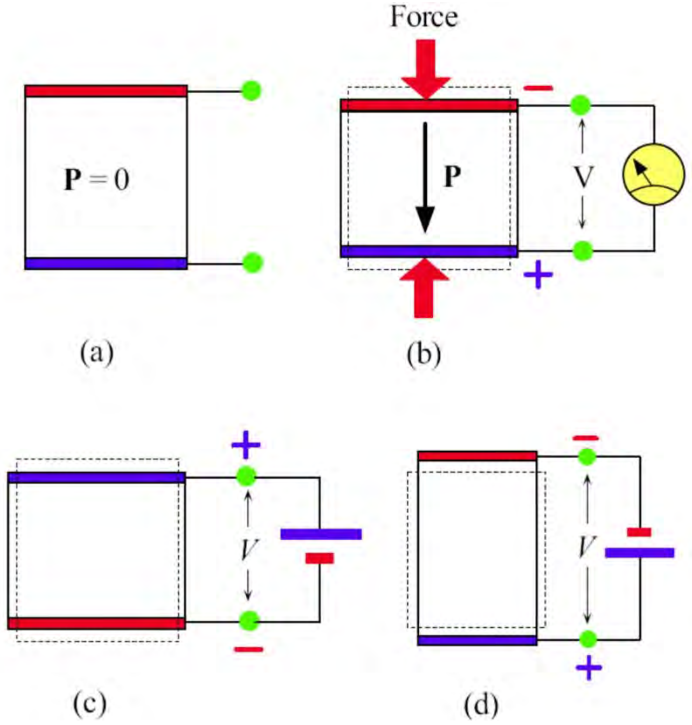
- It was originally discovered in 1880 by Jacques and Pierre Curie.

(a)A crystal with no applied stress or field.

(b) The crystal is strained by an applied force that induces polarization in the crystal and generates surface charges.

(c) An applied field compresses the crystal and causes it to become strained.

(d) The strain changes direction with the applied field and now the crystal is extended



Lecture 4

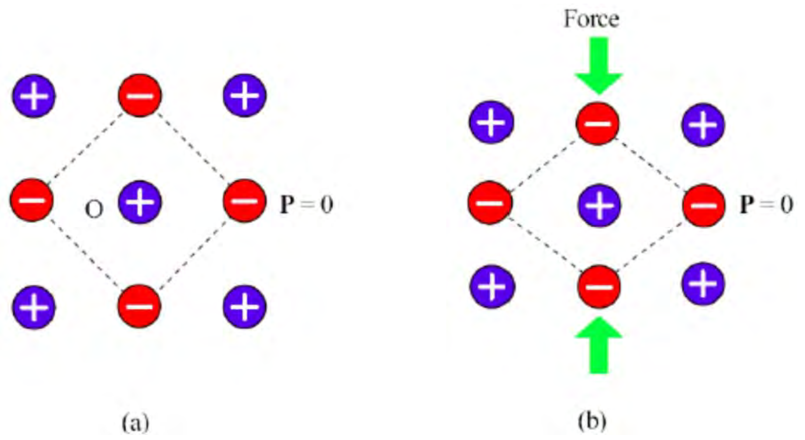
2.13 Crystal Structure

- Only crystal structure with no center of symmetry (noncentrosymmetric) can exhibit piezoelectricity.

☐ *Centrosymmetrical crystal* (Example: NaCl cubic unit cell)

(a) In the absence of an applied force, the centers of mass for positive and negative ions coincide.

(b) This situation does not change when the crystal is strained by an applied force.



(a) (b)

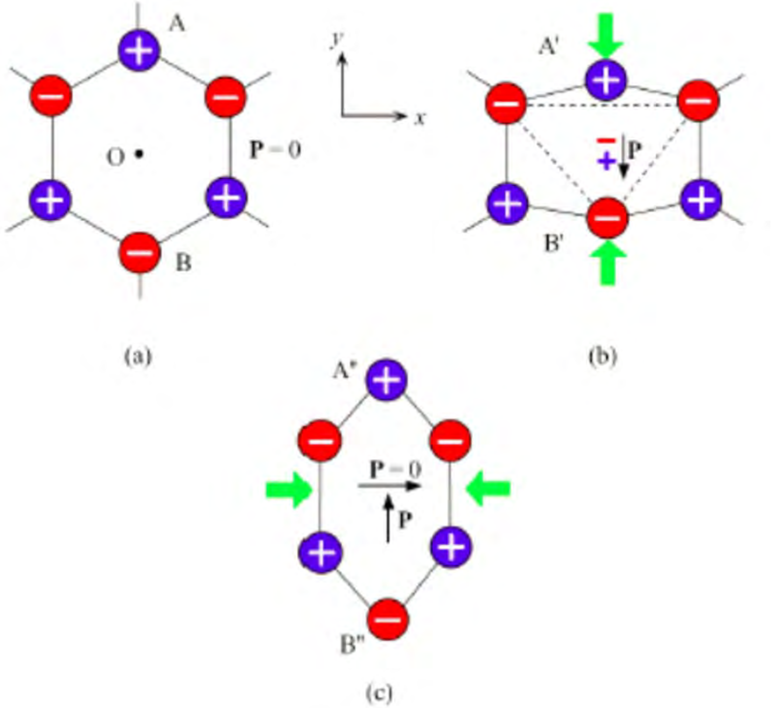
Lecture 4

❑ *Non-Centrosymmetric crystal* (Example: Hexagonal unit cell)

(a)In the absence of an applied force the centers of mass for positive and negative ions coincide.

(b) Under an applied force along y the centers of mass for +ve and –ve ions are shifted which results in a net dipole moment P along y.

(c) When the force is along a different direction, along x, there may not be a resulting net dipole moment in that direction though there may be a net P along a different direction (y).



Lecture 4

2.14 Piezoelectric Coefficients (d_{ij})

- An applied stress in direction *j* can give rise to induced polarization in direction *i* with piezoelectric coefficients d_{ij}.

- Electromechanical transducers

$$P_i = d_{ij} T_j ,$$

$T_j \rightarrow$ Applied mechanical stress (T=F/A)

$P_i \rightarrow$ Induced polarization

The induced strain S_j can as well be expressed as:

$$S_j = d_{ij} E_i$$

where $E_i \rightarrow Applied\ electric\ field$

Lecture 4

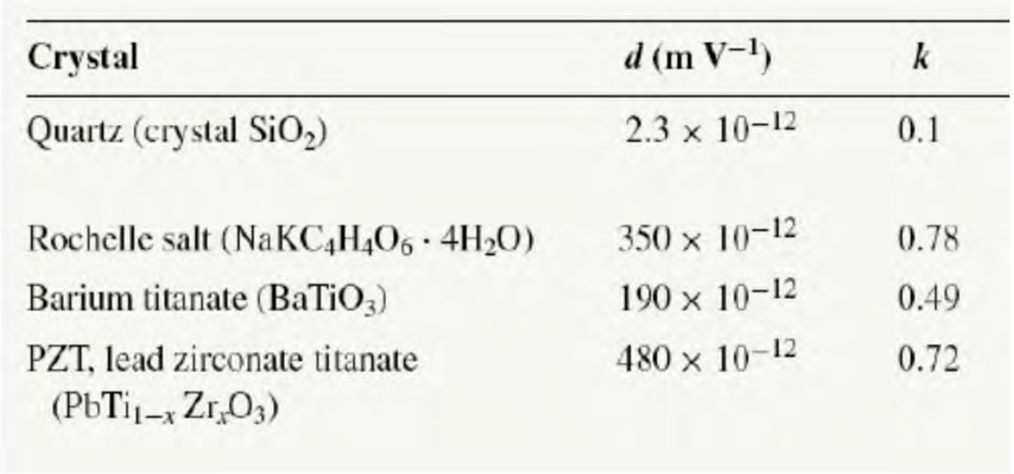
- An engineering factor can be defined by electromechanical coupling factor

$$k^2 = \frac{Electrical\ energy\ converted\ to\ mechanical\ energy}{Input\ of electrical\ energy}$$

- Or equivalently by,

$$k^2 = \frac{Mechanical\ energy\ converted\ to\ Electrical\ \ energy}{Input\ of Mechanical\ \ energy}$$

2.15 Typical Piezoelectric Materials



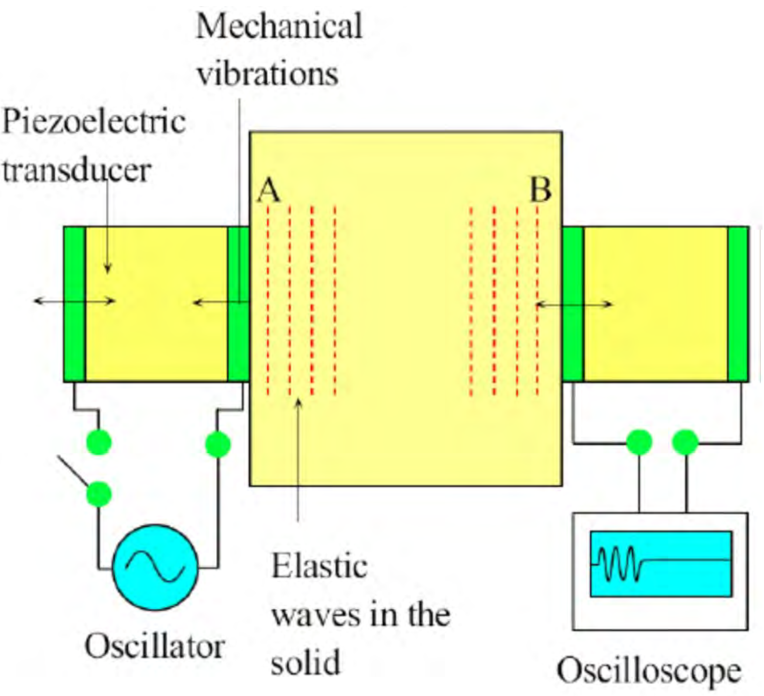
Crystal	***d*** **(m V^{-1})**	***k***
Quartz (crystal SiO_2)	2.3×10^{-12}	0.1
Rochelle salt ($NaKC_4H_4O_6 \cdot 4H_2O$)	350×10^{-12}	0.78
Barium titanate ($BaTiO_3$)	190×10^{-12}	0.49
PZT, lead zirconate titanate ($PbTi_{1-x}Zr_xO_3$)	480×10^{-12}	0.72

Lecture 4

2.16 Applications

❖ Ultrasonic Transducers

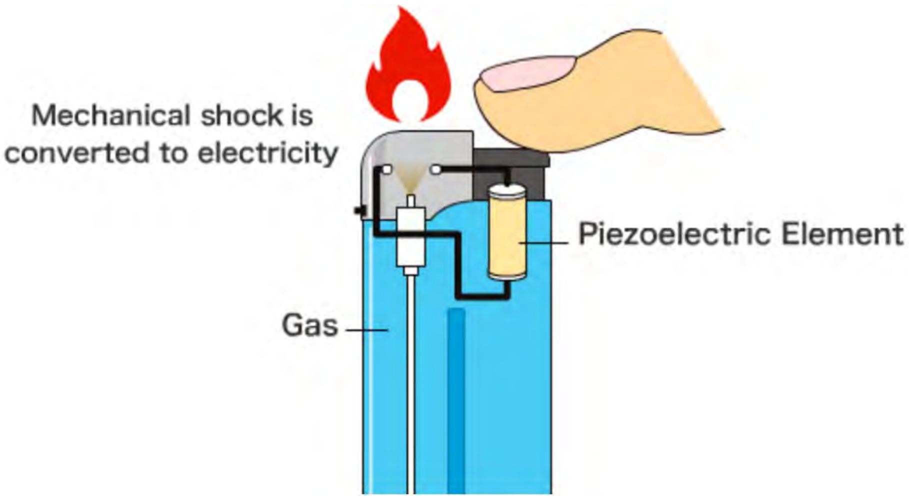
- ❖ The transducer on the left is excited from an ac source and vibrates mechanically.
- ❖ These vibrations are coupled to the solid and generate ultrasonic waves (above audible range).
- ❖ The waves reaches the other end mechanically vibrate the transducer on the right, which converts the vibrations to an electrical signal.
- ❖ It can be used to detect the internal imperfections in the solid.



Lecture 4

❖ Spark Generator

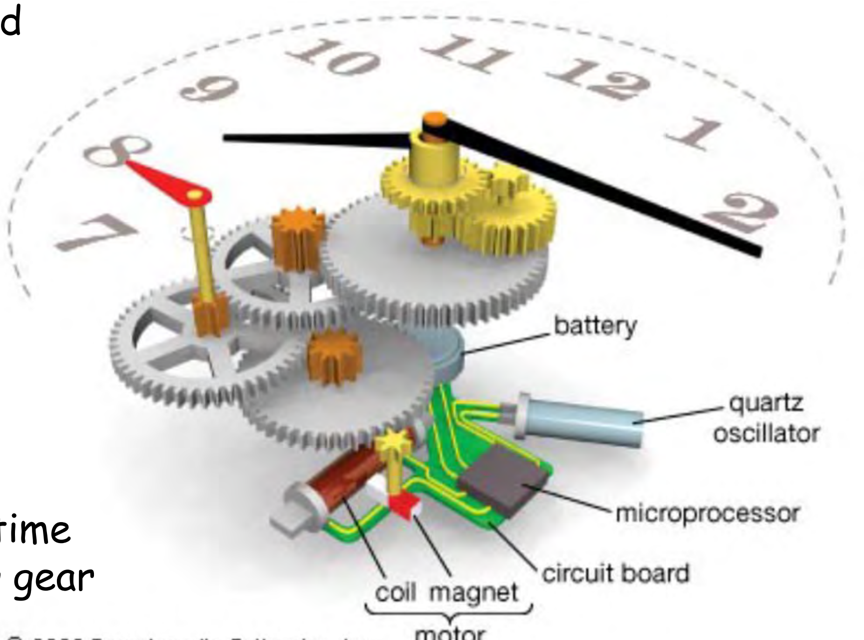
- ❖ The piezoelectric spark generator depends on the phenomenon of dielectric breakdown. It is utilized in lighters, car ignitions, and similar devices.
- ❖ By stressing a piezoelectric crystal, a charge is built up on the electrodes on either side of the spark gap.
- ❖ When the strength of the field across the gap exceeds the dielectric strength of air within the gap, a spark is produced that ignites the fuel.



Lecture 4

❖ Quartz Watches

- ❖ They are battery powered watches different from the old mechanical watches.
- ❖ The battery sends electricity to the quartz crystal through an electronic circuit.
- ❖ The quartz crystal oscillates at a precise frequency: exactly 32768 times each second.
- ❖ The circuit counts the number of vibrations and uses them to generate regular electric pulses, one per second.
- ❖ These pulses can either power an LCD display showing the time numerically or they can drive a small electric motor turning gear wheels that spin the clock's sec, min, and hour hands.



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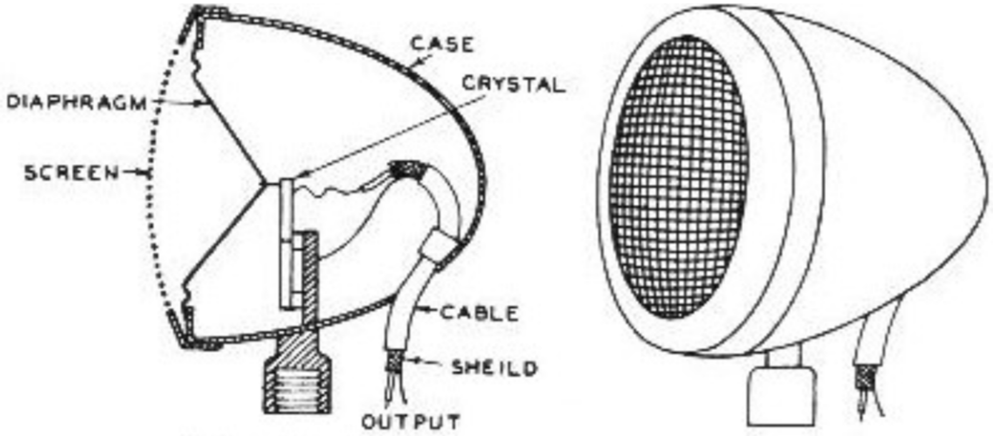
Lecture 4

❖ Microphones



SECTIONAL VIEW PERSPECTIVE VIEW

Lecture 5

Chapter 3: Magnetic Materials

- Many electrical engineering devices utilize the magnetic properties of materials such as inductors, transformers, and rotating machines.

