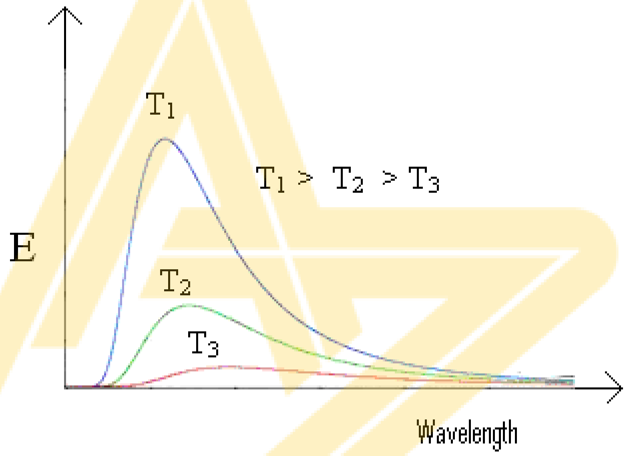
MODULE – IV
QUANTUM MECHANICS

Black Body Radiation:

A body which completely absorbs radiations of all wavelengths incident on it is called **a black body**. When supplied with energy, a black body will radiate electromagnetic waves of all wavelengths. The radiation emitted by a black body is called **black body radiation.**

Black Body Radiation Spectrum:

To study the distribution of radiant energy over different wavelengths, the black body is maintained at a constant temperature. When a graph of intensity versus wavelength was plotted for the radiation emitted by the black body at different temperatures, a set of curves were obtained as shown below.



It can be observed from the graphs that

1. For every temperature there is a curve
2. At a given temperature, a black body emits energy over a continuous range of wavelength
3. Energy is not distributed uniformly throughout the wavelength range
4. At every temperature, there is a particular wavelength at which maximum energy is emitted
5. The wavelength at which maximum emission of energy takes place shifts towards shorter wavelength side with increase in temperature of the black body **(Wein's displacement law)**

Planck's radiation Law:

Max Planck derived an equation which successfully accounted for the spectrum of blackbody radiation.

Planck postulated the following assumptions in his theory:

1. The atomic oscillators in a body cannot have any arbitrary amount of energy. They could have only discrete units of energy given by '$E_n = nh\nu$' where n $\rightarrow$ any positive integer, $\nu \rightarrow$ is the frequency of oscillation, h $\rightarrow$ Planck's constant.

2. The atomic oscillators cannot absorb or emit energy of any arbitrary amount. They absorb or emit energy in indivisible discrete units. The amount of radiant energy in each unit is called a quantum of energy, and carries an energy of '$E = h\nu$'. It represents the smallest quantity of energy of radiation of that frequency.

Based on this quantum theory, Planck derived an expression for the energy density of radiation emitted by a black body in the wavelength range λ and $\lambda + d\lambda$, and is given by

$$\boxed{E_{\lambda} d\lambda = \frac{8\pi hc}{\lambda^5}\left[\frac{1}{e^{\frac{hc}{\lambda KT}} - 1}\right] d\lambda}$$

This is called Planck's radiation law. The law agrees with the experimental observation of black body radiation and is valid for all wavelengths.

Photoelectric Effect:

The phenomenon of emission of electrons from a metal surface when light of suitable frequency falls on it is called photoelectric effect. The material that exhibits photoelectric effect is called photosensitive material. The emitted electrons are called photoelectrons.

Einstein's Explanation:

Einstein realized that the photoelectric effect could be understood if the energy in light is not spread over wave fronts but is concentrated in small packets or photons. According to him, when a photon of energy '$h\nu_0$' falls on a metal surface, the energy of the photon is completely absorbed by a free electron in the metal.

1. A part of this energy is used by the electron to overcome the surface forces and to come out of the metal surface. This minimum energy is called work function (w) of the metal.
2. The remaining part of the energy is used in giving kinetic energy to the emitted photoelectrons.

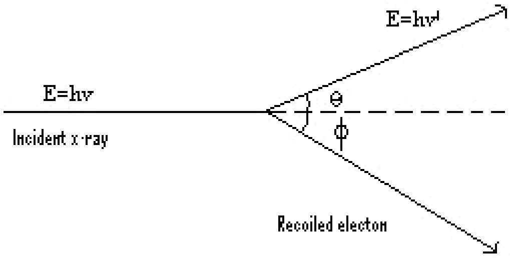
Physical Significance of photoelectric effect:

The photoelectric effect is explained on the basis that the incident light energy appears in small packets called photons and there is one to one interaction between photons and electrons. Thus it signifies the particle nature of light.

Compton Effect:

Compton discovered that when x – rays of given wavelength were incident on a material of low atomic number, the scattered x – rays contain two wavelengths. In addition to the incident wavelength 'λ' there exist a line of longer wavelength 'λ^1', i.e. the incident x – rays suffer a change in wavelength on scattering. This phenomenon in which the wavelength of x – rays show an increase after scattering is called **Compton Effect**.

Compton explained the effect on the basis of quantum theory of radiation. Considering radiations to be made up of photons, he applied the laws of conservation of energy and momentum for the interaction of photon and electron.



Consider an x – ray photon of energy '$h\nu$' incident on an electron at rest. After the interaction, the x – ray photon gets scattered at an angle 'θ' with its energy changed to a value $h\nu^1$ and the electron which was initially at rest recoils at an angle 'ϕ'. The increase in the wavelength of the x –ray photon (known as Compton shift) is given by

$\boxed{\Delta\lambda = \frac{h}{mc}(1 - \cos\theta)}$; Where m $\rightarrow$ mass of electron, $\lambda_C = \frac{h}{mc}$ is a constant called Compton wavelength.

Significance of Compton Effect:

In the Compton Effect, the change in wavelength '$\Delta\lambda$' is explained on the basis that the x – ray photons collide with electrons of the scatterer. During the collision the energy is exchanged between the two as if it is a particle – particle collision. Thus it demonstrates the particle nature of x – rays which are known to be electromagnetic waves.

Wave Particle Dualism:

According to wave theory, light waves leave a source with their energy spread out continuously through the wave pattern. According to the quantum theory, light consists of a stream of photons each small enough to be absorbed by a single electron. Both views have strong experimental support. Hence we can think of light as having a dual character. "The property of light of behaving as both a particle and a wave is called wave – particle duality."

De – Broglie's Hypothesis:

In 1924 Louis de – Broglie put forward a hypothesis that, since nature loves symmetry if radiation behaves as particle under certain circumstances and as waves under certain other circumstances, then one can even expect that entities which ordinarily behave as particles to exhibit properties attributed to only waves under appropriate circumstances.
According to him "**A moving material particle is associated with a wave**." The waves associated with material particles are called matter waves or de-Broglie waves.

For a material paticle mass 'm' moving with a velocity 'v', the deBroglie wavelength is given by

$$\lambda = \frac{h}{p} = \frac{h}{mv}\text{; Where } mv = p\text{, momentum of the particle.}$$

This equation is known as de-Broglie equation.

De –Broglie wavelength of electrons:

If the electrons are accelerated by a potential difference of 'V' so that electrons acquire a velocity 'v' then the work done on the electrons is 'eV'. As a result the kinetic energy gained by the electrons is $\frac{1}{2}mv^2$.

$\therefore$ We can write

$$eV = \frac{1}{2}mv^2 \rightarrow (1)$$

Or $\quad 2eVm = m^2v^2$

$\Rightarrow \quad mv = \sqrt{2meV}$

From de-Broglie's equation,

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

$$\boxed{\lambda = \frac{h}{\sqrt{2meV}} \rightarrow (2)}$$

Or $\quad \boxed{\lambda = \frac{h}{\sqrt{2mE}} \rightarrow (3)}$; $\quad$ (from (1))

Where $E = \frac{1}{2}mv^2$ is the kinetic energy of the electrons.

