

Unit III: Module-1 Quantum Mechanics

Black body radiation (Energy distribution curve of a black body)

Planck's Law (without derivation)

Wien's displacement law and Rayleigh Jeans Law from Planck's theory

De-Broglie concept

Uncertainty principle

Schrödinger's wave equation-Time independent and time dependent equations

Physical significance of wave function

Particle in a one dimensional box

Quantum mechanics also sometimes called wave mechanics, is the one which deals with the investigation of the behavior of micro-particles. Most advances that have taken place in solid state, Atomic and Nuclear physics are based on the principles of quantum mechanics.

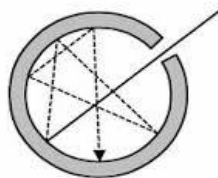
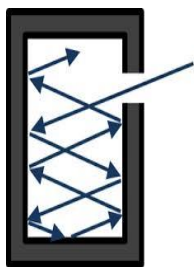
The wave theory of light successfully explained the phenomena of interference, diffraction, polarization etc. But the classical mechanics laws (Corpuscular theory, wave theory of light) failed to explain the newly discovered phenomena like Compton effect, photoelectric effect, Zeeman effect and absorption of light etc.

To explain the above mentioned phenomena resulting due to the interaction of light with matter gave birth to quantum theory of light. This quantum theory of light was first introduced by Max Ludwig Planck of Germany in the year 1900.

➤ Black body radiation

Black body: A perfect black body is one, which absorbs radiation of all wavelength's incident upon it.

The term comes from the fact that a cold blackbody appears visually black. The black body is a composed of atoms and molecules which can emit and absorb light.



As the radiating power of a body is proportional to its absorbing power, a black body would also radiate more strongly at any given temperature than any other surface. They emit light because they are wiggling around due to their heat content (thermal energy). So a blackbody emits a certain spectrum of light that depends only on its temperature. The higher the temperature, the more light energy is emitted and the higher the frequency (shorter the wavelength) of the peak of

the spectrum. The radiations emitted from the black body are independent of the nature of the body

➤ **Black body spectrum(Energy distribution curve of a black body)**

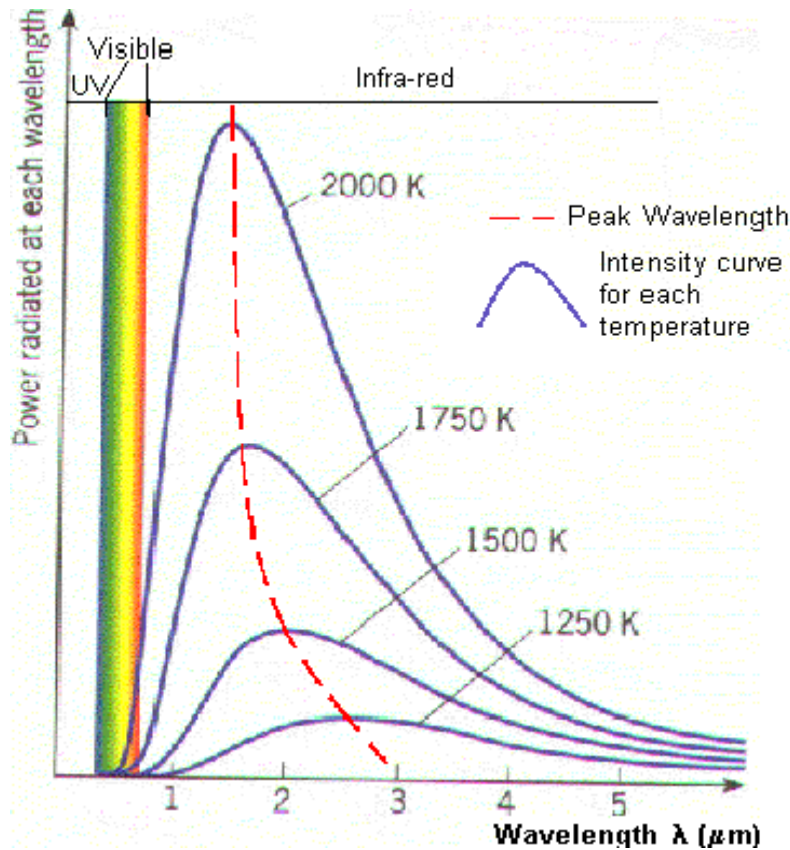


Figure 1 Variation of the energy radiated by black body at different wavelengths for a given temperature

If the temperature of the object is held constant, then the intensity of heat radiation can be plotted as a function of its wavelength, giving a graph of a characteristic shape, called the blackbody spectrum (figure 1). Classical physics was unable to explain these graphs. In fact, it predicted that they would diverge for short wavelengths! This dramatic failure of classical physics was what prompted Max Planck to introduce quantum theory.