3.1 Inductors

- Consider a long solenoid with free-space medium having a length l and a number of turns N.
- From Ampere's law, the magnetic field intensity H due to a conduction current I flowing through the solenoid windings is given by

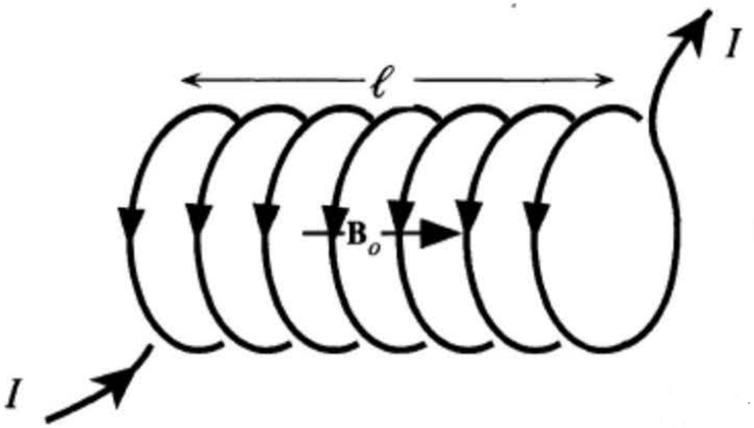
$$H = \frac{NI}{l} = \frac{I_c}{l}$$

where $I_c = NI$ is defined as the conduction current.

- In free-space, the magnetic flux density B_o generated by the current carrying conductor is given by:

$$B_o = \mu_o H = \mu_o (\frac{I_c}{l})$$

where $\mu_o = 4\pi \times 10^{-7} H/m$



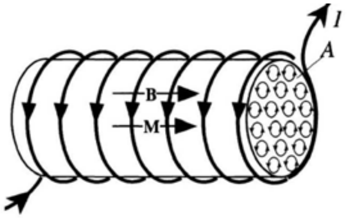
Lecture 5

- The total magnetic flux $N\varphi_o$ threaded per unit current is defined by the inductance

$$L_o = \frac{N\varphi_o}{I} = \frac{NB_oA}{I}$$

- A material medium inserted into the solenoid develops a new magnetic field B along the applied magnetic field B_o. Hence, the inductance becomes

$$L = \frac{N\varphi}{I} = \frac{NBA}{I}$$



- Relative Permeability μ_r

  It is the fractional change in the magnetic field B with respect to the field in free-space B_o. It indicates how easy the material becomes magnetized

$$\mu_r = \frac{B}{B_o} \quad then \quad B = \mu_r\ \mu_o H$$

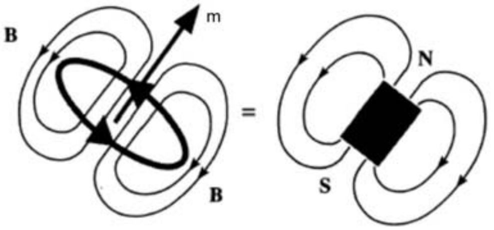
Lecture 5

- Magnetic Permeability $\boldsymbol{\mu}$.

  It is the magnetic field generated per unit magnetizing field.

$$\mu = B/H = \mu_r \ \mu_o$$

3.2. Magnetic Dipole

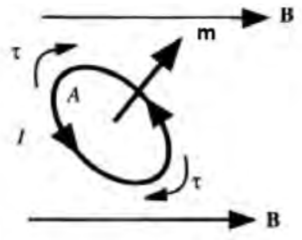


- Consider a loop with area A and carrying current I.
- The current loop creates a magnetic field like a bar magnet.
- The magnetic dipole moment is defined by

$$\mathbf{m} = IA\ \mathbf{a}_n$$

  where $\mathbf{a}_n$ is normal vector.

- When a magnetic moment is placed in a magnetic field, it experiences a torque $\boldsymbol{\tau} = \mathbf{m} \times \mathbf{B}$ that tries to rotate the magnetic moment to align its axis with the magnetic field.



Lecture 5

3.3. Sources of Magnetic Moments

❖ Orbital Magnetic Moment

- Produced due to the electron orbital movement around the nucleus.
- Consider an electron of mass m_e rotate in orbit of radius r with angular frequency ω.
- The electron orbital angular momentum

$$L = m_e v r = m_e \omega r^2$$

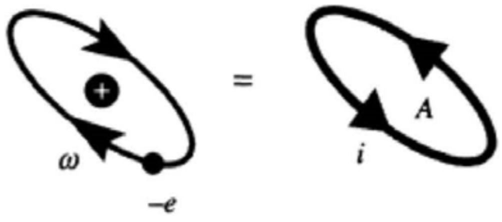
- The orbiting electron behaves like a current loop with current

$$I = e\,\frac{\omega}{2\pi}$$

- The orbital magnetic moment

$$\begin{aligned} m_{orb} &= I A a_n \\ &= -e\frac{\omega r^2}{2}a_n = -\left(\frac{e}{2m_e}\right)L \end{aligned}$$

Where $\left(\frac{e}{2m_e}\right)$ is gyromagnetic ratio

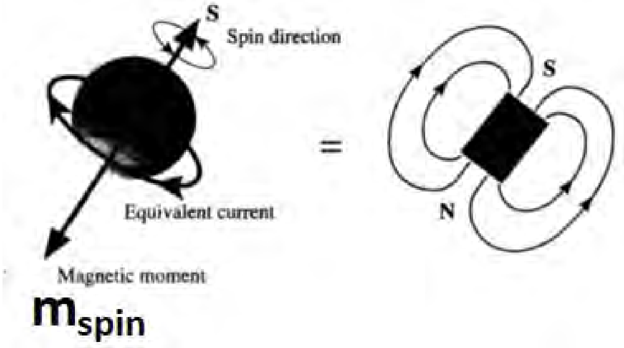


Lecture 5

3.4 Spin Magnetic Moment

- Produced due to the electron spin movement around itself.
- Let **S** be the spin intrinsic angular momentum. The spin magnetic moment

$$m_{spin} = -\left(\frac{e}{m_e}\right)S$$



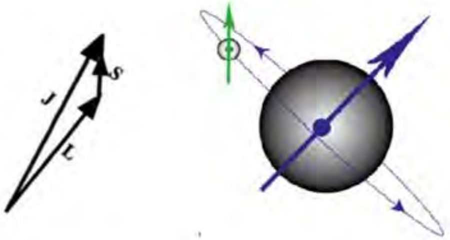
3.6 Total Magnetic Moment

- By vector addition, the total angular momentum

$$\mathbf{J} = \mathbf{L} + \mathbf{S}$$

and the total magnetic moment

$$m = m_{orb} + m_{spin}$$



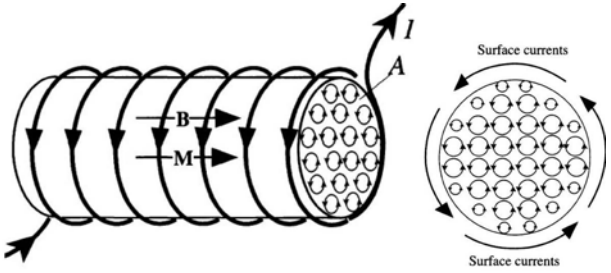
- Noted that: Only incomplete electron shells are considered. For atoms with filled electron shells, total orbital and spin momentums are zero. No magnetic dipole moment.

Lecture 5

3.7 Magnetization Vector

- The magnetic field inside the solenoid due to the conduction current $I_c = NI \; is \; B_o$

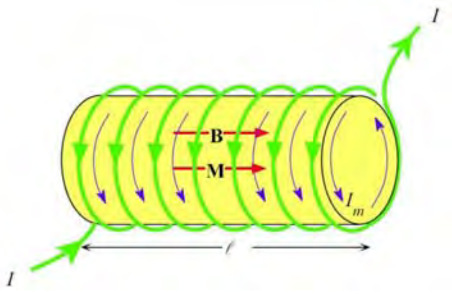
$$B_o = \frac{\mu_o I_c}{l} = \mu_o H$$



- If a material medium is inserted inside the solenoid, each atomic magnetic moment of the material tends to align with the applied field B_o. Thus, a net magnetic moment is developed along B_o and a new field B is built and thus the medium become magnetized.

- Each magnetic moment can be viewed as an elementary current loop circulated in the same direction. Since adjacent currents are in opposite directions and cancel each other. Hence, there is equivalently no internal current and only net induced surface current defined as I_m . Notice that, this is not a flow of free charge carriers.
- The total magnetic moment is

$$\sum_i m_i = I_m A$$



Lecture 5

- The net magnetic moment vector per unit volume of material along B_o is the magnetization vector

$$M = \frac{\sum_i m_i}{vol} = \frac{I_m}{l}$$

3.8 Magnetic Field

- The total field B inside the solenoid arises from the conduction current $I_c = NI$ and the magnetization surface currents I_m.

$$B = B_o + B_m$$
$$= \mu_o \frac{I_c}{l} + \frac{I_m}{l}$$

- Then by definition, the magnetic field is given by,

$$B = \mu_o H + \mu_o M$$

- For linear and isotropic medium (i.e. constant μ_r)

$$B = \mu_o \mu_r H$$

- Then, we have

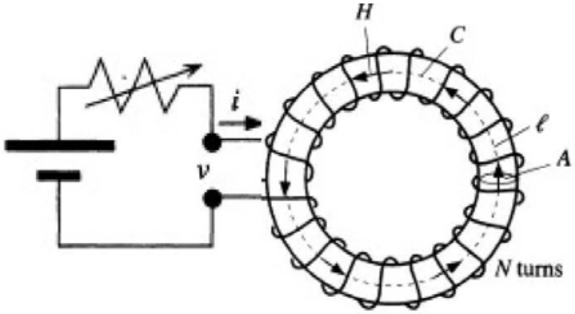
$$M = (\mu_r - 1)H = \chi_m H$$

where χ_m is the magnetic susceptibility.

Lecture 5

3.9 Magnetostatics Energy

- ❖ The **energy** required to establish a magnetic field
- ❖ The potential energy stored in the magnetic field.



- ❖ From Ampere's law:

$$Hl = Ni$$

- ❖ From Faraday's law:

$$v = NA\frac{dB}{dt}$$

Lecture 5

- The electric energy (work) supplied by the battery to increase the field by dB

$$dW = iv\,dt = (Al)\,H\,dB$$

- Work done per unit volume to increase B from B_1 to B_2

$$W_{vol} = \int_{B_1}^{B_2} H dB$$

- For linear magnetic medium (μ_r is constant)

$$B = \mu_o\,\mu_r H$$

- Energy density needed to establish the field B

$$W_{vol} = \frac{1}{2}\mu_r\mu_o H^2 = \frac{B^2}{2\mu_r\mu_o} = \frac{1}{2}HB$$

- This energy is absorbed from the battery and stored as a magnetic potential energy called magnetostatics energy density

Lecture 5

- If the battery is suddenly removed?

- External work comes from stored energy in magnetic field to heat the resistor, current flows for a short while determined by L/R.

3.7 Magnetic Material Classifications

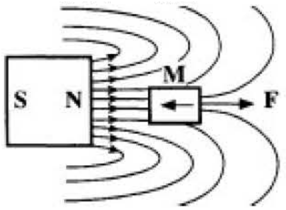
- Magnetic materials are classified into five groups:

- Diamagnetic
- Paramagnetic
- Ferromagnetic
- Antiferromagnetic
- Ferrimagnetic

Lecture 5

Diamagnetism

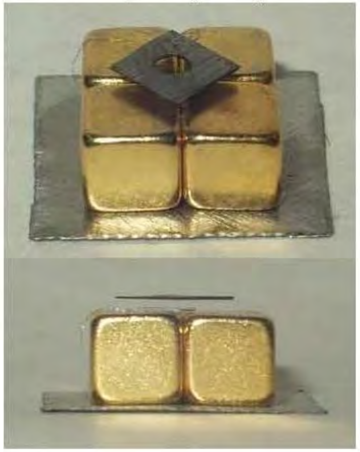
- When a diagnetic substance is placed in a magnetic field B_o, the magnetization vector $\mathbf{M}$ in the material is in the opposite direction to the applied field B_o and the resulting field $\mathbf{B}$ within the material is less than B_o . This repels the diamagnetic material away from a permanent magnet.
- Accordingly, diamagnetic materials have magnetic susceptibility χ_m that is negative and small ~ 10^{-6} Relative permeability $\mu_r = \chi_m$+1 is slightly < 1.
- Atoms of the diamagnetic materials have closed subshells and shells. Example: Neon which has 10 electrons in an atom.



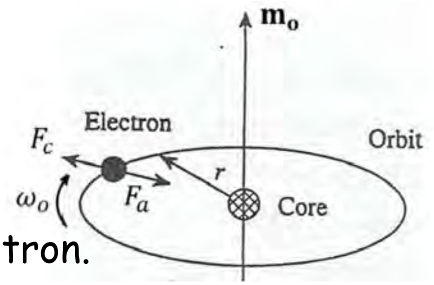
- Covalent and many ionic crystals are examples of diamagnetic materials.
- In absence of applied field $B_o = 0$, each atom in the material has no permanent magnetic moment such that: $m_{atom} = m_{orb} + m_{spn} = 0$.

Lecture 5

- Superconductors are perfect diamagnetic with $\chi_m = -1$ or μ_r = 0 and $\boldsymbol{B}$ = $\mathbf{0}$. Thus, they expel the applied fields, and no field can be established inside the material.
- Application is the diamagnetic Levitation where an object can be made to float in the air above a strong magnet.
  - Simple Model



- Consider a simple atomic model with nuclear charge Ze and an electron in a circular orbit of radius r about the nucleus and having angular frequency ω_o.
- Two forces affected the electron:



1. The coulomb force between e' and nucleus.

$$F_a = \frac{Ze^2}{4\pi\varepsilon_o r^2}$$

2. The centrifugal force F_c of the orbiting electron.

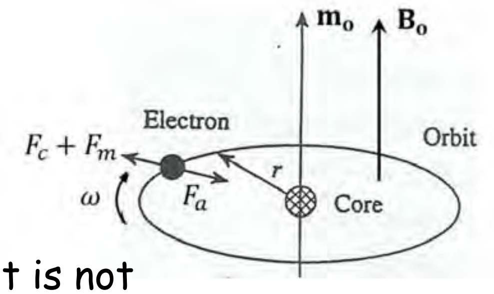
$$F_c = m_e \omega_o^2 r$$

Lecture 5

- With the absence of an applied magnetic field, the attractive coulomb force F_a will be exactly balanced by the centrifugal force F_c . Such that $F_a = F_c$.
- The electron magnetic moment in the absence of the applied field.

$$m_o = \frac{e\omega_o r^2}{2} a_n$$

- Suppose a magnetic field B_o is applied in the same direction of m_o



- The field produces an outward force on the orbiting electron known as the Lorentz force.

$$F_m = e\omega r B_o$$

- Since the orbital radius is quantized, assume that the magnetic field effect is not large enough to cause a change in the radius of the circular orbit. Thus, the inward Coulomb force F_a is also unchanged.
- To balance the outward magnetic force F_m, the orbital angular velocity will change to reduce the outward centrifugal force F_c and becomes ω.

Lecture 5

- By equating the forces, we get

$$F_c + F_m = F_a$$
$$m_e\omega^2 r + e\omega r B_o = m_e\omega_o^2 r$$

- Solving the equation

$$\omega = -\frac{eB_o}{2m_e} + \frac{1}{2}\sqrt{(\frac{eB_o}{m_e})^2 + 4\omega_o^2}$$

- For the case of $\frac{eB_o}{m_e} \ll \omega_o$

$$\therefore \omega = -\frac{eB_o}{2m_e} + \omega_o$$

- The change in the angular frequency due to B results in slow down of the orbiting electron.

- The new magnetic moment

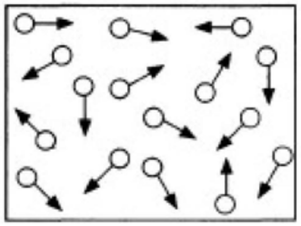
$$m = \frac{e\omega r^2}{2} a_n$$

Lecture 6

Paramagnetism

- Paramagnetic materials have a magnetic susceptibility χ_m that is positive and small ~10^{-5}.
- Each atom has a permanent small net magnetic moment due to unpaired electrons. Example: Al which has 13 electrons in an atom.