Substituting $m = 9.1\times10^{-31}\,kg$; $e = 1.6\times10^{-19}\,C$ and $h = 6.625\times10^{-34}\,J-s$ in equation (2) we get

$$\lambda = \frac{6.625\times10^{-34}}{\sqrt{2\times9.1\times10^{-31}\times1.6\times10^{-19}\times V}} = \frac{12.26\times10^{-10}}{\sqrt{V}} = \frac{12.26\text{A}^0}{\sqrt{V}}$$

Heisenberg's uncertainty principle:

According to deBroglie, a moving material particle is associated with a wave packet, which has a small spread in the space. This wave nature implies that there are fundamental limits to the accuracy with which we can measure particle properties such as position and momentum.

Consider the wave group shown below fig (a)

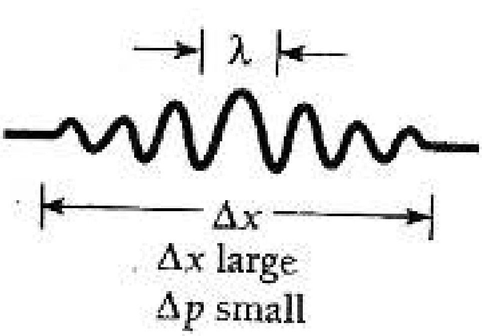


Fig (a)

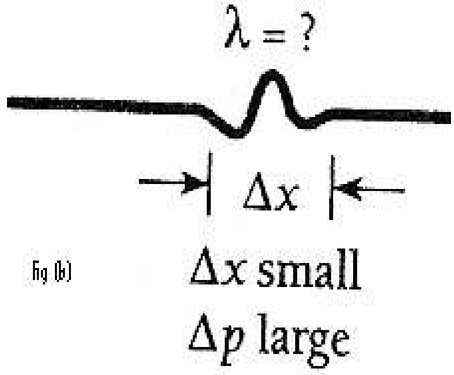


fig (b)

The particle corresponding to this wave group may be located anywhere within the group at a given time. The narrower its wave group, the more precisely a particles position can be specified (fig (b)). But the wavelength λ of the waves in a narrow wave packet is not well defined. This means that, since $\lambda = \frac{h}{p}$, the particle's momentum is not a precise quantity.

On the other hand, a wide wave packet (fig (a)) has a clearly defined wavelength. The momentum that corresponds to this wavelength is therefore a precise quantity. But the width of the group is too large for us to be able to say exactly where the particle is at a given time.

Thus we have the uncertainty principle given by Heisenberg.

"It is impossible to know both the exact position and exact momentum of an object at the same time."

Mathematically $$\Delta x \,.\Delta p \geq \frac{h}{4\pi}$$

Where Δx → uncertainty in the position, Δp → uncertainty in the momentum

ie "In any simultaneous determination of the position and momentum of the particle, the product of the corresponding uncertainties inherently present in the measurement is equal to or greater than $(\frac{h}{4\pi})$."

If we arrange matter, so that Δx is small, corresponding to narrow wave group then Δp will be large. If we reduce Δp in some way, a broad wave group is inevitable and Δx will be large.

Energy-Time uncertainty principle:

It states that "In an simultaneous measurement of energy and time in a physical process, the product of the corresponding uncertainties inherently present in the measurement is equal to or greater than $(\frac{h}{4\pi})$."

ie $$\Delta E \,.\Delta t \geq \frac{h}{4\pi}$$

Where ΔE → uncertainty in the energy, Δt → uncertainty in the time

Angular displacement and Angular momentum uncertainty principle:

It states that "In an simultaneous determination of angular momentum and angular displacement in a physical process the product of the corresponding uncertainties inherently present in the measurement is equal to or greater than $(\frac{h}{4\pi})$."

ie $$\Delta L \,.\Delta \theta \geq \frac{h}{4\pi}$$

Where ΔL → uncertainty in the momentum, $\Delta \theta$ → uncertainty in the displacement

Physical Significance:

The physical significance of the Heisenberg's uncertainty principle is that one should not think of the exact position or an accurate value for momentum of a particle. Instead one should think of the probability of finding the particle at a certain position or of the most probable value for the momentum of the particle. Similar interpretation is made for the conjugate pair ΔE and Δt and ΔLand $\Delta\theta$.

Applications of uncertainty principle:

Non-Existence of electrons in the nucleus:

Heisenberg's uncertainty principle states that $\Delta x\,.\Delta p \geq \frac{h}{4\pi}$ -------------- (1)

The radius of a typical atomic nucleus is about $5\times10^{-15}m$. If the electron is present inside the nucleus, then the uncertainty in its position is atmost equal to the diameter of the nucleus ie $\Delta x = 10^{-14}m$.

Then, from (1) $\quad \Delta p \geq \frac{h}{4\pi.\Delta x}$

$$\geq \frac{6.625\times10^{-34}}{4\times3.14\times10^{-14}}$$

$\Delta p \geq 0.527\times10^{-20}\,kg.m/s$ is the uncertainty in the momentum of the electron. Then the momentum of the electron must at least be equal to the uncertainty in the momentum

i e $\quad p = 0.527\times10^{-20}\,kg.m/s$

The energy 'E' of the electron is given by

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

Substituting for p and m we get

$$E = \frac{(0.527\times10^{-20})^2}{2\times9.1\times10^{-31}}$$

$$E = 95.4 \text{ MeV}$$

This means that in order that an electron may exist inside the nucleus, its kinetic energy must be greater than or equal to 95.4 MeV. But experiments show that the electrons emitted by certain unstable nuclei never have more than a small fraction of this energy (about 3MeV to 4MeV). From this we conclude that electron cannot exist within the nucleus.

Wave function (ψ):

The quantity whose variations make up matter waves is called the wave function ψ (psi). This wave function accounts for the wave-like properties of a particle and contain all possible information about the state of the system. The value of the wave function associated with a moving body at a particular point x, y, z in space at the time't' is related to the likelihood of finding the body there at that time. Wave functions are usually complex with both real and imaginary parts.

Physical significance of wave function (Max Born Approximation):

Probability of occurrence of an event is a real and a positive quantity. Since ψ, the wave function can be complex, it has no attributable physical significance.

The probability that something be in a certain place at a given time must lie between 0 and 1. Intermediate probabilities say 0.3 means that there is a 30% chance of finding the particle. But the amplitude of a wave can be positive as well as negative. A negative probability say -0.2 is meaningless. Hence ψ by itself cannot be an observable quantity.

But the square of the absolute value of the wave function $|\psi|^2$ is always positive and real and is known as **probability density**. This corresponds meaningfully to the definition of probability and is given by $|\psi|^2 = \psi.\psi^*$ where ψ^* is the complex conjugate of ψ.

"The probability of experimentally finding a particle described by the wave function ψ at the point x,y,z at the time 't' is proportional to the value of $|\psi|^2$ there at 't'." A large value of $|\psi|^2$ means the strong possibility of the body's presence, while a small value of $|\psi|^2$ means the slight-possibility of its presence.

Time Independent Schrödinger wave equation:

Consider a particle, moving freely in the positive x-direction in a stationary potential field. The wavelength of the associated deBroglie wave is given by

$$\lambda = \frac{h}{p} \qquad \rightarrow *$$

The wave equation for debroglie wave associated with such a particle can be written in complex notation as

$$\psi = Ae^{-i(wt-kx)} \qquad A \rightarrow \text{Amplitude of the wave}$$

$$\psi = Ae^{+i(kx-\omega t)} \qquad \rightarrow (1)$$

Since the particle is moving in a stationary or steady field, the potential energy of the particle does not depend on time but it varies only with the position of the particle.