Conclusions from the black body spectrum

1. The distribution of the radiated energy is not a uniform
2. For a particular wavelength, the intensity of the radiated energy first increase with increase in temperature and become highest at a certain value of the wavelength, thereafter it decreases with increase in temperature.
3. Rate of emission of black body radiation (area under the curve of a $E-\lambda$ curve) increases with increase in a temperature of the black body.

4. The peak of the curve shifted towards shorter wavelengths as temperature of the black body increases.

➤ Planck's Law of radiation

The Planck law gives the intensity radiated by a blackbody as a function of frequency (or wavelength). Let a blackbody have temperature T . Let be the $E_\lambda d\lambda$ energy density per unit solid angle so that

$$E_\lambda d\lambda = \frac{8\pi hc \lambda^{-5}}{[\exp(\frac{hc}{\lambda kT}) - 1]} d\lambda \dots\dots\dots (1)$$

This relation is known as a Planck's radiation Law

This relation has been derived on the basis of following assumptions

1. A black body is a consist of a large number of oscillation particles which can vibrate with all possible frequencies
2. The energy of a oscillation particle is a quantized and it is given by $E = nh\nu$. For a single photon the energy will be $E = h\nu$.
3. A vibration particle can emit energy only when it goes from one quantized state to another lower quantized state.
4. The absorption and emission of a energy by oscillating particle is always take place in discrete manner.

Special cases of a Planck's Law

1. Wein's distribution law

If we apply Planck's law for the shorter wavelengths (i.e. first half curve of black body spectrum when radiation energy increases with increase in wavelength)

Then, the term

$$\exp\left(\frac{hc}{\lambda kT}\right) - 1 \sim \exp\left(\frac{hc}{\lambda kT}\right)$$

Thus Planck's law becomes

$$E_\lambda d\lambda = 8\pi hc \lambda^{-5} \left[\exp\left(\frac{-hc}{\lambda kT}\right) \right] d\lambda \dots\dots\dots (2)$$

This relation is termed as a Wein's distribution law which is able to explain the black body spectrum for the shorter wavelengths

2. Rayleigh Jean's Law

If we apply Planck's law for the longer wavelengths (i.e. second half curve of black body spectrum when radiation energy decreases with increase in wavelength) Then the denominator of the equation 1 can be solved using exponential series

$$e^x = 1 + x + \frac{1}{2!}x^2 + \frac{1}{3!}x^3 + \dots$$

Thus the denominator of relation 2.1 will be

$$\exp\left(\frac{hc}{\lambda kT}\right) - 1 = \left[1 + \left(\frac{hc}{\lambda kT}\right) + \frac{1}{2!}\left(\frac{hc}{\lambda kT}\right)^2 + \dots\right] - 1$$

as λ is longer the higher terms in the above series can be ignored, thus we obtain

$$\exp\left(\frac{hc}{\lambda kT}\right) - 1 = \left[1 + \left(\frac{hc}{\lambda kT}\right)\right] - 1 = \left(\frac{hc}{\lambda kT}\right)$$

On putting above in 1, we obtain

$$E_\lambda d\lambda = \frac{8\pi hc \lambda^{-5}}{\left(\frac{hc}{\lambda kT}\right)} d\lambda$$

$$= E_\lambda d\lambda = 8\pi kT \lambda^{-4} d\lambda \dots \dots \dots (3)$$

This relation is termed as a Rayleigh Jean's Law

➤ Properties of Photon:

1. The existence of photon and electron are same in nature
2. The energy of one photon is $E = h \nu$
3. The rest mass of the photon is zero and they travel with the speed of light
4. The relation between energy and momentum of a photon

$$E = cp$$

$$h \nu / c = p$$

5. Photons are not affected by either an electric field or magnetic field (i.e. they are electrically neutral)

➤ Scattering of X-rays

The interaction of X-rays with a matter is of two types:

1. Coherent scattering

No change in wavelength after scattering of X-rays by electrons

2. Incoherent scattering (Compton scattering)

The scattered X-rays divided in two components, one having the same wavelength as that of the incident X-rays and other has a slightly larger wavelength.

Compton Effect (theory and experimental verification)

When a monochromatic beam of high frequency radiations (e.g., X-rays and γ rays) is scattered by a substance of less atomic number, the scattered radiations contain the radiations of higher wavelength (lower frequency) along with the radiations of unchanged wavelength (or frequency). This phenomenon is called the Compton Effect.

Theoretical explanation of Compton Effect

The photon move with velocity of light 'c' possess momentum $\frac{h\nu}{c}$ and obey all the laws of conservation of energy and momentum when they strike with electrons of the scattering substances.