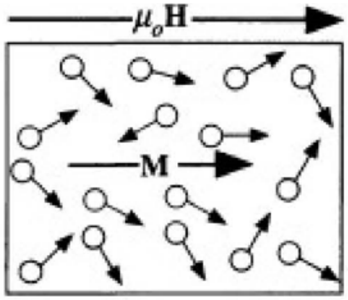
- Many metals are paramagnetic materials.
- In the absence of an applied field **H** = **0**, magnetic moments tend to be randomly oriented due to thermal fluctuations where the average magnetic moment $m_{av} = 0$ and thus magnetization **M** = **0**.



Lecture 6

- In the presence of applied field $\mathbf{H}$, individual magnetic moments tend to be aligned along H and $M = \chi_m H$ is finite and along $\mathbf{H}$.

- Notice that M decreases with increasing temperature due to molecular collisions which destroy the alignments of molecular moments with the applied field.



  - Ferromagnetic Materials
    - Ferromagnetism

- In these materials, the atomic magnetic moments align in the same direction without applying an external magnetic field H. Thus, ferromagnetic materials exhibit permanent magnetization.

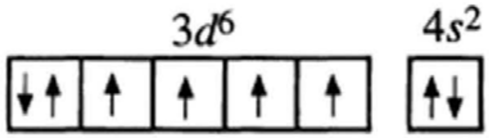
- The susceptibility χ_m is (+ve) and (very large)

- By Hund's rule, electrons try to align their spins.

- By Pauli exclusion principle, parallel spins must occupy different orbitals and hence different spatial distribution.

Lecture 6

- Example: the iron Fe atom [Ar]$3d^6\ 4s^2$.

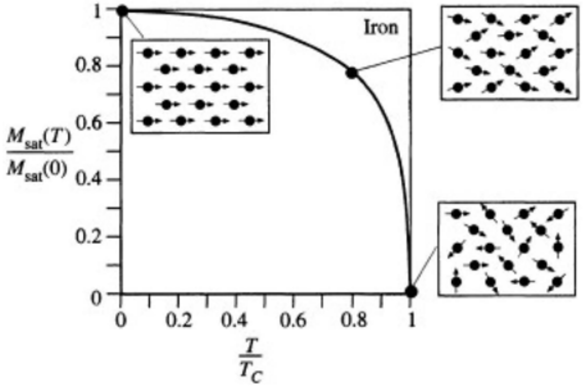


  - Saturation Magnetization

- Maximum magnetization that happens at a given temperature when all the magnetic moments are aligned in the applied field direction.

- As temperature increases, lattice vibrations become more energetic, which leads to a frequent disruption of the alignments of the spins.

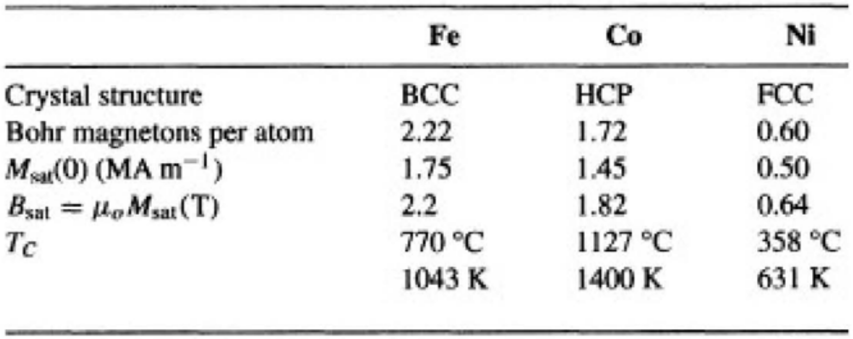
- At temp T = T_c (Curie temp), the thermal energy can overcome the potential energy of the exchange interaction that aligns the spins and hence destroy the spin alignments.



- Above T_c, the ferromagnetic behavior disappears, and the crystal behaves as paramagnetic.

- Some properties of the ferromagnets can be summarized in the following table.

Lecture 6

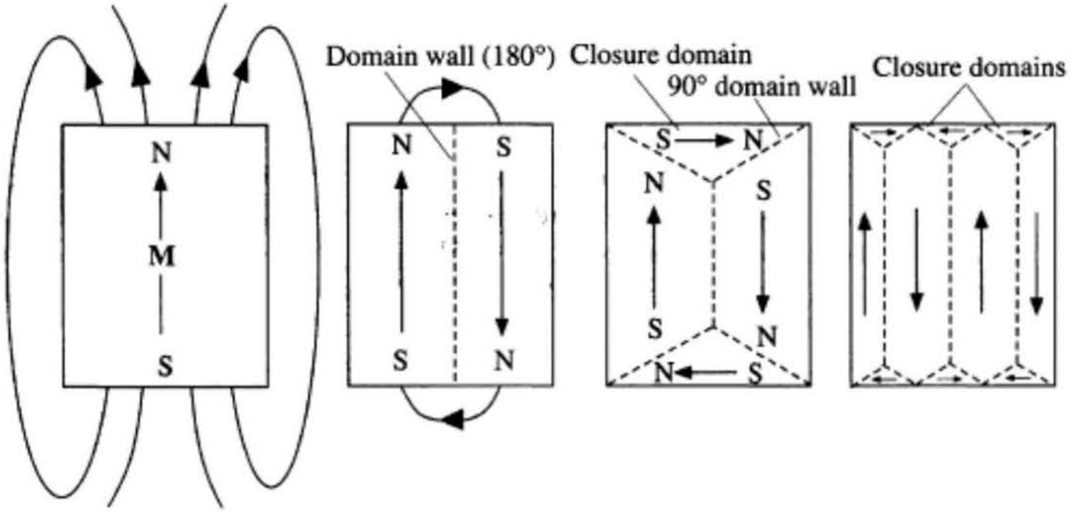


	Fe	Co	Ni
Crystal structure	BCC	HCP	FCC
Bohr magnetons per atom	2.22	1.72	0.60
$M_{sat}(0)$ (MA m^{-1})	1.75	1.45	0.50
$B_{sat} = \mu_o M_{sat}(T)$	2.2	1.82	0.64
T_C	770 °C	1127 °C	358 °C
	1043 K	1400 K	631 K

Magnetic Domain

- A magnetic domain is a region in which all the spin magnetic moments are aligned to produce a magnetic moment in one direction only.
- If a magnetized piece of iron is heated to a temperature about T_c and then allowed to cool in the absence of a magnetic field, it will possess no net magnetization. This is due to the formation of several magnetic domains that effectively cancel each other.

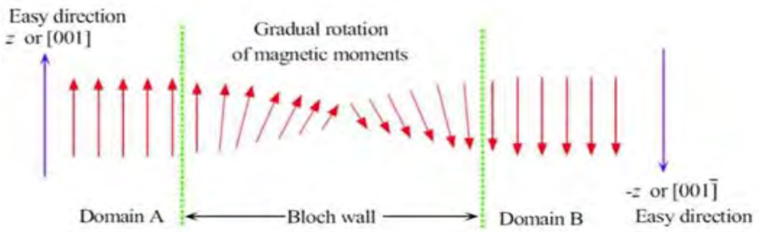
Lecture 6



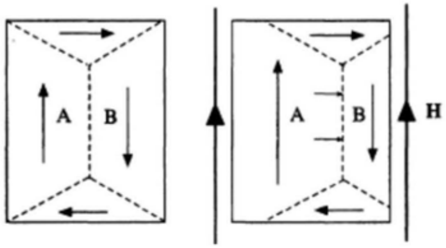
- ❖ For a single domain, the iron crystal is like a bar magnet with external magnetic field.
- ❖ Formation of two domains reduces the external magnetic field lines and there is now less potential energy stored in the magnetic field.
- ❖ Several domains with certain arrangements can eliminate the external fields and the specimen appears unmagnetized.

Lecture 6

Domain Walls



- Domain wall (or Bloch wall), is the region between two domains where the direction of magnetization changes from one direction to the opposite direction.
- In a Bloch wall, the neighboring spin magnetic moments rotate gradually, and it takes several hundred atomic spacings to rotate the magnetic moment by 180^o.
- When an external magnetic field $\mathbf{H}$ is applied, the domains with magnetizations along $\mathbf{H}$ is enlarged due to the rotation of the magnetic moments in the wall by the applied field.
- As a result, the domain wall between A and B migrates into domain B and the specimen now acquires net magnetization.

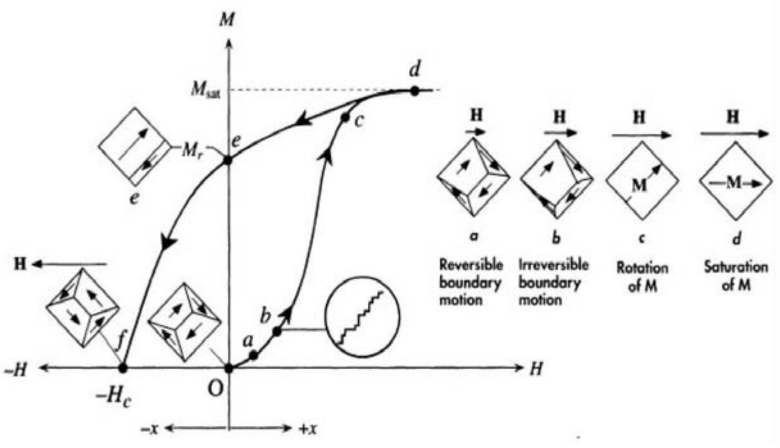


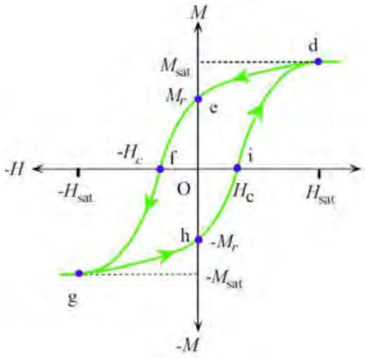
Hysteresis Loop

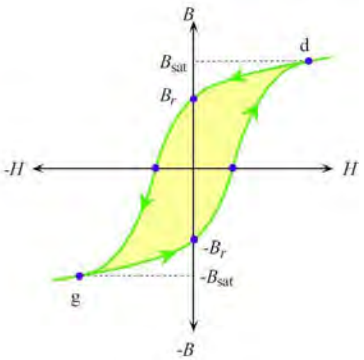
- As discussed before, the structure of the domain in an unmagnetized iron crystal will possess no net magnetization.

Lecture 6

- Consider applying an external magnetic field $\mu_o H$ along some direction. The M or B versus H behavior of a ferromagnetic through one cycle is called the hysteresis loop.
  - (o → d) Increases the applied field (magnetizing)
  - (d) M is aligned along H (saturation magnetization)
  - (d → e) Decrease and remove magnetizing field H
  - (e → f) Applying H in reverse direction
  - An M or B versus H hysteresis curve for a full cycle.

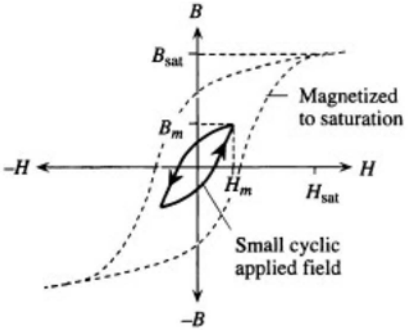






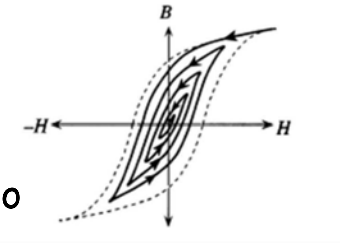
Lecture 6

- ❖ The hysteresis loop depends on the magnitude of the applied field. It can reach some maximum value $B_m\ less\ than\ B_{sat}$.



➢ Demagnetization

- ❖ It can be demagnetized by cycling the field intensity with a decreasing magnitude until the origin is reached.



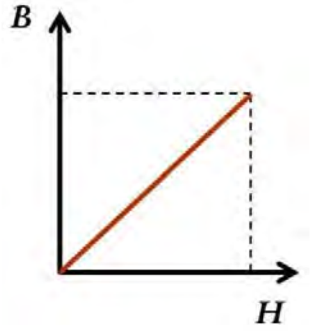
➢ Hysteresis Loss

- ❖ Recall that the energy per unit volume supplied to increase the field by dB is

$$dW_{vol} = H\ dB$$

- ❖ For a linear relation between B and H where μ_r is constant

$$B = \mu_o \mu_r H$$



Lecture 6

- The total energy stored in the magnetic field

$$W_{vol} = \frac{1}{2}HB$$

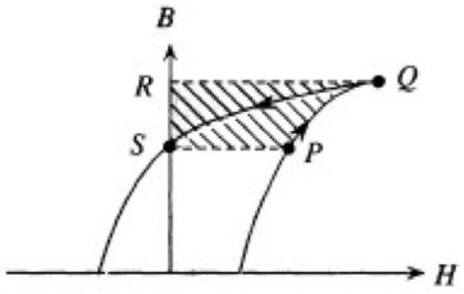
- For ferromagnetic, the total energy density to increase B from $B_r to\ B_{sat}$ = Area (PQRS)

$$W_{vol} = \int_{B_r}^{B_{sat}} HdB$$

- Energy returned from the field = Area (QRS)

- The difference is the energy dissipated in moving and rotating the domain walls.

- Over one full cycle, energy density dissipated (E_h) = total hysteresis loop area



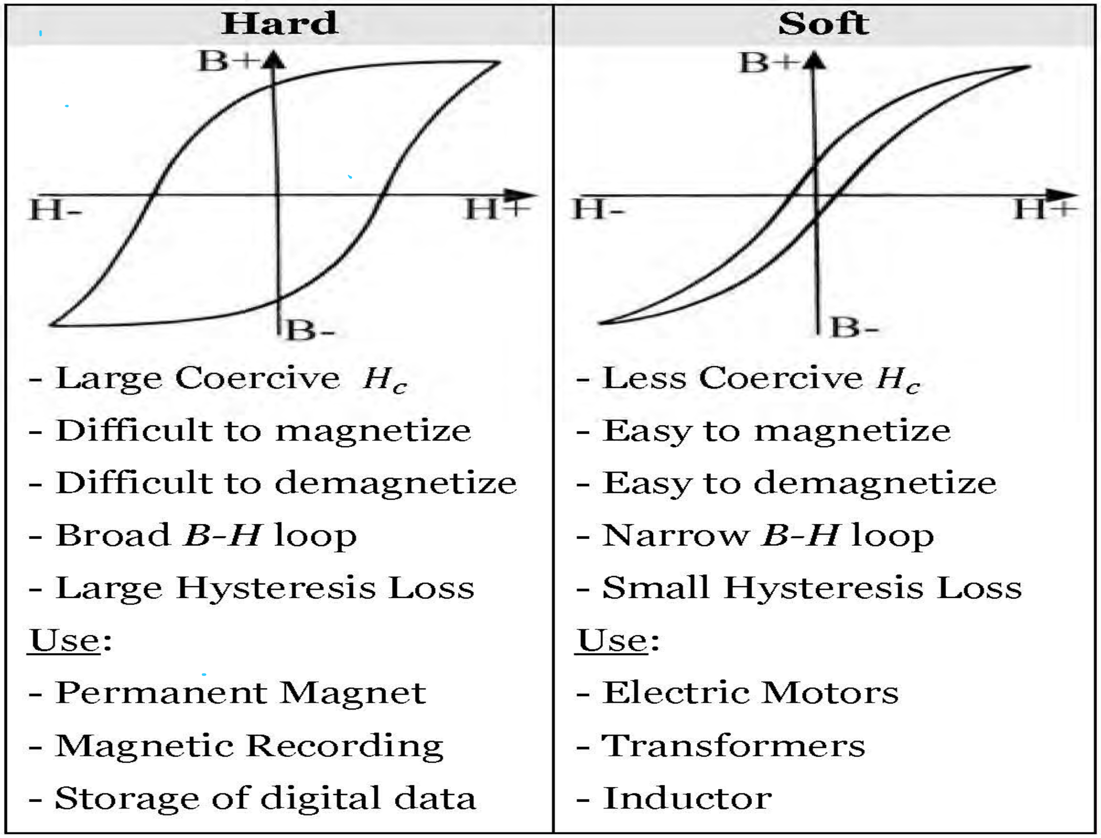
- Hysteresis power loss for AC field of f frequency

$$P_h = E_h f$$

Lecture 6

- Hard and Soft Magnetic Materials

❖ Based on the B-H behavior, engineering ferromagnetic materials are classified into soft and hard magnetic materials.