Differentiating (1) w.r.t x twice we get

$$\frac{d\psi}{dx} = Ae^{i(kx-\omega t)}(ik)$$

$$\frac{d^2\psi}{dx^2} = Ae^{i(kx-\omega t)}(ik)^2$$

$$= -k^2\psi$$

But $k = \frac{2\pi}{\lambda}$, substituting in the above equation we get

$$\frac{d^2\psi}{dx^2}=-\frac{4\pi^2\psi}{\lambda^2}$$

Or $\frac{1}{\lambda^2}=-\frac{1}{4\pi^2\psi}\cdot\frac{d^2\psi}{dx^2}$ ------------ (2)

If 'm' is the mass of the particle moving with a velocity 'v' then K.E is

K.E$=\frac{1}{2}mv^2=\frac{m^2v^2}{2m}=\frac{p^2}{2m}$ ----------- (3)

Where $p=mv$, momentum of the particle. But $p=\frac{h}{\lambda}$; from (*)

$$\therefore \quad \text{K.E}=\frac{h^2}{\lambda^2\cdot 2m}=\frac{h^2}{2m}\cdot\frac{1}{\lambda^2}$$

$$=\frac{h^2}{2m}\times-\frac{1}{4\pi^2\psi}\cdot\frac{d^2\psi}{dx^2}$$

K.E $=-\frac{h^2}{8\pi^2m\psi}\cdot\frac{d^2\psi}{dx^2}$ ------------------------ (4)

Let 'V' be the potential energy of the particle which depends on the position of the particle in the field. Then total energy 'E' of the particle is

$$E=K.E+P.E$$

$$E=-\frac{h^2}{8\pi^2m\psi}\times\frac{d^2\psi}{dx^2}+V$$

ie $\frac{d^2\psi}{dx^2}=-\frac{8\pi^2m}{h^2}(E-V)\psi$

or $$\boxed{\frac{d^2\psi}{dx^2}+\frac{8\pi^2m}{h^2}(E-V)\psi=0}$$

This is the time independent Schrödinger's wave equation in one dimension.

In three dimensions, it becomes

$$\frac{d^2\psi}{dx^2}+\frac{d^2\psi}{dy^2}+\frac{d^2\psi}{dz^2}+\frac{8\pi^2m}{h^2}(E-V)\psi=0$$

Normalization:

If ψ is the wave function associated with a particle, then the probability of finding the particle in a volume dV is $|\psi|^2\,dV$. Since the particle is present somewhere in a particular region, the integral of $|\psi|^2\,dv$ over all space must be finite. If the particle is certainly to be found, in certain region of space then

$\int_{-\infty}^{+\infty}|\psi^2|dV=1$ ------------------- (1)

Any wave function satisfying the equation (1) is said to be normalized wave function.

Very often ψ is not a normalized wave function, i.e. the result of $\int |\psi|^2 dV$ will not be unity, but involves a constant that existed in the equation for ψ. However the actual result obtained is equated to unity and the value of the constant is determined. It is then substituted in the equation for ψ. This process is called **normalization.**

Properties of wave function:

A system is defined by its energy, position, momentum etc. It is postulated in quantum mechanics that a wave function (ψ) corresponding to a system contains all possible information about the system. In order to ψ of a system, the Schrödinger's equation has to be solved. Since it is a second order differential equation it has many solutions. All of them may not be the correct wave functions which correspond meaningfully to a physical system. Only those wave functions which satisfy the following criteria are acceptable wave functions.

1. ψ is single valued, every where. There should be only one probability for the particle to be in a specific location at a specific time.
2. ψ must be normalized, which means that ψ must go to zero as x→ $\pm\infty$, y→ $\pm\infty$, z→ $\pm\infty$ in order that $\int |\psi|^2 dV$ over all space be a finite constant.
3. ψ must be finite every where.
4. ψ and its first derivatives with respect to its variables must be continuous and single valued every where.

Eigen functions:

Eigen functions are those wave functions of quantum mechanics which possess the properties that they are single valued and finite every where and also their first derivatives with respect to their variables are continuous every where.

Eigen values:

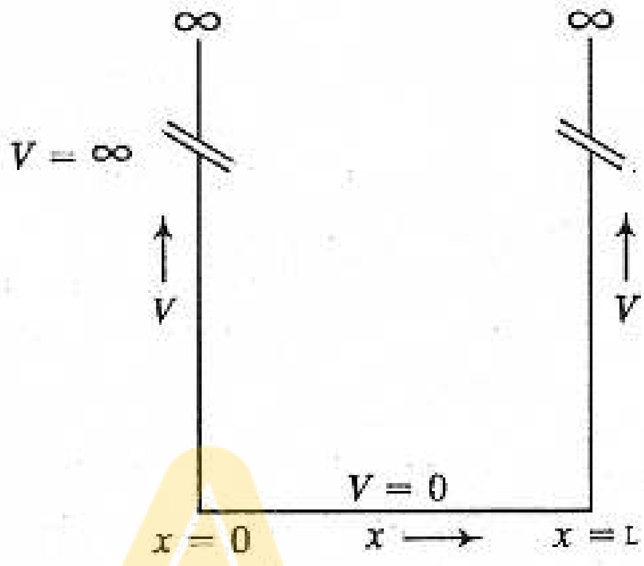
The values of a physical observable such as energy, momentum etc for which Schrödinger's wave equation can be solved are called **Eigen values**.

A wave function ψ contains all the information regarding the state of a system. The wave functions can be obtained by solving Schrödinger's wave equation. Once the correct wave functions called Eigen functions are known, quantum mechanical operators could be used to evaluate the physical observables like energy. But as postulated in quantum mechanics only those values 'λ' for a physical quantity are possible which satisfy the operator equation $\hat{A}\psi = \lambda\psi$ where $\hat{A}$ → operator for the physical quantity , ψ → Eigen function

Thus the eigen functions should be such that the operator operating on it produces back the wave function multiplied by a constant 'λ' such values (λ) for a physical quantity for which scrodinger's equation can be solved are called Eigen values.

Applications of Schrödinger's wave equation:

Energy Eigen values of a particle in one dimensional, infinite potential well (particle in a box):



Consider a particle, which is free to move in the x-direction only in the region x = 0 and x = L. Outside this region the potential energy is taken to be infinite and within this region it is zero ie V = 0 for 0<x<L and $V = \infty$ for $x \geq \infty$ and $x \leq 0$

We have the Schrödinger's time independent wave equation in one dimension

$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2 m}{h^2}(E - V)\psi = 0 \quad \text{------------ (1)}$$

Outside the well, the equation (1) become

$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2 m}{h^2}(E - \infty)\psi = 0 \qquad \text{Since } V = \infty$$

This equation holds good only if $\psi = 0$ for all points outside the well, ie $|\psi|^2 = 0$ which means that the particle cannot be found at all outside the well.

Inside the well, equation (1) becomes

$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2 m}{h^2}E\psi = 0 \quad \text{(Since V =0)}$$

Let $\frac{8\pi^2 m}{h^2}E = k^2$ ---------------- (2)

Then;

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0 \quad \text{------------- (3)}$$

The solution for the above equation is

$$\psi = A\sin kx + B\cos kx \quad \text{------------- (4)}$$

At x = 0, ψ = 0, substituting in (4) we get

$$0 = A\sin 0 + B\cos 0$$

$$\Rightarrow B = 0$$

At x = L, ψ = 0 and equation (4) becomes

$$0 = A\sin kL + B\cos kL$$

$$\Rightarrow A\sin kL = 0 \qquad \text{(Since B=0)}$$

Here ‘A’ need not be zero

$$\therefore \qquad \sin kL = 0$$

i.e. $kL = n\pi$, where n=0, 1, 2, 3……….is an integer called quantum number.

$$\therefore \qquad k = \frac{n\pi}{L} \text{ ---------------(4)}$$

Substituting the values of B and k in (4)

$$\boxed{\psi_n = A\sin\frac{n\pi}{L}x} \text{ ------------------ (6)}$$

which represents the permitted solutions.

