Physics [Module 1]

Notes

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Module-1

Physics

- classical Mechanics ✓
- Thermodynamics and Statistical Mechanics ✓
- Electromagnetism and Electronics ✓
- Relativity
- Quantum Physics ✓
- Optics and Atomic, molecular and Optical Physics ✓
- Condensed matter Physics
- High energy Physics / Nuclear Physics
- Cosmology
- Interdisciplinary Field
  - Astrophysics ✓
  - Biophysics
  - Chemical Physics
  - Computational Physics
  - Econophysics
  - Engineering Physics
  - Geophysics
  - Mathematical Physics ✓
  - Medical Physics
  - Physical Chemistry
  - Quantum Computing

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Visiting student (Under tinker's Lab)
I.I.T. Bombay [Summer-Winter]

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- Modern Physics
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Modern Physics

- Basics of elements of Modern Physics
- Bohr corresponding Principle

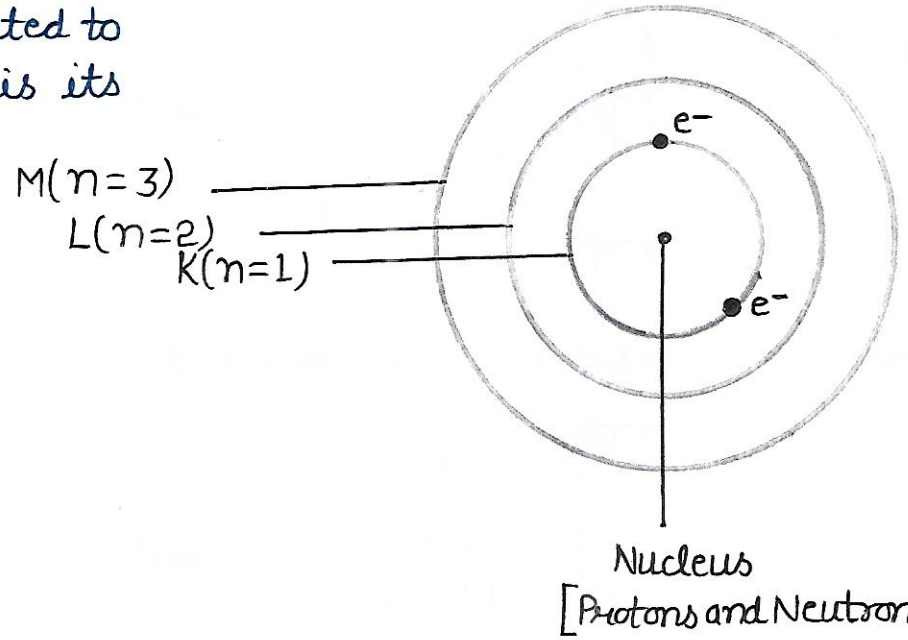
Elements of Modern Physics

⇒ Quick Notes for Exam Preparation-

Atomic Number- The Atomic number is the number of Protons in an atom.

Mass Number- The number of Protons and the number of neutrons determine an element's mass number.

A property closely related to an atom's mass number is its atomic Mass.



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

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

$^{1}_{1}H$ ← Atomic mass

Atomic No. ↑ 1

$^{4}_{2}He$ 4 = no. of protons + no. of Neutrons

No. of e^- = Atomic Number 2

Relation b/w momentum and Energy-

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

$$p = mv \Rightarrow v = \frac{p}{m}$$

Then

$$E_K = \frac{1}{2}m\left(\frac{p^2}{m^2}\right) = \frac{p^2}{2m}$$

Bohr Corresponding Principle-

In micro-universe, the results obtained from Quantum principle are always different from the results on the basis of Classical principle. But if no of Quantums are increasing both principles are correspond with each other. Bohr had given the following principle.

According to classical theory e^- moving in circular orbit has only emitted radiation of special Frequency & It is the frequency of revolution of e^- in that orbit.

We know that

$$\frac{mv^2}{r} = \frac{1}{4\pi\epsilon_0} \cdot \frac{e^2}{r^2} \quad \text{——— (1)}$$

$$mv^2 = \frac{1}{4\pi\epsilon_0} \cdot \frac{e^2}{r}$$

And we know that in Bohr's model the condition for permitted orbit

$$mvr = \frac{nh}{2\pi}$$

$$r = \frac{nh}{2\pi mv} \quad \text{——— (2)}$$

$$mv = \frac{nh}{2\pi r} \quad \text{——— (3)}$$

Squaring eqn (3)

$$m^2v^2 = \frac{n^2h^2}{4\pi^2r^2}$$

$$mv^2 = \frac{n^2h^2}{4\pi^2r^2m}$$

Now in eqn (1)

$$\frac{n^2h^2}{4\pi^2mr^2} = \frac{1}{4\pi\epsilon_0} \cdot \frac{e^2}{r}$$

$$r = \frac{n^2h^2}{4\pi^2m} \cdot \frac{4\pi\epsilon_0}{e^2}$$

$$r = \frac{n^2 h^2 \epsilon_0}{\pi m e^2} \quad \text{——— (4)}$$

Where m = mass of e^-
r = r is radius of Orbit

If v is velocity of e^- then According to classical theory its freq. of revolution,

$$f = \frac{\text{velocity of } e^- \text{ in orbit}}{\text{Circumference of Orbit}}$$

$$f = \frac{v}{2\pi r} \quad \text{——— (5)}$$

From eqn (2)

$$v = \frac{nh}{2\pi m r}$$

$$\frac{v}{2\pi r} = \frac{nh}{4\pi^2 m r^2}$$

Again From eqn (5)

$$f = \frac{nh}{4\pi^2 m r^2} \quad \text{——— (6)}$$

From eqn (4)

$$f = \frac{nh}{4\pi^2 m \left(\frac{n^2 h^2 \epsilon_0}{\pi m e^2}\right)^2}$$

$$f = \frac{nh}{4 \times \pi^2 \times n^4} \left[\frac{\pi^2 m^2 e^4}{n^4 h^4 \epsilon_0^2}\right]$$

$$f = \frac{me^4}{4\epsilon_0^2 n^3 h^3} \times \frac{2C}{2C}$$

$$f = \frac{me^4}{8\epsilon_0^2 C h^3} \times \frac{2C}{n^3}$$

We know that Rydberg Constant is

$$R = \frac{me^4}{8\epsilon_0^2 ch^3}$$

$$f = \frac{2RC}{\cancel{k}n^3}$$

$$\boxed{f = \frac{2RC}{n^3}}$$

It is the frequency which is emitted by moving e^- as in classical Theory.

Now according to Quantum theory the radiation frequency is

$$\nu = \frac{E_i - E_f}{h}$$

$$\nu = \frac{me^4}{8\epsilon_0^2 h^3}\left[\frac{1}{n_f^2} - \frac{1}{n_i^2}\right]$$

$$\nu = \frac{me^4}{8\epsilon_0^2 ch^3} \cdot c\left[\frac{1}{n_f^2} - \frac{1}{n_i^2}\right]$$

Where $R = \frac{me^4}{8\epsilon_0^2 ch^3}$; Rydberg Constant

$$\nu = RC\left[\frac{1}{n_f^2} - \frac{1}{n_i^2}\right]$$

$$\nu = RC\left[\frac{n_i^2 - n_f^2}{n_i^2 n_f^2}\right] = RC\left[\frac{(n_i - n_f)(n_i + n_f)}{n_i^2 n_f^2}\right]$$

We consider a transition for $n_f = n$

$$n_i = n+1$$

$$\nu = RC\left[\frac{(n+1-n)(n+1+n)}{n^2(n+1)^2}\right]$$

$$\nu = RC\left[\frac{2n+1}{n^2(n+1)^2}\right]$$

For large number of quantum numbers we have

$$\Rightarrow 2n+1 \approx n$$
$$\Rightarrow (n+1)^2 \approx n^2$$

$$\nu = \frac{2RC}{n^3} \quad \text{——— (7)}$$

From eqn (6) & (7)

$$\nu = f$$

Thus for very large quantum number, the quantum theory frequency & classical orbit frequency become equal. If transitions are formed then we have

$$n = 2, 3, 4, 5$$

Then

$$\nu = 2f, 3f, 4f$$

It shows that the frequency for quantum principal is corresponding to the frequency for classical theory.

Nuclear Physics

Basics of Nuclear and Atomic Physics

[NUCLEAR PHYSICS]

The Physics of atomic nuclei and their interactions, especially in the generation of nuclear Physics.

⇒NUCLEUS -

* discovered by Ruthorford
* Radius $\approx 10^{-15}$ m
* It is collectively known as nucleous when their are two constituents named neutrons (n) and Protons (p).
* mass of neutron = $1.6749286 \times 10^{-27}$ kg
* mass of Protons = $1.6726231 \times 10^{-27}$ kg
* neutron was discovered by J. Chadwick. It is neutral Particle.
* Proton is Positively charged Particle and it was discovered by Ruthorford.
* $m_p \leq m_n$ [because neutron is nill]

⇒ PROTON-ELECTRON HYPOTHESIS-

Proton was discovered by Ruthorford in 1919. According to this, P^+ and e^- were responsible for mass in neucleus. But this theory was failed after the coming of Bohr.

⇒ Atomic Number = No. of Protons in nucleus = No. of e^-

⇒ Atomic Mass = No. of Neutrons in nucleus + No. of Protons in Nucleus

$A \rightarrow$ Atomic Number

$Z^X \leftarrow$ Element

$Z \rightarrow$ Atomic Mass

$_ZX^A$ or ^A_ZX

e.g. $_1H^1$, $_2He^4$, $_3Li^6$ etc.

⇒ Nucleon = Protons + Neutrons

⇒ Nuclear Dimensions and Nuclear density-

Radius of Nucleus is R Then

$$\frac{4}{3}\pi R^3 \propto A$$

$$\text{Density} = \frac{\text{Mass}}{\text{Volume}}$$

$$\text{Volume} = \frac{\text{Mass}}{\text{Density}}$$

Mass = Volume X density

$\frac{4}{3}\pi R^3 \propto A$ ← Mass number is directly Proposal to Volume.

$R^3 \propto A$

$R \propto (A)^{1/3}$

$$\boxed{R = R_0(A)^{1/3}}$$

R_0 is a constant.

For Helium ${}_2He^4$

$R = R_0(A)^{1/3}$

$R = 1.2 \times 10^{-15} \times (4)^{1/3}$

$$\boxed{R = 1.905 \times 10^{-15} m}$$

Artificial transmutation is used to use for changing one nucleus to another.

* charge on Proton $q = +1.6 \times 10^{-19} C$
* charge on e^- $q = -1.6 \times 10^{-19} C$
* charge on n° = 0 (null)

In 1914, Bainbridge and Scherr used a technique in which they used Hg and bombarded Protons on it, thus they got some temporary gold.

$${}_{80}Hg^{200} + {}_1H^1 \longrightarrow {}_{79}Au^{197} + {}_2He^4$$

discovery of Neutron-

$${}_4Be^9 + {}_2He^4 \longrightarrow {}_6C^{12} + {}_0n^1$$

Outside the nucleus, neutrons are temporary and they ejected β- Particle and an anti-neutron.

$$_0n^1 + {}_1H^1 \longrightarrow {}_{-1}b^0 + \overline{\nu}$$

↑ Anti-neutron

SOME DEFINITIONS-

A. Isotopes;
The nuclei having the same number of protons and but different number of neutrons are called Isotopes.

B. Isotones;
The nuclei with the same neutron number but different atomic number/Protons are called isotons.

C. Isobars:
The nuclei with the same mass number but different atomic number are called isobars.

* Size of Nucleus: Order of 10^{-15} m (Fermi)

Electrodynamics

- Maxwell's equations and Electromagnetic waves
- Radiation from moving charge

UNIT 1

Maxwell's equation and electromagnetic waves

- **Maxwell's equations and their Physical Significance-**

→ A series of four partial diff eq^{n}'s that describe the force of electromag-netism

→ Electromagnetism - Physical Inter-action b/w electrically charged Particles.

→ Mathematician - James clerk Maxwell [1861, 1862]

- Guass Law
- Guass Law of Magnetism
- Faraday's Law
- Ampere's Law

1. $\int \vec{E} \cdot d\vec{A} = \frac{q}{\epsilon_0}$

2. $\int \vec{B} \cdot d\vec{A} = 0$

3. $\mathcal{E} = \frac{d\phi_B}{dt}$

$$\int \vec{E} \cdot d\vec{S} = \frac{d\phi_B}{dt}$$

4. $\int \vec{B} \cdot d\vec{S} = \mu_0 I$

$$\int \vec{B} \cdot d\vec{S} = \mu_0 (I + I_D)$$

↑ displacement current

Maxwell's equations represent one of the most ways to state the fundamentals of electricity and magnetism. From them one can develop most of working relationship in this field. Because of their concise statement, they embody a high level of mathematical sophistication and are therefore not generally introduced in an introductory treatment of the subject.

These basic equations of electricity and magnetism can be used as a starting point of advanced projects

Maxwell equations describe how electric and magnetic fields are generated by charges, currents and changes of the field. One Important consequence of the equations is that they demonstrate how fluctuating electric and magnetic field propogate at the speed of light.

- Differential form with magnetic/Polarizable media;

1. Gauss's law for electricity-

Gauss's law describes the relationship between a static electric field and the electric charge. The field lines begins at positive electric charge and end at negative charge. Counting the number of field lines passing through a closed surface yields the total charge enclosed by the surface, devided by dielectricity of free space [the vaccum permittvity) ϵ_0].

Let us consider a surface S bounding a volume V in a dielectric medium. In a dielectric medium total charge consists of free charge plus polarization charge. If ρ and ρ_p are the charge density of free charge and polarization charge at a point in a small volume element dV.

$$\int_S E \cdot ds = \frac{1}{\epsilon_0} \int_V (\rho + \rho_p)\, dV$$

But polarization charge density $\rho_p = -\operatorname{div} P$

$$\int_S E\, ds = \frac{1}{\epsilon_0} \int_V (\rho - \operatorname{div} P)\, dV$$

$$\int_S \epsilon_0 E\, ds = \int_V (\rho - \operatorname{div} P)\, dV$$

$$\int_V \operatorname{div}(\epsilon_0 E)\, dV = \int_V \rho\, dV - \int_V \operatorname{div} P\, dV$$

$$\int_V \text{div}(\epsilon_0 E + P)\, dV = \int_V \rho\, dV$$

But $\epsilon_0 E + P = D$ = Electric displacement vector

$$\int_V \text{div}\, D\, dV = \int_V \rho\, dV$$

$$\boxed{\nabla D = \rho}$$

2. Gauss law for magnetism –

Gauss law for magnetism states that there are no magnetic charges [magnetic monopoles], analogues to electric charges. In terms of the field lines, this equation states that magnetic field lines neither begin nor end but make loops or extend to infinity or back.

In other words, any magnetic field lines that enters a given volume must somewhere exit that volume. Technical statements are that the sum total magnetic flux through any Gaussian surface is zero.

Since isolated magnetic poles and magnetic currents due to them have no physical Significance. It means that the flux of magnetic Induction B across any closed surface is always zero.

i.e.

$$\int_S B \cdot dS = 0$$

Using guass divergance theorem to change surface Integral into volume Integral,

$$\int_V \text{div}\, B\, dV = 0$$

↖ Surface vanished because it is arbitrary.

$$\text{div}\, B = 0$$

$$\boxed{\nabla B = 0}$$

3. Faraday's Law-

→ The magnetic field creates an electric field.

The maxwell-faraday's law of Induction describes how a time varying magnetic field creates an electric field.

In Integral form, it states that the work per unit charge required to move a charge around a closed loop equals the rate of decrease of the magnetic flux through the closed surface.

According to the Faraday's law of electromagnetic Induction.

$$e = -\frac{d\phi}{dt}$$

But the magnetic flux $\phi = \int_S B \cdot ds$

$$e = -\frac{d}{dt}\int_S B \cdot ds$$

$$e = -\int_S \frac{\partial B}{\partial t} ds \quad \ldots\ldots\ldots (1)$$

According to the definition, emf e can also computed by calculating the work done in carrying a unit charge round the closed loop. C.

$$e = \int_C E \cdot dl \quad \ldots\ldots\ldots (2)$$

comparing both eqn (1) & (2)

$$\int_C E \cdot dl = -\int_S \frac{\partial B}{\partial t} ds$$

$$\int_S \text{curl } E \, ds = -\int_S \frac{\partial B}{\partial t} ds$$

$$\boxed{\text{curl } E = -\frac{\partial B}{\partial t}}$$

4. Ampere's Law -

Ampere's Law with Maxwell's addition states that the magnetic field can be generated in the two ways ; by electric current and by changing electric field.

From Ampere's Law

$$\oint H \cdot dl = I \quad \ldots\ldots (1)$$

$$I = \int_S J \cdot dS \quad \ldots\ldots (2)$$

comparing eqn (1) & (2)

$$\oint H \cdot dl = \int_S J \cdot dS \quad \ldots\ldots (3)$$

And Stoke Theorem

$$\oint H \cdot dl = \int_S \text{curl } H \, dS \quad \ldots\ldots (4)$$

By eqn (3) & (4)

$$\int_S \text{curl } H \, dS = \int_S J \, dS$$

$$\int_S (\text{curl } H - J) \cdot dS = 0 \quad \ldots\ldots (5)$$

$$\text{curl } H - J = 0$$

$$\boxed{\text{curl } H = J}$$

Now

$$\text{div } J = 0$$

$$\text{div } J + \frac{\partial \rho}{\partial t} = 0 \qquad [\because \text{Continuity Equation}]$$

$$\text{div } J = -\frac{\partial \rho}{\partial t}$$

And total current density $C = J + J_d$

$$\text{curl } H = C = J + J_d$$

$$\text{div curl } H = \text{div } (J + J_d)$$

↓ div of curl is always 0.

$$\text{div}(J + J_d) = 0$$

$$\text{div}\, J = -\,\text{div}\, J_d$$

$$\text{div}\, J_d = \frac{\partial \rho}{\partial t}$$

$$\text{div}\, J_d = \frac{\partial}{\partial t}(\text{div}\, D)$$

$$\text{div}\, J_d = \text{div}\left(\frac{\partial D}{\partial t}\right)$$

$$J_d = \frac{\partial D}{\partial t}$$

Therefore

$$\text{Curl}\, H = J + J_d$$

$$\boxed{\text{Curl}\, H = J + \frac{\partial D}{\partial t}}$$

- Physical Significance–

(i) The net outward flux of electric displacement vector through the surface enclosing a volume is equal to the net charge containing within this volume.

$$\text{Since} \int_V \rho\, dv = q$$

(ii) The net outward flux of the magnetic induction B through any closed surface is equal to zero.

$$\int_S B \cdot ds = 0$$

(iii) The e.m.f. $\left(e = \int_C E \cdot dl\right)$ around any closed path is equal to the negative rate of change of magnetic flux linked with the path.

(iv) The m.m.f $\left(\oint_C H \cdot dl = \text{m.m.f.}\right)$ around any closed path is equal to the conduction current plus displacement current through any surface bound by the path.

$$\int_C H \cdot dl = \int_S \left(J + \frac{\partial D}{\partial t}\right) \cdot ds$$

- **Electromagnetic Energy-**

Electromagnetic energy is a form of energy that is reflected or emitted from object in the form of electricity or magnetic waves that can travel through space.

$$U_C = \frac{1}{2}\int_V E \cdot D \, dv$$

$$U_m = \frac{1}{2}\int_V H \cdot B \, dv$$

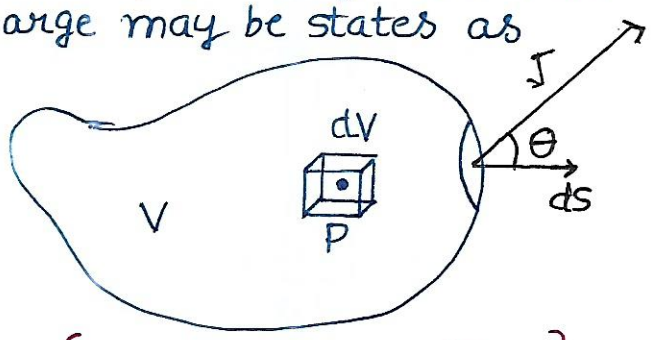
- **Equation of continuity-**

According to principle of conservation of charge the net amount of charge in an isolated system remains constant.

Let us assume that charge density is a function of time. Then the principle of conservation of charge may be states as follows.

The time rate at which charge leaves the volume V bounded by entire surface is given by;

$$\iint_S J \cdot ds$$



$$\left\{ I_{out} = \oint_S \vec{J} \cdot \vec{ds} = \frac{dQ_{in}}{dt} \right\}$$

If q is charge contained is V, then according to charge conservation law, the above integral must be equal to $-dq/dt$, where dq/dt represents the time rate of flow of charge into V, thus

$$\int_S \int J \cdot ds = -\frac{dq}{dt}$$

$$q = \int\int_V \int \rho \, dv$$

$$\int_S \int J \cdot ds = -\frac{d}{dt}\int\int_V \int \rho \, dv$$

$$\int_S \int J \cdot ds = -\int\int_V \int \frac{\partial \rho}{\partial t} dv$$

$$\int_S \int J \cdot ds = \int\int_V \int \text{div} J \, dv$$

$$\int_V \iint \text{div} J \, dv = -\iiint \frac{\partial \rho}{\partial t} dv$$

$$\int_V \iint \left(\text{div} J + \frac{\partial \rho}{\partial t} \right) dv = 0$$

$$\boxed{\text{div} J + \frac{\partial \rho}{\partial t} = 0}$$

– continuity of current Eq^n
– Continuity eq^n

This is required equation of continuity and expresses the conservation of time.

- Relaxation time –

$$\nabla \cdot \vec{J} = -\frac{\partial \rho}{\partial t} \quad \ldots\ldots\ldots (0)$$

For steady state current, $\frac{\partial \rho_v}{\partial t} = 0$

Hence $\nabla \cdot \vec{J} = 0$

Now, Ohm's Law

$$\vec{J} = \sigma \vec{E} \quad \ldots\ldots (1)$$

Guass Law

$$\nabla \vec{E} = \frac{\rho_v}{\epsilon} \quad \ldots\ldots\ldots (2)$$

From eq^n 0, 1, 2

$$\nabla \cdot \sigma \vec{E} = \frac{\sigma \rho_v}{\epsilon} = \frac{-\partial \rho_v}{\partial t}$$

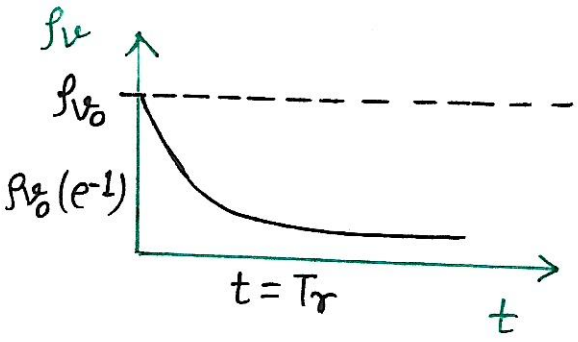
$$\frac{\partial \rho_v}{\partial t} + \frac{\sigma}{\epsilon} \rho_v = 0 \quad \ldots\ldots\ldots (3)$$

eq^n (3) is differential eq^n and the solution is

$$\boxed{\rho_v = \rho_{v_0} e^{-t/T_r}}$$

Where ρ_{v_0} = Initial charge density

T_r = Time constant or Relaxation time



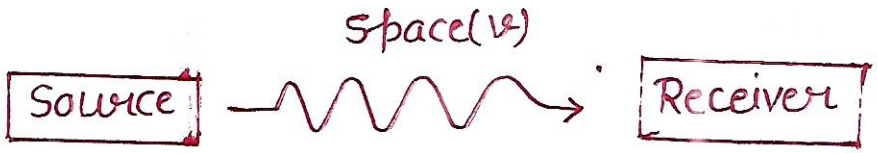
Shows that the introduction of charge at some interior point of the material result in a decay of volume charge density ρ_v.

"Relaxation time is the time it takes a charge placed in the interior of a material to drop to e^{-1} (36.8%) of its initial value."

Note→ T_r = Short time for good conductor.
T_r = long time for dielecric material.

- Poynting Theorem + Poynting vector–

"Poyntime Theorem states that the power flowing out of a given volume V is equal to the time rate of decrease in the energy stored within V without ohmic losses."



using maxwell's eqn

$$\nabla \times \vec{H} = \vec{J} + \frac{\partial \vec{D}}{\partial t}$$

$$\nabla \times \vec{H} = \vec{J} + \epsilon \frac{\partial \vec{E}}{\partial t}$$

$$\vec{J} = \nabla \times \vec{H} - \epsilon \frac{\partial \vec{E}}{\partial t} \quad \ldots\ldots\ldots (1)$$

$\vec{E} \cdot \vec{J} \approx$ dimension of power

$$\vec{E}\cdot\vec{J} = \vec{E}\cdot(\nabla\times\vec{H}) - \underbrace{\varepsilon\vec{E}\cdot\frac{\partial\vec{E}}{\partial t}} \quad \ldots\ldots\ldots (2)$$

vector · vector = scalar

$$\left[\vec{E}\cdot\frac{\partial\vec{E}}{\partial t} = \frac{1}{2}\frac{\partial}{\partial t}E^2\right]$$

using vector Identity,

$$\nabla(\vec{E}\times\vec{H}) = \vec{H}(\nabla\times\vec{E}) - \vec{E}(\nabla\times\vec{H})$$

$$\vec{E}\cdot\vec{J} = \vec{H}\underbrace{(\nabla\times\vec{E})} - \nabla(\vec{E}\times\vec{H}) - \varepsilon\left(\frac{1}{2}\frac{\partial}{\partial t}E^2\right)$$

$$\frac{-\partial B}{\partial t} = -\mu\frac{\partial\vec{H}}{\partial t}$$

$$\vec{E}\cdot\vec{J} = \vec{H}\left(-\mu\frac{\partial\vec{H}}{\partial t}\right) - \nabla(\vec{E}\times\vec{H}) - \varepsilon\left(\frac{1}{2}\frac{\partial}{\partial t}E^2\right)$$

$$\vec{E}\cdot\vec{J} = -\mu\underbrace{\left(\vec{H}\cdot\frac{\partial\vec{H}}{\partial t}\right)} - \nabla(\vec{E}\times\vec{H}) - \varepsilon\left(\frac{1}{2}\frac{\partial}{\partial t}E^2\right)$$

$$\frac{1}{2}\cdot\frac{\partial}{\partial t}H^2$$

$$\boxed{\vec{E}\cdot\vec{J} = -\mu\left(\frac{1}{2}\cdot\frac{\partial}{\partial t}H^2\right) - \nabla(\vec{E}\times\vec{H}) - \varepsilon\left(\frac{1}{2}\frac{\partial}{\partial t}E^2\right)}$$

Integrate over the volume

$$\int_V \vec{E}\cdot\vec{J}\,dv = -\frac{\partial}{\partial t}\int_V\left(\frac{\mu}{2}H^2 + \frac{\varepsilon}{2}E^2\right)dv - \underbrace{\int_V \nabla(\vec{E}\times\vec{H})\,dv}_{\oint_S(\vec{E}\times\vec{H})\cdot d\vec{s}}$$

divergance Theorem

$$\vec{J} = \sigma\vec{E}$$

$$\oint_S(\vec{E}\times\vec{H})\,ds = -\frac{\partial}{\partial t}\int_V\left(\frac{\mu}{2}H^2 + \frac{\varepsilon}{2}E^2\right)dv - \int_V \vec{E}(\sigma\vec{E})\,dv$$

$$\boxed{\oint_S(\vec{E}\times\vec{H})\,ds = -\frac{\partial}{\partial t}\int_V\left(\frac{\mu}{2}H^2 + \frac{\varepsilon}{2}E^2\right)dv - \int_V \sigma E^2\,dv}$$

- Total power leaving the volume
- Rate of decrease in Energy stored in $\vec{E}$ & $\vec{H}$ field
- Ohmic power dissipated

$\vec{E} \times \vec{H} = \vec{P}$ -- Poynting vector (Watt/m2)

is known as poynting vector and is interpreted as the power flux i.e. amount of energy crossing unit area placed perpendicular to the vector, per unit time.

- Hertz Potential-

A general feature of classical electrodynamics is the fact that an electromagnetic field must be a solution of maxwell's equation. The analysis of an electromagnetic field is often facilitated by the use of auxiliary function known as potential function. These sol^n of partial diff^n eq^n. The partial differential eq^n are such, that solving them for the potential functions is equivalent to the more tendious task to solve directly.

The most elegant approach to this is the field represents in term of Green tensors. However, this treatment has the fundamental disadvantage that tensor diff^n eq^n have to be solved. It is only for special kind of media that Green's tensors can be reduced to scalar's green functions.

It was shown by Hertz that an arbitrary electromagnetic field in a source homogenous linear isotopic medium can be defined in terms of single vector potential. The Hertz vector potential notation is an efficient mathematical formulism for solving em... problems.

$$\vec{J} = \frac{\partial \vec{P}}{\partial t}$$

$$\rho = -\vec{\nabla} \cdot \vec{P}$$

The magnetic vector potential $\vec{A}$ and the scalar potential ϕ are related to the Hertz vector potential as follows:

$$\vec{A} = \mu\varepsilon \frac{\partial \vec{\Pi}}{\partial t}$$

$$\phi = -\vec{\nabla} \cdot \vec{\Pi}$$

- Vector potential–

A vector potential is a vector field whose curl is given vector field. Formally

$$V = \nabla \times A$$

Where V = vector field

A = vector potential

Let $V : \mathbb{R}^3 \longrightarrow \mathbb{R}^3$ be a solenoidal vector field which is twice continuously differentiable. Assume that $V(x)$ decreases sufficiently fast as $\|x\| \longrightarrow \infty$.

Define

$$A(x) = \frac{1}{4\pi} \int_{\mathbb{R}^3} \frac{\nabla_y \times V(y)}{\|x-y\|} \, d^3y$$

$$\boxed{\nabla \times A = V}$$

- Scalar potential–

Scalar potential, simply stated, describes the situation where the difference of the potential energies of an object in two different positions depends only on positions, not upon the path taken by the object in travelling from one position to another.

The scalar potential is an example of an scalar field, given a vector field F, the scalar potential P is defined s.t.

$$\boxed{F = -\nabla P = -\left(\frac{\partial P}{\partial x}, \frac{\partial P}{\partial y}, \frac{\partial P}{\partial z}\right)}$$

∇P is a gradient of P.

- Retarded Potential–

In electrodynamics, the retarded potentials are the electromagnetic potentials for the electromagnetic field generated by time varying electric field or charge distribution in the past.

$$\phi = \frac{\rho}{\epsilon_0}$$

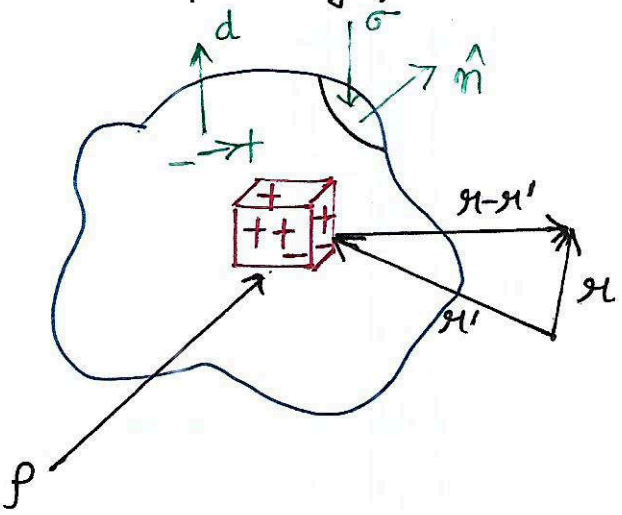
↑ electric potential

- Advanced Potential & Retarded for time-depending field-

$$\phi(r,t) = \frac{1}{4\pi\epsilon_0}\int \frac{\rho(r',t_r)}{(r-r')}\, d^3r'$$

$$A(r,t) = \frac{\mu_0}{4\pi}\int \frac{J(r',t_r)}{(r-r')}\, d^3r'$$

$$t_r = t - \frac{|r-r'|}{c}$$



t_r is retarded time.

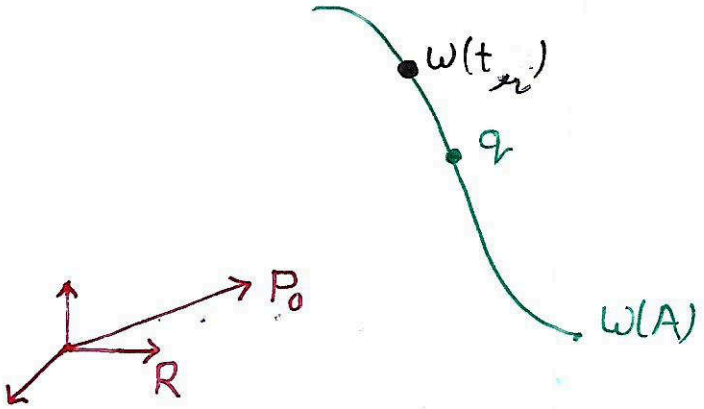
$$-E = \nabla\phi + \frac{\partial A}{\partial B}\,,\quad B = \nabla \times A$$ } Jefimenko's equation

$$t_a = t + \frac{|r-r'|}{c}$$

t_a is advanced time

- Lienard Wiechart Potentials-

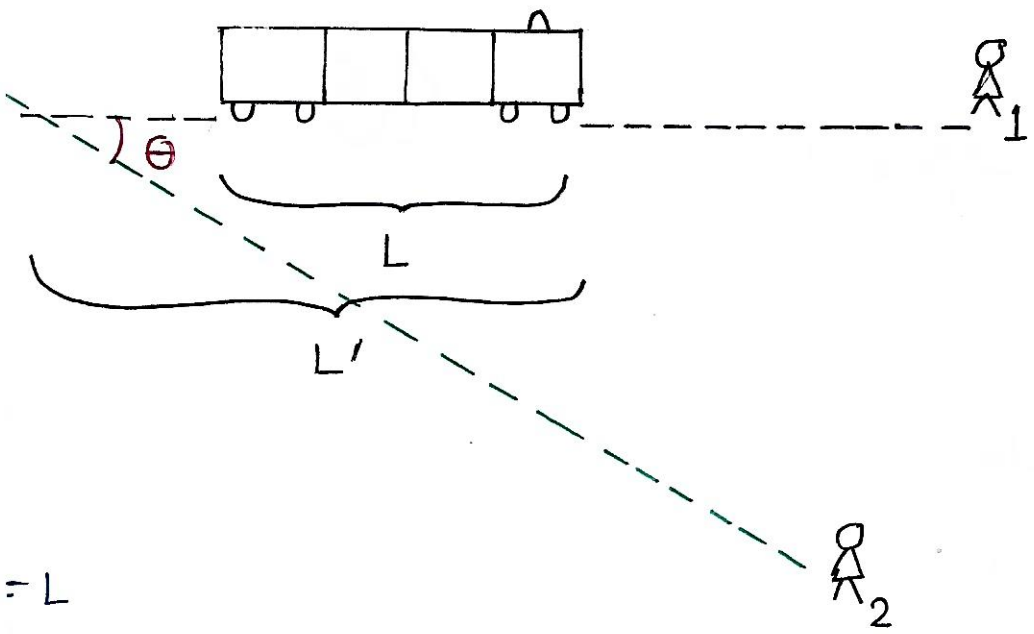
The Lienard wiechert potential are scalar and vector potential produced by moving point charge.



$$t_r = t - \frac{|w(t_r) - \rho_0|}{c}$$

$$r = c(t - t_r)$$

$$V(r,t) = \frac{1}{4\pi\epsilon_0}\int \frac{\rho(r', t_r)}{r}\, dr'$$



$L' = L$

$\frac{L'}{c} = \frac{L'-L}{V}$

$\frac{L'V}{c} = L'-L$

$L' - \frac{L'V}{c} = L$

$$\left(L' = \frac{L}{1-\frac{V}{c}}\right)_1$$

$\frac{L'\cos\theta}{c} = \frac{L'-L}{V}$

$L' = \frac{L}{1-\frac{V\cos\theta}{c}}$

$$\left(L' = \frac{L}{1-\frac{V\hat{r}}{c}}\right)_2$$

$$\tau' = \frac{T}{1-\frac{V\hat{r}}{c}}$$

$$V(r,t) = \frac{1}{4\pi\epsilon_0}\int \frac{\rho(r, t_r)}{1-\frac{\hat{r}V}{c}}\, d\tau$$

$$\boxed{V(r,t) = \frac{qc}{4\pi\epsilon_0\left(r - \frac{\vec{r}\cdot\vec{V}}{c}\right)}}$$

$$A(r,t) = \frac{\mu_0}{4\pi}\int \frac{J(r';tr)}{r}\,d\tau'$$

$$A(r,t) = \frac{\mu_0}{4\pi r}\int \frac{\rho(r,tr)}{1-\frac{\vec{r}\cdot V}{C}}\,d\tau \qquad [\because J=\rho V]$$

$$\boxed{A(r,t) = \frac{\mu_0 q C V}{4\pi(rC-\vec{r}\cdot\vec{V})} = \frac{V}{C^2}V(r,tr)}$$

- Multipole Expansion of the Electromagnetic field-

[Dr. Altan Baykal-Lecturar]

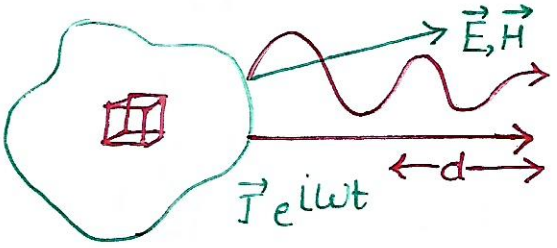
→ Radiation for localized oscalliting Forces

↓

current or charge density

$$\vec{A} = \frac{\mu_0}{4\pi}\int \frac{\vec{J}(\vec{x})}{|\vec{x}-\vec{x}''|}\,e^{ik|x-x^2|}\,d^3x'$$

$$\vec{A} = \frac{\mu_0}{4\pi}\frac{e^{ikr}}{r}\sum_n \frac{(-ik)^n}{n!}\int \vec{J}(\vec{x})(\hat{n}\cdot\vec{x})^n d^3x'$$



$$\vec{A}(\vec{x}) = -\frac{i\mu\omega}{4\pi}\frac{e^{ikr}}{r}\vec{p}$$

↓

$$\vec{p} = \int \vec{x}\rho(\vec{x})d^3x'$$

$\oplus\ qe^{-i\omega t}$

$\ominus\ qe^{-i\omega t}$

$$\vec{H} = \frac{\vec{B}}{\mu_0} = \frac{\vec{\nabla}\times\vec{A}}{\mu_0}$$

$$\vec{H} = \frac{-i\mu_0\omega}{\mu_0 4\pi}\left[\vec{\nabla}\times\left(\frac{e^{ikr}}{r}(\vec{p})\right)\right]$$

$$\vec{\nabla}_r = \frac{\partial}{\partial r}\hat{r}$$

$$\vec{H} = \frac{-i\mu_0\omega}{\mu_0 4\pi}\left[\vec{\nabla}\left(\frac{e^{ikr}}{r}\right)\times\vec{p} + \frac{e^{ikr}}{r}\vec{\nabla}\times\vec{p}\right]$$

$$\vec{H} = \frac{-i\omega}{4\pi}\left[\frac{i}{r}\cdot e^{-ikr} - \frac{e^{ikr}}{r^2}\right]\hat{n}\times\vec{p}$$

$$\vec{H} = \left(\frac{-i\omega}{4\pi}\right) ik\,\frac{e^{-ikr}}{r}\left(1-\frac{1}{ikr}\right)\hat{n}\times\vec{p}$$

$$\boxed{\vec{H} = \frac{ck^2}{4\pi}\left(\frac{e^{ikr}}{r}\right)\left(1-\frac{1}{ikr}\right)\hat{n}\times\vec{p}} \leftarrow \text{Spherical wave}$$

$\leftarrow$ impedance of free space

$$\vec{E} = \frac{iZ_0}{k}\,\vec{\nabla}\times\vec{H}$$

$$\frac{1}{\sqrt{\mu_0\epsilon_0}}$$

$$\vec{E} = i\sqrt{\frac{\mu_0}{\epsilon_0}}\cdot\frac{1}{k}\left[\frac{ck^2}{4\pi}\right]\vec{\nabla}\times\left[\frac{e^{ikr}}{r}\left(1-\frac{1}{ikr}\right)\hat{n}\times\vec{p}\right]$$

$$\vec{E} = \frac{ik}{4\pi\epsilon_0}\vec{\nabla}\times\left[(\hat{n}\times\vec{p})\left(\frac{e^{ikr}}{r}\left(1-\frac{1}{kr}\right)\right)\right]$$

$\Downarrow$

Scalar term

$$\boxed{\vec{E} = \frac{ik}{4\pi\epsilon_0}\left[\vec{\nabla}\left(\frac{e^{ikr}}{r}-\frac{e^{ikr}}{ikr^2}\right)\times(\hat{n}\times\vec{p}) + \left(\frac{e^{ikr}}{r}-\frac{e^{ikr}}{ikr^2}\right)\vec{\nabla}\times(\hat{n}\times\vec{p})\right]}$$

$$\left(ik\frac{e^{ikr}}{r} - \frac{e^{ikr}}{r^2} - \frac{ike^{-ikr}}{ikr^2} + \frac{2e^{ikr}}{ikr^3}\right)\frac{\hat{n}\times(\hat{n}\times\vec{p})}{(\hat{n}\cdot\vec{p})\hat{n}-(\hat{n}\cdot\hat{n})\vec{p}}$$

$$-\frac{\vec{p}}{r} = \frac{(\vec{p}\cdot\hat{n})\hat{n}}{r}$$

$$\frac{ze^{ikr}}{r^2}$$

Now

$$\vec{E} = \frac{1}{4\pi\epsilon_0}\left[k^2(\hat{n}\times\vec{p})\times\hat{n}\,\frac{e^{ikr}}{r} + \left(3\hat{n}(\hat{n}\cdot\vec{p})-\vec{p}\right)\left(\frac{1}{r^2}-\frac{ik}{r^2}\right)e^{ikr}\right]$$

$$\vec{H} = \frac{ck^2}{4\pi}\left(\frac{e^{ikr}}{r}\right)\left(1-\frac{1}{ikr}\right)\hat{n}\times\vec{p}$$

If you go to the far distance, all the dominating terms (much more) faster.

$$kr >>> 1$$

$$\rightarrow \vec{H} = \frac{ck^2}{4\pi}\left(\frac{e^{ikr}}{r}\right)\hat{n}\times\vec{p}$$

$$\rightarrow \vec{E} = \frac{1}{4\pi\epsilon_0}\left(k^2(\hat{n}\times\vec{p})\times\hat{n}\,\frac{e^{ikr}}{r}\right)$$

Combine both of the $\vec{E}$ and $\vec{H}$

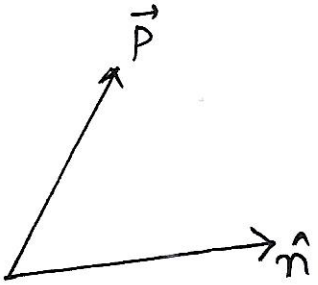
$$\vec{E} = \frac{1}{\epsilon_0 c}\left[\underbrace{\frac{ck^2}{4\pi}(\hat{n}\times\vec{p})\frac{e^{ikr}}{r}}_{\vec{H}}\times\hat{n}\right]$$

$$\frac{1}{\sqrt{\mu_0\epsilon_0}}$$

$$\boxed{\vec{E} = \sqrt{\frac{\mu_0}{\epsilon_0}}\,\vec{H}\times\hat{n}}$$

$$\downarrow$$

$$Z_0$$



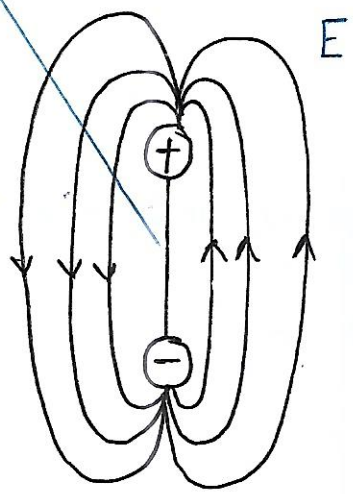


$$\boxed{\vec{E} = Z_0(\vec{H}\times\hat{n})}$$

Now $K_r <<< 1$

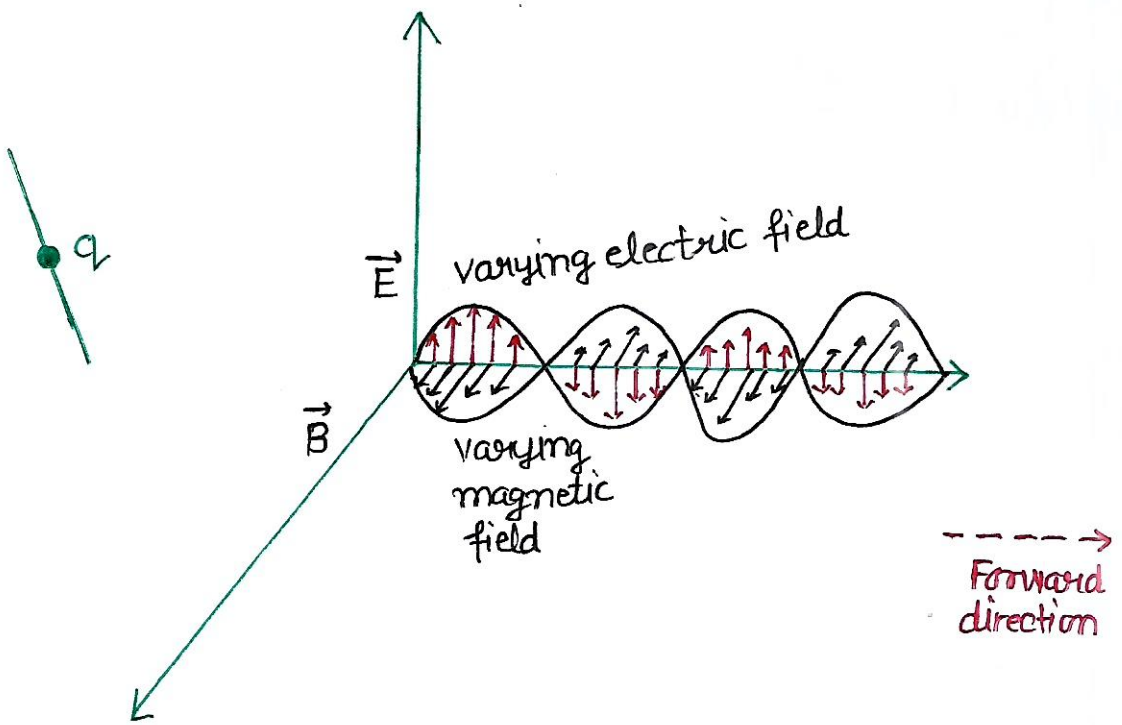
$$\vec{E} = \frac{1}{4\pi\epsilon_0}\left[\frac{3\hat{n}(\hat{n}\cdot\vec{p})\cdot\vec{p}}{r^3}\right]$$

→ near static zone



$$\boxed{|\vec{H}| << 4|\vec{E}|}$$

• Electromagnetic waves in free space-



In free space, there is no charge density and no current density. The maxwell equations in free space are

$$\nabla \cdot E = 0 \quad \ldots\ldots (1)$$

$$\nabla \cdot B = 0 \quad \ldots\ldots (2)$$

$$\nabla \times E = -\frac{\partial B}{\partial t} \quad \ldots\ldots (3)$$

$$\nabla \times B = \underbrace{\mu_0 \rho}_{\Downarrow} + \mu_0 \epsilon_0 \frac{\partial E}{\partial t}$$

$$= 0$$

$$\nabla \times B = \mu_0 \epsilon_0 \frac{\partial E}{\partial t} \quad \ldots\ldots (4)$$

These are four coupled first order differential equations.

Taking curl of eqn (3)

$$\nabla \times (\nabla \times E) = \nabla \times \left(-\frac{\partial B}{\partial t}\right)$$

$$\underbrace{\nabla(\nabla \cdot E)}_{=0} - \nabla^2 E = -\frac{\partial}{\partial t}(\nabla \times B)$$

$$\nabla^2 E = \frac{\partial}{\partial t}\left(\mu_0 \epsilon_0 \frac{\partial E}{\partial t}\right)$$

$$\nabla^2 E = \mu_0 \epsilon_0 \frac{\partial^2 E}{\partial t^2} \quad \ldots\ldots (5)$$

Similarly taking curl of eq^n(4)

$$\nabla\times(\nabla\times B) = \nabla\left(\mu_0\epsilon_0\frac{\partial E}{\partial t}\right)$$

$$\nabla(\nabla\cdot B) - \nabla^2 B = \nabla\left(\mu_0\epsilon_0\frac{\partial E}{\partial t}\right)$$

$$\nabla^2 B = \mu_0\epsilon_0\frac{\partial}{\partial t}(\nabla\times E)$$

$$\nabla^2 B = \mu_0\epsilon_0\frac{\partial}{\partial t}\left(-\frac{\partial B}{\partial t}\right)$$

$$\nabla^2 B = \mu_0\epsilon_0\frac{\partial^2 B}{\partial t^2} \quad \ldots\ldots\ldots (6)$$

Standard wave form

$$\nabla^2\psi = \frac{1}{v^2}\frac{\partial^2\psi}{\partial t^2} \quad \ldots\ldots\ldots (7)$$

comparing the eq^n(5),(6) with (7), we observe that eq^n(5) and (6) are electromagnetic waves eqn in free space representing oscillation of magnetic and electric wave.

Velocity of EM waves in free space-

comparing eq^n(5),(6) and(7), we get

$$\mu_0\epsilon_0 = \frac{1}{v^2}$$

$$v = \frac{1}{\sqrt{\mu_0\epsilon_0}}$$

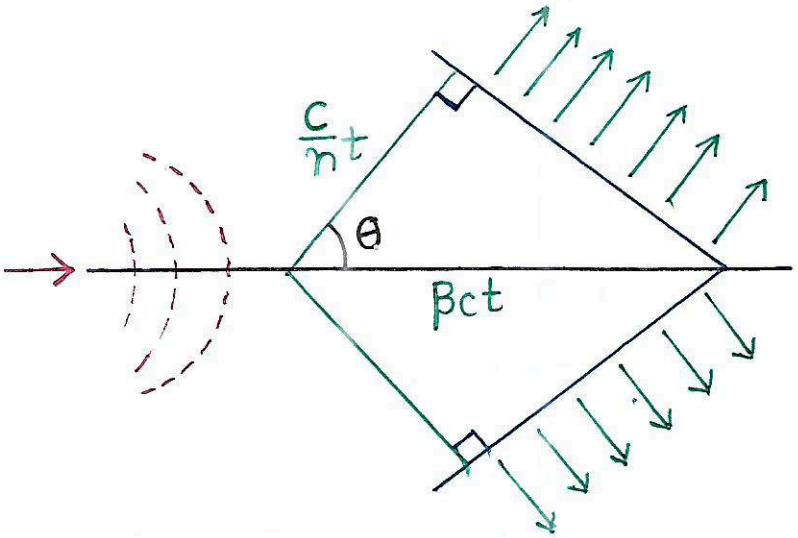
$$v = \frac{1}{\sqrt{4\pi\times10^{-7}\times\frac{1}{4\pi}\cdot\frac{10^{-9}}{9}\times\pi}}$$

$$\boxed{v = 3\times10^8\ m/s = c}$$ speed of Light

UNIT-2
Radiations from Moving Charges

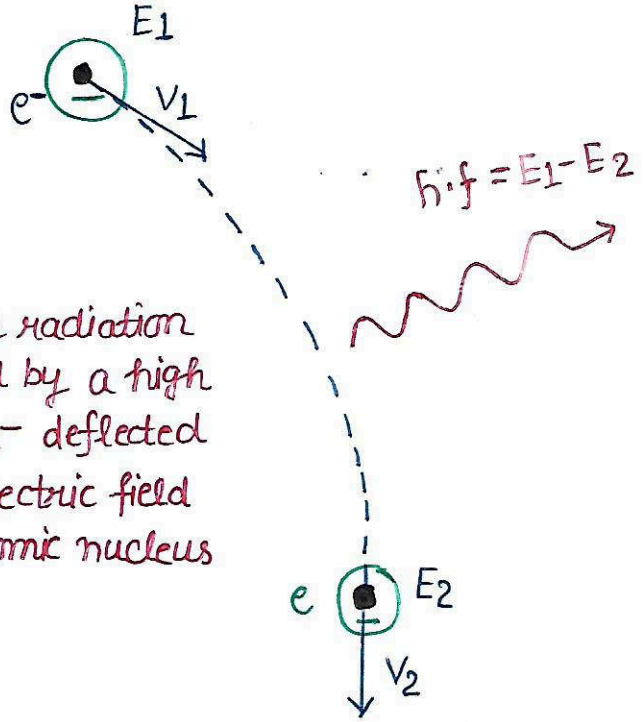
- **Cerenkov Radiation-**

Cerenkov Radiation is an electromagnetic Radiation emitted when a charged particle passes through a dielectric medium at the speed greater than the phase velocity of light in that medium.
The characteristic blue glow of an underwater nuclear reactor is due to cherenkov radiation.



- **Bremsstralung Radiation-**

Bremsstralung Radiation from bremsen "to brake" and Stralung "Radiation", i.e. breaking radiation or dellaration radiation is electromagnetic radiation produced by the declaration of a charged particle when deflected by another charged particle.



Breaking radiation produced by a high energy e⁻ deflected in the electric field of an atomic nucleus

• The Electromagnetic Field of a uniformly moving point charge-

The Electric and magnetic field of a point charge in motion are given by eqn

$$E(r,t) = \frac{q}{4\pi\epsilon_0}\left[\frac{(\mathcal{R}-R\vec{\beta})(1-\beta^2)}{(R-\mathcal{R}\cdot\vec{\beta})^3} + \frac{(\mathcal{R}\times(\mathcal{R}-R\vec{\beta})\times\vec{\beta})}{c(R-\mathcal{R}\cdot\vec{\beta})^3}\right]_{retarded}$$

$$B(r,t) = \frac{\mu_0 c q}{4\pi}\left[\frac{(\vec{\beta}\times n)(1-\beta^2)}{(R-\mathcal{R}\cdot\vec{\beta})^3} + \frac{n\times(\mathcal{R}\times(\mathcal{R}-R\vec{\beta})\times\vec{\beta}}{cR(R-\mathcal{R}-\vec{\beta})^3}\right]_{retarded}$$

$V = c\beta = \text{Constant}$

Then

$\beta = 0$

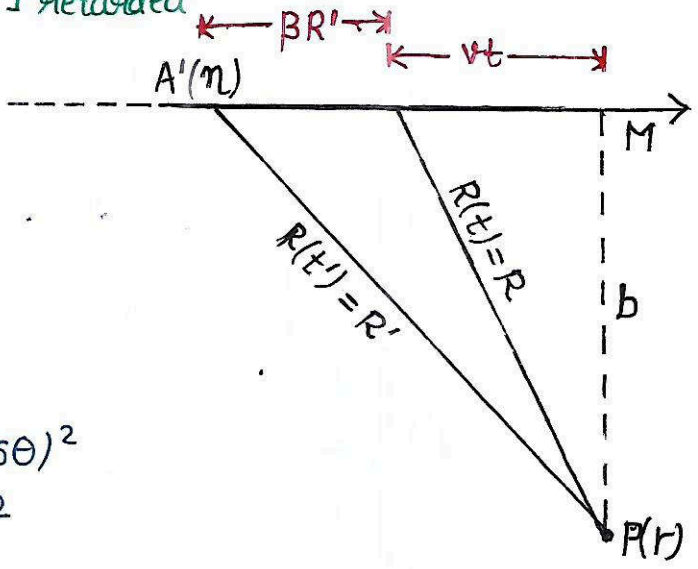
$$E(r,t) = \frac{q}{4\pi\epsilon_0}\left[\frac{(\mathcal{R}-R\vec{\beta})(1-\beta^2)}{(R-\mathcal{R}\cdot\vec{\beta})^3}\right]_{retarded}$$

$$\vec{\beta}_{retarded} = \vec{\beta}$$

$$(1-\vec{\beta}^2)_{retarded} = (1-\beta^2)$$

$$E(r,t) = \frac{q(1-\beta^2)}{4\pi\epsilon_0}\left[\frac{\mathcal{R}-R\vec{\beta}}{(R-\mathcal{R}\vec{\beta})^3}\right]_{retarded}$$

$$B(r,t) = \left[\frac{n\times E(r,t)}{c}\right]_{retarded}$$



$$[\mathcal{R}-R\vec{\beta}]_{retarded} = \mathcal{R}'-R'\vec{\beta} = \mathcal{R}$$

$$b = R'\sin\theta' = R\sin\theta$$

$$\beta^2R'^2\sin^2\theta' = \beta^2R^2\sin^2\theta$$

$$\beta^2R'^2(1-\cos^2\theta') = \beta^2R^2(1-\cos^2\theta)$$

$$\beta^2R'^2-(\beta R'\cos\theta')^2 = \beta^2R^2-(\beta R\cos\theta)^2$$

$$\beta^2R'^2-(\vec{\beta}\cdot\mathcal{R}')^2 = \beta^2R^2-(\vec{\beta}\cdot\mathcal{R})^2$$

$$[\mathcal{R}-R\vec{\beta}^2]_{retarded} = R^2-\beta^2R^2(1-\cos^2\theta)$$

$$[\mathcal{R}-R\vec{\beta}^2]_{retarded} = R^2(1-\beta^2\sin^2\theta)$$

$$E(r,t) = \frac{q}{4\pi\epsilon_0} \cdot \frac{R(1-\beta^2)}{R^3(1-\beta^2\sin^2\theta)^{3/2}}$$

$$B(r,t) = \left[\frac{n \times E}{c}\right] = \frac{\mu_0 c q}{4\pi}\left[\frac{(\vec{\beta} \times R)(1-\beta^2)}{(R-\vec{R}\vec{\beta})^3}\right]$$

$$B(r,t) = \frac{\mu_0 c q}{4\pi}(1-\beta^2)\frac{[\vec{\beta} \times \vec{R}]_{retarded}}{[(R-\vec{R}\cdot\vec{\beta}]_{retarded}]^3}$$

$$\vec{\beta} \times \vec{R}' = \vec{\beta} \times \vec{R}$$

$$[\vec{\beta} \times \vec{R}]_{retarded} = \vec{\beta} \times \vec{R}$$

$$\boxed{B(r,t) = \frac{\mu_0 c q}{4\pi}\left[\frac{(\vec{\beta} \times \vec{R})(1-\beta^2)}{(1-\beta^2\sin^2\theta)^{3/2}}\right]}$$

- **Radiation from an Accelerated charge at Low Velocity - Larmor's Formula!**

The electromagnetic fields of a point charge in motion are

$$E(r,t) = \frac{q}{4\pi\epsilon_0}\left[\frac{(\vec{R}-R\vec{\beta})(1-\beta^2)}{[R-\vec{R}\vec{\beta}]^3} + \frac{\vec{R} \times (\vec{R}-R\vec{\beta}) \times \vec{\beta}'}{c(R-\vec{R}\vec{\beta})^3}\right]$$

$$B(r,t) = \left[\frac{n \times E}{c}\right] = \left[\frac{\vec{R} \times \vec{E}}{Rc}\right]$$

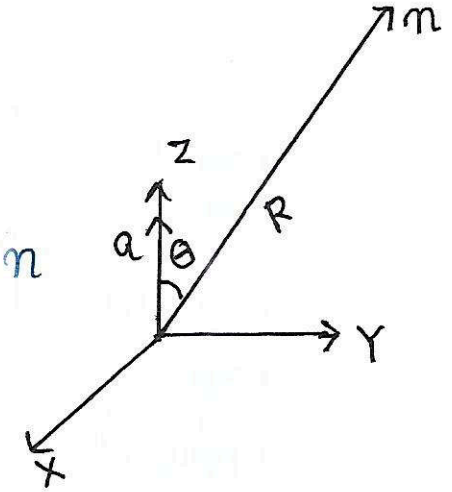
$$E_a(r,t) = \frac{q}{4\pi\epsilon_0 c^2}\left[\frac{(n\cdot a)\, n - a}{R}\right]$$

$$S_a^* = E_a \times H_a = \frac{E_a \times B_a}{\mu_0}$$

$$B = \mu_0 A$$

$$S_a = \frac{1}{\mu_0 c}\left\{\frac{q}{4\pi\epsilon_0 c}\right\}^2 \left|\left[\frac{(n\cdot a)\, n - a}{R}\right]^2\right| n$$

$$S_a = \frac{1}{4\pi\epsilon_0} \cdot \frac{q^2 a^2}{4\pi c^3 R^2}\sin^2\theta\, n$$



Then

$$P = \int_S S_a \cdot n \, da$$

$$\boxed{P = \frac{1}{4\pi\epsilon_0} \cdot \frac{q^2 a^2}{4\pi c^2}\left(\frac{4}{3}\right)(2\pi) = \frac{1}{4\pi\epsilon_0}\frac{2q^2a^2}{3c^3}}$$

• Radiation from an accelerated Charges at High Velocity!

→ Relativistic Generalisation of Larmor formula.

Larmor's non-relativistic formula is

$$P = \frac{1}{4\pi\epsilon_0}\left(\frac{2q^2c^2}{3\cdot c^3}\right)$$

This formula can be generalized for abbitrary velocities of change by using the fact that radiated electromagnetic energy behaves under Lorentz transformation, like the fourth component of a four vector*.

$$P = \frac{dE_{rad}}{dt}$$

$$dE_{rad} = P\,dt$$

Then

$$F = ma \Rightarrow a = \frac{F}{m}$$

$$a = \left(\frac{dP/dt}{m}\right)$$

$$P = \frac{1}{4\pi\epsilon_0}\cdot\frac{2q^2(a\cdot a)}{3c^3}$$

$$P = \frac{1}{4\pi\epsilon_0}\cdot\frac{2}{3}\cdot\frac{q^2}{m^2c^3}\left(\frac{dP_\mu}{dt}\,\frac{dP_\mu}{dt}\right)$$

$$P = \frac{1}{4\pi\epsilon_0}\cdot\frac{2}{3}\cdot\frac{q^2\gamma^2}{m^2c^3}\left[\left(\frac{dP}{dt}\right)^2 - \frac{1}{c^2}\left(\frac{dE}{dt}\right)^2\right]$$

$$E = \frac{mc^2}{\sqrt{1-\beta^2}}$$

$$P = \frac{mv}{\sqrt{1-\beta^2}}$$

Then

$$\boxed{P = \frac{1}{4\pi\epsilon_0}\cdot\frac{2}{3}\frac{q^2\gamma^6}{c}\left[\vec{\beta}^2 - (\vec{\beta}\times\vec{\beta}^2)\right]}$$

Classical Mechanics

- Langrangian formulation and Variational Principle$_1$
- Hamiton's Formulation$_2$
- Principle of Least Action$_3$
- Poisson brackets$_3$
- Mechanics of rigid bodies and Theory of small oscillations$_4$

UNIT - 1

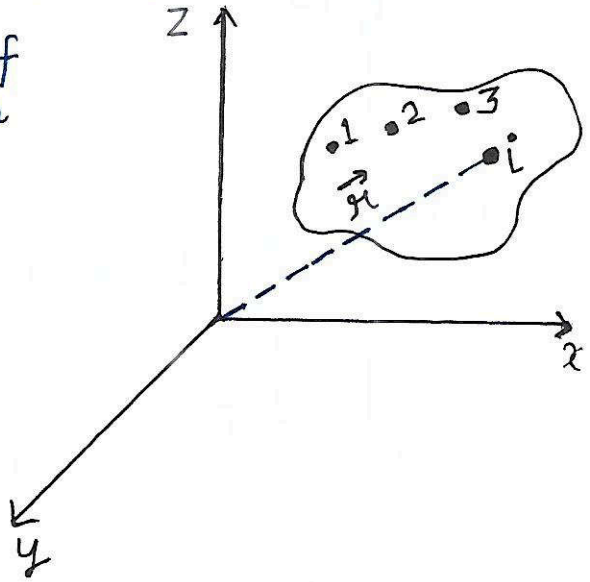
Lagrangian Formulation and Variation Principle

• Mechanics of Particles-

Mechanics is a branch of Physics which deals with physical objects in motion and at rest under the influence of external and Internal interactions. Mechanics had developed since ancient times on the basis of Observations on the motion.

• D'Almbert's Principle -

Suppose that there is a system of n particles.



According to newton's second law of motion, the force on i_{th} particle is given by

$$F = ma$$

$$F = m\left(\frac{dv}{dt}\right)$$

$$F = \frac{d}{dt}(mv)$$

$$F = \frac{dP}{dt}$$

$$F = \dot{P}$$

Then

$$\vec{F_i} = \frac{d\vec{P_i}}{dt} = \dot{\vec{P_i}} \text{ ---}$$ [A virtual (Infinitesimal) displacement of a particle system.]

$$\vec{F_i} = \dot{\vec{P_i}}$$

$$\vec{F_i} - \dot{\vec{P_i}} = 0$$

$\vec{F_i}$ ↑ Actual Force acting on i_{th} particle

$-\dot{\vec{P_i}}$ ← Reserved effective force

This means

$$[\vec{F}_{net}]_i = \vec{F_i} - \dot{\vec{P_i}} = 0 \quad \ldots\ldots\ldots (1)$$

Which is the condition of equilibrium. This means that any particle in equilibrium under force which is equal to the actual force f_i with the reserved effective force.

δr_i is any arbitrary infinitesimal change of the coordinates.

Then by the definition or principle of the virtual work;

$$\sum_{i=1}^{n} (\vec{F}_{net})_i \, \delta\vec{r}_i = 0$$

$$\sum_{i=1}^{n} (\vec{F}_i - \vec{P}_i) \cdot \delta\vec{r}_i = 0 \qquad [\because \text{By equation 1}]$$

But

$$\vec{F}_i = \vec{F}_i^{\,a} + f_i \quad \ldots\ldots\ldots (2)$$

$\vec{F}_i$: force on ith particle

$\vec{F}_i^{\,a}$: Applied force

f_i : force due to constraints

$$\sum_{i=1}^{n} (\vec{F}_i^{\,a} + \vec{f}_i - \dot{\vec{P}}_i) \, \delta r_i = 0$$

$$\sum_{i=1}^{n} \vec{F}_i^{\,a} \, \delta r_i + \sum_{i=1}^{n} \vec{f}_i \, \delta\vec{r}_i + \left(-\sum_{i=1}^{n} \dot{\vec{P}}_i \, \delta r_i \right) = 0 \quad \ldots\ldots (3)$$

Now we restrict ourself to the system for which virtual work of the constraints are zero.

$$\sum_{i=1}^{n} \vec{f}_i \, \delta\vec{r}_i = 0 \quad \ldots\ldots (4)$$

From eqn (3) & (4)

$$\sum_{i=1}^{n} \vec{F}_i^{\,a} \, \delta r_i + \underbrace{\sum_{i=1}^{n} \vec{f}_i \, \delta\vec{r}_i}_{0} - \sum_{i=1}^{n} \dot{\vec{P}}_i \, \delta\vec{r}_i = 0$$

$$\sum_{i=1}^{n} \vec{F}_i^{\,a} \, \delta r_i - \sum_{i=1}^{n} \dot{\vec{P}}_i \, \delta\vec{r}_i = 0$$

For usually notation, $\vec{F}_i^{\,a}$ can be written as $\vec{F}_i$.

So, $\sum_{i=1}^{n} \vec{F}_i \delta\vec{r}_i - \sum_{i=1}^{n} \vec{P}_i \delta\vec{r}_i = 0$

$$\boxed{\sum_{i=1}^{n} (\vec{F}_i - \vec{P}_i)\delta r_i = 0}$$

Which is often called D'Alembert's Principle.

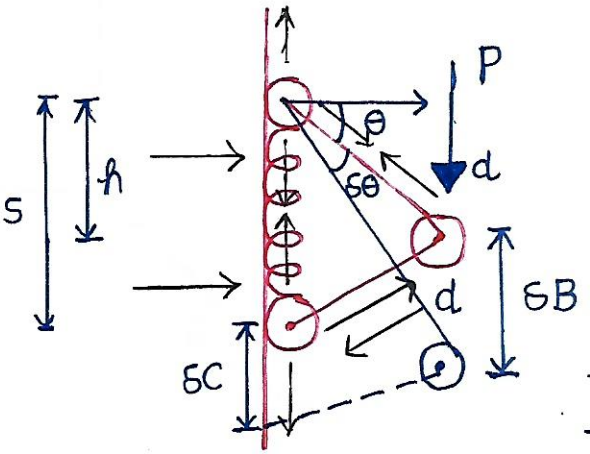
- **Principle of Virtual work-**

Virtual work states that if a system is in equilibrium and the system various forces. Assume a virtual (non-existent) displacement from the equilibrium position.

All forces that do not work on the system are not simply not considered in this analysis. All reaction forces and moments are eliminated from analysis. Only force that do not some (s) work are considered.

This work, caused by a non-existant virtual displacement is called virtual work.

The principle of virtual work states that virtual work will be zero for all virtual displacements. The result from the virtual work principle is the same as that of equilibrium principle.



$B = d\sin\theta$

$\delta B = d\cos\theta\,\delta\theta$

$C = 2d\sin\theta$

$\delta C = 2d\cos\theta\,\delta\theta$

→ h is unstratched height of the spring.

→ $C = h + s$

→ $s = C - h$

→ $s = 2d\sin\theta - h$

The magnitude of spring force is

$$F = Ks = k(2d\sin\theta - h) \quad \ldots\ldots (1)$$

And

$$\delta U = 0$$

$$P\delta B - F\delta C = 0$$

$$P(d\cos\theta\delta\theta) - K(2d\sin\theta - h)[(2d\cos\theta)\delta\theta] = 0$$

$P - K(2d\sin\theta - h)(2) = 0$

Equilibrium Angle;

$$\sin\theta = \frac{P + 2Kh}{4Kd} \quad \ldots\ldots\ldots (2)$$

From eqn (1) & (2)

$$F = K\left(2d\left[\frac{P+2Kh}{4Kd}\right] - h\right)$$

$$\boxed{F = 0.5d}$$

This conclude the that Internal Force is half of external force and on other side the forces are in equilibrium so this ends up with the example and principle of virtual work.

- Newtonian Mechanics: Constraints -

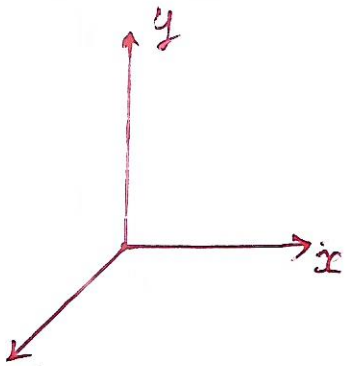
Cause of Acceleration

↓

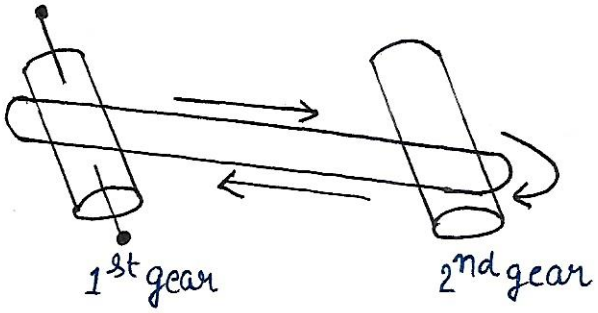
Newton $\longrightarrow \vec{F} = m\vec{a}$

$$(\vec{F}_x, \vec{F}_y, \vec{F}_z) = m(\vec{a}_x, \vec{a}_y, \vec{a}_z)$$

$$\vec{F}_x = m\vec{a}_x$$
$$\vec{F}_y = m\vec{a}_y$$
$$\vec{F}_z = m\vec{a}_z$$



Constraints means restrictions imposed over a particle. The motion of a particle or system of particle is generally restricted in some ways. A constraint motion is a motion which can't proceed arbitrary in any manner. Particle motion is restricted only.



If 1st gear moves forward then 2nd gear will also move forward because it is restricted.