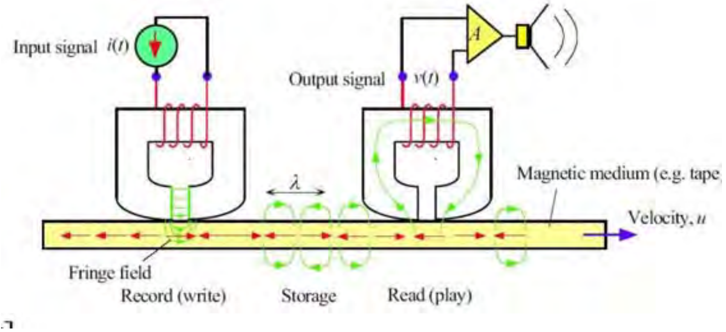


Hard	Soft
- Large Coercive H_c	- Less Coercive H_c
- Difficult to magnetize	- Easy to magnetize
- Difficult to demagnetize	- Easy to demagnetize
- Broad B-H loop	- Narrow B-H loop
- Large Hysteresis Loss	- Small Hysteresis Loss
Use:	Use:
- Permanent Magnet	- Electric Motors
- Magnetic Recording	- Transformers
- Storage of digital data	- Inductor

Lecture 6

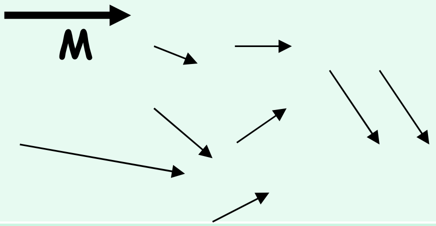
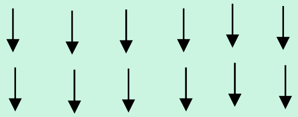
Application – Magnetic Storage

- Storage of data on magnetized medium.
- A form of non-volatile memory.
- Information is stored as
  - ☐ A magnetization pattern (analog form) or
  - ☐ A binary magnetization state (digital form).
- Magnetic materials are found in
  - ☐ Magnetic heads to write, read, and erase.
  - ☐ Magnetic media to store the information.
- Magnetic medium includes hard disks, floppy disks, audio and video tapes … etc.
- Example: Audio cassette



Lecture 6

Summary of Magnetic Materials

Property	**Description**
Diamagnetic	B=0, $m_{orb} = m_{spin}$; net magnetization =0 B is applied, produces a magnetic moment in opposite direction to B. Repelled when brought near a bar magnet. χ_m is negative.
Paramagnetic 	B=0, $m_{orb} \neq m_{spin}$; resulting in a net magnetic moment B is applied, magnetic moment increases. Internal interaction and thermal agitation tend to weaken this increase. (partial alignment only) Attracted when brought near a bar magnet. χ_m is positive.
Ferromagnetic 	Alignment is enhanced quantumly through phenomenon known as exchange coupling or "domains". Above curie temperature T_C, the material becomes a paramagnetic one (magnetic moment of adjacent atoms align in the same direction.)

Lecture 6

Property	Description
Antiferromagnetic ↓ ↑ ↓ ↑ ↓ ↑	Magnetic moment is nil even in the presence of a magnetic field
Ferrimagnetic ↑ ↓ ↑ ↓ ↑ ↓	Adjacent atoms align oppositely, and they have unequal dipole moments. Weaker than ferromagnetic, like ferrite (low electrical conductivity) useful for cores of ac inductors and transformers.
Super ferrimagnetic	It is a ferromagnetic material suspended in dielectric (plastic). Good for Audio, Video, and data recording systems.

Introduction to Quantum Mechanics

Lecture 1

I. Four contradictions between theory and experiment:

1. EM theory: Moving charged particles emit continuous radiations. Experiment: Discrete frequencies
2. EM theory: Moving charged particles emit radiations. Experiment: Electrons on stable orbits do not.
3. Electrons usually come out from a metal surface upon irradiating by light of any frequency. Experiment: Threshold frequency for every metal.
4. Tunneling

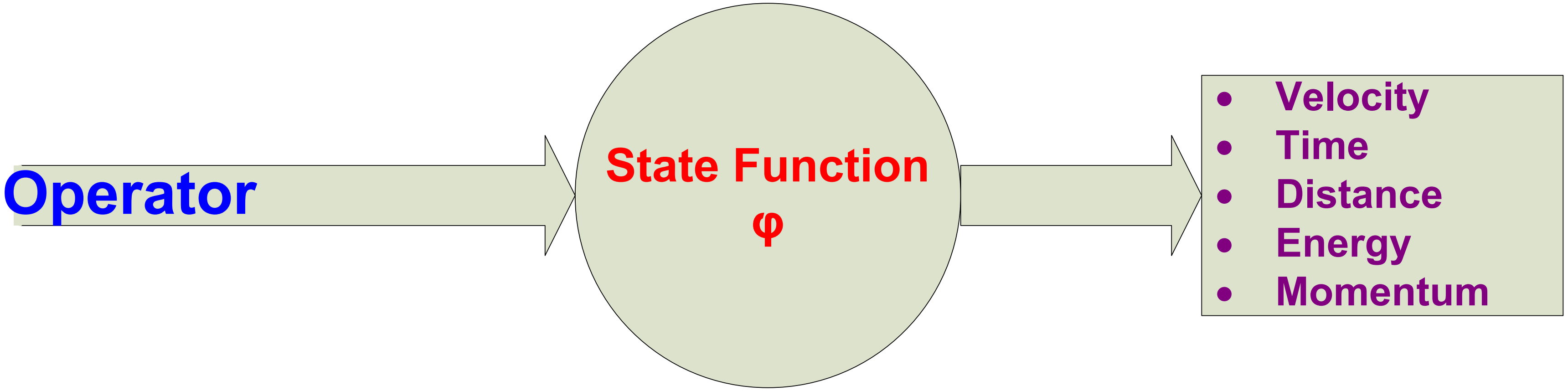
Lecture 1

Classical mechanics: Observables and measurable quantities

Quantum mechanics: Fictitious quantities

There exists a state function φ which contains all information about the system.

Requires operators



Operator

State Function φ

- **Velocity**
- **Time**
- **Distance**
- **Energy**
- **Momentum**

Lecture 1

II. Postulates of quantum mechanics:

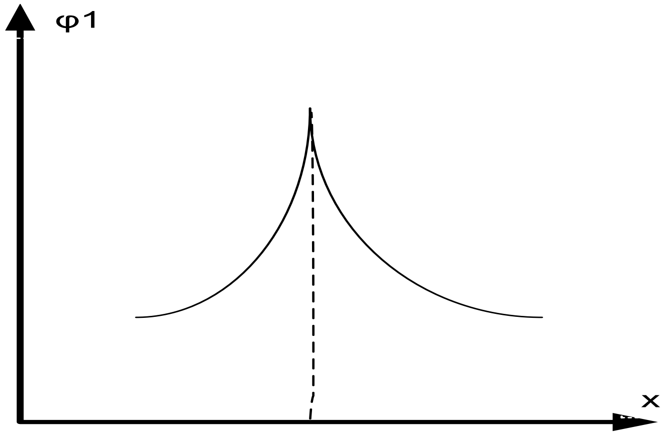
Postulate # 1

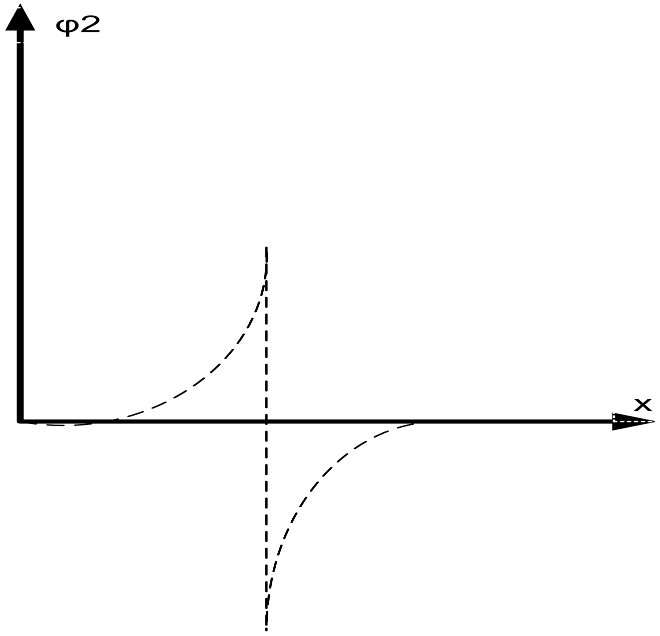
For very dynamical system, there exists a function $\varphi(x, y, z, t)$ which contains all information about the system, this function has to be:

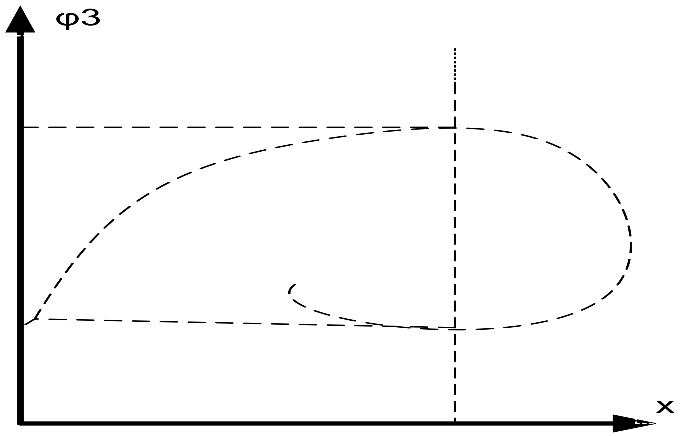
i- finite
ii- single-valued
iii- continuous up to the 1st derivative.

Examples:

Lecture 1





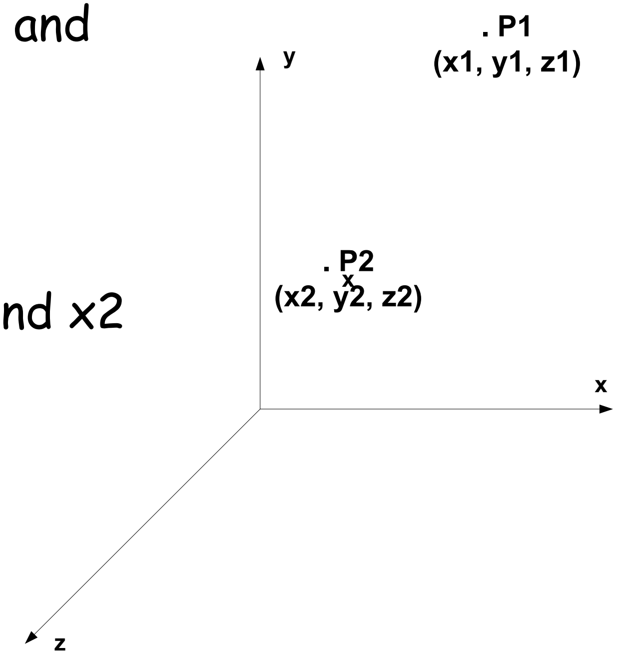


Lecture 1

Configuration space $\boldsymbol{\tau}(\ x, y, z)$:

It is the space containing all valid possible coordinates x, y, and z. i.e. the space through which a given function is defined.

Example: To trace the two particles P1 and P2, we define a configuration space composed of six coordinats (x1, y1. z1 and x2 ,y2, z2)



Lecture 1

The elemental volume of the configuration space:

$$d\tau = dxdydz$$

In a multidimensional system:

$$d\tau = \overset{i}{\pi} dq_i = dq_1 dq_2 dq_3 \dots \dots . .$$

Lecture 1

Postulate # 2

The probability of observing a system at an instant t inside an elemental volume $d\tau$ is the function

$$\varphi\varphi^* d\tau$$

Therefore the integration over the whole configuration is unity

$$\int_\tau \phi\phi^* d\tau = \int |\phi|^2 d\tau = 1$$

$\varphi\ should\ be\ square\ integrable\ \ i.e.\ \ \epsilon$ Hilbert space.

Lecture 1

Postulate # 3

To every dynamic quantity L (energy, position, momentum) there corresponds a linear operator $\underline{L}$ which is Hermitian.

Examples of operators of some basic quantities:

1. Position operator

$$\underline{Q_i}\,\varphi = q_i\,\varphi$$

$$\underline{X}\varphi = x\varphi$$

$$\underline{Y}\varphi = y\varphi$$

Lecture 1

2. Time operator $\underline{T}$

$$\underline{T}\varphi = t\,\varphi$$

3. Linear momentum operator $-j\hbar\vec{\nabla}$

$$-j\hbar\vec{\nabla}\,\varphi = -j\hbar\left(\frac{\partial}{\partial x}\,a_x + \frac{\partial}{\partial y}\,a_y + \frac{\partial}{\partial z}\,a_z\right)\varphi$$

Where:

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

$$and\quad \vec{\nabla}\,F(x,y,z) = \left[\frac{\partial}{\partial x}\,a_x + \frac{\partial}{\partial y}\,a_y + \frac{\partial}{\partial z}\,a_z\right] F(x,y,z)$$

Lecture 1

worth noting that:

Operators are related with the same algebraic formulae which tie the dynamic quantities.

for example

Velocity operator = $\frac{position\ operator}{time\ operator}$

i.e. $\underline{V} = \frac{\underline{Q}}{\underline{T}}$

Lecture 2

So far the systems dealt with are assumed in eigen states.

Eigen state means the operator results directly in its dynamical quantity.

$$\varphi \ \ becomes \ \ \psi$$

and $\underline{L}\ \psi = \lambda\,\psi$

Where λ *is known as the eigen value.*

Lecture 2

Postulate #4

The state function should satisfy the equation:

$$\underline{H}\varphi = j\hbar\frac{\partial\varphi}{\partial t}$$

Which is known an Schrödinger equation. Wave equation or more precisely Schrödinger wave equation. Where $\underline{H}$ is the Hamiltonian (energy) operator.

Hamiltonian Operator:

If a system happens to be in an eigen state of $\underline{H}$ then φ becomes ψ.

$$\underline{H}\psi = j\hbar\frac{\partial\psi}{\partial t}$$

$$\underline{H}\psi = E\psi$$

Lecture 2

Where E is the eigen value of $\underline{H}$. The above equation is known as time-dependent Schrödinger equation and can be rewritten as:

$$\frac{\partial \psi}{\partial t} = - j \frac{E}{\hbar} \psi$$

Postulate #5

The expected or average value <A> of an observable A when a system in a state ,
which is not an eigen state , is given by:

$$< A > = \int_{\tau} \varphi^{*} \underline{A} \, \varphi \, d\tau$$

Lecture 2

III. Functions and operators:

Functions: convert a number into another number

$$F(x) = x^2$$

$$X = 4 \rightarrow \quad F(x) = 16$$

Operators: A recipe to convert a function into another function

1. Multiplication operator $\underline{A}$

$$\underline{A}\, F(x) = x\, F(x).$$

Example:

$$F(x) = a + bx + cx2$$

$$\text{then, } \underline{A}\, F(x) = ax + bx2 + cx3.$$

Lecture 2

2. Differentiation operator $\underline{D}$

$$\underline{D}\, f(x) = \frac{d}{dx}\, f(x)$$

3. Integration operator $\underline{B}$

$$\underline{B}\, f(x) = \int f(x)dx$$

4. Laplacian operator $\underline{\nabla^2}$

$$\underline{\nabla^2}\, f(x,y,z) = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial y^2}$$

Lecture 2

5. Identity operator $\underline{E}$

$$\underline{E}\, f(x) = f(x)$$

6. Inversion operator $\underline{I}$

$$\underline{I}\, f(x) = f(-x)$$

7. Translation operator $\underline{T_a}$

$$\underline{T_a} f(x) = f(x+a)$$

8. Rotation operator $\underline{C_n}$

$$\underline{C_n}\, f(\vartheta) = f(\vartheta + \frac{2\pi}{n})$$

9. Partial derivative operator $\underline{D_x}$

$$\underline{D_x}\, f(x,y) = \frac{\partial\, f(x,y)}{\partial x}$$

Lecture 2

Linear operators:

$\underline{L}$ is called a linear operator if it satisfies the following relation:

$$\underline{L}[af_1(x,y,z)+bf_2(x,y,z)]=a\underline{L}\ f_1(x,y,z)+b\underline{L}\ f_2(x,y,z)$$

Superposition is satisfied.