Since there is only one particle and at any time it is present somewhere inside the well only, the integral of the wave function over the entire space in the well must be equal to unity.

i.e. $$\int_0^L |\psi_n|^2 dx = 1$$

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

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

$$A^2\left[\frac{1}{2}\int_0^L dx - \frac{1}{2}\int_0^L \cos\frac{2n\pi}{L}x\,dx\right] = 1 \qquad [\because \ \sin^2\theta = \frac{1}{2}(1-\cos 2\theta)]$$

Or $$\frac{A^2}{2}\left[x - \frac{L}{2n\pi}\sin\left(\frac{2n\pi}{L}x\right)\right]_0^L = 1$$

Or $$\frac{A^2}{2}\left[L - \frac{L}{2n\pi}\sin(2n\pi) - 0\right] = 1$$

$$\Rightarrow \quad \frac{A^2 L}{2} = 1$$

$$\Rightarrow \quad \boxed{A = \sqrt{\frac{2}{L}}}$$

Substituting in (5) we get

$$\boxed{\psi_n = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi}{L}\right)x} \quad \text{--------------------} \quad (7)$$

which are the normalized wave functions of a particle in a one-dimensional infinite potential well.

Energy Eigen values:

The energy Eigen values can be obtained by substituting $k = \frac{n\pi}{L}$ in equation (2)

$$\frac{8\pi^2 m}{h^2} E = \left(\frac{n\pi}{L}\right)^2$$

Or $$\boxed{E_n = \frac{n^2h^2}{8mL^2}} \quad \text{-------------------------} \ (8)$$

are the energy Eigen values of the particle in an infinite potential well.

Zero-point energy:

The lowest acceptable value for n=1. Because for n=0, $\psi_n = 0$ (from equation (5)), which means that the particle is not present inside the well which is not true.

The lowest energy corresponding to n = 1 is called zero-point energy and it is given by

$$E_{zero-point} = \frac{h^2}{8mL^2}$$

The lowest permitted state of energy is referred to as ground state energy. The energy state for n>1 are called exited states.

Wave functions, Probability densities and Energy levels for particle in an infinite potential well:

The normalized wave functions of a particle in a one dimensional potential well of width 'L' are given by

$$\psi_n = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi}{L}\right)x \quad \text{---------------------} \ (1) \qquad n = 0, 1, 2\ldots\ldots$$

Case1: For n=1:

This is the ground state and the particle is normally found in this state. The Eigen function corresponding to this state

$$\psi_1 = \sqrt{\frac{2}{L}}\sin\left(\frac{\pi}{L}\right)x; \qquad \text{from (1)}$$

Here $\psi_1 = 0$ for x = 0 and x = L and is maximum for $x = \frac{L}{2}$ (fig a)

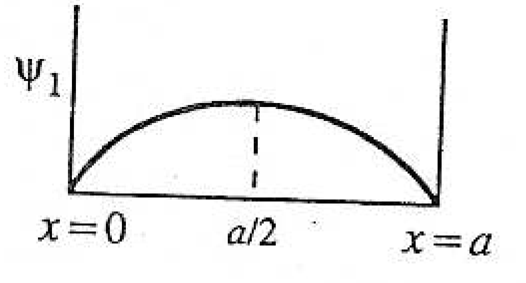


Fig (a)

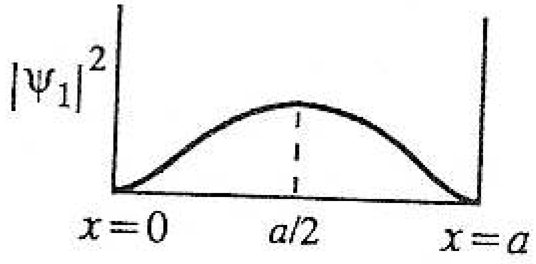


Fig (b)

A plot of $|\psi_1|^2$, the probability density verses **x** is shown in fig (b). It indicates the probability of finding the particle at different locations inside the well. $|\psi_1|^2 = 0$ at x = 0 and x = L and is maximum at $x = \frac{L}{2}$. This means that in the ground state the particle cannot be found at the walls of the box, and the probability of finding it is maximum at the central region.

The energy of the particle in the ground energy state is

$$E_1 = \frac{h^2}{8mL^2} = E_0\text{, Zero-point energy}$$

<u>Case 2</u>: For n=2

This is the first exited state. The Eigen function for this state is

$$\psi_2 = \sqrt{\frac{2}{L}}\sin\left(\frac{2\pi}{L}\right)x$$

Here $\psi_2 = 0$ for x = $0, \frac{L}{2}$, L and maximum for $x = \frac{L}{4}$ and $\frac{3L}{4}$ (fig c)

The plot of $|\psi_1|^2$ verses x is shown in fig (d). As can be seen from the plot, the particle cannot be observed either at the walls or at the center.

The energy of the particle in this state is

$$E_2 = \frac{4h^2}{8mL^2} = 4E_0 \quad ; \qquad \because E_n = \frac{n^2h^2}{8mL^2}$$

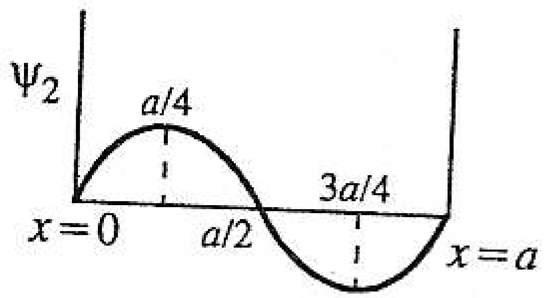


Fig (c)

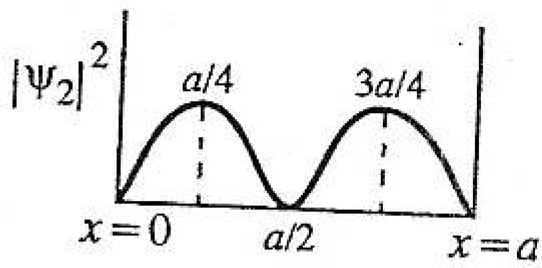


Fig (d)

<u>Csae3:</u> For n=3 (second exited state)

The Eigen function for the second exited state is

$$\psi_3 = \sqrt{\frac{2}{L}}\sin\left(\frac{3\pi}{L}\right)x$$

Here $\psi_3 = 0$ for $x=0, \frac{L}{3}, \frac{2L}{3}$ and L and maximum for $x = \frac{L}{6}, \frac{L}{2}, \frac{5L}{6}$. The plot of ψ_3 and $|\psi_3|^2$ verses x are shown in fig (e) and fig (f). The energy of the particle in this energy state is

$$E_3 = \frac{9h^2}{8mL^2} = 9E_0$$

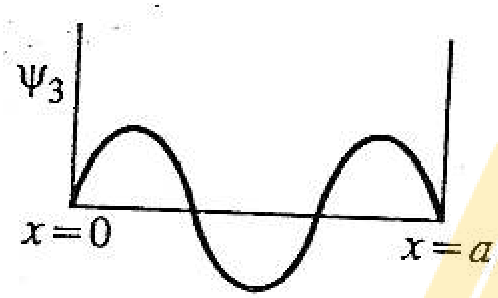


Fig (e)

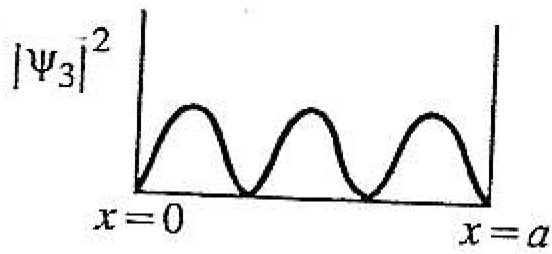


Fig (f)

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QUESTIONS

1. Show that electrons cannot exist inside the nucleus of an atom.
2. State Heisenberg's uncertainty principle in three forms.
3. Set up one dimensional time independent Schrödinger wave equation for an electron.
4. What are the properties of a wave function?
5. Find the Eigen functions and energy Eigen values for a particle in one dimensional potential well of infinite height and discuss the solutions.
6. State and explain Heisenberg's uncertainty principle. Give its physical significance
7. Give an account of wave functions in quantum mechanics.
8. Explain what is meant by normalization.
9. Describe the physical significance of a wave function in respect of probability density.
10. What are Eigen functions and Eigen values?