→Classification of constraints-

1. Holonomic constraints-
   The constraints are presented in the system of N particles so
   $$F(r_1, r_2, \ldots, t) = 0$$
   It is independent to v.
2. Non-Holonomic constraints- can't express in form of $f(r_1, r_2 \ldots t) = 0$
3. Seleronomic constraints - doesn't depend on time
4. Rheonomic constraints - depends on time.
5. Bilateral Constraints- can be in the form of equation.
6. Unilateral Constraints- can be in the form of inequalities.
7. Conservative Constraints- Mechanical energy is conserved.
8. Dissipative Constraints- Mechanical energy of system is not conserved.

- **Lagrange equation of Motion using D'Alembert's Principle-**

$$\sum_{i=1}^{N} (\vec{F_i} - \dot{\vec{P}_i}) \cdot \delta\vec{r} = 0$$

This is D'Alembert's principle. We have achieved our aim, in that forces of constraints no longer (s) appear, and no subscript can now be dropped without ambiguity. It is still not in a useful form to furnish equation of motion for the system. We must now transform the principle into the equation or expression involving virtual displacement using generalized coordinates.

Consider a system of particles N. The transformation equation for the position vectors of the

$$r_i = r_i(q_1, q_2, \ldots q_K, \ldots q_n, t) \ldots\ldots (1)$$

where t is time.
$q_K = (K = 1, 2, \ldots n)$

differenciating eq^n(1) with respect to t, we get the velocity of ith particle.

$$\frac{dr_i}{dt} = \frac{\partial \vec{r_i}}{\partial t} \cdot \frac{\partial q_1}{\partial t} + \frac{\partial \vec{r_i}}{\partial t} \cdot \frac{\partial q_2}{\partial t} + \ldots\ldots + \frac{\partial r_i}{\partial t} \cdot \frac{\partial t}{\partial t}$$

and

$$\frac{d\vec{r_i}}{dt} = v_i$$

so

$$v_i = \frac{\partial r_i}{\partial t} q_j + \frac{\partial r_i}{\partial t} \partial t$$

$$v_i = \dot{r}_i = \frac{\partial r_i}{\partial t} q_j + \frac{\partial r_i}{\partial t} \partial t \quad \ldots\ldots (2)$$

But the last term is zero, since invirtual displacement only coordinate displacement is considered ϕ not on that time.

Therefore,

$$\delta r_i = \sum_j \frac{\partial r_i}{\partial q_j} \delta q_j \quad \ldots\ldots (3)$$

We know de'Alembert Prinaiple,

i.e.

$$\sum_{i=1}^{N} (\vec{F}_i - \vec{p}_i) \delta r_i = 0$$

$$\sum_{ij} F_i \frac{\partial r_i}{\partial q_j} \delta q_j - \sum_{ij} p_i \frac{\partial r_i}{\partial q_j} \delta q_j = 0$$

$\Downarrow$

Q_j

Then

$$\sum_j Q_j \delta q_j - \sum_j \dot{p}_i \frac{\partial r_i}{\partial q_j} \delta q_j = 0 \quad \ldots\ldots (4)$$

Let us evaluate the 2nd term of above eqn

$$\Rightarrow \sum_{ij} \dot{p}_i \frac{\delta q_j}{\partial q_j} \partial r_i = \sum_{ij} m_i \dot{r}_i \frac{\partial r_i}{\partial q_j} \delta q_j$$

$$\Rightarrow \sum_{ij} \left[m_i \dot{r}_i \frac{\partial r_i}{\partial q_j} + m_i \dot{r}_i \frac{d}{dt}\left(\frac{\partial r_i}{\partial q_j}\right) - m_i \dot{r}_i \frac{d}{dt}\left(\frac{\partial r_i}{\partial q_j}\right) \right] \delta q_j$$

$$\Rightarrow \sum_{ij} \left[\frac{d}{dt}\left(m_i \dot{r}_i \frac{\partial r_i}{\partial q_j}\right) - m_i v_i \frac{d}{dt}\left(\frac{\partial r_i}{\partial q_j}\right) \right] \delta q_j \quad \ldots\ldots (5)$$

Further

$$\frac{d}{dt}\left(\frac{\partial r_i}{\partial q_j}\right) = \frac{\partial}{\partial q_K}\left(\frac{\partial r_i}{\partial q_j}\right) \frac{\partial q_K}{\partial t} + \frac{\partial}{\partial t}\left(\frac{\partial r_i}{\partial q_j}\right) \frac{dt}{dt}$$

$$\sum_K \frac{\partial^2 r_i}{\partial q_K \partial r_j} \cdot q_K + \frac{\partial^2 r_i}{\partial t \partial q_j}$$

$$\frac{d}{dt}\left(\frac{\partial r_i}{\partial q_j}\right) = \frac{\partial}{\partial q_j}\left[\frac{\partial r_i}{\partial t}\right] = \frac{\partial}{\partial q_j}[v_i]$$ ——— Equation for Learning

$$\frac{d}{dt}\left(\frac{\partial r_i}{\partial q_j}\right) = \frac{\partial v_i}{\partial q_j} \quad \ldots\ldots\ldots (6)$$

differential eq^n(1) with respect to $\dot{q}_j$

$$v_i = \sum_j \frac{\partial r_i}{\partial q_j} \dot{q}_j + \frac{\partial r_i}{\partial t}$$

$$\frac{\partial v_i}{\partial \dot{q}_j} = \frac{\partial r_i}{\partial q_j} \quad \ldots\ldots\ldots\ldots\ldots (7)$$

Put eq^n(6) & (7) in the eq^n(5)

$$\sum_{ij} \dot{p} \frac{\partial r_i}{\partial q_j} \delta q_j = \sum_{ij} \left[\frac{d}{dt}\left(m_i v_i \frac{\partial v_i}{\partial \dot{q}_j}\right) - m_i v_i \frac{\partial v_i}{\partial q_j}\right] \delta q_j$$

$$\sum_{ij} \dot{p} \frac{\partial r_i}{\partial q_j} \delta q_j = \sum_{ij} \left[\frac{d}{dt}\left\{\frac{\partial}{\partial \dot{q}_j}\left(\sum_j \frac{1}{2} m_i v_i^2\right)\right\} - \frac{\partial}{\partial q_j}\left(\sum_j \frac{1}{2} m_i v_i^2\right)\right]$$

Putting this in eq^n(4)

$$\sum_j Q_j \delta q_j = \sum_j \left[\frac{d}{dt}\left\{\frac{\partial}{\partial \dot{q}_j}\left(\sum_i \frac{1}{2} m_i v_i^2\right)\right\} - \frac{\partial}{\partial q_j}\left(\sum_i \frac{1}{2} m_i v_i^2\right)\right] = 0$$

where $\frac{1}{2} m_i v_i^2 = T$

$$\sum_j Q_j \delta q_j - \sum_j \left[\frac{\partial}{\partial t}\left(\frac{\partial T}{\partial \dot{q}_j}\right) - \frac{\partial T}{\partial q_j}\right] \delta q_j$$

$$\boxed{\left[\frac{d}{dt}\left(\frac{\partial T}{\partial \dot{q}_j}\right) - \frac{\partial T}{\partial q_j}\right] = Q_j} \quad \ldots\ldots\ldots (8)$$

$j = 1, 2, \ldots\ldots n$

- Some data of this chapter is in P¼C3/D204 Physics notebook.

UNIT 2

Hamilton's Formulation

- Need of Formulation-

All the formulations of mechanics discussed in classical Mechanics thus far have been devised for treating systems with a finite, or at most a denumerably infinite, number of degrees of freedom. There are some mechanical problems, however, that involve continuous system.

- Hamilton's Physical Significance-

Here we will discuss Physical significance of H i.e. Hamiltonian.

1. A simple Interpretation of Hamiltonian mechanics comes from its application on a 1-D system consisting of one particle of mass m. The Hamiltonian represents the total energy of the system, which is the sum of Kinetic and potential energy, traditionally denoted T and V respectively. Here q is the space coordinate and p is momentum mv. Then

$$H = T + V \,, \quad T = \frac{p^2}{2m} \,, \quad V = V(q)$$

Like Lagrandre, Hamiltonian 'H' also possessess dimensions of energy but in all circumstances, it is not equal to the total energy E.

2. The system is conservative i.e. potential energy is coordinate dependent & not velocity dependant.
3. Co-ordinate transformation equation be dependent on time so that

$$\sum_j p_j q_j = 2T$$

This condition is necessary condition for Hamiltonian.

- Hamitonian Formulation-

It is possible to obtain a Hamiltonian Formulation for systems with a continueous set of coordinates much as was done for descrete system. To Indicate the method to approach, we return briefly to the linear chain of mass points. conjugate to each field component η_i, there is a canonical momentum.

$$P_i = \frac{\partial L}{\partial \dot{\eta}_i}$$

$$P_i = a \frac{\partial L_i}{\partial \dot{\eta}_i} \quad \ldots\ldots (1)$$

Hamiltonian for a system

$$H = P_i \dot{\eta}_i - L$$

$$H = a\left(\frac{\partial L_i}{\partial \dot{\eta}_i} \dot{\eta}_i - L_i\right) \quad \ldots\ldots (2)$$

$a \longrightarrow 0$
$L_i \longrightarrow L$

Then

$$H = \int dx \left(\frac{\partial L}{\partial \dot{\eta}} \dot{\eta} - L\right) \quad \ldots\ldots (3)$$

The individual canonical momentum P_i, as given by eq^n(1), vanish in the continuous limit, but we can define a momentum density π, that remains finite:

$$\lim_{a \to 0} \frac{P_i}{a} \cong \pi \cong \frac{\partial L}{\partial \dot{\eta}}$$

Equation 3 is in the form of space integral over a Hamiltonian density $\mathcal{H}$ defined by

$$\mathcal{H} = \pi \dot{\eta} - L \quad \ldots\ldots (4)$$

While a Hamiltonian Formulation can thus be introduced in a straightforward manner for classical field, note that the procedure over a time variable for space treatment. It is therefore in contrast to the development we have given for Lagendre formulation where the independant variable of time and space were handled systematically and symattrically. For this reason, the Hamiltonian approach, as least as introduced Here.

• Hamilton's Equation:-

The Hamiltonian, in general, is a function of generalized coordinates q_K, generalized momenta P_K and time t.

i.e.

$$H = H(q_1, q_2, q_3 \ldots\ldots q_n, P_1, P_2 \ldots\ldots P_n, t)$$

We may write

$$dH = \sum_K \frac{\partial H}{\partial q_K} dq_K + \sum_K \frac{\partial H}{\partial P_K} dP_K + \sum \frac{\partial H}{\partial t} dt \quad \ldots\ldots\ldots (1)$$

For a system of N Particles, where r_i does not depend on time. then

$$v_i = \sum_{K=1}^{n} \frac{\partial r_i}{\partial q_K} \dot{q}_K$$

Therefore,

$$T = \sum_{i=1}^{N} \frac{1}{2} m_i v_i^2 = \sum_{i=1}^{N} \frac{1}{2} m_i \left(\sum_{K=1}^{n} \frac{\partial r_i}{\partial q_K} \dot{q}_K \right)$$

$$T = \sum_{i=1}^{N} \frac{1}{2} m_i \sum_K \sum_\ell \left[\frac{\partial r_i}{\partial q_K} \cdot \frac{\partial r_i}{\partial q_\ell} \right] \dot{q}_K \cdot \dot{q}_\ell$$

$$\frac{\partial T}{\partial \dot{q}_K} = \sum_{i=1}^{N} \sum_\ell m_i \left[\frac{\partial r_i}{\partial q_K} \cdot \frac{\partial r_i}{\partial q_\ell} \right] \dot{q}_\ell$$

Multiply by $\dot{q}_K$

$$\sum_K \dot{q}_K \frac{\partial T}{\partial \dot{q}_K} = \sum_{i=1}^{N} \sum_K \sum_\ell m_i \left[\frac{\partial r_i}{\partial q_K} \cdot \frac{\partial r_i}{\partial q_\ell} \right] \dot{q}_K \dot{q}_\ell = 2T$$

K and ℓ run from 1 to n.

But $H = \sum_K P_K \dot{q}_K - L$

$$L = (q_1, q_2, \ldots q_K \ldots q_n, \dot{q}_1, \dot{q}_2, \dot{q}_3, \ldots q_n, t)$$

Therefore

$$dL = \sum_K \frac{\partial L}{\partial q_K} dq_K + \sum_K \frac{\partial L}{\partial \dot{q}_K} d\dot{q}_K + \frac{\partial L}{\partial t} dt$$

But $\dot{P}_K = \frac{\partial L}{\partial q_K}$

$$P_K = \frac{\partial L}{\partial \dot{q}_K}$$

$$dL = \sum_K \dot{P}_K dq_K + \sum_K P_K d\dot{P}_K + \frac{\partial L}{\partial t} dt \quad \ldots\ldots (2)$$

Put the value of dL in eq^n(1)

$$dH = \sum_K \dot{q}_K dP_K - \sum_K \dot{P}_K dq_K - \frac{\partial L}{\partial t} dt \quad \ldots\ldots\ldots (3)$$

comparing the cofficients of dP_K, dq_K and dt,

$$\dot{q}_K = \frac{\partial H}{\partial P_K} \quad \ldots\ldots (4)$$

$$-\dot{P}_K = \frac{\partial H}{\partial q_K} \quad \ldots\ldots (5)$$

$$-\frac{\partial L}{\partial t} = \frac{\partial H}{\partial t} \quad \ldots\ldots (6)$$

Eq^n (4) & (5) are known as Hamilton's canonical equation of motion.

(1) In cylindrical coordinates →

$$x = r\cos\theta$$
$$y = r\sin\theta$$
$$z = Z$$

$$L = T - V$$
$$L = \frac{1}{2} m(x^2 + y^2 + z^2) - V(x, y, z)$$

$$L = \frac{1}{2} m(r^2 + r^2\theta^2 + Z^2) - V(r, \theta, Z)$$

Now

$$H = \sum_K P_K \dot{q}_K - L$$

Where $K = r, \theta, Z$

$$H = P_r \dot{r} + P_\theta \dot{\theta} + P_z \dot{z} - \frac{1}{2}m(r^2 + r^2\theta^2 + z^2) + V(r,\theta,z)$$

$$H = \frac{1}{2m}\left(P_r^2 + \frac{P_\theta^2}{r^2} + P_z^2\right) + V(r,\theta,z)$$

Hamilton's equations are

$$\dot{q}_k = \frac{\partial H}{\partial P_k}$$

$$\dot{P}_k = -\frac{\partial H}{\partial q_k}$$

Therefore

$$\left\{ \begin{array}{l} r = \frac{P_r}{m} \\ P_r = \frac{P_\theta^2}{mr^3} - \frac{\partial V}{\partial r} \end{array} \right\}$$

$$\left\{ \begin{array}{l} \theta = \frac{\partial H}{\partial P_\theta} \\ P_\theta = -\frac{\partial V}{\partial \theta} \end{array} \right\}$$

$$\left\{ \begin{array}{l} z = \frac{\partial H}{\partial P_z} \\ P_z = -\frac{\partial V}{\partial z} \end{array} \right\}$$

These are cylindrical coordinates.

(ii) Spherical coordinates –

$$x = r\sin\theta\cos\phi$$
$$y = r\sin\theta\sin\phi$$
$$z = r\cos\theta$$

$$\dot{x} = r\sin\theta\,\dot{\phi}\cos\phi + r_\theta\cos\theta\cos\phi - r\sin\theta\,\phi\sin\phi$$
$$\dot{y} = r\sin\theta\sin\phi + r_\theta\cos\theta\sin\phi + r\sin\theta\,\phi\cos\phi$$
$$\dot{z} = r\cos\theta - r_\theta\sin\theta$$

$$L = T - V$$

$$L = \frac{1}{2} m(x^2 + y^2 + z^2) - V(x, y, z)$$

$$L = \frac{1}{2} m(\dot{r}^2 + r^2\dot{\theta}^2 + r^2 \sin^2\theta \dot{\phi}^2) - V(r, \theta, \phi)$$

Therefore

$$\dot{r} = \frac{P_r}{m}$$

$$\dot{\theta} = \frac{P_\theta}{mr^2}$$

$$\dot{\phi} = \frac{P_\phi}{mr^2 \sin\theta}$$

$$H = \sum_{K=r,\theta,\phi} P_K \dot{q}_K - L$$

$$H = \frac{1}{2m}\left(P_r^2 + \frac{P_\theta^2}{r^2} + \frac{P_\phi^2}{r^2 \sin^2\theta}\right) + V(r, \theta, \phi)$$

$$\begin{cases} P_r = \dfrac{P_\theta^2}{mr^3} + \dfrac{P_\phi^2}{mr^3 \sin^2\theta} - \dfrac{\partial V}{\partial r} \\ P_\theta = \dfrac{P_\phi^2 \cos\theta}{mr^2 \sin^3\theta} - \dfrac{\partial V}{\partial \theta} \\ P_\phi = -\dfrac{\partial V}{\partial \theta} \end{cases}$$

These are spherical coordinates.

UNIT - 3
Principle of Least action & Poission brackets

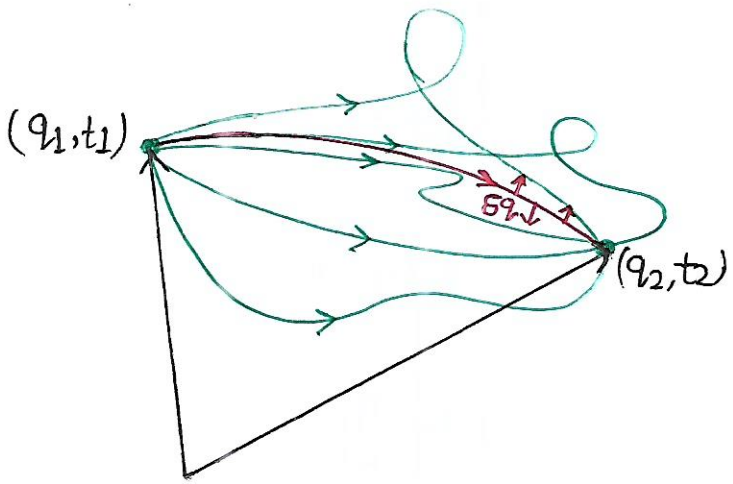
- **Principle of Least Action-**

The principle of Least action or more accurate principle of stationary action is a variational principle that when applied to an action of a mechanical system, can be used to obtain the equation of motion for that system. In relativity, a different action must be minimized or maximized.

The starting point of action denoted S of a physical system.

$$q = (q_1, q_2, q_3 \ldots q_k \ldots q_n)$$

$$q : R \longrightarrow (R^3 \ldots R^N)$$



According to the principle

$$\Delta \int_{t_1}^{t_2} \sum_K p_K \dot{q}_K \, dt = 0$$

$$\Downarrow$$

$$W$$

Where the quantity $W = \int_{t_1}^{t_2} \sum_K p_K \dot{q}_K \, dt$ is something called stationary action.

 # Canonical or contrast Transformation-

In Hamiltonian Mechanics, a canonical Transformation is a change of coordinates $(q, p, t) \longrightarrow (Q, P, t)$ that preserves the form of Hamilton equations. This is something known as invariance.

Hamilton's equation of motion is 1-D eqn.

Here

$$\dot{q} = \frac{\partial H}{\partial p} \qquad [\because H(q,p)]$$

$$\dot{p} = \frac{-\partial H}{\partial q}$$

Hamiltonian $H = \dot{p}\dot{q} - L$

↑ Lagrangian function

$q \longrightarrow Q$
$\dot{p} \longrightarrow P$
} called canonical transformation If $\dot{Q} = \frac{\partial H'}{\partial P}$ and $\dot{P} = \frac{-\partial H'}{\partial Q}$

Now $H'(Q, P)$

- Show that the transformation by

$$q = \sqrt{2P}\sin Q$$
$$\dot{p} = \sqrt{2P}\cos Q \text{ is canonical.}$$

Proof;

$$q = \sqrt{2P}\sin Q \ldots\ldots (1)$$
$$\dot{p} = \sqrt{2P}\cos Q \ldots\ldots (2)$$

deviding eq^n(1) by(2)

$$\frac{q}{\dot{p}} = \frac{\cancel{\sqrt{2P}}\sin Q}{\cancel{\sqrt{2P}}\cos Q}$$

$$\tan Q = \frac{q}{\dot{p}} \ldots\ldots\ldots (3)$$

(dev)^{squaring} eq^n (1) & (2) then add them

$$q^2 + \dot{p}^2 = 2P\sin^2 Q + 2P\cos^2 Q$$
$$q^2 + \dot{p}^2 = 2P(\sin^2 Q + \cos^2 Q)$$
$$q^2 + \dot{p}^2 = 2P$$
$$P = \frac{1}{2}(q^2 + \dot{p}^2) \ldots\ldots\ldots (4)$$

We shall use poission brackets conditions

$$[Q, Q] = [P, P] = 0$$
$$[Q, P] = 1$$

to show

$$[Q, P] = \left(\frac{\partial Q}{\partial q}\frac{\partial P}{\partial \dot{p}} - \frac{\partial Q}{\partial \dot{p}}\frac{\partial P}{\partial q}\right)$$

$$\sec^2 Q \frac{\partial Q}{\partial q} = \frac{1}{p}$$

$$\frac{\partial P}{\partial q} = q$$

$$\sec^2 Q \frac{\partial Q}{\partial p} = -\frac{q}{p^2}$$

$$\frac{\partial P}{\partial p} = p$$

Then

$$[Q,P] = \left[\left(\frac{1}{p}\cos^2 Q\right)p + \left(\frac{q}{p^2}\cos^2 Q\right)q\right]$$

$$[Q,P] = \left[\cos^2 Q\left(1 + \frac{q^2}{p^2}\right)\right]$$

$$[Q,P] = \cos^2 Q\left[(1 + \tan^2 Q)\right]$$

$$[Q,P] = \cos^2 Q \sec^2 Q$$

$$\boxed{[Q,P] = 1}$$

So the transformation is canonical and the condition for a transformation to canonical has been proved.

- Poission Brackets-

The poission brackets of two functions u, v with respect to the canonical variables (q,p) is defined as

$$[u,v]_{(q,p)} = \frac{\partial u}{\partial q_i}\cdot\frac{\partial v}{\partial p_i} - \frac{\partial u}{\partial p_i}\frac{\partial v}{\partial q_i}$$

In this bilinear expression we have a typical symplectic structure, as in Hamilton's equation.

→Properties-

1. Poission bracket does not obey commutative law.

$$[u,v]_{q,p} \neq [v,u]_{q,p}$$

Proof :- $[u,v]_{q,p}$

$$= \sum_k \left[\frac{\partial u}{\partial q_k}\frac{\partial v}{\partial p_k} - \frac{\partial u}{\partial p_k}\frac{\partial v}{\partial q_k} \right]$$

$$= -\sum_k \left[\frac{\partial u}{\partial p_k}\cdot\frac{\partial v}{\partial q_k} - \frac{\partial u}{\partial q_k}\frac{\partial v}{\partial p_k} \right]$$

$$= -\sum_k \left[\frac{\partial v}{\partial q_k}\frac{\partial u}{\partial p_k} - \frac{\partial v}{\partial p_k}\frac{\partial u}{\partial q_k} \right]$$

$$= -[v,u]_{q,p}$$

Hence

$$\boxed{[u,v]_{q,p} = -[v,u]_{q,p}}$$

2. Poission brackets obey distributive law :-

$$[u+v,w]_{q,p} = [u,w]_{q,p} + [v,w]_{q,p}$$

Proof :-

$$[u+v,w]_{q,p} = \sum_k \left[\frac{\partial(u+v)}{\partial q_k}\frac{\partial w}{\partial p_k} - \frac{\partial(u+v)}{\partial p_k}\frac{\partial w}{\partial q_k} \right]$$

$$= \sum_k \left[\left\{ \frac{\partial u}{\partial q_k} + \frac{\partial v}{\partial q_k} \right\}\frac{\partial w}{\partial p_k} - \left\{ \frac{\partial u}{\partial p_k} + \frac{\partial v}{\partial p_k} \right\}\frac{\partial w}{\partial q_k} \right]$$

$$= \sum_k \left[\frac{\partial u}{\partial q_k}\cdot\frac{\partial w}{\partial p_k} + \frac{\partial v}{\partial q_k}\cdot\frac{\partial w}{\partial p_k} - \frac{\partial u}{\partial p_k}\frac{\partial w}{\partial q_k} - \frac{\partial v}{\partial p_k}\frac{\partial w}{\partial q_k} \right]$$

$$= \sum_k \left[\frac{\partial u}{\partial q_k}\frac{\partial w}{\partial p_k} - \frac{\partial u}{\partial p_k}\frac{\partial w}{\partial q_k} \right] + \sum_k \left[\frac{\partial v}{\partial q_k}\frac{\partial w}{\partial p_k} - \frac{\partial v}{\partial p_k}\frac{\partial w}{\partial q_k} \right]$$

$$= \sum_k [uw]_{q,p} + [v,w]_{q,p}$$

$$= [uw]_{q,p} + [v,w]_{q,p}$$

3. Distribution law of Multiplication :

$$[uv,w]_{q,p} = u[v,w]_{q,p} + v[u,w]_{q,p}$$

Proof :

$$[uv,w] = \sum_K \left[\frac{\partial}{\partial q_K}(uv)\frac{\partial w}{\partial p_K} - \frac{\partial}{\partial p_K}(uv)\frac{\partial w}{\partial q_K}\right]$$

$$= \sum_K \left[\left(u\frac{\partial v}{\partial q_K} + \frac{\partial u}{\partial q_K}\cdot v\right)\frac{\partial w}{\partial p_K} - \left(u\frac{\partial v}{\partial p_K} + \frac{\partial u}{\partial p_K}v\right)\frac{\partial w}{\partial q_K}\right]$$

$$= \sum_K \left[u\frac{\partial v}{\partial q_K}\frac{\partial w}{\partial p_K} + \frac{\partial u}{\partial q_K}\cdot v\frac{\partial w}{\partial p_K} - u\frac{\partial v}{\partial p_K}\frac{\partial w}{\partial q_K} - v\frac{\partial u}{\partial p_K}\frac{\partial w}{\partial q_K}\right]$$

$$= \sum_K \left[u\left(\frac{\partial v}{\partial q_K}\frac{\partial w}{\partial p_K} - \frac{\partial v}{\partial p_K}\frac{\partial w}{\partial q_K}\right) + v\left(\frac{\partial u}{\partial q_K}\frac{\partial w}{\partial p_K} - \frac{\partial u}{\partial p_K}\frac{\partial w}{\partial q_K}\right)\right]$$

$$= u[v,w]_{(q,p} + v[u,w]_{(q,p)}$$

4. Jacobi Identity :

$$[u,(v,w)] + [v(u,w)] + [w(u,v)] = 0$$

5. $[p_j, p_K] = 0$

Proof :

$$[p_j,p_K]_{q,p} = \sum_K \left[\frac{\partial p_j}{\partial q_K}\cdot\frac{\partial p_K}{\partial p_K} - \frac{\partial p_j}{\partial p_K}\frac{\partial p_K}{\partial q_K}\right]$$

$$= \sum_K [0\times 1 - 0\times 0]$$

$$= 0$$

6. $[q_j, q_K] = 0$

Proof :

$$[q_j,q_K]_{q,p} = \sum_K \left[\frac{\partial q_j}{\partial q_K}\frac{\partial q_K}{\partial p_K} - \frac{\partial q_K}{\partial q_K}\frac{\partial q_j}{\partial p_K}\right]$$

$$= \sum_K \left[\frac{\partial q_j}{\partial p_K} - \frac{\partial q_j}{\partial p_K}\right]$$

$$= 0$$

7. $[q_j, p_k]_{q,p} = -\delta_{jk}$

$$[q_j, p_k]_{q,p} = \sum_k \left[\frac{\partial q_j}{\partial q_k} \cdot \frac{\partial p_k}{\partial p_k} - \frac{\partial q_j}{\partial p_k} \cdot \frac{\partial p_k}{\partial q_k} \right]$$

$$= \sum \left[\frac{\partial q_j}{\partial q_k} - \frac{\partial q_j}{\partial p_k} \frac{\partial p_k}{\partial q_k} \right]$$

$$= \delta_{jk}$$

And $\delta_{jk} = 0$ If $j \neq k$

$\delta_{jk} = 1$ If $j = k$

- Condition for Canonical Transformation-

Suppose $F = F(q_k, Q_k)$

$$\frac{\partial F}{dt} = 0$$

and $H = H'$

Then $p_k = \frac{\partial F}{\partial q_k}$ and $P_k = \frac{-\partial F}{\partial Q_k}$

$$dF = \sum_k \frac{\partial F}{\partial q_k} dq_k + \sum_k \frac{-\partial F}{\partial Q_k} dQ_k$$

$$dF = \sum_k p_k dq_k + \sum_k -P_k dQ_k$$

$$dF = \sum_k p_k dq_k - \sum_k P_k dQ_k \quad \ldots\ldots\ldots (1)$$

The left hand side of eq^1 is an exact differential, Hence for a given transformation to be canonical, the right hand side of eq^n(1), i.e. $\sum_k p_k dq_k - \sum_k P_k dQ_k$ must be an exact differential.

UNIT-4

Mechanics of Rigid bodies and theory of small oscillations

- The Eular's Angle-

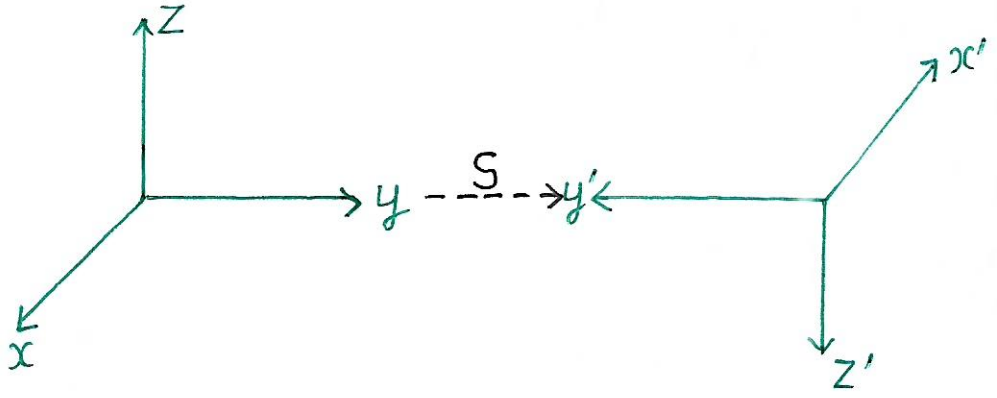
Consider the simplest 3X3 matrix with determinant -1:

$$S = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix} = -1$$

The transformation S has the effect of changing the sign of each of the components or coordinates axes. Such an operation transforms a right handed coordinate system into a left handed one and it is known as an inversion of the coordinate axes.

One method of performing an inversion is to rotate about a coordinate axis by 180° and then reflect in that coordinate axis direction. For the Z-axe(direction), this gives

$$\begin{pmatrix} \text{rotate} \\ \text{by } 180^\circ \\ \text{about Z} \end{pmatrix} \begin{pmatrix} \text{reflect} \\ \text{in the} \\ xy \text{ plane} \end{pmatrix} = \text{Inversion}$$



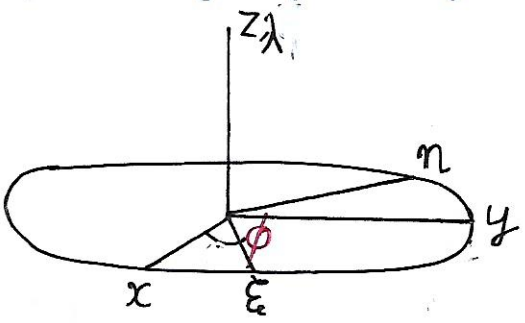
In matrix notation, this has the form

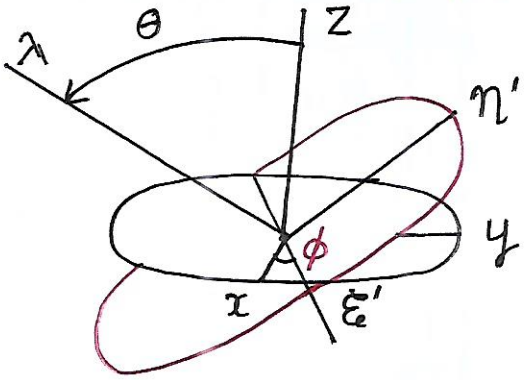
$$\begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix} = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

Where the 180° rotation is obtained by setting $\phi = 180^\circ$

We can carry out the transformation from a given cartesian coordinate system to another by means of three successive rotation performed in a specific sequence. The eular angles are then defined as the three successive angle of rotation.

The sequence employed here is started by rotating the initial system of axes xyz by an angle ϕ counterclockwise about the z axes.





The initial rotation about z can be described by the matrix D.

$$\xi = Dx$$

Then transformation

$$\xi' = C\xi$$

Hence

$x' = Ax$ is the product of the successive matrix.

$$A = BCD$$

Now

$$D = \begin{bmatrix} \cos\phi & \sin\phi & 0 \\ -\sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$C = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & \sin\theta \\ 0 & -\sin\theta & \cos\theta \end{bmatrix}$$

$$B = \begin{bmatrix} \cos\psi & \sin\psi & 0 \\ -\sin\psi & \cos\psi & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Then Product $A = BCD$

$$A = \begin{bmatrix} \cos\psi\cos\phi - \cos\theta\sin\phi\sin\psi & \cos\psi\sin\phi + \cos\theta\cos\phi\sin\psi & \sin\psi\sin\theta \\ -\sin\psi\cos\phi - \cos\theta\sin\phi\cos\psi & -\sin\psi\sin\phi + \cos\theta\cos\phi\cos\psi & \cos\psi\sin\theta \\ \sin\theta\sin\phi & -\sin\theta\cos\phi & \cos\theta \end{bmatrix}$$

This is..... Eulars Angle.

• Eular equation of motion for a rigid body-

If a rigid body is rotating under the action of a torque τ with one point fixed then the torque is expressed as

$$\tau = \left[\frac{dJ}{dt}\right]_S$$

where J is Angular momenta
S is subscript

The body coordinate system is rotating with an instantanous angular velocity ω. The time derivates of angular momentum J in the body coordinate and space coordinate system are related as

$$\left[\frac{dJ}{dt}\right]_S = \left[\frac{dJ}{dt}\right]_b + \omega \times J$$

$$\tau = \frac{dJ}{dt} + \omega \times J$$

$$\text{If } J = I_1\omega_1\hat{i} + I_2\omega_2\hat{j} + I_3\omega_3\hat{k}$$
$$\omega = \omega_1\hat{i} + \omega_2\hat{j} + \omega_3\hat{k}$$

$$\tau = I_1\omega_1\hat{i} + I_2\omega_2\hat{j} + I_3\omega_3\hat{k} + (\omega_1\hat{i} + \omega_2\hat{j} + \omega_3\hat{k}) \times (I_1\omega_1\hat{i} + I_2\omega_2\hat{j} + I_3\omega_3\hat{k})$$

Then

$$\left.\begin{aligned} \tau_1 &= I_1\omega_1 + (I_3 - I_2)\,\omega_2\omega_3 \\ \tau_2 &= I_2\omega_2 + (I_1 - I_3)\,\omega_1\omega_3 \\ \tau_3 &= I_3\omega_3 + (I_2 - I_1)\,\omega_1\omega_2 \end{aligned}\right\} \ldots\ldots\ldots\ldots (1)$$

Eq^n(1) is known as eular equation of motion of a rigid body for one point fixed under the action of a torque.

MATHMATICAL PHYSICS

- Differential equations
- Group Theory
- Complex Variable
- Matrix and tensors

UNIT-1
Differential Equations

- Besell's Equation-

$$x^2\frac{d^2y}{dx^2}+x\frac{dy}{dx}+(x^2-n^2)y=0$$

OR

$$\frac{d^2y}{dx^2}+\frac{1}{x}\frac{dy}{dx}+\left(1-\frac{n^2}{x^2}\right)y=0 \quad \ldots\ldots\ldots (1)$$

Let us consider that eqⁿ solution of Beselle's diffⁿ equation on asending power of x.

$$y=x^K(a_0+a_1x+a_2x^2+\ldots\ldots+a_rx^r)$$

$$y=\sum_{r=0}^{\infty}a_rx^{K+r}$$

$$\frac{dy}{dx}=\sum_{r=0}^{\infty}(K+r)a_rx^{K+r-1}$$

$$\frac{d^2y}{dx^2}=\sum_{r=0}^{\infty}a_r(K+r)(K+r-1)x^{K+r-2}$$

substitute $\frac{d^2y}{dx^2}$, $\frac{dy}{dx}$ and y values in eqⁿ (1)

$$\sum_{r=0}^{\infty}a_0(K+r)(K+r-1)x^{K+r-2}+\frac{1}{x}\sum_{r=0}^{\infty}a_r(K+r)x^{K+r-1}+\left(1-\frac{n^2}{x^2}\right)\sum_{r=0}^{\infty}a_rx^{K+r}=0$$

$$\sum_{r=0}^{\infty}a_r\left[(K+r)(K+r)-n^2\right]x^{K+r-2}+\sum_{r=0}^{\infty}a_rx^{K+r}=0 \quad \ldots\ldots\ldots (2)$$

This eqⁿ is identical & we can evaluated the diffⁿ power of x in eqⁿ(2). Let us first start with the smallest power i.e. x^{K+r-2}.

$$\sum_{r=0}^{\infty}a_r[(K+r)(K+r)-n^2]=0 \quad \ldots\ldots\ldots (3)$$

Putting $r=0$

$$a_0[(K)(K)-n^2]=0$$

$$a_0[K^2-n^2]=0$$

$$[K^2-n^2]=0$$

$$K^2 = n^2$$

$$\boxed{K = \pm n}$$

Putting $r = 1$

$$a_1[(K+1)^2 - n^2] = 0$$

$$(K+1)^2 = n^2 \neq 0$$

Then

$$\boxed{a_1 = 0}$$

$r \longrightarrow r+2$

Putting in eqn (2)

Then $$\sum_{r=0}^{\infty} a_{r+2}[(K+r+2)^2 - n^2]\, x^{K+r} + \sum_{r=0}^{\infty} a_{r+2}\, x^{K+r+2} = 0$$

Now comparing,

$$a_{r+2} = \frac{a_2}{(K+r+2)^2 - n^2}$$

$$= \frac{a_r}{(K+r+2+n)(K+r+2n)}$$

$r = 1, 3, 5 \ldots\ldots a_5$

→CASE I :

When $K = n$

$$a_{r+2} = \frac{-a_r}{(2n+r+2)(r+2)}$$

Now substituting $r = 0, 2, 4, 6, \ldots$

$r = 0$, then

$$a_2 = \frac{-a_0}{2(2n+2)} = \frac{-a_0}{(2)^2(n+1)}$$

$r = 2$, then,

$$a_4 = \frac{-a_2}{4(2n+4)} = \frac{a_0}{2 \cdot 4(2n+2)(2n+4)}$$

$r = 4$, then,

$$a_6 = \frac{-a_4}{(2)^4 \cdot 2!(2n+1)(2n+2)} = \frac{-a_0}{2 \cdot 4 \cdot 6(2n+2)(2n+4)(2n+6)}$$

Now,

$$y = x^n \left[a_0 + \frac{a}{2^2(n+1)} x^2 + \frac{a_0}{2^4 2!(n+1)(n+2)} x^4 + \dots \right]$$

$$y = x^n a_0 \left[1 + \frac{(-1)^1}{2^2 1!(n+1)} x^2 + \frac{(-1)^2}{2^4 2!(n+1)(n+2)} x^4 + \dots \right]$$

$$y = x^n a_0 \sum_{r=0}^{\infty} \frac{(-1)^r x^{2r}}{2^{2r} r! [(n+1)(n+2)\dots(n+r)]}$$

If $a_0 = \frac{1}{2^n \lceil n+1}$

The above eqn is known as Bessel's differential eqn solution of (1) kind where a_0 is constant

$$J_n(x) = x^n \frac{1}{2^n \lceil n+1} \sum_{r=0}^{\infty} \frac{(-1)^r \cdot x^{2r}}{2^{2r} r! (n+1)(n+2)\dots(n+r)}$$

$$J_n(x) = \sum_{r=0}^{\infty} \frac{(-1)^r}{r! \lceil n+r+1} \left(\frac{x}{2}\right)^{n+2r} \left\{ (n+1)\lceil n+1 - \lceil n+r+1 \right\}$$

This is required solution of this is 1st kind solution.

→ Case II :

$K = -n$

Then

$$J_r(x) = \sum_{r=0}^{\infty} \frac{(-1)^r}{r \lceil (-n)(r)+1} \left(\frac{x}{2}\right)^{-n+2r}$$

The second above solution is known as Beselle eqn of second kind.

Then

$$y = J_n(x) + J_{-n}(x)$$

• Beta and Gamma Function-

$\gamma \rightarrow$ Lower case gamma

$\Gamma \rightarrow$ Upper case gamma (In grik)

$$\Gamma n = \int_0^\infty e^{-x} x^{n-1} dx$$

$n > 0$

$$\Gamma n+1 = \int_0^\infty \underbrace{e^{-x} x^n}_{\text{By parts}} dx = \Pi(n)$$

$$\Pi(n) = \Gamma n+1$$

$$\Pi(n) = \frac{e^{-x}}{-1} x^n + \int e^{-x} \frac{d}{dx}(x^n)$$

$$\Pi(n) = \Gamma n+1 = -e^{-x} x^n + \int e^{-x} . n x^{n-1} dx$$

$$\Pi(n) = -e^{-x}[x^n]_0^\infty + n \int e^{-x} x^{n-1} dx$$

$$\Pi(n) = 0 + n \Gamma n$$

$$\boxed{\Gamma n+1 = n \Gamma n = \Pi(n)}$$

β = Lower case beta

B = Upper case beta

$$B(m,n) = \int_0^1 x^{m-1} (1-x)^{n-1} dx \ldots\ldots\ldots (1)$$

$$B(m+1, n+1) = \int_0^1 x^m (1-x)^n dx$$

$$B(m,n) = \int_0^\infty \frac{x^{m-1}}{(1+x)^{n+1}} dx \ldots\ldots\ldots (2)$$

Put $x = \sin^2\theta$

$dx = 2\sin\theta\cos\theta\, d\theta$

$$\begin{bmatrix} x & 0 & 1 \\ \theta & 0 & \pi/2 \end{bmatrix}$$

$$B(m,n) = \int_0^{\pi/2} \sin^{2m-2}\theta \cos^{2n-2}\theta \cdot 2\sin\theta\cos\theta\, d\theta$$

$$B(m,n) = 2\int_0^{\pi/2} \sin^{2m-1}\theta \cos^{2m-1}\theta\, d\theta \ldots\ldots (3)$$

Properties;

(i) $B(m,n) = B(n,m)$

(ii) $B(m,n) = \dfrac{\lceil m \lceil n}{\lceil m+n}$

- Poisson Equations-

Study this unit from classical Mechanics section

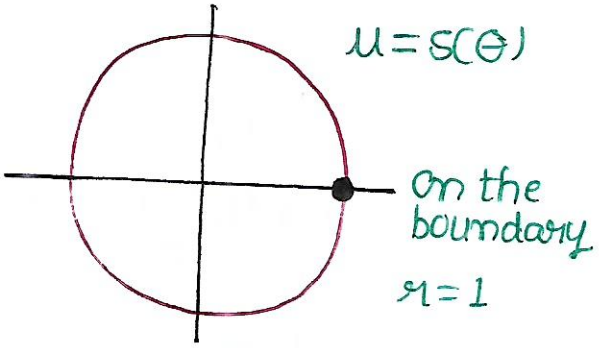
- Fourier Series of Laplace equation-

$$u(r,\theta) = \sum_{n=0}^{\infty} a_n r^n \cos n\theta + \sum_{n=0}^{\infty} b_n r^n \sin n\theta$$

$u(1,\theta)$ = delta function $\delta(\theta)$

$$\sum_{n=0}^{\infty} a_n \cos n\theta + \sum_{n=0}^{\infty} b_n \sin n\theta = \delta(\theta)$$

odd function cancelled



$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0$$

$$a_0 = \frac{1}{2\pi}\int_{-\pi}^{\pi} \delta(\theta)\, d\theta = \frac{1}{2\pi}$$

$$a_n = \frac{1}{\pi}\int \delta(\theta)\cos n\theta\, d\theta = \frac{1}{\pi}$$

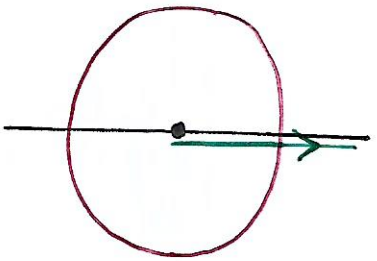
$$u(r,\theta) = \sum_{n=0}^{\infty} \frac{1}{2\pi} + \frac{1}{\pi}\cos n\theta \cdot r^n$$

$$u(r,\theta) = \frac{1}{2\pi} + \sum_{n=1}^{\infty} \frac{r^n}{\pi}\cos n\theta = \frac{1}{2\pi}\cdot\frac{1-r^2}{1+r^2-2r\cos\theta}$$

Ray $\theta = 0$, $\cos\theta = 1$

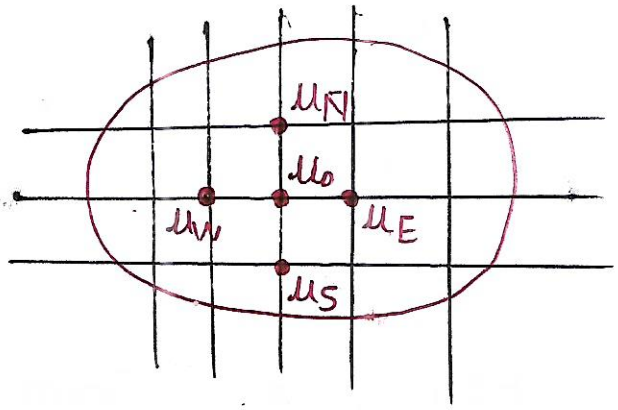
$$u(r,\theta) = \frac{1}{2\pi} \cdot \frac{1-r^2}{(1-r)^2}$$

$$\boxed{u(r,\theta) = \frac{1}{2\pi} \cdot \frac{1+r}{1-r}}$$



$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0$$

$$\rightarrow u_0 = \frac{1}{4}\left(u_E + u_W + u_N + u_S\right)$$



- Legendre differential Equation-

$$(1-x^2)\frac{d^2y}{dx^2} - 2x\frac{dy}{dx} + n(n+1)y = 0$$

$$\Rightarrow \frac{d}{dx}\left\{(1-x^2)\frac{dy}{dx}\right\} + n(n+1)y = 0$$

$$[\because n = 0, 1, 2, 3, \ldots.]$$

$x = \pm 1$ are the singular points and $x = 0$ is the ordinary point of the differential equation.

- $P_n(1) = 1$
- $P_n(-1) = (-1)^n$
- $P_n(x)$ = even function if n is even
- $P_n(x)$ = odd function if n is odd

} Properties of Legendre Polynomial

- Hermite differential equation–

$$\frac{d^2y}{dx^2} - 2x\frac{dy}{dx} + 2ny = 0$$

$$[\because n = 0, 1 \ldots .]$$

$x = 0$ is an ordinary point of the Hermite differential eqn.

Solution:

The solution of the Hermite differential eqn is a terminating series, so it is called Hermite polynomial of order n i.e. $H_n(x)$

$$H_n(x) = \sum_{r=0}^{P} \frac{(-1)^r n! (2x)^{n-2r}}{r!(n-2r)!}$$

$$\Rightarrow P = \frac{n}{2}$$

if $n = 2, 4, 6, 8, \ldots .$

$$\Rightarrow P = \frac{n-1}{2}$$

if $n = 1, 3, 5, 7, 9, \ldots .$

- Lagauerre Equation of differenciation–

$$x\frac{d^2y}{d} + (1-x)\frac{dy}{dx} + ny = 0$$

$x = 0$ is a regular singular point of Laguerre differential eqn.

Solution:

The solution

$$L_n(x) = \sum \frac{(-1)^r n! x^r}{(r!)^2 (n-r)!}$$

The solution of Lagauerre differential eq^n is known as Lagauerre polynomial of order n i.e. $L_n(x)$.

UNIT-2
Group Theory

- **Group –**

A group is an algebric structure $(G, *)$ consisting of a set of elements equipped with a binary operation which combines any two elements to form a third element. To be a group, this operation must satisfy four following axioms.

1. Closure Axioms –

$$a, b \in G \Rightarrow a * b \in G \quad \forall a, b \in G$$

2. Associative Axioms –

$$a, b, c \in G \Rightarrow$$

$$\boxed{a * (b * c) = (a * b) * c}$$

3. Identity Axioms –

$$a, b \in G \Rightarrow$$

There exist an element $e \in G$ s.t.

$$\boxed{a * e = e = e * a}$$

4. Inverse Axiom –

For each element of G possesses inverse.

$$a, b \in G \Rightarrow$$

$$a * b = b * a = e$$

And

$$b = a^{-1}$$

Then

$$\boxed{a * a^{-1} = a^{-1} * a = e}$$

If any groupic algebric structure $(G, *)$ satisfies these five conditions, it will be a group.

5. Commutative group –

$$a, b \in G$$

$$\boxed{a * b = b * a \in G}$$

so it is called an abelian group.

- History of Group theory-

The original motivation for group theory was the quest for solution of polynomial equations of degree higher than 4. In 19th century Evariste Galois gave a criterion (गैलोइस) for the solvability of a particular polynomial equation in terms of the symmetrical group of its roots. The elements of such a galois group corresponding a certain permutations of the roots.

- Subgroup-

A subgroup H of a group G is a non-empty subset of G that forms a group under the binary operation of G. Equivalenty, H is a non-empty subset of G s.t. If $a, b \in H$, so does ab^{-1}.

$$1 = aa^{-1} \in H$$

Also

$$ab = a(b^{-1})^{-1} \in H$$

→ Properties of subgroup.

(i) The Intersection of two subgroup is a subgroup of G.
(ii) The union of two subgroup is not necessary a subgroup.

→ Necessary and sufficient condition-

For a subgroup H of a group G to be a subgroup:

(i) $a \in H, b \in H \Rightarrow a * b \in H$
(ii) $a \in H, a^{-1} \in H$
(iii) $a \in H, b \in H \Rightarrow a \cdot (b^{-1})^{-1} \in H$

- Cyclic group-

A group G is cyclic group if $G = \langle a \rangle$ for some $a \in G$ and $\langle a \rangle$

$$\langle a \rangle = \{ a^k \mid k \in \mathbb{Z} \}$$

Such an element is called a generator of G.

OR

In Mathematics, a cyclic group is a group that is generated by a single element.

- **Homomorphism-**

Let $(G,*)$ and $(G',*')$ are groups then a mapping $f: g \longrightarrow g'$ is said to be homomorphism if

$$f(a*b) = f(a)*'f(b)$$

where $a,b \in G$ and $f(a), f(b) \in G'$

- **Isomorphism-**

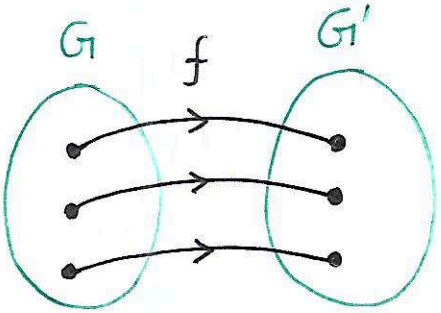
Let $(G,*)$ and $(G',*')$ are two groups. Then a mapping $f: G \longrightarrow G'$ is called isomorphism if

(i) f is one-one.

(ii) f is onto.

(iii) f is homomorphism

$f(a*b) = f(a)*'f(b)$ $\forall$ $a,b \in G$



→ $G = [1, \omega, \omega^2]$ of order 3 under multiplication.

$*$	1	ω	ω^2
1	1	ω	ω^2
ω	ω	ω^2	1
ω^2	ω^2	1	ω

- **Representation Theory of finite group-**

Let G be a finite group. Let k be a field. We will assume that characteristic of k is 0 e.g. $\mathbb{C}, \mathbb{R}$ or $\mathbb{Q}$ though often $\text{char}(K) \nmid |G|$ is enough.

A representation of G over k is a homomorphism,

$$\rho: G \longrightarrow GL(V)$$

where V is a vector space of finite dimension over field k. The vector space V is called a representation space of G and its dimension the dimension of representation.

- **Reducible Representation–**
A representation (ρ, V) is called completely reducible if it is a direct sum of irreducible ones. Equivalently if $V = W_1 * \dots * W_n$, where each W_i is G-invariant Irreducible representations.

- **Irreducible Representation –**
A representation (ρ, V) of G is called irreducible if it has no proper invariant subspace i.e. only invariant subspaces are 0 and V.

Let (ρ, V) and (ρ', V') be two representations of G over field k.

$$\rho * \rho' : G \longrightarrow GL(V * V')$$
$$(\rho * \rho')(g)(v, v') = (\rho)(g)(v), \rho'(g)(v')$$

In matrix notation

$$g \longrightarrow \begin{bmatrix} \rho(g) & 0 \\ 0 & \rho'(g) \end{bmatrix}$$

This motivates us to look at those nice representations which can be obtained by taking direct sum of irreducible ones.

- **Schur's Lemma Theorem–**

Definition– Let (ρ, V) and (ρ', V') be two representations of G over field k. A linear map

$$T : V \longrightarrow V'$$

is called a G-map if it satisfies the following;

$$\rho'(t)\, T = T[\rho(t)] \quad \forall t \in G$$

G-map

- **Statement–**
Let (ρ, V) and (ρ', V') be two irreducible representations of G. (of dimension ≥ 1)
Let $T : V \longrightarrow V'$ be a G-map.
Then
$T = 0$ or T is isomorphism.

Moreover
If T is nonzero
Then T is isomorphism.

$\therefore$ If and only If two representations are equivalent.

Proof -

Let us consider the subspace $Ker(T)$. We claim that it is a G-invariant subspace of V.

$$v \in Ker(T)$$

Then

$$T\rho(t)(v) = \rho'(t)T(v) = 0$$

$$\rho(t)(v) \in Ker(T) \quad \forall\ t \in G$$

Now applying Maschke's Theorem on irreducible representation V. we get,

$$Ker(T) = 0 \quad or \quad Ker(T) = V$$

Now assume $Ker(T) = 0$

$\therefore$ T is injective

Now we consider

$$Im(T) \subset V'$$

And It is also a G-varient.

Let $y = T(x) \in Im(T)$

$$\rho'(t)(y) = \rho'(t)T(x) = T\rho(t)(x) \in Im(T) \quad \forall\ t \in G$$

Hence Im is G-invarient

Again, applying Maschke's Theorem on irreducible representation V'. we get,

$$Im(T) = 0 \quad or \quad Im(T) = V'$$

T is Injective.

$Im(T) \neq 0$

Hence

$Im(T) = V'$

It proves that,

T is an isomorphism.

- Orthogonality Relations-

The Schur Orthogonality relation, which proves by Issai schur through schur's Lemma, express a central fact about representation of finite groups. They admit that a generalization to the case of compact groups in general and in particular compact Lie groups, such as the rotation group $(SO)_3$.

$$\langle \alpha, \beta \rangle := \frac{1}{|G|} \alpha(g)\overline{\beta(g)}$$

↑ complex conjugate

$$\langle \chi_i, \chi_j \rangle = \begin{cases} 0 & \text{If } i \neq j \\ 1 & \text{If } i = j \end{cases}$$

$$\sum_{\chi_i} \chi_i(g)\overline{\chi_i(h)} = \begin{cases} |C_G(g)| \text{ , If } g, h \text{ are conjugate} \\ 0 \text{ , otherwise} \end{cases}$$

- Statement- The set of irreducible character $\{\chi_1, \chi_2, \ldots\}$ form an orthonormal set of $(C(G), \langle , \rangle)$ That is,

(1) If χ is a character of an irreducible representation then $\langle \chi, \chi \rangle = 1$

(2) If χ and χ' are two irreducible characters of non isomorphic representation then $\langle \chi, \chi' \rangle = 0$

- Proof-

Let ρ and ρ' be non isomorphic irreducible representations. $\langle a_{ij} \rangle$ and $\langle b_{ij} \rangle$ be the corresponding matrix elements.

Then

$$\chi(g) = \Sigma_i \, a_{ii}(g)$$

$$\chi'(g) = \Sigma_j \, b_{jj}(g)$$

Then

$$\langle \chi, \chi' \rangle = \langle \chi, \chi' \rangle = \left(\Sigma_i \, a_{ii}, \Sigma_j \, b_{jj} \right) = \left(\Sigma_{ij} \left(a_{ii}, b_{jj} \right) \right) = 0$$

If $\frac{1}{|G|} \sum_{t \in G} a_{il}(t) \, a_{mj}(t^{-1}) = \frac{1}{n} \delta_{lm} \delta_{ij}$ and $\forall f \in C(G)$ then $(f, \chi) = \langle f, \chi \rangle$

Then

$$\langle \chi, \chi \rangle = \langle \chi, \chi \rangle = \left(\Sigma_i \, a_{ii}, \Sigma_j \, b_{jj} \right) = \Sigma_i (a_{ii}, b_{jj}) = \Sigma_{i=1}^{n} \frac{1}{n} = 1$$

↑ dimension of representation ρ

- **Character of Representation-**

Let (ρ, V) be a representation of G. The character of (Corresponding to) representation ρ is a map $\chi: G \longrightarrow C$ defined by $\chi(t) = t_r(\rho(t))$

↑ trace of corresponding matrix.

Strictly speaking it is χ_ρ but for the simplicity of notation, we write χ only when it is clear which representation it corresponds to.

- **Class-**

In mathematics, especially group Theory, the elements of any group may be partitioned into conjugacy classes; members of the same conjugacy class share many properties, and study of conjugacy classes of non abelian groups reveals many Important features of their structure. For an abelian group, each conjugacy class is a set containing one element.

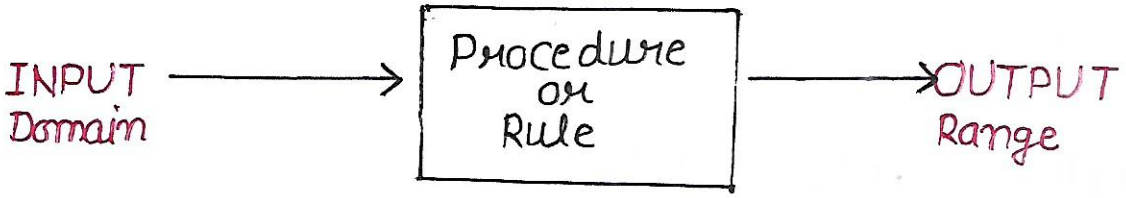
$$cl(a) = \{b \in G \mid \text{there exists } g \in G \text{ with } b = gag^{-1}\}$$

and is called the conjugacy class of a.

UNIT-3
Complex Variables

- Functions of complex Variables-

A function is a procedure which gives a unique output for any suitable inputs is called the domain of the function while the set of outputs which are possible is called the range of the function.



e.g. Squareroot ; the square of the output is equal to the input.

INPUT 4, 9 $\longrightarrow \sqrt{\quad} \longrightarrow$ OUTPUT 2, 3

$Z = x+iy \longrightarrow$ Function Machine $\longrightarrow W = f(z) = u+iv$

- Analytic Function-

In mathematical Physics, an analytic function is a function that totally given by a convergent series. There exist both real and complex analytic Function.
A function $f(z)$ is said to be analytic function if it is defined and differenciable at each point of a Region R. This function is called regular or holomorphic function.

Mathematically,

$$f(x) = \sum_{n=0}^{\infty} a_n (x - x_0)^n$$

Where f is real analytic Function
$x_0 \in R$
a_n is real number

$$T(x) = \sum_{n=0}^{\infty} \frac{(f^n)(x_0)}{n!} (x - x_0)^n$$

↑ Infinite diff^n funt.^{n}

• Cauchy's Integral Theorem-

In mathematics, the cauchy's Integral Theorem (formally known as the Cauchy-Goursat Theorem) in complex analysis, named after Augustin-Louis Cauchy is an important statement about line integrals for holomorphic function in complex plane.

↑ Function of one or more complex variables

→ Statement- If $f(z)$ is an analytic function of z and if $f'(z)$ is continuous at each point (of) within, an, close contour c then

$$\int_c f(z)\,dz = 0$$

→ Proof: Let $f(z)$ is a function of complex variables.

$$f(z) = u + iv$$
$$z = x + iy$$
$$dz = dx + i\,dy$$

Then

$$\int_c f(z)\,dz = \int_c (u+iv)(dx+i\,dy)$$

$$= \int_c (u\,dx + iu\,dy + iv\,dx - v\,dy)$$

$$= \int_c (u\,dx - v\,dy) + i\int_c (v\,dx + u\,dy)$$

(P, Q, P, Q)

• Green's Theorem

$$P\,dx + Q\,dy = \iint_S \left(\frac{\partial Q}{\partial x} - \frac{\partial P}{\partial y}\right) dx\,dy$$

$$\int_c f(z)\,dz = \iint_S \left(-\frac{\partial v}{\partial x} - \frac{\partial u}{\partial y}\right) dx\,dy + i\iint_S \left(\frac{\partial u}{\partial x} - \frac{\partial v}{\partial y}\right) dx\,dy$$

$$\int_C f(z)\,dz = \iint_S \left(\frac{-\partial v}{\partial x} - \frac{\partial u}{\partial y}\right) dx\,dy + i\iint_S \left(\frac{\partial u}{\partial x} - \frac{\partial v}{\partial y}\right) dx\,dy$$

- CR eqn's

$$\left.\begin{aligned} \frac{\partial u}{\partial x} &= \frac{\partial v}{\partial y} \\ \frac{\partial u}{\partial y} &= -\frac{\partial v}{\partial x} \end{aligned}\right\} \text{Apply in } \int_C f(z)\,dz$$

$$\int_C f(z)\,dz = \iint_S \left(\frac{\partial u}{\partial y} - \frac{\partial u}{\partial y}\right) dx\,dy + i\iint_S \left(\frac{\partial v}{\partial y} - \frac{\partial v}{\partial y}\right) dx\,dy$$

$$\boxed{\int_C f(z)\,dz = 0}$$

This is desired result.

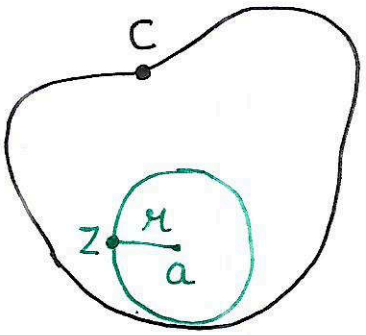
- Cauchy's Integral Formula-

In mathematics, cauchy's Integral Formula, named after Augustin-Louis Cauchy, is a cauchy's central statement in complex analysis. It expresses the fact that a holomorphic function defined on a disk is completely determined by its value of boundary of the disk.

→Statement→

If $f(z)$ is analytic & single valued within and on close contour 'C' and 'a' is any point on 'C' then,

$$f(a) = \frac{1}{2\pi i}\oint \frac{f(z)}{z-a}\,dz$$



→Proof; Let $z=a$ in a closed contour C. consider a circle r with center at $(z=a)$ and radius ρ.

consider the function

$$\oint_C \frac{f(z)}{z-a}\,dz = \oint_{C_1} \frac{f(z)}{z-a}\,dz$$

--- Integral Theorem

$$|z-a| = r$$

$$z-a = re^{i\theta}$$

$$z = a + re^{i\theta} \quad \ldots\ldots(1)$$

$$dz = rie^{i\theta}\,d\theta \quad \ldots\ldots(2)$$

$$\oint_C \frac{f(z)}{z-a}\,dz = \oint_{C_1} \frac{f(a+re^{i\theta})}{re^{i\theta}}\, rie^{i\theta}\,d\theta$$

$$\oint_C \frac{f(z)}{z-a}\,dz = i\oint_{C_1} f(a+re^{i\theta})\,d\theta$$

$$r \ll\ll\ll\ll\ll a$$

Then

$$\oint_C \frac{f(z)}{z-a}\,dz = i\oint_{C_1} f(a)\,d\theta$$

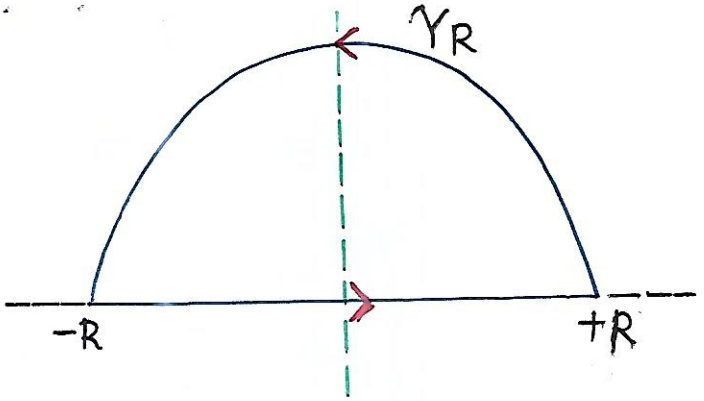
$$\oint_C \frac{f(z)}{z-a}\,dz = if(a)\oint_{C_1} d\theta = if(a)\left[\theta\right]_0^{2\pi} = 2\pi i f(a)$$

$$\oint_C \frac{f(z)}{z-a}\,dz = 2\pi i f(a)$$

$$\boxed{f(a) = \frac{1}{2\pi i}\oint_C \frac{f(z)}{z-a}\,dz}$$

This is desired expression.

- Contour Integration- Contour Integration is the process of calculating the value of a contour Integration around a given contour in a complex plane. As a result of a truly amazing property of



holomorphic function, such integrals can be computed easily simply by summing the value of the complex residue inside the contour.

Let $P(x)$ and $Q(x)$ be polynomials of polynomial degree n and m with cofficients $b_n \ldots\ldots b_0$ and $c_m, \ldots\ldots c_0$. Take that contour in the upper half plane, replace x by z and $z = Re^{i\theta}$ Then

$$\int_{-\infty}^{\infty} \frac{P(z)}{Q(z)}\,dz = \lim_{R\to\infty} \int_{-R}^{R} \frac{P(z)}{Q(z)}\,dz$$

$$\lim_{R\to\infty} \int_{\gamma R} \frac{P(z)}{Q(z)}\,dz = \lim_{R\to\infty} \int_{-R}^{R} \frac{P(Re^{i\theta})}{Q(Re^{i\theta})}\, iRe^{i\theta}\,d\theta$$

$$= 2\pi i \sum_{I\,|z|>0} \text{Res} \left| \frac{P(z)}{Q(z)} \right|$$

$$\lim_{R\to\infty} \int_{-R}^{R} \frac{P(z)}{Q(z)}\,dz = 2\pi i \sum_{I|z|>0} \text{Res}\left[\frac{P(z)}{Q(z)}\right] - \lim_{R\to\infty} \int_{0}^{\pi} \frac{P(Re^{i\theta})}{Q(Re^{i\theta})}\, iRe^{i\theta}\,d\theta$$

$$I_R = \lim_{R\to\infty} \int_{0}^{\pi} \frac{P(Re^{i\theta})}{Q(Re^{i\theta})}\,d\theta \cdot iRe^{i\theta}$$

$$I_R = \lim_{R\to\infty} \int_{0}^{\pi} \frac{b_n(Re^{i\theta})^n + \ldots\ldots + b_0}{c_m(Re^{i\theta})^m + \ldots\ldots + c_n}\, iR\,d\theta$$

$$I_R = \lim_{R\to\infty} \int_{0}^{\pi} \frac{b_n}{c_m}(Re^{i\theta})^{n-m}\, iR\,d\theta$$

$$I_R = \lim_{R\to\infty} \int_{0}^{\pi} \frac{b_n}{c_m}(R)^{n+1-m}(e^{i\theta})^{n-m}\,d\theta$$

$$\epsilon \equiv -(n+1-m)$$

Then

$$\boxed{I_R = \lim_{R\to\infty} \frac{i}{R^{\epsilon}} \cdot \frac{b^n}{c_m} \int_{0}^{\pi} e^{i(n-m)\theta}\,d\theta}$$

• CR^n or necessary and sufficient condition for $f(z)$ to be analytic-

→Necessary condition;

The necessary condition for a function $f(z) = u(x+y) + iv(x,y)$ to be analytic in domain D is that

$$f'(z) = \lim_{\Delta z \to 0} \frac{f(z+\Delta z) - f(z)}{\Delta z}$$

$$z = x+iy$$
$$f(z) = u+iv$$
$$\Delta z = \Delta x + i\Delta y$$
$$z+\Delta z = (x+iy) + [(\Delta x) + (i\Delta y)]$$
$$= (x+\Delta x) + i(y+\Delta y)$$

$$= \lim_{\Delta z \to 0} \frac{f(z+\Delta z) - f(z)}{\Delta z}$$

$$= \lim_{\Delta z \to 0} \frac{[u(x+\Delta x, y+\Delta y) + iv(x+\Delta x, y+\Delta y)] - [u+iv]}{\Delta z}$$

case 1-

$$= \lim_{\Delta z \to 0} \frac{[u(x+\Delta x, y) - u(x,y) + i[v(x+\Delta x, y)] - v(x,y)}{\Delta x}$$

$$f'(z) = \frac{\partial u}{\partial x} + i\frac{\partial v}{\partial x} \quad \ldots\ldots (1)$$

case 2;

$$= \lim_{\Delta z \to 0} \frac{[u(x,y+\Delta y) - u(x,y)]}{i\Delta y} + i\left[\frac{v(x,y+\Delta y) - v(x,y)}{i\Delta y}\right]$$

$$f'(z) = \frac{1}{i}\frac{\partial u}{\partial y} + \frac{\partial v}{\partial y} \quad \ldots\ldots (2)$$

by eq^n (1) & (2)

$$\frac{\partial u}{\partial x} + i\frac{\partial v}{\partial x} = \frac{1}{i}\frac{\partial u}{\partial y} + \frac{\partial v}{\partial y}$$

$$\left.\begin{aligned} \frac{\partial u}{\partial x} &= \frac{\partial v}{\partial y} \\ -\frac{\partial v}{\partial x} &= \frac{\partial u}{\partial y} \end{aligned}\right\} \text{ necessary cond}^n$$

→ Sufficient condition –

$$\frac{f(z+\Delta z)-f(z)}{\Delta z} = \frac{\left[\frac{\partial u}{\partial x}\Delta x+\frac{\partial v}{\partial y}\Delta y\right]+i\left[\frac{\partial v}{\partial x}\Delta x+\frac{\partial u}{\partial y}\Delta y\right]}{\Delta z}$$

$$= \frac{\frac{\partial u}{\partial x}(x+iy)+\frac{\partial v}{\partial x}(i\Delta x-\Delta y)}{\Delta z}$$

$$= \frac{\frac{\partial u}{\partial x}(\Delta x+i\Delta y)}{\Delta z} + i\frac{\partial v}{\partial x}$$

$$= \frac{\partial u}{\partial x}+i\frac{\partial v}{\partial x}$$

$z \longrightarrow 0$

Then

$$\lim_{z\to 0}\frac{f(z+\Delta z)-f(z)}{\Delta z} = \frac{\partial u}{\partial x}+i\frac{\partial v}{\partial x}$$

- Residue Theorem –

An analytic $f(z)$ whose Laurent series is given by

$$f(z) = \sum_{n=-\infty}^{\infty} a_n (z-z_0)^n$$

It can be integrated term by using a closed γ encircling z_0

$$\int_\gamma f(z)\,dz = \sum_{n=-\infty}^{\infty} a_n (z-z_0)^n dz$$

$$\int_\gamma f(z)dz = \sum_{n=-\infty}^{-2} a_n (z-z_0)^n dz + a_{-1}\int_\gamma \frac{1}{z-z_0}dz + \sum_{n=0}^{\infty} a_n \int_\gamma (z-z_0)^n dz$$

$$\int_\gamma f(z)\,dz = a_{-1}\int_\gamma \frac{1}{z-z_0}dz$$

↑ complex residue

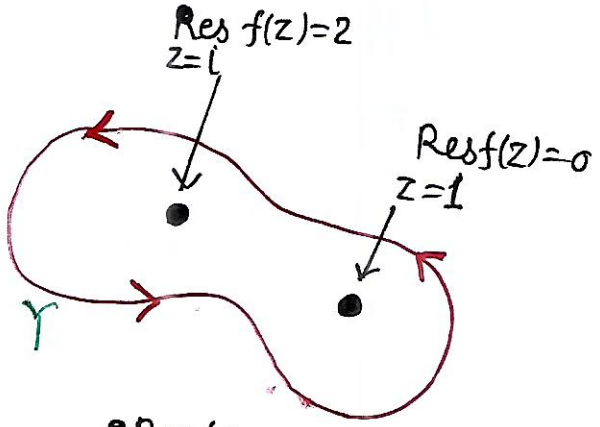
$$z = \gamma(t) = e^{it} + z_0$$

$$\int_\gamma \frac{dz}{z-z_0} = \int_0^{2\pi} \frac{ie^{it}\,dt}{e^{it}} = 2\pi i$$

$$\int_\gamma f(z)\,dz = 2\pi i a_{-1}$$

$$\boxed{\int_\gamma f(z)dz = 2\pi i \sum_{a\in A} \operatorname*{Res}_{z=a_i} f(z)}$$

$\operatorname*{Res}_{z=3+2i} f(z)=i$



$\operatorname{Res} f(z)=-2$
$z=-i$

$\operatorname{Res} f(z)=5$
$z=-1-2i$

$$f(z)=\frac{3}{(z-1)^2}+\frac{2}{z-i}-\frac{2}{z+i}+\frac{i}{z+3-2i}+\frac{5}{z+1+2i}$$

$$\int_\gamma f(z)\,dz = 2\pi i(0+2)$$

$$\boxed{\int_\gamma f(z)dz = 4\pi i}$$

UNIT-4
Matrix and Tensors

- **Matrix:**
  - **Definition -**
    A matrix is an $m \times n$ array of scalars from a given field F. The Individual values in the matrix are called entries

    e.g.

$$A = \begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix}_{2\times 2 = m\times n}$$

    where m is number of rows
    n is number of columns

    Notation of matrix is

$$A = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ a_{m1} & a_{m2} & & a_{mm} \end{bmatrix}$$

    Rows

    Column

    A = denotes of matrix
    a = entries of matrix where $a \in F$

  - **Types -**
    (1) Square matrix -
    A matrix having same no. of rows and columns is called square matrix.