When a photon of energy $h\nu$ collides with the free electron of the scattering substance initially at rest, it transfers some of the energy to electron. Due to this energy, the electron gains kinetic energy and recoils with velocity v . Hence the scattered photon will have lower energy i.e. lower frequency or longer wavelength than incident one.

$$\downarrow E = h\nu \quad \downarrow = \frac{hc}{\lambda \uparrow}$$

Basic assumption adopted for Compton scattering:

1. Compton effect is a result of interaction of a individual photon and free electron of target
2. The collision is relativistic and elastic
3. The laws of conservation of linear momentum and energy are valid

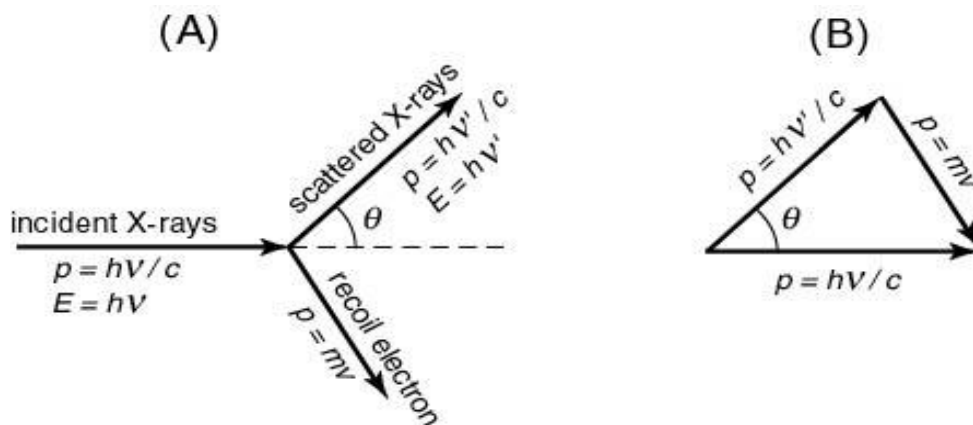


Figure: 2; Schematic figure of Compton scattering

The de Broglie Hypothesis

Since light seems to have both wave and particle properties, it is natural to ask whether matter (electrons, protons) might also have both wave and particle characteristics.

In 1924, a French physics student, Louis de Broglie, suggested this idea in his doctoral dissertation.

For the wavelength of electron, de Broglie chose:

$$\lambda = h/p$$

$$f = E/h$$

where E is the total energy, p is the momentum, and λ is called the de Broglie wavelength of the particle.

➤ Heisenberg's Uncertainty principle

In classical mechanics, a moving particle at any instant has (a) fixed position in space and a definite momentum which can be determined if the initial values are known. However, in wave mechanics, the particle is described in terms of a wavepacket. Particle may be found anywhere within the wavepacket. When the wavepacket is large, the velocity can be fixed but there is large indefiniteness in position. In this way the certainty in position involves uncertainty in momentum or velocity and certainty of momentum involves the uncertainty in position. This shows that it is impossible to know where within the wavepacket the particle is and what is its exact momentum.

The principle states that ‘The order of magnitude of the product of the uncertainties in the knowledge of two variables must be at least Planck’s constant h .

Considering the pair of physical variables as position and momentum,

$\Delta p \Delta x \approx h$ where Δp is corresponding to momentum and Δx corresponds to position.

Similarly we have,

$\Delta E \Delta t \approx h$ and $\Delta J \Delta \theta \approx h$

➤ Schrödinger's wave equation-Time independent and time dependent equations

Schrödinger equation is the one of the basic equation in the quantum mechanics. This equation can be applied for both macroscopic and microscopic particles.

Schrödinger derived a mathematical equation to describe the dual nature of the matter waves.

The equation that describes the wave nature of a particle in mathematical form is known as *Schrödinger's wave equation*

Schrödinger wave equation is the composite equation of a De-Broglie wavelength relation and classical differential equation of a progressive wave.

De-Broglie wavelength relation is given by.....

$$\lambda = \frac{h}{mv} \dots\dots\dots (1)$$

Classical differential equation of a progressive wave is given by

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} = \frac{1}{v^2} \frac{\partial^2 \psi}{\partial t^2} \dots\dots\dots (2)$$

(a). Time-independent Schrödinger Wave Equation

The solution of above equation 2 is given by-

$$\psi = \psi_o e^{-i\omega t} \dots\dots\dots (3)$$

Taking differentiation of 3 w.r.t 'time' we get

$$\frac{\partial \psi}{\partial t} = \psi_o e^{-i\omega t} (-i\omega)$$

Again taking differentiation

$$\frac{\partial^2 \psi}{\partial t^2} = [\psi_o e^{-i\omega t} (-i\omega)] (-i\omega)$$

$$\frac{\partial^2 \psi}{\partial t^2} = -\omega^2 \psi \dots\dots\dots (4)$$

On replacing $\frac{\partial^2 \psi}{\partial t^2}$ in equation 2 by above value (equation 4), equation 2 becomes-