MODULE -IV

LASERS

LASER is the acronym of "**L**ight **A**mplification by **S**timulated **E**mission of **R**adiation".

Properties of Lasers:

1. The laser light is very nearly monochromatic.
2. The laser light is coherent with the waves all exactly in phase with one another.
3. Directionality**:** Laser beam is highly directional. It hardly diverges. This property is useful to measure long distance with higher accuracy.
4. Intensity: Laser is extremely intense; hence by Laser we can achieve very high energy density.

Basic Principle:

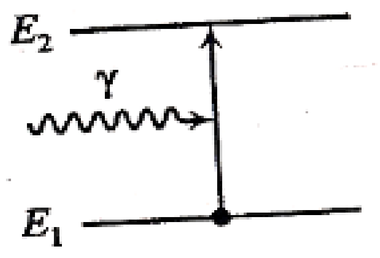
When radiation interacts with matter, it leads to the transition of a quantum system such as atom or molecule from one energy state to another.

Consider two energy states E_1 and E_2, $(E_2 > E_1)$ of a system. An electron at the energy state E_1 is exited to E_2, when it absorbs a light photon of energy ΔE = (E_2-E_1). If an electron makes a transition from the higher energy state E_2 to E_1, a light of photon of energy ΔE = E_2-E_1 is emitted. In both the case the frequency of the photon involved is $\nu = \frac{\Delta E}{h} = \frac{E_2 - E_1}{h}$

There are three possible ways in which interaction of radiation and matter can take place.

1. Induced (stimulated) absorption:

"The process in witch an atom in a lower energy state is raised to a higher energy state by absorbing a suitable photon is called stimulated absorption."



INDUCED ABSORPTION

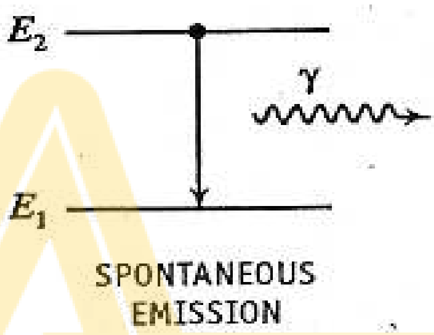
Consider two energy states with energies E_1 and E_2. Let a photon of energy, $\Delta E = E_2 - E_1$ be incident on the atom. The atom absorbs the energy of the photon and its energy becomes equal to $E_1 + \Delta E = E_2$. Hence it makes a transition to the exited state E_2. This is called induced absorption.

Induced absorption can be represented as

atom + photon $\rightarrow$ atom* (* represents the excited state)

2. Spontaneous emission:

"The process in which an atom in the higher energy state falls to the lower state by emitting a photon on its own is called spontaneous emission."



Consider an atom in the excited state, the atom voluntarily emits a photon of energy ΔE equal to $(E_2 - E_1)$ and falls to the energy state E_1. The emission where an atom emits a photon without any aid by external agency is called spontaneous emission. The photons emitted may have any direction and phase. Hence they are incoherent.

This process can be represented as

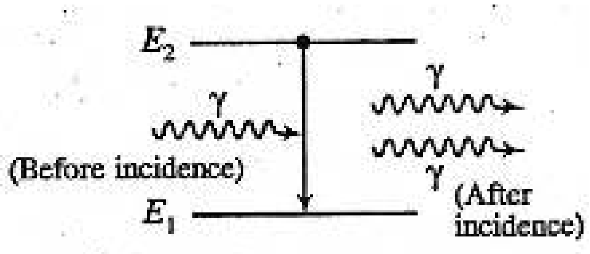
atom* $\rightarrow$ atom + photon

Note: 1) Life time of atoms in higher energy state is usually very small of the order of 10^{-8} sec.

2) If there is an assembly of atoms, the radiation emitted spontaneously by each atom has a random direction and random phase. Therefore radiation emitted by spontaneous emission is incoherent. (Eg: glowing electric bulb)

3. Stimulated emission:

"The process of the emission of a photon by a system under the influence of a incident photon of suitable energy, due to which the system transits from a higher energy state to a lower energy state is called stimulated emission."



STIMULATED EMISSION

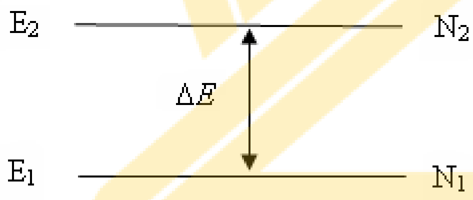
Consider an atom in the exited state with energy E_2. Let a photon of energy $\Delta E = E_2 - E_1$ interacts with this atom. As a result, the atom emits a photon and transits to the lower energy state. The emitted photon will have same phase, energy and direction of movement as that of the incident photon." The electromagnetic waves associated with the two photons will have same phase and thus they are coherent.

This kind of emission is responsible for laser action.

This process can be represented as

$$\text{atom}^* + \text{photon} \rightarrow \text{atom} + 2\,\text{photon}$$

Einstein's coefficients - Expression for energy density



Consider two energy states E_1 and E_2 of a system of atoms ($E_1 < E_2$). Let N_1 be the number of atoms in the energy state E_1 and N_2 be in E_2 per unit volume of the system. Then N_1 and N_2 are called the number density of atoms in the energy states E_1 and E_2 respectively. Let $U_\upsilon d\nu$ be the energy of the incident radiation per unit volume of the system where radiations lie in the frequency range ν to $\nu + d\nu$, then 'U_υ' is called the energy density of frequency "ν".

Case (1): Induced absorption:

In this case an atom in the energy level E_1 can undergo a transition to the level E_2 by absorbing a radiation of suitable frequency $\nu = \dfrac{E_2 - E_1}{h}$

The number of such absorptions per unit time per unit volume is called the rate of absorption.

It depends on (a) the number density of lower energy state

(b) The energy density 'U_υ'.

$\therefore$ Rate of absorption $\propto N_1 U_\upsilon$

Or Rate of absorption = $B_{12} N_1 U_\upsilon$ $\rightarrow$ (1)

Where B_{12} → Einstein's Coefficient of induced absorption.

Case (2): Spontaneous emission:

In this case, an atom in the higher energy state E_2 undergoes a transition to the lower energy state E_1, by itself, emitting a photon. It is independent of energy density of any frequency. The number of such spontaneous emission per unit time per unit volume is called the rate of spontaneous emission. It depends only on the number density of higher energy state ie N_2.

Therefore Rate of spontaneous emission = $A_{21}N_2$ ------------ (2)

where A_{21} → Einstein's coefficient of spontaneous emission.

Case 3: Stimulated emission:

In this case an external photon of frequency $\nu = \frac{E_2 - E_1}{h}$ stimulate an atom for the downward transition and thereby cause emission of stimulated photons. The number of stimulated emission per unit time per unit volume is called rate of stimulated emission.

It depends on a) Number density of higher energy state

b) The energy density 'U_υ'.

Therefore rate of stimulated emission $\propto N_2 U_\upsilon$

$$= B_{21} N_2 U_\upsilon \quad \text{---------------} \quad (3)$$

where B_{21} is the Einstein's coefficient of stimulated emission.