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}_{3\times 3}$$

→ a_{11}, a_{21}, a_{33} are called diagonal matrix elements.
→ Diagonal elements of square matrix are called the trace of the matrix.

(ii) Diagonal matrix –
If all the elements of a square matrix are zero, except those in the leading diagonal then the matrix is said to be diagonal matrix.

e.g.
$$\begin{bmatrix} a_{11} & 0 & 0 & \dots & 0 \\ 0 & a_{22} & 0 & \dots & 0 \\ 0 & 0 & a_{33} & \dots & 0 \\ 0 & 0 & 0 & \dots & a_n \end{bmatrix}$$

(iii) Scalar Matrix –
A diagonal matrix in which all the diagonal elements are equal arecalled scalar matrix.
$$A = \begin{bmatrix} \lambda & 0 & 0 & .. & 0 \\ 0 & \lambda & 0 & .. & 0 \\ 0 & 0 & \lambda & .. & 0 \\ 0 & 0 & 0 & .. & \lambda \end{bmatrix}_{n \times n}$$

(iv) Identity or Unitary Matrix –
A scalar matrix in which each diagonal element is unitary.

e.g.
$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Thus on square matrix $[a_{ij}]$ is an unitary matrix if.
$$a_{ij} = \begin{cases} 1 & \text{for } i=j \\ 0 & \text{for } i \neq j \end{cases}$$

(v) Row matrix –
$$[x]_{1 \times n} = [a_{11}, a_{12} \dots a_{1n}]_{1 \times n}$$

(vi) Column matrix –
$$[x]_{m \times 1} = \begin{bmatrix} a_{11} \\ a_{21} \\ \dots \\ \dots \\ a_{m1} \end{bmatrix}_{m \times 1}$$

(vii) Null and Zero matrix–

If all the elements of matrix will be zero

$$[X]_{3\times3} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}_{3\times3}$$

- Inverse of a matrix–

$$A = \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix}_{2\times2}$$

$$A^{-1} = ?$$

$$A^{-1} = \frac{1}{|A|} \text{adj } A$$

$$|A| = \begin{vmatrix} 1 & -1 \\ 1 & 1 \end{vmatrix} = 1 + 1$$

$$|A| = 2 \neq 0$$

$$\text{adj } A = \left(\begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix} \right)^{t} =$$

$$\text{adj } A = \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix}$$

$$A^{-1} = \frac{1}{2} \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix}$$

$$A^{-1} = \begin{bmatrix} 1/2 & -1/2 \\ 1/2 & 1/2 \end{bmatrix}$$

- Trace of a matrix–

$$\begin{bmatrix} 1 & 2 & 1 \\ 1 & 4 & 3 \\ 3 & 3 & 4 \end{bmatrix} = 1 + 4 + 4 = 9$$

- Orthogonality –

A matrix A is said to be orthogonal if $AA^T = I$

e.g.

$$A = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$A^T = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$A \cdot A^T = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$A \cdot A^T = \begin{bmatrix} 0+1+0 & 0+0+0 & 0+0+0 \\ 0+0+0 & 0+1+0 & 0+0+0 \\ 0+0+0 & 0+0+0 & 0+0+1 \end{bmatrix}$$

$$A \cdot A^T = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$\boxed{A \cdot A^T = I}$$

- Eigen value and Eigen Vectors :

$$AX = \lambda X \quad \ldots\ldots (1)$$

$$A(X) = \lambda X$$

$$(A - \lambda I)X = 0$$

↑ It may be written as $(A - \lambda I)X = 0$

e.g. $$A = \begin{bmatrix} 2 & -1 & 1 \\ -1 & 2 & -1 \\ 1 & -1 & 2 \end{bmatrix}$$

$$A-\lambda I = 0$$

$$\begin{bmatrix} 2 & -1 & 1 \\ -1 & 2 & -1 \\ 1 & -1 & 2 \end{bmatrix} - \lambda \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = 0$$

$$\begin{bmatrix} 2 & -1 & 1 \\ -1 & 2 & -1 \\ 1 & -1 & 2 \end{bmatrix} - \begin{bmatrix} \lambda & 0 & 0 \\ 0 & \lambda & 0 \\ 0 & 0 & \lambda \end{bmatrix} = 0$$

$$\begin{bmatrix} 2-\lambda & -1 & 1 \\ -1 & 2-\lambda & -1 \\ 1 & -1 & 2-\lambda \end{bmatrix} = 0$$

$$\Rightarrow (2-\lambda)\left[(2-\lambda)(2-\lambda)-(1)\right] - (-1)\left[(-1)(2-\lambda) - (-1)(1)\right] + 1\left[(-1)(-1) - 2-\lambda(1)\right] = 0$$

$$\Rightarrow (2-\lambda)[\lambda^2 - 4\lambda + 3] + 1[\lambda - 1] + \lambda - 1 = 0$$

$$\Rightarrow -\lambda^3 - 6\lambda^2 - 9\lambda + 4 = 0$$

$$\Rightarrow (\lambda - 4)(\lambda^2 - 2\lambda + 1) = 0$$

$$\Rightarrow (\lambda - 4)(\lambda - 1)(\lambda - 1) = 0$$

$$\boxed{\lambda = 4, 1, 1}$$

- Find Eigen Vectors-

$$A = \begin{bmatrix} 2 & 1 & 0 \\ 1 & 2 & 1 \\ 0 & 1 & 2 \end{bmatrix}$$

$$(A - \lambda I)\, X = 0$$

$\lambda_1 = 2$

$$\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

$$y = 0$$

$$x + z = 0 \Rightarrow 1 - 1 = 0$$

$$y = 0$$

$$x_i = \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}$$

$$|x_i| = \sqrt{(1)^2+(0)^2+(-1)^2}$$

$$|x_i| = \sqrt{2}$$

$$|\hat{x}_i| = \begin{pmatrix} 1/\sqrt{2} \\ 0 \\ -1/\sqrt{2} \end{pmatrix}$$

same process for λ_2 and λ_3.

- Find adj A = ?

$$A = \begin{bmatrix} 2 & -1 & 0 \\ 0 & 1 & 2 \\ 1 & 1 & 0 \end{bmatrix}$$

$$\text{adj}A = \begin{bmatrix} +A_{11} & -A_{12} & +A_{13} \\ -A_{21} & +A_{22} & -A_{23} \\ +A_{31} & -A_{32} & +A_{33} \end{bmatrix}'$$

$$\text{adj}A = \begin{bmatrix} +(2-0) & -(2-0) & +(1-0) \\ -(0+1) & +(0-0) & -(-1-2) \\ +(0+2) & -(0-4) & +(0-2) \end{bmatrix}'$$

$$\text{adj}A = \begin{bmatrix} 2 & -2 & 1 \\ -1 & 0 & 3 \\ 2 & 4 & -2 \end{bmatrix}'$$

$$\boxed{\text{adj}A = \begin{bmatrix} 2 & -1 & 2 \\ -2 & 0 & 4 \\ 1 & 3 & -2 \end{bmatrix}}$$

• Cayley Hamilton Theorem–

Every square matrix have its own characteristic eq^n } Statement
i.e. if for a square matrix $(n \times n)$ of order n.

The characteristic Polynomial is

$$|A-\lambda I| = a_0+a_1\lambda+a_2\lambda^2+\ldots.+a_n\lambda^n$$

Then the matrix eq^n

$$a_0+a_1X+a_2X^2+\ldots\ldots+a_nX^n=0$$

Proof;

The characteristic polynomial is

$$|A-\lambda I| = a_0+a_1\lambda^1+a_2\lambda^2+a_3\lambda^3+\ldots..+a_n\lambda^n \ldots\ldots\ldots(1)$$

The characteristic of A is

$$|A-\lambda I| = a_0+a_1\lambda^1+a_2\lambda^2+a_3\lambda^3+\ldots..+a_n\lambda^n=0 \ldots\ldots(2)$$

The matrix eq^n is

$$a_0+a_1X^1+a_2X^2+\ldots.+a_nX^n=0 \ldots\ldots\ldots(3)$$

If this eq^n is satisfied by A then we have to show that

$$a_0I+a_1A+a_2A^2+\ldots\ldots+a_nA^n=0 \ldots\ldots\ldots(4)$$

Since the each element of characteristic matrix $|A-\lambda I|$ is an ordinary polynomial of degree n.

The cofactor of each and every element of $|A-\lambda I|$ is an ordinary polynomial of degree $n-1$, then;

$$B = \text{adj}\,|A-\lambda I|$$

$$B = \text{adj}\,|A-\lambda I| = B_0+B_1\lambda^1+B_2\lambda^2+\ldots\ldots+B_{n-1}\lambda^{n-1}\ldots(5)$$

Where $B_0, B_1 \ldots B_{n-1}$ are the square matrix of same order n.

By eq^n(5) & (1)

$$|A-\lambda I|(B_0+B_1\lambda^1+B_2\lambda^2+\ldots+B_{n-1}\lambda^{n-1}) = (a_0+a_1\lambda+a_2\lambda^2+a_3\lambda^3\ldots a_n\lambda^n)I$$

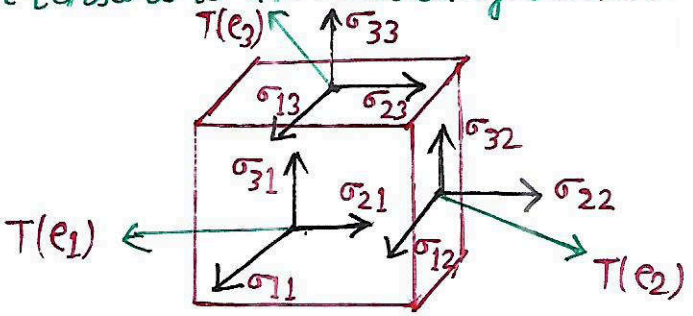
compare the cofficient

$$AB_0 = a_0I$$
$$A(B_1-B_0) = a_1I$$
$$A(B_2-B_1) = a_2I$$
$$\ldots\ldots\ldots,$$
$$A(B_{n-1}-B_{n-2}) = a_{n-1}I$$

$$a_0I+a_1A+a_2A^2+\ldots\ldots+a_nA^n=0$$

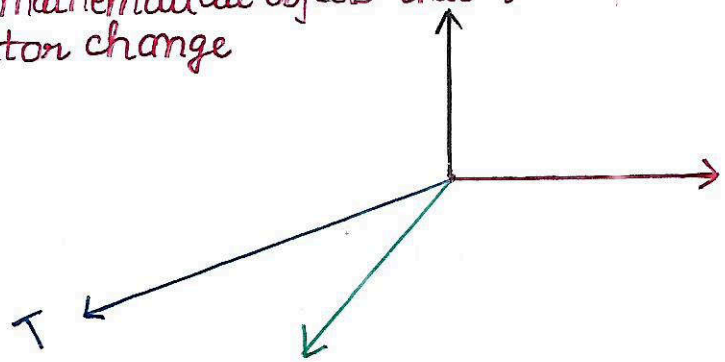
- Tensors-

In mathematics, a tensor is an arbitrary complex geomatric object that maps in a multilinear manner geomatric vectors and scalars and other tensors to an resulting tensor.



$$T = \begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{bmatrix}$$ → Cauchy second order tensor

Tensors are mathematical objects that transform in a special way when the basis vector change



- Multiplications of tensors-

$$\left\{ \begin{array}{l} g^{ij} A_j = A^i \\ g^{ij} A^j = A_i \end{array} \right\}$$ [Afriken 1985]

- contravarient Tensors-

A contravarient tensor is a tensor having specific transformation property.

$$dr = dx_1 \hat{x}_1 + dx_2 \hat{x}_2 + dx_3 \hat{x}_3$$

for which

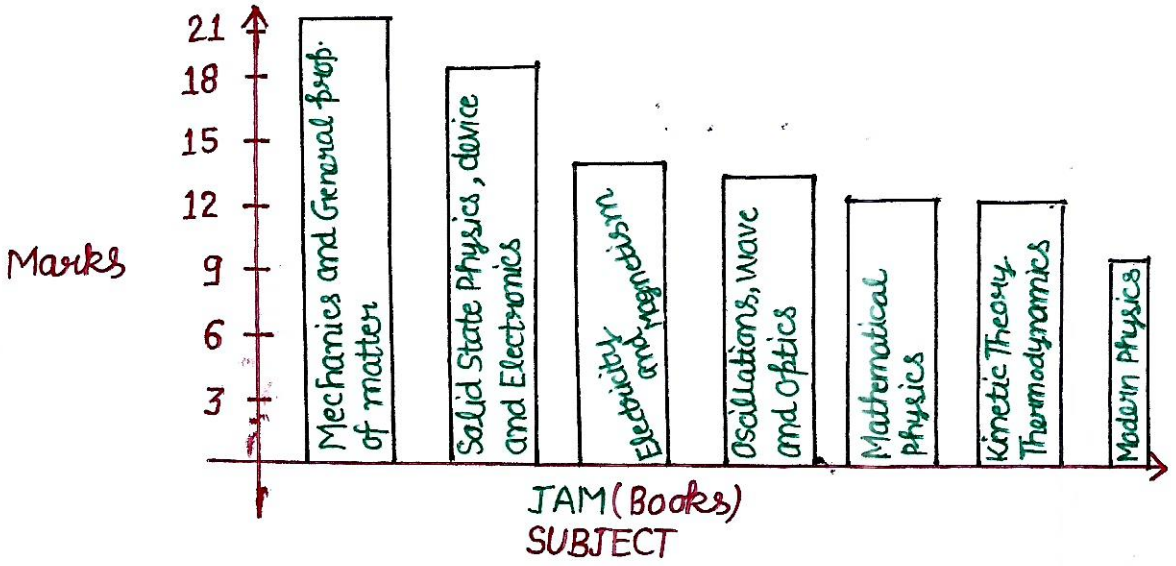
$$dx_i' = \frac{\partial x_i'}{\partial x_j} dx_j$$

- Convarient Tensor-

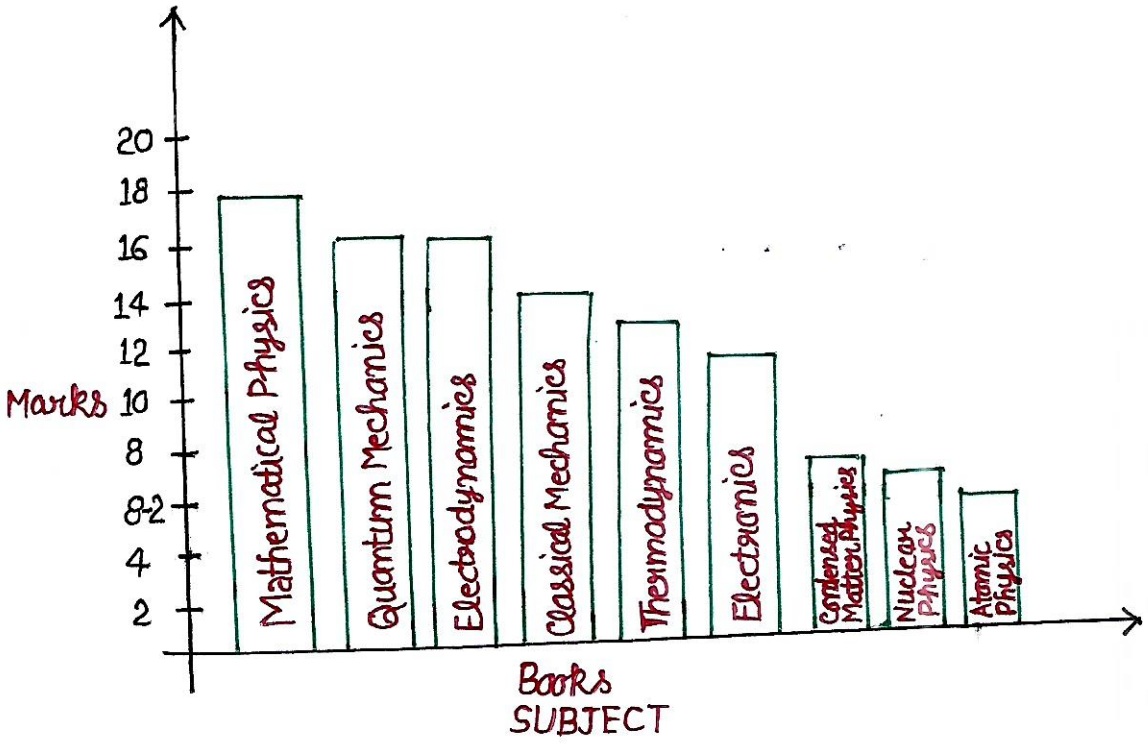
A convarient tensor denoted with lowered index (e.g. a_{ij}) is a tensor having specific property

$$\nabla \phi = \frac{\partial \phi}{\partial x_1} \hat{x}_1 + \frac{\partial \phi}{\partial x_2} \hat{x}_2 + \frac{\partial \phi}{\partial x_3} \hat{x}_3 \quad \text{for which} \quad \frac{\partial \phi'}{\partial x_i'} = \frac{\partial \phi}{\partial x_j} \cdot \frac{\partial x_j}{\partial x_i'}$$

IIT-JAM


Marks
21
18
15
12
9
6
3
Mechanics and General Prop. of matter
Solid State Physics, device and Electronics
Electricity and magnetism
Oscillations, Wave and Optics
Mathematical Physics
Kinetic Theory. Thermodynamics
Modern Physics
JAM (Books)
SUBJECT

IIT- CSIR-UGC-NET



Astrophysics-1

- The Solar System
- The Stellar System

UNIT-1
The Solar system

- Rings of the planet (2007)
- Comets (2007)
- Solar Wind (2008)
- Classification of galaxies
- Jupiter, Sitturn, Uranus, Naptune
- Hubble's Law
- Kepler's laws of Planetary Motion
- Surface Feature, Interior, Composition, Atmosphere, Satellite and different rings of Saturn, Jupiter
- Asteriods
- List of Planets in order of Increasing mass
- Active galaxies
- Comets
- Celestial Coordinates
- Telescopes
- Origin, Feature and motion of minor planets

Questions?

- Mars- The Red Planet -
  - → First successful flyby to Mars in 1965 by Mariner 4
  - → Rovers exploring life on Mars
  - → 4th Planet
  - → Minor Planet
  - → Iron Oxide
  - → Roman God [Mars]
  - → Core is made up of Metal [Iron, Nickel, Sulpher]
  - → 96% CO_2, 3.82% Ar and Other traces like O_2, H_2O
  - → 25° tilt on Axis
  - → 1 Year = 687 days of earth
  - → -143 °C → Lowest temp on poles

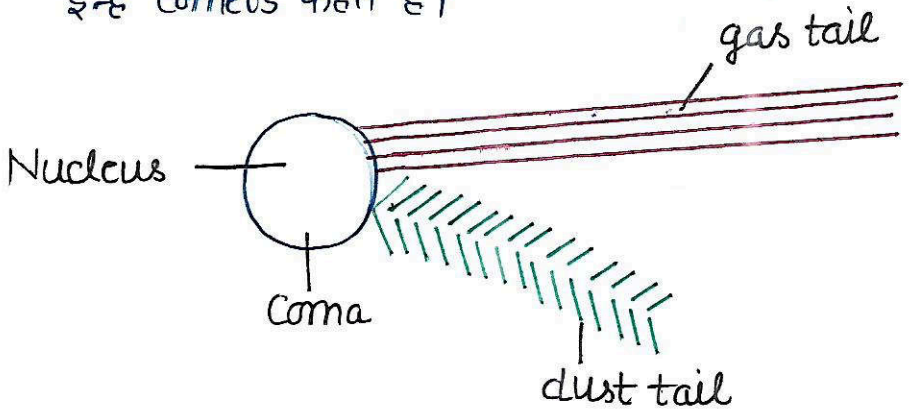
→ Cold planet
→ Ice caps on poles
→ -35°C minimum temp.
→ Sublimation -- Ice → Gas
→ Inside Rover will search H_2O under surface.
→ Olumpus Mones → Valcano
↓
Biggest Valcano of our solar system

• Asteroids- Asteroids generally बड़े पत्थर होते हैं जो सूर्य का चक्कर लगाते हैं जो पृथ्वी से टकरा चुके हैं। Mainly Asteroid mars or jupitor के बीच Asteroid belt में मौजूद हैं जो 200 से भी ज्यादा हैं जिनका diameter 100Km से अधिक हैं।

1801
↓
G. Pieze
↓
Serus

→ C type Cabonaceous, dark / 75%
→ M type Metallic (Rock) / Reddish colour / 8% (Iron/Nickle ↑)
→ S type Silicate / Reddish colour / 17%

• Comets- Comets generally asteroids ही होते हैं जो बर्फ, पत्थर के मिश्रण से बने होते हैं। लेकिन ये हमारे solar system के बाहर से आते हैं इसलिए इन्हें comets कहते हैं।

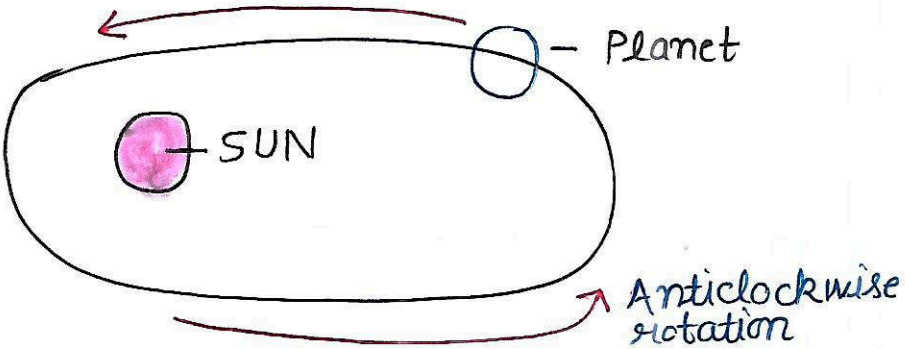


- Meteroids -

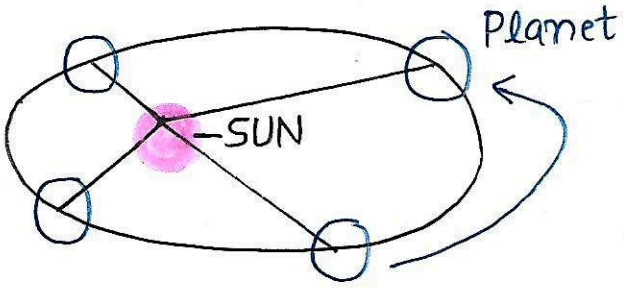
ये Space Rock हैं जो dust particles से बना होता है और Asteroids से छोटे होते हैं। Meteroids का अर्थ है - छोटे पिण्ड। जब कोई पिण्ड पृथ्वी पर गिरता है तो उसे meteroid कहते हैं।

- Laws of Planetery Motion -

In Asteronomy, Kepler's law of Planetery motion are three scientific laws describing the motion of Planets around SUN.



Law 1. The orbits of the planets are ellipse, with the sun at focus.



Law 2. The Line joining a planet to the sun sweeps out equal areas in the equal time as the planet travels around the ellipse

$$\frac{dA}{dt} = \frac{1}{2} r^2 \frac{d\theta}{dt}$$

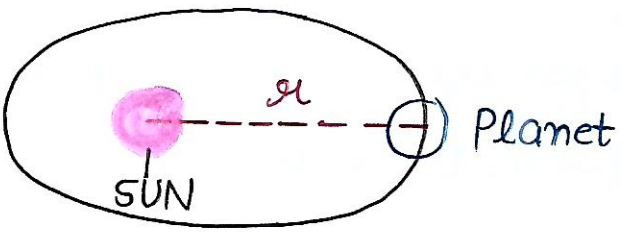
elliptical orbit $= \pi ab$

$$\text{P.} \quad \frac{1}{2} r^2 \frac{d\theta}{dt} = \pi ab$$

$$n = \frac{2\pi}{P}$$

satisfies

$$\boxed{r^2 d\theta = ab\, n\, dt}$$



Law 3. The square of the total time period [T] of the orbit is propotional to the cube of the avarage distance of the planet.

$$mr\omega^2 = G\frac{Mm}{r^2}$$

$$mr\left(\frac{2\pi}{T}\right)^2 = G\frac{Mm}{r^2}$$

$$T^2 = \left(\frac{4\pi^2}{GM}\right) r^3$$

$$\boxed{T^2 \propto r^3}$$

- Jupiter (बृहस्पति) –
  - → 5th सबसे बड़ा ग्रह (सबसे बड़ा Gas gaint)
  - → Romans ने अपने देवता के नाम पर इसका नाम रखा।
  - → काफी चमकीला
  - → अजीब सरंचना
  - → Ring system
  - → 1610/Gallilio → Setallite
  - → diameter → 142984 Km
  - → density → 1.326 gms cm^{-3}
  - → 24% He, 75% H , 1% Other
  - → Methane, Amonia
  - → 67°C – Surface temp.
  - → Great Red Spot
    - ↓
    - Storm → Robert Hook

→ हवा की Speed – 360 Km/H

→ पथरीली Core, Hydrogen (Liquid), Ordinary Hydrogen, Helium

↓

electrical conductive

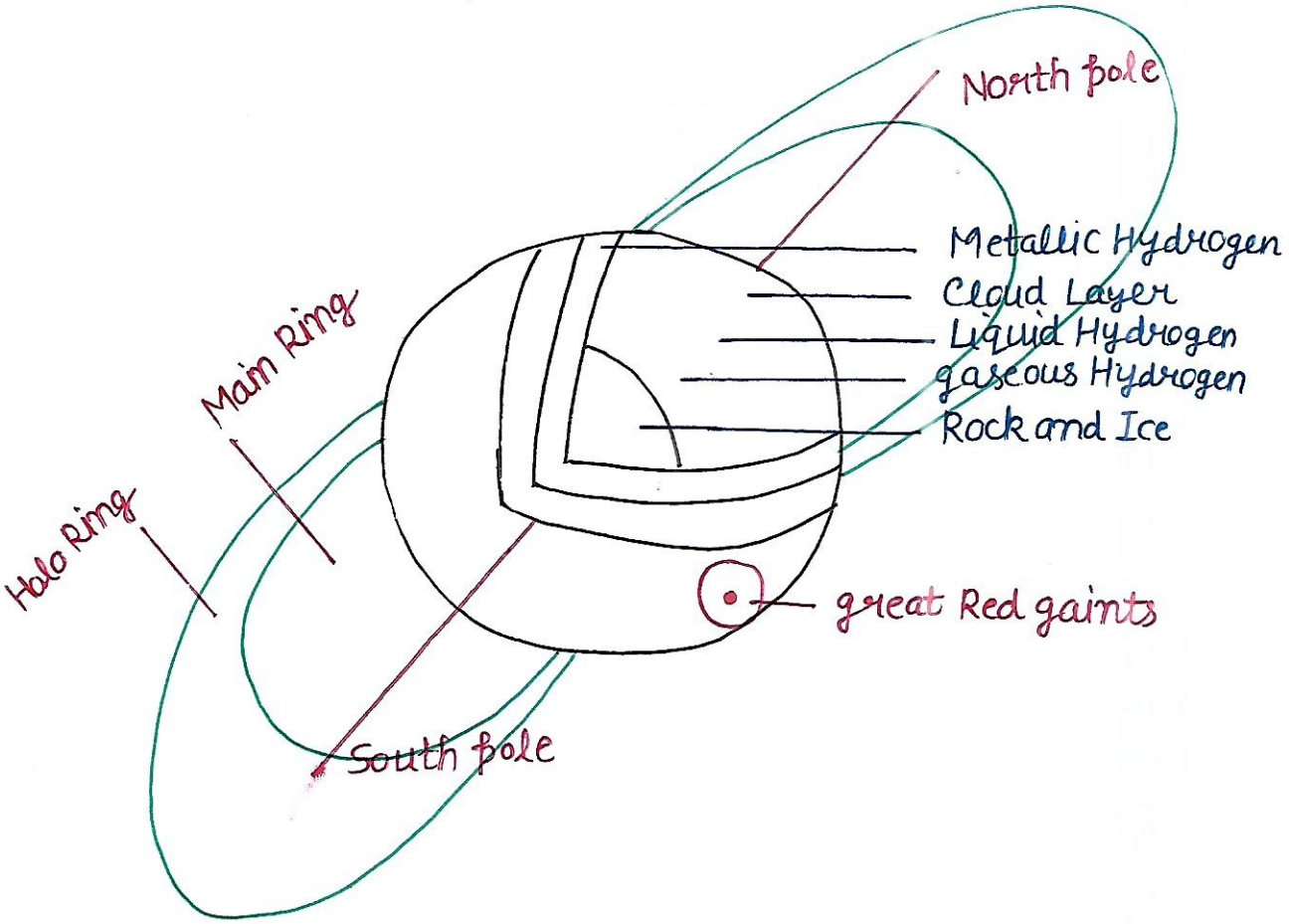
↓

Strongest magnetic field

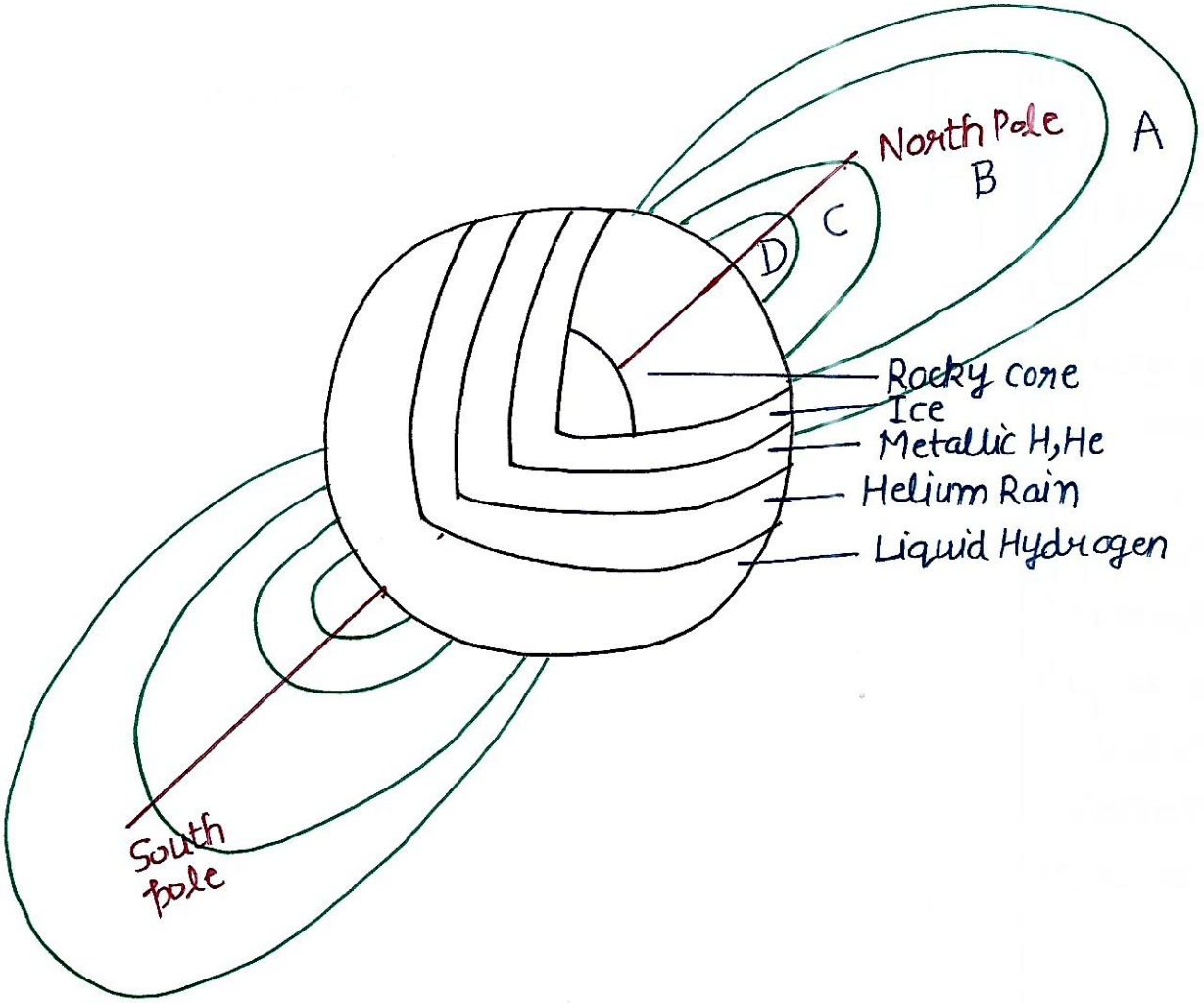
→ 1 दिन – 9 Hour, 50 min, 30 Sec.

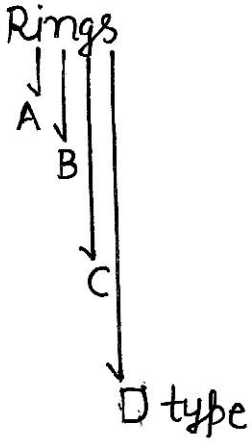
→ 1 year – 11.8 Year में एक चक्कर लगाता है (सूर्य का)

→ 79 setallite



- Saturn (♄)
  - → 6th Planet
  - → 120536 Km – diameter
  - → Roman god of Agriculture
  - → Gas planet
  - → 96.3% H, 3.25% He
  - → Satellite – 62
  - → Rainfall of diamonds


North Pole
A
B
C
D
Rocky core
Ice
Metallic H,He
Helium Rain
Liquid Hydrogen
South pole

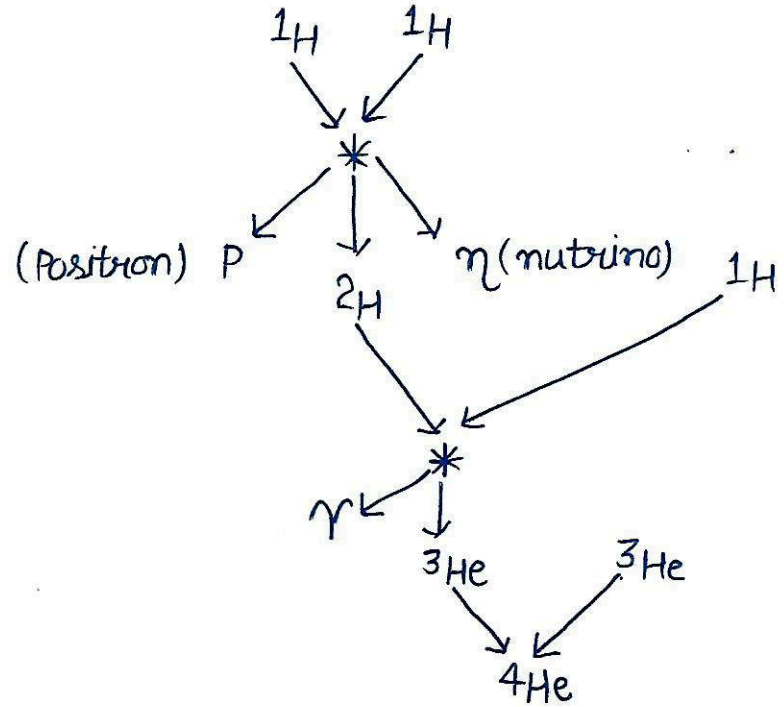

Rings
A
B
C
D type

UNIT- 2
Stellar System

- SUN atmosphere
- SUN Gravity
- SUN SPOT
- Type of galaxies
- HR diagram
- Solar Wind
- Algol paradox
- Nuclear Reactions
- Butterfly diagram
- Star Clusters
- Types of Clusters
- Evolution of Stars

} ?

- SUN –
  - → Massive star of our solar system
  - → 15 million °C
  - → The Pressure is a crushing 260 Billions times the earth's atmosphere pressure.
  - → Nuclear Fusion



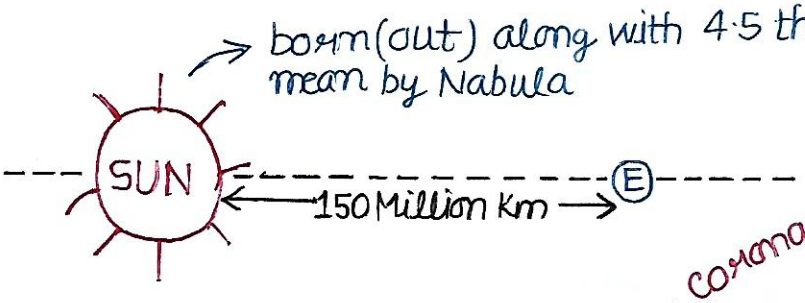
Energy

$E = mc^2$

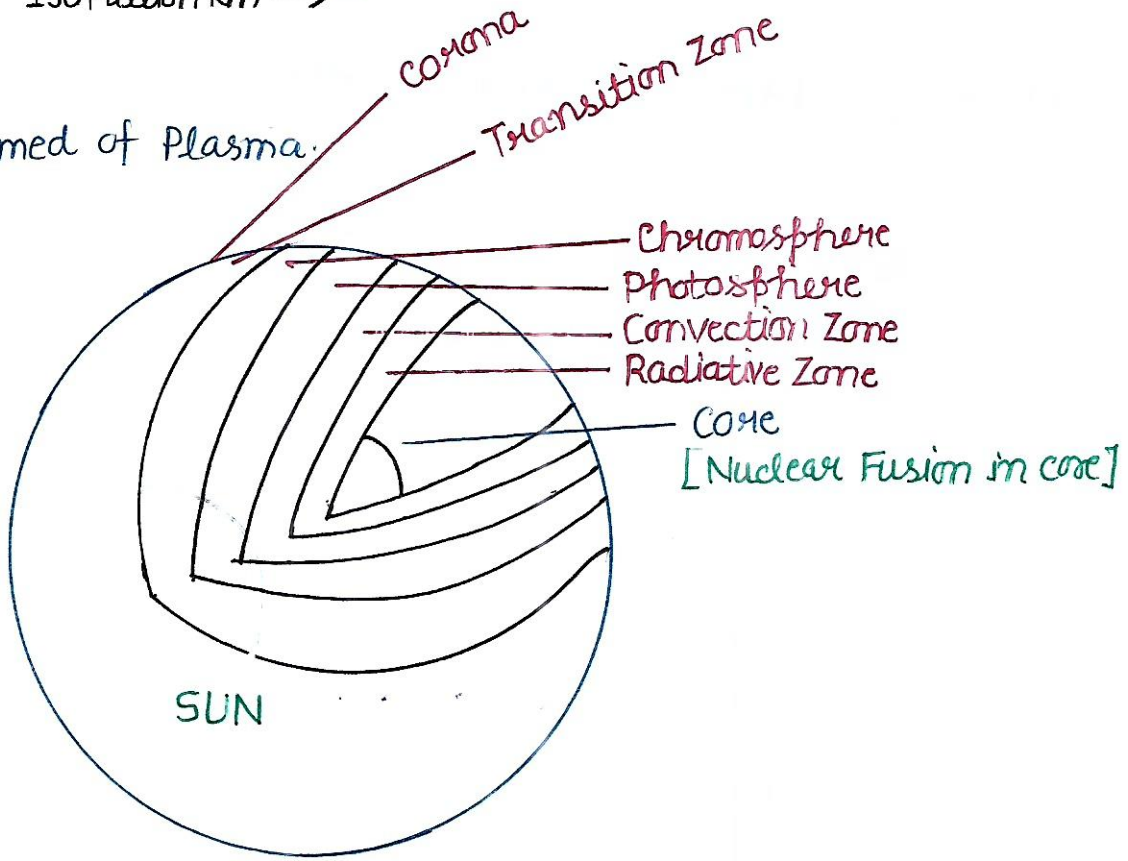
mass

Speed of Light

- Every second of every day, the sun converts 700 million tons of Hydrogen into 695 million tons of Helium.
- It's equivalent to detonating 400 Billion one megaton nuclear bombs every single second.
- 150 Million Km distance from earth



- SUN 70% formed of Plasma.



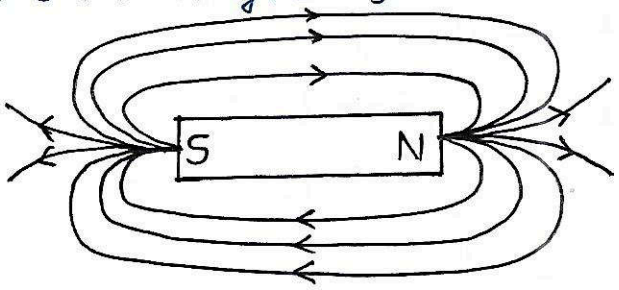
- Convection Zone is an efficient way of transferring heat.

- Photosphere -
  1. Thin Layer
  2. Sphere of Light

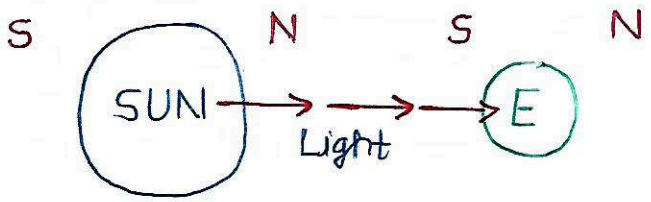
→ SUN is a gas, doesn't have a solid surface.

- Corona -
  → Solar wind

- Moving Electric charge create magnetic field.



- Coronal Mass Ejection -
  Flares like tornado occurs in corona.

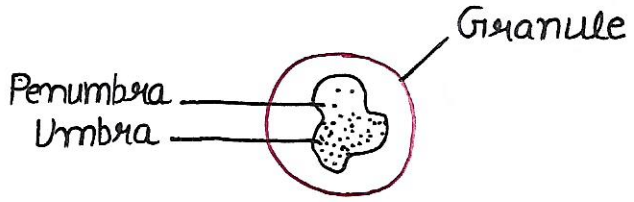


- SUN is a star powered by Nuclear Fusion.
- Hot Plasma moving inside the SUN, creating magnetic field which can create sunspot, solar flare and coronal mass ejection.

- Squarespace → e-source

• Nebula Theory - SUN was formed 4 thousand billion years ago.

• SUN SPOT-



• SUN

The sun is the star at the center of the solar system. It is nearly perfect sphere of hot plasma, with internal convective motion that generates a magnetic field via a dynamo process.

It is by far the most important source of energy for life on Earth. Its diameter is about 1.39 millions km or 109 times of earth and its mass is about 330,000 times of the earth. It accounts for about 99.86% of the total mass of the solar system. Roughly three quarters of the sun's mass consists of 73% Hydrogen, the rest of mostly 25%.

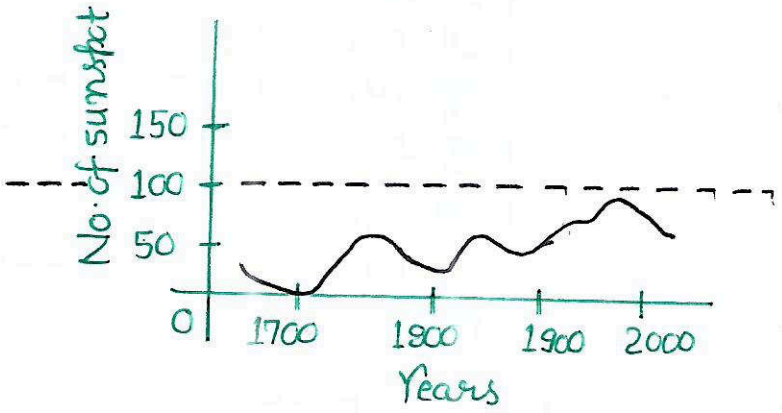
The solar dynamo is the physical process that generates the SUN's magnetic field. A dynamo, essentially a naturally occuring electric generator in the sun's interior, produces electric currents and a magnetic field, following the laws of Ampere, Faraday and Ohm, as well as the laws of hydrodynamics, which together form the laws of megatohydrody--namics. In short a dynamo converts E_K into electric-magnetic energy

• Physical characteristic-

→ radius = 695700 Km
→ Area = 6.09×10^{12} Km^2
→ Mass = 1.9×10^{30} Kg
→ Gravity = 274 m/s^2
→ Temp. = $\approx 5 \times 10^6$ K (Corona)
→ = $\approx 1.5 \times 10^7$ K (Core)
→ Colour = 0.69
→ Age = ~10 billion year (Predicted)
→ $Velocity_{escape}$ = 617.7 Km/s
→ Volume = 1.41×10^{18} km^3

- SUN SPOT –
  - Black dots on the sun surface.
  - Maximum magnetic field (Strongest).
  - Low temperature than other places.
  - Low light emitted from spots.
  - Blocking the convective zone of SUN.
  - Cooler Reagion of SUN.

Sunspots are temporary phenomena on the SUN's photosphere that appear as spots darker than the surrounding areas. They are region of reducing surface temperature caused by concentration of magnetic field flux that inhibit convection. Sunspot usually appear in pairs of opposite magnetic polarity. Their number varies according to the approximately 11 years solar cycle.



Solar cycle is an avarage duration of about 11 years.

- STAR CLUSTER –

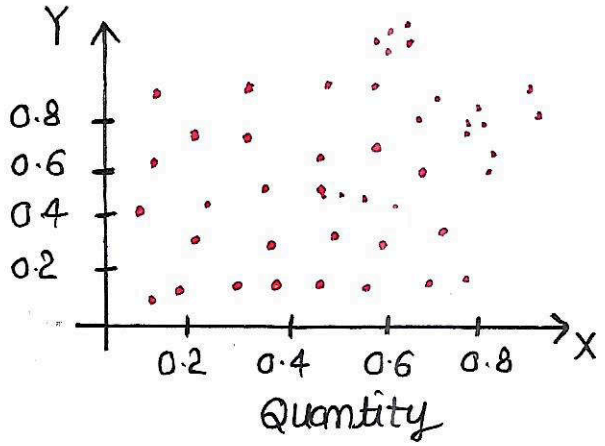
Star clusters are groups of stars. 2 Types of star clusters can be distinguished. Globular clusters are tight groups of hundereds or thousands of very old stars which are gravitationally bound, while open clusters more loosly clusters groups of stars, generally contain fewer than a few hundred members, are often very young.

A globular cluster is a spherical collection of stars that orbits a galactic core as a satellite. There are very tight bound by g, which gives them their spherical shape.

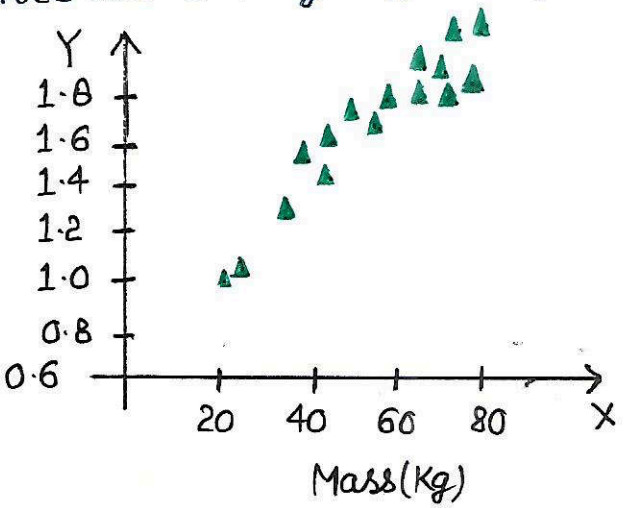
An open cluster is a group to a few thousand stars that were formed from the same giant molecule cloud.

- HR diagram-

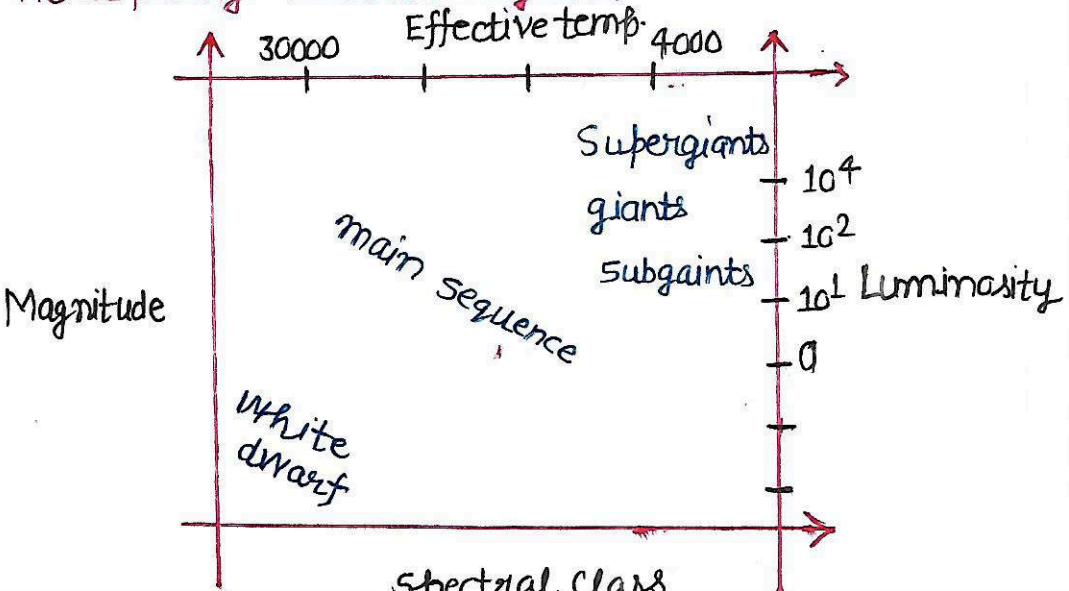
Graphing or plotting data is an essential tool used by scientists. In attempting to make sense of data and see if two quantities are related we can plot them and seek trends. If we have a look at the two examples below the first shows two quantities X and Y that an object may have. There is no discernable relationship between X and Y In fact in this example, there is no relationship, the data is purely random.



If we plot data for height versus mass for a small group of people, however, wee see a very different pattern as shown below.



Hertzprung-Russell diagram-

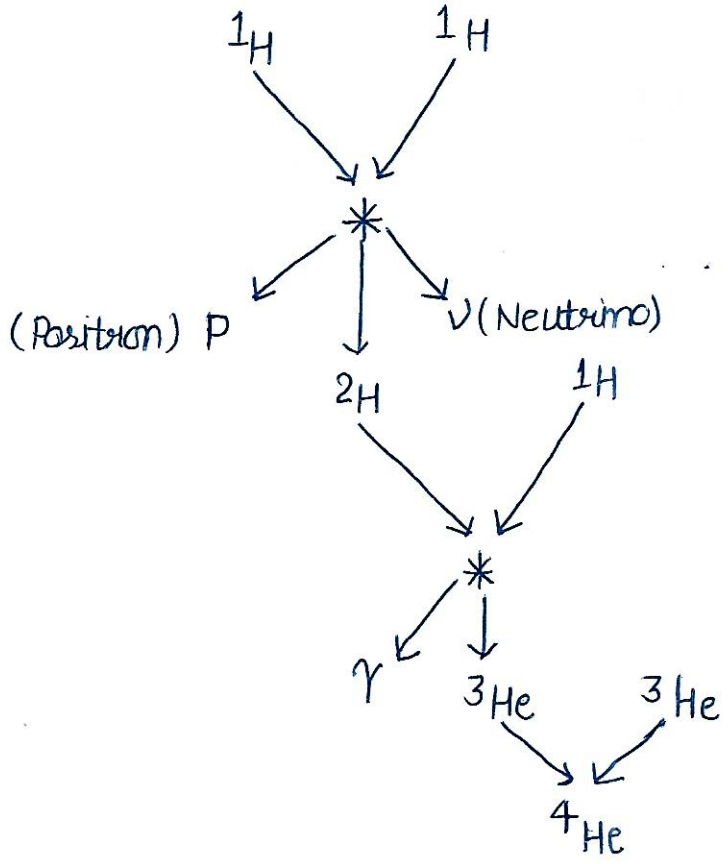


UNIT-4[2]
Stellar System[2]

This page is a content of Astrophysics section. It is just written here by mistake. Go to the tagged page with flap paper of Pink colour.

- SUN's Atmosphere
- SUN's gravitational Field
- SUN spot
- Type of galaxies
- HR diagram
- Solar Wind
- Algol Paradox
- Nuclear Reactions in stars
- Butterfly diagram
- Star Clusters
- Types of clusters
- Evolution of Star

- SUN -
  - → Massive star in our solar system
  - → The pressure is a crushing 260 Billions times the earth's atmosphere pressure
  - → 15 Million °C
  - → Nuclear Fusion



Electronics

- Power Amplifiers
- Feedback in Amplifiers
- Operational Amplifiers
- Optoelectronics
  1. Optical Source
  2. Optoelectric
  3. Optical detectors

Power Amplifiers

- Class B Push Pull Amplifier and efficiency is 78.5%
- Class D and efficiency
- Feedback in Amplifier, Negative, Positive Feedback, Best way (-ve) or (+ve)
- Amplification of Signal
- Class D Amplifier
- Class A, B, C, AB Amplifier and their characteristic

↓

Improve stability
Reduce distortion

- Power Amplifier-

Power Amplifier are designed to obtain maximum power at the output. The main function of Power amplifier is to feed large amount of power to the Load.

Where Voltage amplification are used to range the voltage table of the signal or for maximum voltage amplification.



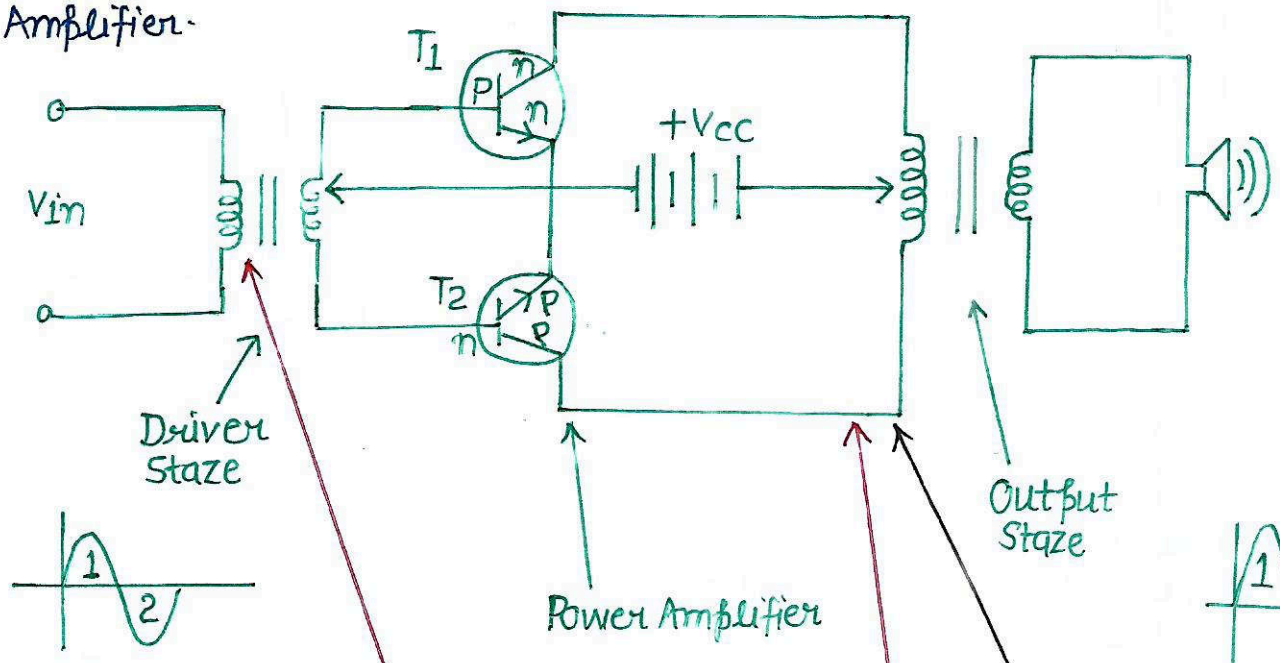
→ Characteristic-

Performance Parameter
- efficiency (η)
- Distortion
- Power dissipation Capacity

Staze of practical Power Amplifier
- Voltage Amplification
- Driver Staze
- Power staze

- Push Pull Amplifier-

Class B Amplifier is used in this arrangement because its efficiency is very much higher. Two transistors are used here T_1 and T_2. I_C is zero if input signal is not applied. Transformer winding provide proper impedance matching. $+V_{CC}$ is supplied at the center taping of this Amplifier.



Input power/signal is applied accross the secondary terminal of the driver.

T_1 = Reverse bias
T_2 = Forward bias- next half cycle due to T_2 during -ve half cycle

during +ve half cycle
T_1 = forward bias - current will conduct in this
T_2 = Reverse bias

→ Efficiency-

Since here, we are using two identical transistors

$$I_C = \frac{I_{C\,max}}{2}$$

$$I_{dc} = 2I_C = 2\,\frac{I_{C\,max}}{\pi}$$

$$(P_{ac})_{I/p} = V_{cc} \times I_{dc} = 2V_{cc} \times \frac{I_{c\,max}}{\pi}$$

$$(P_{ac})_{o/p} = V_{rms} \times I_{rms} = \frac{V_{cc}}{\sqrt{2}} \times \frac{I_{cmax}}{\sqrt{2}}$$

$$(P_{ac})_{o/p} = \frac{V_{cc} \times I_{cmax}}{2}$$

$$\eta = \frac{(P_{ac})_{o/p}}{(P_{dc})_{I/p}}$$

$$\eta = \frac{\frac{V_{cc}\, I_{cmax}}{2}}{\frac{2 \cdot I_{cmax}\, V_{cc}}{\pi}}$$

$$\eta = \frac{\pi}{4}$$

$$\eta = 0.785$$

$$\boxed{\eta = 78.5\%}$$

Power dissipation $= (P_{ac})_{I/p} - (P_{ac})_{o/p}$

$$= 2V_{cc}\frac{I_{cmax}}{\pi} - \frac{V_{cc}\, I_{cmax}}{2}$$

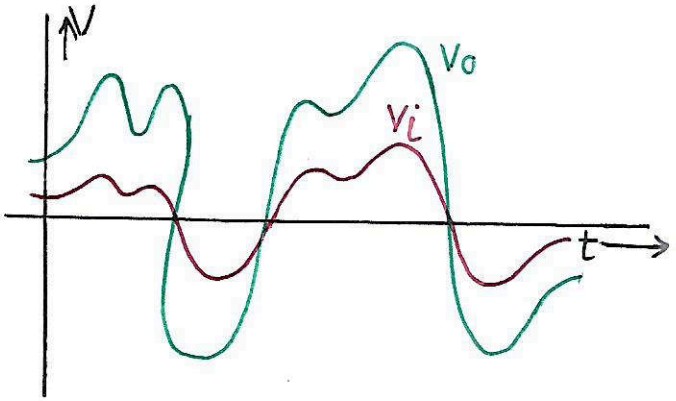
$$= V_{cc}\, I_{cmax}\left[\frac{2}{\pi} - \frac{1}{2}\right]$$

→ Advantages-
(i) High Efficiency
(ii) Distortion free output
(iii) Provide more AC output power

→ Disadvantages-
(i) To use two identical transistor
(ii) Requires two equal and opposite voltage at input.

- Amplification of Signal -

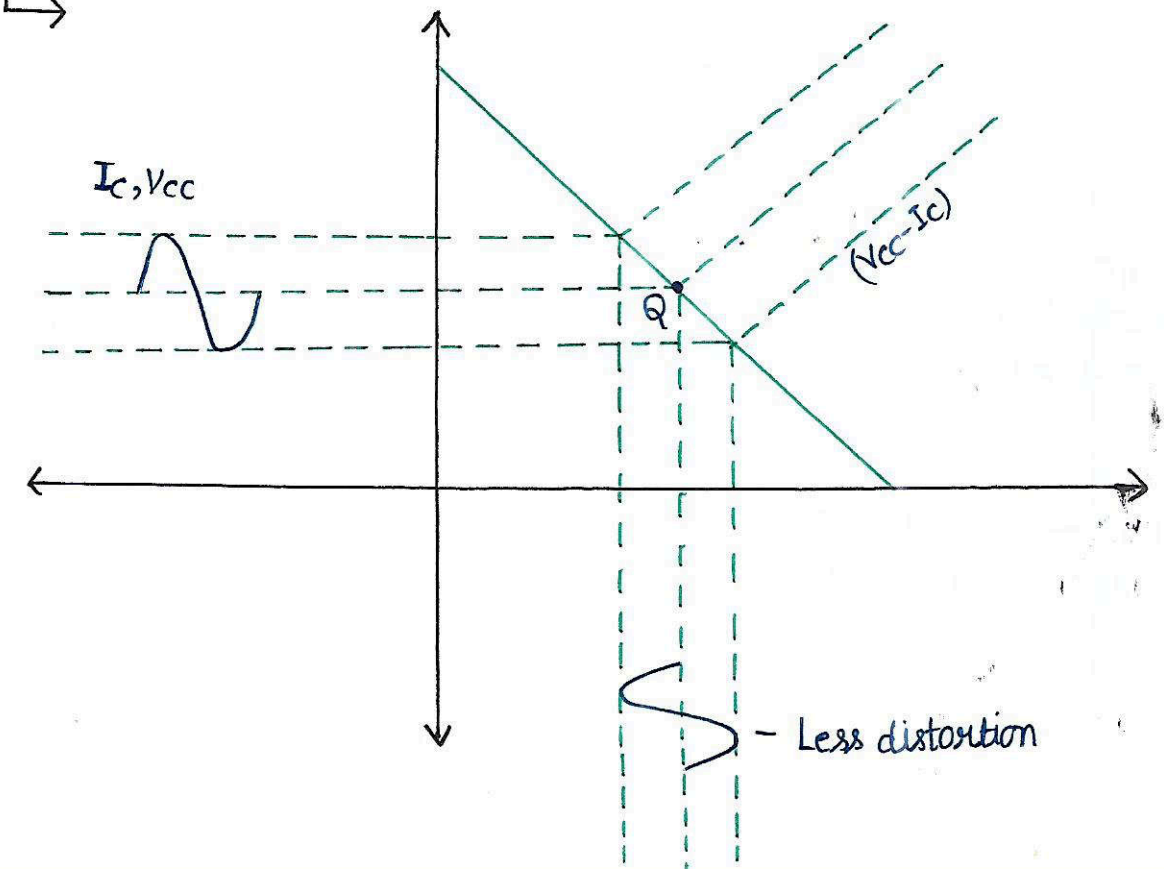
An Amplifier, electronic amplifier or amp is an electronic device that can Increase the power of a signal (a time varying voltage or current). It is a two port electronic circuit that uses electric power from the power supply to increase the amplitude of the signal applied to its input terminals.



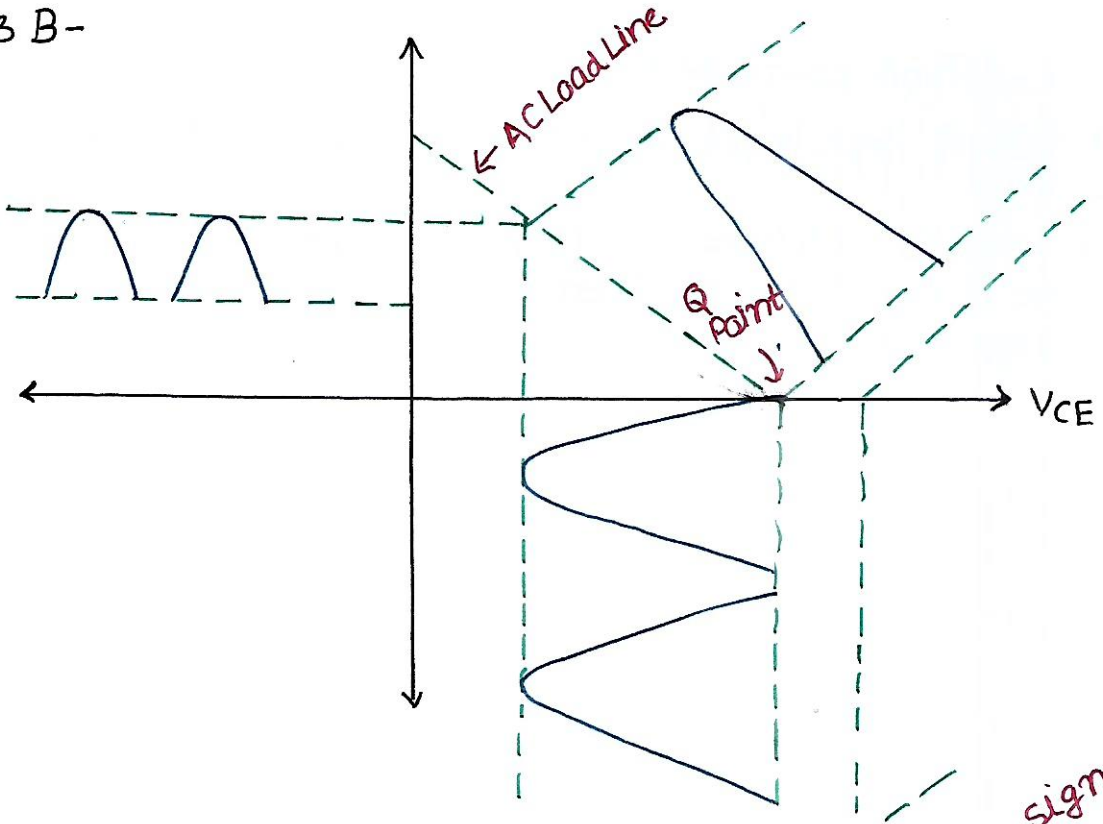
Amplification means increasing the amplitude (V or I) of a time varying signal by a given factor.

Power Amplifier

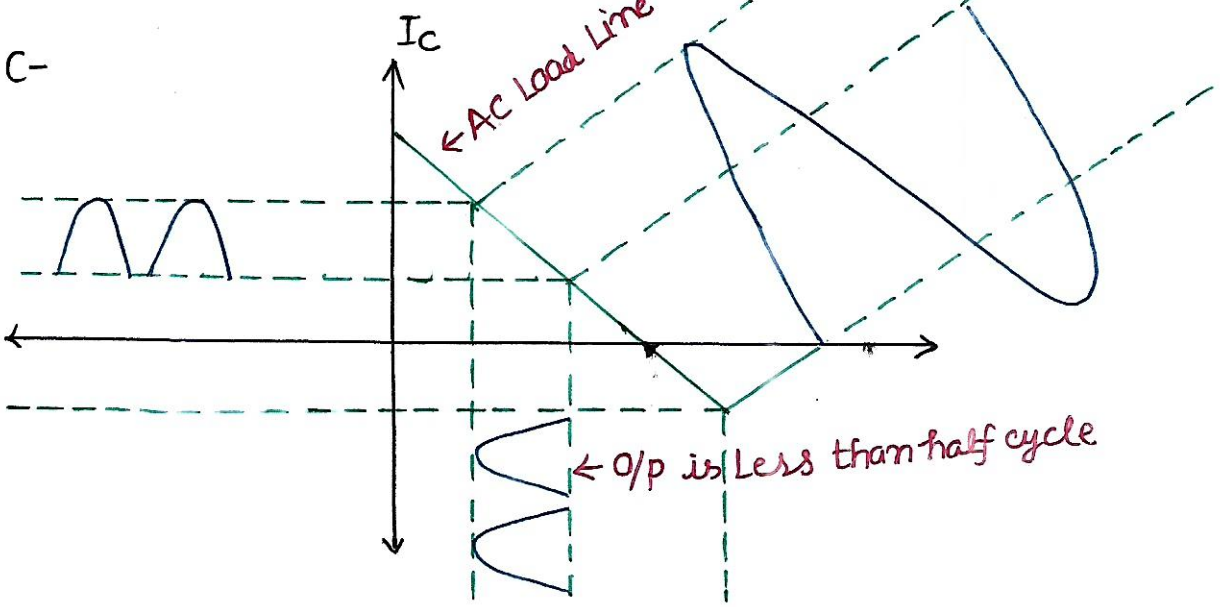
CLASS A	CLASS B	CLASS C	CLASS AB
current flows during whole cycle of O/P	I_C flows only in positive half cycle	I_C flows for less than half cycle	I_C flows more than half but less than full



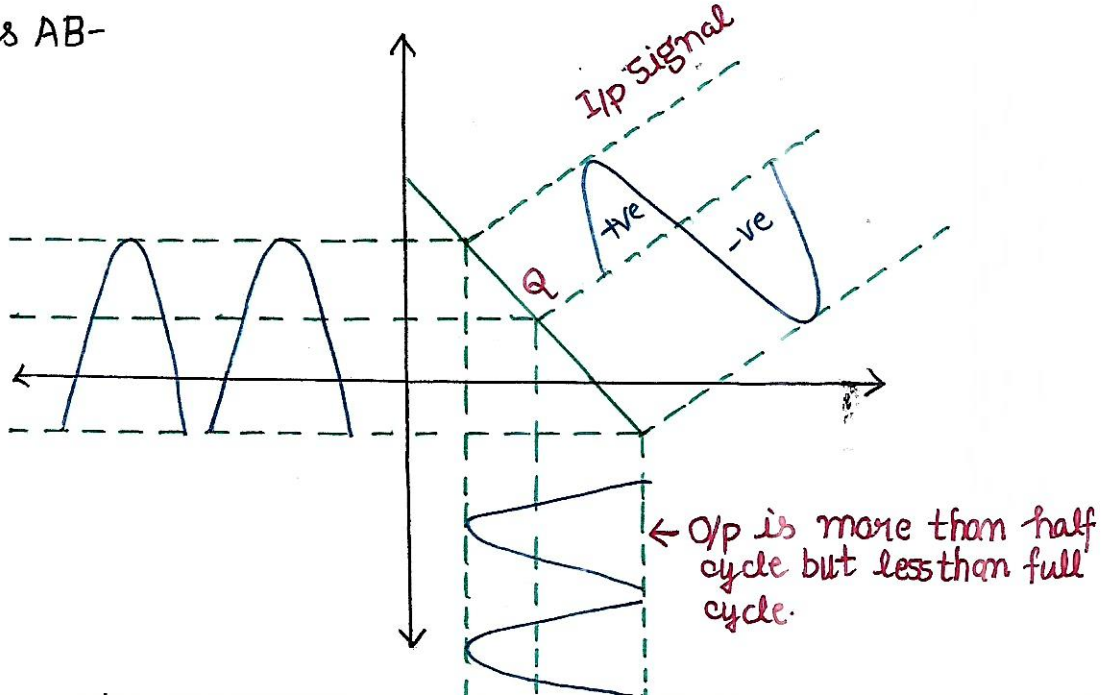
• Class B-



• Class C-



• Class AB-



- Power Amplifier-
  (i) It has high power gain.
  (ii) It has a significant current gain which results the power gain.
  (iii) It require additional cooling mechanism because it dissipate more than voltage amplifier has low power efficiency than voltage amplifier.