Example of linear operators:

$$\underline{D_x}\ (ax+bx^2+cd)=a+2bx$$

$$a\underline{D_x}\ x+b\underline{D_x}x^2+\ \underline{D_x}bc=a+2bx+0=a+2bx$$

Lecture 2

Example of a nonlinear operator:

Assume an operator $\underline{G}$

$$\underline{G}\, f(x) = f(x)\,\frac{df(x)}{dx}$$

Let $f_1(x) = ax \qquad and \qquad f_2(x) = b(x^2 + \mathrm{c})$

$$\begin{aligned} \underline{G}[f_1(x) + f_2(x)] &= \underline{G}[ax + b(x^2 + c)] \\ &= [ax + bx^2 + bc][a + 2bx] \\ &= 2b^2x^3 + 3abx^2 + (a^2 + 2b^2c)x + abc \end{aligned}$$

Lecture 2

Now applying $\underline{G}$ to each function separately,

$$f_1(x) = ax$$
$$f_2(x) = b(x^2 + \mathrm{c})$$

$$\underline{G}\, f_1(x) + \underline{G}\, f_2(x) = axa + b(x^2 + c).2bx$$

$$= 2b^2x^3 + (a^2 + 2b^2c).x$$

$$\neq \underline{G}[f_1(x) + \ f_2(x)]$$

Lecture 2

Operators' Properties:

Two main properties usually encountered on quantum mechanics.
Let $\underline{A}\ and\ \underline{B}$ be two linear operators

1. Distributive law

If,

$$\left(\underline{A} + \underline{B}\right) f(x) = \underline{A}\, f(x) + \underline{B}\, f(x)$$

Then,

$\underline{A}$ and $\underline{B}$ are associative.

2. Commutative law

If,

$$\underline{A}\,\underline{B}\ f(x) = \underline{BA}\ f(x)$$

Then,

$\underline{A}$ and $\underline{B}$ commute

Lecture 2

Generally linear operators do not commute

$$\underline{A}\,\underline{B} \neq \underline{B}\,\underline{A}$$

$$\underline{A}\,\underline{B} - \underline{B}\,\underline{A} \neq 0$$

$$[\underline{A},\ \underline{B}] = \underline{A}\,\underline{B} - \underline{B}\,\underline{A}$$

Commutator = $[\underline{A},\ \underline{\boldsymbol{B}}]$ = 0 operators commute, $\neq 0$ *operators do not commute*

Example of non commuting operators

$$\underline{A} = \frac{d}{dx}, \underline{B} = x$$

$$\underline{AB}y = \frac{d}{dx}(\underline{B}y) = \frac{d}{dx}(x.y) = x.\frac{d}{dx} + y$$

$$\underline{BA}y = x.\frac{dy}{dx} \neq \underline{AB}y$$

$$so, [A, B] = y \neq 0$$

Lecture 3

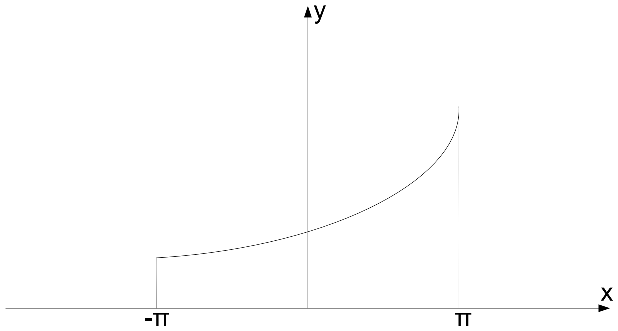
IV. Eigen functions and eigen values:

The state function φ is an eigen function ψ of an operator $\underline{L}$ if $\underline{L}\,\psi = \lambda\,\psi$, where λ is a constant.

$$\psi \text{ is called the eigen function of } \underline{L}$$
$$\text{and } \lambda \text{ is the eigen value}$$

Example:

Consider a function $y_k = e^{\lambda_k x}$ defined over a configuration space $-\pi \le x \le \pi$



Lecture 3

This function y_k is an eigen function of the derivative operator $\underline{L} = \frac{d}{dx}$.

$$\underline{L}\, y_k = \lambda_k e^{\lambda_k x} = \lambda_k y$$

Eigen values could be real or imaginary.

$$y_k = e^{j\lambda_k x}$$

For the 1st derivative operator $\underline{D}$ $the\ eigen\ value\ is\ imaginary$:

$$\underline{D}\, y_k = j\lambda_k\, y_k$$

While for the 2nd derivative operator $\underline{M} = \frac{d^2}{dx^2}\ it\ is\ real$

$$\underline{M}\, y_k = -\lambda_k^2\, y_k$$

For the function $y_k = e^{-j\lambda_k x}$, $\underline{M}\, y_k = -\lambda_k^2\, y_k$.

Which means that the eigen value $-\lambda_k^2$ belongs to two different eigen functions $e^{\pm j\lambda_k x}$.

Lecture 3

Such an eigen value is called a two-fold degenerate eigen value, it belongs to two different eigen functions.

In general one can find n-fold degenerate eigen value.

V. Hermetian operators:

If φ_1 and φ_2 are two functions belonging to the same class of functions and $\underline{L}$ is a linear operator , acting on these two functions, is said to be Hermetian if:

$$\int_{\tau} \phi_1^*(\underline{L}\phi_2)d\tau = \int_{\tau} \phi_2(\underline{L}^*\phi_1^*)d\tau$$

The integration is carried out over the whole configuration space τ . A different simpler way to express the Hermeticity of an operator is to write:

$$(\phi_1, \underline{L}\phi_2) = (\underline{L}\phi_1, \phi_2)$$

The quantity to the left of the comma is always complex conjugate

Lecture 3

Example:

The operator $\underline{L} = aj\frac{d}{dx}$ is Hermetian when applied to square integrable functions, i.e. functions which belong to Hilbert space.

$$(\varphi_1, \underline{L}\,\varphi_2) = \int_\tau \varphi_1^*(\underline{L}\,\varphi_2)\, d\tau$$

$$= \int_{-\infty}^{\infty} \varphi_1^*\,(a\,j\frac{d\varphi_2}{dx})\,dx$$

$$= a\,j\int_{-\infty}^{\infty} \varphi_1^*(d\,\varphi_2)$$

$$= a\,j\,\left[(\varphi_1^*\,\varphi_2)\,\Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \varphi_2\,d\,\varphi_1^*\right]$$

Lecture 3

φ_1 and φ_2 are assumed to be square integrable functions , i.e. their values go to zero as x goes to infinity.

$$(\varphi_1, \underline{L}\varphi_2) = -aj \int_{-\infty}^{+\infty} \varphi_2 \frac{d\varphi_1^*}{dx}\, dx$$

$$= \int_{-\infty}^{+\infty} \varphi_2 \left(-aj \frac{d\varphi_1^*}{dx}\right) dx$$

$$= \int_{-\infty}^{+\infty} \varphi_2 (\underline{L}^* \varphi_1^*)\; dx$$

$= (\underline{L}\, \varphi_1, \varphi_2)$ Therefore $\underline{L}$ is Hermetian

Lecture 3

Theorem:

The eigen values of Hermetian operators are real.

Proof:

$$\underline{L}\psi = \lambda\psi \qquad (1)$$

Taking the complex conjugate of the last equation results in

$$\underline{L}^*\psi^* = \lambda^*\psi^* \qquad (2)$$

Pre-multiply equation (1) by ψ^* gives:

$$\psi^*\underline{L}\psi = \psi^*\lambda\psi \qquad (3)$$

Lecture 3

Integrating equation (3) over the whole configuration space

$$\int_\tau \Psi^* \underline{L} \Psi \, d\tau = \int_\tau \Psi^* \lambda \, \Psi d\tau$$

$$= \lambda \int_\tau \Psi^* \; \Psi d\tau \qquad (4)$$

Pre-multiply Equation (2) by Ψ :

$$\Psi \underline{L}^* \, \Psi^* = \Psi \lambda^* \Psi^* \qquad (5)$$

Integrate equation (5) over the whole configuration space

$$\int_\tau \psi L^* \psi^* d\tau = \int_\tau \psi \lambda^* \psi^* d\tau = \lambda^* \int \psi \psi^* d\tau \qquad (6)$$

Lecture 3

Comparing equation 4 and equation 6 and Since L is a Hermetian operator, then

$$\int_{\tau} \psi^* L \psi d\tau = \int_{\tau} \psi L^* \psi^* d\tau$$

$$\lambda^* \int_{\tau} \psi^* \psi d\tau = \lambda \int_{\tau} \psi^* \psi d\tau$$

$$\lambda = \lambda^* \therefore \lambda\, is\; real$$

we are ultimately interested in observable quantities i.e. real values, here comes the importance of Hermetian operators.

Lecture 3

Hamiltonian (ENERGY) Operator $\underline{H}$:

Consider a single particle of mass M moving with a velocity v in a potential field V (x,y,z,t) in a conservative system and get its energy

$$E = \frac{1}{2} m v^2 + V(x, y, z, t)$$

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

$$\therefore E = \frac{p^2}{2m} + V(x, y, z, t)$$

$$\underline{p} = -j\hbar\nabla$$

Lecture 3

$$\underline{H} = \frac{p^2}{2m} + V(x,y,z,t)$$

$$\underline{H} = \frac{-\hbar^{-2}\nabla^2}{2m} + V(x,y,z,t)$$

The last equation is known as the Hamiltonian operator

Angular Momentum Operator:

L is the linear momentum $= m\overline{v}$
The angular momentum = Iω
I is the rotational moment of inertia = $m\,r^2$

Lecture 3

$$V_r = v\cos\alpha$$

$$V_\theta = v\sin\alpha$$

$$L = mr^2\,\omega$$

$$= mr\,.\,r\omega$$

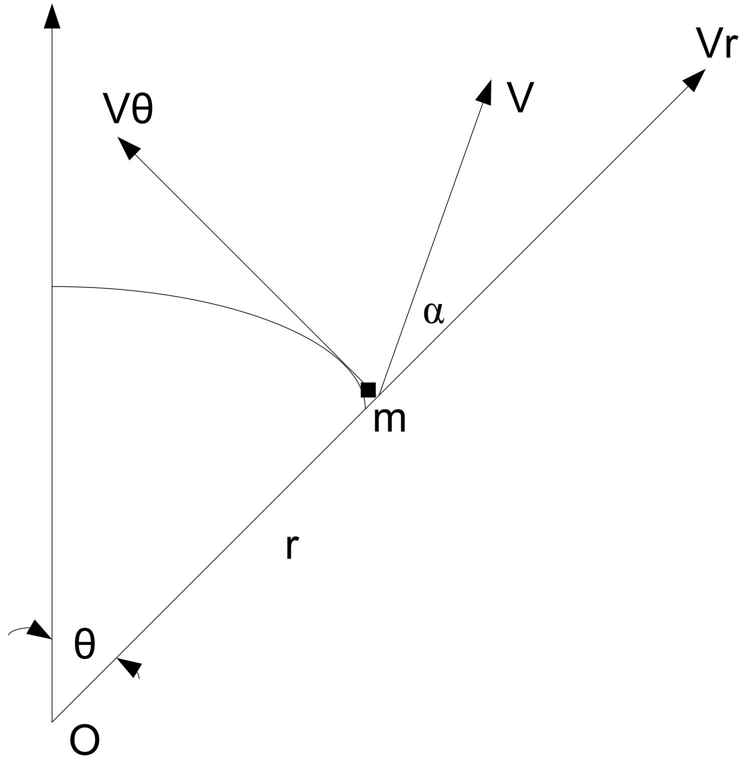
$$= mr\,.\,V_\theta$$

$$L = mr\ v\ sin\ \alpha$$

$$L = p.r.\sin\alpha = \vec{r}\times\vec{p}$$

$$\underline{\underline{L}} = \underline{r}\times\underline{p} = rx(-j\hbar\nabla)$$

$$= -j\hbar\,(\vec{r}\times\vec{\nabla})$$



Lecture 3

Components and properties of Angular momentum operator:

$$\underline{L} = \underline{L}_x a_x + \underline{L}_y a_y + \underline{L}_z a_z$$

$$= -j\hbar \underline{r} \times \underline{\nabla}$$

$$= -j\hbar \begin{bmatrix} a_x & a_y & a_z \\ x & y & z \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \end{bmatrix}$$

$$\therefore \ \underline{L}_x = -j\hbar \left[y \frac{\partial}{\partial z} - z \frac{\partial}{\partial y} \right]$$

$$\underline{L}_y = -j\hbar \left[z \frac{\partial}{\partial x} - x \frac{\partial}{\partial z} \right]$$

$$\underline{L}_z = -j\hbar \left[x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right]$$

Lecture 3

The commutator:

$$[\underline{L}_x, \underline{L}_y] = \underline{L}_x\,\underline{L}_y - \underline{L}_y\,\underline{L}_x$$

$$\underline{L}_x\;\underline{L}_y = -\hbar^2\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)$$

$$= -\hbar^2\left[y\frac{\partial}{\partial z}z\frac{\partial}{\partial x} - z^2\frac{\partial}{\partial x}\frac{\partial}{\partial y} - xy\frac{\partial^2}{\partial z^2} + xz\frac{\partial}{\partial y}\frac{\partial}{\partial z}\right]$$

$$\underline{L}_y\,\underline{L}_x = -\hbar^2\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)$$

$$= -\hbar^2\left(zy\frac{\partial}{\partial x}\frac{\partial}{\partial z} - xy\frac{\partial^2}{\partial z^2} - z^2\frac{\partial}{\partial x}\frac{\partial}{\partial y} + x\frac{\partial}{\partial z}z\frac{\partial}{\partial y}\right)$$

$$\underline{L}_x\underline{L}_y - \underline{L}_y\underline{L}_x = -\hbar^2\left[y\frac{\partial}{\partial z}z\frac{\partial}{\partial x} - yz\frac{\partial}{\partial x}\frac{\partial}{\partial z} + xz\frac{\partial}{\partial y}\frac{\partial}{\partial z} - x\frac{\partial}{\partial z}z\frac{\partial}{\partial y}\right]$$

Lecture 3

$$\underline{L}_x \underline{L}_y - \underline{L}_y \underline{L}_x = -\hbar^2 \left\lfloor y\frac{\partial}{\partial z} z \frac{\partial}{\partial x} - yz\frac{\partial}{\partial x}\frac{\partial}{\partial z} + xz\frac{\partial}{\partial y}\frac{\partial}{\partial z} - x\frac{\partial}{\partial z} z\frac{\partial}{\partial y} \right\rfloor$$

$$= -\hbar^2 \left\lfloor z\frac{\partial}{\partial z}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) + \frac{\partial}{\partial z} z \left(y\frac{\partial}{\partial x} - x\frac{\partial}{\partial y}\right) \right\rfloor$$

$$= -\hbar^2 \left(z\frac{\partial}{\partial z}\left(\frac{j\underline{\underline{L}}_z}{\hbar}\right) - \frac{\partial}{\partial z}\left(\frac{z\,j\underline{\underline{L}}_z}{\hbar}\right)\right)$$

$$= -j\hbar \left\lfloor z\frac{\partial \underline{\underline{L}}_z}{\partial z} - z\frac{\partial \underline{\underline{L}}_z}{\partial z} - \underline{L}_z \right\rfloor = j\hbar \underline{L}_z$$

$$\therefore \left[\underline{L}x, \underline{L}y\right] = j\hbar \underline{L}_z$$

$$\underline{L} \times \underline{L} = j\hbar \underline{L}$$

Lecture 3

Inner product of the angular momentum operator:

$$\underline{L}\,.\,\underline{L} = \underline{L_x^2} + \underline{L_y^2} + \underline{L_z^2}$$

$$\left\lfloor \underline{L}^2, \underline{L}_{x,y,z} \right\rfloor = 0$$

Lecture 4

If a system is in a state φ:

$$\underline{H}\varphi = j\hbar\frac{\partial\varphi}{\partial t}$$

In an eigen state Ψ:

$$\underline{H}\psi = E\psi = j\hbar\frac{\partial\psi}{\partial t}$$

then

$$\frac{\partial\psi}{\partial t} = -j\frac{E\psi}{\hbar}$$

Whose solution is

$$\psi = \psi(x.y.z)e^{\frac{-jEt}{\hbar}}$$

which means that we can solve the time independent equation and eventually we multiply by

$$e^{\frac{-jEt}{\hbar}}$$

Lecture 4

For a system in a state φ *you can get the average of any physical dynamical quantity* A *as such*:

$$< A >= \int_{\tau} (\varphi^{*} \underline{A} \varphi) d\tau$$

We need now to prove that the above equation indeed represents a probabilistic average of A. i.e. it resembles throwing a die a very large number of times. If the number 1 through 6 represents a temperature in degree Celsius, the probabilistic average of temperature would be:

$$< T >= 1 * \frac{1}{6} + 2 * \frac{1}{6} + 3 * \frac{1}{6} + 4 * \frac{1}{6} + 5 * \frac{1}{6} + 6 * \frac{1}{6} = 3.\frac{1}{2}\, o_{C}$$

Lecture 4

V. Orthogonal Functions:

A set of functions is said to be orthogonal in the interval (a , b) if for any two members of the set

$$\int_a^b f_i^*(x)\, f_j(x)\, dx = a_j\ \delta_{ij}$$

$$\delta_{ij} = 1 \quad \text{for } i = j$$

and 0 elsewhere

a_j is a non-zero positive constant and δ_{ij} is the Kronecker δ

If a_j =1 the set is an orthonormal set, and we can always normalize an orthogonal set by dividing each function by $\sqrt{a_j}$

$$\frac{1}{a_j^{1/2} a_j^{1/2}} \int f_i^*(x)\, f_j(x)\, dx = \frac{a_j}{a_j^{1/2} a_j^{1/2}}\, \delta_{ij} = \delta_{ij}$$

Lecture 4

Fourier series → periodic function → sum of sines and cosines.