At thermal equilibrium,

Rate of absorption = Rate of spontaneous emission+ Rate of stimulated emission.

ie $B_{12} N_1 U_\upsilon = A_{21}N_2 + B_{21} N_2 U_\upsilon$

ie $U_\upsilon (B_{12} N_1 - B_{21} N_2) = A_{21} N_2$

$$\therefore U_\upsilon = \frac{A_{21} N_2}{B_{12} N_1 - B_{21} N_2}$$

Or $$U_\upsilon = \frac{A_{21}}{B_{21}}\left[\frac{1}{\frac{B_{12}}{B_{21}}\frac{N_1}{N_2}-1}\right]$$ ---------------------- (4)

According to Boltzmann's law we have

$$N_2 = N_1 e^{-\left(\frac{E_2-E_1}{KT}\right)} = N_1 e^{-\frac{h\upsilon}{KT}}$$

$$\therefore \frac{N_1}{N_2} = e^{h\nu/kT}$$ ------------- (5)

Therefore equation (4) becomes

$$U_\upsilon = \frac{A_{21}}{B_{21}}\left[\frac{1}{\frac{B_{12}}{B_{21}}e^{\frac{h\upsilon}{KT}}-1}\right]$$ ---------------- (6)

According to Planck's law of radiation

$$U_\nu = \frac{8\pi h\nu^3}{C^3}\left[\frac{1}{e^{\frac{h\nu}{KT}}-1}\right]$$ -------------------- (7)

Comparing equation (6) and (7) we have

$$\frac{A_{21}}{B_{21}} = \frac{8\pi h\nu^3}{C^3}, and\ \frac{B_{12}}{B_{21}} - = 1$$

➔ $B_{12}=B_{21}=B$ ---------- (8) and $A_{21} = A$

The identity (8) implies that the probability of induced absorption is equal to the probability of stimulated emission.

Therefore we can write the expression for energy density in terms of Einstein's A & B coefficients as

$$\boxed{U_\upsilon = \frac{A}{B\left[e^{\frac{h\nu}{kT}}-1\right]}}$$

Condition for Laser action

1. **Population inversion:**

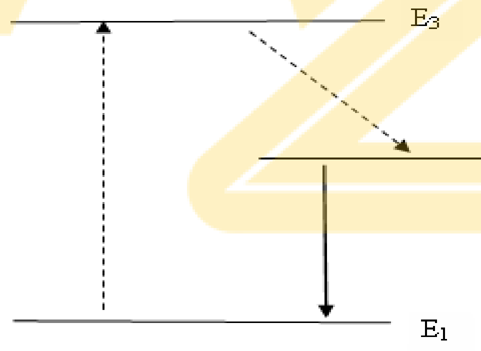
"It is the state of a system in which the number of atoms in the higher energy level is greater than the number of atoms in the lower energy state."

Under normal condition, the population is more in lower state. But for stimulated emission and hence for lasing action more atoms must be present in the exited state. This can be achieved by some artificial means i.e. by providing energy in to the active medium of the laser system.

2: Metastable state:

Under normal condition, population inversion doesn't exist. However it is possible to achieve the population inversion in certain systems which posses a special exited state called **metastable state.**

It is an exited state different from the ordinary exited state. The atoms which are excited to the higher energy states remain for a short duration of 10^{-8} sec and return to lower energy state. In case the state at which the atom is exited is a metastable state, then it stays there for a longer time of about 10^{-3} to 10^{-2} sec. This property helps in achieving population inversion.



Consider 3 energy levels E_1, E_2, and E_3 of an atomic system. Let E_2 be a metastable state. By supplying suitable external energy, the atoms are exited from E_1 to E_3. The atoms in E_3 undergo spontaneous transition to E_1 and E_2 rapidly. Since E_2 is a metastable state, the atoms in this state stay for a longer time duration because of which the population in E_2 increases and population inversion is created. Once the population of E_2 exceeds that of E_1, the stimulated emission takes place. The photons emitted are all identical in respect of phase, wavelength and direction; grow to a large number which is the laser light.

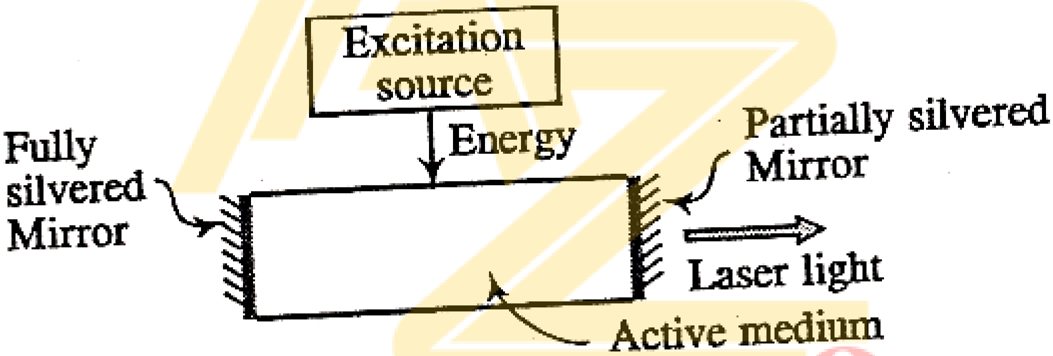
Requisites of a laser system.

1) An excitation source for pumping action.
2) An active medium which supports population inversion.
3) A laser cavity.

1) An **excitation source** provides energy in an appropriate from for pumping the atoms to higher energy levels If the pumping is achieved by light energy input then it is called optical pumping (Ruby laser). If the pumping is achieved by electrical energy input then it is called electrical pumping (He-Ne laser).

2) **Active medium**. A medium in which light gets amplified is known an active medium. The medium may be solid, liquid or a gas. Out of the different atoms in the medium, only a small fraction of atoms of particular species are responsible for stimulated emission and consequent light amplification. They are called active centres. The remaining bulk of the active medium acts the role host which supports active centres.

3) Laser cavity:

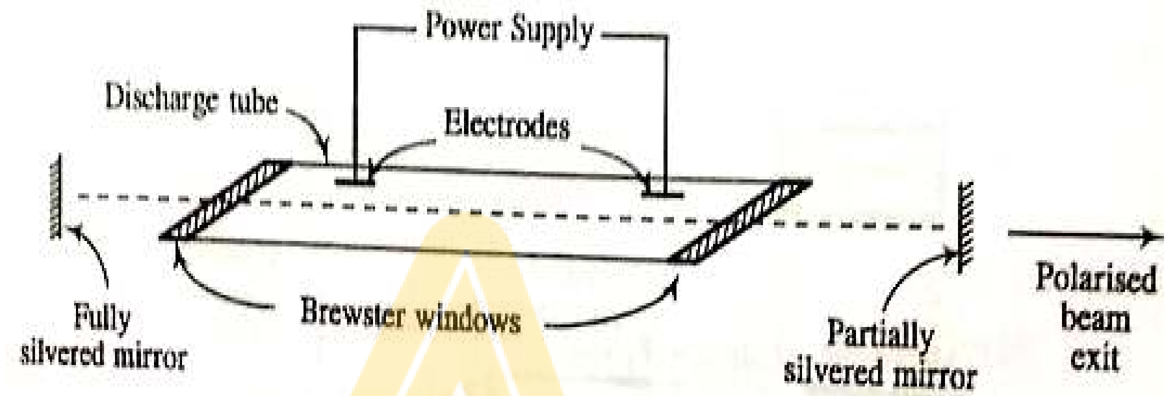


A laser device consists of an active medium bound between two parallel mirrors of high reflectivity. The mirrors reflect the photon to and fro through the active medium. Thus the two mirrors along with the medium is called cavity. Inside the cavity two types of waves exist, one moving towards the right and other to the left. These waves interfere constructively or destructively depending on the phase difference. In order to arrange for constructive interference, the distance 'L' between the two mirrors should be such that the cavity should support an integral number of half wavelength, i.e. $L = m\frac{\lambda}{2}$, where m→ an integer. This results in the amplification of stimulated emission of radiation which is the laser light.