Feedback in Amplifier

- Wein bridge Oscillator
- Relation of frequency of osillator
- Phase Shift Principle, circuit
- Crystel Oscillator definition
- Advantage and disadvantage of oscillator
- Feedback principle / Mono, bistable Multiviberator

- Feedback- The process is combining if reaction of output energy back to input is known as feedback.

- Type of feedback
  - # Negative feedback
  - # Positive feedback

#Its magnitude increase output is in same phase shift.

$V_i = V_s + \beta V_o$

Non stabilize gain distortion increase, noise increase, gain reduce in R_i reduce.

Its magnitude reduce.
Output is 180° phase shifted

$V_i = V_s - \beta V_o$

Stablize gain, distortion reduce, gain increase, R_i increase, noise reduce

- Basic theory of negative feedback-

The feedback amplifier mainly uses two parts :-

(i) Amplifier
(ii) Feedback circuit

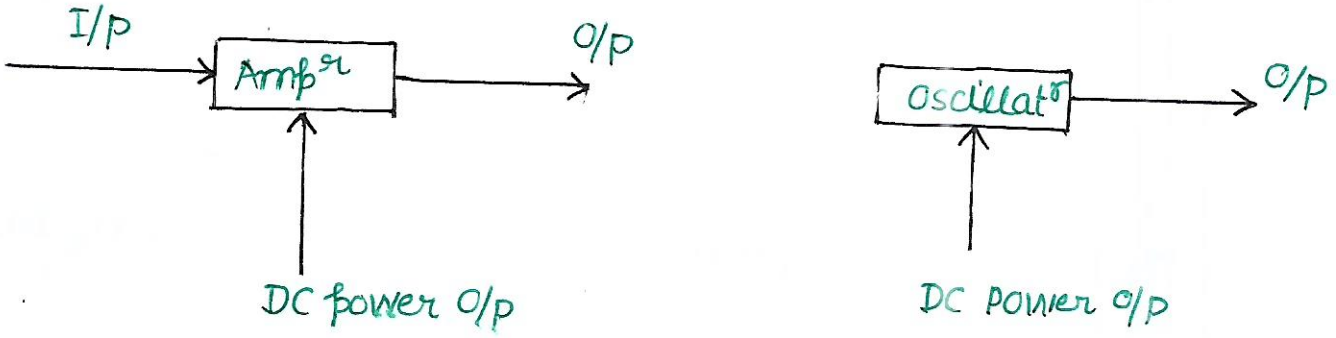
- Advantages-

(i) Stabilization of gain
(ii) Reduction in distortion
(iii) Reduce noise
(iv) Change in input impedance
(v) Stabilization of gain

$$A_f = \frac{A}{1+A\beta}$$

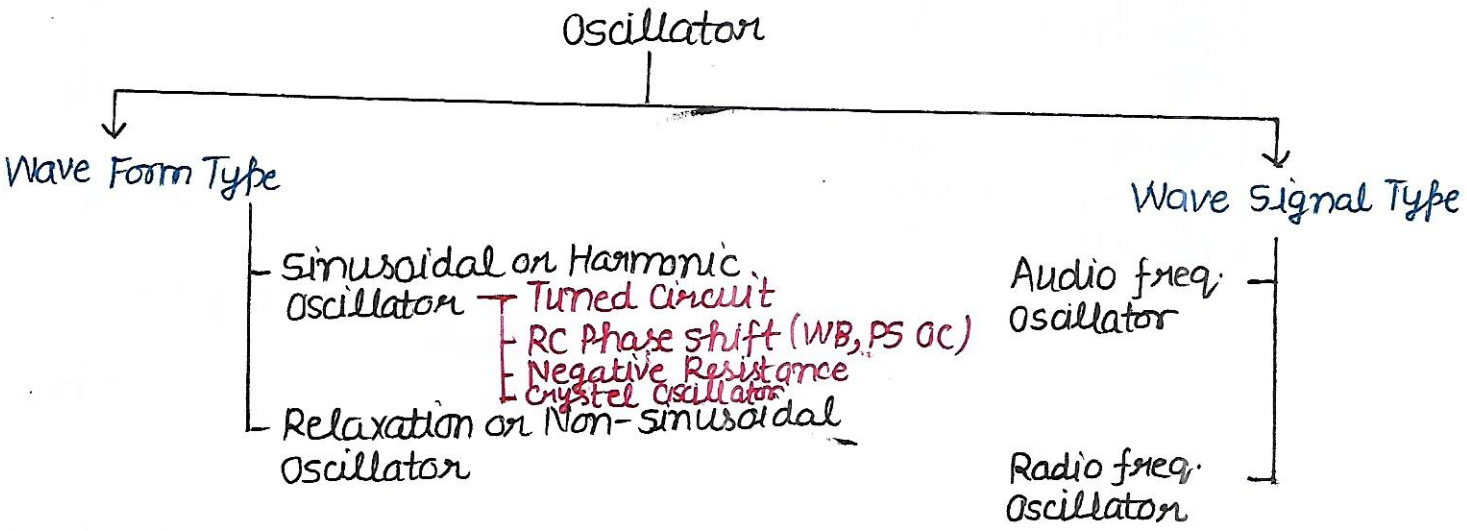
• Oscillator –

It converts dc signal into AC signal at very high frequency. It's operation is just reverse of rectifier converts AC into dc. Oscillators are different from the Amplifiers only when Amplifier has input signal but the oscillators do not have any external input.



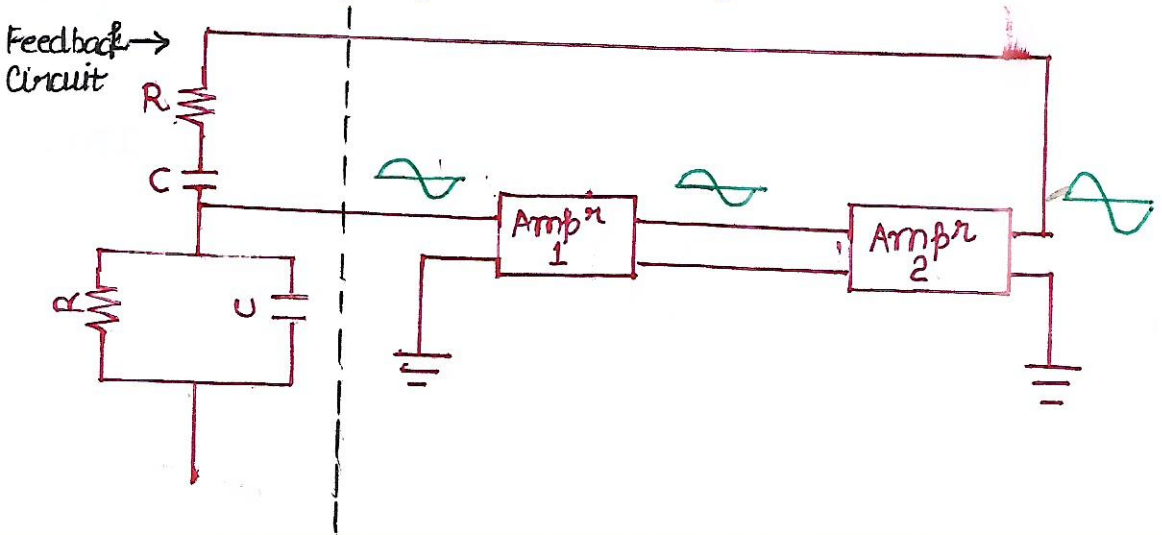
The frequency of the oscillator output is determined by the passive component used in the oscillator such as

$$f_o = \frac{1}{2\pi\sqrt{LC}}$$



• Wein Bridge Oscillator –

This is the Audio frequency RC oscillator. The advantage of this oscillator is that the range of this frequency lies from 10 Hz to 1 MHz.



It consists of two stazes of RC coupled Amplifier and a feedback network. The net phase shift of this oscillator is zero.

As shown in the figure that two RC circuit are used one is in parallel and other one is in series will not be directly feedback section to avoid the looses due to direct coupling so we will use here a bridge consists of both of these circuit.

→ Two staze Amplifier with RC bridge circuit.

→ Bridge has four Arms

* R_1C_1 in series.
* R_2C_2 in parallel.

→ T_1 serve as an oscillator and Amplifier.

→ T_2 act as inverter

→ F_o is given by R_1C_1 & R_2C_2

When switch is closed.

$$F_o = \frac{1}{2\pi\sqrt{R_1C_1\,R_2C_2}}$$

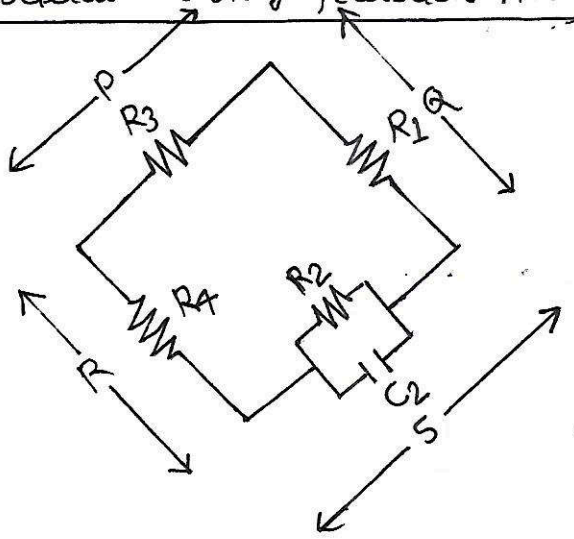
$$R_1 = R_2 = R$$
$$C_1 = C_2 = C$$

Then

$$F_o = \frac{1}{2\pi\sqrt{RC}\sqrt{RC}}$$

$$F_o = \frac{1}{2\pi RC}$$

→ Frequency of oscillator using feedback network of wein bridge oscillator



$$\frac{P}{Q} = \frac{R}{S}$$

Then

$$\frac{R_3}{R_1 + \frac{1}{j\omega C_1}} = \frac{R_4}{\frac{R_2 \cdot \frac{1}{j\omega C_2}}{R_2 + \frac{1}{j\omega C_2}}}$$

$$\frac{R_3 j\omega C_1}{R_1 j\omega C_1 + 1} = \frac{R_4(R_2 j\omega C_1 + 1)}{R_2}$$

Then Put $j^2 = -1$

Then Put $j^2 = 1$

Now the oscillation will be possible only when the phase shift is zero.

$$\Rightarrow R_4 = -R_1 R_2 R_4 C_2 C_1 \omega^2$$

$$\omega^2 = \frac{1}{R_1 R_2 C_1 C_2}$$

$$\boxed{f = \frac{1}{2\pi\sqrt{R_1 R_2 C_1 C_2}}}$$

Condition for oscillation:-

$$R_2 R_3 - R_1 R_4 - R_2 R_4 \frac{C_2}{C_1} = 0$$

$$\frac{R_3}{R_4} - \frac{R_1}{R_2} = \frac{C_2}{C_1}$$

$$R_1 = R_2 = R \text{ \& } C_1 = C_2 = C$$

Then

$$\frac{R_3}{R_4} - 1 = 1$$

$$\boxed{\frac{R_3}{R_4} = 2}$$

Gain:-

$$\beta = \frac{V_f}{V_o}$$

$$V_f = V_o \frac{R_4}{R_3 + R_4} = V_o \frac{R_4}{2R_4 + R_4} = V_o \frac{R_4}{3R_4}$$

$$\frac{V_f}{V_o} = \frac{R_4}{3R_4} \Rightarrow \boxed{\beta = \frac{1}{3}}$$

• Crystel Oscillator-

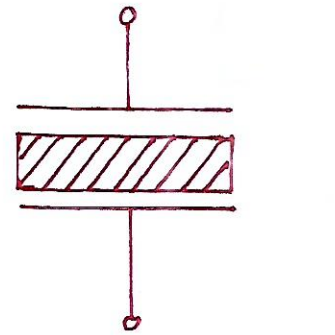
→Due to the limitation of RC and LC oscillators, crystel oscillators are used.

→The limitation which effect dominently is changed of the frequency due to the change in the temperature.

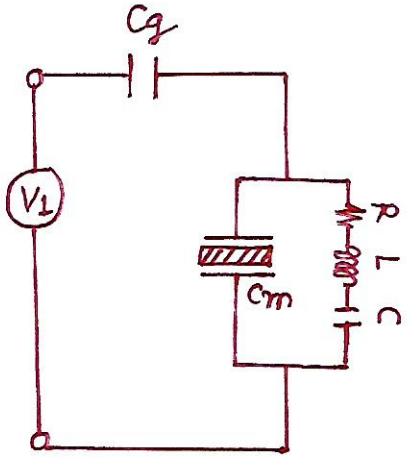
→ LC and RC oscillators are positive temperature cofficient.

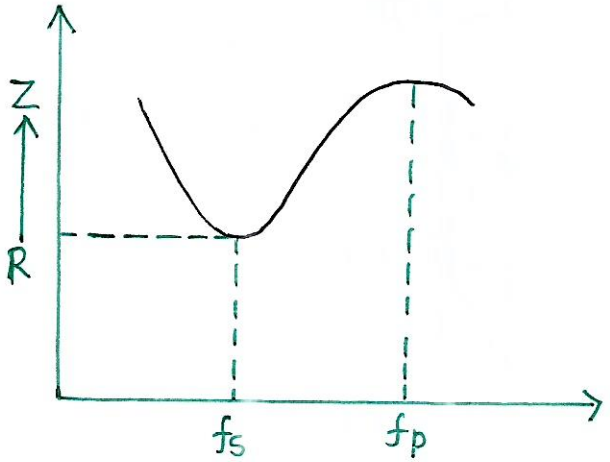
→So the solution of this problem to maintain the constant frequency within extremely low tolarance for temperature.

→This solution is done by crystel oscillator.



crystel mounted b/w two plates





$$Q = \frac{\omega L}{R}$$

$$f_s = \frac{1}{2\pi\sqrt{LC}} \text{ and } f_p = \frac{1}{2\pi\sqrt{LC_T}}$$

$$C_T = \frac{C \times Cm}{C + Cm}$$

C_T → Total Capacitance

• Advantage or disadvantage of Oscillator-

The Advantage of Oscillator is that they all have good stability at high frequency and have a good wave purity. The disadvantage is that it is hard to design.

• Phase shift Oscillator-

→ The essential requirement for the oscillation is that there must be 180° Phase shift around the feedback network and gain should be greater than unity.

→ In the phase shift oscillator RC network is selected in such a way that for the frequency the phase angle is 60°.

→ So to maintain the angle of 180°. Circuit with RC selections are used here.

→ Here npn transistor is used and common emitter configuration is there. R_1 and R_2 provide dc ammeter phase bias R_L is the load control collection voltage V_C.

$$R' = R - h_{fe}$$

→ Applying KVL

$$\left(2R + \frac{1}{j\omega C}\right) I_1 - R I_2 + h_{fe} I_b R = 0 \quad \ldots\ldots (1)$$

$$-R I_1 + \left(2R + \frac{1}{j\omega C}\right) I_2 - R I_b = 0 \quad \ldots\ldots (2)$$

$$-R I_2 + \left(2R + \frac{1}{j\omega C}\right) I_b = 0 \quad \ldots\ldots (3)$$

$$\begin{vmatrix} I_1 & I_2 & I_3 \\ 2R+X_C & -R & h_{fe}R \\ -R & 2R+X_C & -R \\ 0 & -R & 2R+X_C \end{vmatrix}$$

$$= 6R^3 + 2RX_C^2 + 8R^2X_C + 3X_CR^2 + X_C^3 + 4RX_C^2$$

$$-2R^3 - X_CR^2 + h_{fe}R^3 = 0$$

Put $X_C = -jX_C$

Then

$$X_C^3 - 10R^2X_C = 0$$

$$X_C^3 = 10R^2X_C$$

$$X_C^2 = 10R^2$$

$$X_C = \sqrt{10}R$$

$$\frac{1}{\omega_C} = \sqrt{10}R$$

$$\frac{1}{\omega} = \sqrt{10}RC$$

$$\omega = 2\pi f$$

$$\frac{1}{2\pi f} = \sqrt{10}RC$$

$$\boxed{f = \frac{1}{2\sqrt{10}RC}}$$

Now Imaginary part = 0

$$4R^3 - 6RX_C^2 + h_{fe}R^3 = 0$$

$$h_{fe}R^2 = 6X_C^2 - 4R^2$$

$$h_{fe} = \frac{6X_C^2}{R^2} - 4$$

$$X_C^2 = 10R^2$$

$$h_{fe} = \frac{6 \times 10R^2}{R^2} - 4$$

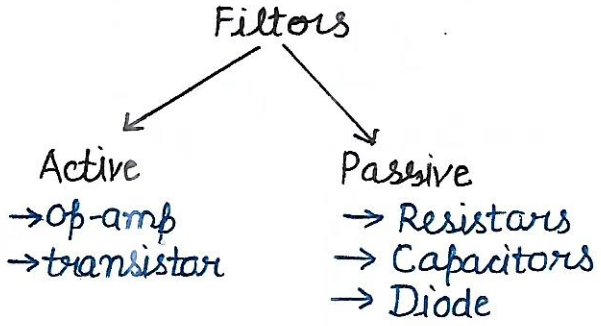
$$h_{fe} = 60 - 4$$

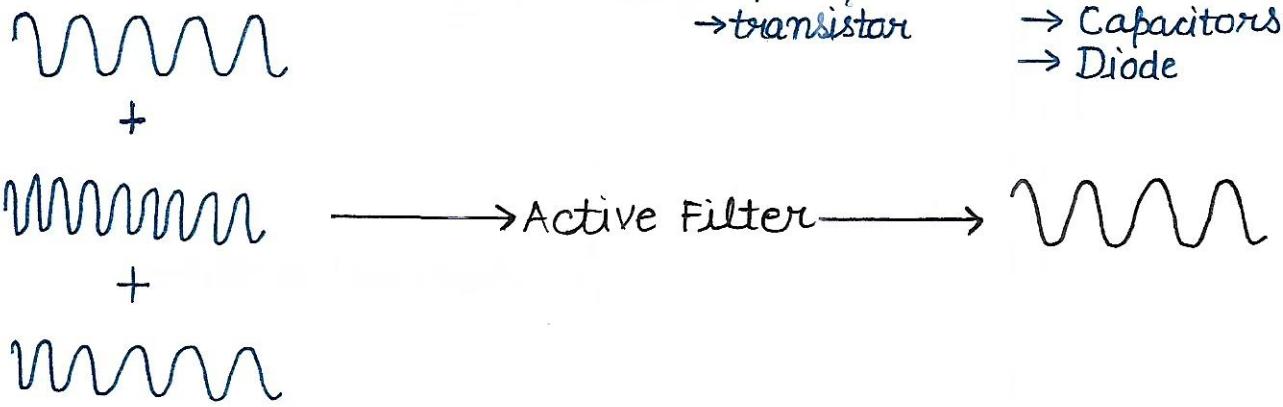
$$\boxed{h_{fe} = 56}$$

Operation Amplifiers

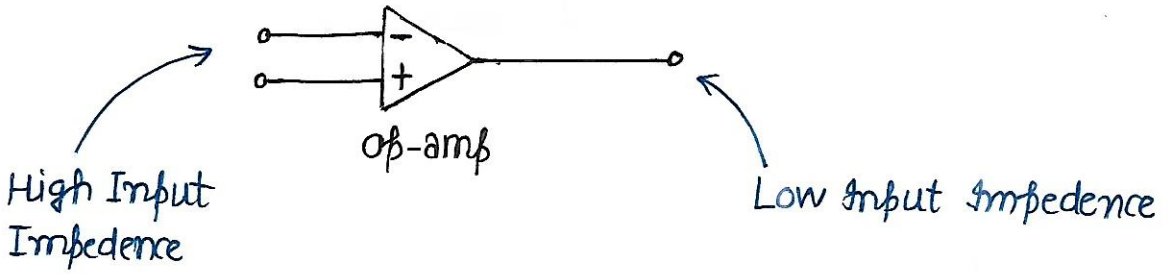
- Operation Amplifier / An Inverter / An Adder / An differenciator
- Block diagram of Inverting and Non-Inverting terminal
- H circuit - Voltage Regulator
- Active Filters

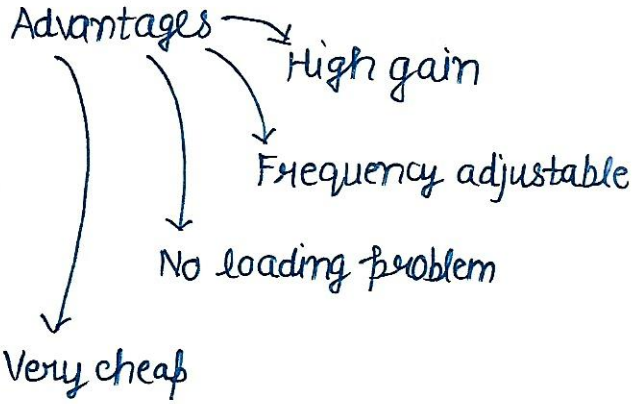
- Active Filters -
  - Application of op-Amp
  - Vout < Vin





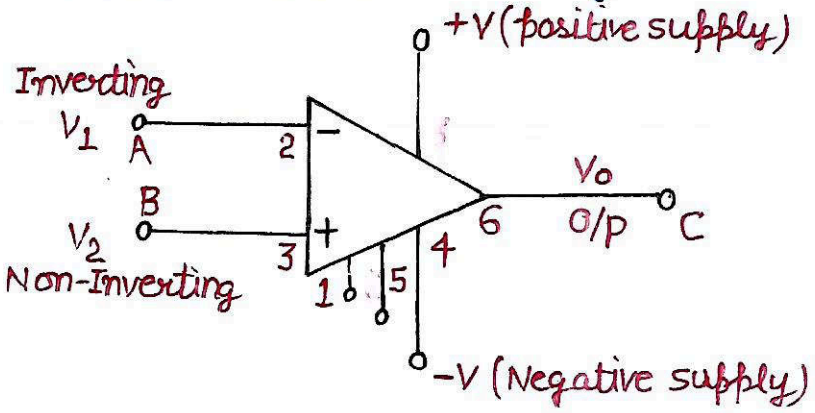
Active Filter provide gain to the input signals and selectively passes certain band of frequency.



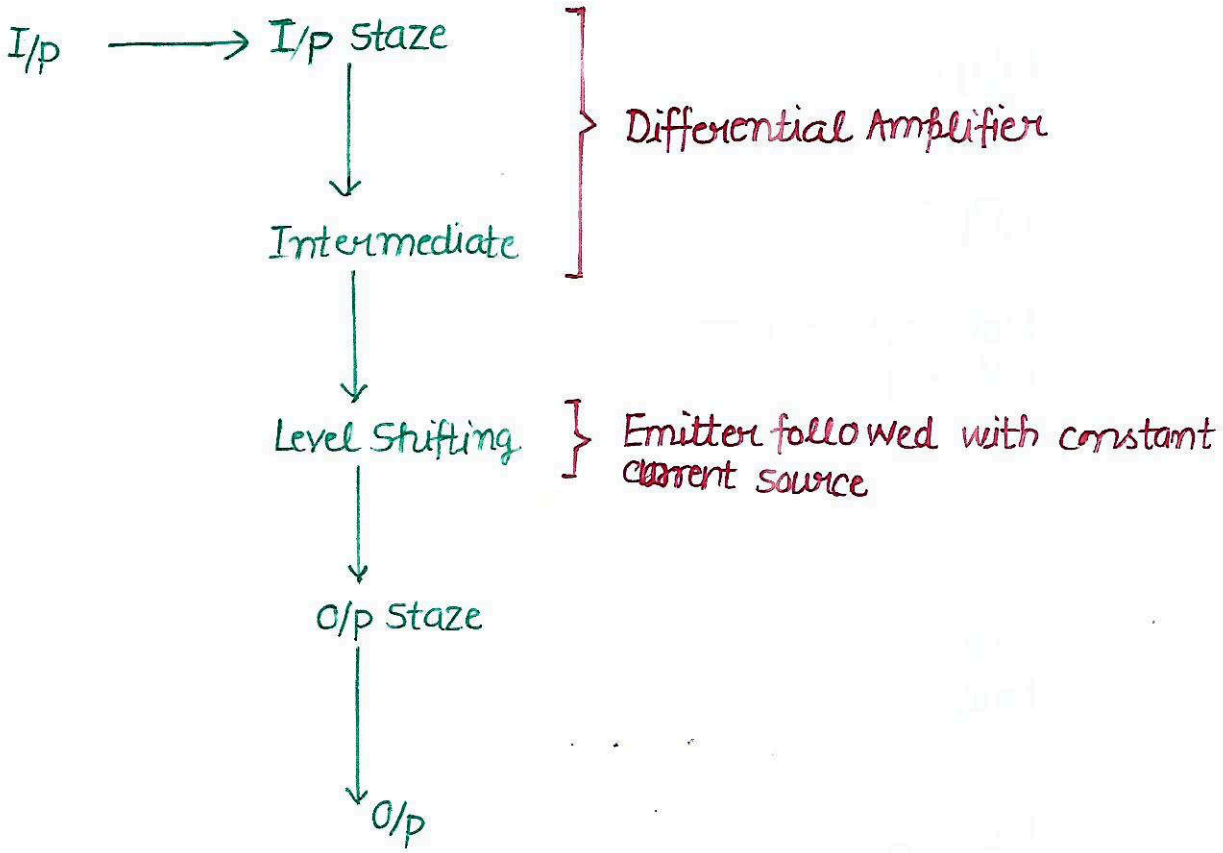


• Operational Amplifier-

→ Commonly known as op-amp.
→ High gain
→ directly coupled
→ -ve feedback amplifier
→ 0Hz to 1MHz → Filtering



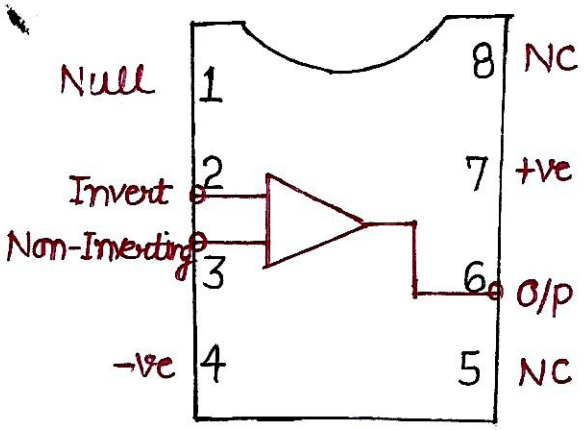
#Stages-



• CMRR (common Mode Rejection Ratio)-

$$CMRR = \frac{A_{DM}}{A_{CM}}$$

• Block diagram of Inverting and Non-Inverting Terminal:-



Optoelectronics

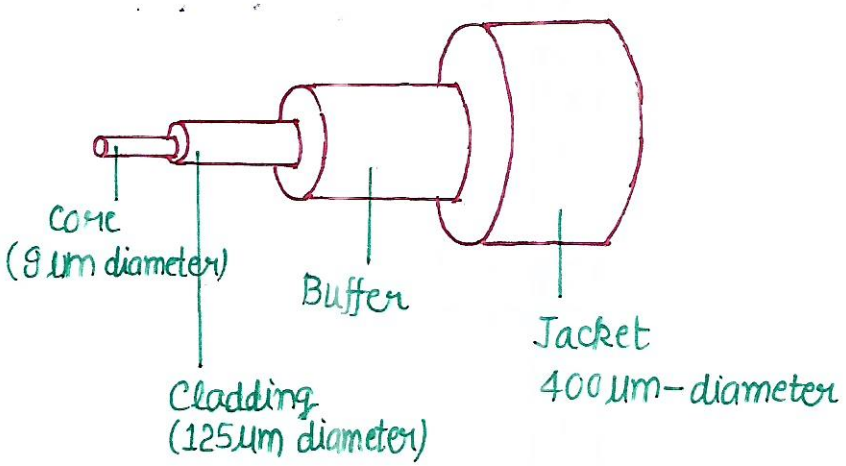
- Photodiode
- Step Index and Graded Index Fibre
- LED
- Optical Fibre
- Avalanche Photodiode

• Optical Fibre –

A thin flexible and transparent wire prepared for light propagation is called optical Fibre. The optical fibre has been constructed for the following reasons;

- The light wave cannot transerve long distance in air without any losses.
- To make loss less light wave communication, the optical fibre wave can be guided through optical fibre
- Additional advantage of high bandwidth.

physically optical fibre is very thin and flexible. The optical fibre can be used for many of Industrial application and medical application as well. The Optical Fibre consists of two media kept one inside the other. The center transparent medium of Optical Fibre is called core and the outer is cladding. The refractive index of core will be always higher than the refractive index of cladding.



Having cylindrical shape with three sections.

1. Core
2. Cladding
3. Buffer
4. Jacket

The core of a conventional Optical Fibre is a cylinder of glass or Plastic that runs along the fibre length. The core is surrounded by a medium with a lower refrective index known as cladding of a different glass or plastic. Light travelling in the core reflects from the core cladding boundary due to the total internal reflection. The core is characterised by the diameter or cross section area.

Cladding in optical fibre is one or more layers of materials of lower refrective index with the core material of high referective index.

Buffer is a component use to incapsulate one or more optical fibres for the purpose of providing such function such as mechanical isolation protection from physical damage and other.

The Jacket is the outer most portion of a Optical Fibre. Jacket is made from Polymer(PVC, plastic etc.) to protect the core and cladding from mechanical lose or damage. Fibre Optical Jacket are made in different colours for colour coating Identification.

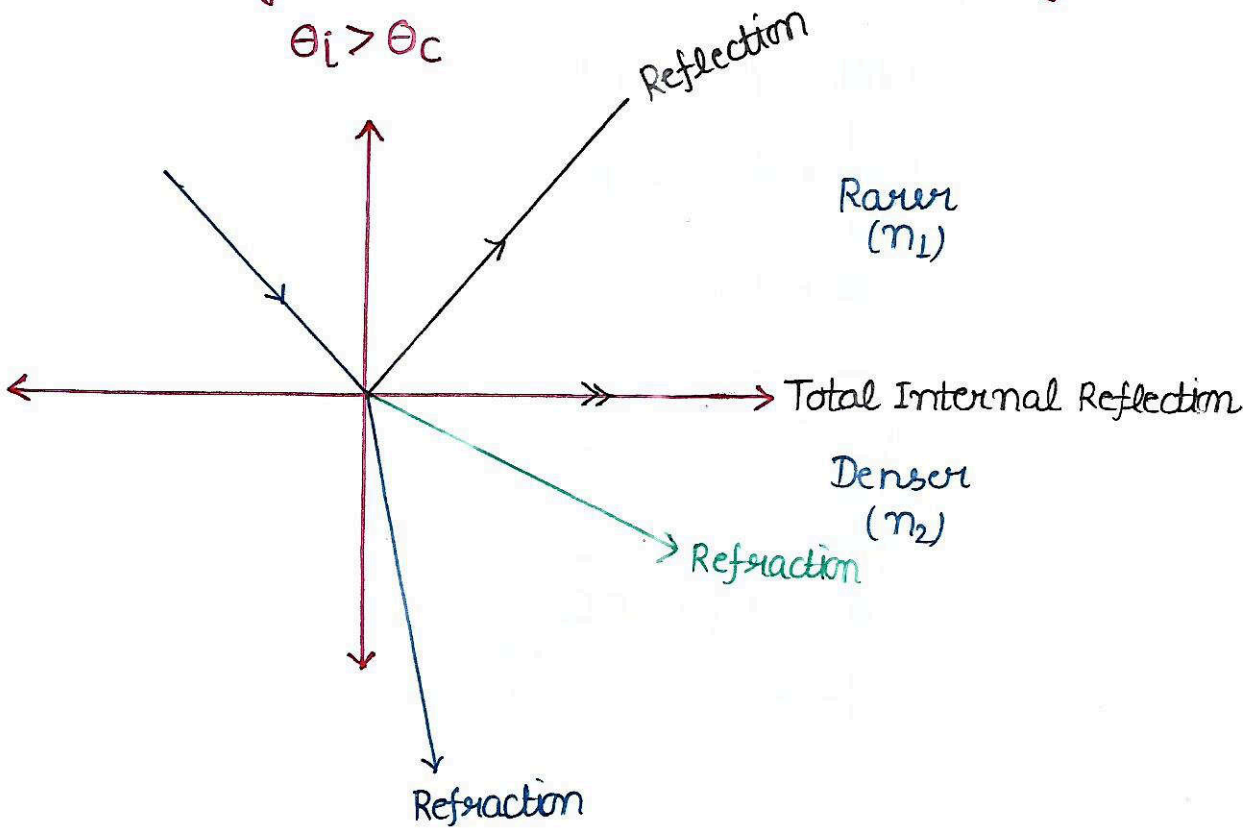
- Importance of Optical Fibre-
  (i) Attanuation is lower than the coaxial cable.
  (ii) Smaller size and light weight.
  (iii) No physical, electric connection is required between sender and receiver.
  (iv) Realiblity is high.
  (v) Higher data rate
  (vi) cost effective

- The Propagation of Light in optical fibre-
  The light propagates through optical fibre through "Total Internal reflection". The TIR reflection appears due following reasons.

- When light travers from optically rarer medium (like air) to denser medium (glass) the refracted ray moves towards the normal drawn on the interface of media as in snell's law. Conversly, if light traverse from denser to optically rarer medium, the refracted ray moves away from the normal drawn on the interface of the medium.

Conditions for Total Internal Reflection :

1. The ray of Light should be transerve from denser to rarer medium.
2. The incident angle should be more than the critical angle



Parameters –

(i) Radius of core

(ii) Numerical Aparture

$$n_0 \sin\theta_i = n_1 \sin\theta_r$$

$$\sin\theta_i = \frac{n_1}{n_0} \sin\theta_r$$

$$\sin\theta_i = \frac{n_1}{n_0}\sqrt{1-\cos\theta_r} \quad \ldots\ldots\ldots (1)$$

Snell's rule

$$n_1 \sin\theta = n_2 \sin 90^\circ$$

$$n_1 \sin(90-\theta) = n_2 \sin 90^\circ$$

$$n_1 \cos\theta = n_2$$

$$\cos\theta_r = \frac{n_2}{n_1} \quad \ldots\ldots (2)$$

From eqn (1) & (2)

$$\sin\theta_i = \frac{n_1}{n_0}\sqrt{1-\left(\frac{n_2}{n_1}\right)^2}$$

$$\checkmark \left(NA = \sin\theta_i = \frac{1}{n_0}\sqrt{n_1^2 - n_2^2}\right)$$

(iii) Acceptance Angle

$$NA = \sin\theta_i = \frac{1}{n_0}\sqrt{n_1^2 - n_2^2}$$

$$\sin\theta_i = \frac{1}{n_0}\sqrt{n_{01}^2 - n_2^2}$$

$$\theta_i = \sin^{-1}\left(\frac{1}{n_0}\sqrt{n_1^2 - n_2^2}\right)$$

$$\boxed{\theta_i = \sin^{-1}(NA)}$$

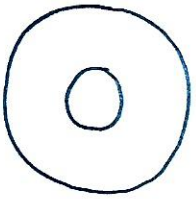
(iv) Attenuation

$$\boxed{\alpha = -\log\left(\frac{I_{out}}{I_{in}}\right)}$$

#Classification

- Material based
  - Plastic made OFC
  - Glass made OFC
- Refractive Index
  - Step / Single Index OFC
    - Single mode
    - Multimode
  - Graded Index OFC
    - Single mode
    - Multi mode

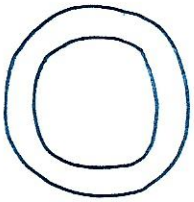
Single Index / Step Index -



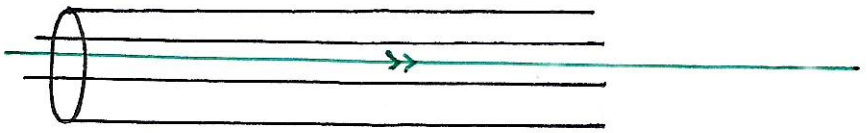
core << cladding

If the refractive index of core remains the same from the center of the core to the core cladding Interface.

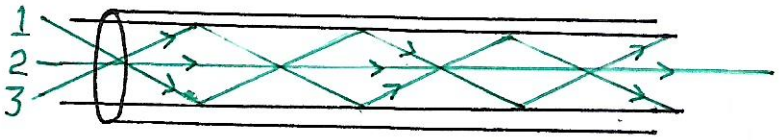
Graded Index -



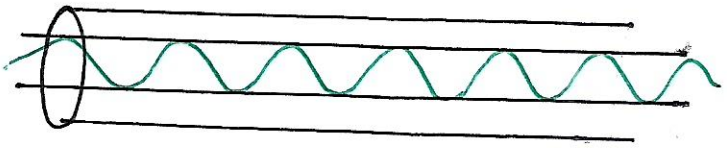
core < cladding



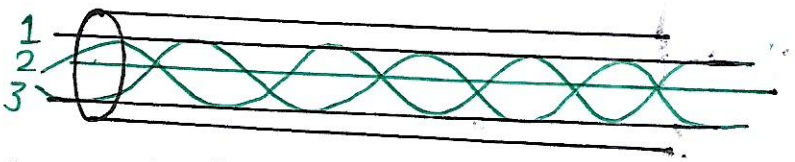
Step Index single Index mo



Step
Index Multimode

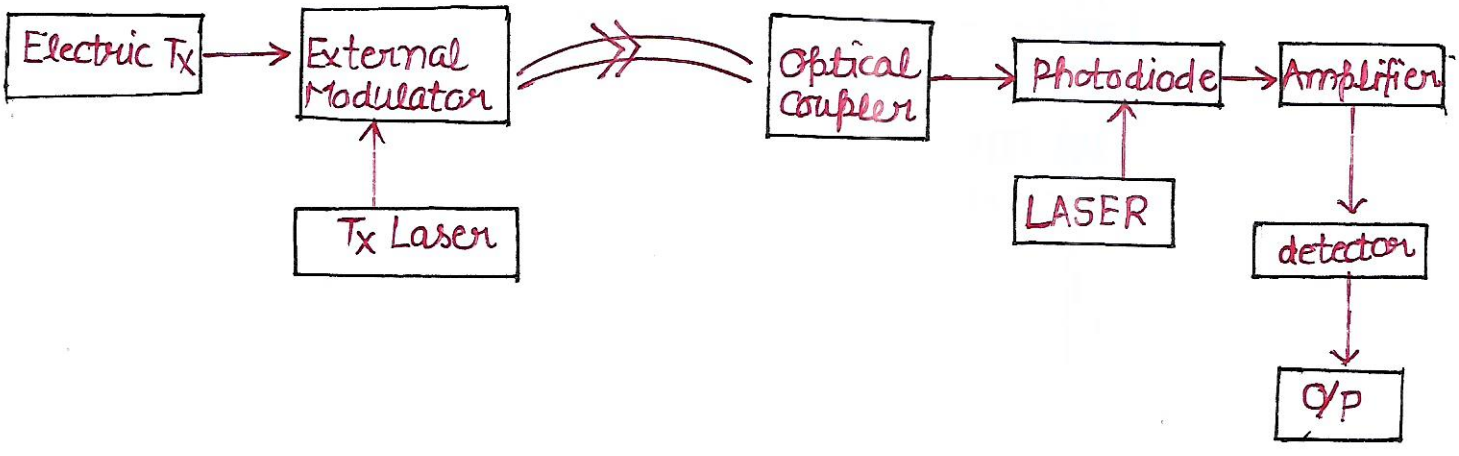


Graded
Index Single Mode



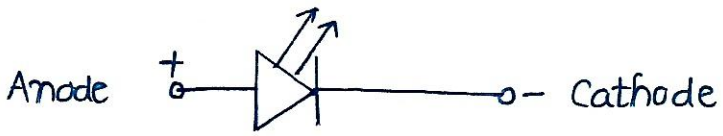
Graded Index Multimode

Communication -

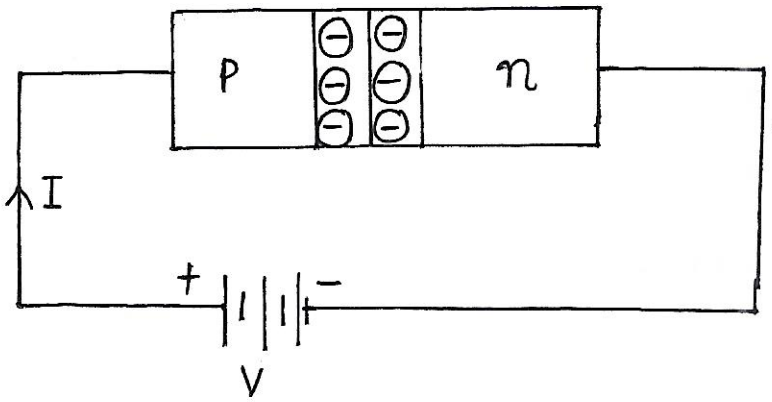


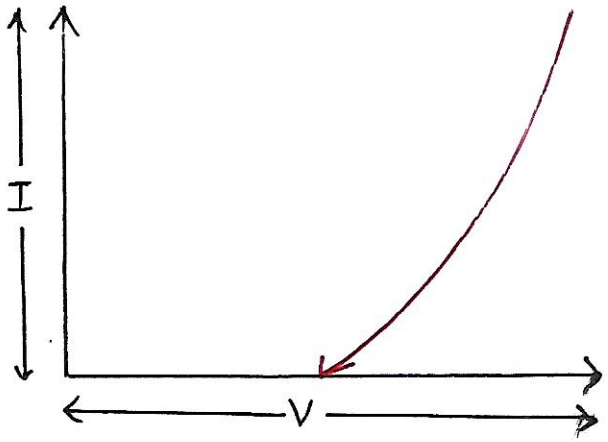
- LED-

Light Emitting Diode



Heavilty doped P-n junction
In Foorward bias, emit radiation
transparent cover





#Application-

- Remote control
- Optical communication.

#Advantages-

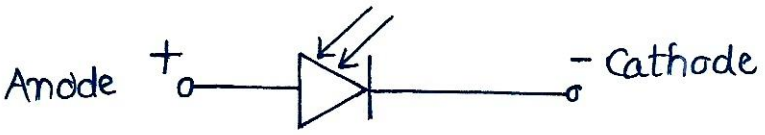
- Low power and no warm up time required
- Long life
- More Efficient
- Fast action

• PD-

Photodiode

Reverse biased Si/Ge Pn junction

Reverse current ∝ Intensity of Light



(A) pplication

(i) Alarm circuit

(ii) Counter circuit

Solid State Physics

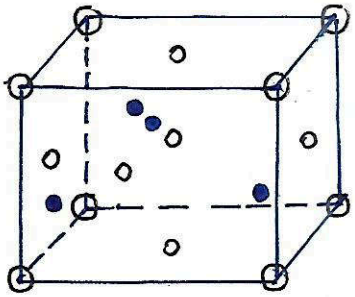


Diamond Structure–

→ Exhibits both cubic and Hexagonal type structure.
→ dc structure is more common and is described here.
→ Space lattice of the diamond cubic structure is fcc.
→ Basically consisting of two carbon atoms

Location
- Lattice Point
- other at a distance of one quarter of the body diagonal from Lattice point along body diagonal.

→ The unit all of the dc structure is shown in figure



○ C atom occupied fcc position
● C atom occupied tetrahedral position

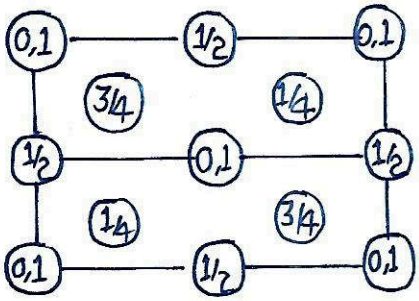
→ The Packing Efficiency of the dc stcture is only 34% as compared to 74% for the fcc structure.

→ Coordination number for carbon = 4

→ Nearest neighbour distance = $\frac{\sqrt{3}}{4}a$

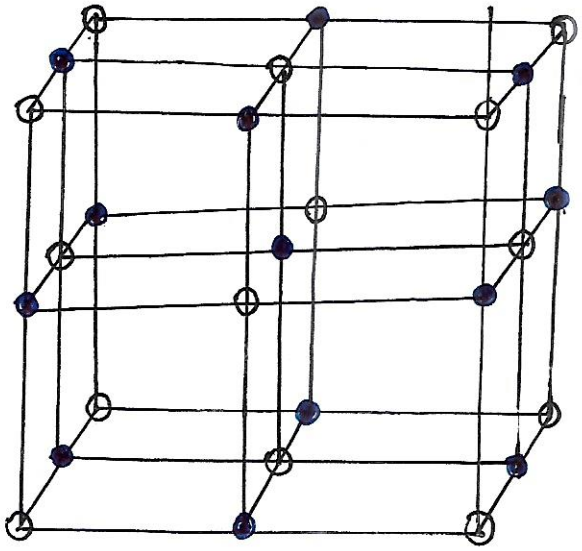
a ↑ Lattice parameter

The dc structure may also be viewed as an interpenetration of two fcc sublattice with their origin at (0,0,0) and (1/4, 1/4, 1/4)



NaCl Structure-

→ The Unit cell of NaCl structure is shown in figure



→ In NaCl structure, the radii of Na^+ and Cl^- ions are such that each Na^+ ion is octahedrally coordinated to 6 Cl^- ions.

→ The Unit cell is fcc with four Cl^- ions occupying all the four fcc positions and Na^+ ions occupying the fcc octahedral voids.

→ The NaCl Structure can be viewed as two interpentrating fcc sublattice, one belong to Na^+ with origin (0,0,0) and Cl^- with origin $(a/2, 0, 0)$.

* The position of various ions in the unit cell are as follows:

Na^+ : $0,0,0 ; \frac{1}{2},\frac{1}{2},0 ; \frac{1}{2},0,\frac{1}{2} ; 0,\frac{1}{2},\frac{1}{2}$

Cl^- : $\frac{1}{2},\frac{1}{2},\frac{1}{2} ; 0,0,\frac{1}{2} ; 0,\frac{1}{2},0 ; \frac{1}{2},0,0$

Lecture : Crystal structure

Matter

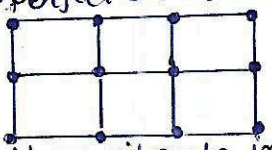
1. Bose Einstein condensation
2. Solid ✓
3. Liquid
4. Gases
5. Plasma

→ Solid

Crystalline

Naturally, maximum energy release

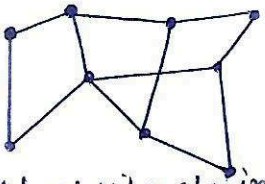
- Perfect order Arrangement



→ Atoms vibrate in place in fixed pattern

→ Low energy state

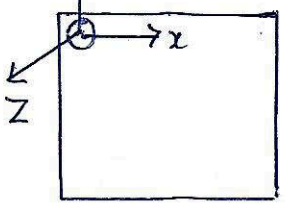
Amorphous



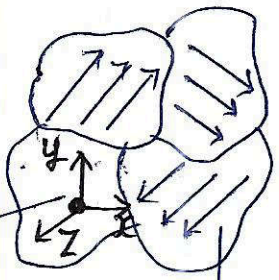
- Atoms vibrate in place in more random Arrangment
- Arbitrary arrangement



y Single



Poly crystal

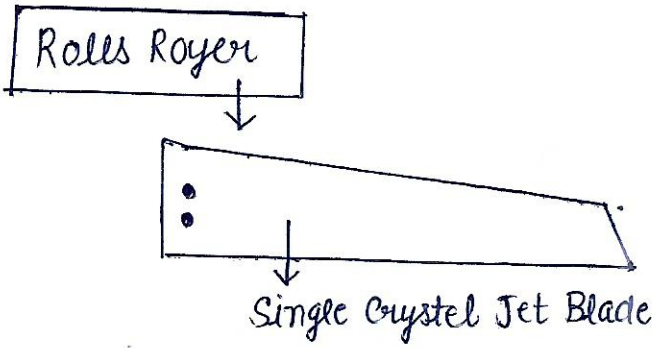


⇐ Microscopically watching

grains or Crystallite

Vibrational Orientation

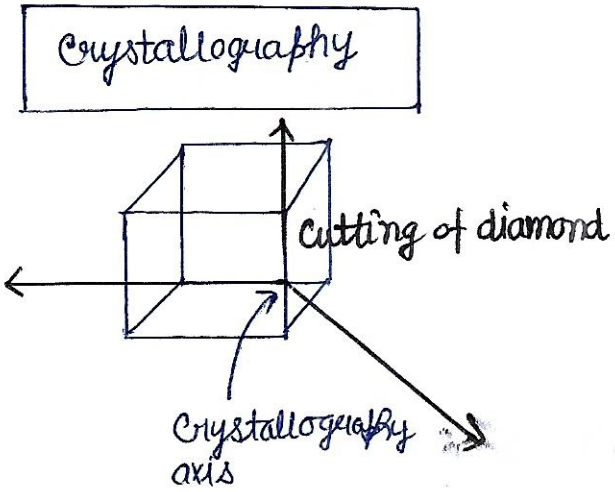
→ Single crystalline have (heavy) good strength.



→ Single crystel

- Quartz crystel
- Gems
- Jet blades

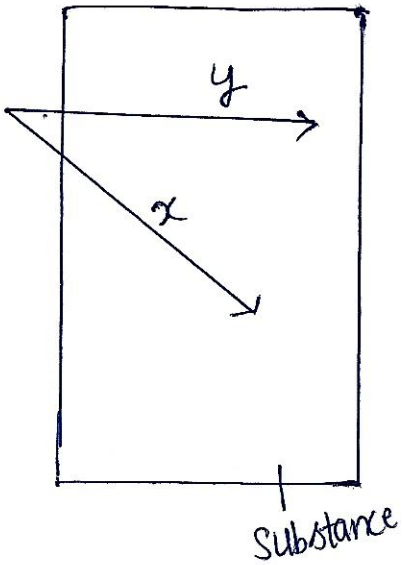
→ Single crystels are very important.



Crystallography is a science in which we study about geometery, geometrical orientation and physical property.

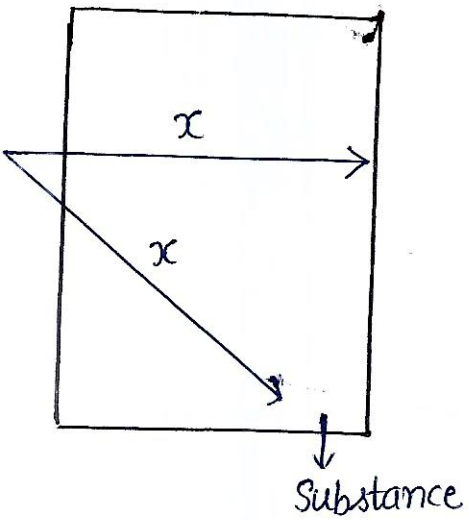
- Anisotropic
- Isotopic

Anisotropic



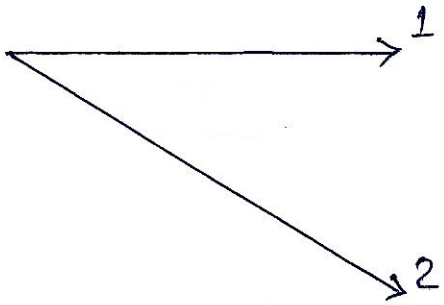
This substance is Anisotropic

Isotropic



This substance is Isotropic

Finding λ



$\lambda_1 = ?$

$\lambda_2 = ?$

$\lambda_1 \neq \lambda_2$

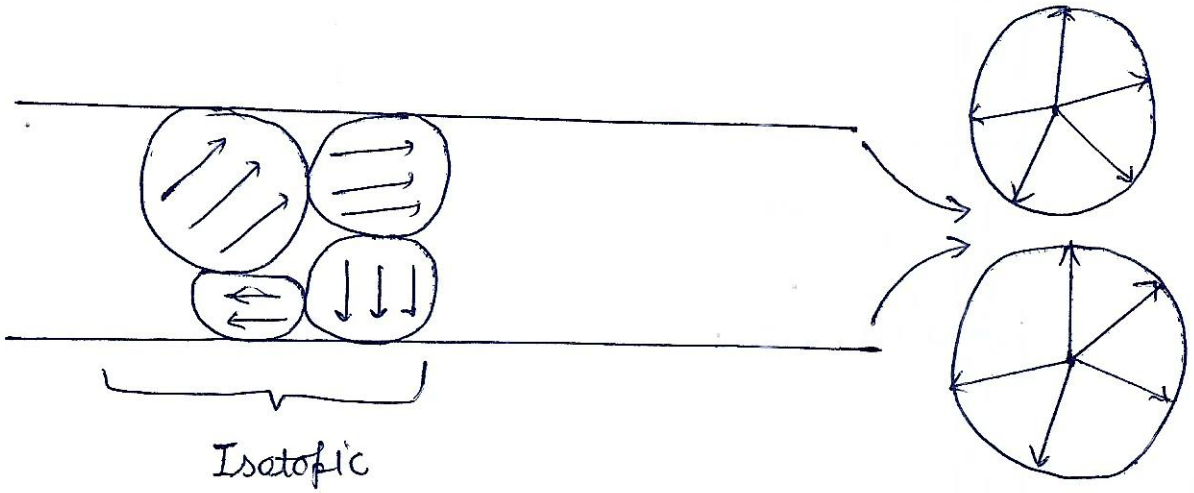
Crystalles are iso-ani-tropic
i.e. Anisotropic

Amorphous are isotropics.

Crystel and Amorphous

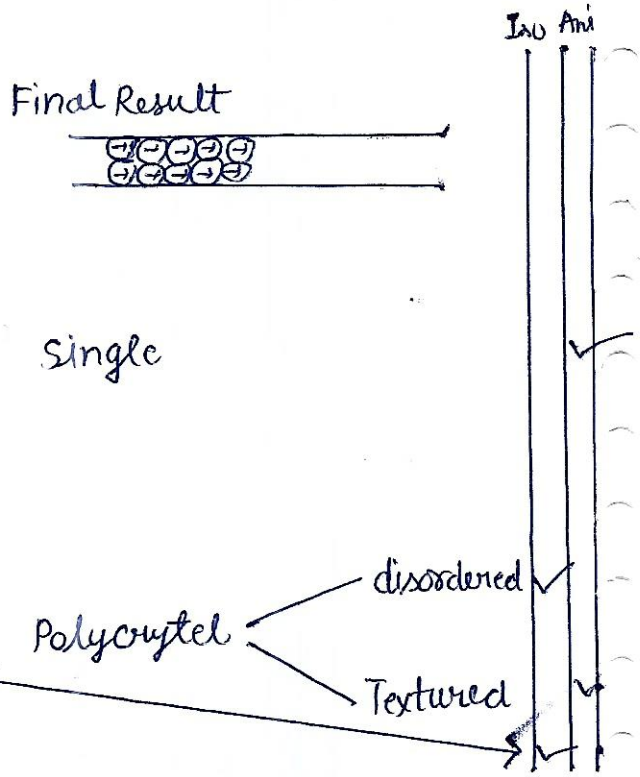
single crystel → Anisotropic

Poly crystel → Isotropic



Poly crystel

Isotopic



Crystel

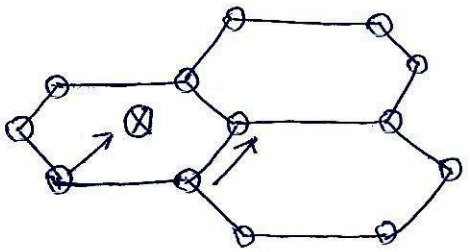
Single

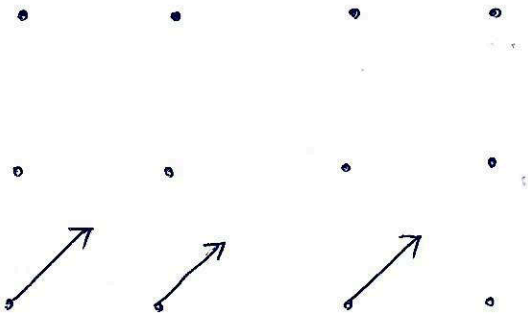
Amorphous

- Space Lattice
- Translational Vector
- Unit Cell
- Wigner Cell
- Basis

} Outline

→ Space Lattice-





→ 2D
→ 3D

→ Translation Operation-

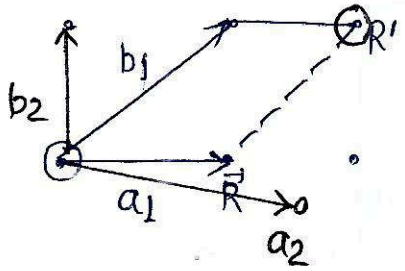
$$T = n_1\vec{a} + n_2\vec{b} + n_3\vec{c}$$

Funamental translational Vector
or
Crystel Axes
or
Basis Vector

$R' = R + T$

$R' = R + 0\,a_1 + 1\,b_1$

$\boxed{T = 0a_1 + 1b_1}$ ..... (1)



$R' = R + T$

$R' = R + \frac{1}{2}a_2 + \frac{1}{2}b_2$

$\boxed{R' = R + \frac{1}{2}a_2 + \frac{1}{2}b_2}$ ..... (2)

General translation

$T = n_1 a + n_2 b + n_3 b$

0, 1-Integers

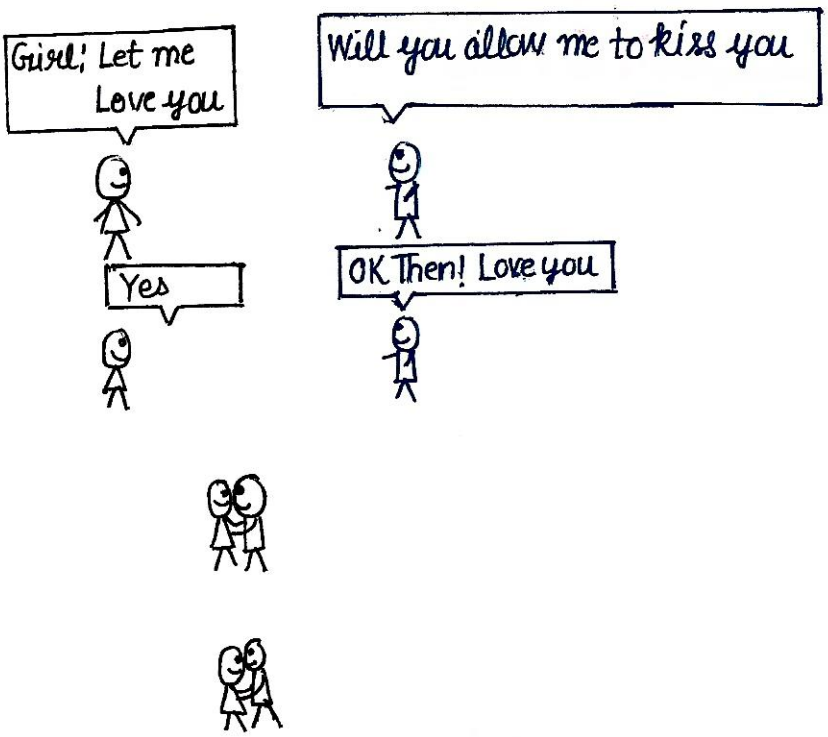
Primitive Translation

$T = \frac{1}{2}a + \frac{1}{2}b$

Statistical Physics

Important Questions

⇒ Liouville's Theorem (7) ✓✓
⇒ Ensembles (13) ✓✓
⇒ Maxwell Boltzmann Distributions (5) ✓✓
⇒ Partition Function (7) ✓
⇒ Gibb's Paradox (9) ✓✓
⇒ Sakur-tetrode Equation (6) ✓
⇒ Difference b/w ideal and Real Gas (5) ✓✓
⇒ Vander Waal's Equation (3) ✓
⇒ MB, FD, BE distributions (6) ✓✓
⇒ BE Condensation (6) ✓✓
⇒ Application & Properties of liquid He (10) ✓
⇒ Plank Law of blackbody Radiation using BE statistics (8) Wein & Stefan's Law ✓✓
⇒ Rayleigh Jean's Formula (3) ✓✓
⇒ Wein's Law & Wein displacement Formula ✓✓
⇒ Stefan's Law (1)
⇒ Debye Theory (2)
⇒ Equipartition Energy Theory (4)
⇒ Bason & Fermion (3) ✓✓
⇒ Chemical Potential (2) ✓✓
⇒ Entropy (2) ✓✓
⇒ Phase Space (4) ✓✓
⇒ Degree of freedom ✓✓

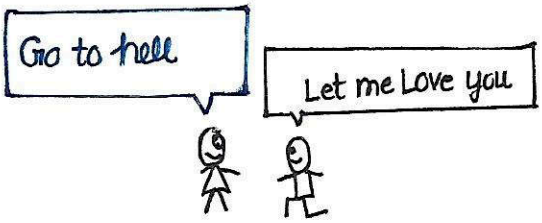


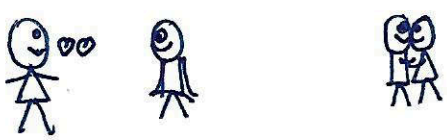
Properties of liquid He -

1. The 2 e^- of He occupy the 1S orbital with opposite spin The filled orbital makes this nobel gas inert
2. He remains in a liquid state at ordinary pressure.
3. The lighter isotope of He^3 has three nucleons and obeys fermi statistics
3. He(II) flows through capillary without resistance.

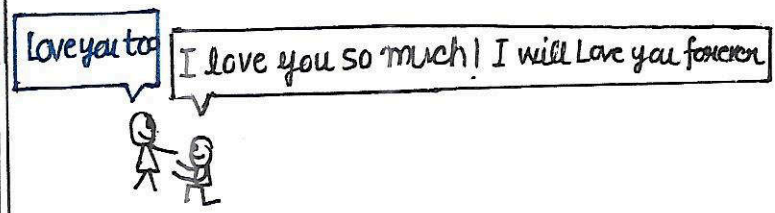
Difference between Fermion & Boson-

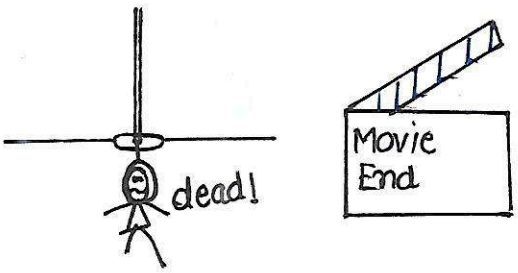
Fermion	Boson
On the basis of spin	
$S = \frac{1}{2}, \frac{3}{2}$	$S = 0, 1, 2$
→ half-integer spin quantum number	→ Integer Spin quantum number
→ Fermion obey Pauli Exclusion principle	→ Bosons don't obey Pauli Exclusion principle
→ e^-, p^+, n°	→ Photons, α- Particles
→ If we add two of fermions together, you can get boson.	
→ If you add three fermions together, you can get fermion..	
→ Fermions can't co-exist in the same location at the same time because it follows Pauli Exclusion principle.	













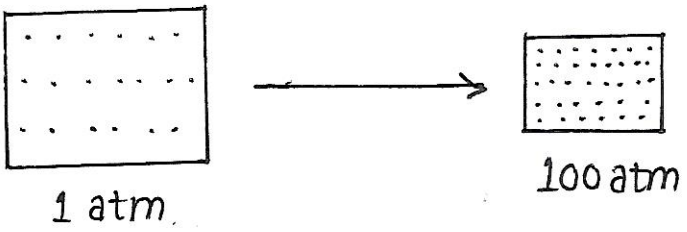
#Vander Waals Gas Equation-

- At low pressure (or high temperature), the gas molecules are far away from one another. In addition, the volume of container is much larger than volume of molecules.

$$PV = nRT$$

Where P = Pressure
V = Volume
R = Gas Constant
n = No. of moles
T = Temperature (in °K)

- Ideal Gas



But at high Pressure (or low temperature):
(1) Molecule are much closer to the one another (Electrical Forces)
(2) Volume of molecule compared to the volume of container is no longer negligible.

- Ideal gas is not useful under such condition

b = Unavailable volume per mole.

- If we multiply b by n, we obtain the volume that

$$P \propto \frac{1}{V}$$

$$P = \frac{a}{V^2}$$

$$\left(P + \frac{a}{V^2}\right)(V - b) = RT$$

Liouville's Theorem–

→ In classical Mechanics, the complete state of particle can be given by its position and momentum.

→ In 3D, there are 3 dimensions and 3 momentum. If we consider a 6 dimensional Phase space, a point in that space represent the state of a particle

→ A Particle will follow the determined path through space.

→ Now consider a large no. of particles in a beam. These particle can be described by one point in Phase space for particle.

→ For really large no. of particles, a system can be described as $D(q_i, p_i)$ density which is a function of position in space.

→ Liouville's Theorem state that the density of particles in phase space is a constant

$$\frac{dD}{dt} = 0$$

According to the theorem, the Phase space distribution is constant along the trajectories of the system

Proof:

Let us suppose that the distribution with its time dependance is known as (q, p, t)

So we can write

$$dD = \sum_j \frac{\partial D}{\partial q_i} \frac{dq_i}{dt} + \sum_i \frac{\partial D}{\partial p_i} \frac{dp_i}{dt} + \frac{\partial D}{\partial t} \frac{dt}{dt}$$

if we recall the theorem from classical mechanics using chain rule and Poission bracket.

$$\frac{dD}{dt} = \frac{\partial D}{\partial q_i} \dot{q_i} + \frac{\partial D}{\partial p_i} \dot{p_i} + \frac{\partial D}{\partial t} = 0$$

using Hamiltonian equation

$$\dot{q_i} = \frac{\partial H}{\partial p_i}$$

$$\dot{p_i} = \frac{-\partial H}{\partial q_i}$$

$$\frac{dD}{dt} = \frac{\partial D}{\partial q_i}\frac{\partial H}{\partial p_i} + \frac{\partial D}{\partial p_i}\frac{\partial H}{\partial q_i} + \frac{\partial D}{\partial t} = 0$$

$$\frac{dD}{dt} = [D,H] + \frac{\partial D}{\partial t} = 0$$

under the condition of equilibrium, Poission bracket will be zero

$$[D,H] = 0$$

so

$$\frac{dD}{dt} = \frac{\partial D}{\partial t} = 0$$

$$\frac{\partial D}{\partial t} = 0$$

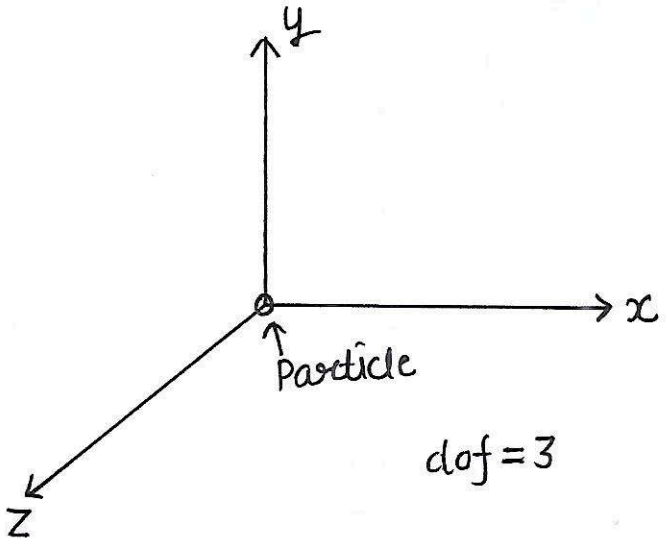
$$\Rightarrow \boxed{D \text{ is constant}}$$

Difference b/w Real and Ideal Gas

Real Gas	Ideal Gas
→ They are non hypothetical Gasses	→ There are hypothetical Gases.
→ There is ~~no~~ weak intermolecular Force	→ There is no intermolecular Force.
→ Volume (Small)	→ No Volume
→ Non Perfectly elastic	→ Elastic collision
→ It has mass	→ It has no mass
→ Whose molecule occupy space	→ Occupy negligible space.
→ Pressure is low	→ Pressure is high
→ Real Gas eqn $\left(P+\frac{a}{V^2}\right)(V-b) = nRT$	→ Ideal Gas equation $PV = nRT$

Phase Space-

In Classical Mechanics,



When Particle is in motion



$$\frac{dx}{dt} = \dot{x}$$

$$\frac{dy}{dt} = \dot{y}$$

$$\frac{dz}{dt} = \dot{z}$$

Momentum $P_x = m\dot{x}$, $P_y = m\dot{y}$, $P_z = m\dot{z}$ } Momentum coordinates

$x \quad y \quad z$

$P_x \quad P_y \quad P_z$ } 6 dimentional Phase space

In classical mechanics, the state of a system of particles at any given time is completely specified by the knowledge of Position and momentum (or velocity) of each of the particle. The instantanous position of a single particle is determined by 3 independent coordinates x, y, z and instantanous motion of

a particle is described by velocity component (v_x, v_y, v_z) or more conventiently by momentum (p_x, p_y, p_z). Therefore the state of a single particle is then completely specified by position coordinates x, y, z and momentum coordinates p_x, p_y, p_z. As a purely mathematical concept we may imagine 6 dimensional space in which $dx\,dy\,dz\,dp_x dp_y dp_z$ is an element of volume and position of a point particle in this space will be described by a set of 6 coordinates x, y, z, p_x, p_y, p_z. This six dimensional space for a single particle is termed as phase space, and particularly the μ-space.

If the system contains a large no. of particles such that the state of system is represented by f independent position coordinates $q_1, q_2, q_3 \ldots q_f$ and f momentum coordinates $p_1, p_2, \ldots p_f$, then mathematically these $2f$ combined position momentum coordinate may be allowed to define $2f$ dimentional space in which the configuration of the system is represented by $2f$ coordinates i.e. $q_1, q_2, q_3, \ldots q_f; p_1, p_2 \ldots p_f$. This $2f$ dimentional space is called Phase-space or Γ-space.

#Entropy–

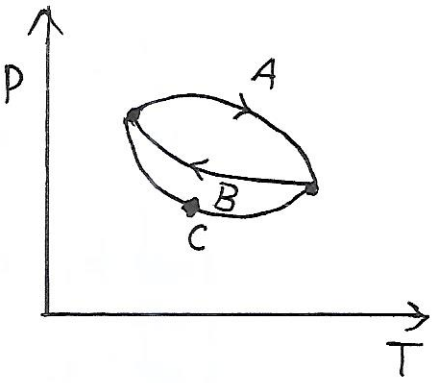
→ In statistical Mechanics, entropy is an extensive property of a thermodynamical system.

→ Thermodynamic entropy is a part of science of heat energy. It is a measure of how organise and disorganise energy is in a system of atom and molecule.

→ symbol S

→ Unit JK^{-1}

→ Clausius explain the entropy is a measure of variable of heatenergy per change in work. It can't be defined directly. Thus to explain the term entropy, we take the help of term "change in entropy". Generally it is denoted by S. If at absolute temp. T, The amount of Heat Q is either absorbed or given to a gas.