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} = \frac{-\omega^2 \psi}{v^2} \dots\dots\dots (5)$$

We know that $\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} = \Delta^2$

And $\omega = 2\pi\nu = 2\pi\frac{v}{\lambda}$

so, $\frac{\omega}{v} = \frac{2\pi}{\lambda}$

on putting above in equation 5,

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

Now, on putting value of λ from equation 1,

$$\Delta^2\psi = \frac{-4\pi^2 m^2 v^2}{h^2}\psi$$

On rearranging above term

$$\Delta^2\psi = - \left[\frac{2\pi}{h} \right]^2 m^2 v^2 \psi$$

$$\Delta^2\psi + \left[\frac{2\pi}{h} \right]^2 m^2 v^2 \psi \dots\dots\dots(6)$$

Now, as we know the total energy of a particle is sum of potential energy and kinetic energy,

TE=PE+KE

$$E = U + \frac{1}{2}mv^2$$

$$E - U = \frac{1}{2}mv^2$$

$$2(E - U) = mv^2$$

$$2m(E - U) = m^2 v^2 \dots\dots\dots(7)$$

On putting equation 7 in equation 6

$$\Delta^2\psi + \left[\frac{2\pi}{h} \right]^2 2m(E - U) \psi = 0$$

But as \hbar (h prime) = $\frac{h}{2\pi}$

So,

$$\Delta^2\psi + \frac{2m(E - U)}{\hbar^2} \psi = 0 \dots\dots\dots(8)$$

This equation is known as Time-independent Schrödinger Wave Equation

(b). Time-dependent Schrödinger Wave Equation

The wave function is given by (from equation 3)

$$\psi = \psi_o e^{-i\omega t}$$

Taking differentiation of 3 w.r.t 'time' we get

$$\frac{\partial \psi}{\partial t} = \psi_o e^{-i\omega t} (-i\omega)$$

From 3, we get

$$\frac{\partial \psi}{\partial t} = \psi (-i\omega) \dots\dots\dots(9),$$

As we know, $E = h\nu$

$$\gg \nu = \frac{E}{h}$$

$$\text{So we can write } \omega = 2\pi\nu = 2\pi\frac{E}{h} = \frac{2\pi}{h} E = \frac{E}{\hbar}$$

On putting above values in equation 9, we get

$$\frac{\partial \psi}{\partial t} = \psi \left(-i \frac{E}{\hbar}\right)$$

$$\gg \frac{\partial \psi}{\partial t} = \psi \left(-i \frac{E}{\hbar}\right)$$

$$\gg \frac{\partial \psi}{\partial t} = \frac{E\psi}{i\hbar}$$

$$i\hbar \frac{\partial \psi}{\partial t} = E\psi \dots\dots\dots(10)$$

On putting value of $E\psi$ from equation 10 in equations 8, we get

$$\Delta^2 \psi + \frac{2m(\frac{i\hbar \partial \psi}{\partial t} - U\psi)}{\hbar^2} = 0$$

On rearranging the above equation, we get

$$\Delta^2 \psi = -\frac{2m(i\hbar \frac{\partial \psi}{\partial t} - U\psi)}{\hbar^2}$$

$$-\frac{\hbar^2}{2m} \Delta^2 \psi = i\hbar \frac{\partial \psi}{\partial t} - U\psi$$

$$-\frac{\hbar^2}{2m} \Delta^2 \psi + U\psi = i\hbar \frac{\partial \psi}{\partial t}$$

$$\left[-\frac{\hbar^2}{2m} \Delta^2 + U \right] \psi = i\hbar \frac{\partial \psi}{\partial t}$$

This equation is known as Schrödinger Time-dependent Wave Equation which further can be written as-

$$H \psi = E \psi$$

Here $H = -\frac{\hbar^2}{2m} \Delta^2 + U$, that is termed as a Hamiltonian Operator

And $E = i\hbar \frac{\partial}{\partial t}$, that is termed as a Energy Operator

➤ Physical significance of wave function

1. Schrödinger wave equation relates particle and wave nature of a matter statistically.
2. Wave function (ψ) is complex quantity and hence we can not measure it.
3. It is a single valued and continuous everywhere
4. The probability density or charge density $\psi \psi^*$ (or $|\psi|^2$) is the measure of particle density
5. The probability of finding the particle in a volume element $d\tau = dx dy dz$ about any point r at time is expressed as

$$P(r) d\tau = |\psi(r, t)|^2 d\tau$$

6. The function ψ is sometimes called probability amplitude for the position of the particle.
7. If the particle is certainly to be found somewhere in space, then $P(r) d\tau = |\psi(r, t)|^2 d\tau = 1$

➤ Particle in a one dimensional box (square well potential)

The particle in a box problem is a common application of a quantum mechanical model to a simplified system consisting of a particle moving horizontally within an infinitely deep well from which it cannot escape. The solutions to the problem give possible values of E and ψ that the particle can possess. E represents allowed energy values and $\psi(x)$ is a wave function, which when squared gives us the probability of locating the particle at a certain position within the box at a given energy level.