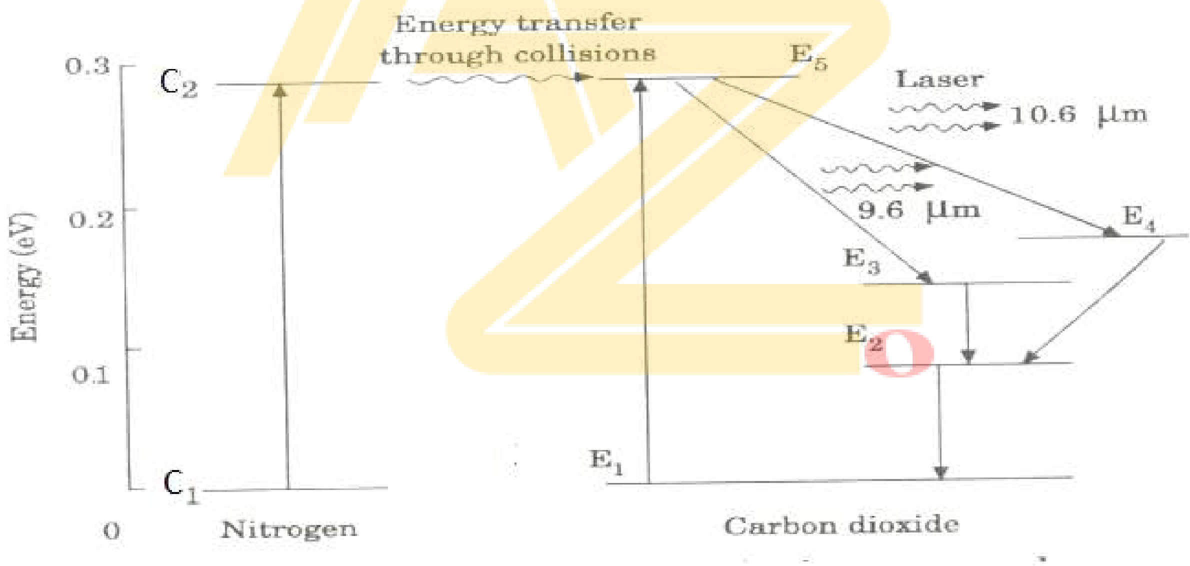
Carbon Dioxide Laser:

The carbon dioxide gas laser is a four level molecular laser which operates at 10.6 μm in a far IR region. It operates in a continuous wave (CW) mode and is capable of generating very high power of 100 kilo watts at relatively high efficiency of 40%. Therefore it is the most widely used laser in communications, weaponry and laser fusion.

Construction:

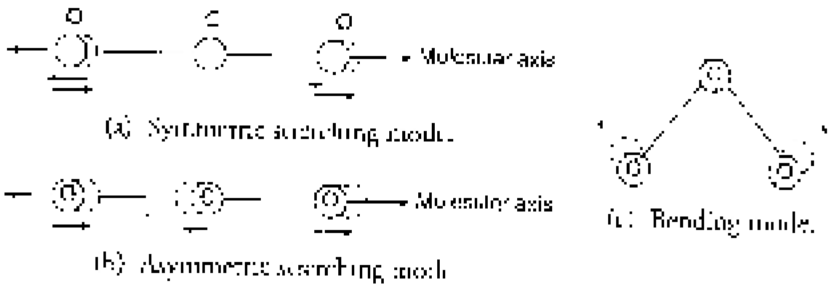


Energy Level Diagram



The CO_2 laser has a discharge tube of length 5 m and diameter 2.5 cm. The ends of the tube are closed with Brewster windows. Outside the ends of tube, confocal silicon mirrors coated with aluminium are arranged. This forms the resonant cavity. The discharge tube is filled with a mixture of carbon dioxide, nitrogen and helium gases in 1:2:3 respectively. A high DC voltage is applied to the mixture. The pumping mechanism based on electric discharge is used to create population inversion.

Fundamental modes of vibration in CO_2 molecule:



In CO_2 molecule there are three fundamental modes of vibration

1. Symmetric stretching mode: In this mode, the Carbon atom is stationary and oxygen atoms oscillates simultaneously to and fro along the molecular axis
2. Asymmetric stretching mode : In this mode both oxygen atoms move in one direction and carbon atom moves in opposite direction along the molecular axis
3. Bending mode: The oxygen atoms and the carbon atom move perpendicular to the molecular axis. The internal vibrations of CO_2 molecule are the linear combination of the above three modes.

In CO_2 laser, the energy transition takes place between the rotational sublevel of an upper and lower vibrational level.

Working: (Excitation mechanism and lasing action)

When electric discharge takes place in the gas mixture both N_2 and CO_2 atoms absorb energy and are excited to higher energy levels. The energy level C_2 of nitrogen matches with one of the vibrational – rotational level of CO_2 (E_5 shown in diagram). Therefore more CO_2 atoms are raised to E_5 level by colliding with nitrogen molecules in C_2 state. There is an efficient transfer of energy between C_2 level of nitrogen and E_5 level of CO_2. This kind of energy transfer is called ***resonant energy transfer.***

This energy transfer results in the population inversion between E_5 and E_4 and between E_5 and E_3. The transition from E_5 to E_4 produces a radiation of wavelength 10.6 μm and from level E_5 to E_3 produces radiation of wavelength 9.6

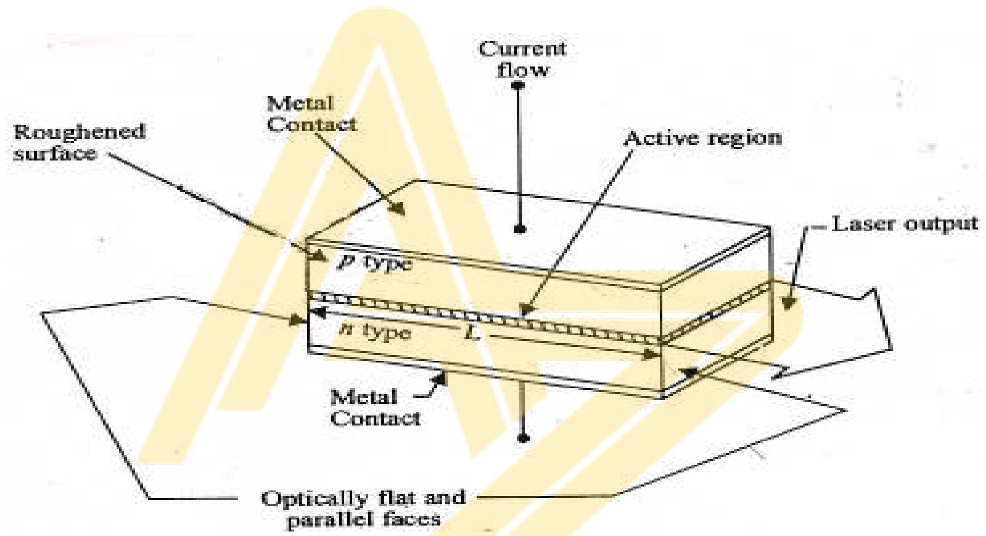
μm both lying in IR region. The other transition from E_3 to E_2 and E_2 to E_1 is accomplished through inelastic collision with helium atoms. The helium atoms help to depopulate the lower energy levels. Also due to high thermal conductivity of He, the heat is conducted away from laser cavity.

Applications:

1. CO_2 lasers are extensively used in industries for welding, cutting and drilling.
2. CO_2 lasers are extensively used in communication systems.

Semiconductor Diode laser:

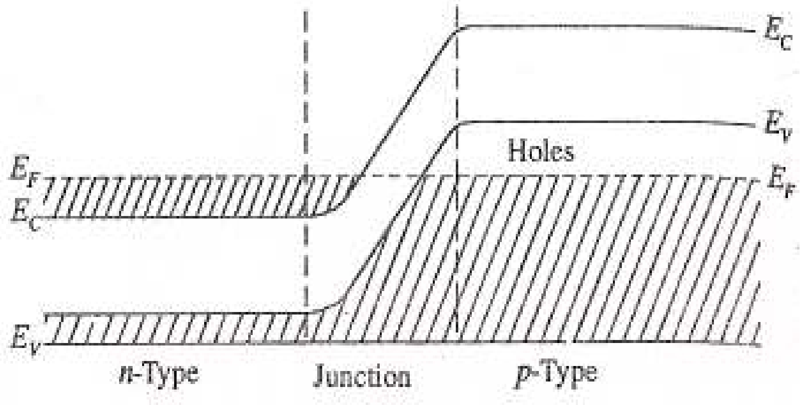
Construction:



A semiconductor diode laser is a specially fabricated p-n junction device that emits coherent light when it is forward biased.