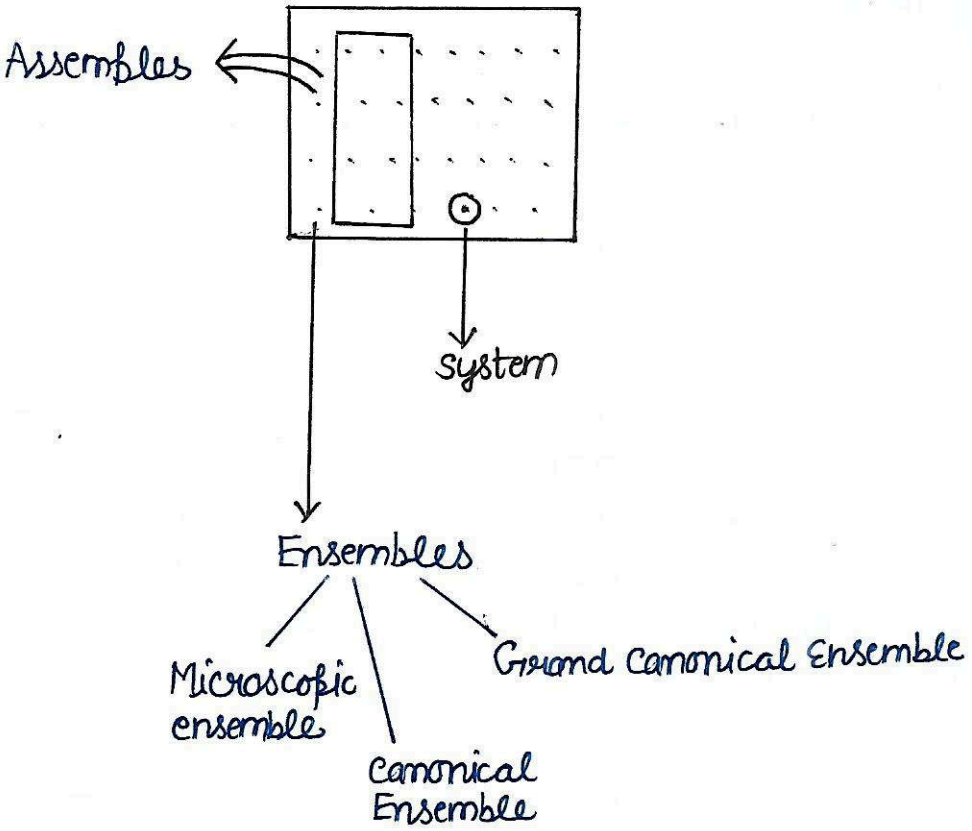


$$S = \frac{Q}{T} \quad \text{in reversible Process}$$

$$\text{Change in entropy } \Delta S = \int \frac{\Delta Q}{\Delta t}$$

$$\Delta S = \int \frac{dQ}{T}$$

Ensembles -



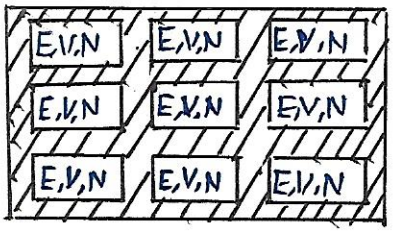
→ A system is defined as the collection of no. of particles but an ensemble is defined as collection of large no. of microscopic identical and esentially identical and independent systems.

→ It satisfies macro conditions like V, E, P, total no. of particle.

→ Identical means system's every system is identical

→ Independent means that the system is non-interacting.

Microscopic Ensemble

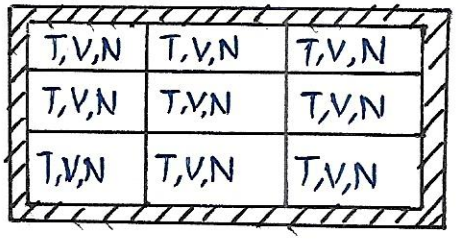


→ Collection of large number of independent system having same E,V,N.

→ All particles are identical

→ The individual systems are separated by rigid, impermeable and well insulated walls.

Canonical Ensemble

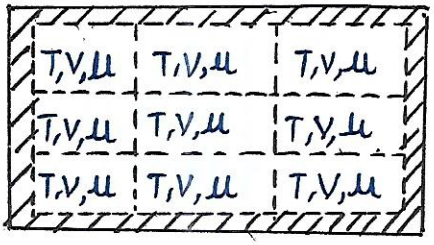


→ Collection of Large no. of systems having same T,V,N.

→ The equality of the temp of all the systems can be achieved by bringing each in thermal contact with a large heat reservoir at constant T.

→ All system are separated by rigid, impermeable but conducted Walls.

Grand Canonical Ensemble



→ Collection of large no of independent system having T,V, μ

→ As the separation walls are conducting and permiable, the exchange of heat energy as well as that the of particles b/w the systems take place in such a way that the all the system arrive at common T and μ chemical potential μ. These ensemble can be had after a complete study of Liouville's Theorem.

Degree of freedom-

→ It is defined as the smallest no. of independent Variables (such as temperature, pressure and concentration) that are required to define the system completely.

e.g. A system consisting of one phase of water (Solid, liquid, Gas) requires temperature and pressure to be specified to define the state of system completely and hence it has two dof.

Chemical Potential-

The workdone in bringing a change from a position of potential V_1 to a potential V_2 is a given by

$$W = q(V_2 - V_1)$$

↑ Capacity factor

Similarly, we define the capacity and potential quantities for a chemical system in which mole is taken as the capacity factor and molal free energy as the potential. This molal free energy is called Chemical Potential.

$$W = n(F_2 - F_1)$$

F_2 → State 1 of molal free energy

F_1 → State 2 of molal free energy

Let us consider any thermodynamic property for homogenous system. Thus extensive property X may be represented as

$$X = f(T, P, \underbrace{N_1, N_2, N_3, \ldots, N_i}_{\text{No. of moles.}})$$

Then the change in dX, then the extensive property can be written

$$dX = \left(\frac{\partial X}{\partial T}\right)_{P,N_1,N_2} dT + \left(\frac{\partial X}{\partial P}\right)_{T,N_1,N_2} dP + \left(\frac{\partial X}{\partial N_1}\right)_{T,P,N_2} dN_1 + \left(\frac{\partial X}{\partial N_2}\right)_{T,P,N_1} dN_1 \ldots$$

$$dX = \left(\frac{\partial X}{\partial T}\right)_{P,N_1,N_2} dT + \left(\frac{\partial X}{\partial P}\right)_{T,N_1,N_2} dP + \sum_i \left(\frac{\partial X}{\partial N_i}\right)_{T,P} dN_i \quad \ldots\ldots\ldots (1)$$

The internal energy of a system may be expressed

$$U = f(S, V, N_1, N_2, \ldots N_i)$$

For small change in entropy, Volume and composition

$$dU = \left(\frac{\partial U}{\partial S}\right)_{V,N_1,N_2} dS + \left(\frac{\partial U}{\partial V}\right)_{S,N_1,N_2} dV + \left(\frac{\partial U}{\partial N_1}\right)_{V,S,N_2} dN_1 + \left(\frac{\partial U}{\partial N_2}\right)_{S,V,N_1} dN_2 + \ldots$$

$$dU = \left(\frac{\partial U}{\partial S}\right)_{V,N_1,N_2} dS + \left(\frac{\partial U}{\partial V}\right)_{S,N_1,N_2} dV + \sum_i^N \left(\frac{\partial U}{\partial N_i}\right)_{S,V} dN_i \quad \ldots\ldots (2)$$

When the composition is constant,
Then,

$$dU = T\,dS - P\,dV \quad \ldots\ldots (2)$$

comparing eq^n ② & ③

$$T = \left(\frac{\partial U}{\partial S}\right)_{V,N_1,N_2}$$

$$P = -\left(\frac{\partial U}{\partial V}\right)_{S,N_1,N_2}$$

Now we introduce a new system μ_i to a partial derivative.

$$\left(\frac{\partial U}{\partial N_i}\right)_{S,N_i} dN_i = \mu_i$$

μ_i → Chemical Potential in the form of Halmoltz free energy (F)

$$F = f(T, V, N_1, N_2, \ldots N_i)$$

so

$$\mu_i = \left(\frac{\partial F}{\partial N_i}\right)_{T,V,N_i}$$

Which predicts the chemical potentials are the rate of change in free energy per mole at constant temperature & Pressure.

Maxwell Boltzmann Distribution/Statistics-

Let the Identical, distinguisible particle obey maxwell-Boltzmann distribution Law which tells us how a total fixed amount of energy is distributed among the various members of the assembly of identical particles in the most probable distribution.

Let us consider a system of particles $n_1, n_2, \ldots n_K$ having energy $\varepsilon_1, \varepsilon_2, \ldots \varepsilon_N$

The total no. of particles is constant i.e.

$$N = n_1 + n_2 + n_3 + \ldots + n_K = \text{Constant} \quad \text{——— (1)}$$

$$\delta N = \delta n_1 + \delta n_2 + \delta n_3 + \ldots + \delta n_K = 0$$

$$\sum_i \delta n_i = 0 \quad \ldots\ldots\ldots\ldots\ldots\ldots (2)$$

The total energy of the system is constant i.e.

$$E = \varepsilon_1 n_1 + \varepsilon_2 n_2 + \ldots\ldots + \varepsilon_K n_K = \text{Constant} \quad \ldots\ldots (3)$$

$$\delta E = \delta\varepsilon_1 \delta n_1 + \delta\varepsilon_2 \delta n_2 + \ldots\ldots + \delta\varepsilon_K \delta n_K = 0$$

$$\sum \varepsilon_1 \delta n_i = 0 \quad \ldots\ldots\ldots\ldots (4)$$

When the gas is in equilibrium, the probability is maximum.

$$\delta P = 0$$

When P is maximum, log P is maximum

$$\delta(\log P) = 0$$

But $P = \dfrac{N!}{n_1! n_2! \ldots n_k!} g_1^{n_1} g_2^{n_2} g_3^{n_3} \ldots g_K^{n_K} \quad \ldots\ldots\ldots (5)$

g_i is Prior probability.

Taking natural log of this equation

$$\log P = \log N! - \log n_i! + n_i \log g_i$$

Using stiriling formula

$$\log P = N \log N - N - \sum_i n_i \log n_i + \boxed{n_i} + n_i \log g_i$$

$\boxed{n_i} \rightarrow N$

$$\log P = N\log N - \sum_i n_i \log n_i + \sum_i n_i \log g_i$$

$\downarrow \delta$

According to eq^n(5), we get

$$\delta(\log P) = -\sum_i n_i\, \delta(\log n_i) - \sum \log n_i \delta n_i + \sum \log g_i \delta n_i = 0 \quad \ldots\ldots(6)$$

But $\delta(\log n_i) = \dfrac{1}{n_i}\, \delta n_i$

$$n_i\, \delta(\log n_i) = \delta n_i$$

$$n_i \delta(\log n_i) = \delta n_i = 0 \quad [\because \text{from eq}^n(1)]$$

Therefore from eq^n(6)

$$\sum_i \log n_i \delta n_i - \sum_i \log g_i \delta n_i = 0 \quad \ldots\ldots\ldots(7)$$

Let us consider α, β are two undeterminstic quantities

$$\sum_i \log n_i \delta n_i - \sum_i \log g_i \delta n_i + \sum_i \delta\alpha n_i + \sum_i \beta\epsilon_i \delta n_i = 0$$

$$\sum_i \left[\log n_i - \log g_i + \alpha + \beta\epsilon_i\right] \delta n_i = 0$$

Then

$$\log n_i - \log g_i + \alpha + \beta\epsilon_i = 0$$

Take antilog

$$n_i - g_i + e^{\alpha} + e^{+\beta\epsilon_i} = 0$$

$$\boxed{n_i = g_i e^{-\alpha} e^{-\beta\epsilon_i}}$$

This result determines the most probable distribution of molecules among the various possible individual states and is known as Maxwell Boltzmann distribution Law.

• Drawbacks of Maxwell Boltzmann Statistics-

→ To derive particle speed in an ideal gas
→ Temp. is high
→ Density is low
→ Expected no. of particles with energy

$$\frac{\langle N_i \rangle}{N} = \frac{g_i}{e^{(\varepsilon_i - \mu)/KT}} = \frac{1}{Z} g_i e^{-\varepsilon_i/KT}$$

(g_i → degeneracy; Temp.)

Avarage no. of Particles; Total no of Particles; Chemical Potential; Boltzmann constant

→ Provide non-physical result for entropy.
→ No real particle
→ Useful for gases that are not very dense.

Bose-Einstein ~~con~~ distribution-

Identical and Indistinguishable particles of zero or integral spin. The helium atoms at low temperature and the photons are the particles of this kind. This particles are called Bosons and do not obey the pauli Exclusion principle.

In maxwell Boltzmann statistics, the particles are distinguishable from each other. Thus if the particles interacting their position or energy state, a new state is generated. But in the case of BE statistics, the particles are indistinguishable so the interchange of two particles between two energy state will not produce any new state.

We consider a general case!

Approximate constant energies $\varepsilon_1, \varepsilon_2, \varepsilon_3 \ldots \varepsilon_i$ respectively
occupation number $n_1, n_2, n_3 \ldots n_i \ldots n_K$
Degeneracy $g_1, g_2, g_3 \ldots g_i \ldots g_K$

In case of ~~boltzmann~~ Bose Einstein statistics, we have the problem of assiging n indistinguishable particle to g_i distinguishable levels when there is no restrictions as to the no. of particles that can occupy one level.

Thus in B.E. statistics, the conditions are;

1. The particles are indistinguishable from each other so that there is no distinction between the different ways in which n_i particles can be choosen.
2. Each cell or sublevel of ith quantum state may contain 0,1,2.. n_i identical particles.
3. The sum of energies of all the particles in the different quantum groups, taken together constitutes the total energy of the system.

Let us imagine a box.

#g_i sections
g_i ways of distribution
(g_i-1) Remaining compartments
$(n_i+g_i-1)!$ no. of ways

$$\text{distribution} = g_i(n_i+g_i-1)! \quad \ldots\ldots\ldots (1)$$

$$\text{No. of ways} = \frac{g_i(n_i+g_i-1)!}{n_i!\,g_i!}$$

$$G_1 = \frac{(n_i+g_i-1)!\,g_i}{n_i!\,g_i(g_i-1)!}$$

$$G_1 = \frac{(n_1+g_1-1)!}{n_1!(g_1-1)!} \times \frac{(n_2+g_2-1)!}{n_2!(g_2-1)!} \times \ldots\ldots$$

$$G_1 = \sum \frac{(n_i+g_i-1)!}{n_i!(g_i-1)!}$$

Postulate of prior postulate

$$W = G_1 \times \text{Constant}$$

$$\omega = G \times \text{constant}$$

$$\omega = \frac{(n_i+g_i-1)!}{n_i!(g_i-1)!} \times \text{constant}$$

taking log into both sides

$$\log \omega = \sum_i \left[\log(n_i+g_i-1)! - \log n_i - \log(g_i-1)! \right] + \text{constant}$$

Using stirling Approximation

$$\log \omega = \sum_i \left[(n_i+g_i)\log(n_i+g_i) - \cancel{n_i} - \cancel{g_i} - n_i \log n_i + \cancel{n_i} - g_i \log g_i + \cancel{g_i} \right] + C$$

diff^n $\longrightarrow$

$$\delta \log \omega = \sum_i \left[(n_i+g_i)\log(n_i+g_i) - n_i \log n_i - g_i \log g_i \right] + C$$

$g_i \longrightarrow$ constant, $\Downarrow$ 0

$$\delta \log \omega = \sum_i \left[\delta n_i \log(n_i+g_i) + \frac{\cancel{(n_i+g_i)}}{\cancel{(n_i+g_i)}} \delta \cancel{n_i} - \delta n_i \log n_i - \frac{\cancel{n_i}}{\cancel{n_i}} \delta \cancel{n_i} \right] + \cancel{C}$$

$$\delta \log \omega = \sum_i \left[\delta n_i \log(n_i+g_i) - \delta n_i \log n_i \right]$$

$$\delta \log \omega = \sum_i \left[\log \left[\frac{n_i}{n_i+g_i} \right] \right] \delta n_i$$

n is constant

$(\delta n_i = 0) \times \alpha$

E is constant

$(\delta E = \sum E_i \delta n_i = 0) \times \beta \epsilon_i$

$$\sum_i \left[\log \left(\frac{n_i}{n_i+g_i} \right) + \alpha + \beta \epsilon_i \right] \delta n_i = 0$$

$$\log \left(\frac{n_i}{n_i+g_i} \right) = e^{-\alpha} e^{-\beta \epsilon_i}$$

$$\frac{n_i+g_i}{n_i} = e^{\alpha + \beta \epsilon_i}$$

$$1+\frac{g_i}{n_i}=e^{\alpha+\beta\epsilon_i}$$

$$\frac{g_i}{n_i}=-1+e^{\alpha+\beta\epsilon_i}$$

$$\boxed{n_i=\frac{g_i}{e^{\alpha+\beta\epsilon_i}-1}}$$

Fermi Dirac Distribution/Statistics-

(g_i-1) ways

$$G_1=\frac{g_i!}{n_i!(g_i-n_i)!}$$

$$\omega = C\times G=\sum\frac{g_i!}{n_i!(g_i-n_i)!}\times \text{constant}$$

Take log into both sides

$$\log\omega=\sum[\log g_i!-\log n_i!-\log(g_i-n_i)!]+C$$

$$\log\omega=\sum[g_i\log g_i-g_i-n_i\log n_i+n_i-(g_i-n_i)\log(g_i-n_i)+g_i-n_i]+C$$

$$\log\omega=\sum[g_i\log g_i-n_i\log n_i+(n_i-g_i)\log(g_i-n_i)]+C$$

diff^n $\longrightarrow$ $g\longrightarrow$ constant

$$\delta\log\omega=\sum\left[\delta n_i\log(g_i-n_i)+\frac{(n_i-g_i)}{(g_i-n_i)}\delta n_i-\delta n_i\log n_i-\frac{n_i}{n_i}\delta n_i\right]$$

$$\delta\log\omega=[\log(g_i-n_i)-\log n_i]\delta n_i$$

$$\delta n_i[\log(g_i-n_i)-\log n_i]=0$$

$$\log\left[\frac{n_i}{g_i-n_i}\right]\delta n_i=0$$

$(\delta n=\delta n_i=0)\times\alpha$

$(\delta E=\delta n_i\delta\epsilon_i=0)\times\beta$

$$\left[\log \frac{n_i}{g_i - n_i} + \alpha + \beta \epsilon_i\right] = 0$$

$$\log \frac{n_i}{g_i - n_i} = e^{-\alpha - \beta \epsilon_i}$$

$$\frac{n_i}{g_i - n_i} = e^{-(\alpha + \beta \epsilon_i)}$$

$$\frac{g_i - n_i}{n_i} = e^{\alpha + \beta \epsilon_i}$$

$$\boxed{n_i = \frac{g_i}{e^{\alpha + \beta \epsilon_i + 1}}}$$

Bose Einstein Condensation -

The equation of gas degeneracy is taken. Bose Einstein condensation was first predicted by S.N. Bose and A. Einstein in 1925. In 1955, the first gas of BE condensation was produced.

For an Ideal Bose gas, N particles in a volume V, the most probable no. of particles

$$n_i = \frac{g_i}{e^{\alpha + \beta \epsilon_i} - 1}$$

$$\alpha = \frac{\mu}{KT}$$

$$\beta = \frac{1}{KT}$$

$$n_i = \frac{g_i}{e^{(\epsilon_i - \mu/KT)} - 1}$$

$$N = \sum_i n_i = \sum \frac{g_i}{e^{\alpha + \beta \epsilon} - 1}$$

$$N = \int_0^\infty \frac{g(\epsilon)\, d\epsilon}{e^{\alpha + \beta \epsilon} - 1}$$

$$g(\epsilon)d\epsilon = 2\pi V\left(\frac{2m}{h^2}\right)^{3/2} \epsilon^{1/2}\, d\epsilon$$

Put in eqn

$$N = 2\pi V\left(\frac{2m}{h^2}\right)^{3/2} \int_0^{\infty} \frac{\epsilon^{1/2}\, d\epsilon}{e^{\alpha} e^{\beta\epsilon} - 1}$$

Let $Z = e^{-\alpha}$

$$N = 2\pi V\left(\frac{2m}{h^2}\right)^{3/2} \int_0^{\infty} \frac{\epsilon^{1/2}\, d\epsilon}{\frac{1}{Z} e^{\beta\epsilon} - 1}$$

Put $\beta\epsilon = x$

$$\beta = \frac{1}{KT}$$

$$\frac{\epsilon}{KT} = x$$

$$\epsilon = xKT$$

$$d\epsilon = KT\, dx$$

$$N = 2\pi V\left(\frac{2m}{h^2}\right)^{3/2} \int_0^{\infty} \frac{x^{1/2}(KT)^{1/2} KT\, d\epsilon}{\frac{1}{Z} e^{x} - 1}$$

$$N = 2\pi V\left(\frac{2m}{h^2}\right)^{3/2} (KT)^{3/2} \int_0^{\infty} \frac{x^{1/2}\, dx}{\frac{1}{Z} e^{x} - 1}$$

$$N = V\left(\frac{2\pi m KT}{h^2}\right)^{3/2} \left[\frac{2}{\sqrt{\pi}} \int_0^{\infty} \frac{x^{1/2}\, dx}{\frac{1}{Z} e^{+x} - 1}\right]$$

$$N = V\left(\frac{2\pi m KT}{h^2}\right)^{3/2} B(Z) \quad \ldots\ldots (1)$$

$$B(z) = \frac{2}{\sqrt{\pi}} \int_0^{\infty} \frac{x^{1/2}\, dx}{\frac{1}{z} e^{+x} - 1}$$

$$B(z) = \frac{2}{\sqrt{\pi}} \int_0^{\infty} \frac{z x^{1/2} dx}{e^{x} - z}$$

$$B(z) = \frac{2}{\sqrt{\pi}} \int_0^{\infty} \frac{z x^{1/2} dx}{e^{x}(1 - e^{-x} z)}$$

$$B(z) = \frac{2}{\sqrt{\pi}} \int_0^{\infty} z e^{-x} x^{1/2} (1 - z e^{-x})^{-1}$$

$$B(z) = \frac{2}{\sqrt{\pi}} \int_0^{\infty} z e^{-x} x^{1/2} dx (1 + z e^{-x} + z e^{-2} + z e^{-3} + \ldots)$$

$$B(z) = \frac{2}{\sqrt{\pi}} \int_0^{\infty} z e^{-x} x^{1/2} dx + \frac{2}{\sqrt{\pi}} \int_0^{\infty} z^2 e^{-2x} x^{1/2} dx + \ldots\ldots$$

$$B(z) = z + \frac{z^2}{2^{3/2}} + \frac{z^3}{3^{3/2}} + \ldots\ldots$$

$$B(z) = \sum_{n=1}^{\infty} \frac{z^n}{n^{3/2}}$$

At limiting maximum

$$B(z) = \frac{1}{n^{3/2}}$$

$$B = 1 + \frac{1}{2^{3/2}} + \frac{1}{3^{3/2}}$$

$$B = 2.612 \ldots\ldots\ldots (2)$$

From eqn (1) & (2)

$$T = T_b$$

$$N = V\left(\frac{2\pi mKT_b}{h^2}\right)^{3/2} \times 2.612$$

$$\left(\frac{2\pi mKT_b}{h^2}\right)^{3/2} = \frac{N/V}{2.612}$$

$$T_b = \frac{h^2}{2\pi mK}\left(\frac{1}{2.612}\right)^{2/3}\left(\frac{N}{V}\right)^{2/3}$$

↓

Bose Temp.

$T < T_b$

$T \downarrow \quad N \downarrow$

$E = 0$

$T > T_b$

The particle tends to occupy space.

$$N = N_0 + N_e$$

$$N_e = N - N_0$$

$$N_e = V\left(\frac{2\pi mKT}{h^2}\right)^{3/2} \times 2.612$$

$$\frac{N_e}{N} = \left(\frac{T}{T_b}\right)^{3/2}$$

$$N_0 = N - N_b$$

$$\boxed{N_0 = N\left[1 - \left(\frac{T}{T_b}\right)^{3/2}\right]}$$

Plank, Wein, Rayleigh, Stefan's Law using BE distribution-

$$g(p)dp = \frac{4\pi p^2 dp}{h^3/V}$$

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

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

$$dp = h\frac{d\nu}{c}$$

$$g(\nu)d\nu = \frac{4\pi V}{h^3} \cdot \frac{h^2\nu^2}{c^2} \frac{h}{c} d\nu$$

$$g(\nu)d\nu = \left(\frac{4\pi V \nu^2 d\nu}{c^3}\right) \times 2 = \frac{8\pi V \nu^2 d\nu}{c^3}$$

$$dn = \frac{g(\nu)d\nu}{e^{\alpha+\beta\epsilon}-1}$$

$$dn = \frac{8\pi V \nu^2}{c^3} \frac{d\nu}{e^{\alpha+\beta\epsilon}-1}$$

$$\frac{dn}{V} = \frac{8\pi \nu^2}{c^3} \frac{d\nu}{e^{\alpha+\beta\epsilon}-1}$$

$$\left[hc\frac{dn}{V} = u_\nu d\nu\right]$$

$$u_\nu d\nu = h\nu \frac{8\pi\nu^2}{c^3} \frac{d\nu}{e^{\alpha+\beta\epsilon}-1}$$

$$\beta = \frac{1}{KT}, \alpha = 0$$

$$\boxed{u_\nu d\nu = \frac{8\pi\nu^3 h}{c^3} \frac{d\nu}{e^{h\nu/KT}-1}}$$

Plank Law

$h\nu << KT$

$$u(\nu)d\nu = \frac{8\pi\nu^3 h}{c^3}\frac{d\nu}{h\nu/KT}$$

$$\boxed{u(\nu)d\nu = \frac{8\pi\nu^2 KT}{c^3}\,d\nu}$$ Rayleigh Law

$h\nu >> KT$

$$\boxed{(u)\nu\, d\nu = \frac{8\pi\nu^3 h}{c^3}\, e^{-hc/KT}\, d\nu}$$ Wein's Law

$$\frac{U}{V} = \frac{8\pi h}{c^3}\left(\frac{KT}{h}\right)^4 \frac{\pi^4}{15}$$

$$\frac{U}{V} = \sigma T^4$$

$$\boxed{E = \sigma T^4}$$ Stefan's Law

Gibb's Paradox-

- Paradox- A paradox is a statement in which it seems that if one part of its true then other part of it is not true.

- Gibb's Paradox-

The Partition function of a perfect gas

$$Z = \frac{V}{h^3}(2\pi mKT)^{3/2} \quad \ldots\ldots\ldots (1)$$

Entropy of perfect gas

$$S = NK\log Z + \frac{3}{2}NK \quad \ldots\ldots\ldots (2)$$

substituting the value of Z

$$S = NK\log\left[\frac{V}{h^3}(2\pi mKT)^{3/2}\right] + \frac{3}{2}NK$$

$$S = NK\left[\log V + \frac{3}{2}\log m + \frac{3}{2}\log T + C\right] \quad \ldots\ldots (3)$$

C: constant part for h and K

The entropy given by above eqn does not satisfy additional property.

Consider two system denoted by a & b at same temp.

$$T_a = T_b = T$$

a		b
N_a, V_a, T		N_b, V_b, T
m_a, S_a		m_b, S_b

Parameters sepated by a barrier as shown in figure. If the particle of two system are different then using eqn (3), the entropy of system a and b are given by

$$S_a = N_aK\left[\log V_a + \frac{3}{2}\log m_a + \frac{3}{2}\log T_a + C\right] \quad \ldots\ldots (4)$$

$$S_b = N_bK\left[\log V_b + \frac{3}{2}\log m_b + \frac{3}{2}\log T_a + C\right] \quad \ldots\ldots (5)$$

Where N_a, N_b = No. of Particles
V_a, V_b = Volume of systems
m_a, m_b = mass of system

As the entropy is extensive property, it must satisfy the additional properties.

$$S_{ab} = S_a + S_b$$

$$S_{ab} = N_aK\left[\log V_a + \frac{3}{2}\log m_a + \frac{3}{2}\log T_a + C\right] + N_bK\left[\log V_b + \frac{3}{2}\log m_b + \frac{3}{2}\log T_b + C\right]$$

Take $V_a = V_b = V$

~~$m_a = m_b = m$~~

$N_a = N_b = N$

$S_a = S_b = S$

$S_{ab} = 2NK$

$$S_a = S_b = N_K \left[\log V + \frac{3}{2} \log m + \frac{3}{2} \log T + C \right] \quad \ldots\ldots (6)$$

Thus the entropy of combined system

$$S_{ab} = S_a + S_b$$

$$S_{ab} = 2N_K \left[\log V + \frac{3}{2} \log m + \frac{3}{2} \log T + C \right] \quad \ldots\ldots (7)$$

Now we find the actual entropy of combined system using eq^n(3). Let the partition be removed to allow the molecular of gas to mixed free. Now, we consider the mixed system having 2N particles in volume 2V. Using eq^n (3)

$$S_{ab} = 2NK \left[\log 2V + \frac{3}{2} \log m + \frac{3}{2} \log T + C \right]$$

$$S_{ab} = 2NK \left[\log V + \frac{3}{2} \log m + \frac{3}{2} \log T + C \right] + 2N_K \log 2$$

↑ The entropy of joint system may be obtained.

$$S_{ab} = S_a + S_b + 2N_K \log 2 \quad \ldots\ldots (8)$$

Which is not equal to eq^n (7). $2NK \log 2$ indicates that by mixing diff. gases. Each containing same no. of molecules and by the entropy of joint system increased by multiple of $2NK \log 2$. This addition entropy is called the entropy of mixing. Thus if we use eq^n (3) for entropy, we get Paradox result. Entropy being an extensive therodynamical function, this particular behaviour of entropy gives gibb's Paradox.

#Sackur Tetrode Equation-

The entropy of a substance is given by

$$S = k \ln \Omega \quad \ldots\ldots (1)$$

Where Ω is the no. of microstate accessible to substance

For a 3D Ideal Gas

$$\Omega = \frac{V^N (2\pi m U)^{3N/2}}{h^{3N} N! (3N/2)!} \quad \ldots\ldots (2)$$

Where V = Volume
U = Internal Energy
N = No. of molecule
m = Mass of single molecule
h = Plank constant

$$N! = \sqrt{2\pi N}\, N^N e^{-N} \quad \ldots\ldots (3)$$

$$\left(3N/2\right)! = \sqrt{3\pi N}\left(\frac{3N}{2}\right)^{3N/2} e^{-3N/2}$$

$$\text{Hence } \Omega = \frac{V^N (\pi m U)^{3N/2}\, 2^{3N}\, e^{5N/2}}{h^{3N}\sqrt{6}\; 3^{3N/2}\, \pi\, N^{5N/2}} + 1$$

Where N is very large we can throw away a couple of factor and take

$$\Omega = \frac{V^N (\pi m U)^{3N/2}\, 2^{3N}\, e^{5N/2}}{h^{3N}\, 3^{3N/2}\, N^{5N/2}}$$

$$\ln\Omega = N \ln\left(V\left(\frac{\pi m U}{3}\right)^{3/2}\left(\frac{2}{h}\right)^3 \frac{1}{N^{5/2}}\right) + \frac{5N}{2}$$

$$\ln\Omega = N\left[\ln\left(\frac{V}{N}\left(\frac{4\pi m U}{3N h^2}\right)^{3/2}\right) + \frac{5}{2}\right]$$

$$\boxed{S = K\ln\Omega = NK\left[\ln\left(\frac{V}{N}\left(\frac{4\pi m U}{3N h^2}\right)^{3/2}\right) + \frac{5}{2}\right]}$$

This is sackur Tetrode Equation.

Partition Function-

For developing the concept of Partition Function. Let us consider an assembly of gas molecule obeying classical statistics. Let the distribution of gas molecule be such that n_i molecule occupy the 1st state with energy b/w $\epsilon_i + d\epsilon_i$ and degeneracy g_i. Then from MB distribution law

$$n_i = g_i e^{-\alpha} e^{-\epsilon_i/KT} \quad \ldots\ldots (1)$$

$$n_i = g_i A e^{-\epsilon_i/KT} \qquad [\because e^{-\alpha} = A]$$

$$N = \sum_i n_i = \sum_i g_i A e^{-\epsilon_i/KT}$$

$$N = A \sum_i g_i e^{-\epsilon_i/KT} \quad \ldots\ldots (2)$$

$$\frac{N}{A} = \sum_i g_i e^{-\epsilon_i/KT} = Z \quad \ldots\ldots (3)$$

↓ Boltzmann Partition Function

$$Z = \sum_i e^{-\epsilon_i/KT}$$

$$g(p)dp = \frac{V \cdot 4\pi p^2 dp}{h^3}$$

$$g(\epsilon)d\epsilon = \frac{V \cdot 4\pi\, 2m\epsilon}{h^3} \cdot \frac{m d\epsilon}{\sqrt{2mE}}$$

$$g(\epsilon)d\epsilon = \frac{2\pi V}{h^3} (2m)^{3/2} \epsilon^{1/2} d\epsilon \quad \ldots\ldots (5)$$

$$Z = \sum_i g_i e^{-\epsilon_i/KT}$$

$$Z = \int_0^\infty \frac{2\pi V}{h^3} (2m)^{3/2} \epsilon^{1/2} d\epsilon \cdot e^{-\epsilon_i/KT}$$

$$Z = \frac{2\pi V (2m)^{3/2}}{h^3} \int_0^\infty \epsilon^{1/2} e^{-\epsilon_i/KT} d\epsilon$$

$$\boxed{Z = \frac{2\pi V (2m)^{3/2}}{h^3} \frac{\sqrt{\pi}}{2} (KT)^{3/2}}$$

Atomic and Molecular Physics

- Atomic Spectroscopy
- Molecular Spectroscopy

- Important Questions
  - LS and jj coupling
  - H_α line Fine Structure
  - Raman Effect
  - Stark Effect
  - Born Oppenheimer Approximation
  - Heilter London Treatment
  - Zeeman Effect
  - Frank Condon Principle and Condon Parabola
  - Spin Orbit Interaction
  - Pauli Exclusion Principle
  - Pure Rotational/Vibrational Spectra

Atomic Spectroscopy

#Fine structure of Hydrogen Lines - 4

The first order perturbation corrections due to different effects combine linearly. Therefore, the net term-shift due to spin orbit interaction and the relativistic effect in a Hydrogen-like atom is

$$\Delta T = \Delta T_{l,s} + \Delta T_r$$

$$\Delta T = ?$$

→ SPIN ORBIT INTERACTION

$$\Delta T_{l,s} = -\frac{\Delta E_{l,s}}{hc}$$

$$\Delta T_{l,s} = \frac{R_\infty \alpha^2 Z^4}{2n^3 l\left(l+\frac{1}{2}\right)(l+1)}\left[j(j+1)-l(l+1)-s(s+1)\right]$$

→ QUANTUM-MECHANICAL RELATIVITY CORRECTION

$$\Delta T_r = -\frac{\Delta E_r}{hc}$$

$$\Delta T_r = \frac{R_\infty \alpha^2 Z^4}{n^3}\left[\frac{1}{l+\frac{1}{2}} - \frac{3}{4n}\right]$$

$$\Delta T = \frac{R_\infty \alpha^2 Z^4}{2n^3 l\left(l+\frac{1}{2}\right)(l+1)}\left[j(j+1)-l(l+1)-s(s+1)\right] + \frac{R_\infty \alpha^2 Z^4}{n^3}\left[\frac{1}{l+\frac{1}{2}} - \frac{3}{4n}\right]$$

$$\Delta T = \frac{R_\infty \alpha^2 Z^4}{n^3}\left[\frac{1}{l+\frac{1}{2}} - \frac{j(j+1)-l(l+1)-s(s+1)}{2l\left(l+\frac{1}{2}\right)(l+1)} - \frac{3}{4n}\right]$$

$$s = \frac{1}{2}$$

$$j = l + \frac{1}{2}$$

$$j = l - \frac{1}{2}$$

$$\Delta T = \frac{R_\infty \alpha^2 Z^4}{n^3}\left[\frac{1}{l+1} - \frac{3}{4n}\right]$$

$$\Delta T = \frac{R_\infty \alpha^2 Z^4}{n^3}\left[\frac{1}{l} - \frac{3}{4n}\right]$$

Since $j = l + \frac{1}{2}$ and $j = l - \frac{1}{2}$, the last two equation can be replaced by a single equation

$$\Delta T = \frac{R_\infty \alpha^2 Z^4}{n^3}\left[\frac{1}{j+\frac{1}{2}} - \frac{3}{4n}\right]$$

Where $K = j + \frac{1}{2}$

$$\Delta T = \frac{R_\infty \alpha^2 Z^4}{n^3}\left[\frac{1}{K} - \frac{3}{4n}\right]$$

This equ^n was independently obtained by Dirac from a completely relativistic quantum mechanical treatment of Hydrogen Atom obtained from atoms, and hence known as Dirac eq^n.

Let us now compare the energy levels of the Hydrogen Atom obtained from sommerfold's theory with dirac's theory.

$$\Delta T = \frac{5.84}{n^3}\left[\frac{1}{K} - \frac{3}{4n}\right]$$

$$\Delta T = \frac{5.84}{n^3}\left[\frac{1}{j\left(j+\frac{1}{2}\right)} - \frac{3}{4n}\right]$$

Here $R_\infty = 1.097 \times 10^7\ m^{-1}$

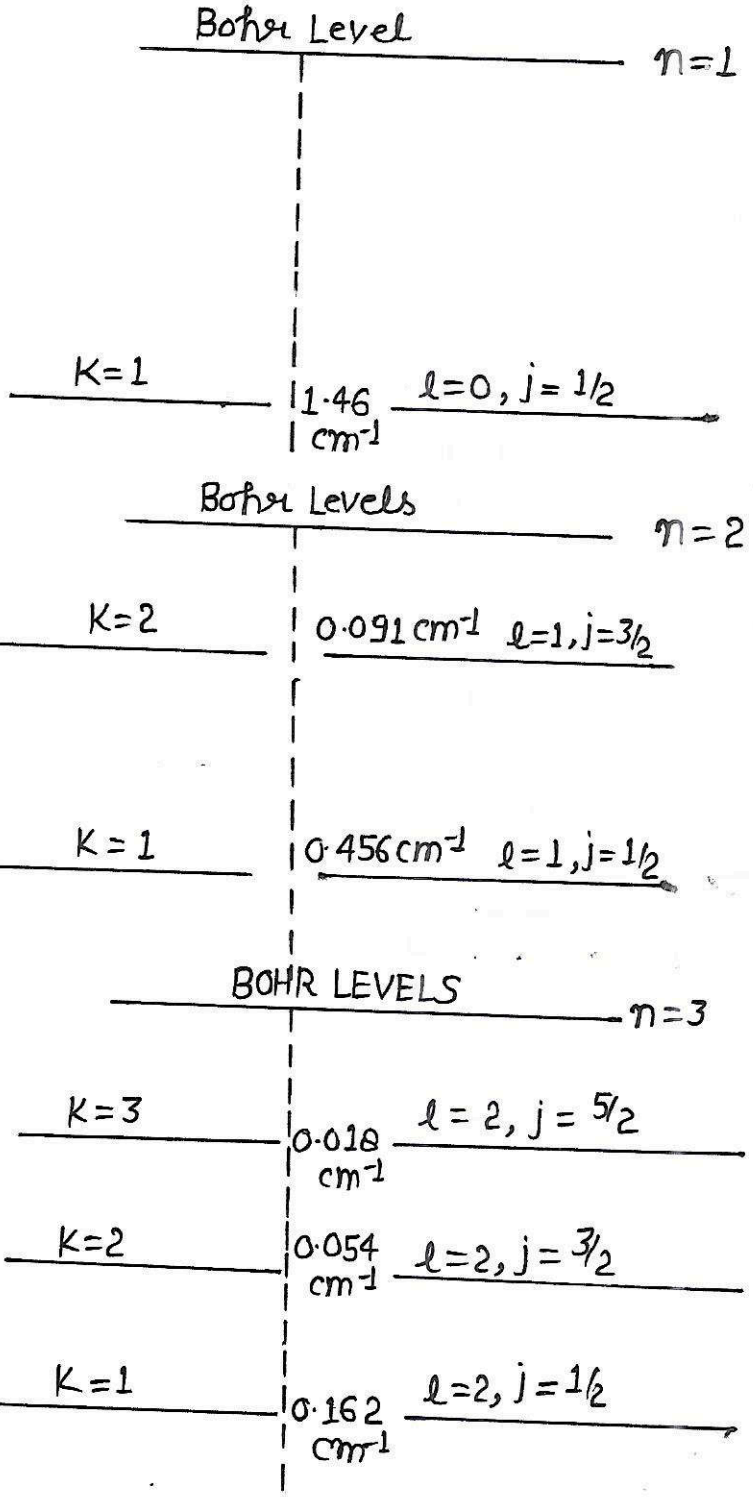
$\alpha = \frac{1}{137}$

$Z = 1$ (For H]

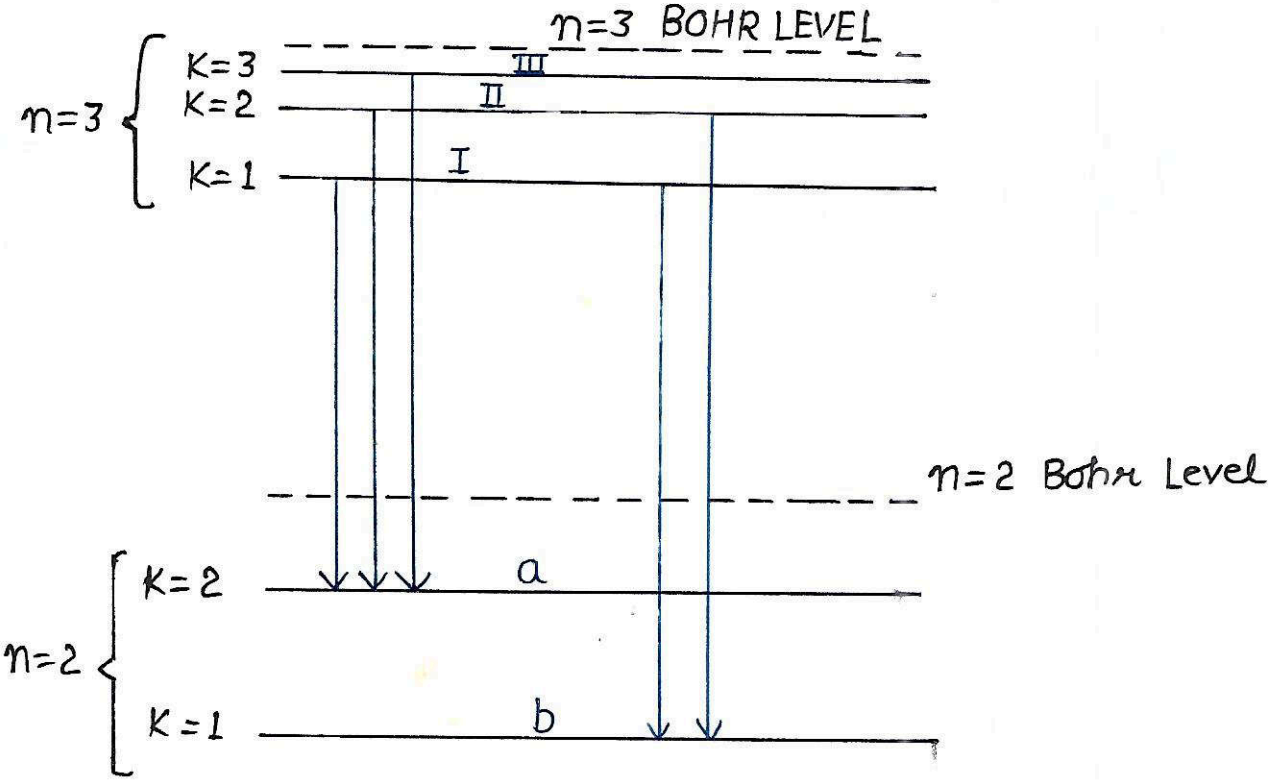
ΔT is a term shift from the Bohr level

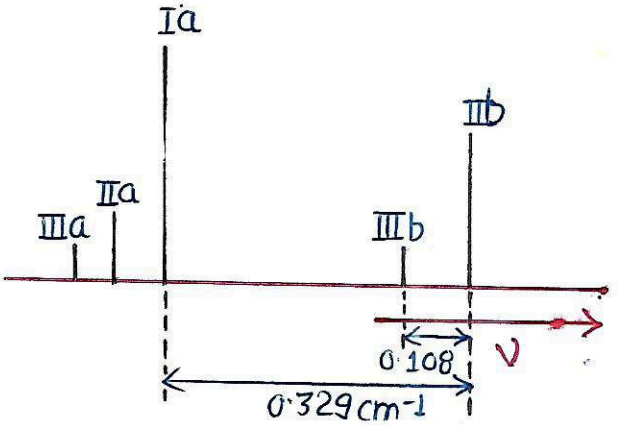
Bohr Level n	Sommerfeld Levels $\Delta T\,(cm^{-1})$	Dirac Levels $\Delta T\,(cm^{-1})$
1	1·46	1·46
2	0·091 0·456	0·091, 0·456 0·456
3	0·018 0·054 0·162	0·018, 0·054 0·054, 0·162 0·162

The energy Levels of Hydrogen Atom, as predicted by bohr, sommer-feld and dirac for $n=1,2,3$



We see that the energy levels due to sommerfeld and those due to dirac are esentially same. This coincidence occurs for the Hydrogen Atom because the errors made by sommerfeld in ignoring the spin orbit interaction and in using classical mechanics to evaluate the energy shift due to relativity happen to cancel for the case of Hydrogen Atom.
Let us consider the fine structure of H_α-lines ($n=3 \longrightarrow n=2$) on the basis of dirac theory.





This is theoritical structure of H_α as predicted by spin-relativity quantum mechanical theory.
Selection Rule for transition

$$\Delta l = \pm 1$$
$$\Delta j = 0, \pm 1$$

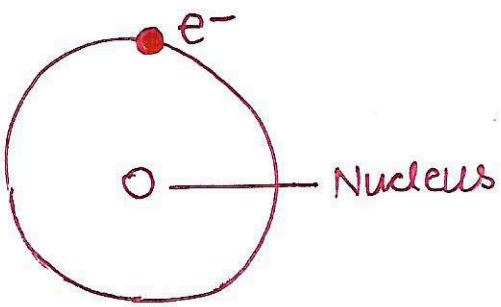
This rule allows 5 transitions as shown above in figure.

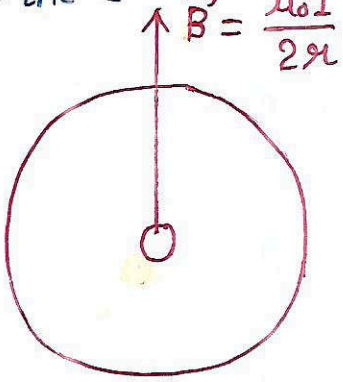
Spin-Orbit Interaction-[1]

Sommarfeld was the first who attempted to explain the observed fine structure of H_α lines. The mass of e^- is moving in elliptic orbits. As we have seen, sommerfeld was fairly successful in his mission. A more perfect account of observed fine structure is given by quantum mechanics taking spin orbit interaction as well as relativity correlation into account.

The spin-Orbit interaction is an interaction b/w e^- spin's magnetic dipole moment and the internal magnetic field of an atom which arises from the orbital motion of e^- through the nuclear electric field. Since the internal magnetic field is related to e^- orbital angular momentum, this is called spin-orbital interaction.

Suppose that we are in the reference frame of the e^-. The nucleus in such a case will be seen orbitting the e^-.





As the positively charged nucleus orbits the e^-, it creates a positive charge loop that in turn create a magnetic field $\vec{B}$. Each e^- has an intrinstic property called e^- spin that induces a spin angular momentum. The e^- spin also creates a spin magnetic dipole moment μ_S. Then it feels Torque and change the energy of e^-.

$$\Delta E = -\vec{\mu}_S \cdot \vec{B}$$

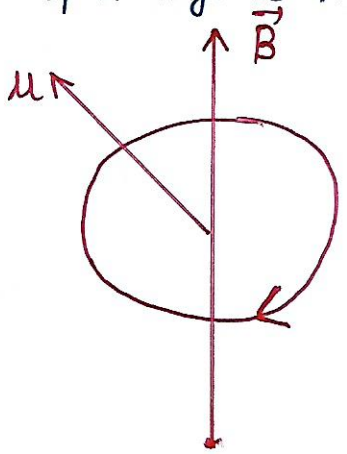
The relative motion of the nucleus of the atom creates a magnetic field that is related to orbital angular momentum ($\vec{L}$).

$$\vec{B} = \frac{\mu_0 Z_e \vec{L}}{4\pi m_e r^3}$$

The spin magnetic moment $\vec{\mu}_s$ is related to angular momentum $\vec{L}$.

$$\boxed{\Delta E \propto S \cdot \vec{L}}$$

The interaction b/w the orbital angular momentum of the nucleus and e^- spin angular momentum is known as spin orbit interaction.



$$\Delta U = -\vec{\mu} \cdot \vec{B}$$

Let us write the electric field $\vec{E}$, in which the e^- is moving, as a gradient of potential function $V(r)$.

$$\vec{E} = \text{grad } V(r)$$

$$\vec{E} = \frac{\vec{r}}{r} \cdot \frac{d(V(r))}{dr} \qquad \left[\because \text{grad } V(r) = \frac{\vec{r}}{r} \right]$$

Magnetic field

$$\vec{B} = \frac{1}{c^2} (\vec{E} \times \vec{v})$$

$$\vec{B} = \frac{1}{c^2 r} \frac{dV(\vec{r})}{dr} (\vec{r} \times \vec{v})$$

multiply m on both sides

$$m \cdot \vec{B} = \frac{1}{c^2 r} \frac{dV(\vec{r})}{dr} [m(\vec{r} \times \vec{v})]$$

$$\vec{B} = \frac{1}{mc^2} \frac{1}{r} \cdot \frac{d[V(\vec{r})]}{dr} \vec{L} \qquad \text{——— (1)}$$

Magnetic potential energy-

$$\Delta E_{l,s} = -\vec{\mu}_s \cdot \vec{B}$$

But

$$+\vec{\mu}_s = -g_s \left(\frac{e}{2m}\right)\vec{S} \quad \text{and } g_s = 2$$

$$\Delta E_{l,s} = +\cancel{g_s}\left(\frac{e}{\cancel{2}m}\right)\vec{S}\cdot\vec{B}$$

$$\Delta E_{l,s} = +\frac{e}{m}\vec{S}\cdot\vec{B}$$

$$\vec{B} = \Delta E_{l,s}\ \vec{S}^{-1}\left(\frac{m}{e}\right)$$

Put the value of $\vec{B}$ in eq^n(1)

$$\Delta E_{l,s}\ \vec{S}^{-1}\left(\frac{m}{e}\right) = \frac{1}{mc^2}\cdot\frac{1}{r}\frac{dV(r)}{dr}\vec{L}$$

$$\Delta E_{l,s} = \frac{e}{\cancel{2}m^2c^2}\frac{1}{r}\frac{dV(\vec{r})}{dr}\vec{S}\cdot\vec{L}$$

$$\Delta E_{l,s} = \frac{e}{2m^2c^2}\cdot\frac{1}{r}\frac{dV(\vec{r})}{dr}\vec{S}\cdot\vec{L} \qquad \text{——— (2)}$$

$$\vec{S}\cdot\vec{L} = \frac{1}{2}\left[\vec{J}\cdot\vec{J} - \vec{L}\cdot\vec{L} - \vec{S}\cdot\vec{S}\right] = \frac{1}{2}\left[J^2 - L^2 - S^2\right]$$

$$\vec{S}\cdot\vec{L} = \frac{1}{2}\left[j(j+1) - l(l+1) - s(s+1)\right]\frac{\hbar^2}{4\pi^2}$$

Then Put the value of $\vec{S}\cdot\vec{L}$ in eq^n (2)

$$\Delta E_{l,s} = \frac{e\hbar^2}{16\pi^2m^2c^2}\left[j(j+1) - l(l+1) - s(s+1)\right]\underbrace{\frac{1}{r}\frac{dV(\vec{r})}{dr}}$$

This term is not constant during the e⁻ motion.

This is the general expression of spin-orbit interaction energy of the atom. The avarage value of $\frac{1}{r}\frac{dV(\vec{r})}{dr}$ is calculated using $V(\vec{r})$.

$$\frac{dV(\vec{r})}{dr} = \frac{1}{4\pi\epsilon_0}\cdot\frac{Ze}{r^2} \quad \text{Hence} \quad \boxed{\Delta T = 5.84\frac{Z^4}{n^3l(l+1)}\ \text{cm}^{-1}}$$

Pauli Exclusion Principle-

When dealing with the hydrogen Atom which has only one (1) e^-, it is pretty simple to tell in which orbital the e^- will go; In the ground state, it will go to the most stable and lowest in energy quantum state given by

$$n=1,\ l=0,\ m_e=0,\ m_s=X$$

Where n = Principle qn
l = Orbital qn
m_e = magnetic qn
m_s = Spin qn

The individual e^- can then be characterized by four quantum number

$$n=1,2,3,\ldots\ldots,n$$
$$l=0,1,2,\ldots\ldots,n-1$$
$$m_e=-l,\ldots\ldots+l$$
$$m_s=\pm\frac{1}{2}$$

However for more complex atoms that have many e^-, it is difficult to know which e^- goes in which orbital. A rule was invented by Wolfgang Pauli, that becomes known as Pauli exclusion principle. It states that each e^- has a unique set of four quantum no. that describes its quantum state.

Why?

The basic of this principle lies in the fact that each e^- carries a negative charge. This means that e^- in close proximity will repel one another, leading to an increasing energy and instability Therefore e^- naturally want to be as far as possible from one another.

e.g.

determine the quantum state for all e^- in the ground state of boron.

In its neutral state,

$$^{10}_{5}B$$

Boron contains $5e^-$.

$$\hat{H} = \left\{\frac{-h^2}{8\pi^2 m}\nabla_1^2 + V\right\} + \left\{\frac{-h^2}{8\pi^2 m}\nabla_2^2 + V\right\}$$

$$\hat{H} = \hat{H}_1 + \hat{H}_2$$

$$\psi(1,2) = \psi(1)\psi(2)$$

$$\psi_{ab}(1,2) = \psi_a(1)\,\psi_b(2)$$

$$\psi_{ba}(1,2) = \psi_b(1)\,\psi_a(2)$$

$$\psi(1,2) = \frac{1}{\sqrt{2}}\left[\psi_a(1)\,\psi_b(2) \pm \psi_b(1)\,\psi_a(2)\right]$$

$$\psi_{BOSE}(1,2) \neq 0$$

$$\psi_{FERMI}(1,2) = 0$$

#	n	ℓ	m_e	m_s	
1	1	0	0	$+1/2$	$\rightarrow (1,0,0,+1/2)$
2	1	0	0	$-1/2$	$\rightarrow (1,0,0,-1/2)$
3	2	0	0	$+1/2$	$\rightarrow (2,0,0,+1/2)$
4	2	0	0	$-1/2$	$\rightarrow (2,0,0,-1/2)$
5	2	1	0	$+1/2$	$\rightarrow (2,1,0,+1/2)$

Notice that each one of the 5 e^- corresponds to the own unique set of four quantum number. This is in accordance with the Pauli exclusion principle.

> Hund's Rule-

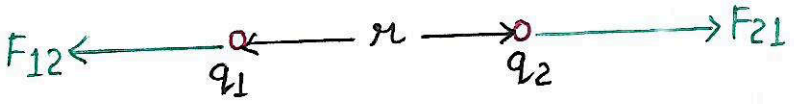
→ e^- configuration of Atoms

facts ?

- Opposite charges attaract each other.
- Like charges repel each other

Opposite charges will repel one another according to columb rule.

$$F = K\frac{q_1 q_2}{r_1^2}$$



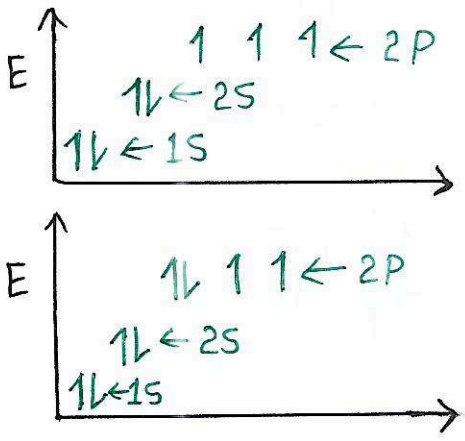
Placing e^- in the same orbital in a subshell will create repulsive force.

→ This is why a maximum of 2 e^- can go into an orbital.

→ Hund's rule states that e^- will not go into an occupied orbital until all orbitals in the subshell are filled.

$_7N$ $\quad 1s^2, 2s^2, 2p_x^1, 2p_y^1, 2p_z^1$

$_8O$ $\quad 1s^2, 2s^2, 2p_x^2, 2p_y^1, 2p_z^1$



According to Hund's rule, one e^- is placed in all the degenerate orbitals, such as p_x, p_y, p_z before a second e^- is placed in any of them, and that the electrons in the singly-occupied orbital have parallel spins.

Rule:

(1) For a given e^- configuration, the term with maximum multiplicity has the lowest energy.

$\uparrow$

$2S+1$

(2) For given multiplicity, L has lowest energy.

(3) $J = L+S$

$\downarrow$

J has lowest energy.

Central Field Approximation[1] → Hatress self consistent Theory[2]

Let us consider an atom or ion containing a nucleus of charge Z and N electrons.

It is clear that such a detailed study of many-electron atom is a very difficult task, in which approximations must be maide.

In what follow we will neglect columb attaractive force, repulsive force of e^-, spin orbit interaction, spin-spin Interaction.

Hamiltonian of N-electron atom in the absence of external field as

$$H = \sum_{i=1}^{N} \left(\frac{-\hbar^2}{2m} \nabla_{r_i}^2 - \frac{Ze^2}{4\pi\epsilon_0 r_i} \right) + \sum_{i<j=1}^{N} \frac{e^2}{4\pi\epsilon_0 (r_{ij})}$$

Where r_i = relative coordinate of e^-

$$H = \sum_{i=1}^{N} \left(-\frac{1}{2} \nabla_{r_i}^2 - \frac{Z}{r_i} \right) + \sum_{i<j=1}^{N} \frac{1}{r_{ij}}$$

Schrodinger equation of N electron Atom

$$\left[\sum_{i=1}^{N} \left(-\frac{1}{2} \nabla_{r_i}^2 - \frac{Z}{r_i} \right) + \sum_{i<j=1}^{N} \frac{1}{r_{ij}} \right] \psi(q_1, q_2, \ldots q_n) = E\psi(q_1, q_2, \ldots q_n)$$

Let us moment ignore the spin of electrons. The schrodinger eqn

$$H\psi(r_1, r_2, \ldots r_N) = E\psi(r_1, r_2 \ldots r_N)$$

Then

$$\left[\sum_{i=1}^{N}\left(-\frac{1}{2}\nabla_i^2 - \frac{Z}{r_i}\right) + \sum_{i<j=1}^{N}\frac{1}{r_{ij}}\right]\psi(r_1, r_2 \ldots r_N) = E\psi(r_1, r_2 \ldots r_N) \quad \text{---(1)}$$

This equation is partial differential equation in 3N dimensions involving the coordinates $r_1, r_2 \ldots r_N$ of the electrons. $1/r_{ij}$ represents the repulsive force b/w e⁻. This equation is not separate. $1/r_{12}$ can be treated by Perturbation Theory. $1/r_{ij}$ seems very large.

Thus if we want to apply Perturbation Theory in a meaningful way to present problem, we must define a new unperturbed Hamiltonian which is not just the sum of hydrogenic Hamiltonians repulsion b/w e⁻. On the other Hand it should be efficient. Thus an approximation is considered. This approximation is based on the independent particle model. A good approximation to be effective potential energy of an e⁻

$$V(r) = -\frac{Z}{r} + S(r)$$

Approximate Potential

$$-\frac{Z}{r_i} + \sum_{j=1}^{N-1}\frac{1}{r_i} = \frac{Z-N+1}{r_i}$$

$$-\frac{Z}{r_i} + \left\langle \sum_{j=1}^{N-1}\frac{1}{r_j} \right\rangle = -\frac{Z}{r_i} + C$$

Effective central potential

$$V(r) \longrightarrow -\frac{Z}{r_i}, \quad r \to 0$$

$$V(r) \longrightarrow \frac{Z-N+1}{r}, \quad r \to \infty$$

For neutral Atom $V(r) \longrightarrow -\frac{1}{r}, \quad r \to \infty$

Thus Put All the values in equation (1)

$$H_c \psi_c = \sum_{i=1}^{N} \left[-\frac{1}{2} \nabla_{r_i}^2 + V(r_i) \right] \psi_c = E_c \psi_c$$

$-\frac{1}{2} \nabla_{r_i}^2 + V(r_i)$ is the Hamiltonian corresponding to the central field Approximation.

$$E = \frac{-\mu e^4}{8 \epsilon_0^2 h^2}$$

Total energy of outermost shell

Hartree's self-consistent field Theory (Central field Approximation) is, however, not free from limitations.

(i) Hartree considered only the strongest interaction felt by the atomic electrons.

(ii) Having no definite symmetry.

> Thomas Fermi Statistical Model[1]

Determination of Potential $V(r)$ is the basic problem of central field Approximation. This problem will be analyzed by using two approaches. One is Hartree self consistent theory and other one is Thomas Fermi model, which is based on statistical and semi-classical considerations.

Before we analyse the theory developed by Thomas and Fermi for the ground state of multielectron, it is convenient to consider a simple problem of Fermi electron gas.

Suppose that there are N free electrons of our system are confined to a large cube of side L. Each of e^- is moving independently.

Schrodinger eq^n for free particles

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

$\psi = 0$ is boundary.

Eigenfunction for a spinless particle.

$$\psi_{n_x n_y n_z}(r) = C \sin\left(\frac{n_x \pi}{L} x\right) \sin\left(\frac{n_y \pi}{L} y\right) \sin\left(\frac{n_z \pi}{L} z\right)$$

Where $C = \left(\frac{8}{L^3}\right)^{1/2}$, normalized constant

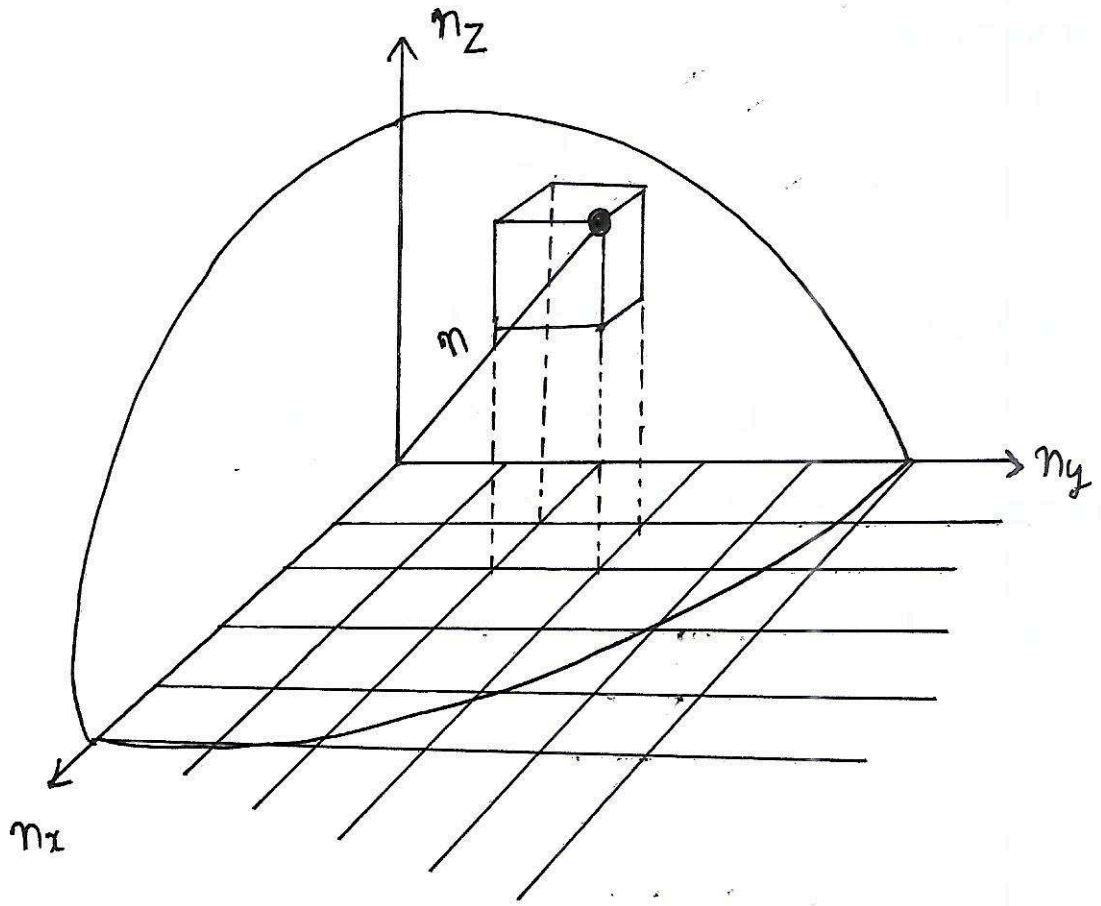
$$E = \frac{\pi^2 \hbar^2}{2mL^2}(n_x^2 + n_y^2 + n_z^2)$$

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

Where $n^2 = n_x^2 + n_y^2 + n_z^2$

Spin Orbitals

$$\psi_{n_x n_y n_z m_s} = \psi_{n_x n_y n_z}(r) \chi_{1/2\, m_s}$$



Hence Fermi Energy may be evaluated

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

$$D(E) = \frac{dN_S}{dE} = \frac{1}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} V E^{1/2}$$

The thomas-Fermi Theory for multielectron atom and ions developed independently by Thomas and Fermi for the ground state of complex atoms having a large number of electrons is based on statistical and semi-classical consideration. The N electrons of a system are treated as fermi electron gas in the ground state, confined to a region of space by a central potential $V(r)$ which vanishes at Infinite. It is assumed that the potential is slowly varying over a distance which is large compared to de broglie wavelength of the e⁻.

The Aim of the Thomas Fermi model is to provide a method of calculating the potential $V(r)$ and the electron density $\rho(r)$.

Total energy of e⁻

$$\left\{ \frac{p^2}{2m} + V(r) \right\}$$ and this energy can not be positive

Total energy of most energatic electron of the system

$$E_{max} = E_F + V(r) \quad \text{——— (1)}$$

E_{max} is independent to r. k_F is now a function of r.

$$k_F^2(r) = \frac{2m}{\hbar^2}\left[E_{max} - V(r)\right]$$

$$E_F = \frac{\hbar^2}{2m}(3\pi^2\rho)^{2/3}$$

Then

$$\rho(r) = \frac{1}{3\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\left[E_{max} - V(r)\right]^{3/2}$$

$$\phi(r) = -\frac{1}{e}V(r)$$

$$V(r) = \frac{-ze^2}{(4\pi\epsilon_0)r} \chi$$

The Spectra of Alkali -

The structure of the ground state of the alkali metals Li, Na and K is that of a single valance electron moving in an orbital outside a core consisting of a closed (sub)shell system.

$$^{3}Li \longrightarrow 1s^2\ 2s^1$$

$$^{11}Na \longrightarrow 1s^2,\ 2s^2,\ 2p^6,\ 3s^1$$

$$^{19}K \longrightarrow 1s^2,\ 2s^2,\ 2p^6,\ 3s^2,\ 3p^6,\ 4s^1$$

In Li, Na, P case the total angular momentum and total spin angular momentum of the core are zero, designated as $^1S_0$. The core of other alkali metals are also $^1S_0$. Because the core is spherically symmetric, the valence electron of a neutral alkali atom (N=Z) moves in an effective central potential $V(r)$, which at large distance approaches the coulomb potential

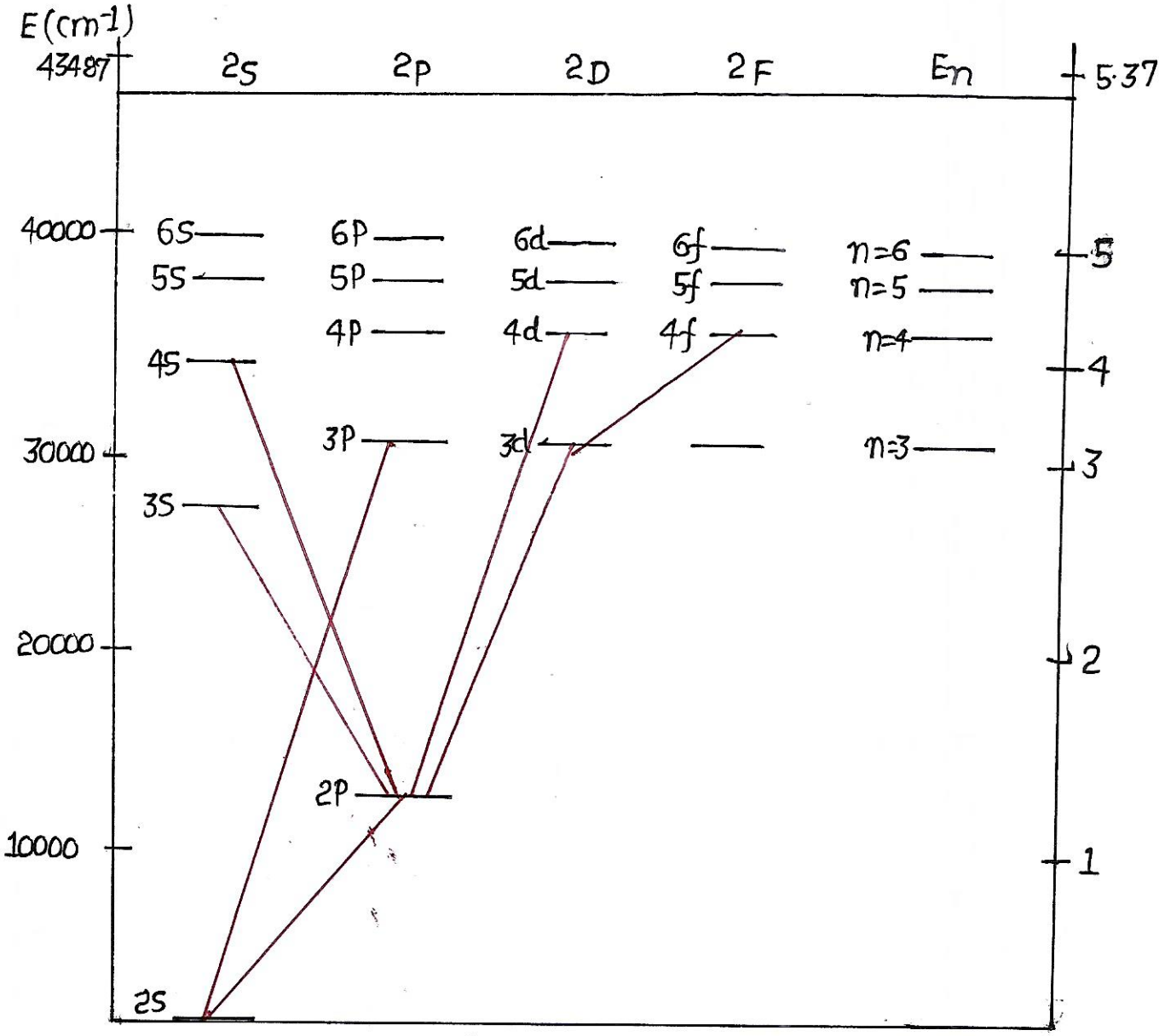
$$V(r) \xrightarrow[r\to\infty]{} -\frac{e^2}{(4\pi\epsilon_0)r} \qquad \text{---------- (1)}$$

Since the nuclear charge Ze is screened by the core which contains $(Z-1)\ e^-$. The lowest state of the valence e^- has zero orbital angular momentum and corresponding orbital is designated (n_0S), where to satisfy the Pauli principle $n_0 = 2$ for Li, 3 for Na, 4 for K, and so on. For small r, the potential $V(r)$ is more attractive than $-e^2/(4\pi\epsilon_0)r$, so the binding energy of the orbital is always greater than that of the level of Hydrogen.

For heighly excited state, for which the charge density of the orbital is almost entirely outside the region of the core, the orbitals approximate closely to true hydrogenic wave function and the energy levels are very close to those of Hydrogen.

As $V(r)$ is not columbic at short distance, the energy levels are not degenerate in l, for a given n. Thus the $2s^1$ level in Li lies well below the 2P level, and for sodium the $3s^1$ Level is below the 3P level, which in turn is below to 3d level.