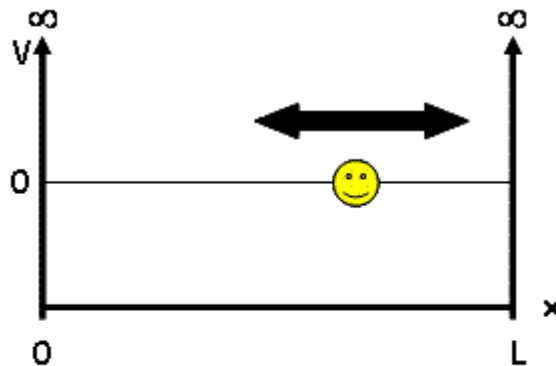


Figure:5; 1D box (Potential box)

The potential energy is 0 inside the box ($V=0$ for $0 < x < L$) and goes to infinity at the walls of the box ($V=\infty$ for $x < 0$ or $x > L$). We assume the walls have infinite potential energy to ensure that the particle has zero probability of being at the walls or outside the box. Doing so significantly simplifies our later mathematical calculations as we employ these **boundary conditions** when solving the Schrödinger Equation.

The time-independent Schrödinger equation for a particle of mass m moving in one direction with energy E is

$$\left[-\frac{\hbar^2}{2m} \Delta^2 + U \right] \psi = i\hbar \frac{\partial \psi}{\partial t}$$

Here

- \hbar is the reduced Planck Constant where $\hbar = h/2\pi$
- m is the mass of the particle
- $\psi(x)$ is the stationary time-independent wave function
- $V(x)$ is the potential energy as a function of position
- E is the energy, a real number

This equation can be modified for a particle of mass m free to move parallel to the x-axis with zero potential energy ($V = 0$ everywhere) resulting in the quantum mechanical description of free motion in one dimension:

From Schrödinger time independent equation

$$\Delta^2 \psi + \left[\frac{2\pi}{h} \right]^2 2m(E - U) \psi$$

For a free particle $U=0$ so

$$\Delta^2 \psi + \left[\frac{2\pi}{h} \right]^2 2mE \psi \dots\dots\dots(1)$$

On rearranging above

$$\Delta^2 \psi + \frac{8\pi^2 mE}{h^2} \psi$$

$$\text{Taking } k^2 = \frac{8\pi^2 mE}{h^2} \dots\dots\dots(2)$$

The equation 1 gives a general solution of:

$$\psi(x) = A \sin(kx) + B \cos(kx) \dots\dots\dots(3)$$

where A , B , and k are constants.

The solution to the Schrödinger equation we found above is the general solution for a 1-dimensional system. We now need to apply our **boundary conditions** to find the solution to our particular system. According to our boundary conditions, the probability of finding the particle, $\psi(x)$ at $x=0$ or $x=L$ is zero.

When $x=0$ $\sin(0)=0$ and $\cos(0)=1$; therefore, B must equal 0 to fulfill this boundary condition giving:

From equation 3

$$0 = A\sin(k0) + B\cos(k0) = 0 + B$$

$$\gg B = 0$$

On putting above in 3, we get

$$\psi(x) = A\sin(kx) \dots\dots\dots(4)$$

$$\text{at } x = L \text{ also } \psi(x) = 0$$

$$\text{so } 0 = A\sin(kx) \text{ but } A \neq 0 \text{ so}$$

$$\sin(kL) = 0 \text{ which gives}$$

$$kL = n\pi$$

$$k = \frac{n\pi}{L} \dots\dots\dots (5) \text{Where } n=1, 2, 3 \dots\dots\dots$$

On putting above value of k in equation (4), we get

$$\psi(x) = A\sin\left(\frac{n\pi}{L}x\right) \dots\dots\dots(6)$$

To determine A, recall that the total probability of finding the particle inside the box is 1, meaning there is no probability of it being outside the box. When we find the probability and set it equal to 1, we are *normalizing* the wave function.

$$\int_0^L \psi \psi^* dx = 1$$

Here ψ^* is the conjugate eigen function,

$$\text{Since } \psi \psi^* = \psi^2 \text{ so}$$

$$\int_0^L \psi^2 dx = 1$$

For our system, the normalization looks like:

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

On using formula $\sin^2\theta = \frac{1 - \cos 2\theta}{2}$, we can further solve it as follows

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

$$\frac{A^2}{2} \left[\int_0^L dx - \int_0^L \cos \frac{2n\pi x}{L} \right] = 1$$

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

$$\frac{A^2}{2} \{L - 0\} - \{0 - 0\} = 1$$

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

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

On putting above value in equation 6, we get

$$\psi(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right) \dots\dots\dots(7)$$

The function $\psi(x)$ denoted by above equation 7 is called normalized wave function and a value $A = \sqrt{\frac{2}{L}}$ is called normalization constant for a particle in a 1-dimensional box:

Step 4: Determine the Allowed Energies

On equating equations 2 and 5, we get

$$k^2 = \frac{8\pi^2 mE}{h^2}$$

$$\left[\frac{n\pi}{L} \right]^2 = \frac{8\pi^2 mE}{h^2}$$

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

The above equation gives the allowed values of energy values for different values of n. The possible values of the energy E are called Eigen-values and the corresponding values of ψ are called Eigen-functions.