Orthogonal functions → sines and cosines.

Likewise: A state function → sum of orthogonal functions.

$$\varphi = \sum_{i=1}^{n} C_i\, f_i(x) \qquad C_i \quad \text{is a constant}$$

If C_i are all zeros except one this means that φ belongs to the set and cannot be expressed in terms of the orthogonal function

Multiply both sides of the above equation by f_i^* and integrate from a to b

$$\int_a^b f_j^*(x)\varphi \mathrm{dx} = \int_a^b f_j^*(x) \sum^{n} C_i f_i(x) dx$$

Lecture 4

$$\int_a^b f_j^* (x)\varphi \mathrm{dx} = \int_a^b f_j^*(x) \sum_{i=1}^{n} C_i f_i(x) dx$$

$$= C_j a_j$$

$$\mathrm{c}_j = \frac{1}{\mathrm{a}_j} \int_a^b \mathrm{f}_j^* \phi \, \mathrm{dx}$$

$$\phi = \sum_{i=1}^{n} \left(\frac{1}{\mathrm{a}_j} \int_a^b \mathrm{f}_j^* . \varphi \, \mathrm{dx} \right) \mathrm{f}_i(\mathrm{x})$$

Lecture 4

THEOREM:

Any two different eigen functions with non-degenerate eigen values of a Hermetian operator are orthogonal

PROOF:

Let ψ_1 and ψ_2 be two eigen functions of a Hermetian operator $\underline{L}$ with eigen values

$$\lambda_1 \text{ and } \lambda_2 \ (\lambda_1 \text{ is not equal } \lambda_2)$$

$$\underline{L}\,\Psi_1 = \lambda_1\Psi_1$$
$$\underline{L}\,\Psi_2 = \lambda_2\Psi_2$$

Lecture 4

Pre-multiply the first equation by Ψ_2^* *and integrate over the whole configuration space*

$$\int_\tau \Psi_2^* \, \underline{L}\Psi_1 d\tau = \lambda_1 \int_\tau \Psi_2^* \, \Psi_1 d\tau$$

Taking the complex conjugate of the second equation and premutiply by Ψ_1 and integrate over the whole configuration space

$$\int_\tau \psi_1 \left(\underline{L}\psi_2\right)^* d\tau = \lambda_2 \int_\tau \psi_1 \psi_2^* d\tau$$

$\underline{L}$ *is a Hermetian operator*

$$\int_\tau \psi_2^* \underline{L} \psi_1 d\tau = \int_\tau \psi_1 \left(\underline{L}\psi_2\right)^* d\tau$$

Lecture 4

One can now write from the last two equations

$$\therefore(\lambda_1 - \lambda_2)\int_{\tau}\psi_1\psi_2^{*}d\tau = 0$$

and from the quantum mechanical postulate

$$\therefore\int_{\tau}\psi_1^{*}\psi_1 d\tau = 1$$

Therefore Ψ_1 *and* Ψ_2 are orthonormal functions

So any well behaved function can be expressed as a sum of non-degenerate eigen functions of a Hermetian operator

Lecture 4

Exercise:

Prove that the state function $\varphi = C_1\psi_1 + C_2\psi_2$ is not an eigen function of an operator $\underline{L}$ whose nondegenerate eigen functions are ψ_1 and ψ_2 .

$$\phi = c_1\psi_1 + c_2\psi_2$$

$$\underline{L}\phi = \underline{L}\left(c_1\psi_1 + c_2\psi_2\right)$$

$$= c_1\underline{L}\psi_1 + c_2\underline{L}\psi_2$$

$$= c_1\lambda_1\psi_1 + c_2\lambda_2\psi_2$$

Lecture 4

Since λ_1 *is not equal to* λ_2 *.then*

$$\underline{L}\,\varphi \neq \lambda\phi$$

and φ *is not an eigen function of* $\underline{L}$.

From the QM postulates $\int_\tau \varphi^*\varphi d\tau = 1$

$$\int_\tau \left(c_1\psi_1 + c_2\psi_2\right)^* \left(c_1\psi_1 + c_2\psi_2\right) d\tau = 1$$

$$\int_\tau \left(c_1^*\psi_1^* + c_2^*\psi_2^*\right)\left(c_1\psi_1 + c_2\psi_2\right) = 1$$

Lecture 4

$$c_1^* c_1 \int_\tau \psi_1^* \psi_1 \, d\tau + c_1^* c_2 \int_\tau \psi_1^* \psi_2 \, d\tau + c_2^* c_1 \int_\tau \psi_2^* \psi_1 \, d\tau + c_2^* c_2 \int_\tau \psi_2^* \psi_2 \, d\tau = 1$$

$$c_1^* c_1 + c_2^* c_2 = 1$$

$$|c_1|^2 + |c_2|^2 = 1$$

Lecture 4

$$\phi = \sum_{i=1}^{n} c_i \psi_i$$

Where $c_i = \int_\tau \psi_i^* \phi \, d\tau$

$$\int_\tau \phi^* \underline{A} \phi \, d\tau = \int_\tau \sum_{i=1}^{n} c_i^* \psi \, d\tau \left(\underline{A} \sum_{i=1}^{n} c_i \psi i \right) d\tau$$

$$= \int_\tau \sum_{i=1}^{n} \left(c_i^* \psi_1^* \right) \left(\underline{A} \sum_{i=1}^{n} c_i \psi_i \right) d\tau$$

$$= \int_\tau \sum_{i=1}^{n} c_i^* \psi_1^* \left(\sum_{i=1}^{n} c_i \lambda_i \psi_i \right) d\tau$$

$$\therefore \int_\tau \phi^* \underline{A} \phi \, d\tau = \sum_{i=1}^{n} c_i c_i^* \lambda_i$$

Lecture 4

<A>

Knowing that

$$\int_\tau \psi_i^* \psi_i \, d\tau = 1$$

$$\int_\tau c_i^* c_j \lambda_j \psi_i^* \psi_j \, d\tau = 0$$

$$= \int_\tau \phi^* \underline{A} \, \phi \, d\tau = \sum_{i=1}^{n} |c_i|^2 \lambda_i$$

$$\sum_{i=1}^{n} |c_i|^2 = 1$$

$$\therefore \int_\tau \varphi^* \, \underline{A} \, \varphi \, d\tau \;\; \textit{is indeed a probablistic average.}$$

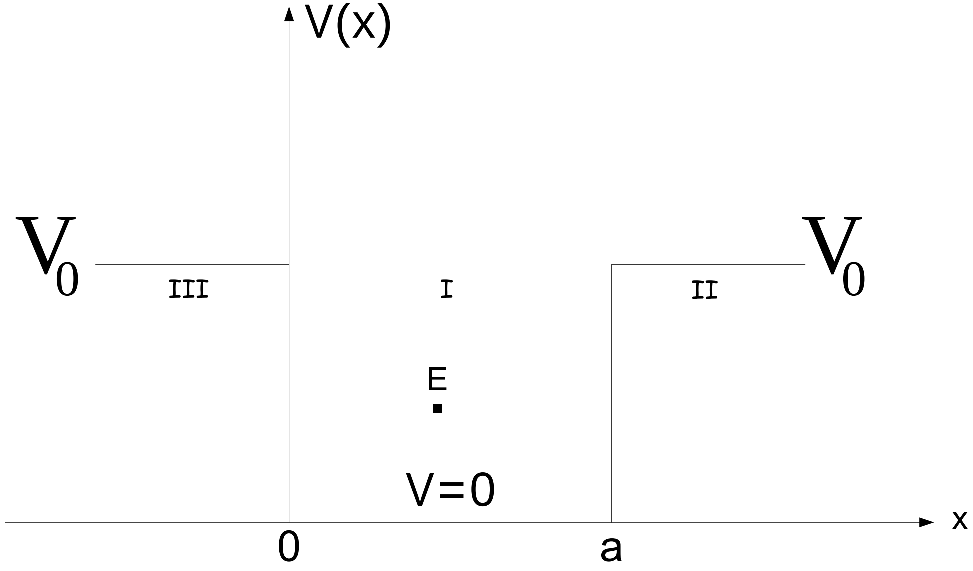
Lecture 5

VI. Applications

Assume a particle of energy E inside the shown one dimensional well.

1. The possible energy the particle can possess
2. The possible locations of the particle.

$$\underline{H}\psi = E\psi$$



Lecture 5

$$\left[\frac{-\hbar^2}{2m}\nabla^2 + V\right]\psi = E\psi$$

$$\nabla^2 = \frac{\partial^2}{\partial x^2}$$

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

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

Lecture 5

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

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

Region I: $0<x<a, and\ \ V=0$

$$\frac{\partial^2\psi_1}{\partial x^2}+\frac{2m}{\hbar^2}(E)\psi_1=0$$

$$\frac{\partial^2\psi_1}{\partial x^2}+\alpha^2\psi_1=0, \qquad \alpha=\sqrt{\frac{2mE}{\hbar^2}}$$

Lecture 5

$$\therefore \psi_1 = A_1 \cos ax + A_2 \sin ax$$

Region II: $x \geq a, \quad V = V_o, \quad and \quad E < V_o$

$$\frac{\partial^2 \psi_2}{\partial x^2} + \frac{2m}{\hbar^2}(\mathrm{E} - V_o)\,)\,\psi_2 = 0$$

$$\frac{\partial^2 \psi_2}{\partial x^2} - \frac{2m}{\hbar^2}(V_o - \; E\,)\psi_2 = 0$$

$$\frac{d^2 \psi_2}{dx^2} - \; \beta^2 \psi_2 = 0$$ Where $\beta = \sqrt{\frac{2m}{\hbar^2}\,(V_0 - \; E)}$

Lecture 5

$$\therefore\ \psi_2 = B_1 e^{\beta x} + B_2 e^{-\beta x}$$

Region III: $x \leq 0, \quad V = V_o, \quad and \quad E < V_o$

$$\therefore \psi_3 = C_1 e^{\beta x} + C_2 e^{-\beta x}$$

$$\psi_1 = A_1 \cos \alpha x + A_2 \sin \alpha x$$

$$\psi_2 = B_1 e^{\beta x} + B_2 e^{-\beta x}$$

$$\psi_3 = C_1 e^{\beta x} + C_2 e^{-\beta x}$$

Lecture 5

Since ψ has to be finite:

$$\therefore \; B_1 = C_2 = 0$$

$$\psi_1 = A_1 \cos \alpha x + A_2 \sin \alpha x$$

$$\psi_2 = B_2 e^{-\beta x}$$

$$\psi_3 = C_1 e^{\beta x}$$

Boundary conditions: ψ has also to be continuous up to the first derivative

$$\psi_1(0) = \psi_3(0) \Rightarrow A_1 = C_1$$

$$\frac{d\psi_1(0)}{dx} = \frac{d\psi_3(0)}{dx}$$

Lecture 5

$$\therefore -A_1\alpha\, sin\,\alpha\, x + A_2\alpha\, cos\,\alpha x\Big|_{x=0} = \beta C_1\, e^{\beta x}\Big|_{x=0}$$

$$A_2\alpha = C_1\beta = A_1\beta$$

$$therefore \qquad \frac{A_1}{A_2} = \frac{\alpha}{\beta}$$

Boundary conditions at x = a:

$$\psi_1(a) = \psi_3(a)$$

$$\frac{d\psi_1(a)}{dx} = \frac{d\psi_3(a)}{dx}$$

$$A_1\cos\alpha a + A_2\sin\alpha a = B_2\, e^{-\beta a} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots..(1)$$

$$-A_1\alpha\, sin\,\alpha a + A_2\alpha\cos\alpha a = -\beta B_2 e^{-\beta a} \ldots\ldots\ldots\ldots \quad \ldots\ldots \quad ..(2)$$

Lecture 5

Dividing (1) over (2) results in:

$$\frac{A_1 \cos \alpha a + \ A_2 \sin \alpha a}{-A_1 \alpha \sin \alpha a + \ \ A_2\, \alpha \cos \alpha a} = \frac{-1}{\beta}$$

Dividing numerator and denominator by $A_2\, cos\, \alpha\, a$ yields:

$$\frac{\alpha/\beta + tan\, \alpha\, a}{-\alpha^2/\beta\, tan\, \alpha\, a + \alpha} = \frac{-1}{\beta}$$

$$\frac{\alpha^2}{\beta} tan\, \alpha\, a - \alpha = \alpha + \beta\, tan\, \alpha\, a$$

$$2\alpha = (\frac{\alpha^2}{\beta} - \beta)\, tan\, \alpha\, a$$

Lecture 5

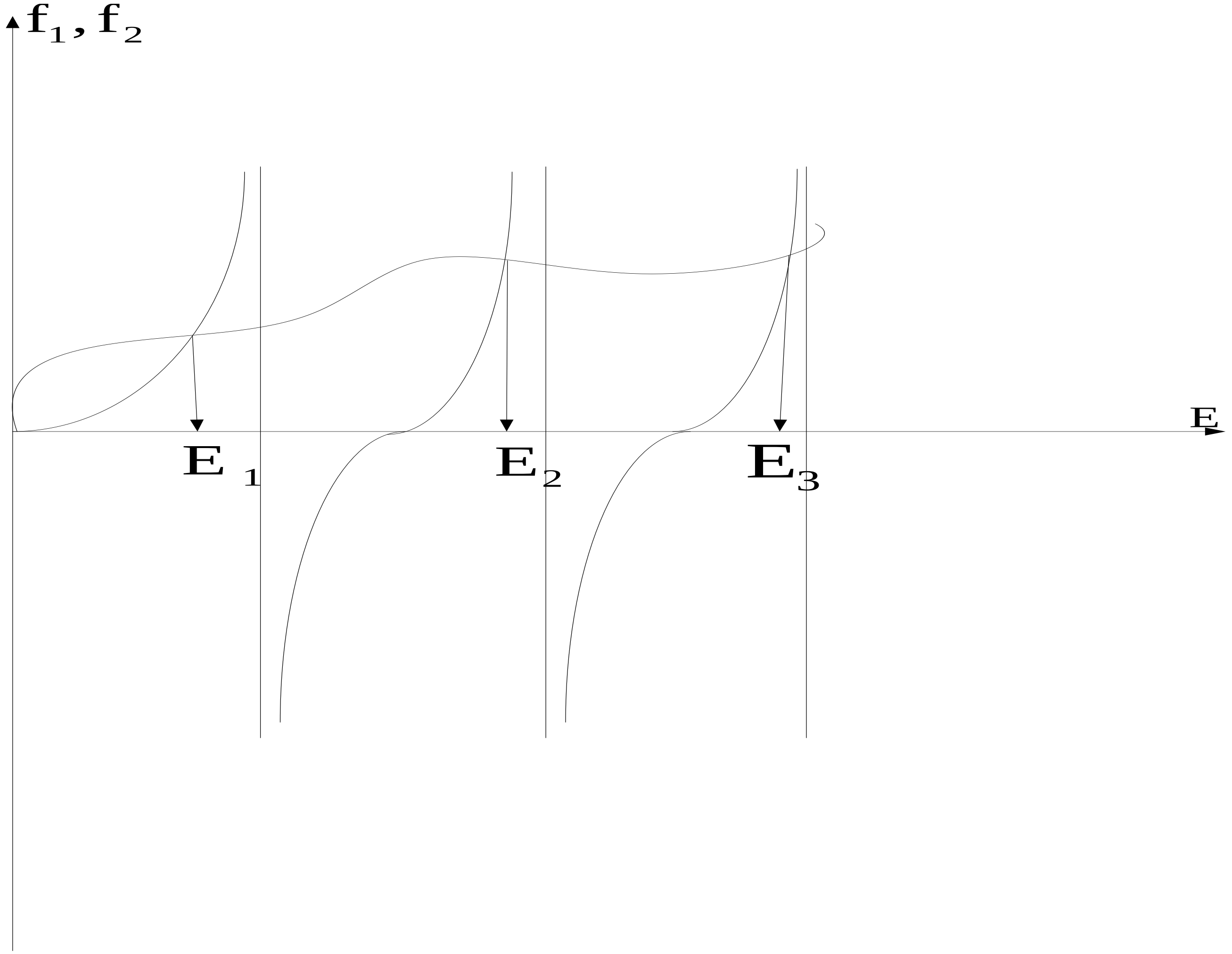
$$\tan \alpha a = \frac{2\alpha\beta}{(\alpha^2 - \beta^2)}$$