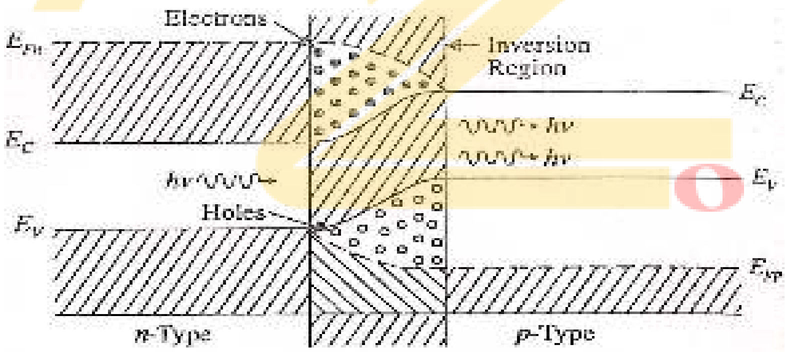
The diode is extremely small in size with sides of the order of 1mm. The junction lies in the horizontal plane through the centre. The top and bottom faces are metallized and ohmic contacts are provided to pass current through the diode. The front and rear faces perpendicular to the plane of the junction are polished and silvered to form the laser cavity. The other two faces are roughened to prevent lasing action in that direction. The active region consists of a layer of about 1 μm thickness.

Working:



(a)

The population inversion can be achieved in a semiconductor by using it in the form of a heavily doped p-n junction and forward biasing it. With very high doping on n-side, the donar levels as well as a portion of the conduction band (CB) are occupied by electrons and the Fermi level lies within the CB. On the heavily doped p-side, the accepter levels are unoccupied and holes exist in the valence band (VB) and the Fermi level lies within the VB. At equilibrium the Fermi level is uniform across the junction [fig (a)].



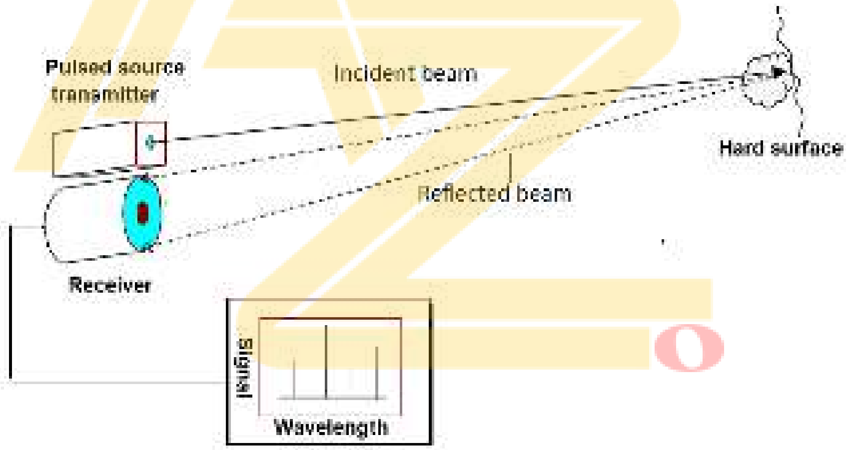
(b)

When a forward bias is applied, the energy levels shifts and the new distribution will be as shown in fig (b). Electrons and holes are injected in to the depletion region, where they appear in large number. At low forward current, the electron-hole recombination cause spontaneous emission of photons. As the current increased and reaches a threshold value, the carrier-concentration in the depletion region will reach very high values. The upper levels in the depletion region are having high population of electrons while the lower levels are having large number of holes. This is the state of population inversion. The narrow region where the state of population inversion is achieved is called inversion or active region. Thus the forward bias current plays the role of pumping agent in semiconductor laser. The photons that propagate in the junction plane induce the conduction electrons to jump in to the vacant state of VB. The stimulated electron hole recombination causes emission of coherent radiation.

Applications of Laser:

Laser Range finder:

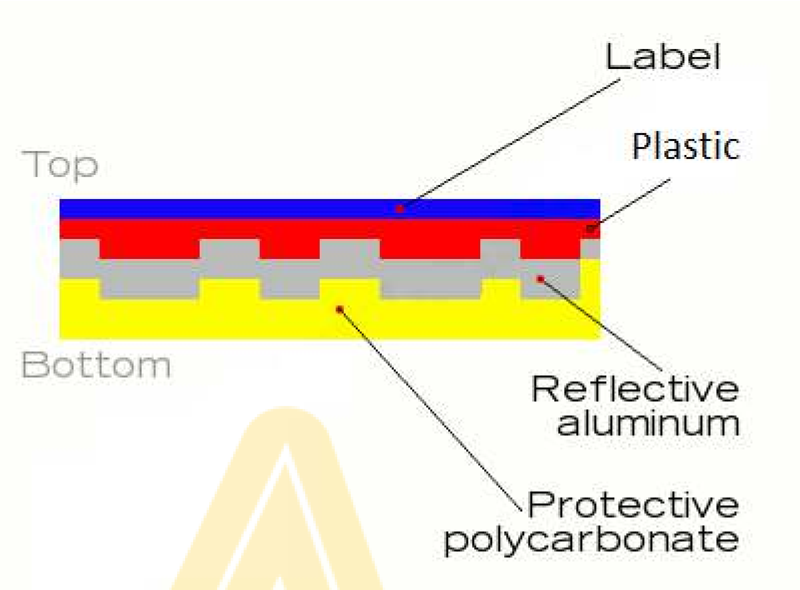
A rangefinder is a device that measures the distance from the observer to a target for the purposes of surveying, auto-focusing or accurately aiming a weapon. The excellent directionality of laser makes it ideal for ranging applications. Laser range finders are used to get accurate information about the enemy target without the knowledge of the enemy personals. The computer interfaced rangefinders can calculate the distance of the target within 1% of the actual distance.



A high power laser pulse is directed towards the enemy target from the transmitting part of the range finder. The beam gets reflected from the surface of the target which is collected by a receiver. A suitably tuned optical interference filter present in the receiver eliminates the background noise. The pure signal is amplified by the photomultiplier tube. The time for to and fro motion of beam is measured by a built-in clock which is then converted in to the distance.

LASERS IN DATA STORAGE

A compact disc is a thin, circular disc of metal and plastic. It consists of three layers, a tough, brittle plastic called **polycarbonate** at the bottom, a protective layer of plastic and lacquer at the top. A thin layer of aluminum is sandwiched in between these two layers.



The information is created in digital form using a laser beam. A series of microscopic holes/bumps known as **pits** are formed by burning the surface at certain specified intervals. The presence of this pit or bump in a fixed length indicates the number **'zero'**. The unburnt flat area on the disc is called **land** and it represents the number **'one'**. Thus the information is stored by burning some lengths of the surface (zeroes) and leaving some length unburnt (ones) in binary form.

While reading the CD, the surface is scanned by a laser beam. As the beam bounces, it follows the pattern of pits and lands. Laser light reflected from pit represents binary zero and from the land represents binary number one. The reflected light is converted in to electric pulses by a photo detector. An electronic circuit generates zeroes and ones from these pulses. These binary numbers are converted into an analog electrical signal using decoder.

IMPORTANT QUESTIONS

1) What is Laser?
2) Explain with sketches the basic principle of operation of laser
3) What is metastable state?

4) Describe the construction and working of CO_2 laser with energy level diagram.

5) Derive the expression for energy density of radiation using Einstein's coefficient.

6) Describe with energy band diagram the construction and working of semiconductor diode laser.

7) What are the conditions and requisites of a laser system?

8) Explain induced absorption, spontaneous and stimulated emissions.

9) Explain the application of laser in

i) Range Finders

ii) Data storage