For ground state, n=1

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

For first excited state

$$E_1 = \frac{2^2 h^2}{8mL^2} = \frac{4h^2}{8mL^2} = 4E_0$$

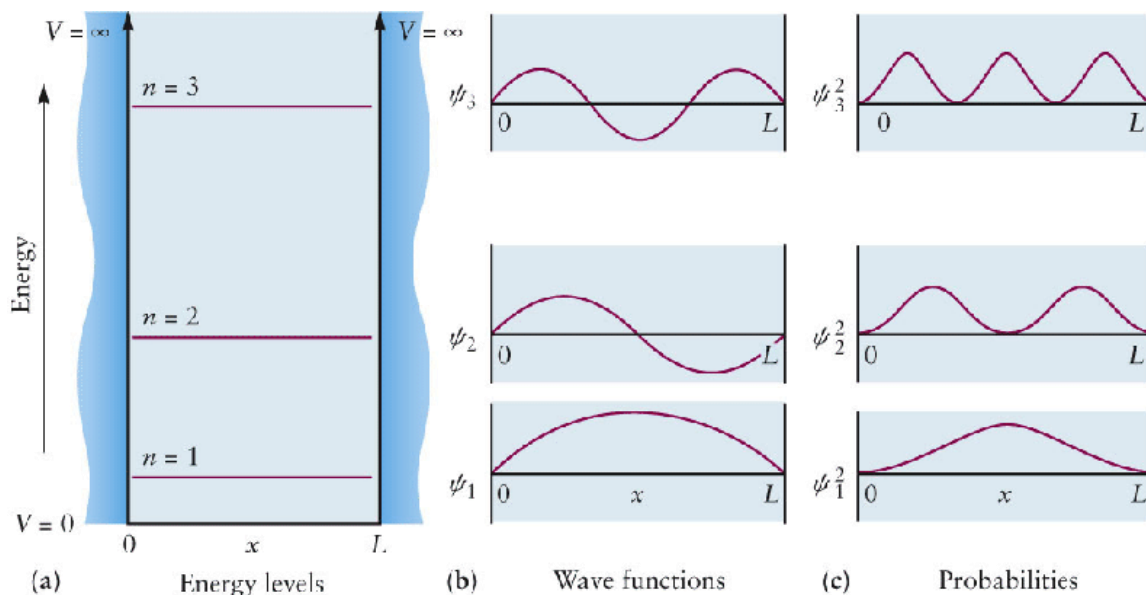
For second excited state

$$E_2 = \frac{3^2 h^2}{8mL^2} = \frac{9h^2}{8mL^2} = 9E_0$$

This is a very important result; it tells us that:

1. The energy of a particle is quantized.
2. The lowest possible energy of a particle is **NOT** zero. This is called the **zero-point energy** and means the particle can never be at rest because it always has some kinetic energy.

This is also consistent with the Heisenberg Uncertainty Principle: if the particle had zero energy, we would know where it was in both space and time.



The wave function for a particle in a box at the n=1 and n=2 energy levels is shown in figure (b). The probability of finding a particle at a certain spot in the box is determined by squaring ψ . The probability distribution for a particle in a box at the n=1 and n=2 energy levels is shown in figure (c).

Notice that the number of **nodes** (places where the particle has zero probability of being located) increases with increasing energy n. Also note that as the energy of the particle becomes greater, the quantum mechanical model breaks down as the energy levels get closer together and

overlaps, forming a continuum. This continuum means the particle is free and can have any energy value. At such high energies, the classical mechanical model is applied as the particle behaves more like a continuous wave. Therefore, the particle in a box problem is an example of Wave-Particle Duality.