$$= \frac{2\sqrt{E(V_o - E)}}{2E - V_o}$$

$$\tan \sqrt{\frac{2m}{\hbar^2}E}.a = \frac{2\sqrt{E(V_o - E)}}{2E - V_o}$$

$$f_1(E) = f_2(E)$$

Lecture 5



Quantized energy levels,
answer to the first question

Lecture 5

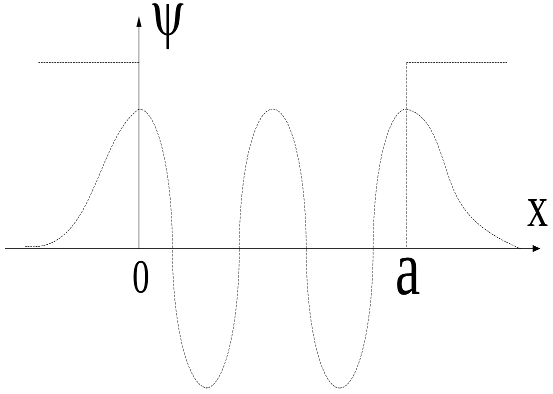
Now the second question: where the particle can most likely be located?

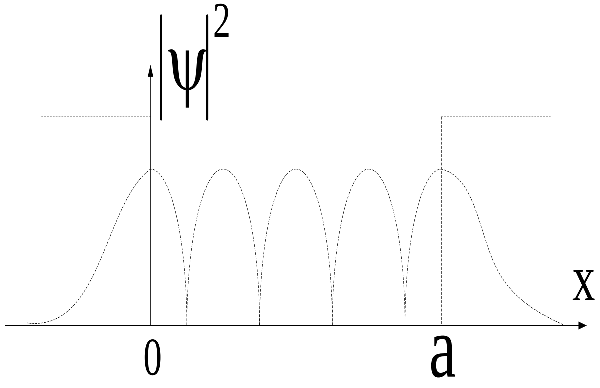
This is obtained by integrating the probability density function $|\psi|^2$over a region within which the particle is searched for. Because we know:

$$\int_{-\infty}^{\infty} \psi\psi^* \, dx = \int_{-\infty}^{0} \psi_3\psi_3^* dx + \int_{0}^{a} \psi_1\psi_1^* dx + \int_{a}^{\infty} \psi_2\psi_2^* dx = 1$$

Let us plot a sketch of the wave function ψ for a given energy value E and the associated probability density function $|\psi|^2$.

Lecture 5





Remarks:

1. $|\psi|^2$ gives the probability of finding the particle in a distance dx within the configuration space. Integrating $|\psi|^2$dx over a distance (x_1, x_2) gives the probability that the particle can be located within this distance.

2. Even though E is less than V_o, there is a nonzero probability of finding the particle in regions III and II.

Lecture 5

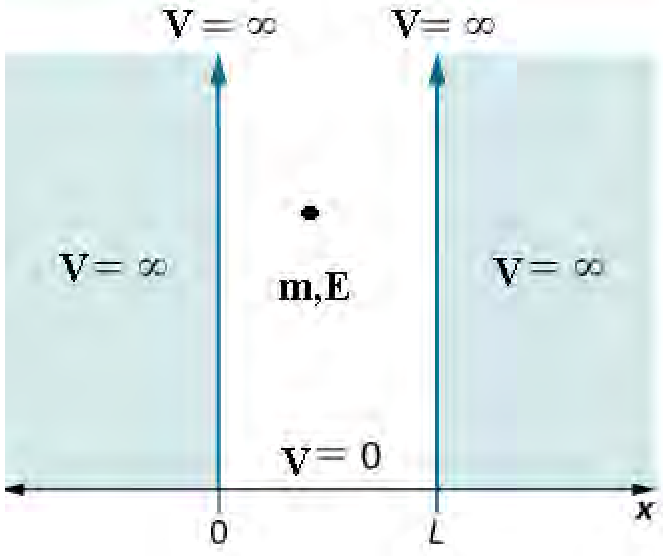
Example: Infinite potential well

Let us assume that $V_o = \infty$. Recall the solution we obtained before and get its limit when $V_o \quad goes\ to \quad \infty$.

$$\tan a\sqrt{\frac{2mE}{\hbar^2}} = \left.\frac{2\sqrt{E(V_o - E)}}{2E - V_0}\right|_{V_o \to \infty} = 0$$

$$\tan a\sqrt{\frac{2mE}{\hbar^2}} = 0$$ Which means

$$\sin a\sqrt{\frac{2mE}{\hbar^2}} = 0$$



Lecture 5

$$\text{hence,} \qquad a\sqrt{\frac{2mE}{\hbar^2}} = n\pi, \qquad n = 1,2,3,4,\ldots\ldots\ldots\ldots\ldots\ldots$$

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

$$E = n^2\,\frac{\hbar^2\pi^2}{2ma^2}\,, \qquad n = 1,2,3,..$$

$$E_n = n^2\,\frac{\hbar^2\pi^2}{2ma^2}\,, \qquad n = 1,2,3,..$$

Which confirms the quantization of energy.

Lecture 5

Now, what about ψ_2 and ψ_3

$$\beta = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}\Bigg|_{V_0 \to \infty} = \infty$$

$$\therefore \psi_2 = \psi_3 = 0$$

Which means the particle can neither be found in region I nor in region II.

Agrees with the classical theory

Lecture 5

Boundary conditions:

$$at \;\; x = 0, \qquad \psi_1 = \psi_3 = 0 \quad \Rightarrow A_1 = 0$$

$$at \;\; x = a, \qquad \psi_1(a) = \psi_2(a) = 0 \qquad \Rightarrow \alpha = \frac{n\pi}{a}$$

$$\therefore \psi_1 = A_2 \, sin \frac{n\pi}{a} . x$$

A_2 can be obtained by integrating the probability density function over the whole configuration space:

$$\int_\tau \psi_1 \psi_1^* \, d\tau = 1$$

Lecture 5

$$\int_0^a A_2^2 \sin^2 \alpha x dx = 1$$

$$\int_0^a \frac{A_2^2}{2}(1 - \cos 2\,\alpha x) dx = 1$$

$$\frac{A_2^2}{2}(a) = 1$$

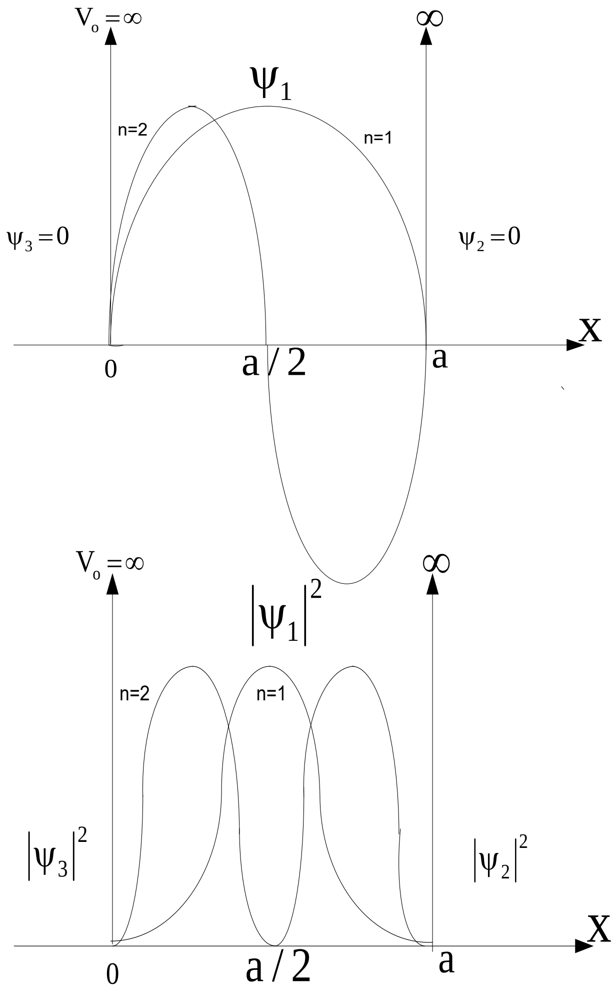
Which gives:

$$A_2^2 = \frac{2}{a}$$

$$A_2 = \sqrt{\frac{2}{a}}$$

Lecture 5

$$\therefore \psi_1 = \sqrt{\frac{2}{a}} sin \frac{n\pi}{a} x$$



Sketch of ψ *and* $|\psi|^2$ for n = 1 and n = 2.

Curve of $|\psi|^2$ shows locations of maximum and minimum probability

Example:

For n=1, the energy $E_1 = \frac{\hbar^2}{2ma^2}$,

and the likelihood is to find the particle at $\frac{a}{2}$.

Lecture 6

VII. Probability current density:

$$\frac{\partial P}{\partial t} + \nabla . J = 0$$

P is the probability and J is the number of particles crossing a unit area per unit time.

From the QM postulates:

$$\underline{H}\psi = j\hbar\frac{\partial \psi}{\partial t}$$

$$\left(\frac{-\hbar^2}{2m}\nabla^2 + V\right)\psi = j\hbar\frac{\partial \psi}{\partial t} \qquad \times\,\psi^* \qquad (1)$$

$$\left(\frac{-\hbar^2}{2m}\nabla^2 + V\right)\psi^* = j\hbar\frac{\partial \psi^*}{\partial t} \qquad \times\,\psi \qquad (2)$$

Lecture 6

Subtract (2) from (1)

$$\frac{-\hbar^2}{2m}\left[\,\psi^*\,\nabla^2\psi\;-\;\psi\nabla^2\psi^*\right]=j\hbar\left[\psi^*\frac{\partial\psi}{\partial t}+\psi\frac{\partial\psi^*}{\partial t}\right]$$

$$\frac{-\hbar^2}{2m}\nabla.\left[\,\psi^*\nabla\psi\;-\;\psi\nabla\psi^*\right]=j\hbar\left[\psi^*\frac{\partial\psi}{\partial t}+\psi\frac{\partial\psi^*}{\partial t}\right]$$

$$\frac{-\hbar^2}{2m}\nabla.\left[\,\psi^*\nabla\psi\;-\;\psi\nabla\psi^*\right]=j\hbar\frac{\partial(\psi.\psi^*)}{\partial t}$$

$$\frac{\partial(\psi.\psi^*)}{\partial t}+\frac{-j\hbar}{2m}\nabla.\left[\,\psi^*\nabla\psi\;-\;\psi\nabla\psi^*\right]=0$$

Lecture 6

Comparing the last equation with the continuity equation yields:

$$J = \frac{-j\hbar}{2m}[\,\psi^*\nabla\psi \;-\; \psi\nabla\psi^*]$$

In one dimensional case

$$J_x = \frac{-j\hbar}{2m}\left[\psi^*\frac{d\psi}{dx} - \psi\frac{d\psi^*}{dx}\right]$$

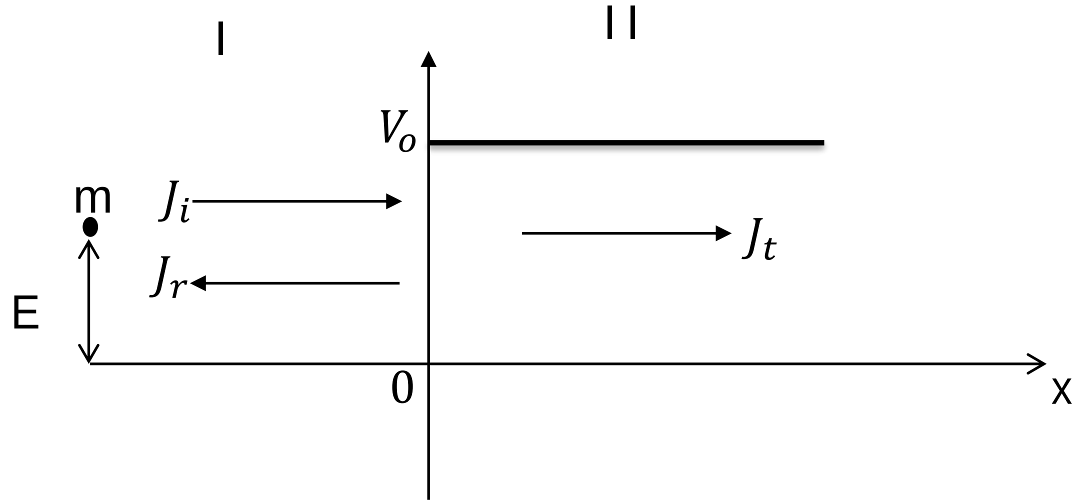
Which is the probability per unit time that a particle passes through the unit area placed perpendicular to the direction of J.