As the excitation increases and the level becomes more hydrogenic in character, there is near degeneracy in l, for a given n.
The valence e^- is bound weakly compared to the core electrons.
The energy levels can be-configuration.

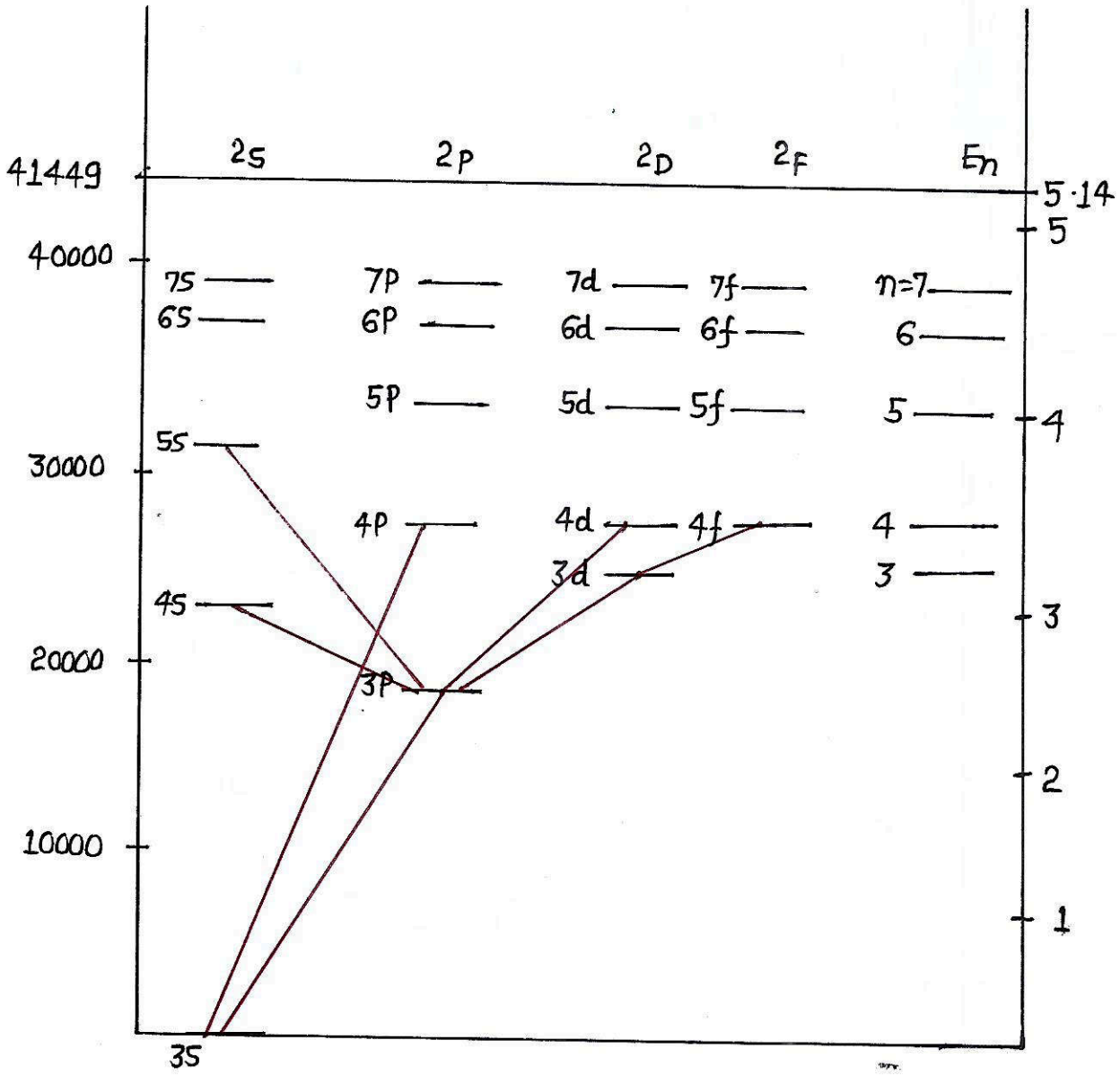


represented by the empirical formula

$$E_{nl} = -\frac{1}{2}\cdot\frac{1}{(n-\mu_{nl})^2} \text{ a.u.} \quad \text{——— (2)}$$

The quantities μ_{nl} are known as quantum defects. To a good approximation μ_{nl} is a function of l only. Thus we can write the effective quantum no; in the form of Rydberg, as

$$n^* = n - \alpha(l) \quad \text{——— (3)}$$



For Li, Na, K · A small (amount) (of) correction to this formula was made by Ritz, who wrote

$$n^* = n - \alpha(l) - \beta(l)/n^2$$

The observed series in the emission spectrum arises from the following transitions:

$np \rightarrow 3s$, $n>2$	Principal Series
$ns \rightarrow 3p$, $n>3$	Sharp Series
$nd \rightarrow 3p$, $n>2$	Diffuse Series
$nf \rightarrow 3d$, $n>3$	Fundamental Series

The absorption spectra can be obtained by passing light through the vapour of the alkali metal. Except at very high temperature, most atoms will be in the ground state, and the series of absorption lines correspond to transition from the $(n_0 s)$ ground state to the (np) levels, with frequencies

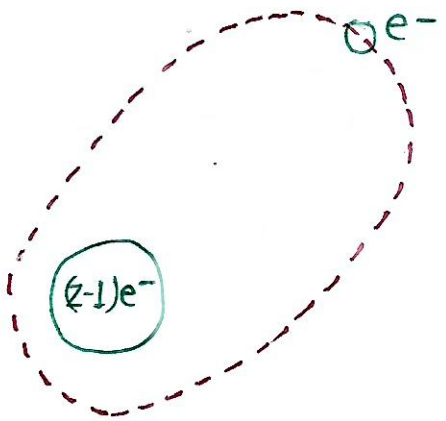
$$\nu = R\left[\left(\frac{1}{n^*_{n_0 s}}\right)^2 - \left(\frac{1}{n^*_{np}}\right)^2\right]$$

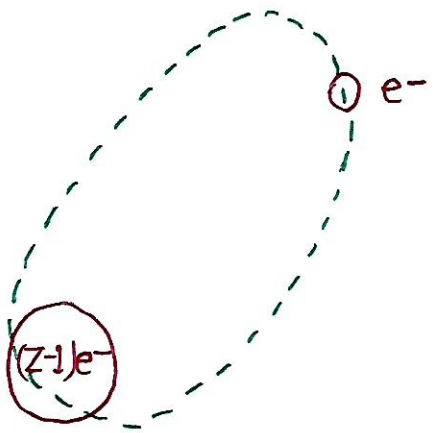
Rydberg Constant ↓

This series is called Principal series.

> Pentrating and Non-pentrating orbits-[2]

The first in the case when the outer e⁻ has a non pentrating orbit, as in the figure. It its accepted that the mean symmetry of the doud formed by $(z-1)$ e⁻ is similar, the e⁻ experiences the electrostatic potential of the nuclear charge $(z-1)$. The discussion presented for the Hydrogen atom remains valid.





On the other hand, if the orbit of the outer e⁻ penetrates inside the core of the atom, the problem is much more complex, simple solution by sommerfeld, is this

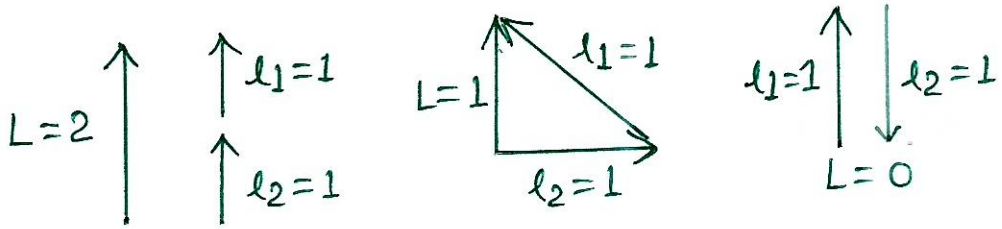
$$V_{ext} = \frac{1}{4\pi\epsilon_0}\frac{e}{r}$$ For 'r' Large

$$V_{in} = \frac{1}{4\pi\epsilon_0}\cdot\frac{ze}{r} + \text{constant}$$ For 'r' small

>L-S coupling-

→ known as Russell- Saunders coupling
→ Two Astronomers used it in studying the atomic spectrum emitted by stars.

If the interaction b/w the (s_i, l_i) b/w the spin and orbital angular momentum of the individual e^- is smaller than the mutual interaction of the spin and orbital angular momentum l_i combined vectorically to a total orbital angular momentum L and spin angular momentum S. L couples with S to form the total angular momentum J.



For many e^- system, the orbital angular momenta

$$L = l_1 + l_2 \quad \ldots\ldots\ldots (1)$$

$$|L| = \sqrt{L(L+1)}\,\hbar = \sqrt{L(L+1)}\,\frac{h}{2\pi}$$

Then

$L = l_1+l_2, l_1+l_2-1, \ldots\ldots l_1-l_2, \ldots\ldots$ where $l_1 \geqslant l_2$

The quantum no. L determines the term characteristic

$L = 0, 1, 2, \ldots\ldots$ indicates S, P, D, ... terms

It should be noted here that with L=1 is called a P term but does not necessary.

For optical transitions, the following selection rule hold:

$\Delta l = \pm 1$, For single e^-

$\Delta l = 0, \pm 1$, For the total system

$\Delta L = 0$ means that the quantum state of 2 e^- change simultaniously, and in opposite direction. This is only possible when caupling is strong.

Total Spin

$$S = s_1 + s_2$$

$$|S| = \sqrt{S(S+1)}\hbar = \sqrt{S(S+1)}\frac{h}{2\pi}$$

The total spin quantum no.

$$S = \frac{1}{2} + \frac{1}{2} = 1$$

$$S = \frac{1}{2} - \frac{1}{2} = 0$$

i.e. $S = 0, 1$

The selection rule for optical dipole radiation is $\Delta S = 0$, spin flipping is not associated with optical dipole radiation.

Finally

Total Angular momentum

$$J = L + S$$

$$J = \sqrt{J(J+1)}\hbar = \sqrt{J(J+1)}\frac{h}{2\pi}$$

The quantum no. J can have following values;

$S = 0$, $J = L$

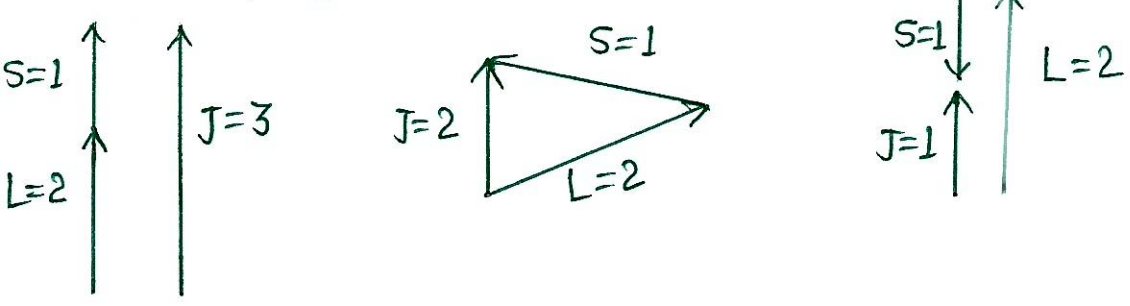
$S = 1$, $J = L+1, L, L-1$

in which all terms are triplets.

The individual angular momenta are combined according to the exactly same quantum rule. In the general case of several e^- system, there are $2S+1$ possible orientation of S with respect to L.

For e.g

Possible coupling of $S=1, L=2$



$_2He^4 = 2$

$1s^2$

$n_1 = n_2 = 1$

$l_1 = l_2 = 0$

$s_1 = s_2 = \frac{1}{2}$

The resultant quantum no. of the atom are either

$L = 0$

$S = 0$

$m_{s_1} = -m_{s_2}$

$J = 0$

or the singlet ground state $^1S_0$, or

$L = 0$

$S = 1$

$m_{s_1} = m_{s_2}$

$J = 1$

However, where 1 e^- remains in the shell with $n=1$, the other region with the state $n=2$

$n_1 = 1, n_2 = 2$

$l_1 = l_2 = 0$

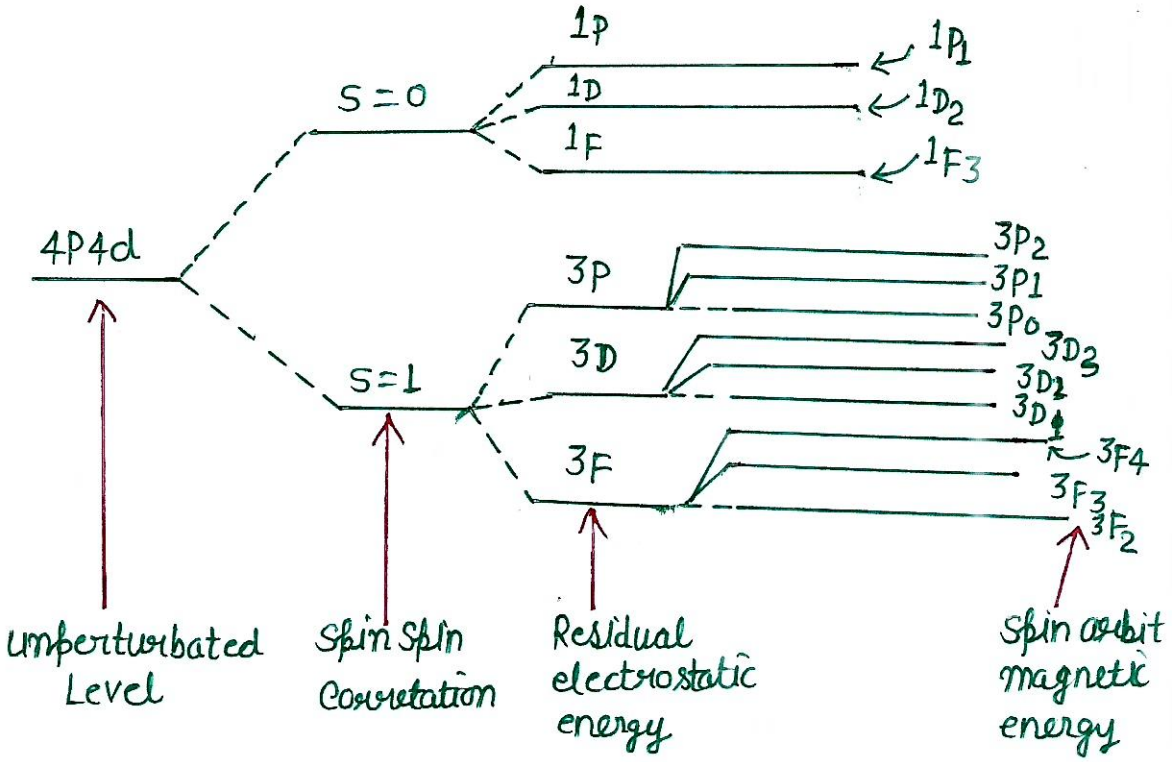
$s_1 = 1/2$

$s_2 = 1/2$

The yield either $L=0, S=0, J=0$ for singlet $^1S_0$.

$L=0, S=1, J=1$ for triplet $^3S_0$.





> J-J Coupling -

→ J-J coupling is an opposite extreme to the ideal L-S coupling

→ Approached by heiver atoms

The J-J coupling is an opposite exterme to the ideal L-S coupling and is approached by heavier atoms, for which the spin-orbit (magnetic) interaction term in the Hamiltonian predominates over the residual electrostatic interaction and the spin-spin correlation.

Therefore, in this case the splitting of the unperturbated energy level due to the introduction of the various perturbations takes place in this order!

(a) Spin-~~Spin~~ Orbital Interaction

(b) Residual electrostatic Interaction or spin-spin correlation

(a) As a result of the stronger spin-orbit Interaction, the orbital and the spin angular momentum vectors of each individual electron are strongly coupled together to form a resultant angular momentum vector $\vec{j}$ of magnitude $\sqrt{j(j+1)}\,\hbar$ or $\sqrt{j(j+1)}\,\frac{h}{2\pi}$ i.e. $\sqrt{j(j+1)}\,\frac{h}{2\pi}$

where $j = l - \frac{1}{2}$ and $j = l + \frac{1}{2}$, that is, j takes half-integral values only.

(b) As a result of the residual electrostatic interaction and spin-spin correlation, the resultant angular momentum vector $\vec{j}$ of the individual e^- are less strongly coupled with one another to form the total angular momentum vector $\vec{J}$ of the atom of magnitude

$$\sqrt{J(J+1)}\frac{h}{2\pi}.$$

The total angular momentum quantum numbers takes values:

$$J = |\vec{j}_1 + \vec{j}_2 + \ldots|_{min}, |\vec{j}_1 + \vec{j}_2 + \ldots|_{min+1}, \ldots (j_1 + j_2 + \ldots)$$

As the illution, let us consider the term for the electron configuration 4P 4d, under j-j coupling

For P-e^- ; $l_1 = 1$, $s_1 = 1/2$ and so $j_1 = \frac{1}{2}, \frac{3}{2}$

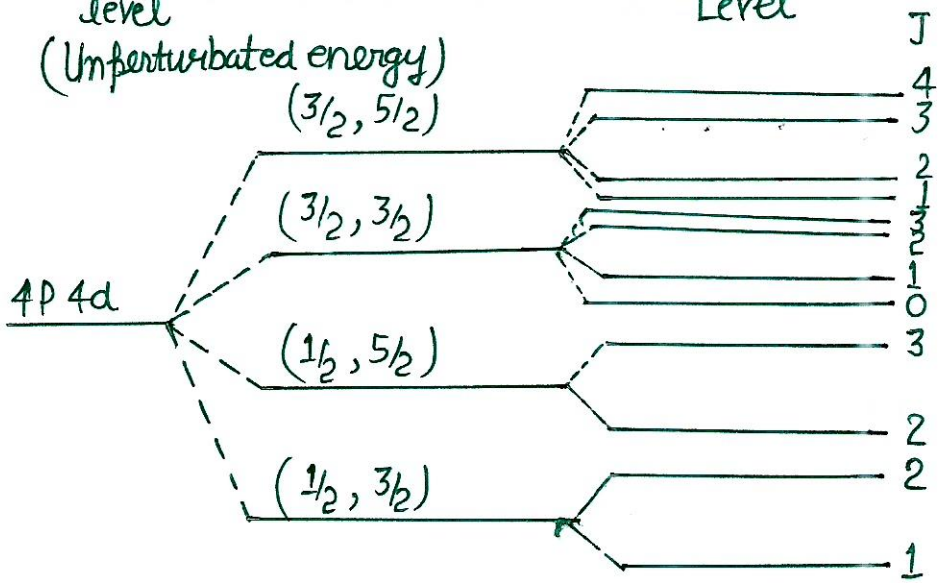
For d e^- ; $l_2 = 2$, $s_2 = 1/2$ and so $j_2 = \frac{3}{2}, \frac{5}{2}$

Thus gives four (j_1, j_2) combinations of possible j_1, j_2.
These are

$$\left(\frac{1}{2}, \frac{3}{2}\right), \left(\frac{1}{2}, \frac{5}{2}\right), \left(\frac{3}{2}, \frac{3}{2}\right), \left(\frac{3}{2}, \frac{5}{2}\right)$$

↑ Lowest level (Unperturbated energy)

↑ Highest Level

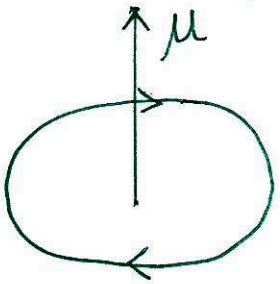


Selection Rule → $\Delta J = 0, \pm 1$ but $J = 0 \not\leftrightarrow J = 0$

> Zeeman Effect [4]

There are two types of zeeman effect →
- → Normal Zeeman Effect
- → Anomalous Zeeman Effect

The magnetic dipole moment of an e^- is caused by e^- spin.



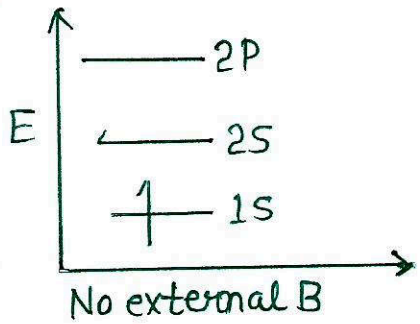
If an atom is placed into an external magnetic field $\vec{B}$ that points along the Z-axis, then the $\vec{B}$ will create a torque on the magnetic dipole moment of an e^- and will orient it along Z axis.

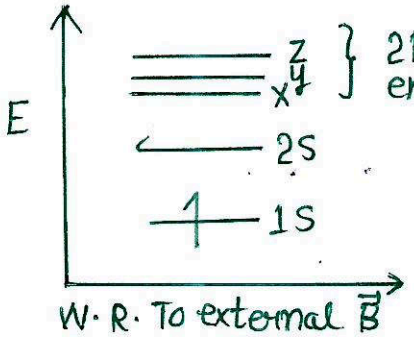
$$\mu_z = \mu_B \cdot m_l$$

m_l ← Magnetic quantum no.

μ_B ← Bohr magneton

Spectral Splitting happens:
The orbital of any given atom has the ability to undergo splitting when in the presence of an external magnetic field $\vec{B}$. The number of splits of any orbital depends on the orbital quantum no.



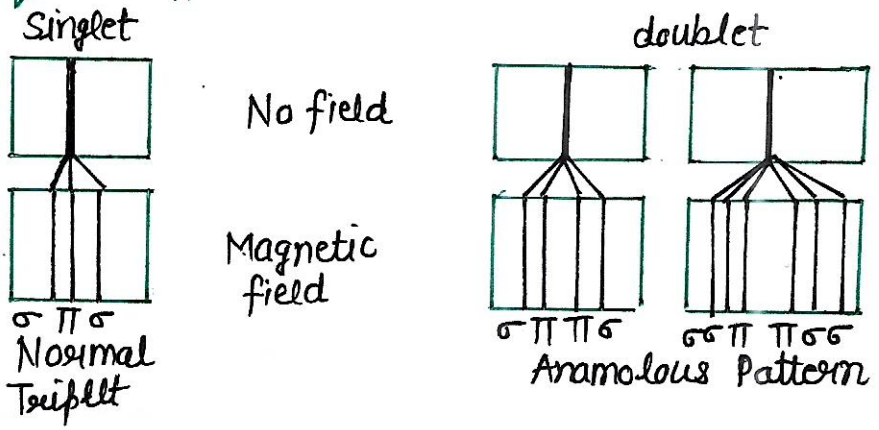


No. of splitting = $2l+1$

The splitting of P orbital within an atom in presence of an external magnetic field is known as Zeeman Effect.

Why Splitting?

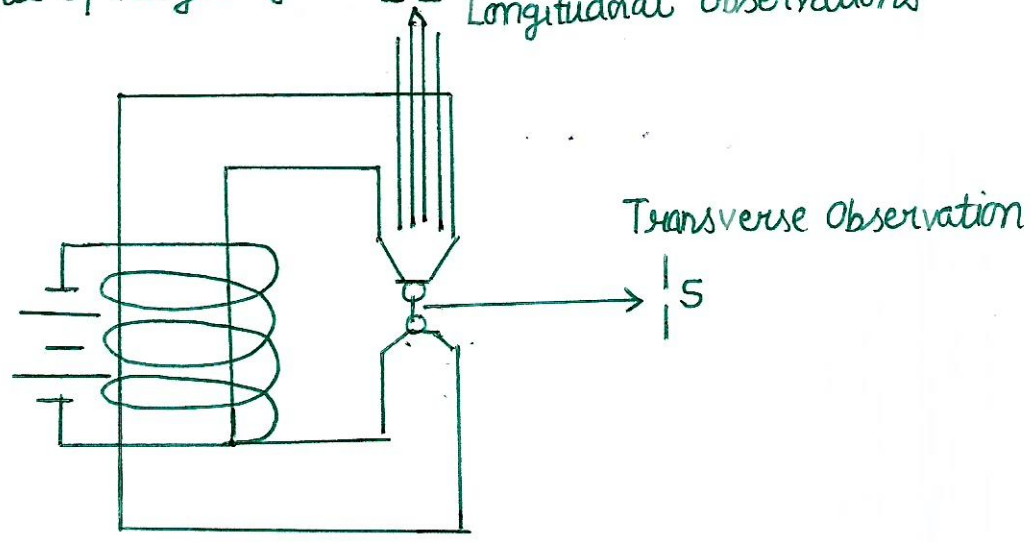
Every e^- contains its own magnetic dipole moment μ that points in same direction when placed into an $\vec{B}$; the torque that acts on μ must do work to orient that e^- μ along the same direction as the magnetic field lines. Any 2 e^- clouds with μ that have different orientation will require different amount of work to rotate it.



In 1896, ~~Orb~~ Zeeman observed that the spectral lines of Atoms were split in the presence of an external magnetic field.

#Experimental Setup of Zeeman Effect-

The splitting of the energy terms of atoms in a magnetic field can also be observed as a splitting of the frequencies of transitions in a optical spectra. A splitting of this type of spectral lines in a magnetic field was observed for the first time in 1896 by Zeeman. This effect is small, for its observation, spectral apparatus of very high resolution is required.



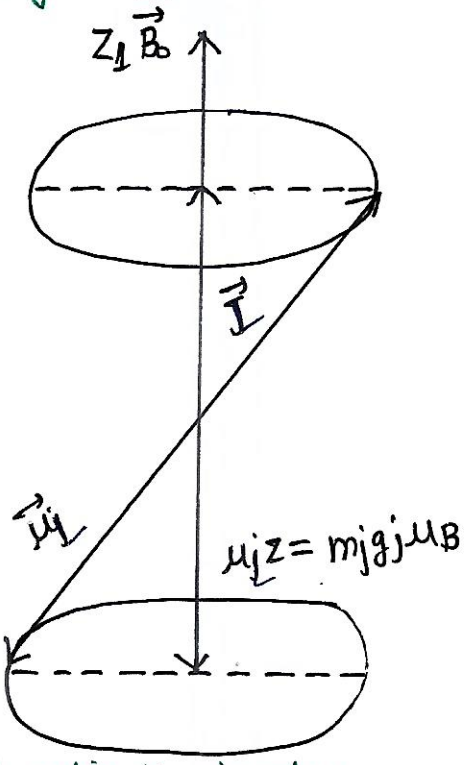
The zeeman effect may be understood to a large extent using classical electron Theory as was shown by Lorentz shortly after its discovery. The splitting of states with pure orbital angular momentum. The normal zeeman effect describes states in which no spin magnetism occures.

A complete quantum Mechanical treatment will be given. The angular momentum vector j and the magnetic moment μ_j which is coupled to j, process together the field B_0. The additional energy of the atom due to magnetic field is :-

$$V_{mj} = -(\mu_j)_z B_0 = + m_j g_j \mu_B B_0$$

The distance b/w two components with $\Delta m_j = 1$ is

$$\Delta E = g_j \mu_B B_0$$



- **Normal Zeeman Effect**-

In the term of quantum Theory, the gyromagnetic ratio is given by

$$\frac{|\vec{\mu}_L|}{|\vec{L}|} = \frac{e}{2m}$$

e and m are charge and mass of e- respectively.

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

M_L is magnetic quantum no.

$$M_L = L, L-1, \ldots -L$$

The By Larmor formula

$$\omega = \frac{|\vec{\mu}_L|}{|\vec{L}|} B = \frac{e}{2m} B$$

The Interaction energy

$$\Delta E = \omega L_z = \frac{e}{2m} B \cdot M_L \frac{h}{2\pi}$$

$$\Delta E = \frac{eh}{4\pi m} B M_L$$

In wave no.

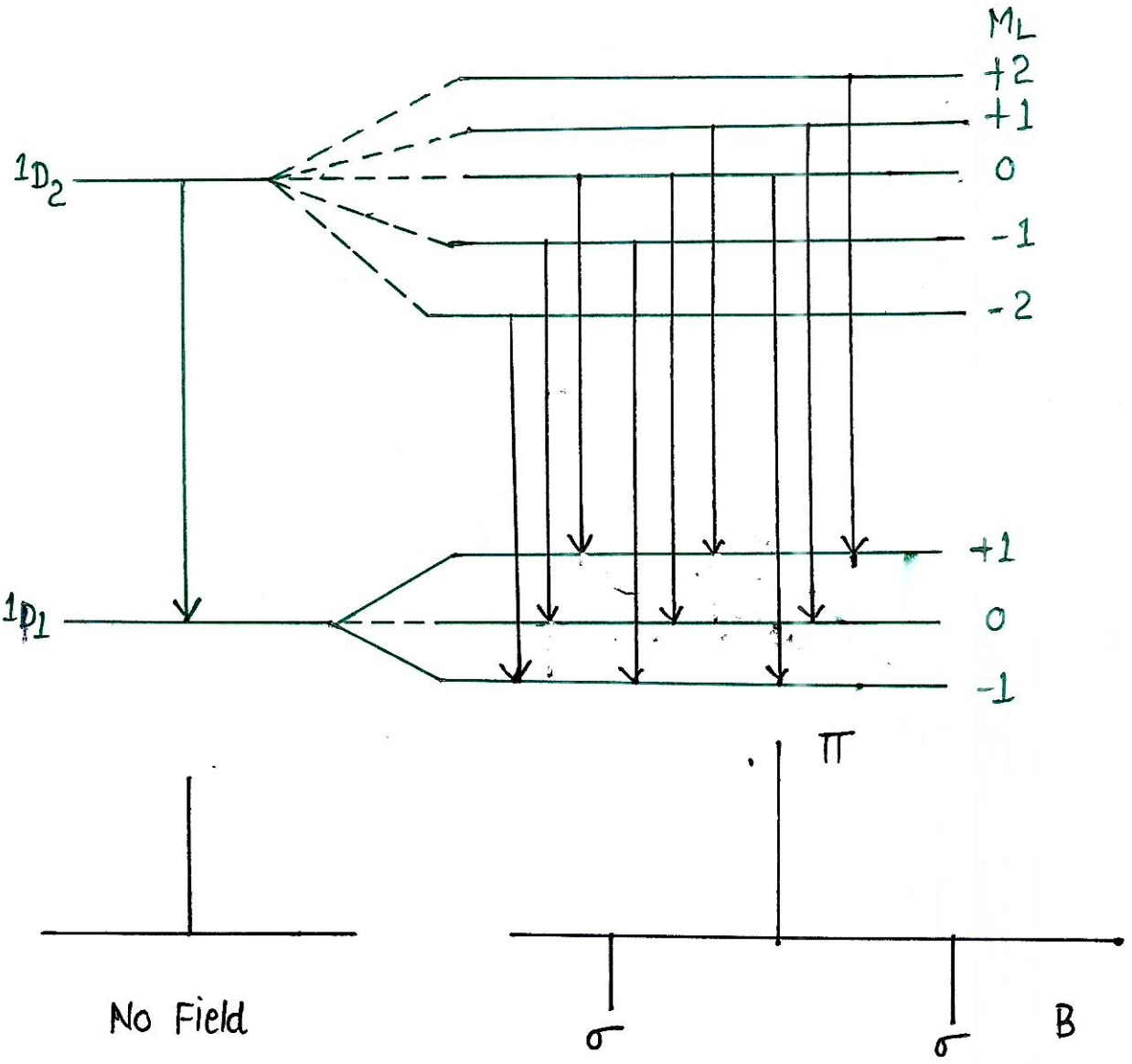
$$\frac{\Delta E}{hc} = -\Delta T \Rightarrow \frac{\Delta E}{hc} = \frac{eB}{4\pi m} M_L \frac{h}{hc}$$

$$\Rightarrow -\Delta T = \frac{eB}{4\pi mc} M_L$$

$$\boxed{-\Delta T = M_L L'}$$

Where L' is Lorentz Unit

ΔT is the change in energy for each M_L level from the original level.

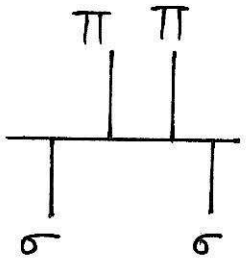


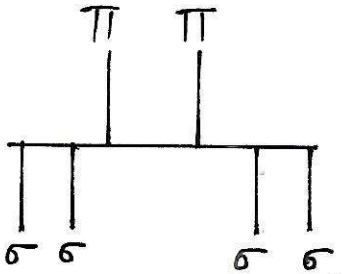
The magnitude of the splitting is thus the same as in classical theory. For optical transitions, one must also make use of selection rule.

$$\boxed{\Delta M_L = 0, \pm 1}$$

- **Anomalous Zeeman Effect-**

The Anomalous zeeman Effect occurs when the angular momentum and magnetic moment of the two terms b/w which an optical transition occurs cannot be described just one of the two quantum no. (s and l) but are determined by both.



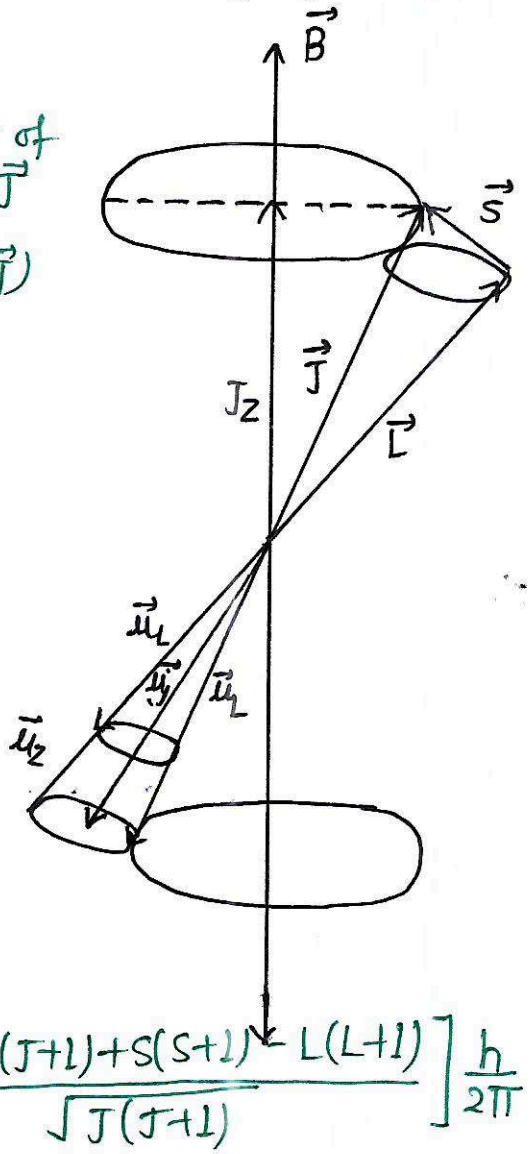


μ_j = Component of $\vec{\mu}_L$ along $\vec{J}$ + component of $\vec{\mu}_S$ along $\vec{J}$

$$\mu_j = \frac{e}{2m}|\vec{L}|\cos(\vec{L},\vec{J}) + \frac{2e}{2m}|\vec{S}|\cos(\vec{S},\vec{J})$$

$$\vec{L} = \sqrt{L(L+1)}\frac{h}{2\pi}$$

$$\vec{S} = \sqrt{S(S+1)}\frac{h}{2\pi}$$



Then

$$\mu_j = \frac{e}{2m}\left[\sqrt{L(L+1)}\frac{h}{2\pi}\cos(\vec{L},\vec{J}) + 2\sqrt{S(S+1)}\frac{h}{2\pi}\cos(\vec{S},\vec{J})\right]$$

$$\mu_j = \frac{e}{2m}\left[\frac{J(J+1)+L(L+1)-S(S+1)}{2\sqrt{J(J+1)}} + \frac{J(J+1)+S(S+1)-L(L+1)}{\sqrt{J(J+1)}}\right]\frac{h}{2\pi}$$

Lande 'g' factor

$$g = 1 + \frac{J(J+1) + S(S+1) - L(L+1)}{2J(J+1)}$$

Then

$$\mu_j = g \frac{e}{2m} \sqrt{J(J+1)} \frac{h}{2\pi}$$

$$\mu_j = g \frac{e}{2m} |\vec{J}|$$

$$\boxed{\frac{\mu_j}{|\vec{J}|} = g \frac{e}{2m}}$$

By Larmor Formula

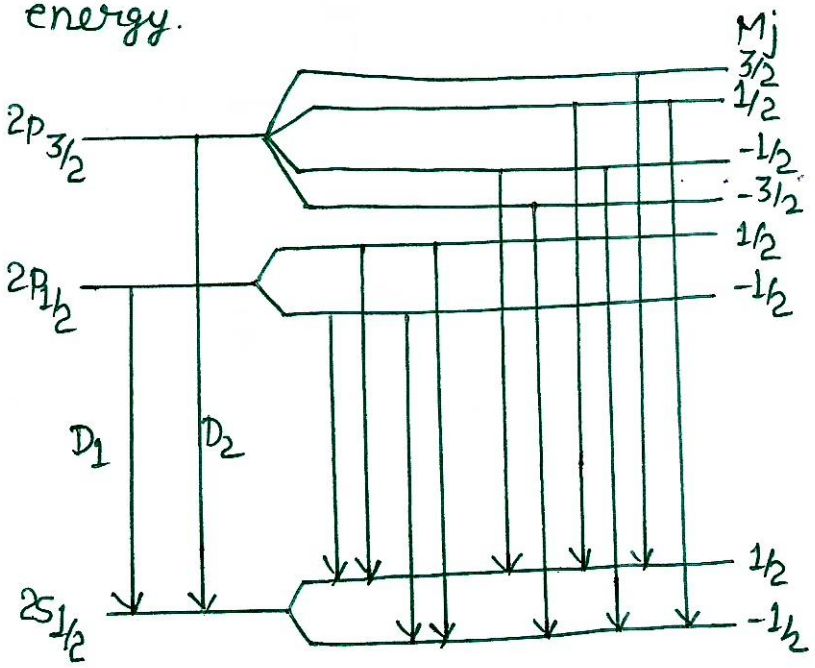
$$\omega = \frac{\mu_j}{|\vec{J}|} B = g \frac{e}{2m} B$$

$$\boxed{\Delta E = g M_J \frac{eh}{4\pi m} B}$$

And

$$\boxed{-\Delta T = g M_J L'}$$

This is the expression for the weak field magnetic interaction energy.



Selection rule

$\Delta M_j = 0, \pm 1$

but $M_j = 0 \not\leftrightarrow M_j = 0$ if $\Delta J =$

> Paschen Back effect

In the zeeman effect, the external magnetic field is weak as compared to internal field due to the spin and (angular) orbital motions of the valence e^-. However, the ~~strong~~ strength of the external field is increased, the separations b/w zeeman components increase until they becomes greater than the separations b/w multiplet fine-structure components. The anomalous zeeman pattern then changes over to like a normal zeeman pattern. This phenomenon is known as Paschen Back Effect. It can be explained by following derivation.

$$M_L = L \ldots\ldots -L$$
$$M_S = S \ldots\ldots -S$$

By Larmor formula,

$$\omega_L = \frac{e}{2m} B$$

$$\omega_S = 2\frac{e}{2m} B$$

$$\Delta E_L = \omega_L L_Z = \frac{e}{2m} B M_L \frac{h}{2\pi}$$

$$\Delta E_S = \omega_S S_Z = 2\frac{e}{2m} B M_S \frac{h}{2\pi}$$

$$\Delta E = \Delta E_L + \Delta E_S$$

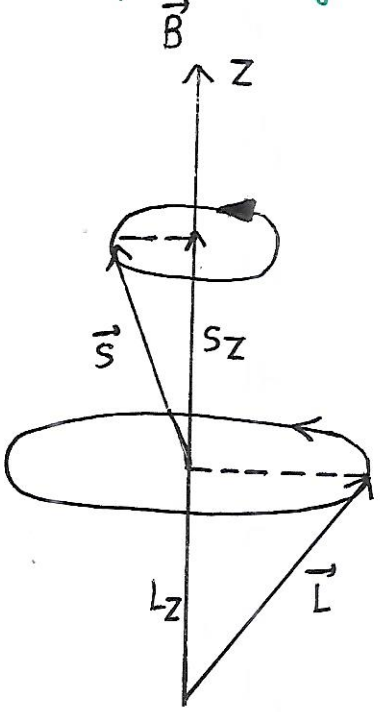
$$\Delta E = (M_L + 2M_S)\frac{eh}{4\pi m} B$$

The shift in wave no.

$$-\Delta T = \frac{\Delta E}{hc}$$

$$-\Delta T = (M_L + 2M_S)\frac{eB}{4\pi mc}$$

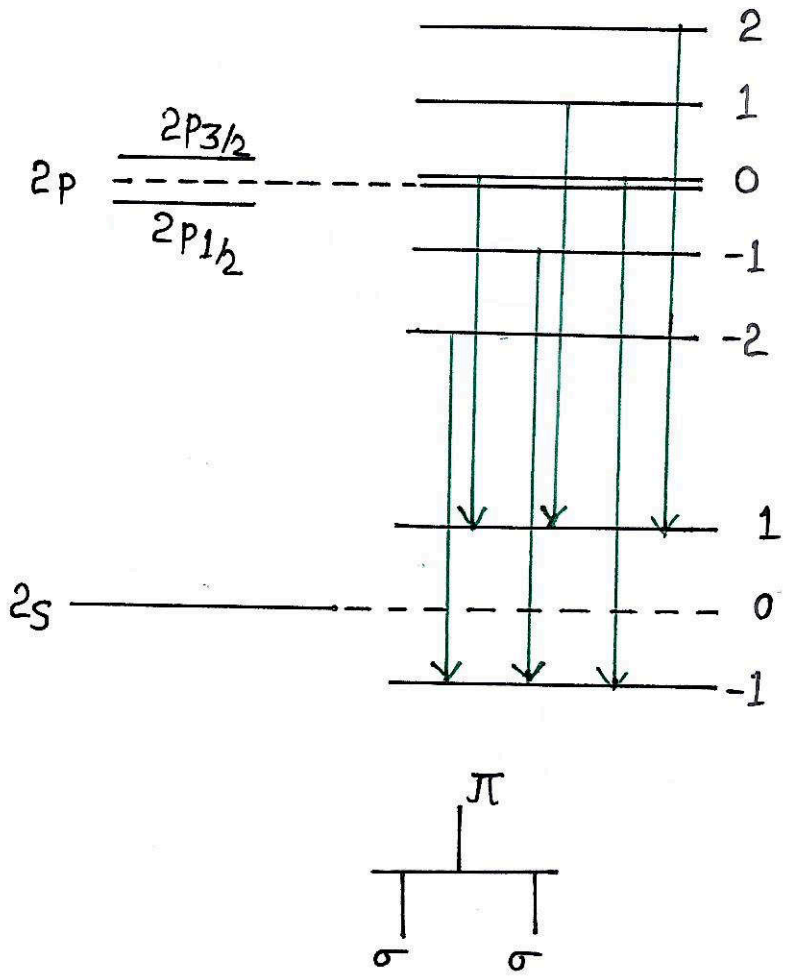
$$\boxed{-\Delta T = (M_L + 2M_S) L'}$$



When the external field $\vec{B}$ becomes stronger as compared with the internal field, the magnetic coupling b/w $\vec{J}$ and $\vec{B}$ exceeds that b/w $\vec{L}$ and $\vec{S}$, and the precession of $\vec{J}$ about $\vec{B}$ becomes faster than the $\vec{L}$ and $\vec{S}$ about $\vec{J}$. Under these conditions the coupling between $\vec{L}$ and $\vec{S}$ is partially broken down and $\vec{J}$ is no longer fixed in magnitude, As the field $\vec{B}$ is further increased, $\vec{L}$ and $\vec{S}$ start processing independently about $\vec{B}$.

Then magnitude of components are $M_L\frac{h}{2\pi}$ and $M_S\frac{h}{2\pi}$ respectively.

The strong-field splittings of the term ^2p and ^2s have been shown.



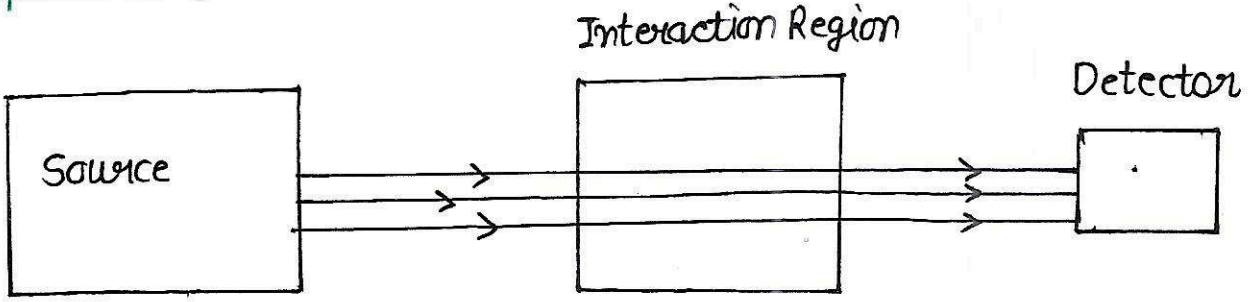
Selection Rule

$$\Delta M_L = 0$$
$$\Delta M_L = \pm 1$$
$$\Delta M_S = 0$$

> Lamb Shift-

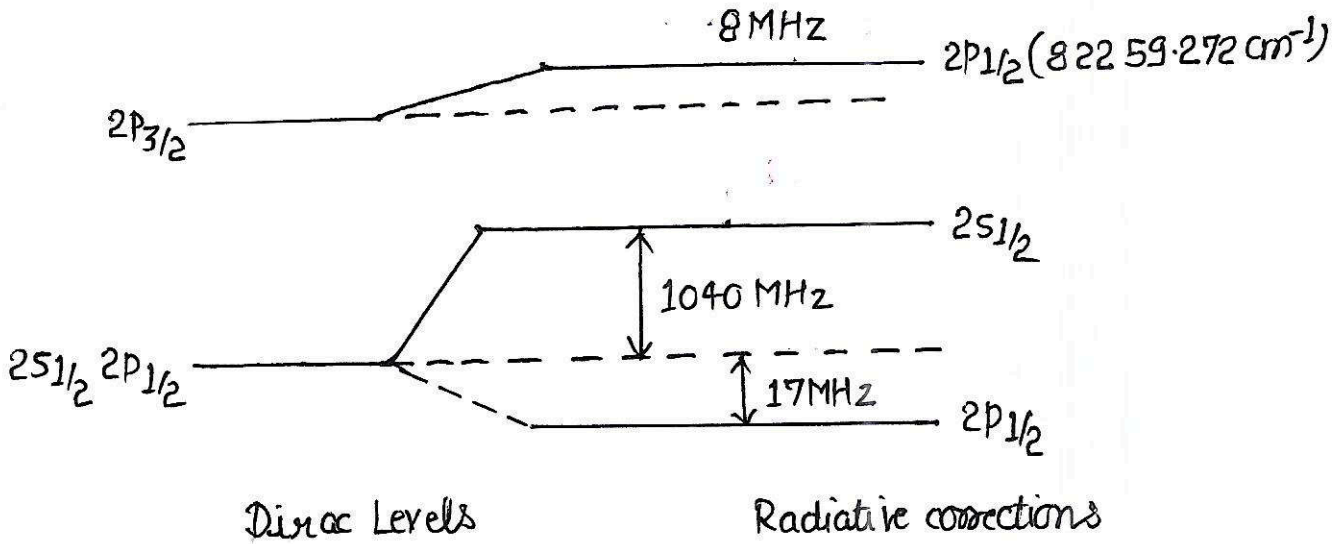
According to dirac theory, energy levels of one electron atoms with the same value to the quantum no. j but different value of l should coincide. Husuton and Williams, are found no discrepancy with the dirac theory. The question was settled in 1947 by W.E. Lamb and R.C. Retherford who performed a brilliant experiment which we shall now briefly describe. Instead of attempting to resolve the fine structure of hydrogen by investigating its optical spectrum, Lamb and Retherford used microwave techniques to stimulate the direct radio frequency transition b/w the $2S_{1/2}$ and $2P_{1/2}$ levels.

The experimental method of Lamb and Retherford is based on the fact that the $2S_{1/2}$ level is metastable. Indeed, as we have seen, the electric dipole transition from the state $2S_{1/2}$ to the ground state $1S_{1/2}$ is forbidden by selection rule $\Delta l = \pm 1$. The most probably decay mechanism of the $2S_{1/2}$ state is two-photon emission, with a lifetime of 1/7s. Thus, in the absense of perturbations, the lifetime of the $2S_{1/2}$ state is very long compared to that of the 2p state, which is about 1.6×10^{-9} s. In the apparatus of Lamb and Retherford is shown below.



The source produces an atomic beam of Hydrogen containing a small fraction of atoms in the $2S_{1/2}$ level. The beam is passed through a region of a radio-frequency electric field and a variable magnetic field and is detected by an apparatus which records only atoms in the $n=2$ levels.

The energy shift for the $2S_{1/2}$, $2P_{1/2}$ and $2P_{3/2}$ levels with respect to the dirac theory are illustrated for the case of atomic hydrogen. The theoritical value of 1057.91 MHz for the lamb shift is an excellent agreement with the experimental value (1057.77 ± 0.10 MHz) obtained by Lamb and with a more recent measurement by Robiscoe and Shyn giving the result (1057.90 ± 0.06) MHz. The Lamb shift has also measured and calculated for other levels of atomic hydrogen and also for other hydrogenic systems such as deuterium He^+, Li^{2+} and so on.



> Stark Effect -

This effect of static electric field on the spectrum of Hydrogen and other atoms was studied by J. Stark and also by A. Lo Surdo in 1913. The splitting of spectral lines observed his become known as the stark effect. We shall assume that the external electric field is constant over a region of atomic dimensions and directed along the z axis.

- **Main-Features -**

The main features of the observed stark effect are;

(i) All Hydrogen lines (are) form symmetrical patterns, but the pattern depends markedly on the quantum number n of term involved. The number of Stark lines, and the total width of the pattern increase with n.

(ii) The wave no. shifts are integral multiple of a unit which is proportional to the strength of the electric field, and is same for all hydrogen lines.

(iii) Except for the absence of circular polarization in longitudinal observation, the polarization properties of stark effect lines resemble those of the zeeman lines. But, in contrast to zeeman lines, the π components show greater shift than the σ- compo.

(iv) The hydrogen lines involving the lower energy states (small n) such as H_α, H_β show only a symmetrical splitting proportional to the field strength about their field strength about their field free positions. This is known as linear stark effect.

- **Linear Stark Effect -**

Since the ground state is non-degerate, the first-order correction to its energy is given by

$$E^1 = e\mathcal{E}_0 \langle \psi | z | \psi \rangle$$

$$E^1 = e\mathcal{E} \int |\psi(x)|^2 z \, dx$$

- **Quadratic Stark Effect -**

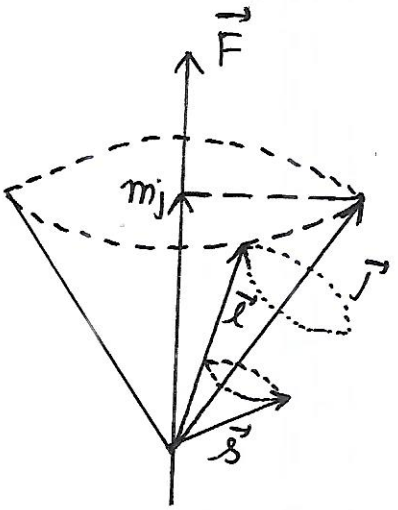
the second order correction

$$E^2 = e^2 \mathcal{E}^2 \sum_{\substack{n \neq 1 \\ l,m}} \frac{\langle 1 | \psi_{nlm} | z | \psi_{nlm} | 1 \rangle^2}{E_1 - E_n}$$

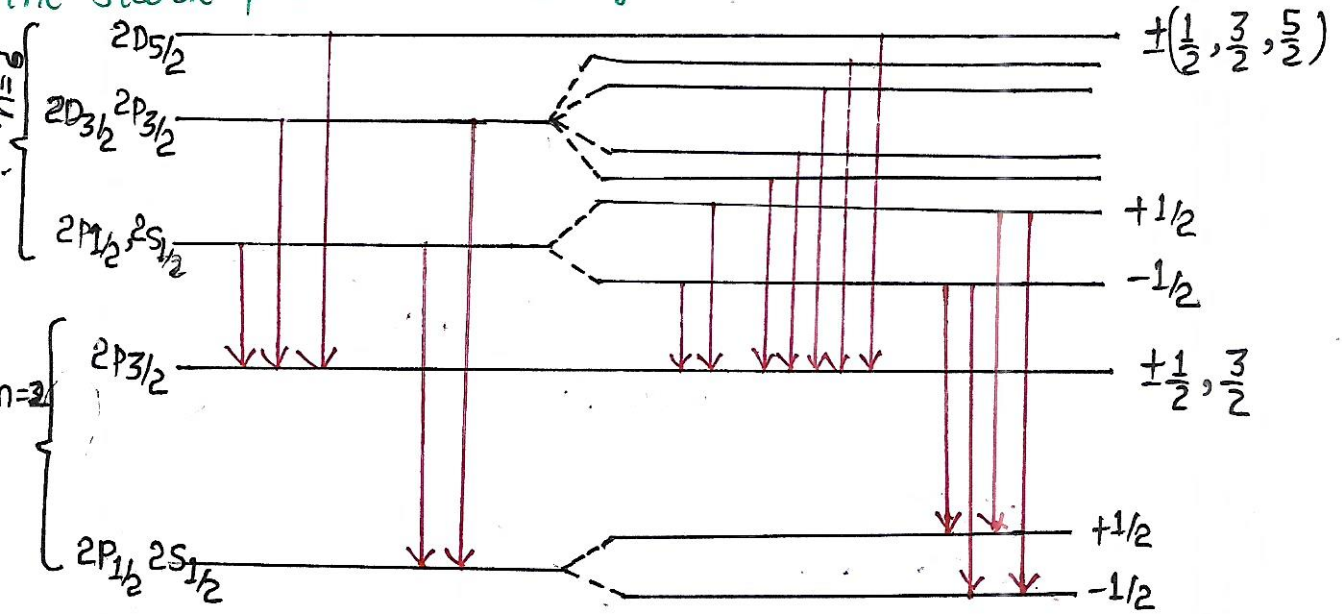
- Weak Field Stark effect in Hydrogen-

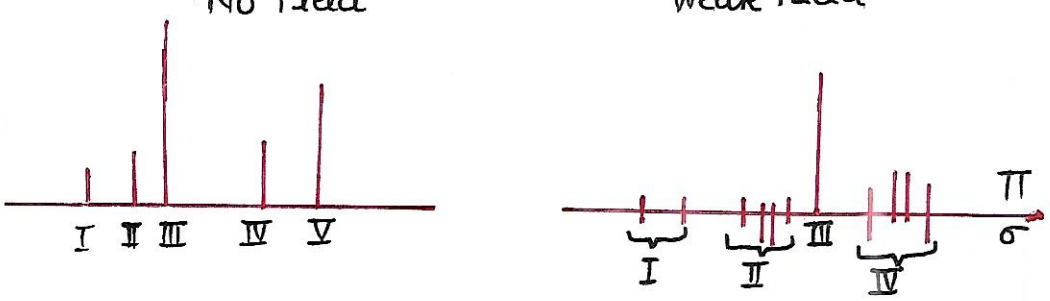
A weak electric field for Hydrogen is one for which the interaction energy between the electron's total angular momentum $\vec{j}$ and the field $\vec{F}$ is less than the magnetic interaction energy b/w orbital momentum I and spin momentum $\vec{s}$, that is, for which the stark splitting is smaller compared with the fine-structure splitting. In such a field, as shown in figure. $\vec{I}$ and $\vec{s}$ couple to form j which processes around $\vec{F}$ with projection $m_j h/2\pi$ where

$$m_j = +j, j-1, j-2, \ldots\ldots -j$$



The energy level of Hydrogen atom for the two states $n=2$ and $n=3$ are shown in figure. The field free levels and theoritical pattern for H_α are given at the left and the weak field levels and the stark pattern at the right.





selection rules

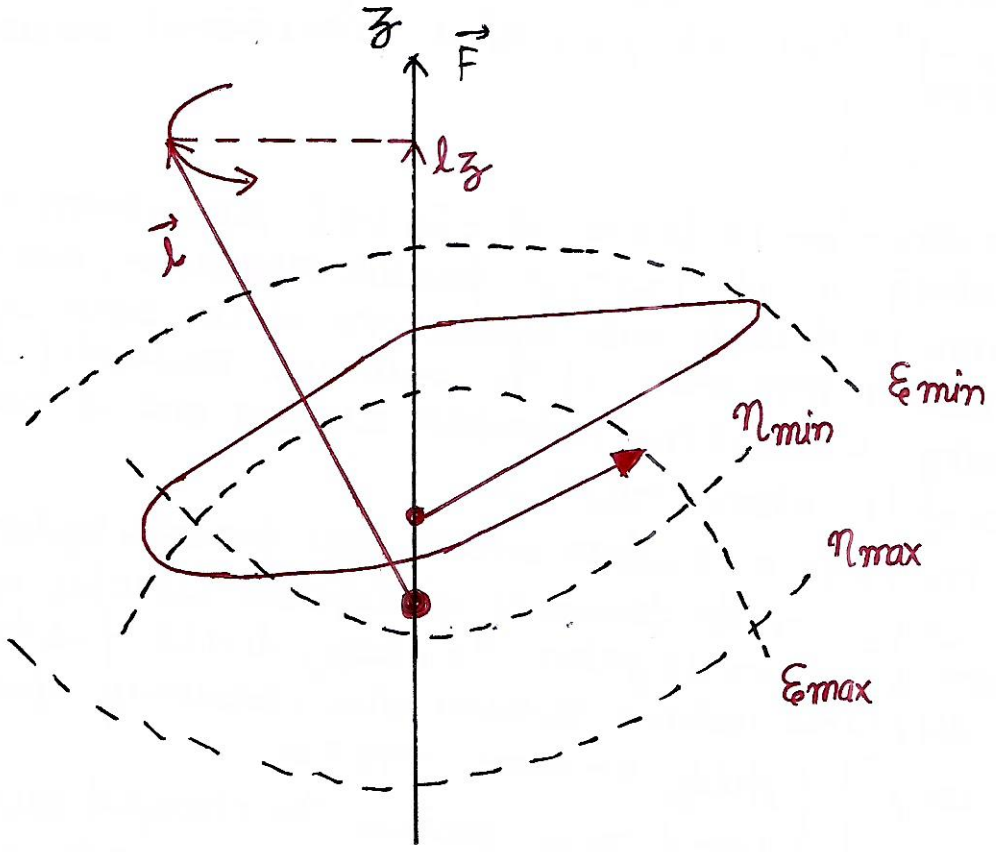
$$\Delta m_j = 0 \text{ for } \pi$$
$$\Delta m_j = \pm 1 \text{ for } \sigma$$

- **Strong-Field Stark Effect in Hydrogen-**

A strong electric field for Hydrogen is one for which the interaction energy b/w the electron's total angular momentum $\vec{J}$ and the field $\vec{F}$ is greater than the magnetic interaction energy b/w e^- orbital momentum $\vec{I}$ and spin momentum $\vec{S}$.
This effect is homogenous electric field $\vec{F}$, parallel to the Z-axis, one an e^- moving in the Kepler ellipse is different from that of a magnetic field. For the Kepler motion, the center of gravity of the e^- avaraged over its orbit does not coincide with the nucleus and thus forms an electric dipole. The torque on the orbital dipole exerted by the electric field causes a precession the orbital about Z axis. However the orbital angular momentum $\vec{I}$ is not constant and it is no longer good quantum number.

$$\text{Energy value } E = E_0 - \frac{3 a_0 e}{2Z} Fn(n_2 - n_1)$$

↳ Free Field energy of atom



• Stark shifting of Hydrogen energy level-

$$-\Delta T = \frac{\Delta E}{hc}$$

$$-\Delta T = \frac{3a_0 e}{2Zhc} F n(n_2 - n_1)$$

Putting the known values of a_0, e, h, c, we get

$$-\Delta T = \frac{3(0.53\times10^{-10})(1.6\times10^{-19})}{2Z(6.63\times10^{-34})(3\times10^{8})} F n(n_2 - n_1)$$

$$-\Delta T = \frac{6.40\times10^{-5}}{Z} F n(n_2 - n_1)$$

$$\boxed{-\Delta T = \frac{6.40\times10^{-5}}{Z} F n(n_2 - n_1) \ cm^{-1}}$$

Thus the stark effect levels in a hydrogen-like Atom are all shifted by integral multiples of a fundamental amount from the original level.

> Hyperfine Structure-[1]

Many fine-structure components of spectral lines, when examined under instruments of highest possible resolution, are further splitted into components with separations of the order of $1cm^{-1}$. which is very smaller than those of the ordinary multiplet structure. This splitting is called the hyperfine structure and is caused by properties of the atomic nucleus

There are two types of nuclear effects that produce hyperfine structure. The first is due to the presence of different isotopic species in the element under investigation. The energy levels of isotopes are slightly displaced relative to each other, producing spectral transitions at slightly different wave no.

The second type of effect arises because the charged nucleus possesses as spin angular momentum and the associated magnetic dipole moment. An Interaction between the internal magnetic field produced by the orbital motion of the electrons in the atom and the spin magnetic dipole moment of the nucleus causes a hyperfine splitting of the spectral terms.

→ Isotope Effects-

Many e- are composed of isotopic atoms. Different isotopes of an element have the same number and arrangement of extranuclear electrons, but differ from one another in mass.

e.g. Let us examine and calculate shift for H_β lines (4861.33 Å).

For this transition, we have from Balmar formula.

$$\frac{1}{\lambda_H} = R_H\left(\frac{1}{2^2} - \frac{1}{4^2}\right)$$

$$\frac{1}{\lambda_D} = R_D\left(\frac{1}{2^2} - \frac{1}{4^2}\right)$$

$$\frac{\lambda_D}{\lambda_H} = \frac{R_H}{R_D}$$

$$\frac{\lambda_D - \lambda_H}{\lambda_H} = \frac{R_H - R_D}{R_D}$$

$$\Delta\lambda = \lambda_D - \lambda_H = -\lambda_H\left(\frac{R_D - R_H}{R_D}\right)$$

$$= -4861.33\ \text{Å}\left(\frac{109707.4 - 109677.6}{109707.4}\right)$$

$$= -1.32\ \text{Å}$$

Many cases of isotopic shift are not as simple as that of Hydrogen. In fact, for the rare earths and heavier atoms, the main contribution in isotope-shift is not due to a different mass but due to a change in nuclear radius with mass and derivation of the nuclear magnetic field from being purely a coulombian one.

→ Nuclear Spin and Hyperfine Splitting-

In 1924, Pauli pointed out that hyperfine splitting structure could be explained when it is assumed that the atomic nucleus possesses

an intrinstic spin angular momentum $\vec{I}$ with which is associated a magnetic dipole moment $\vec{\mu}_I$.

Thus the magnitude of nuclear angular momentum

$$|\vec{I}| = \sqrt{I(I+1)}\frac{h}{2\pi}$$

Then

$$I_z = M_I \frac{h}{2\pi}$$

$$M_I = I, \ldots\ldots :-1.$$

This motion of the nuclear protons produces a magnetic moment $\vec{\mu}_I$.

$$\vec{\mu}_I = g_I \left(\frac{e}{2m_p}\right)\vec{I}$$

$$\vec{\mu}_I = g_I \left(\frac{e}{2m_p}\right)\sqrt{I(I+1)}\frac{h}{2\pi}$$

$$\vec{\mu}_I = g_I \sqrt{I(I+1)}\frac{eh}{4\pi m_p}$$

$\frac{eh}{4\pi m_p}$ is natural unit of nuclear magnetic momentum i.e. nuclear magneton μ_N.

$$\vec{\mu}_I = g_I \sqrt{I(I+1)}\,\mu_N$$

$$\boxed{\vec{\mu}_{Iz} = g_I M_I \mu_N}$$

→ Selection Rule –

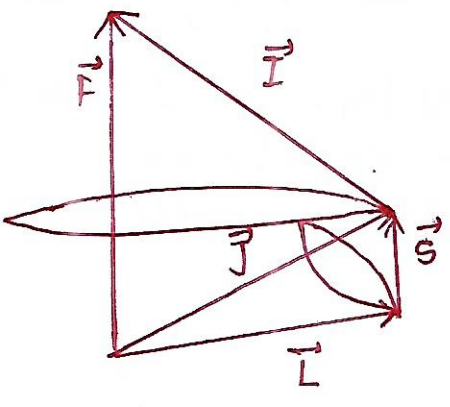
The selection Rule for F for electric dipole transition

Atomic Model – $\Delta F = 0, \pm 1$ but $F=0 \not\leftrightarrow F=0$

$\vec{F} = J+1, \ldots\ldots\ldots |J-I|$

$$\Delta E = \frac{1}{2}A'[(F+1)(F+2) - F(F+1)]$$

$$\boxed{\Delta E = A'(F+1)}$$



UNIT-2

Molecular Spectroscopy

→ Raman Effect, Raman Spectroscopy, QT ✓
→ Born Oppenheimer Approximation ✓
→ Heitler- Loudon Treatment for H-ion and H-molecule ✓
→ Franck Condon Principle, Condon parabola ✓
→ Molecular Orbital Theory
→ Vibration Spectra and Rotational Spectra

• Heitler-Loudon Treatment for Hydrogen H_2

The H_2 molecule is held by a covalent bond b/w two neutral H atoms.

H-H

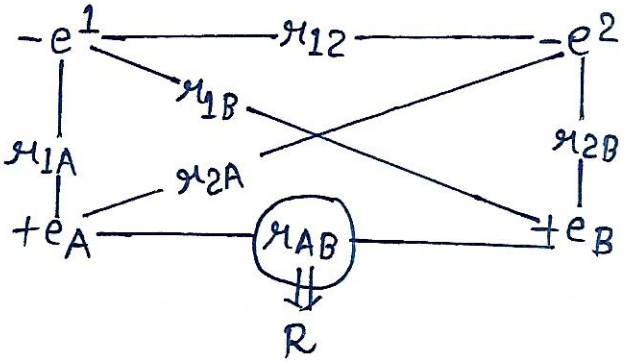
The bond is provided by a pair of e⁻ which is shared by two atoms. H_2 is more compact and more tightly bound. Its equilibrium internuclear separation is 0.74Å. with a binding energy of 4.74eV. The wave function of H_2 are different than those of H_2^+ because of the electrostatic repulsion b/w the two e⁻ in H_2, a factor absent in H_2^+.

Heitler Loudon treated the stability of H_2 molecule by starting out from the state of two separated normal H atoms as zero approximation and then introducing the interaction of the two atoms as a perturbation

The normal H atoms in the 2S state give rise to two molecular state $^1\Sigma_g^+$ and $^3\Sigma_u^+$. Heitler and Loudon showed that $^1\Sigma_g^+$ which is the ground state of the molecule, is stable while $^3\Sigma_u^+$ is unstable.

According to Heitler Loudon theory, the strong binding force b/w two H atoms arises from "exchange degeneracy". Hence they are called exchange forces. That is, the two configurations are degenerate. When the atoms approach each other, an interaction b/w them takes place which removes the degeneracy. The exchange force b/w the two atoms are attractive for the configuration of smaller energy which is therefore a stable state; while they are repulsive for the configuration of greater energy which is therefore an unstable state.

Let us consider an H_2 molecule, a system consisting of two e^- 1 & 2 in the field of two protons A and B.



The total potential energy of the system

$$V = \frac{1}{4\pi\epsilon_0}\left[-\frac{e^2}{r_{1A}} - \frac{e^2}{r_{2A}} - \frac{e^2}{r_{1B}} - \frac{e^2}{r_{2B}} + \frac{e^2}{r_{12}} + \frac{e^2}{R}\right] \ldots\ldots (1)$$

The schrodinger eqn of the H_2 molecule with the proton considered fixed at the distance R is

$$\nabla_1^2\psi + \nabla_2^2\psi + \frac{8\pi^2 m}{h^2}(E-V)\psi = 0 \ldots\ldots\ldots (2)$$

Let us first suppose that R is very large. Then the potential energy reduces to

$$V = \frac{1}{4\pi\epsilon_0}\left[\frac{-e^2}{r_{1A}} - \frac{e^2}{r_{2B}}\right]$$

The eigenfunction of the system in the product

$$\psi_A(1)\,\psi_B(2)$$

↑ Hydrogen eigenfunction of e^- 1 moving about Proton A.

↑ Hydrogen eigenfunction of e^- 2 moving about the Photon B.

If the two H atoms are in their groundstate, then

$$\psi_A(1) = \frac{1}{\sqrt{\pi a_0^3}} e^{-r_{1A}/a_0}$$

$$\psi_B(2) = \frac{1}{\sqrt{\pi a_0^3}} e^{-r_{2B}/a_0}$$

The energy of the system for large R is then simplified $2E_H$. Where E_H is the groundstate energy of H atom.

We may use

$$V = \frac{1}{4\pi\epsilon_0}\left[\frac{-e^2}{r_{2A}} - \frac{e^2}{r_{1B}}\right]$$

Which would lead us to the eigenfunction

$$\psi_A(2)\psi_B(1)$$

Any linear combination of the two eigenfunction $\psi_A(1)\psi_B(2)$ and $\psi_A(2)\psi_B(1)$ would also be a solution of the wave eqn.

Now we have to substitude the entire potential energy V given in eqn (i) and the wave in eqn (ii)

Linear combination of above

$$\psi_S = N_S[\psi_A(1)\psi_B(2) + \psi_A(2)\psi_B(1)] \rightarrow \text{symmetric}$$

$$\psi_a = N_a[\psi_A(1)\psi_B(2) - \psi_A(2)\psi_B(1)] \rightarrow \text{Anti-symmetric}$$

The normalization factor is given by

$$N_S = \frac{1}{\sqrt{2+2S}}$$

$$N_a = \frac{1}{\sqrt{2-2S}}$$

Where $S = \int \psi_A(1)\psi_B(2)\psi_A(2)\psi_B(1)\, d\tau_1 d\tau_2$

↑ overlap integral and is always less than 1.

Where first order perturbation calculation is carried out using the derivation from the potential energy for large R as perturbation function W, that is,

$$W=\frac{1}{4\pi\epsilon_0}\left[\frac{-e^2}{r_{2A}}-\frac{e^2}{r_{1B}}+\frac{e^2}{R}+\frac{e^2}{r_{12}}\right]$$

The following eigenvalue (energies) corresponding to the eigenfunction ψ_S and ψ_a are found;

$$E_S = 2E_H + \frac{K-J}{1+S}$$

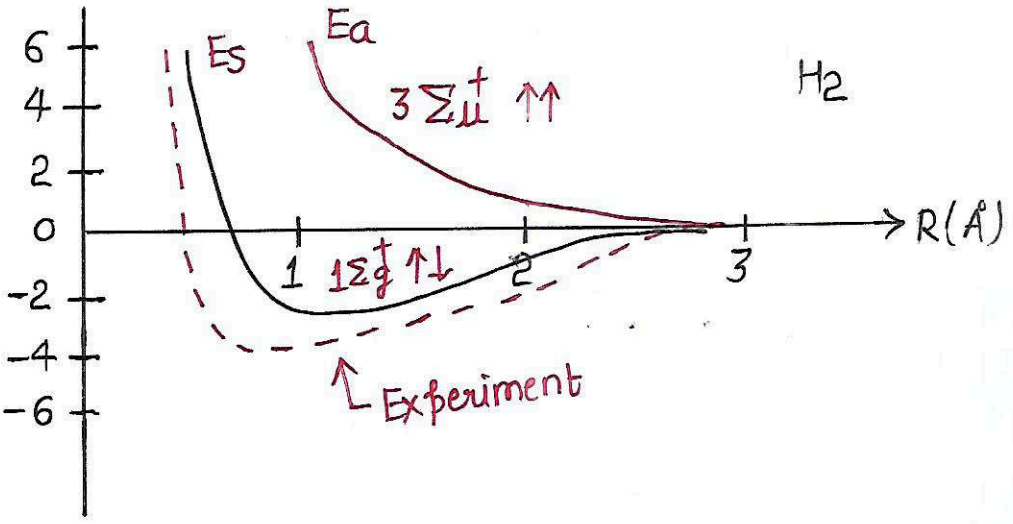
$$E_a = 2E_H + \frac{K-J}{1-S}$$

Where

$K = \int \psi_A(1)\psi_B(2) W \psi_A(a1)\psi_B(2) d\tau_1 d\tau_2$
Columb Integral

$J = \int \psi_A(1)\psi_B(2) W \psi_A(2)\psi_B(1) d\tau_1 d\tau_2$
Exchange Integral

The variation of E_S and E_a with R, as calculated Heilter Loudon, is shown below.