Important Facts from the Particle in the Box

- The energy of a particle is quantized. This means it can only take on discrete energy values.
- The lowest possible energy for a particle is **NOT** zero (even at 0 K). This means the particle *always* has some kinetic energy.
- The square of the wavefunction is related to the probability of finding the particle in a specific position for a given energy level.
- The probability changes with increasing energy of the particle and depends on the position in the box you are attempting to define the energy for
- In classical physics, the probability of finding the particle is independent of the energy and the same at all points in the box

Assignments:

Definitions:

Black Body

Black Body radiation

Planck's law

Wien's law of Black Body Radiation

Rayleigh Jean's Law of Black body Radiation

DeBroglie Wavelength

Scattering

Wave

Wave function

Short Questions:

- **Explain energy distribution plot of Energy density for a black body radiation.**
- **What is Planck's law of Black Body Radiation?**
- **Derive Wien's law formula for a shorter wavelength**

- Derive the energy density formula from Planck's law , applied for a longer wavelength.
- Mention few properties of photon.
- Explain DeBroglie hypothesis.
- Explain Uncertainty principle.

Long Questions:

- Derive time independent Schrödinger wave equation for a particle having mass m and moving with velocity v .
- Derive time dependent Schrödinger wave equation for a particle having mass m and moving with velocity v .
- Derive the formula for energy and wave function for a particle moving in one dimensional potential box.

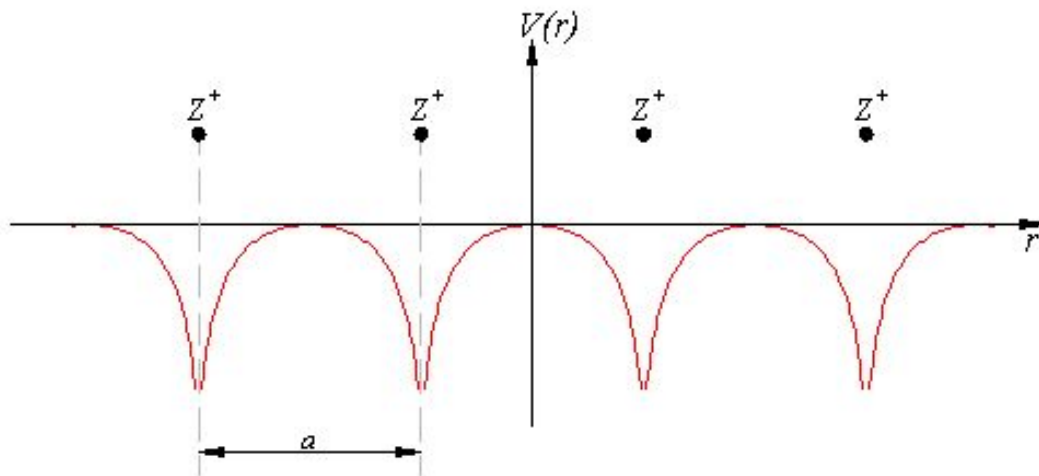
Examples for practices:

1. Calculate the energy in eV for a photon of wavelength 0.1×10^{-9} m. What is the momentum of this photon?
2. Calculate the number of photons emitted by a 100 watt sodium lamp. The wavelength of emitted light is 5893 \AA .
3. Calculate the energy density per unit wavelength in a black body cavity at a temperature of 1500K at a wavelength of 4000 \AA .
4. Compute the first 3 permitted energy values for an electron in a box of width 4 \AA .
5. What is the lowest energy that a neutron of mass 1.67×10^{-27} kg can have if it is confined to move along the edge of an impenetrable box of length 10^{-15} m.
6. Calculate the frequency and wavelength of a photon whose energy is 75 eV.
7. Find the number of quanta of energy emitted per second if a radio station operates at a frequency of 98 MHz and radiates power of 2×10^5 W.
8. How many photons of yellow light of wavelength 5500 \AA constitute 1.5 J of energy?
9. Calculate the deBroglie wavelength associated with the automobile of mass 2×10^3 kg which is moving with a speed 96 km/hr.

Unit III (Module 2) – Introduction to Solids and Semiconductor Physics

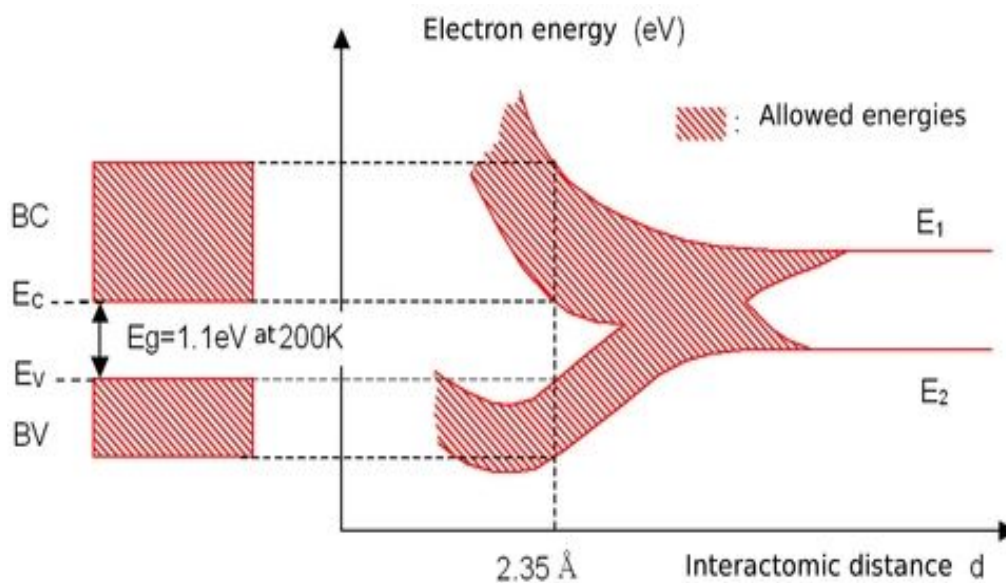
Band Theory of Solids :