Lecture 6

A particle in a potential step:

Case I $E < V_o$

Region I: $\boldsymbol{V = 0 \;\; and \;\; x < 0}$



$$\frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi = E\psi$$

$$\frac{d^2\psi}{dx^2} - \frac{2m}{\hbar^2}(V - E)\psi = 0$$

$$\frac{d^2\psi}{dx^2} - \frac{2m}{\hbar^2}(V - E)\psi = 0$$

For Region I, V = 0 and $\psi = \psi_1$

$$\frac{d^2\psi_1}{dx^2} + \frac{2m}{\hbar^2}E\psi_1 = 0$$

Lecture 6

The solution of the last equation can be written as:

$$\psi_1(x) = A_1 e^{j\alpha x} + A_2 e^{-j\alpha x} \qquad where \quad \alpha = \sqrt{\frac{2m}{\hbar^2}E}$$

Region II: $\boldsymbol{V = V_o \ and \ x \geq 0}$

$$\frac{d^2\psi_2}{dx^2} - \frac{2m}{\hbar^2}(V_o - E)\psi_2 = 0$$

Whose solution can be written as:

$$\psi_2(x) = B_1 e^{\beta x} + B_2 e^{-\beta x} \qquad where \quad \beta = \sqrt{\frac{2m}{\hbar^2}(V_o - E)}$$

Lecture 6

ψ_2 *has to be finite which means goes to* 0 *as* x *goes to* ∞ *, so* $B_1 = 0.$

$$\psi_2(x) = B_2 e^{-\beta x}$$

Boundary condition at x = 0:

$$\psi_1(0) = \psi_2(0)$$

$$A_1 + A_2 = B_2 \qquad (1)$$

$$\frac{d\psi_1(0)}{dx} = \frac{d\psi_2(0)}{dx}$$

$$j\alpha(A_1 - A_2) = -\beta B_2$$

$$(A_1 - A_2) = \frac{-\beta B_2}{j\alpha} \qquad (2)$$

Lecture 6

Add (1) to (2):

$$2A_1 = B_2\left(1 - \frac{\beta}{j\alpha}\right)$$

$$\therefore B_2 = \frac{2j\alpha A_1}{j\alpha - \beta}$$

Back into equation (2):

$$A_2 = B_2 - A_1 = A_1\left(\frac{2j\alpha}{j\alpha - \beta} - 1\right) = A_1\frac{j\alpha + \beta}{j\alpha - \beta}$$

$$\therefore \psi_1(x) = A_1\left(e^{j\alpha x} + e^{-j\alpha x}\frac{j\alpha + \beta}{j\alpha - \beta}\right)$$

incident

reflected

Lecture 6

$$\psi_2(x) = \frac{2j\alpha A_1}{j\alpha - \beta}\, e^{-\beta x}$$

Transmission (T) and reflection (R) coefficients:

$$T = \frac{J_t}{J_i} \qquad and \;\; R = \frac{J_r}{J_i}$$

$$J_x = \frac{-j\hbar}{2m}\left[\psi^* \frac{d\psi}{dx} - \psi \frac{d\psi^*}{dx}\right] = 0$$

Use the incident wave for J_i:

$$J_i = \frac{-j\hbar}{2m}\left[A_1^* e^{-j\alpha x} . j\alpha A_1 e^{j\alpha x} - A_1 e^{j\alpha x} . (-j\alpha) A_1^* e^{-j\alpha x}\right]$$

Lecture 6

$$J_i = \frac{-j\hbar|A_1|^2}{2m}(j\alpha + j\alpha) = \frac{\hbar|A_1|^2\alpha}{m} = \frac{\hbar|A_1|^2}{m}\sqrt{\frac{2m}{\hbar^2}E}$$

$$J_i = \frac{\hbar|A_1|^2}{m}\sqrt{\frac{2m}{\hbar^2}\frac{P^2}{2m}}$$

$$J_i = \frac{|A_1|^2 P}{m}$$

$$J_i = v|A_1|^2$$

Similarly, $J_r = -v|A_1|^2$, $\left|\frac{j\alpha + \beta}{j\alpha - \beta}\right| = 1$

Lecture 6

$$\therefore R = \frac{J_r}{J_i} = -1$$

$$let\ A = \frac{2j\alpha}{j\alpha\ -\ \beta} A_1 \Rightarrow \psi_2 = Ae^{-\beta x}$$

$$J_t = \frac{-j\hbar}{2m}\left[A^* e^{-\beta x} . A(-\beta)\, e^{-\beta x}\ - Ae^{-\beta x} . A^*(-\beta) e^{-\beta x}\right]$$

$$J_t = \frac{-j\hbar}{2m} |A|^2\, \beta\left[-e^{-2\beta x} + e^{-2\beta x}\ \right] = 0$$

i.e. no resultant transmission, those particles which were able to be transmitted to region II would get reflected back, $T = \frac{J_t}{J_i} = 0.$

Lecture 6

Case II $E > V_o$

Region I : solution is the same

$$\psi_1(x) = A_1 e^{j\alpha x} + A_2 e^{-j\alpha x} \qquad where \quad \alpha = \sqrt{\frac{2m}{\hbar^2}E}$$

Region II

$$\frac{d^2\psi_2}{dx^2} + \frac{2m}{\hbar^2}(E - V_o)\psi_2 = 0 \qquad let \qquad \beta' = \sqrt{\frac{2m}{\hbar^2}(E - V_o)}$$

$$\psi_2(x) = B_1 e^{j\beta' x} + B_2 e^{-j\beta' x}$$

No reflection in region II $\Rightarrow B_2 = 0 \quad \therefore \psi_2(x) = B_1 e^{j\beta' x}$

Lecture 6

Solution as before with replacing $-\beta \;\; with \; j\beta'$

$$\therefore \psi_1(x) = A_1\left(e^{j\alpha x} + \frac{j\alpha - j\beta'}{j\alpha + j\beta'} e^{-j\alpha x}\right)$$

$$\therefore \psi_1(x) = A_1\left(e^{j\alpha x} + \frac{\alpha - \beta'}{\alpha + \beta'} e^{-j\alpha x}\right)$$

incident

reflected

$$\psi_2(x) = \frac{2\alpha A_1}{\alpha + \beta'} e^{j\beta' x}$$

transmitted

Lecture 6

Following the same procedure we get J_i , $J_r \; and \; J_t$

$$\therefore R = \frac{J_r}{J_i} = -\left(\frac{\alpha - \beta'}{\alpha + \beta'}\right)^2$$

and $$T = \frac{\beta'}{\alpha}\left(\frac{2\alpha}{\alpha + \beta'}\right)^2$$

It is clear now that:

$$T + |R| = 1$$

Lecture 7

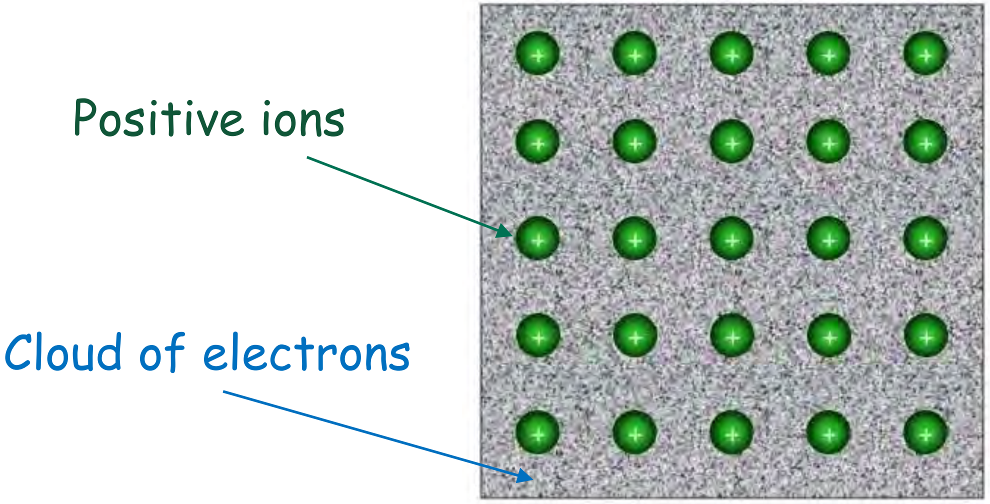
VIII. Energy Band Theory

Free Electron Fermi Gas:

Electrons move freely inside metals. This is because the potential inside metals is zero and the wave nature of electrons make them propagate freely inside metals.

Metallic bond:

Cloud of electrons move freely inside the crystal and are hindered by frequent scattering with th4 lattice and other electrons



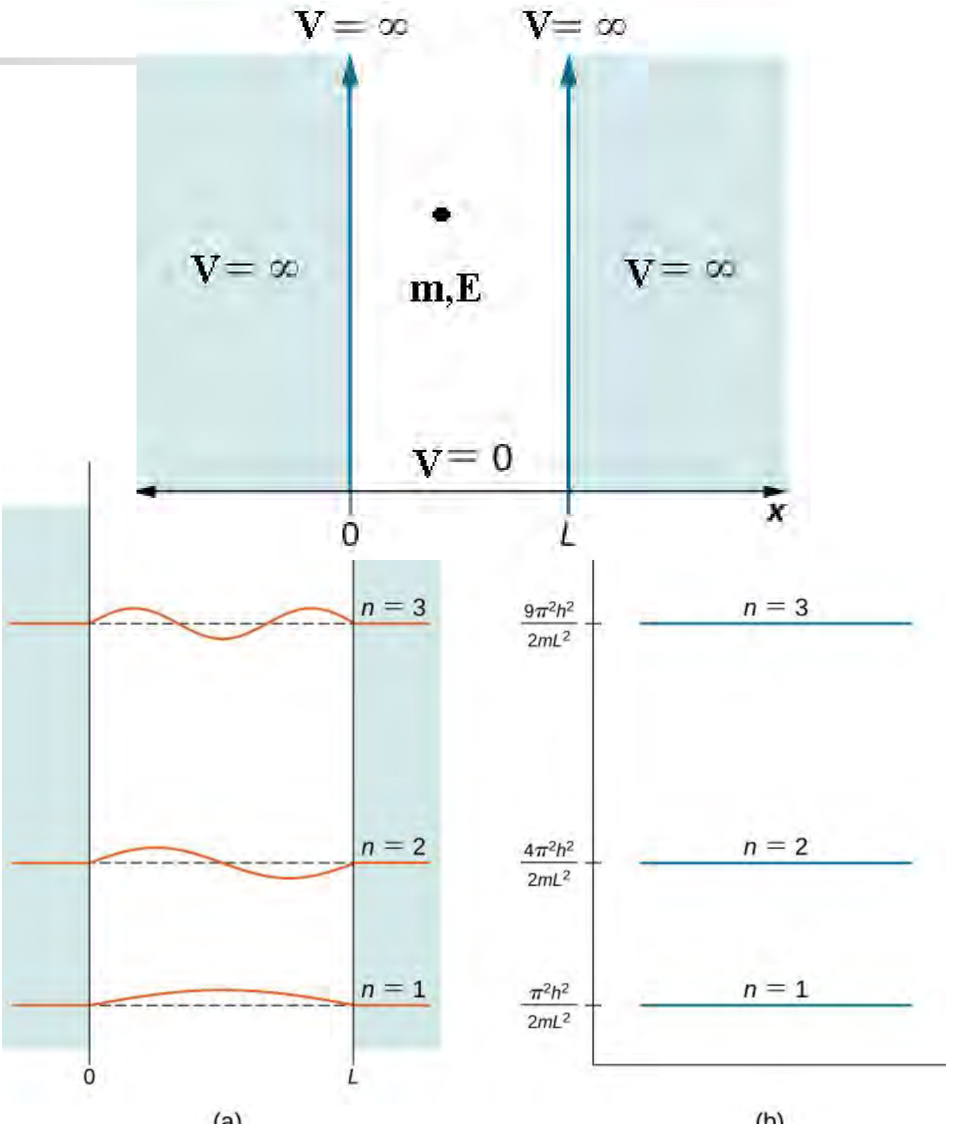
Positive ions

Cloud of electrons

Lecture 7

Energy Levels in one dimension

Electrons inside metals are considered to move inside an infinite potential well

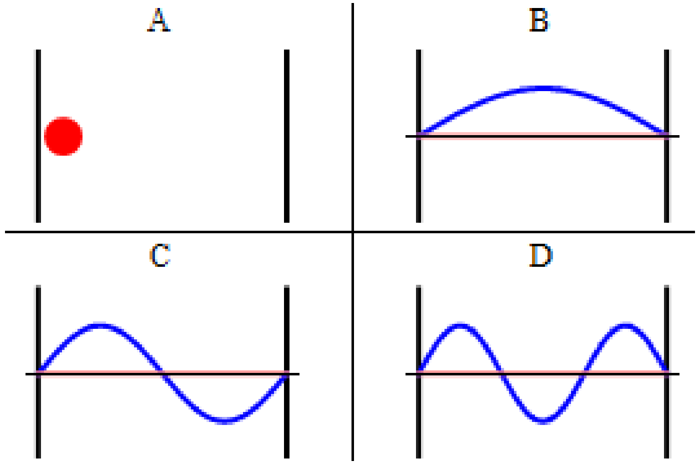


The solution Schrodinger wave equation has been previously obtained and confirm the existence of quantized energy levels.

$$\psi_1(x) = \sqrt{\frac{2}{L}}\,sin\frac{n\pi}{L}x$$

$$E_n = n^2\frac{\hbar^2\pi^2}{2mL^2}\,, \qquad n = 1,2,3,..$$

Lecture 7

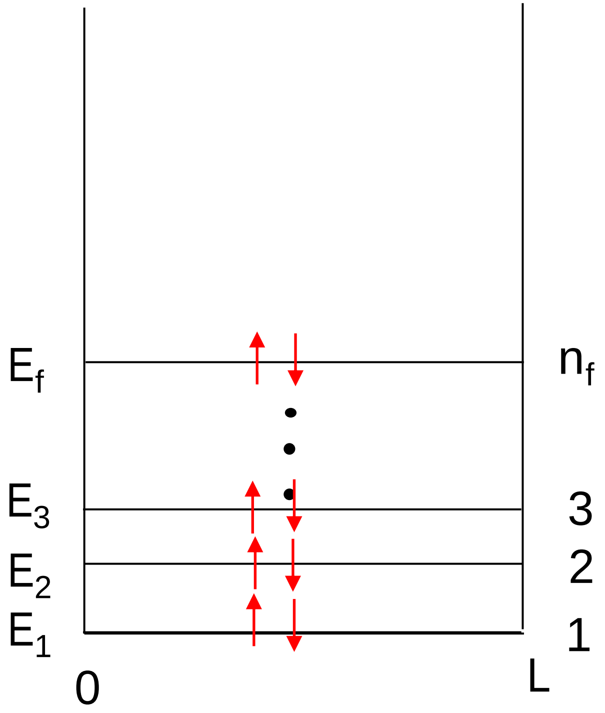


Maximum energy an electron can possess inside metals (Fermi Level)

$$E_f = n_f^2 \frac{\hbar^2 \pi^2}{2mL^2}$$

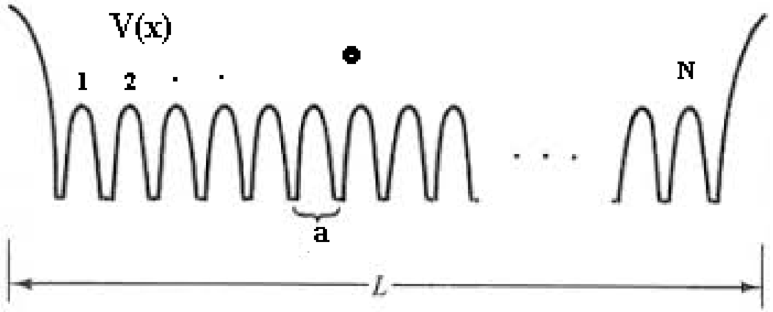
Consider each atom contributes a single free electrons and N is the number of free electrons per unit volume.

$$\therefore N = 2n_f$$



Lecture 7

Bloch Theorem:



Inside a metal the potential can be considered periodic as shown, i.e.:

$$V(x+a) = V(x)$$

and therefore $$\psi(x+a) = e^{jkx}\psi(x)$$

and $$\psi(x) = e^{jkx}u(x)$$

Where $u(x)$ is the unit cell solution, a region of an extension equal to the lattice constant a.

The solution $\psi(x)$ is a plane wave e^{jkx} modulated by the unit cell solution $u(x)$ which has the same periodicity of $V(x)$.

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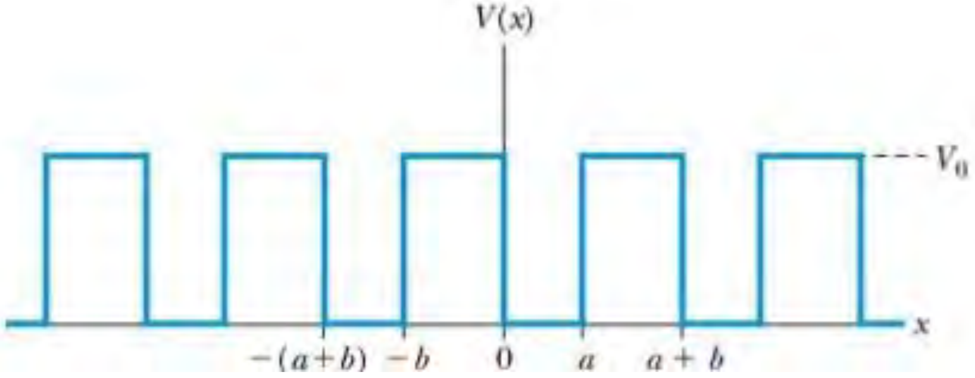
Kronig-Penny model

They simplified the periodic potential inside metal, assumed by Bloch, to look like the shown figure.



Solving now Schrodinger wave equations one can write:

$$\psi_a(x) = A_1 \sin \alpha x + A_2 \cos \alpha x \qquad for \qquad 0 \le x \le a$$

$$\psi_b(x) = B_1 \sin \beta x + B_2 \cos \beta x \qquad for \qquad -b \le x < 0$$

$$where \quad \alpha = \sqrt{\frac{2m}{\hbar^2} E} \ \ and \qquad \beta = \sqrt{\frac{2m}{\hbar^2}(V_o - E)}$$

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Applying the boundary conditions and taking care of the periodicity one can reach to the following transcendental equation:

$$-\frac{\alpha^2+\beta^2}{2\alpha\beta}\sin\alpha a\sin\beta b+\cos\alpha a\cos\beta b=\cos k(a+b)$$

$$f(E)=\cos k(a+b)$$