The product of a spatical eigenfunction ψ_S and ψ_A, which describes the coordinates of the e^- and a spin function β_S or β_a which describes the orientation of their spins.

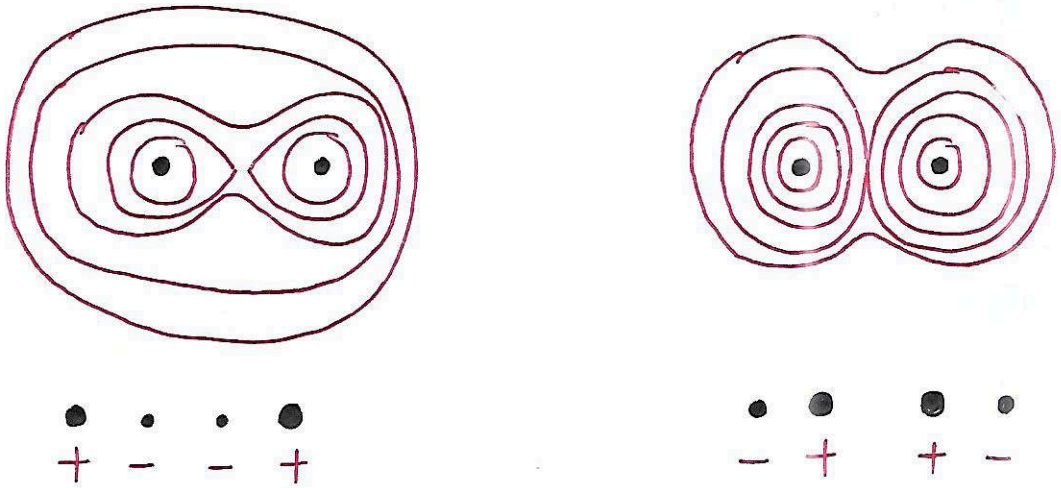
The acceptable total eigenfunction would be formed only as;

$$\Psi_{total} = \Psi_s \beta_a$$

$$\Psi_{total} = \Psi_a \beta_s$$

Which can also say that the Hydrogen atoms attaract each other when their electrons spins are antiparallel, and repel each other when the e^- spins are parallel.

The probability density distribution of the e^- of the H_2 molecule, calculated for $^1\Sigma$ and $^3\Sigma$ is shown graphically.



$^1\Sigma$ state (attaraction) the e^- clouds of the atoms (2) blend into each other.

$^3\Sigma$ state (repulsive), the e^- clouds remains almost completely separated.

> Born-Oppenheimer Approximation[5]

A dioatomic molecule is a stable arrangement of two atoms (nuclei and e^-) separated by a distance. If the two atoms forming the molecule are similar, the molecule is said to be homonuclear molecule, such as H_2, N_2, O_2, ... molecule. On the other hand; if the atoms are different, the makecule is said to be hetronuclear molecule such as HCl, CO, CN, ... molecule.

The energy levels in a molecule are much more than in an atom. Therefore, to a first approximation, the motion of the e^- at any instant is the same as if nuclei were fixed in space. Born and Oppenheimer presented quantum-mechanical equivalent of this approximation. They showed that the molecular schrodinger equation can be solved in two steps;

(i) Wave eqn showed in which nuclear coordinate appear simply as parameter.

(ii) Wave eqn for the motion of the nuclei(along) solved alone in which the characteristic eigenvalue of the electronic eqn occurs as part of the potential energy function of nuclear motion.

Let us formulate this approximation;

The complete Hamiltonian operator $\left(\frac{-h^2}{8\pi^2 m}\nabla^2 + V\right)$ for a molecule consisting of α-nuclei and i electrons is

$$H = \underbrace{-\sum_{\alpha}\frac{h^2}{8\pi^2 m_\alpha}\nabla_\alpha^2}_{\text{Kinetic energy of nuclei}} \underbrace{-\sum_{i}\frac{h^2}{8\pi^2 m}\nabla_i^2}_{\text{Kinetic energy of } e^-} + \underbrace{V_{nn} + V_{ne} + V_{ee}}_{\text{Potential energy function nuclear-electronic; nuclear-nuclear; electronic-electronic interaction}} \quad \ldots\ldots\ldots (1)$$

Wave equation

$$H\psi = E\psi \quad \ldots\ldots\ldots (2)$$

Hamiltonian for e^-

$$H_e = -\sum_{i}\frac{h^2}{8\pi^2 m}\nabla_i^2 + V_{ne} + V_{ee} \quad \ldots\ldots\ldots (3)$$

Let us represent the remaining term

$$H_n = -\sum_{\alpha}\frac{h^2}{8\pi^2 m_\alpha}\nabla_\alpha^2 + V_{nn} \quad \ldots\ldots\ldots (4)$$

$$H = H_n + H_e \quad \ldots\ldots\ldots (5)$$

Now Born and Oppenheimer make an assumption that the eigenvalues function ψ for the whole system may be expressed as a product $\psi_e\psi_n$

Hence

$$H\psi_e\psi_n = E\psi_e\psi_n \quad \ldots\ldots\ldots\ldots (6)$$

Then Put the values from eq^n(3)(4) and (5) in equation (6)

$$-\sum_\alpha \frac{\hbar^2}{8\pi^2 m_\alpha}\nabla_\alpha^2 \psi_e\psi_n - \sum_i \frac{\hbar^2}{8\pi^2 m}\nabla i^2\,\psi_e\psi_n + (V_{nn}+V_{ne}+V_{ee})\,\psi_e\psi_n = E\psi_e\psi_n$$

$\ldots\ldots\ldots (7)$

Now

$$\nabla_\alpha^2 \psi_e\psi_n = \psi_n \nabla_\alpha^2 \psi_e + \psi_e \nabla_\alpha^2 \psi_n + 2\nabla_\alpha \psi_e \nabla_\alpha \psi_n$$

$$\nabla_i^2\,\psi_e\psi_n = \psi_n \nabla_i^2\,\psi_e^*$$

Thus

$$\nabla_\alpha^2 \psi_e\psi_n = \psi_e \nabla_\alpha^2 \psi_n$$

$$\nabla_i^2\,\psi_e\psi_n = \psi_n \nabla_i^2 \psi_e$$

Then Put all values in eq^n(7)

Hence

$$-\psi_e \sum_\alpha \frac{\hbar^2}{8\pi^2 m_\alpha}\nabla_\alpha^2 \psi_n - \psi_n \sum_i \frac{\hbar^2}{8\pi^2 m}\nabla i^2\,\psi_e + (V_{nn}+V_{ne}+V_{ee})\,\psi_e\psi_n = E\psi_e\psi_n$$

$$-\frac{\psi_e}{\psi_e}\sum_\alpha \frac{\hbar^2}{8\pi^2 m_\alpha}\nabla_\alpha^2 \psi_n + \left[-\sum_i \frac{\hbar^2}{8\pi^2 m}\nabla i^2\,\psi_e + (V_{ne}+V_{ee})\,\psi_e\right] + V_{nn}\psi_e = E\psi_e$$

$$\left[\sum_\alpha \frac{-\hbar^2}{8\pi^2 m_\alpha}\nabla_\alpha^2 + E_e' + V_{nn}\right]\psi_n = E\psi_n$$

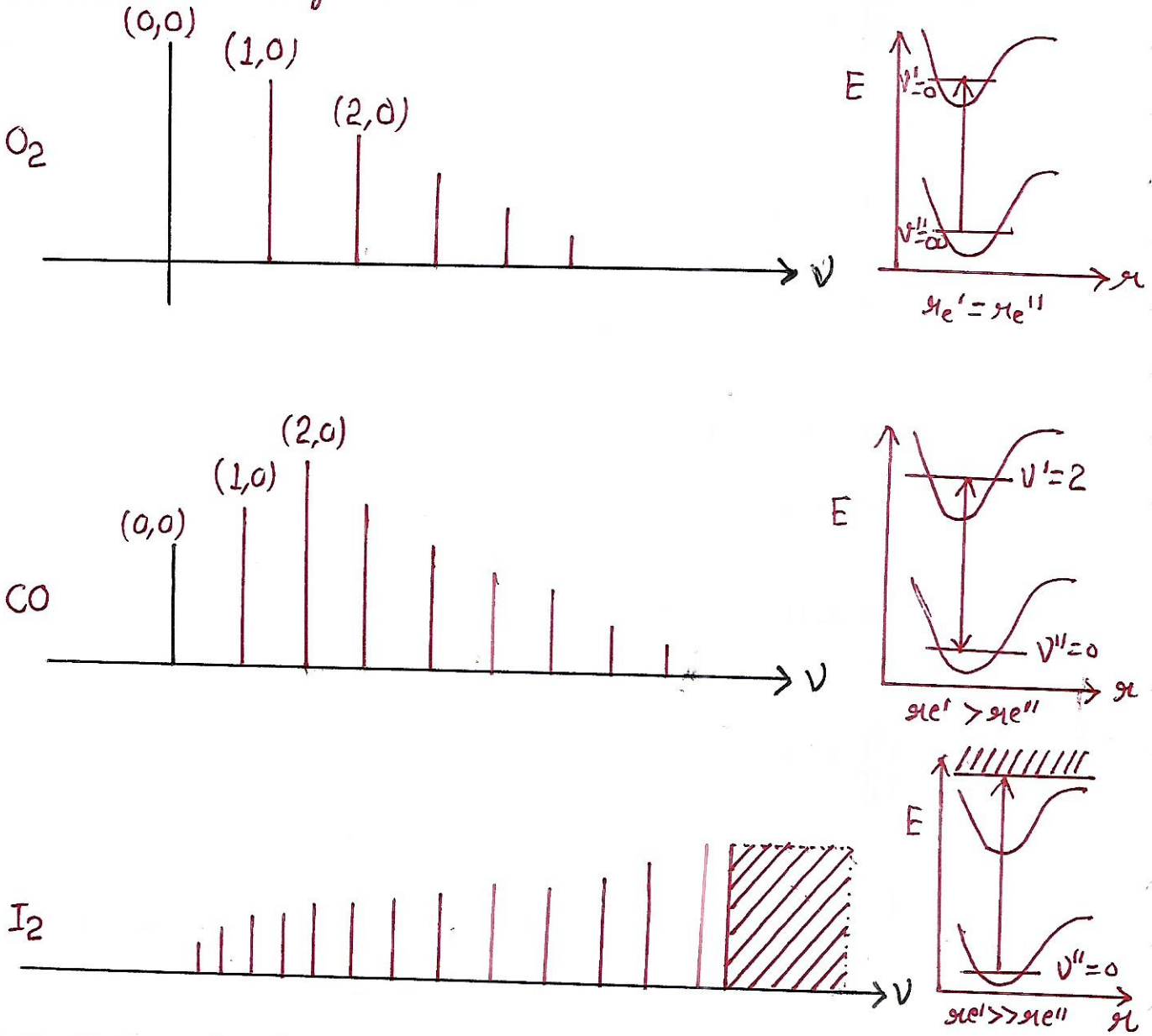
$$\boxed{[H_n + E_e']\psi_n = E\psi_n}$$

Thus the Born and oppenheimer approximation enables us to solve the complete molecular wave equation in molecular physics.

• Frank Condon Principle-

The distribution of intensity among the bands of electronic band system varies greatly from one molecule to other molecule.

There are three intensity distributions observed in the absorption ...



bands of O_2, CO, I_2 molecule.

In case of O_2, the (0,0) band is maximum intense while the successive band of the v' progressive (v''=0) appears with rapidly decreasing intensity.

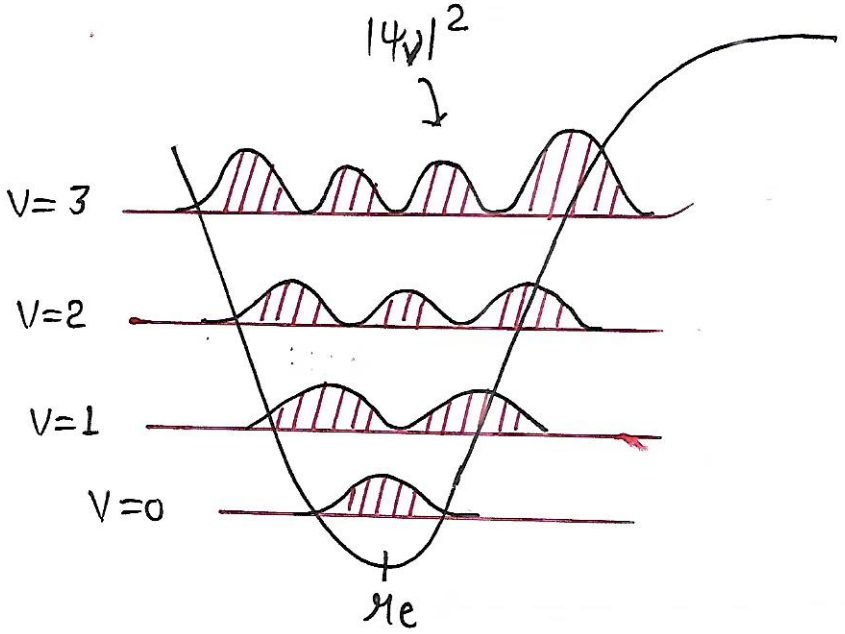
In the spectrum of CO, the intensity of bands along the progression first increase rapidly to the maximum and then gradually decreases.

In the case of I_2 molecule, a long progression is observed. Then intensity rises gradually and maximum reaches at very high v'-value sometimes in the continuum.

A different type of intensity distributions are explained by frank condon principle whose basis semi-classical idea is as follows;

A electronic transition in a molecule takes place so rapidly compared to the viberational motion of the nuclei that at the instantanious internuclear distance and the velocity of nuclei can be considered remaining unchanged during the electronic transition.

The diagram showing the potential energy curves of the two electronic states, the transitions must be represented by vertical lines:



Another important factor to be considered is the distributions of the probability density $|\psi_v|^2$ in various levels of each electronic state

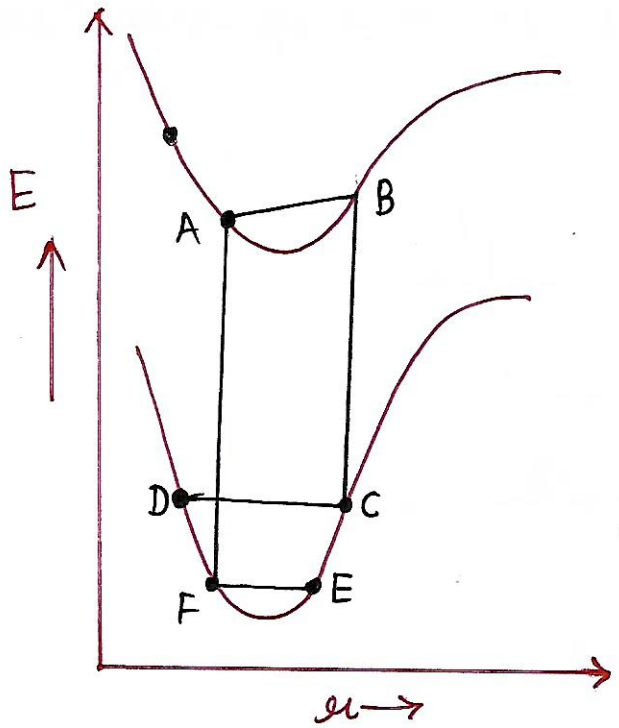
figure shows graphs of $|\psi_v|^2$ along the various viberational levels of the ground electronic state of a typical diatomic molecule.

Evidently, $|\psi_v|^2$ is a maximum at the mid-point of the $v=0$ level, and the near the turning points of the heigher viberational levels. Hence those transitions are more probabile which begin from or end at, the mid point of $v=0$ level and either turning point of the $v=1,2,3,..$ levels. This idea can be incorporated in the frank condon idea in the following statement :-

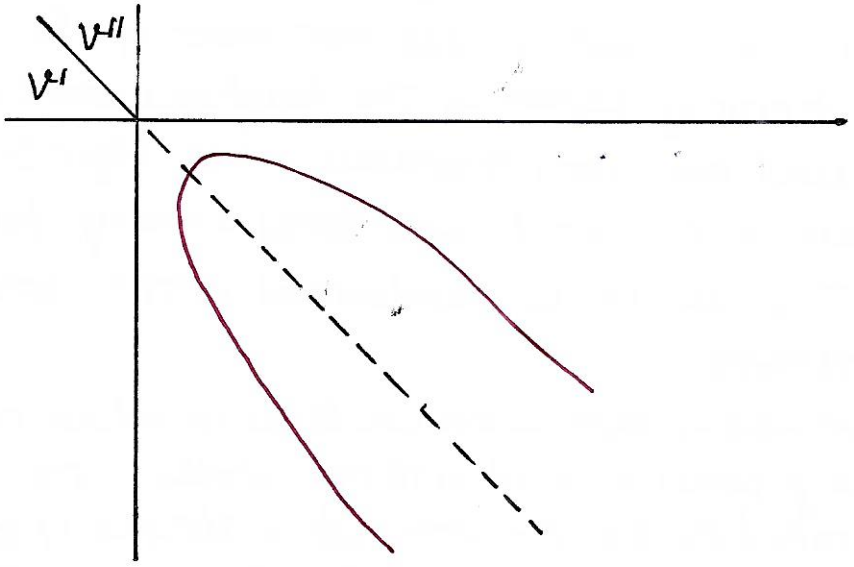
The most probable viberational transitions are those in which one of the following two turning points of a viberational levels of one electronic state lies at approximately the same internuclear distance at one of the two turning points of a level of other electronic state, except in case of $v=0$ levels for which the mid point rather than the turning point must be substituted.

#Condon Parabola-2

According to Frank Condon principle, the distribution in a band progression with $v'=0$ in emission corresponds exactly to that of a progression with $v''=0$ in absorption. There is an intensity maximum at a v'' value depending on relative position of a minima of the two potential curves. The greater the difference $r_e' - r_e''$, the larger the v'' value for the intensity maximum.

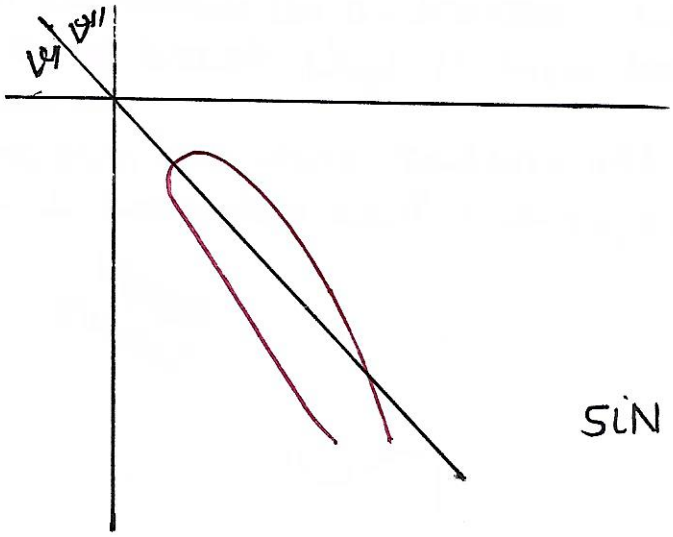


v' and v'' arrays are similar to a deslandres table and joint up the most intense bands, we obtain a parabolic curve whose axis is the principle diagonal. It is called condon parabola.



It represents the distribution characteristic deduced above.

e.g. :-



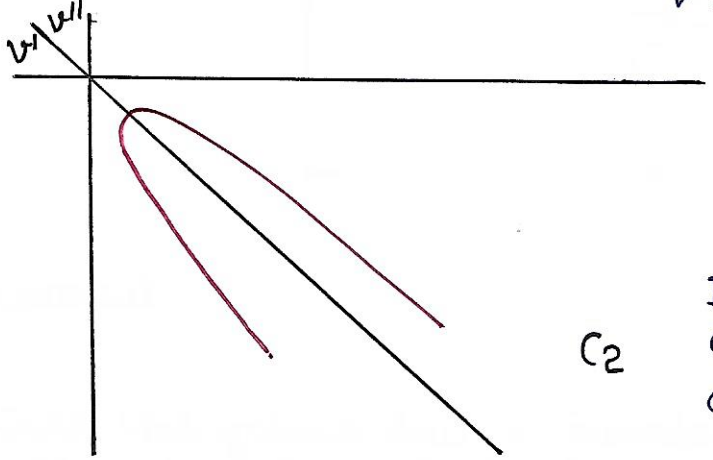
SiN

$\Delta v = ?$

⇓

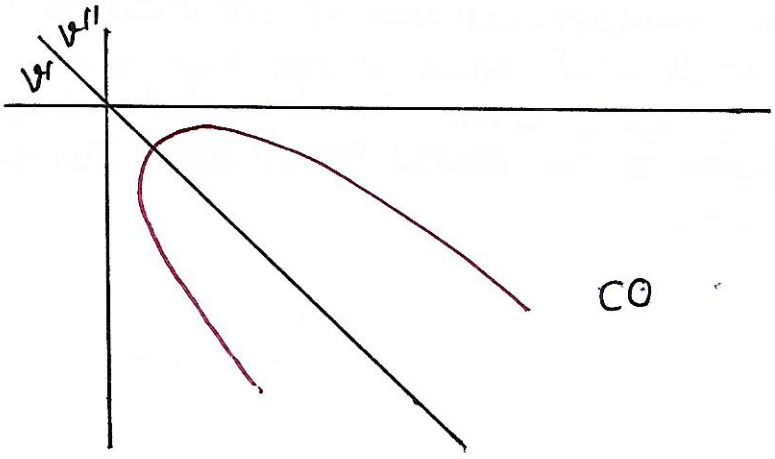
Thus we can obtain many informations about a molecule from a study of its condon parabola.

In cases like SiN ($r_e' = r_e''$), where the two maxima in each progression $v' =$ constant

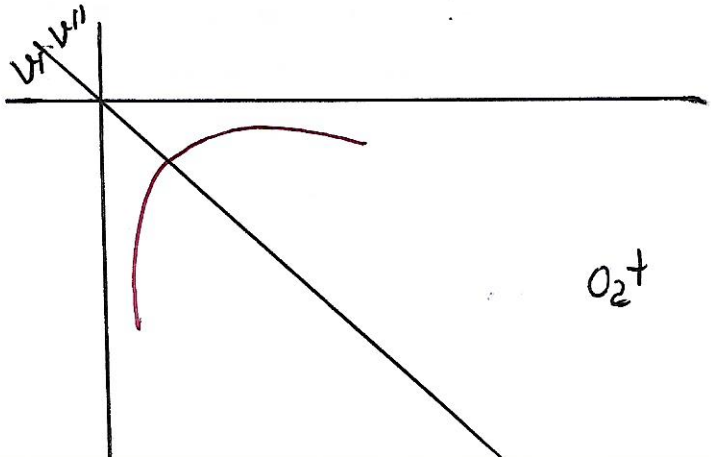


C_2

In cases like C_2, CO, $\Delta v = 0$ sequence appears quite strong but with only first few band detectable



CO

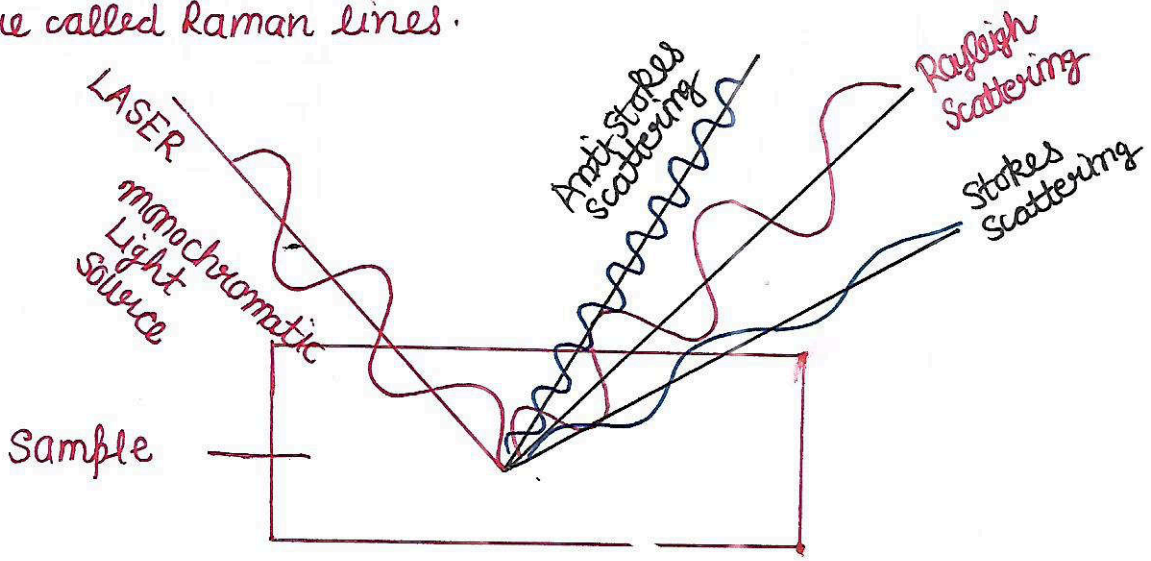


O_2^+

For O_2^+, the difference $r_e' \sim r_e''$ is appreciatly large

#Raman Effect-

When a strong beam of (light) visible or UV line-spectral light illuminates a gas, a liquid, or a transparent crystal, a small fraction of light scattered in all directions. The spectrum of the scattered light is light found to consist of changed frequencies as the incident beam and also certain weak lines of changed frequencies. These additional lines are called Raman lines.

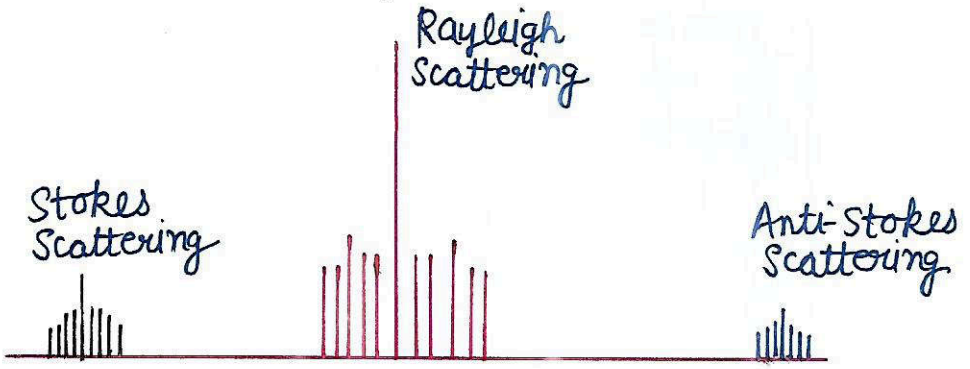


Fluoroscense

The Raman lines corresponding to each exciting line (Rayleigh) line occurs symmetrically on the both sides of exciting lines. The lines on the low frequencies side of the exciting line are called Stokes lines while those on the high frequencies side are called Anti-Stokes lines. The Anti Stokes lines are much weaker compared to the stokes Raman lines. This phenomena is called Raman Effect.

The wave no. displacements $\Delta\nu$ of the Raman lines from the corresponding exciting line are independent of the frequency of the exciting line. If another line source with a different line spectrum is used, other Raman lines are obtained for the same scattering substance. However, the displacement from the exciting lines are the same. For different scattering substance, however, the displacement are different. Thus the Raman displacement are characteristic of the scattering substance.

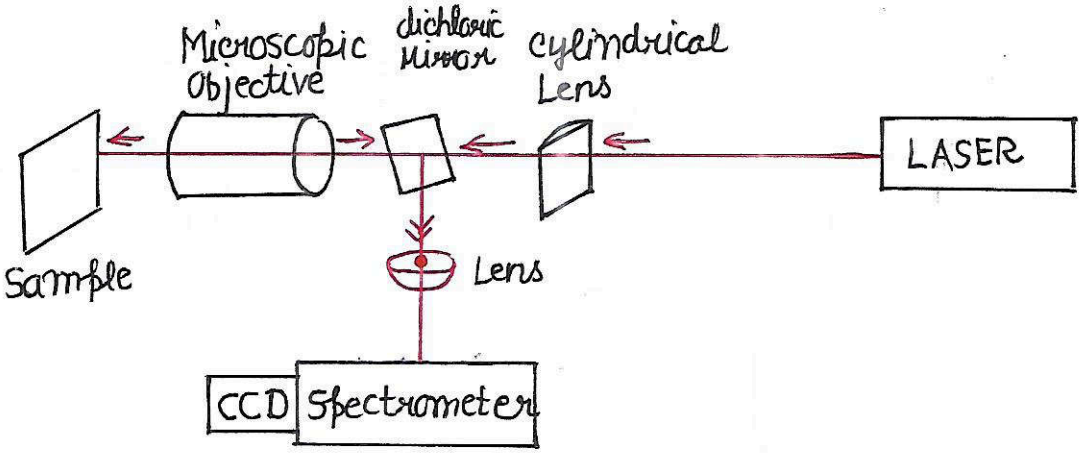
A typical Raman Effect spectrum is shown below.



1. Under low resolution, there are one stoke raman line and one anti-parallel Stokes Raman line, each having the same wave no. displacement $\Delta\nu$ w.r.to the exciting line. This is Viberational Raman Spectrum.
2. Under high resolution, the exciting line is formed to have on both side approximately equidistant lines. This is pure rotational Raman Spectrum. The spration b/w ~~b/w~~ successive rotational lines is very nearly twice the sepration b/w successive lines as far as IR spectrum of the molecule. The stokes and anti-stokes lines are referred above are also found to be bands composed of rotational fine structure. They constitute the viberational Raman spectra of this molecule.

>Experimental Arrangement-

Schematic of Raman Spectrometer is as following!

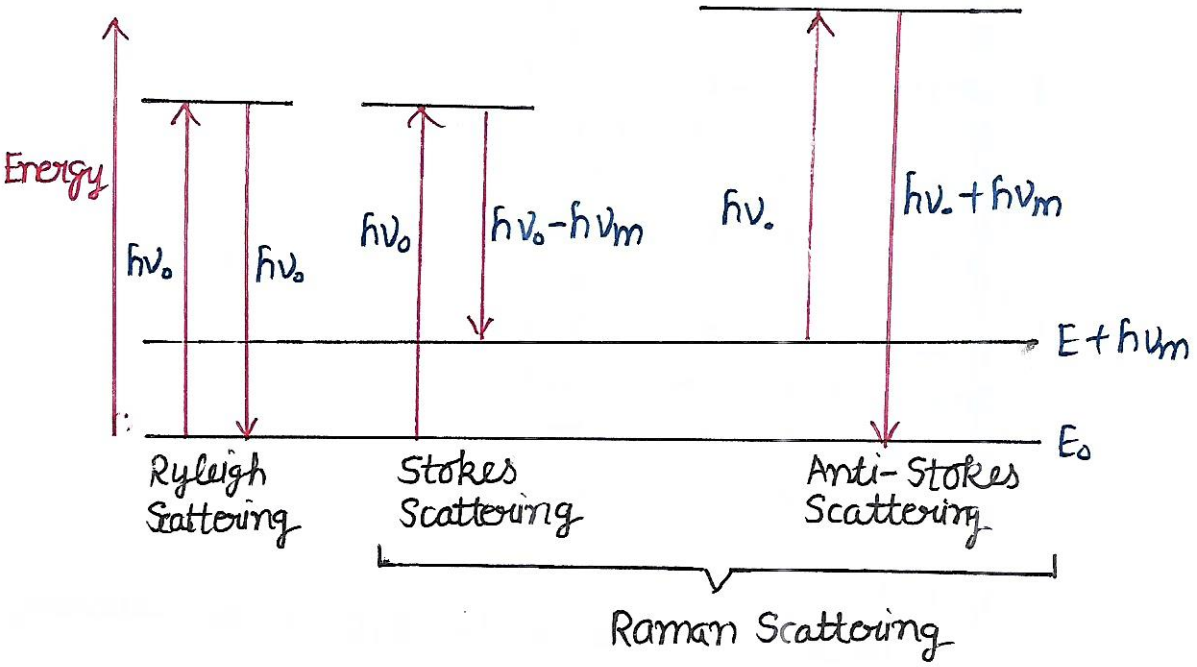


The displayed set-up focuses the illuminating LASER (colour Green) down to a line on the sample (Slit scanning mode), which can be replaced by a spot by removing cylindrical Lens. When a spot is illuminated at the sample, the Raman shifted light is filtered out from the LASER light by a dichloric mirror, and dispersed along a vertical on the

two dimensional CCD detector. In slit-scanning mode, many spectra are equired simultaniously: each position along the line on the sample produces a spectrum along the CCD detector.

> Quantum Theory of Raman Effect-

Raman Effect can be explained from quantum theory. According to this theory, light of wave no. ν is a bundle or packet of photons, each of energy $h c \nu$. When light falls on a scatterer, the photon collide with the molecule of the scatterer. There are three posibillities in such a collision.



(1) The collision may be elastic, this is, the scatterer molecule maintain its initial energy state and the photon is scattered with its energy unchanged giving rise to the Rayleigh line at wave no. ν.

(ii) The collision may be inelastic, in which the molecule in its initial energy state E'' takes energy from the photon and goes to a heigher energy state E', and the photon is consequently scattering with a smaller energy $hc\nu - \Delta E$ where

$$\Delta E = E'' - E'$$

This gives rise to a Raman line with a frequency

lower than the spectral line at a wave no. $\frac{h\nu - \Delta E}{hc}$, the wave no. shift being $\frac{\Delta E}{hc}$, such a raman line is called a stokes line.

(iii) The photon may collide with the scatterer molecule already in the exciting energy state E' and takes energy ΔE from it.

Wave no. $\frac{h\nu + \Delta E}{hc}$

Raman Shift $\Delta\nu = \frac{\Delta E}{hc}$

Such a Raman line is called Anti-Stokes Line.

Viberational Raman Spectra

$$R^{nm} = \int \psi_n^* P \psi_m \, d\tau$$

$$P = \alpha E$$

$$R^{nm} = E \int \psi_n^* \alpha \psi_m \, d\tau$$

$$\alpha = \alpha_0 + \left(\frac{d\alpha}{dx}\right)_0 x + \ldots\ldots$$

$$R^{v'v''} = E\alpha_0 \int \psi_{v'}^* \psi_{v''} \, dx + E\left(\frac{d\alpha}{dx}\right)_0 \int x \psi_{v'}^* \psi_{v''} \, dx$$

$$v' = v'' \pm 1$$

$$\Delta v = \pm 1$$

$$\boxed{\nu^{\nu}_{\text{Raman}} = \nu + \omega}$$

$$\frac{\text{Anti-Stokes intensity}}{\text{Stokes intensity}} = e^{-\omega hc/kT}$$

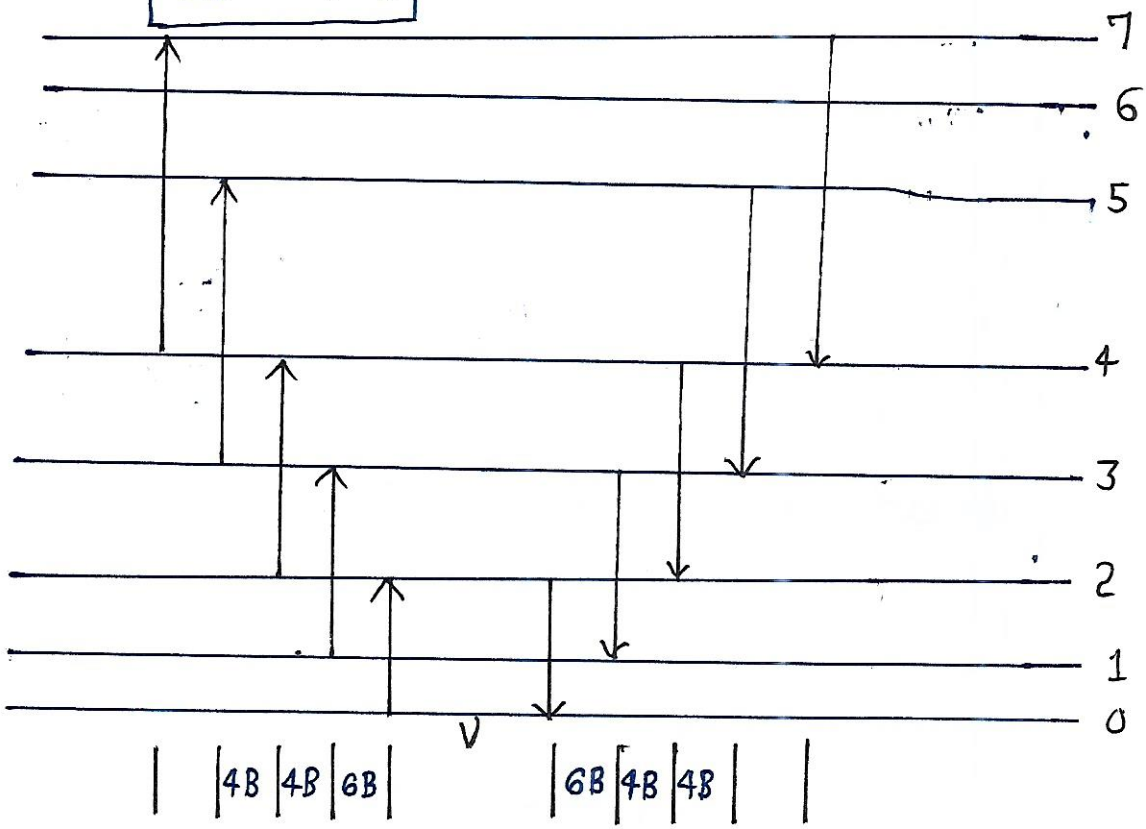
Viberational Raman Shift

$$|\Delta\nu|^{\nu}_{Raman} = \omega$$

Pure Rotational Raman Shift

$$J' = J'' \text{ or } J' = J'' \pm 2$$

$$\boxed{\Delta J = 0, \pm 2}$$



ν

Stokes Line

Anti-Stokes Line

$$|\Delta\nu|'_{Raman} = 4B\left(J + \frac{3}{2}\right) = 6B, 10B, 14B, 18B, \ldots\ldots$$

Quantum Mechanics

Origin and Introduction of Quantum Mechanics

1.
Origin and Introduction of Quantum Physics

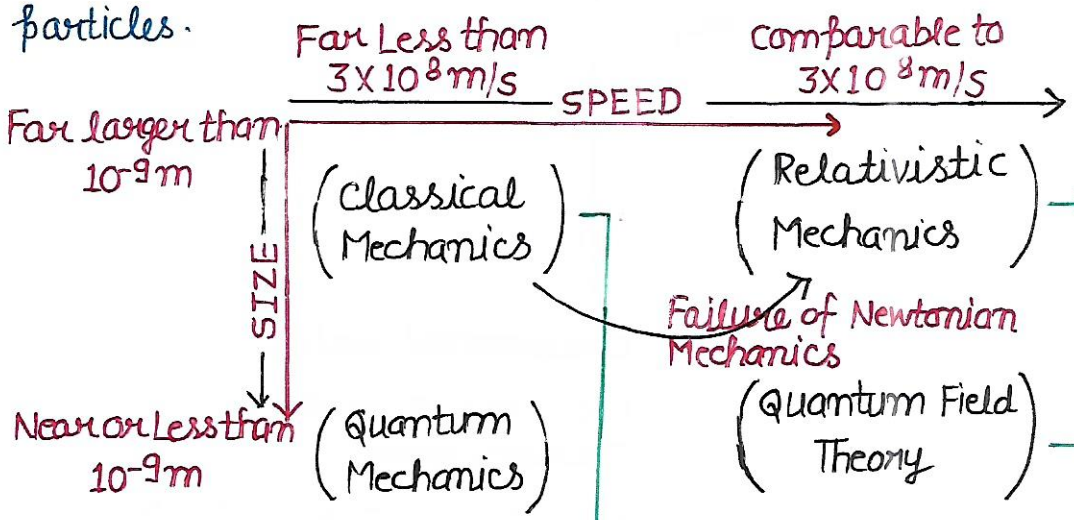
→ Quanta ÷ Invisible manifestation of a physical property, such as a force or angular momentum.

↓

Quantum Mechanics.

• Quantum Mechanics–

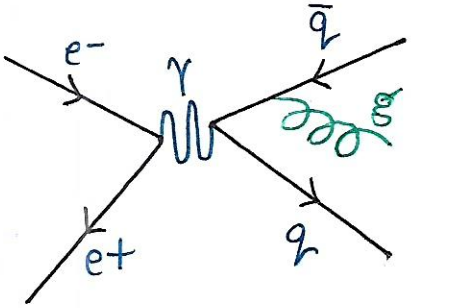
Quantum Mechanics (QM; also known as Quantum Mechanics, Quantum Physics, Quantum theory, Wave Mechanical Model or matrix mechanics), including quantum field theory, is a fundamental theory in physics which describes nature at the smallest scale of energy levels of atoms and subatomic particles.



In Physics, relativistic Mechanics refers to mechanical compatible with Special relativity and general relativity.

Quantum Field theory is the mathematical and conceptual framework for contemporary elementry particle physics

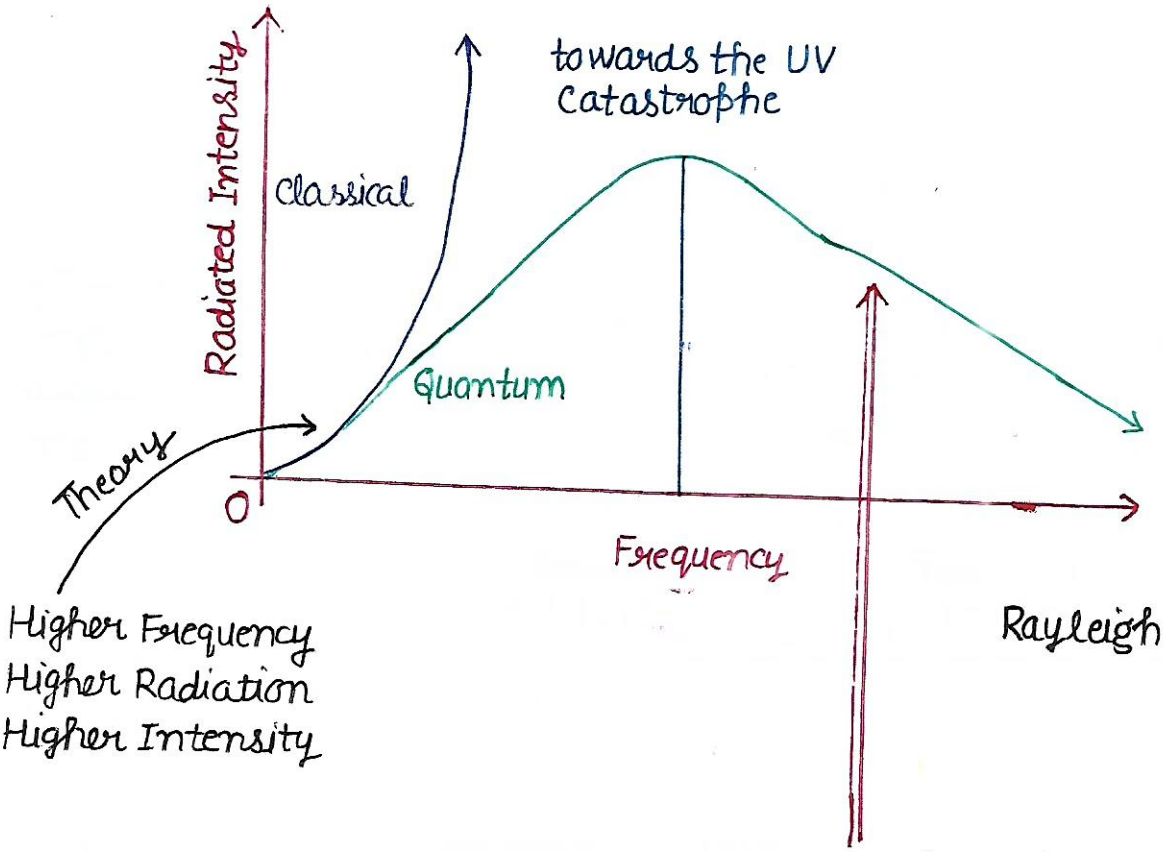
Classical Physics refers to the theories of Physics that predate modern, more complete or more widely acceptable theories.



Feynman diagram

• Development of QM-

Light is wave → before (Huygens)
Light is particle → later (Newton Prism experiment)
→ QM



Experimental Result

Frequency Increase
Intensity draw

• There is always a peak, this is UV catastrophe.

Higher Frequency ∝ Higher Intensity

↓

Contradition of conservation of Law of Energy

Missing eqn

↓

Max Plank

↓

Plank's Law

$E = hf$

Where E = Energy of Photon

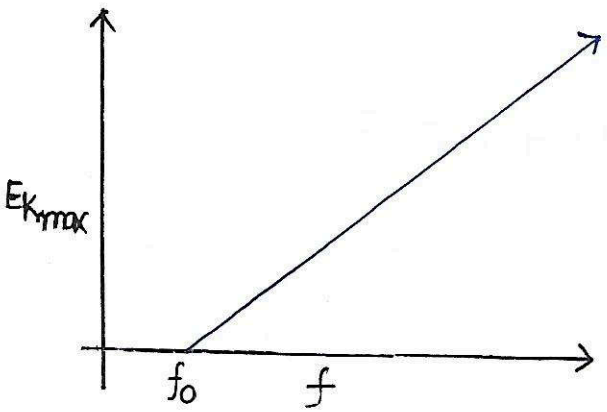
h = Plank's constant = $6.626 \times 10^{-34} m^2 Kg s^{-1}$

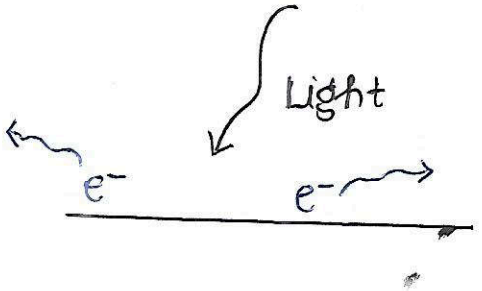
f = Frequency

DNA HELIX, VIRUS, WAVELENGTH	$10^{-9}m$
WAVELENGTH OF Y, X Rays	$10^{-12}m$
Atomic Nucleus, P, n	$10^{-15}m$
e^-, Quark, String	$10^{-35}m$
Quantum Foam	$10^{-35}m$

Quantum Foam → Quantum Physics

- Photoelectric Effect-





$K = h\nu - W$

$K + W = h\nu$

Both the wave theory and the particle theory of light predict that Light knocks e^- out of the metal.

- The failure of classical physics to explain several microscopic phenomena- such as blackbody Radiation, the photoelectric effect, atomic stability and atomic spectroscopy.

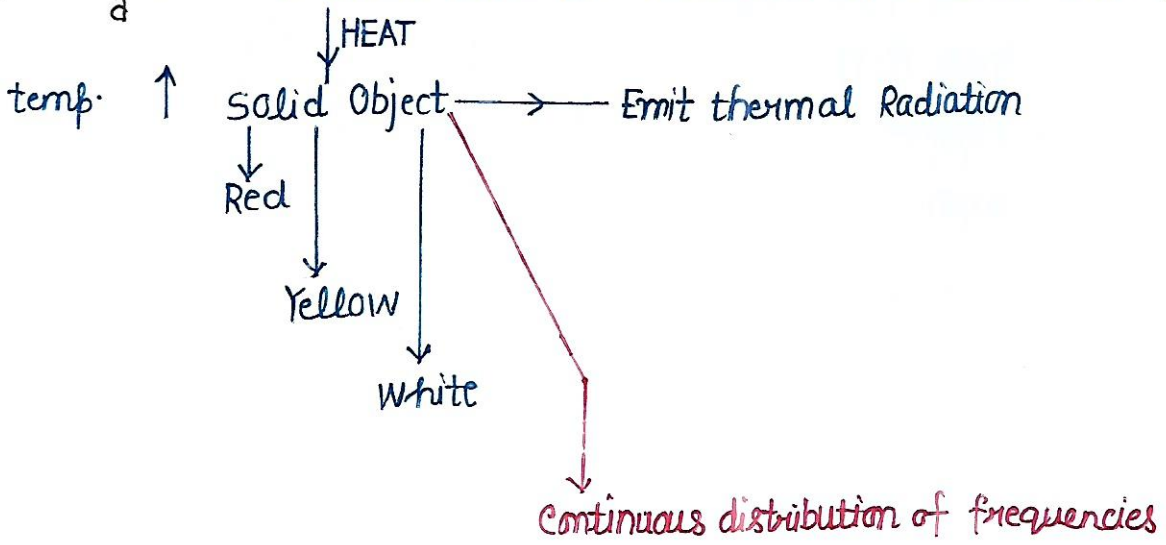
1900 ⟶ New Concept

↓

Quantum of Energy

• Particle Aspect of Radiation-

Blackbody Radiation- At issue here how radiation interacts with matter-

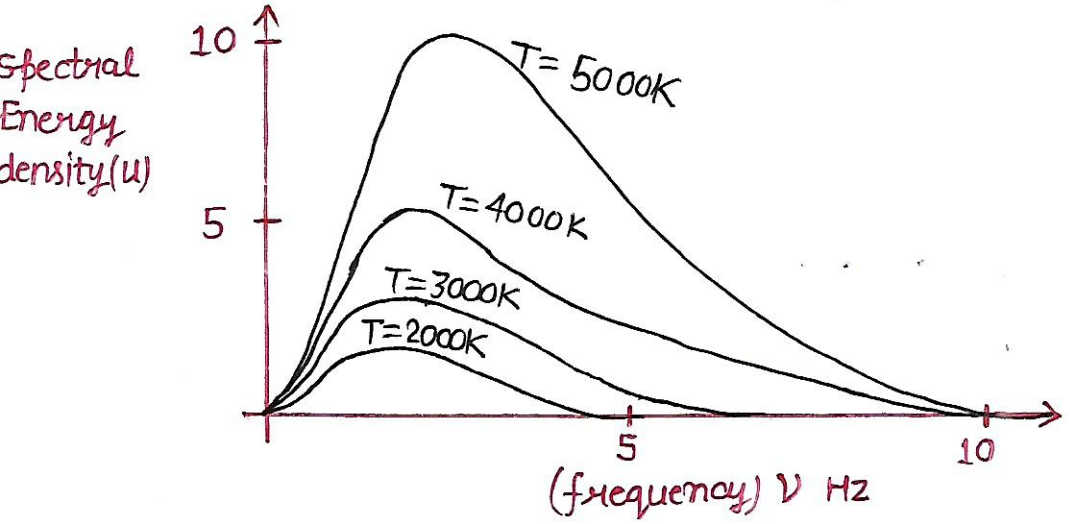


Problem ?
How energy gets exchanged between radiation and matter?

When radiation falls on an object, some of it might be absorbed and some reflected. An idealized blackbody is a material object that absorbs all the radiation falling on it, and hence appears as black under reflected when illuminated from outside.

Theoritically, blackbody is a perfect absorber as well as a perfect emitter of radiation.

A practical blackbody can be constructed by taking a hollow cavity whose internal walls perfectly reflect EM radiation.



Total intensity radiated by glowing object of temperature T.

$$P = a\sigma T^4$$

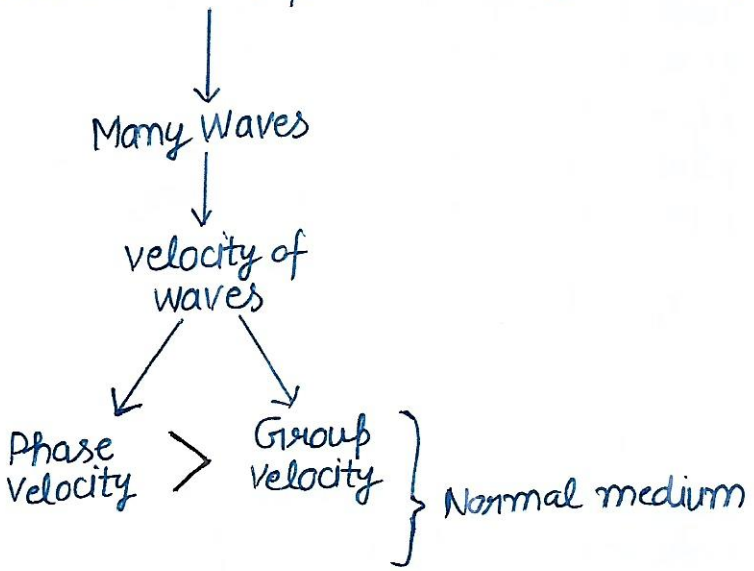
↓

Stephan Boltzmann Law

$\sigma = 5.67 \times 10^{-8}\ W m^{-2} K^{-4}$

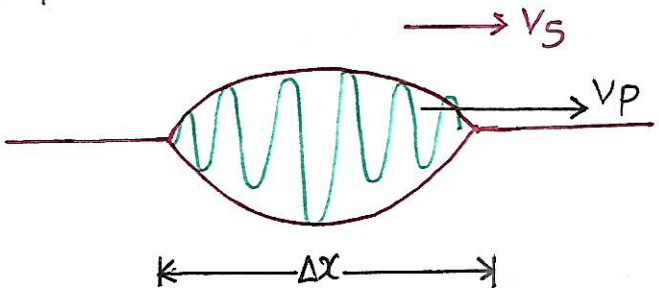
• Difference b/w Phase Velocity and Group Velocity-

According to quantum mechanics, particles sometimes behave like waves. In some cases, waves behave like particles. This property of particles and waves is known as wave particle duality. This dual nature of particles and wave allow us to represent a particle in terms of wave. Based on this concept, waves are used to represent particle as it is an essential step when we deal with particle in quantum physics.



#Group Velocity-

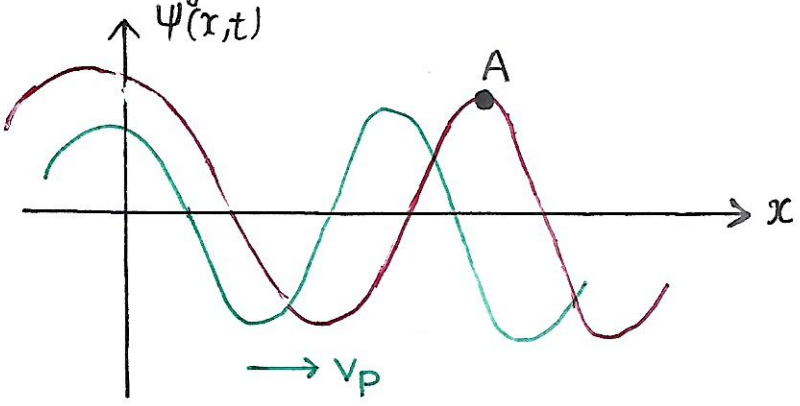
In quantum Mechanics, the idea of group velocity comes with the idea of wave packets or pulses. A wave packet can be obtained by adding up many waves having different wave no. and amplitude. So the position of the particle can be localized within a specific region.



The velocity of the group or wave packet is called the group velocity.

$$\text{Group velocity } v_g = \frac{d\omega}{dk}$$

Phase Velocity-



The phase velocity (Wave Velocity) of a wave is the velocity with which any given phase of the wave travels.

Mathematically, $V_p = \omega/k$

→ Normal medium $V_p > V_g$

→ Anomalous medium $V_g > V_p$

→ The concept of group velocity is very important when a particle is represented by waves. The phase velocity is important when we deal with individual waves.

→ In a wave packet, the envelope travels with the group velocity. Otherwhere the carrier wave travels with phase velocity.

→ $V_g = \frac{d\omega}{dk}$ and $V_p = \omega/k$

• Schrodinger Equation-

Imagine of particle of mass m, constrained to move along the x-axis, subject to some specific force $F(x,t)$. This program of classical mechanics is to determine the position of the particle at any given time $x(t)$. Once we know that, we can figure out the velocity ($v = dx/dt$), the momentum ($p = mv$), the kinetic energy ($T = (1/2)mv^2$) or any other dynamical variable of interest. And how do we get to go about determining $x(t)$. We apply newton's second Law $F = ma$

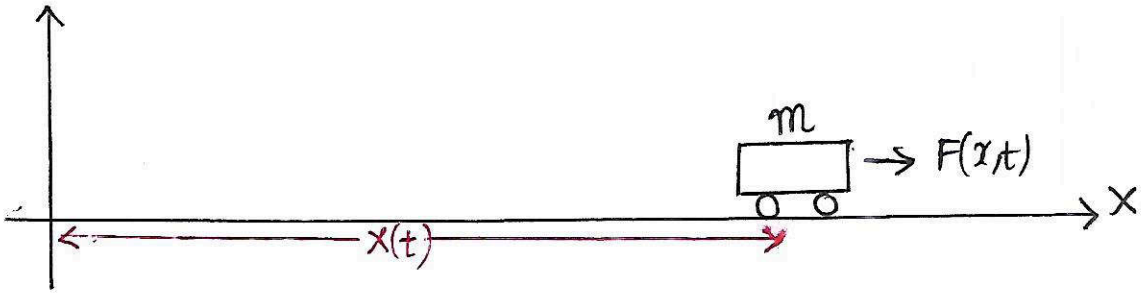
$$F = -\frac{\partial V}{\partial x} \leftarrow \text{As potential energy Function}$$

$$m\frac{d^2x}{dt^2} = -\frac{\partial V}{\partial x}$$

This together with approach and appropriate initial condition (typically the position and velocity at $t = 0$), determining $x(t)$.

Quantum Mechanics approaches this same problem quite differently. In this case what we're looking for the particle wave function, $\psi(x,t)$ and we get it by solving the schrodinger eqn

$$i\hbar\frac{\partial \psi}{\partial t} = -\frac{\hbar}{2m}\frac{\partial^2 \psi}{\partial x^2} + V\psi \ldots\ldots\ldots (1)$$



Here i is the square root of -1 and $\hbar$ is Plank constant - or rather, his original constant (h) is devided by 2π

$$\hbar = \frac{h}{2\pi} = 1.054572 \times 10^{-34}\ J \cdot S$$

The schrodinger equation plays a role logically analogue to Newton's second law; giving suitable initial conditions ($\psi(x,0)$), the schrodinger equation determines $\psi(x,t)$ for all the future time, just as in classical mechanics, newton's law determines $x(t)$ for all the future time

- **The Ehrenfest Theorem–** If quantum mechanics is to be more general than classical mechanics, it must contain classical mechanics as a limiting case. To illution the idea, let us look at the time evolution of the expectation values of the position and momentum operators, $\hat{\vec{R}}$ and $\hat{\vec{P}}$, of a particle moving in a potential $\hat{V}(\vec{r})$, and then compare these relations with their classical counterparts.

Since the position and the momentum observables do not depend explicitly on time, within the context of wave mechanism, the terms $(\partial\hat{\vec{R}}/\partial t)$ and $(\partial\hat{\vec{P}}/\partial t)$ are zero. Hence, inserting

$$\hat{H} = \frac{\hat{\vec{P}}^2}{2m} + \hat{V}(\hat{\vec{R}},t) \quad \ldots\ldots\ldots (1)$$

Time evolution of expectation values

$$\frac{d}{dt}\langle\hat{A}\rangle = \frac{1}{i\hbar}\langle[\hat{A},\hat{H}]\rangle + \left\langle\frac{\partial\hat{A}}{\partial t}\right\rangle \quad \ldots\ldots\ldots (2)$$

From eq^n (1) & (2)

$$\frac{d}{dt}\langle\hat{\vec{R}}\rangle = \frac{1}{i\hbar}\langle[\hat{\vec{R}},\hat{H}]\rangle = \frac{1}{i\hbar}\left\langle\left[\hat{\vec{R}},\frac{\hat{\vec{P}}^2}{2m}+\hat{V}(\hat{\vec{R}},t)\right]\right\rangle = \frac{1}{2im\hbar}[\hat{\vec{R}},\hat{\vec{P}}^2]$$

$$[\hat{\vec{R}},\hat{\vec{P}}^2] = 2i\hbar\vec{P}$$

$$\frac{d}{dt}\langle\hat{\vec{R}}\rangle = \frac{1}{m}\langle\hat{\vec{P}}\rangle \quad \ldots\ldots\ldots (3)$$

As $\frac{d\langle\hat{\vec{P}}\rangle}{dt}$, we can infer its expression from a treatment analogous to $\frac{d\langle\hat{\vec{R}}\rangle}{dt}$, using

$$[\hat{\vec{P}}, \hat{V}(\vec{R},t)] = -i\hbar\vec{\nabla}\hat{V}(\vec{R},t)$$

$$\frac{d}{dt}\langle\hat{\vec{P}}\rangle = \frac{1}{i\hbar}\langle[\hat{\vec{P}}, \hat{V}(\hat{\vec{R}},t)]\rangle = -\langle(\vec{\nabla}\hat{V}(\hat{\vec{R}},t))\rangle \quad \ldots\ldots\ldots(4)$$

Eq^{n}(3) & (4), expressing the time evolution of the expectation values of the position and momentum operator, are known as the Ehrenfest Theorem, or Ehrenfest equations. Their respective form are reminiscent of the Hamilton-Jacobi eq^{n} of classical mechanics,

$$\frac{d\vec{r}}{dt} = \frac{\vec{P}}{m}$$

$$\frac{d\vec{P}}{dt} = -\vec{\nabla}[V(\vec{r})]$$

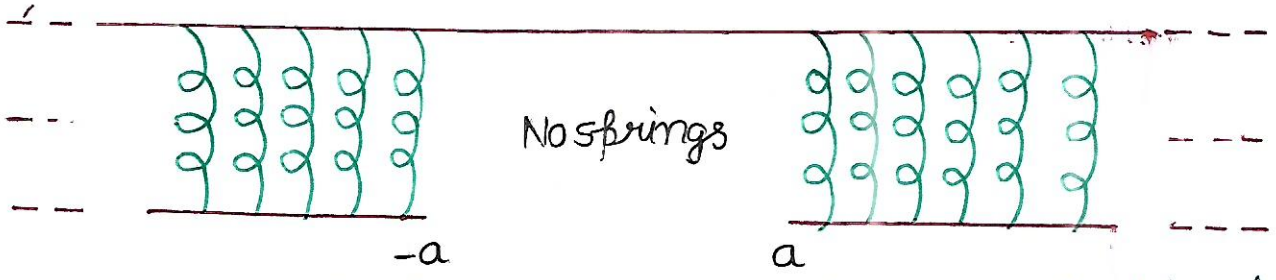
Which reduce to Newton's equation of motion for a classical particle of mass m, position $\vec{r}$, and momentum $\vec{P}$.

$$\frac{d\vec{P}}{dt} = m\frac{d^2\vec{r}}{dt^2} = -\vec{\nabla}V(\vec{r})$$

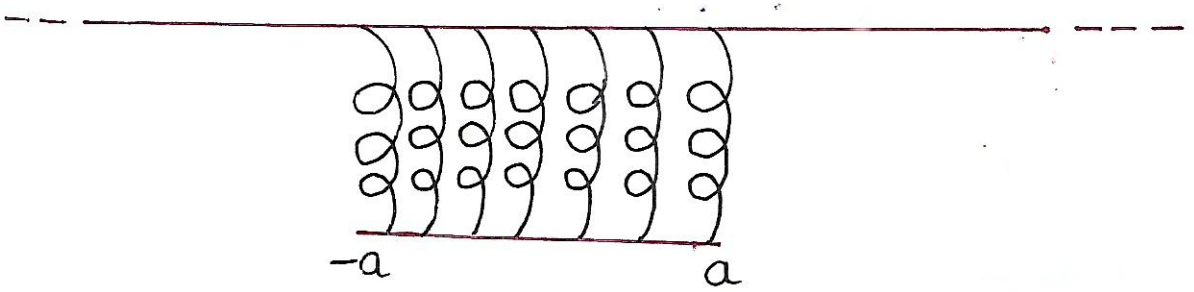
The center of the wave packet as moving like a classical particle when subject to a potential $V(\vec{r})$.

- Tunneling- APPLICATION ⇝

Consider a string/spring system that is the opposite of the system.



So now have springs in the middle region, and a normal string in the outer system region.



If a rightward tunneling wave comes in from the left, and if the frequency ω is less than the cut off frequency ω_s, then we will have an evanescent wave in

the middle region. And we will also rightward tunneling wave in the right region so the wave in the three regions like the general form,

$$x<-a \;:\; \psi_1(x) = A_1 e^{ikx} + B_1 e^{-ikx} \quad \ldots\ldots\ldots (1)$$

$$-a<x<a \;:\; \psi_2(x) = A_2 e^{kx} + B_2 e^{-kx} \quad \ldots\ldots\ldots (2)$$

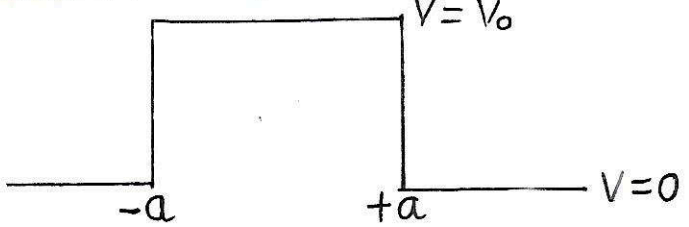
$$x>a \;:\; \psi_3(x) = A_3 e^{ikx} \quad \ldots\ldots\ldots (3)$$

We've given only the x dependance here. All of these waves are multiplied by the same function of t, namely $e^{-i\omega t}$. The ratio B_1/A_1 is the reflection cofficient, and the ratio A_3/A_1 is the transmission cofficient. Note that we can have both the exponentially growing and decaying terms in the middle region, because the boundary condition at $\pm\infty$ don't apply.

The frequency ω can take on any value. It need not take on certain discrete values as it did in the opposite string/Spring system analogues to the finite well above. There are two ways of seeing why this is true. First, it makes physical sense, because you are free to wiggle the string at whatever ω you want, when creating the incoming waves, $A_1 e^{i(kx-\omega t)}$. Second, it make mathematical sense if we count the number of unknowns and equations. In the finite-well case, we had seven unknowns; $A_1, A_2, A_3, B_1, B_2, B_3$, and E (or equivalently ω); And we had seven equations: Six boundary conditions and normalization condition. so we could solve for everything. In the present case, we have six unknowns A_1, A_2, A_3, B_1, B_2 and ω and have four eq^n. We have boundary conditions at each $x=\pm a$. So, we are free to give the incoming wave whatever amplitude and frequency we want it to have, which making sense. We can therefore solve for the reflection and transmission cofficients B_1/A_1 and A_3/A_1 in terms of ω. The calculation is rather messy, so we won't do it here. The situation isn't symmetric, since we're throwing things in front of the left, so we can't make easy use of the even/odd trick from problems or apps.

The important cofficients and points to note is that the cofficients A_3 is not equal to zero. This is unbelievable, because the string the middle region will move at least a little, so the right end of the wiggle the string in the right region, creating a rightward-traveling $A_3 e^{i(kx-\omega t)}$ wave. Intuitively, if the springs are weak, or if the width $2a$ of the middle region is small. Then virtually, all of the wave will make it through, so $A_3 \approx A_1$.

Let's now consider the analogue quantum system which is shown in figure.



$V(x)$ equals zero except for the $-a<x<a$ region where it equals V_0. If we send a particle in from the left, and if the energy is less than the height V_0 of the bump, then we have exactly the same situation as with the string/spring system. A_3 is non zero. This phenomenon is known as tunneling. The main application of tunneling, including α decay, flash memory and scanning tunneling microscopes.

- **Uncertainty Relations and Wave Packets-**

We want to show that the width of the wave packet $\psi_0(x)$ and the width of its amplitude $\phi(K)$ are not independent; they are correlated by a reciprocal relationship. As it turns out, the reciprocal relationship b/w the width in the x and K spaces has a direct connection to Heigenburg's uncertainity relation.

For simplicity, Let us illustrate the main ideas on the Gaussian wave packet treated in the previous example like

$$\phi(K) = \left(\frac{a^2}{2\pi}\right)^{1/4} \exp\left[-\frac{a^2}{4}(K-K_0)^2\right] \quad \ldots\ldots (1)$$

$$\psi_0(x) = \left(\frac{2}{\pi a^2}\right)^{1/4} e^{-x^2/a^2} e^{iK_0 x} \quad \ldots\ldots (2)$$

As displayed in

$$\frac{8\pi hc}{\lambda^6}\left[-5(1-e^{-hc/\lambda KT}) + \frac{hc}{\lambda KT}\right]\frac{e^{hc/\lambda KT}}{(e^{hc/\lambda KT}-1)^2} = 0$$

$|\psi_0(x)|^2$ and $|\phi(K)|^2$ are centered at $x=0$ and $K=K_0$, respectively. It is convenient to define the half width Δx and ΔK are corresponding to the half-maxima of $|\psi_0(x)|^2$ and $|\phi(K)|^2$. In this way, when x varies from 0 to $\pm\Delta x$ and K and K_0 to $K_0 \pm \Delta K$ the function $|\psi_0(x)|^2$ and $|\phi(K)|^2$ drop to $e^{-1/2}$

$$\frac{|\psi(\pm\Delta x, 0)|^2}{|\psi(0,0)|^2} = e^{-1/2}$$

$$\frac{|\phi(\pm K_0 \pm \Delta K)|^2}{|\phi(K_0)|^2} = e^{-1/2} \quad \ldots\ldots (3)$$

These equation combined with eq^n (1) & (2), lead to $e^{-2\Delta x^2/a^2} = e^{-1/2}$ and $e^{-a^2\Delta K^2/2} = e^{-1/2}$ respectively, or to

$$\Delta x = \frac{a}{2}$$

$$\Delta K = \frac{1}{a}$$

$$\Delta x \cdot \Delta K = \frac{1}{2}$$

Since $\Delta K = \Delta p/\hbar$, we have

$$\boxed{\Delta x \, \Delta p = \frac{\hbar}{2}}$$

This relationship shows that if the packet's width is narrow in x-space, its width in momentum space must be very broad, and vice versa.
The uncertainity principle makes a statement about the uncertainities in the position and momentum of a particle.

- Schrodinger 3D time dependent Equation (Mathematical Only) -

$$\nabla^2 \psi = \frac{1}{v^2} \frac{\partial^2 \psi}{\partial t^2} \quad \ldots\ldots \text{wave eq}^n$$

C.R. $$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} = \frac{1}{v^2} \cdot \frac{\partial^2 \psi}{\partial t^2} \quad \ldots\ldots (1)$$

v ↑ wave velocity

$$\psi(\vec{r}, t) = \psi_0(\vec{r})\, e^{-i\omega t}$$

$$\frac{\partial \psi}{\partial t} = -i\omega \psi_0(\vec{r})\, e^{-i\omega t}$$

$$\frac{\partial^2 \psi}{\partial t^2} = i^2 \omega^2 \psi_0(\vec{r}) e^{-i\omega t}$$

$$\frac{\partial^2 \psi}{\partial t^2} = -\omega^2 \psi \quad \ldots\ldots \text{Put in eq}^n (1)$$

$$\nabla^2 \psi = \frac{1}{v^2} (-\omega^2 \psi)$$

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

$$\nabla^2 \psi = -K^2 \psi \qquad \left[\because v = \frac{\omega}{K} \;\; K = \frac{\omega}{v} \right]$$

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

$$\nabla^2\psi = -\frac{4\pi^2}{\lambda^2}\psi$$

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

$$\nabla^2\psi = -\frac{4\pi^2}{h^2}p^2\psi$$

$\Rightarrow p = mv$

$$\nabla^2\psi = -\frac{4\pi^2 m^2 v^2}{h^2}\psi$$

We know

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

$$m^2v^2 = 2m(E-V)$$

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

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

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

Schrodinger time Independent Equation

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

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

$$\psi = \psi_0 e^{-i\omega t}$$

$$\frac{\partial\psi}{\partial t} = -i\omega\psi_0 e^{-i\omega t}$$

$$\omega = 2\pi\nu$$

$$E = h\nu$$

$$\nu = \frac{E}{h}$$

$$\frac{\partial \psi}{\partial t} = -i\left(2\pi\nu\right)\psi = -i\left(\frac{2\pi E}{h}\right)\psi$$

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

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

$$i\hbar\frac{\partial \psi}{\partial t} = E\psi$$

$$\boxed{\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = i\hbar\frac{\partial \psi}{\partial t}}$$ Schrodinger time depending Equation

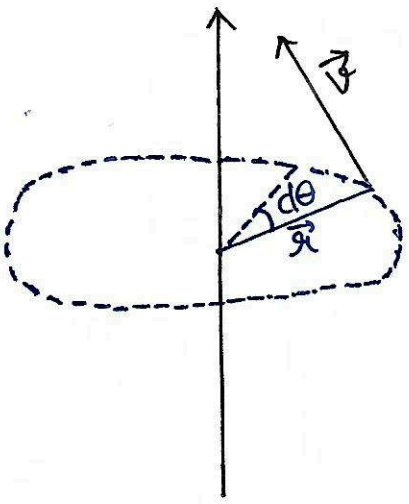
- Hydrogen Atom-

1. Orbital Magnetic Moment-

→ e^- revolve in orbits
↓
Motions of 2 type
↙ Orbital motion ↘ Axial motion

→ two magnetic moments
↙ Orbital magnetic moment ↘ Spin magnetic moment

- mass of e^- is m.
- Orbit radius is r.
- Charge on e^- is e considered.
↓
magnetic field generated



$$i = \frac{e}{T} \quad \ldots\ldots\ldots (1)$$

- Area of Loop is A

Then magnetic dipole moment

$$\mu_l = i \cdot A$$

$$\mu_l = \frac{e}{T} A$$

Areal Velocity

$$A = \frac{1}{2} r^2 \frac{d\theta}{dt}$$

$$A = \int_0^T \frac{1}{2} \left(r^2 \frac{d\theta}{dt} \right) dt$$

$$l = m r^2 \omega$$

$$\omega = \frac{d\theta}{dt}$$

$$l = m r^2 \frac{d\theta}{dt}$$

$$\frac{l}{m} = r^2 \frac{d\theta}{dt}$$

$$A = \int_0^T \frac{1}{2} \left(\frac{l}{m} \right) dt$$

$$A = \frac{1}{2} \frac{LT}{m}$$

$$A = \frac{LT}{2m}$$

Orbital magnetic moment

$$\mu_l = \frac{e}{T} \left(\frac{LT}{2m} \right)$$

$$\mu_l = \frac{e}{2m} (L)$$

$$\vec{\mu}_l = \left(\frac{e}{2m} \right) \vec{L}$$

$$L = \frac{lh}{2\pi}$$ [According to Quantum mechanics]

$$\mu_l = \frac{e}{2m}\left(\frac{lh}{2\pi}\right)$$

$$\mu_l = l\left(\frac{eh}{4\pi m}\right)$$

$$\frac{\mu_l}{L} = \frac{e}{2m}$$ } Gyromagnetic Ratio

$\frac{\mu_l}{L}$ ↓ constant

2. Bohr Magneton-

$$\mu_B = \frac{\mu_l}{l} = \frac{eh}{4\pi m}$$

$$\mu_B = 9.28 \times 10^{-24}\ Amp \cdot m^2$$

3. Spin magnetic moment-

$$\mu_S = 2\left(\frac{e}{2m}\right) L_S$$

$$L_S = S\frac{h}{2\pi}$$

$$\mu_S = 2\left(\frac{e}{2m}\right) S\frac{h}{2\pi}$$

$$\mu_S = 2S\left(\frac{eh}{4\pi m}\right)$$

$\left(\frac{eh}{4\pi m}\right)$ ↓ μ_B

$$\boxed{\mu_S = 2S\mu_B}$$

↓

$$S = \frac{1}{2}$$

$$\boxed{\mu_B = \mu_S}$$

- Linear Harmonic Oscillator (B.Sc. Basic)-
  - There is a particle called Linear Harmonic oscillator which start one dimensional motion in linear restoring force.

$F \propto x$ → displacement

↑

{ Linear Harmonic Oscillator Restoring Force }

$F = -Kx$ → Force constant

$F = -\frac{dV}{dx}$

- Classical eqn of particle of motion

$$m\frac{d^2x}{dt^2} = -Kx$$

$$\frac{d^2x}{dt^2} = -\frac{K}{m}x$$

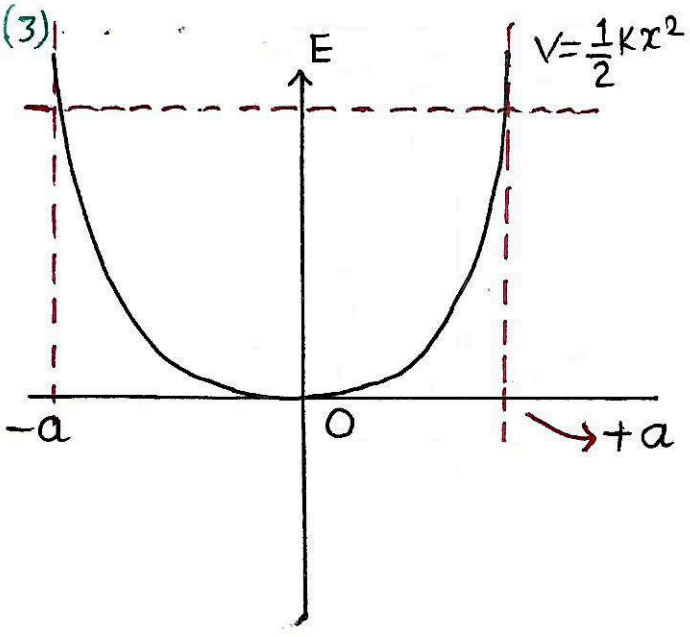
$$\frac{d^2x}{dt^2} + \omega^2 x = 0 \quad \ldots\ldots\ldots (1)$$

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

$$\nu = \frac{1}{2\pi}\sqrt{\frac{K}{m}} \quad \ldots\ldots\ldots (2)$$

- Potential Energy of particle

$$V = \frac{1}{2}Kx^2 \ldots (3)$$



One dimentional oscillator

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E-V)\psi = 0 \quad \ldots\ldots (4)$$

$$V = \frac{1}{2}Kx^2$$

$$\omega^2 = \frac{K}{m}$$

$$V = \frac{1}{2} m\omega^2 x^2 \quad \ldots\ldots (5)$$

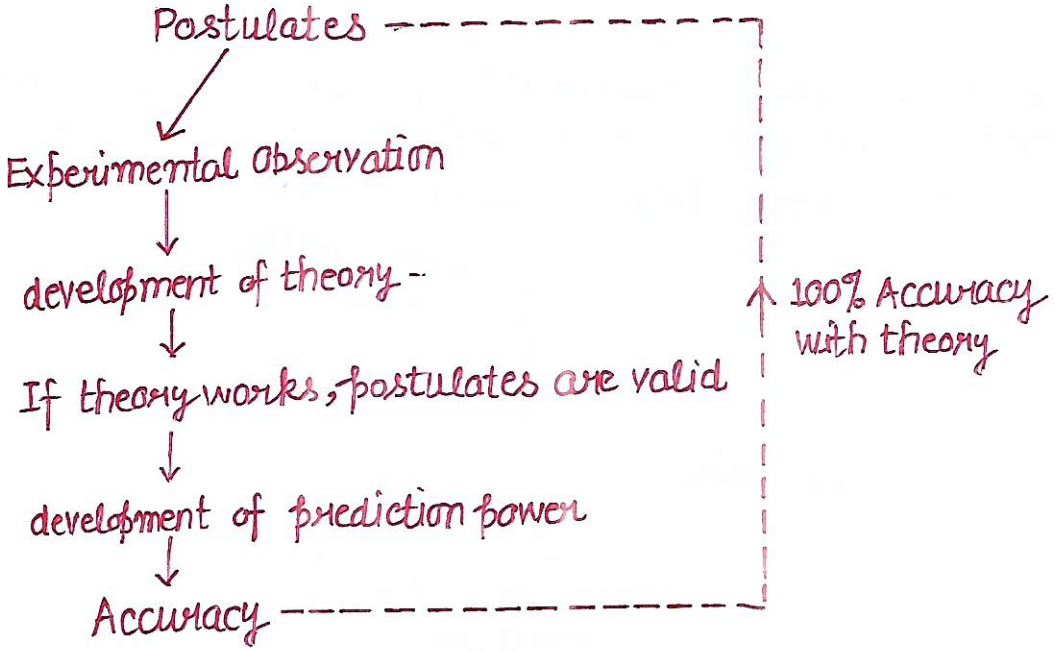
$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E - V)\psi = 0$$

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}\left(\frac{2mE}{\hbar^2} - \frac{m^2\omega^2 x^2}{\hbar^2}\right)\psi = 0$$

It is shrodinger eqn of oscillator.

- **Postulates of quantum Mechanics-**

The formulism of quantum Mechanics is based on a number of Postulates. These postulates are based on experimental observations. We will discuss how can be used to extract quantitative information about microphysical system. These postulates cannot be derived. They represent the minimal set of assumptions needed to develop theory of quantum mechanics.



↝ The basic posulates of Quantum Mechanics-

According to classical mechanics, the state of a particle is specified, at any time t, by two fundamental dynamical variables: the position $\vec{r}(t)$ and the momentum $\vec{p}(t)$. Any other physical quantity, relavant to the system, can be calculated in terms of these two dynamical variables. In addition, knowing these variables at a time t, we can predict, using for instance Hamilton's equation $dx/dt = \partial H/\partial p$ and $dp/dt = -\partial H/\partial x$, the values of these variables at any later time t'.

The quantum mechanics counterparts to these ideas are specified by postulates, which enable us to understand:

→ how a quantum state is described mathematically at a given time t,

→ how to calculate the various physical quantities from the quantum state and

→ knowing the system's state at a time t, how to find the state at any time t'; that is how to describe the time evolution of a system.

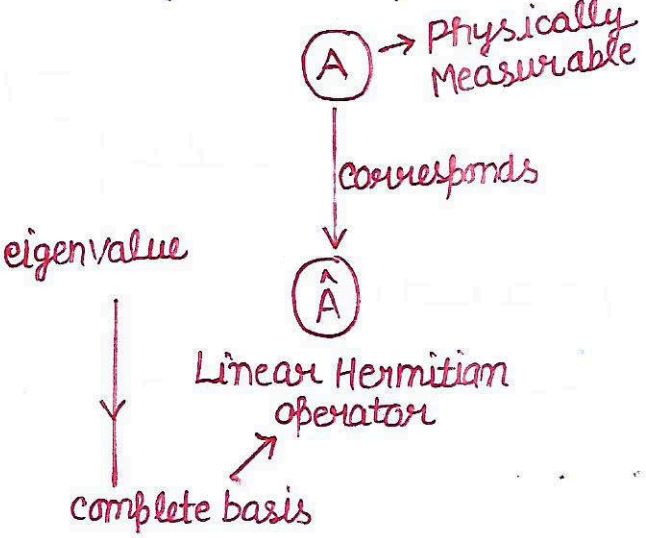
There are five postulates:

1. Postulates 1: State of a system

The state of any physical system is specified, at each time t, by a state vector $|\psi(t)\rangle$ in a Hilbert space $\mathcal{H}$; $|\psi(t)\rangle$ contains (and serves as the basic to extract) all the needed information about the system; Any superposition of state vector is also a state vector.

2. Postulate 2: Observables and operators

To every physically measurable quantity A, called an observable or dynamical variable, there corresponds a linear Hermitian operator $\hat{A}$ whose eigenvectors from a compelete basis.



3. Postulate 3: Measurements and eigenvalues of Operators

The measurement of an observable A may be represented formally by the action of $\hat{A}$ on a state vector $|\psi(t)\rangle$. The only possible result of such a measurement is one of the eigenvalues a_n (which are real) of an operator $\hat{A}$. If the result of a measurement of A on a state $|\psi(t)\rangle$ is a_n, the state of the system immediately after the measurement changes to $|\psi_n\rangle$:

$$\hat{A}|\psi(t)\rangle = a_n|\psi_n\rangle$$

$$\downarrow$$

$$a_n = \langle\psi_n|\psi(t)\rangle$$

$$\downarrow$$

a_n is the component of $|\psi(t)\rangle$ when projected onto the eigen vector $|\psi_n\rangle$.

Postulate 4 | Probabilistic outcome of measurements

- Discrete Spectra | When measuring an observable A of a system in a system state $|\psi\rangle$, the probability of obtaining one of the nondegenerate eigenvalues a_n of the corresponding operator $\hat{A}$ is given by

$$P_n(a_n) = \frac{|\langle\psi_n|\psi\rangle|^2}{\langle\psi|\psi\rangle} = \frac{|a_n|^2}{\langle\psi|\psi\rangle}$$

Where $|\psi\rangle$ is an eigenstate of $\hat{A}$ with eigenvalue a_n

m-degenerate

$$P_n(a_n) = \sum_{j=1}^{m} \frac{|\langle\psi_n^j|\psi\rangle|^2}{\langle\psi|\psi\rangle} \quad \ldots\ldots\ldots (1)$$

$$\boxed{P_n(a_n) = \frac{\sum_{j=1}^{m} |a_n^{(j)}|^2}{\langle\psi|\psi\rangle}}$$

- Continuous Spectra |

For $P_n(a_n)$ in eq^n(1), which is valid for discrete spectra, can be extended to determine the probability density that is measurement of $\hat{A}$ yields a value between a and a+da on a system which is initially in a state $|\psi\rangle$:

$$\frac{dP(a)}{da} = \frac{|\psi(a)|^2}{\langle\psi|\psi\rangle}$$

$$\frac{dP(a)}{da} = \frac{|\psi(a)|^2}{\int_{-\infty}^{+\infty} |\psi(a')|^2 da'}$$

Postulate 5 | Time Evolution of a system

The time evolution of the vector space $|\psi(t)\rangle$ of a system is governed by the time-dependent schrodinger equation

$$\boxed{i\hbar \frac{\partial |\psi(t)\rangle}{\partial t} = \hat{H} |\psi(t)\rangle}$$

where $\hat{H}$ is the Hamiltonian operator corresponding to the total energy of the system.

Remark |

The First four describes the system at a given time. The fifth postulate shows how this description evolves in time.

- The Superposition Principle |

The state of a system does not have to be represented by a single wave function; it can be represented by a superposition of two or more wave functions.

$$|\psi\rangle = \sum_i a_i |\psi_i\rangle$$

(a_i: complex number)

$$P = \left| \sum_i a_i |\psi_i\rangle \right|^2$$

$$P = \sum_i |a_i|^2$$

$$P = P_1 + P_2 + P_3 + \ldots\ldots$$

where $P_i = |a_i|^2$; P_i is the probability of finding the system in the state $|\psi_i\rangle$.

• A brief review of the foundation of quantum Mechanics-

Quantum mechanics is viewed most remarkable development in 20th century physics. Its point of view is completely different from classical mechanics. Its predictions are often probabilistic. It is development. It will develop the mathematical formulism and some applications. It will emphasize vector space (to which wavefunction) (belong to). These vector space are some time finite dimensional, but more often infinite dimensional. The pure mathematical basis for these is in Hilbert space but (fortunately!) no knowledge of this area is required now.

1. Wavefunction-

A wavefunction $\psi(x) : \mathbb{R}^3 \longrightarrow \mathbb{C}$ is associated with the single particle in 3D. ψ represents the state of a physical system for a single particle. If ψ is normalised, that is

$$|\psi|^2 = \int \underbrace{d^3x\,|\psi^2|}_{\text{Probability of finding a particle in the infinitesimal region } d^3x} = 1$$

Wave function is variable quantity that mathematically describes the wave characteristic of a particle

$\psi \rightarrow$ Greek

↘ No physical significance

$|\psi^2 \Rightarrow$ Physical significance

Statistical interpretation of a wave function which says that $|\psi(x,t)|^2$ is the probability density for finding the particle at point x, at time t. It follows that the integral of $|\psi|^2$ must be 1.

$$\int_{-\infty}^{+\infty} |\psi(x,t)|^2 \, dx = 1$$

① If $\psi(x,t)$ is a solution, so too is $A\psi(x,t)$, where is any constant. What we must do, then, is pick this undetermined multiplicative factor so as to ensure this eqn is satisfied

$$i\hbar \frac{\partial \psi}{\partial t} = \frac{-\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V\psi \quad \text{①}$$

$$\frac{d}{dt}\int_{-\infty}^{+\infty}|\psi(x,t)|^2\,dx = \int_{-\infty}^{+\infty}\frac{\partial}{\partial t}|\psi(x,t)^2|\,dx \quad \ldots\ldots(1)$$

By product rule

$$\frac{\partial}{\partial t}|\psi|^2 = \frac{\partial}{\partial t}(\psi^* \times \psi) = \psi^*\frac{\partial \psi}{\partial t} + \frac{\partial \psi^*}{\partial t}\psi \quad \ldots\ldots(2)$$

Schrodinger eqn

$$\frac{\partial \psi}{\partial t} = \frac{i\hbar}{2m}\frac{\partial^2 \psi}{\partial x^2} - \frac{i}{\hbar}V\psi \quad \ldots\ldots(3)$$

$$\frac{\partial \psi^*}{\partial t} = \frac{i\hbar}{2m}\frac{\partial^2 \psi^*}{\partial x^2} - \frac{i}{\hbar}V\psi^* \quad \ldots\ldots(4)$$

so put the value from eqn (3) & (4) in eqn (2)

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

$$\frac{\partial}{\partial t}|\psi|^2 = \frac{\partial}{\partial x}\left[\frac{i\hbar}{2m}\left(\psi^*\frac{\partial \psi}{\partial x} - \frac{\partial \psi^*}{\partial x}\psi\right)\right]$$

$$\frac{d}{dt}\int_{-\infty}^{+\infty}|\psi(x,t)|^2\,dx = \frac{i\hbar}{2m}\left[\psi^*\frac{\partial \psi}{\partial x} - \frac{\partial \psi^*}{\partial x}\psi\right]_{-\infty}^{+\infty}$$

$$\Downarrow$$

$$0$$

$$\boxed{\frac{d}{dt}\int_{-\infty}^{+\infty}|\psi(x,t)|^2\,dx = 0}$$

$$\Downarrow$$

And Hence that the integral is constant (independent to time); If ψ is normalized at $t=0$, it says that it will stay normalized for all future time.

$$\Downarrow$$

$$\boxed{\int_{-\infty}^{+\infty}|\psi(x,t)|^2\,dx = 1}$$

2. Superposition principle-

It is written on Left written Page.

3. Time dependence- |> depending on 5th Postulate

This is governed by the schrodinger Equation.

$$i\hbar\frac{\partial\psi}{\partial t} = H\psi$$

↑ Hamiltonian

$$i\hbar\frac{\partial\psi}{\partial t} = H\psi$$

$$i\hbar\frac{\partial}{\partial t}(\psi,\psi) = (\psi,H\psi)-(H\psi,\psi) = 0$$

Hamiltonian

If H is Hermition. H must be Hermition for the consistency of quantum mechanics.

$$(\psi,\psi) = 1 \text{ for all time.}$$

If we consider eigenfunction ψ_i of H with the eigenvalue Ei we can expand a general wavefunction as

$$\psi(x,t) = \sum_i a_i e^{\frac{-iEi}{\hbar}t}\psi_i(x)$$

↑

If ψ is normalized then the probability of finding the system with energy Ei is $|a_i|^2$.

Uncertainty Relations b/w two operators-

Let us consider two operators $\hat{A}$ and $\hat{B}$. Now it is given a formal derivation of Heigenberg's uncertainty relations. Let $\langle\hat{A}\rangle$ and $\langle\hat{B}\rangle$ denote the expectation values of two Hermitian operators $\hat{A}$ and $\hat{B}$ with respect to a normalized state vector.

$$|\psi\rangle : \langle\hat{A}\rangle = \langle\psi|\hat{A}|\psi\rangle \text{ and } \langle\hat{B}\rangle = \langle\psi|\hat{B}|\psi\rangle.$$

Then

$$\Delta\hat{A} = \hat{A} - \langle\hat{A}\rangle$$
$$\Delta\hat{B} = \hat{B} - \langle\hat{B}\rangle \quad \ldots\ldots\ldots (1)$$

$$(\Delta\hat{A})^2 = \hat{A}^2 - 2\hat{A}\langle\hat{A}\rangle + \langle\hat{A}\rangle^2$$
$$(\Delta\hat{B})^2 = \hat{B}^2 - 2\hat{B}\langle\hat{B}\rangle + \langle\hat{B}\rangle^2$$

$$\langle\psi|\Delta\hat{A}|\psi\rangle = \langle(\Delta\hat{A})^2\rangle = \langle\hat{A}^2\rangle - \langle\hat{A}\rangle^2$$
$$\langle\psi|\Delta\hat{B}|\psi\rangle = \langle(\Delta\hat{B})^2\rangle = \langle\hat{B}^2\rangle - \langle\hat{B}\rangle^2$$

$$\Delta A = \sqrt{\langle (\Delta \hat{A}^2) \rangle} = \sqrt{\langle \hat{A}^2 \rangle - \langle \hat{A} \rangle^2}$$
$$\Delta B = \sqrt{\langle \Delta \hat{B}^2 \rangle} = \sqrt{\langle \hat{B}^2 \rangle - \langle \hat{B} \rangle^2}$$

Let us write the action of the operator on any staze as follows:

$$\langle x \rangle = \Delta \hat{A} |\psi\rangle = (\hat{A} - \langle \hat{A} \rangle) |\psi\rangle$$
$$\langle \phi \rangle = \Delta \hat{B} |\psi\rangle = (\hat{B} - \langle \hat{B} \rangle) |\psi\rangle$$

The schwarz inequality for the state $|x\rangle$ and $|\phi\rangle$ is given by

$$\langle x|x\rangle \langle \phi|\phi\rangle \geq |\langle x|\phi\rangle|^2 \quad \ldots\ldots\ldots (2)$$

Since ΔA and ΔB are Hermitian.
$\Delta \hat{A}$ and $\Delta \hat{B}$ also be Hermition.

$$\Delta \hat{A}^\dagger = \hat{A}^\dagger - \langle \hat{A} \rangle = \hat{A} - \langle \hat{A} \rangle = \Delta \hat{A}$$
$$\Delta \hat{B}^\dagger = \hat{B}^\dagger - \langle \hat{B} \rangle = \hat{B} - \langle \hat{B} \rangle = \Delta \hat{B}$$

Thus we can show the following relations:

$$\langle x|x\rangle = \langle \psi | (\Delta \hat{A})^2 | \psi \rangle$$
$$\langle \phi|\phi\rangle = \langle \psi | (\Delta \hat{B})^2 | \psi \rangle$$
$$\langle x|\phi\rangle = \langle \psi | \Delta \hat{A} \Delta \hat{B} | \psi \rangle \quad \ldots\ldots\ldots (3)$$

Now by eqn (2)

$$\langle (\Delta \hat{A})^2 \rangle \langle (\Delta B)^2 \rangle \geq |\langle \Delta \hat{A} \Delta \hat{B} \rangle|^2$$

$$\Delta A \Delta B = \frac{1}{2} [\Delta \hat{A}, \Delta \hat{B}] + \frac{1}{2} [\Delta \hat{A}, \Delta \hat{B}]$$

↑ Hermition Operator — ↑ Real Value

↑ Anti Hermitian Operator — ↑ Imaginary value

$$\Delta B \Delta A = \frac{1}{2} [\hat{A}, \hat{B}] + \frac{1}{2} [\Delta \hat{A}, \Delta \hat{B}]$$

$$|\Delta \hat{A} \Delta \hat{B}| = \frac{1}{4} |\langle [\hat{A}, \hat{B}] \rangle|^2 + \frac{1}{4} |\langle \{\Delta \hat{A}, \Delta \hat{B}\} \rangle|^2$$

$$|\langle \Delta\hat{A}\Delta\hat{B} \rangle|^2 \geq \frac{1}{4}|\langle [\hat{A},\hat{B}] \rangle|^2$$

$$\langle (\Delta\hat{A})^2 \rangle \langle (\Delta\hat{B})^2 \rangle \geq \frac{1}{4}|\langle [\hat{A},\hat{B}] \rangle|^2$$

$$\boxed{\Delta A \, \Delta B \geq \frac{1}{2}|\langle [\hat{A},\hat{B}] \rangle|^2}$$

The uncertainty relations plays an important role in the formulism of quantum mechanics. Its application to position and momentum operator leads to the Heigenberg uncertainty relation which represents the open cornerstones of quantum mechanics.

? Find the components of Heigenburg uncertainty relation;

$\hat{X}$ → Position operator

$\hat{P}_x$ → Momentum operator

$$\Delta x \, \Delta p_x \geq \frac{1}{2}|\langle (\hat{X},\hat{P}_x) \rangle|$$

$$= i\hbar I$$

$$\Delta x \, \Delta p_x \geq \frac{1}{2} i\hbar I$$

$$\boxed{\Delta x \Delta p_x \geq \frac{\hbar}{2}}$$

The schrodinger Equation-

A system of N particles is characterised by the position and momentum variables $x_1, x_2, x_3, \ldots x_N$ and $p_1, p_2, p_3, \ldots p_N$. Its energy is given by the Hamiltonian function H depending in general on all the position and momentum variables.

$$E = H(x_1, x_2, \ldots x_N, p_1, p_2, \ldots p_N, t) \quad \ldots\ldots (1)$$

Time depending external force is acting on the system.

$$E \longrightarrow i\hbar \frac{\partial}{\partial t}$$

$$p_i \longrightarrow i\hbar \nabla_i$$

↑ gradient operator taken with respect to the position

$$\nabla_i = \left(\frac{\partial}{\partial x_i}, \frac{\partial}{\partial y_i}, \frac{\partial}{\partial z_i}\right)$$

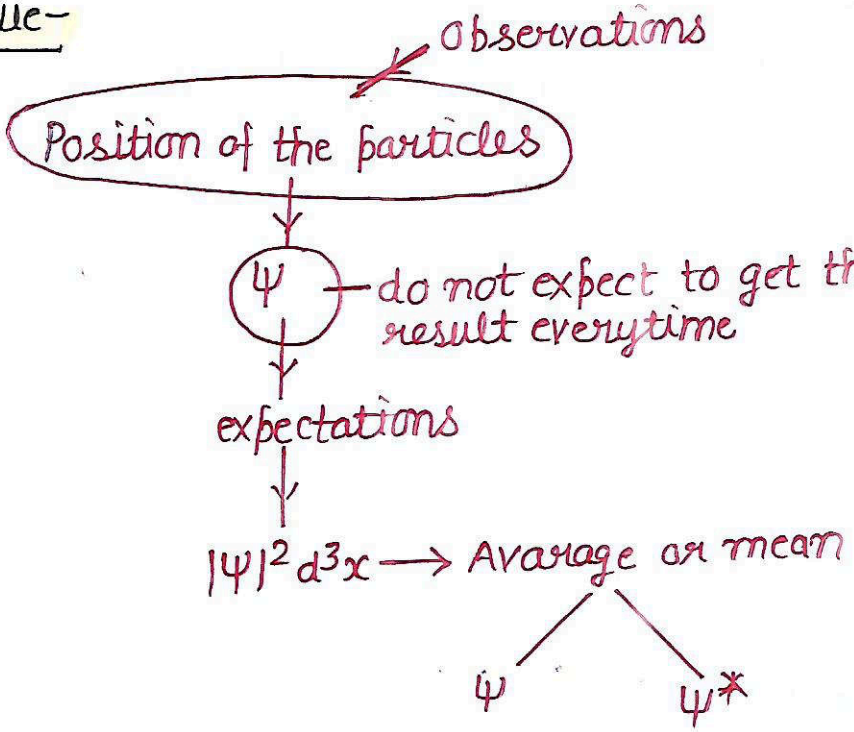
Using the operator correspondance, we can write down the eqn for the wave function ψ as

$$i\hbar \frac{\partial \psi(x_1, x_2, x_3 \ldots . x_N; t)}{\partial t}$$

$$E = H(x_1, x_2, \ldots . x_N, -i\hbar\nabla_1 - i\hbar\nabla_2, \ldots . -i\hbar\nabla N)\, \psi(x_1, x_2, \ldots x_N; t)$$

This is general form of the schrodinger equation.

#Expectation Value-



Suppose now, we can make a large no. of observations of the position of the particle. Through we can take care to ensure that the particle has the same wave function ψ before each observation, we do not expect to get the same result each time. What is expected is that, of all the observations, a fraction equal to $|\psi|^2 d^3x$ will show the particle as show

the particle as being within the volume element d^3x. Therefore if we take the mean or average of the observed values of the position vectors, the result is expected to be

$$\langle x \rangle = \int x |\psi|^2 d^3x = \int \psi^* x \psi \, d^3x$$

This eqn shows the expected mean value of the particle.

One dimensional Potential Step-

A Particle that is free everywhere, but beyond a particular point, say $x=0$, the potential increases sharply (i.e., it becomes repulsive or attaractive). A potential of this type is called a potential step.

$$V(x) = \begin{cases} 0 \, , & x<0, \\ V_0 \, , & x \geq 0, \end{cases}$$

We try to analyze the dynamics of the flux of particles (all having the same mass m and moving with the same velocity) moving from left to the right. We are going to consider two cases.

$E > V_0$ $E < V_0$

(a) Case $E > V_0$

The particle is free everywhere for $x<0$ and feel a repulsive potential V_0 that starts at $x = 0$ and stays flat for $x>0$. Let us analyze the dynamics of this flux of particles classically and then quantum mechanically.

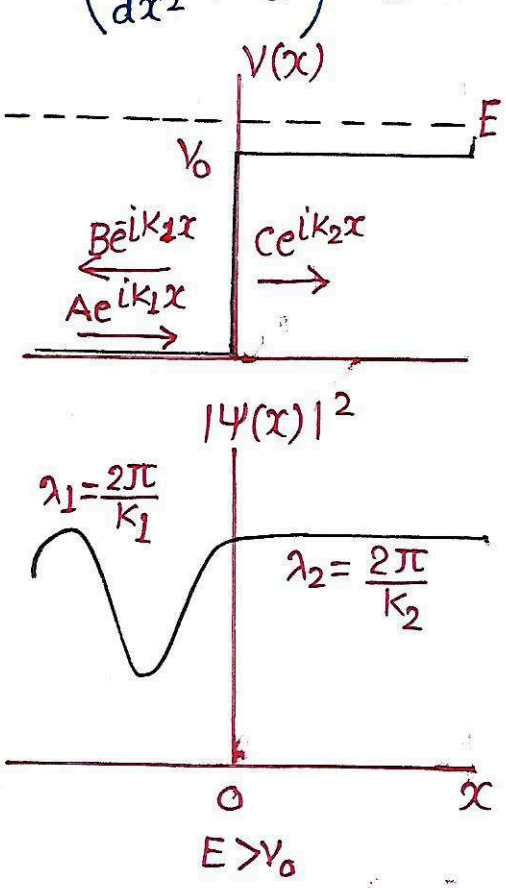
clasically,

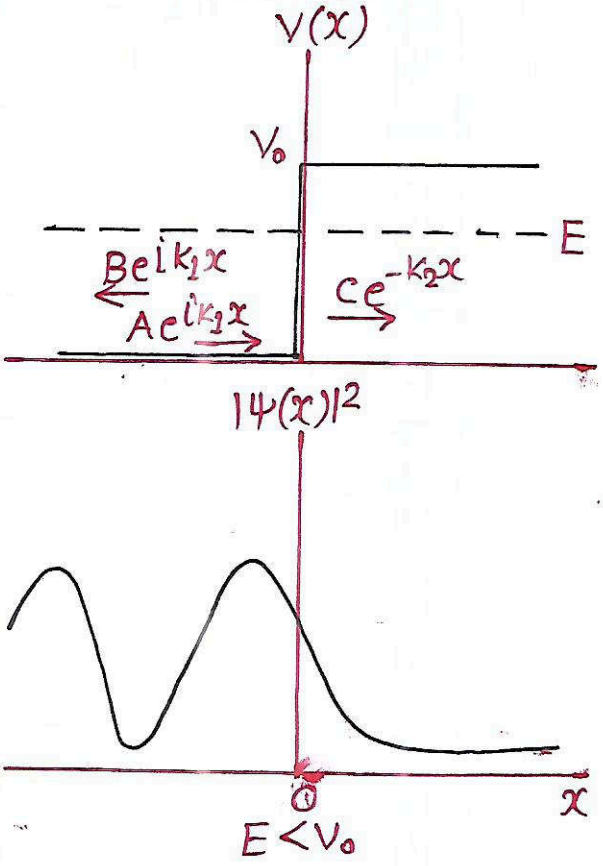
Particle
↓ momentum
$\sqrt{2mE}$
↓ enters the region $x \geq 0$
$\sqrt{2m(E-V_0)}$ ⟶ conserve momentum

Total transmission
↑
Particle have sufficient energy to penetrate into the region $x \geq 0$

Quantum Mechanically, the dynamics of the particles is regulated by the Schrodinger equation, which is these two region by

$$\left(\frac{d^2}{dx^2} + K_1^2\right)\psi_1(x) = 0 \qquad (x<0) \quad \ldots\ldots (1)$$





$$\left(\frac{d^2}{dx^2} + K_2^2\right)\psi_2(x) = 0 \qquad (x>0) \quad \ldots\ldots (2)$$

Then

$$\psi_1(x) = Ae^{iK_1x} + Be^{-iK_1x}$$
$$\psi_2(x) = Ce^{iK_2x} + De^{-iK_2x}$$

Incident wave ↑ Reflected wave ↑

$$\psi(x,t) = \begin{cases} \psi_1(x)e^{-i\omega t} = Ae^{i(K_1x-\omega t)} + Be^{-i(K_1x+\omega t)} \\ \psi_2(x)e^{-i\omega t} = Ce^{i(K_2x-\omega t)} \end{cases}$$

↓ Transmitted wave

$$\text{Reflected coefficient } R = \left|\frac{J_{reflected}}{J_{Incident}}\right| = \frac{|B|^2}{|A|^2} = \frac{(K_1-K_2)^2}{(K_1+K_2)^2}$$

$$\text{Transmission coefficient } T = \left|\frac{J_{transmitted}}{J_{Incident}}\right| = \frac{|C|^2}{|A|^2} = \frac{4K_1K_2}{(K_1+K_2)^2}$$

(b) Case $E<V_0$

Clasically, the particle arriving at the potential step from the left will come to a stop at $x=0$ and then all will bounce back to the left with the magnitude of their momenta unchanged. None of the particle will make it into the right side of the barrier $x=0$; there is total reflection of the particle. So the motion of the particle is reserved by the potential barrier.

Quantum mechanically, the picture is somehow different. In this case, the schrodinger eqn and the wave function in the region $x<0$ are given and $x>0$, are given

$$\left(\frac{d^2}{dx^2} - K_2'^2\right)\psi_2(x) = 0 \qquad (x \geq 0) \quad \ldots\ldots\ldots (3)$$

$$\downarrow$$

$$K_2'^2 = \frac{2m(V_0 - E)}{\hbar^2}$$

$$\psi_2(x) = Ce^{-iK_2'x} + De^{-iK_2'x}$$

$$\psi(x,t) = \begin{cases} Ae^{i(K_1x - \omega t)} + Be^{-i(K_1x + \omega t)} & x<0 \\ Ce^{-K_2'x}e^{-i\omega t} & x \geq 0 \end{cases}$$

$$\downarrow$$

Transmitted wave function $=0$

$$J_{transmitted} = 0$$

$$R = \frac{|B|^2}{|A|^2}$$

$$R = \frac{K_1^2 + K_2'^2}{K_1^2 + K_2'^2} = 1$$

Quantum mechanically, there is a nonzero probability that the wave function penetrate this classically forebidden region.

Relative probability density $P(x) = |\psi_t(x)|^2 = |C|^2 e^{-2K_2'x} = \frac{4K_1^2|A|^2}{K_1^2 + K_2'^2} e^{-2K_2'x}$

$$\downarrow$$

shown in figures.

*Hydrogen Atom-

Now, we take up the wave equation for a (1-D) 1 e^- atom like Hydrogen. This is a two particle system, consisting of a atom nucleus of charge Ze, and the electron of charge $-e$. But if the nucleus is superposed to remain static, the schrodinger eq^n is just that for a single particle, the e^-, moving in the potential $V_r(r) = \frac{-Ze^2}{r}$

$$V(r) = \frac{-Ze^2}{r}$$

This is just the electrostatic potential energy of interaction of two charges.

Actually when the atom as a whole is at rest, it is not the nucleus, but the center of mass of the two particle system which remain static.

→ Solution of the Radial Eq^n ; Energy Levels-

Since the potential is spherically symmatric, our task is just to solve the radial wave equation

NOT WRITTEN

$$h\nu_1 \equiv E_1 - E_{l-1} = \frac{l\hbar^2}{\mu r_0^2} \longrightarrow \nu_1 \equiv \frac{l\hbar}{4\pi^2 \mu r_0^2}$$

$$\nu = \frac{\omega}{2\pi} = \left(\frac{k}{2\pi^2\mu}\right)^{1/2}$$

Hamiltonian $H = \frac{p^2}{2\mu} + V(r)$

$$u(r,\theta,\phi) = R(r)Y_{lm}(\theta,\phi)$$

$$Hu = Eu$$

Then

$$\left[\frac{\hbar^2}{2\mu}\nabla^2 + V(r)\right]u = Eu$$

$$\frac{-\hbar^2}{2\mu r^2}\left[\frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} - \frac{L^2}{\hbar^2}\right]u + V(r)u = Eu$$

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\frac{2\mu}{\hbar^2}\left[E+\frac{Ze^2}{r}-\frac{l(l+1)\hbar^2}{2\mu r^2}\right]R=0 \quad \ldots\ldots(1)$$

Let us consider a bound state, for which $E<0$, and define the position real parameters α and λ through

$$\alpha^2=\frac{-8\mu E}{\hbar^2}$$

$$\lambda=\frac{2\mu Ze^2}{\alpha\hbar^2}=\frac{Ze^2}{\hbar}\left(\frac{\mu}{-2E}\right)^{1/2}$$

Write dimensionless,

$$\frac{1}{\rho^2}\frac{d}{d\rho}\left(\rho^2\frac{dR}{d\rho}\right)+\left[\frac{\lambda}{\rho}-\frac{1}{4}-\frac{l(l+1)}{\rho^2}\right]R=0 \quad \ldots\ldots(2)$$

$$R(\rho)=R(r) \text{ with } \rho=\alpha r$$

Examine behaviour of R in the asymptotic region.

$$\rho\longrightarrow\infty$$

So

$$R(\rho)=K(\rho)e^{-\frac{1}{2}\rho} \quad \ldots\ldots(3)$$

$$R(\rho)=\rho^l e^{-\frac{1}{2}\rho}L(\rho) \quad [\text{Put the value of } R \text{ in eq}^n(2)]$$

$$\rho\frac{d^2L}{d\rho^2}+(2[l+1]-\rho)\frac{dL}{d\rho}+[\lambda-(l+1)]L=0 \quad \ldots\ldots(3\cdot1)$$

$$L(\rho)=c_0+c_1\rho+c_2\rho+\ldots\ldots=\sum_{s=0}^{\infty}c_s\rho^s \quad \ldots\ldots(4)$$

Since we know that $R(\rho)$ behaves like ρ^l for small ρ, $L(\rho)$ must tend to a constant as $\rho\to0$, according to eq^n (3). This is why the series has been taken a start with a constant term.

On substituting the eq^n(4) in (3·1) eq^n

Recurrance Relation

$$c_{s+1}=\frac{s+l+1-\lambda}{(s+1)(s+2l+2)}c_s$$

$$\frac{c_{s+1}}{c_s} \longrightarrow \frac{1}{s}$$

$$L(\rho) \xrightarrow[\rho \to \infty]{} \text{const.} \; e^{\rho}$$

$$R(\rho) \longrightarrow \text{const.} \; \rho^{1} \cdot e^{\frac{1}{2}\rho}$$

i.e. it diverges. To avoid this, we have to make the series terminate. This can be done by choosing

$$\lambda = n = \text{integer} \quad \ldots\ldots\ldots (5)$$

so that when s reaches the value n' given by

$$n' = n - l - 1$$

The factor $(s + l + 1 - \lambda)$ vanishes.

$$n = 1, 2, 3, \ldots$$
$$l = 0, 1, \ldots\ldots, n-1$$

The condition eq^n(5) which determines the admissible solution also gives us the energy eigenvalue E_n: on substituting $\lambda = n$ in eq^n, we get

$$E_n = (-|E_n|)$$

$$\boxed{E_n = -|E_n| = -\frac{\mu z^2 e^4}{2\hbar^2 n^2}}$$

$n = 1, 2, 3, \ldots\ldots$

According to the Bohr's Theory of Hydrogen like Atom in Modern Physics

$$E_n = \frac{-mz^2 e^4}{8\varepsilon_0^2 h^2}\left(\frac{1}{n^2}\right)$$

- **Particle in a three dimensional box -**

In this simple case of a free particle, the schrodinger equation reduces to three eqn. Similarly to $V_x = 0$, $V_y = 0$ and $V_z = 0$.

Then X equation

$$\frac{d^2X}{dx^2} = -K_x^2 X(x) \quad \ldots\ldots (1)$$

$$K_x^2 = \frac{2mE_x}{\hbar^2}$$

$$E_x = \frac{\hbar^2 K_x^2}{2m} \quad \ldots\ldots (2)$$

$$X(x) = \frac{1}{\sqrt{2\pi}} e^{iK_x x} \quad \ldots\ldots (3)$$

Put the values from eqn (3) & (2) in eqn (1)

$$\psi_{\vec{K}}(x,y,z) = (2\pi)^{-3/2} e^{iK_x x} e^{iK_y y} e^{iK_z z} = (2\pi)^{-3/2} e^{i\vec{K}\vec{r}}$$

$$E = E_x + E_y + E_z = \frac{\hbar^2}{2m}(K_x^2 + K_y^2 + K_z^2) = \frac{\hbar^2}{2m}\vec{k}^2$$

$$|\vec{K}| = \sqrt{K_x^2 + K_y^2 + K_z^2} = \text{Constant}$$

$$\psi_{\vec{K}}(\vec{r},t) = \psi(\vec{r}) e^{i\omega t} = (2\pi)^{-3/2} e^{i(\vec{K}\cdot\vec{r} - \omega t)}$$

And

$$\omega = \frac{E}{\hbar}$$

$$\int \psi^*_{\vec{K}'}(\vec{r},t)\, \psi_{\vec{K}}(\vec{r},t)\, d^3r = \int \psi^*_{\vec{K}'}(\vec{r})\, \psi_{\vec{K}}(\vec{r})\, d^3r = (2\pi)^{-3} \int e^{i(\vec{K}-\vec{K}')}\, d^3r = \delta(\vec{K}-\vec{K}')$$

which can be written as dirac's notation as

$$\boxed{\langle \psi_{\vec{K}'}(t) | \psi_{\vec{K}}(t) \rangle = \langle \psi_{\vec{K}'} | \psi_{\vec{K}} \rangle = \delta(\vec{K}-\vec{K}')}$$

2. Matrix Formulation of Quantum Mechanics

- **The state of a system-**

To describe a system in quantum mechanics, we use a mathematical entity (a complex function) belonging to a Hilbert space, a state vector $|\psi(t)\rangle$, which contains all the information we need to know about the system and from which all needed physical quantities can be computed. As we know, the state vector $|\psi(t)\rangle$ may be represented in two ways:

A wave function $\psi(\vec{r},t)$ in the position space.

$$\psi(\vec{r},t) = \langle \vec{r} | \psi(t) \rangle$$

A momentum wave function $\psi(\vec{p},t)$ in the momentum space:

$$\psi(\vec{p},t) = \langle \vec{p} | \psi(t) \rangle$$

So, for instance, to describe the state of a 1-D particle in quantum mechanics we use a complex function $\psi(x,t)$, instead of two real numbers (x,p) in classical physics.

The wave function to be used are only those that correspond to physical systems. What are the mathematical requirements for that a wave function must satisfy to represent a physical system?

$\psi(x) \rightarrow$ Wave function

$\downarrow$ Physically Acceptable

$\frac{d\psi(x)}{dx} \rightarrow$ Finite, continuous and single valued

- **Probability Density-**

- Physical meaning of ψ?

$\downarrow$

$|\psi|^2 \rightarrow$ has a meaning

According to born's probabilistic interpretation, the square of the norm of $\psi(\vec{r},t)$

$$P(\vec{r},t) = |\psi(\vec{r},t)|^2$$

This represents a position probability density; that is, the quantity $|\psi(\vec{r},t)|^2 d^3r$ represents the probability ability of finding the particle at t time in a volume element d^3r located between $\vec{r}$ and $\vec{r}+d\vec{r}$. Therefore, the total probability of finding the system somewhere in space is equal to 1.

$$\int |\psi(\vec{r},t)|^2 d^3r = \int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dy \int_{-\infty}^{+\infty} |\psi(\vec{r},t)|^2 dz = 1$$

A wave function $\psi(\vec{r},t)$, satisfying this relation is said to be normalized.

$\psi(\vec{r})$ ⟶ Physical dimension → $1/\sqrt{L^3}$

↓

$|\psi(\vec{r})|^2$ ⟶ Physical dimension → $1/L^3$

#Hilbert Space-

A Hilbert space H consists of a set of vectors $\psi, \phi, \chi, \ldots$ and a set of scalars $a, b, c, \ldots$ which satisfy following four properties.

(a) H is a linear Space-

→ Vectors ψ, ϕ, χ

→ Scalars a, b, c

- Addition properties:
  1. Commutativity $\psi + \phi = \phi + \psi$
  2. Associativity $(\psi + \phi) + \chi = \psi + (\phi + \chi)$
  3. Existance $0 + \psi = \psi + 0 = \psi$
  4. Inverse $\psi + (-\psi) = (-\psi) + \psi = 0$

- Multiplication rule:
  1. $a(\psi + \phi) = a\psi + a\phi$
  2. $a(b\psi) = (ab)\psi$
  3. $I\psi = \psi I = \psi$
  4. $0\psi = \psi 0 = 0$

(b) H has a defined scalar product that is strictly positive-

The scalar product of an element ψ with another element ϕ is in general a complex number denoted by (ψ, ϕ).

$$(\psi, \phi) = \text{complex number}$$

$$(\psi, \phi) = (\phi, \psi)^*$$

$$(\phi, a\psi_1 + b\psi_2) = a(\phi, \psi_1) + b(\phi, \psi_2)$$

$$(a\phi_1 + b\phi_2, \psi) = a^*(\phi_1, \psi) + b^*(\phi_2, \psi)$$

$$(\psi, \psi) = \|\psi\|^2 \geq 0$$

(c) H is separate-

There exist a Cauchy sequence

$$\psi_n \in H (n = 1, 2, \ldots)$$

Then

$$\|\psi - \psi_n\| < \epsilon$$

(d) H is complete-

Every cauchy sequence

$$\psi_n \in H$$

Then

$$\lim_{m, n \to \infty} \|\psi_n - \psi_m\| = 0$$

defined a unique limit

$$\boxed{\lim_{n \to \infty} \|\psi - \psi_m\| = 0}$$

- **Physical significance of Hilbert Space-**

1. Hilbert Space is used in theories of Partial diff. eq^n and Fourier Analysics.
2. Hilbert Space is an infinite dimensional Space which is complete and closed.
3. Hilbert space is an interface to understand QM more clearly.

- De-broglie- Wavelength-

Particle / Particle \ Wave

$E = h\nu$ (Max Plank)
$E = mc^2$ (Einstein)

$$mc^2 = h\nu$$
$$mc = \frac{h\nu}{c}$$
$$p = \frac{h}{\lambda} \quad \left[\because \lambda = \frac{c}{\nu}\right]$$

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

$\lambda \propto \frac{1}{p}$

λ ↓ Wave, p ↓ Particle

0 ⟶ v

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

$$\lambda = \frac{h}{mv}$$
$$\lambda = \frac{h}{m\sqrt{\frac{2E}{m}}}$$

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

$\frac{1}{2}mv^2 = \frac{3}{2}KT$

$mv = \sqrt{3mKT}$

$$\lambda = \frac{h}{\sqrt{3mKT}}$$

$E = qV$

$$\lambda = \frac{h}{\sqrt{2mqV}}$$ Accelerated Charged Particle

$\psi = \psi_0 \sin \omega t$

$\psi = \psi_0 \sin 2\pi\nu t$

$$\psi = \psi_0 \sin \frac{2\pi V\left(t' + \frac{Vx'}{c^2}\right)}{\sqrt{1-\frac{V^2}{c^2}}} \qquad t = \left[\frac{t' + \frac{Vx'}{c^2}}{\sqrt{1-\frac{V^2}{c^2}}}\right]$$

$$\psi = \psi_0 \sin \frac{2\pi}{T}\left(t' + \frac{x'}{u'}\right)$$

$$u' = \frac{c^2}{V}$$

$$\frac{1}{T} = \nu' = \frac{V}{\sqrt{1-V^2/c^2}}$$

$E = m_0c^2 = mv$

$v = \frac{m_0c^2}{h}$

$$\nu' = \frac{\frac{m_0c^2}{h}}{\sqrt{1-\frac{V^2}{c^2}}}$$

$\nu' = \frac{mc^2}{h}$

$\lambda = \frac{\text{Velocity}}{\text{Frequency}}$

$\lambda = \frac{u'}{\nu'}$

$\lambda = \frac{c^2}{\frac{V}{\frac{mc^2}{h}}}$

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

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

• Time Evolution and the schrodinger Equation

Acting on a wave function ψ with an operator has nothing what so ever to do measuring the associated observable.

1. configuration – $\psi(x,t)$
2. Observables – Operators $\hat{A}\phi_a(x) = a\phi_a(x)$
   - ↓ Physical quantity that can be measured
   - $\hat{A}$: operator; $\phi_a(x)$: Eigen function

The Operator acting on a wave function gives the same function times a.

3. Superposition – $\psi(x) = \sum_a c_a \phi_a(x)$

Fourier Theorem

$$S_N(x) = \sum_{n=-N}^{N} c_n \cdot e^{i\frac{2\pi n x}{P}}$$

This is the statement that any arbitrary function (when observable is the momentum) can be expended as a superposition or a sum of exponantials. and that's the fourier theorem.

4. $TP(A=a) = |c_a|^2$

$$c_a = \left(\frac{\phi_a}{\psi}\right) \equiv \int_{-\infty}^{+\infty} dx\ \phi_a^*(x)\,\psi(x)$$

5 collapse –

Measure $A = a \Rightarrow \psi(x) = \phi_a(x)$

$\psi(x, t_*) = \phi_a(x)$

6. Schrodinger Equation –

$$\partial_t \psi(x,t) = \frac{1}{i\hbar} \cdot \hat{E}\,\psi(x,t)$$

- Linear

- Linear $\psi_1(x,t)$, $\psi_2(x,t)$ Solve SE

  $\Rightarrow \alpha\psi_1 + \beta\psi_2 = \psi$ solves SE

- Unitary ; conserves $\mathbb{P}$
- Deterministic

$$\psi(x,0) = \phi_E(x) \qquad \hat{E}\,\phi_E(x) = E\phi_E(x)$$

$$\nearrow \psi(x,0) = e^{i\alpha}\,\phi_E(x)$$

Illusion

$$i\hbar\,\partial_t\,\psi(x,0) = E\,\psi(x,0) \Rightarrow \boxed{\partial_t\psi = -\frac{iE}{\hbar}\psi}$$

$$\psi(x,t) = e^{\frac{-iE}{\hbar}}\,\phi_E(x)$$

$$[\hbar] = [E][t] = [p][x]$$

$$\psi(x,t) = e^{-i\omega t}$$

$$\omega = \frac{E}{\hbar}$$

$\phi_E(x)$ = "Stationary State"

$$\mathbb{P}(x,t) = |\psi(x,t)|^2 = |\phi_E(x)|^2$$

↑ independent to time

3.

Symmetry in Quantum Mechanics

Wigner-Eckart Theorem-

Let us now focus only on the representation of irreducible tensor operator and we can easily generalized these two relation to any spherical tensor of Rank K, $\hat{T}_q^{(K)}$ Thus;

$$[\hat{J}_z, \hat{T}_q^{(K)}] = \hbar q \hat{T}_q^{(K)}$$

Taking matrix element of this equation

$$\langle j', m' | [\hat{J}_z, \hat{T}_q^{(K)}] = \hbar q \hat{T}_q^{(K)} | j, m \rangle = 0$$

or $\quad (m' - m - q) \langle j', m' | \hat{T}_q^{(K)} | j, m \rangle = 0 \qquad [\because m' = m + q]$

$\langle j', m' | \hat{T}_q^{(K)} | j, m \rangle$ must be propotional to Clebsh-Gordon cofficient $\langle j', m' | j, K ; m, q \rangle$, hence leads to

$$(m' - m - q) \langle j', m' | j, K ; m, q \rangle = 0$$

Now, taking the matrix element of irreducible tensor between $|j, m\rangle$ and $|j', m'\rangle$, we obtain

$$\sqrt{(J' \pm m')(J' \mp m' + 1)} \langle j', m' \mp 1 | \hat{T}_q^{(K)} | j, m \rangle$$

$$= \sqrt{(J' \mp m')(j \pm m + 1)} \langle j', m' | \hat{T}_q^{(K)} | j, m \pm 1 \rangle +$$

$$\sqrt{(K \pm q)(K \pm q + 1)} \langle j', m' | \hat{T}_{q \pm 1}^{(K)} | j, m \rangle$$

This equation has a structure which is identical to the recursion relation. For instance,

$$j = j'$$
$$m = m'$$
$$j_1 = j$$
$$m_1 = m$$
$$j_2 = K$$
$$m_2 = q$$

$$\sqrt{(J' \pm m')(J' \mp m'+1)}\,\langle J', m' \mp 1 \mid j, k; m, q\rangle =$$

$$\sqrt{(J \mp m)(J' \mp m' + 1)}\,\langle J', m', j, k; m \pm 1, q\rangle$$

$$+\sqrt{(K \mp q)(K \mp q + 1)}\,\langle j, m' \mid j, k; m, q \pm 1\rangle$$

A comparison b/w eqn can be suggesting that dependance through clebsh gordan cofficient has yet to be determined.

The matrix elements of spherical tensor operator $\hat{T}_q^{(K)}$ with respect to angular momentum eigenstate $|j, m\rangle$ are given by

$$\boxed{\langle j', m' \mid \hat{T}_q^{(K)} \mid j, m\rangle = \langle j, K; m, q \mid j', m'\rangle \langle j' \| \hat{T}^{(K)} \| j\rangle}$$

When dealing scalar operator $\hat{B}$, tensor of rank $k=0$, hence $q=0$ as well, thus, equation yield.

$$\boxed{\langle j', m' \mid \hat{B} \mid j, m\rangle = \langle j, 0, m, 0 \mid j', m'\rangle \langle j', m' \rangle \langle j' \| \hat{B} \| j' \rangle \delta j' j \delta m' m}$$

Clebsh-Gordon Cofficients and properties-

Let us now return to the addition of angular momentum $\vec{J}_1$ and $\vec{J}_2$. The problem consists in essence of obtaining the eigenvalues of $\vec{J}^2$. This problem consists in essence :-

$$\vec{J} = \vec{J}_1 + \vec{J}_2 \quad \ldots\ldots\ldots (1)$$

$$|j, m\rangle = |j_1, j_2; m_1, m_2\rangle$$

$|j, m\rangle$ is the state in which $\hat{\vec{J}}^2$ and $\hat{\vec{J}}_z$ has fixed values $j(j+1)$ and m.

The $\{|j_1, j_2; m_1, m_2\rangle\}$ and $\{|j, m\rangle\}$ bases can be connected by means of a transformation as follows.

$$|j,m\rangle = \left(\sum_{m_1=-j_1}^{j_1} \sum_{m_2=-j_2}^{j_2} |j_1,j_2;m_1,m_2\rangle\langle j_1,j_2;m_1,m_2| \right) |j,m\rangle$$

$$= \sum_{m_1 m_2} \langle j_1,j_2;m_1,m_2|j,m\rangle |j_1,j_2;m_1,m_2\rangle,$$

Now use normalized condition

$$\boxed{\langle j_1,j_2;m_1,m_2|j,m\rangle = \langle j,m|j_1,j_2;m_1,m_2\rangle}$$

These cofficients are called Clebsh-Gordon cofficients.

Orthonormal relation of Clebsh-Gordon cofficients

$$\sum_{m_1 m_2} \langle j',m'|j_1,j_2;m_1,m_2\rangle\langle j_1,j_2;m_1,m_2|j,m\rangle = \delta_{j',j}\delta_{m;m}$$

This relation can be written as

$$\sum_{m_1 m_2} \langle j_1,j_2;m_1,m_2|j',m'\rangle\langle j_1,j_2;m_1,m_2|j,m\rangle = \delta_{j',j}\delta_{m',m}$$

which leads to

$$\sum_{m_1 m_2} \langle j_1,j_2;m_1,m_2|j,m\rangle^2 = 1$$

Likewise

$$\sum_{j} \sum_{m=-j}^{j} \langle j_1,j_2;m_1',m_2'|j,m\rangle\langle j_1,j_2;m_1,m_2|j,m\rangle = \delta_{m_1',m_1}\delta_{m_2',m_2}$$

And in Particular

$$\boxed{\sum_{j} \sum_{m} \langle j_1,j_2;m_1,m_2|j,m\rangle^2 = 1}$$

In Physics, C-G cofficient are numbers that arises in angular momentum coupling in quantum Mechanics.

The coupling states can be exponded via the completeness relation (resolution of identity) in the uncoupled basis.

$$|JM\rangle = |j_1 m_1 j_2 m_2\rangle\langle JM\rangle$$

→ Properties :

1. Symmetry properties of CG cofficients;

Clebsh-Gordon coefficients in which the angular momentum j_1, j_2, j_3 are recorded may be simply related to each other. The most trivial case involves to exchange of the order of the quantum number $j_1 m_1$ and $j_2 m_2$. The state vector $|j_1 j_2 j_2 m_2\rangle$ is a direct product of two vectors involving separate subspace of the full Hilbert space. Thus $\langle j_1 j_1 j_2 m_2 | j_3 j_3 \rangle$ must be positive by our phase convenstion.

$$m_1 = j_3 - j_2$$

Also $\langle m_1, m_2 | j, m \rangle = 0$

Angular momentum matrices of J_+, J_-, J_z, J^2 –

→ Total Angular momentum operators–

The total angular momentum which may include the spin contribution is conveniently denoted by $J \longrightarrow (J_x, J_y, J_z)$ and is defined as the the generalized angular momentum operator J as any Hermition operator whose components, satisfy commutation rules.

$$[J_x, J_y] = i\hbar J_z$$
$$[J_y, J_z] = i\hbar J_x$$
$$[J_z, J_x] = i\hbar J_y$$

Thus

$$[J \times J] = i\hbar J$$

Angular momentum

$$J = \hbar^{-1}(r \times p)$$

Thus $\hbar = 1$

Then writing eqn

$$[J_x, J_y] = iJ_z$$
$$[J_y, J_z] = iJ_x$$
$$[J_z, J_x] = iJ_y$$

equivalenty

$$\boxed{J \times J = iJ}$$

→ Commutation relations of total Angular momentum with components.

The total Angular momentum

$$J^2 = J_x^2 + J_y^2 + J_z^2$$

commutation relation with J_x, J_y, J_z

$$[J^2, J_x] = [J_x^2, J_y^2, J_z^2, J_x] = [J_x^2, J_x] + [J_y^2, J_y] + [J_z^2, J_z]$$

$$[J_x^2, J_x] = [J_x, J_x, J_x]$$
$$= J_x[J_x, J_x] + [J_x, J_x]J_x = 0$$

$$[J^2, J_x] = [J_y^2, J_x] + [J_z^2, J_x]$$
$$= 0$$

$$[J^2, J_x] = 0$$
$$[J^2, J_y] = 0$$
$$[J^2, J_z] = 0$$

Ladder Operators

$$J_+ = J_x + iJ_y$$
$$J_- = J_x - iJ_y$$

Commutation Relation J_z with J_+ and J_-

$$[J_z, J_+] = [J_z, J_x, +iJ_y]$$
$$= [J_z, J_x] + i[J_z, J_y]$$
$$= [J_z, J_x] - i[J_y, J_z]$$
$$= \hbar J_+$$

$$[J_z, J_-] = -\hbar J_-$$

$$[J_z, J_\pm] = \hbar J_\pm$$

Commutation Relation of J_+, J_- mutually

$$[J_+, J_-] = [J_x + iJ_y, J_x - iJ_y]$$
$$= [J_x, J_x] - [J_x, J_y] + i[J_y, J_x] + [J_y, J_y]$$
$$= 2\hbar J_z$$

Commutation Relation of J^2 with J_+ , J_-

$$[J^2, J_+] = [J^2, J_x + iJ_y]$$

$$= [J^2, J_x] + i[J^2, J_y]$$

$$= 0$$

$$[J^2, J_-] = 0$$

$$\boxed{J^2, J_\pm = 0}$$

4.
Approximation Methods for Bound States

WKB Approximation-

The Wentzal-Karmers-Brillouin method of Approximation is a technique for obtaining approximate solution to time independing schrodinger equation in one-dimension.

It is particularly useful in calculating band state energies and tunneling rate through potential barrier.

↓

Applications of WKB Approximation

The WKB method is useful for treatments of approximate of systems with slowly varying potential; that is potentials which remain almost constant over a region of the order of the de-Broglie wavelength. In the case of classical systems, this property is always satisfied since the wavelength of a classical system, approaches zero. The WKB method can thus be viewed as a semiclassical Approximation.

- General Formalism-

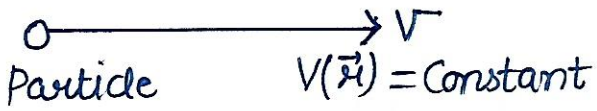
Consider the motion of particles in a time independing potential $V(\vec{x})$; the schrodinger equation for the corresponding stationary state is

$$\frac{-\hbar^2}{2m}\nabla^2\psi(\vec{x}) + V(\vec{x})\psi(\vec{x}) = E\psi(\vec{x}) \quad \ldots\ldots\ldots (1)$$

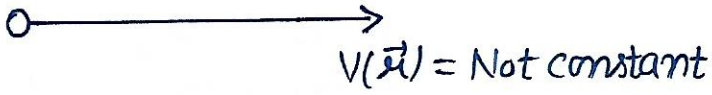
$$\nabla^2\psi(\vec{x}) + \frac{1}{\hbar^2}p^2(\vec{x})\psi(\vec{x}) = 0 \quad \ldots\ldots\ldots (2)$$

Where $\vec{p}(\vec{r})$ is the classical momentum at $\vec{r}$.

$$P(\vec{r}) = \sqrt{2m(E-V)}$$



Then $\psi = A e^{\pm i\vec{p}\cdot\vec{r}/\hbar}$



How does one deal with those cases where $V(\vec{r})$ is not constant? The WKB method provides an approximation treatment for systems whose potential, while not constant, are slowly varying function of $\vec{r}$.

$V(\vec{r})$ is almost constant in a region which extends over several de-broglie wavelength; we may recall that the de-broglie wavelength of a particle of mass m and energy E that is moving in a potential $V(\vec{r})$ is given by

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

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

$$\psi = A(\vec{r})\, e^{iS(\vec{r})/\hbar} \quad \ldots\ldots\ldots (3)$$

Where $A(\vec{r})$ is amplitude
$S(\vec{r})$ is Phase

Put the value of ψ from eq^n(3) to eq^n(2)

$$A\left[\frac{\hbar^2}{A}\nabla^2 A - (\vec{\nabla}S)^2 + p^2(\vec{r})\right] + i\hbar\left[2(\nabla\vec{A})\cdot(\vec{\nabla}S) + A\nabla^2 S\right] = 0$$

The real and imaginary parts of this equation must vanish separately.

$$(\nabla \vec{S})^2 = p^2(\vec{r}) = 2m(E - V(\vec{r})) \quad \ldots\ldots\ldots (4)$$

$$2(\vec{\nabla} A)\cdot(\vec{\nabla} S) + A\nabla^2 S = 0 \quad \ldots\ldots\ldots (5)$$

$\frac{\hbar^2}{A}\nabla^2 A$ is very small hence it is neglected.

To illusion the various aspects of the WKB method, Let us consider the small simple case of one dimensional motion of a single particle. We can then reduce eq^n(4) & (5)

$$\frac{dS}{dx} = \pm p(x) = \pm\sqrt{2mE - V(\vec{r})} \quad \ldots\ldots\ldots (6)$$

$$2\left(\frac{d}{dx}\ln A\right)p(x) + \frac{d}{dx}p(x) = 0 \quad \ldots\ldots\ldots (7)$$

Let us find the solution of eq^n (6) & (7).

Then

$$S(x) = dS = \pm\int dx\sqrt{2mE - V(\vec{x})} = \pm\int p(x)\,dx \quad \ldots\ldots\ldots (8)$$

$$\frac{d}{dx}[2\ln A + \ln p(x)] = 0$$

Which in turn leads to

$$A(x) = \frac{C}{\sqrt{|p(x)|}} \quad \ldots\ldots\ldots (9)$$

C is arbitrary constant.

Eq^n(8),(9) give the amplitude A(x) and phase S(x) of the WKB Approximation's wave function (eq^n 3)

Inserting eq^n(8),(9) in eq^n(3)

$$\psi\pm(x) = \frac{C\pm}{\sqrt{|p(x)|}}\exp\left[\pm\frac{i}{\hbar}\int^x p(x')\,dx'\right]$$

Now we can examine two separate cases.

$E > V(x)$ [Classically Allowed Region]

$$\psi(x) = \frac{C+}{\sqrt{p(x)}} \exp\left[\frac{i}{\hbar}\int^{x} p(x')dx'\right] + \frac{C^-}{\sqrt{p(x)}} \exp\left[\frac{i}{\hbar}\int^{x} p(x')dx'\right]$$

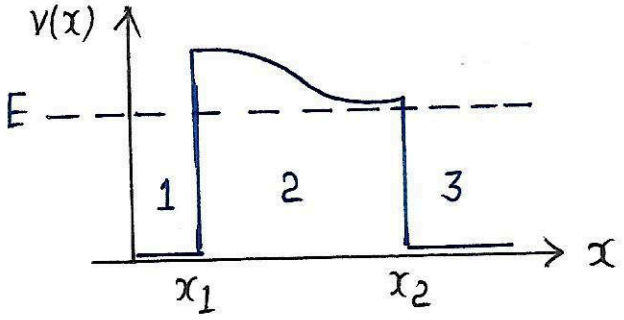
$E > V(x)$ [Classically Forbidden Region]

$$\psi(x) = \frac{C'-}{\sqrt{|p(x)|}} \exp\left[-\frac{i}{\hbar}\int^{x} |p(x')|dx'\right] + \frac{C'+}{\sqrt{|p(x)|}} \exp\left[\frac{i}{\hbar}\int^{x} |p(x')|dx'\right]$$

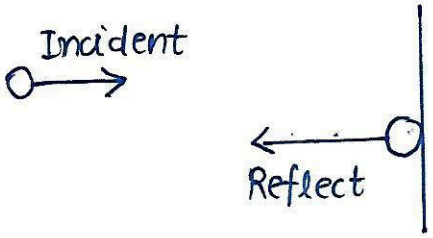
Both equations give the system's wave function in the allowed and forbidden regions.

- Application-

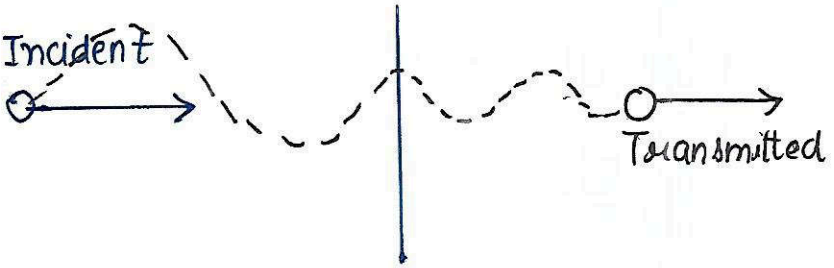
Consider the motion of particle of momentum $P_0 = \sqrt{2mE}$ incident from left onto a potential Barrier $V(x)$.



The energy E that is very small than the potential maximum value V_{max}. Classically, the particle can in no way pentrate inside the barrier



Quantum Mechanically



$$\psi_1(x) = \psi_{incident} + \psi_{reflected} = Ae^{ip_0 x/\hbar} + Be^{-ip_0 x/\hbar}$$

$$\psi_3(x) = \psi_{transmitted} = Ee^{ip_0 x/\hbar}$$

A, B, E are amplitudes of waves

What about the wave function in classically forbidden Region.

$$\psi_2(x) = \frac{C}{\sqrt{|p(x)|}} \exp\left[-\frac{i}{\hbar}\int_{x_1}^{x} |p(x)'dx'\right] + \frac{D}{\sqrt{|p(x)|}} \exp\left[\frac{i}{\hbar}\oint_{x_1}^{x} |p(x')dx'\right]$$

$D \simeq 0$

$$\psi_2(x) = \frac{C}{\sqrt{|p(x)|}} \exp\left[-\frac{i}{\hbar}\int_{x_1}^{x} |p(x')|dx'\right]$$

$$T = \frac{E^2}{A^2}$$

$$\frac{E}{A} = \frac{2}{1 - a_0/ip_0}\sqrt{\frac{a_1}{a_2}}\, e^{ip_0(x_1 - x_2)/\hbar} \exp\left[-\frac{i}{\hbar}\int_{x_1}^{x_2} |p(x)|dx\right]$$

$$\frac{E^2}{A^2} = \frac{4}{a_2/a_1 + a_1^{a_2}/p_0^2} \exp\left[-\frac{2}{\hbar}\int_{x_1}^{x_2} |p(x)|dx\right]$$

Yield

$$T \sim e^{-2\gamma}, \quad \gamma = \frac{1}{\hbar}\int_{x_1}^{x_2} \sqrt{2m(V(x) - E)}dx$$

Time Indefendent Perturbation Theory-

$$\hat{H} = \hat{H}_0 + \hat{H}_p$$

$$\hat{H}_p = \lambda W$$

$$(\hat{H}_0 + \lambda W)|\psi_n\rangle = E_n|\psi_n\rangle$$

$$\hat{H}_0 |\phi_n\rangle = E_n^{(0)} |\psi_n\rangle$$

$$E_n = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \ldots\ldots$$

$$|\psi_n\rangle = |\phi_n\rangle + \lambda |\psi_n^{(1)}\rangle + \lambda^2 |\psi_n^{(2)}\rangle + \ldots\ldots$$

$$(\hat{H}_0 + \lambda \hat{W})(|\phi_n\rangle + \lambda |\psi_n^{(1)}\rangle + \lambda^2 |\psi_n^{(2)}\rangle + \ldots) =$$

$$(E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \ldots)(|\phi_n\rangle + \lambda |\psi_n^{(1)}\rangle + \lambda^2 |\psi_n^{(2)}\rangle + \ldots)$$

0th order – $\hat{H}_0 |\phi_n\rangle = E_n^{(0)} |\phi_n\rangle$

1th order – $\hat{H}_0 |\psi_n^{(1)}\rangle + \hat{W} |\phi_n\rangle = E_n^{(1)} |\psi_n^{(1)}\rangle + E_n^{(1)} |\phi_n\rangle$

2nd order – $\hat{H}_0 |\psi_n^{(2)}\rangle + \hat{W} |\psi_n^{(1)}\rangle = E_n^{(2)} |\psi_n^{(2)}\rangle + E_n^{(1)} |\psi_n^{(1)}\rangle + E_n^{(2)} |\phi_n^{(0)}\rangle$

$$\langle \phi_n | \psi_n \rangle = 1$$

$$\lambda \langle \phi_n | \psi_n^{(1)} \rangle + \lambda^2 \langle \phi_n | \psi_n^{(2)} \rangle + \ldots = 0$$

$$\langle \phi_n | \psi_n^{(1)} \rangle = \langle \phi_n | \psi_n^{(2)} \rangle = \ldots\ldots = 0$$

$$\boxed{E_n^{(1)} = \langle \phi_n | \hat{W} | \phi_n \rangle}$$