In crystals, the value of a lattice constant is of order of linear dimensions of atoms ($\sim 1\text{\AA}$). Obviously at such a short separation between various neighboring atoms, electrons in an atom can not only be subjected to the Coulomb force of the nucleus of this atom but also by Coulomb forces due to nuclei and electrons of the neighboring atoms. In fact it is this interaction which results in the bonding between various atoms which leads to the formations of crystals.



Consider an isolated hydrogen atom. Assume that two such atoms are brought together. Let u_1 and u_2 denote the electronic wave functions for the two atoms when they are far apart and are not influenced by one another. As the separation between the atoms is decreased, the wave function u_1 and u_2 overlap and the resultant electronic wave function due to the two nuclei may be either $u_1 + u_2$ or $u_1 - u_2$. For the wave function $u_1 + u_2$, the electron has a finite probability of existing midway between the two nuclei. For the wave function $u_1 - u_2$, the probability density is zero midway. Thus there is a

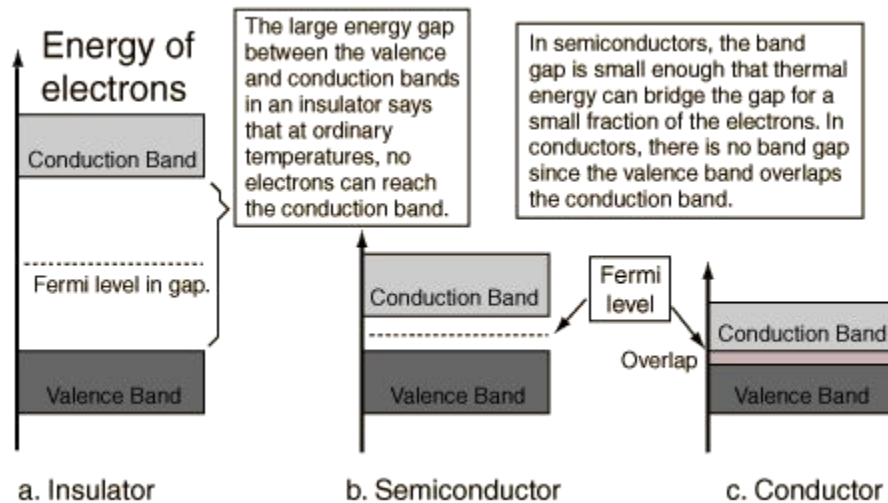
difference in energy between the states $(u_1 + u_2)$ and $(u_1 - u_2)$. This means that as the two atoms are brought close together, each energy state splits into two distinct energy states. If N no. of atoms are brought together, each energy state splits into N distinct energy states. When N is large, the separation between these energy states is small and they may be thought to produce a quasi-continuous band. That is each energy level may be considered to split into a band of energy levels. The width of a band depends on the strength of interaction and overlap between the neighboring atoms.



Valence Band : The band of energies occupied by the valence electrons is called as valence band. This is the highest occupied band below which all the lower bands are fully occupied. The electrons in the outermost orbit of an atom are known as valence electron.

Conduction Band : The band, above the valence band, occupied by conduction electrons is known as conduction band. This is the uppermost band and all electrons in the conduction band are free electrons. The conductor band is empty for insulators and partially filled for conductors.

Forbidden Energy Gap : The gap between the valence band and the conduction band is known as forbidden band or energy gap.



On the basis of band gap solids are divided in three categories.

Conductor	Semiconductor	Insulator
Good Conductor of electricity	Behave as a Insulator at 0 K Temperature	Bad conductor of Electricity
CB and VB are partially filled	VB is completely filled CB is completely empty	VB is completely filled CB is completely empty
Energy gap = 0 eV	Energy gap ~ 1 eV	Energy gap ~ 6 - 7 eV
Conductivity decreases with increase in Temperature (Linearly)	Conductivity increases with increase in Temperature (Exponentially)
Exp : Cu, Ag, Au	Exp : Si, Ge	Exp : Diamond, Glass

Note: Energy gap for Ge. = 0.7 eV , Si. = 1.1 eV

Intrinsic Semiconductor :

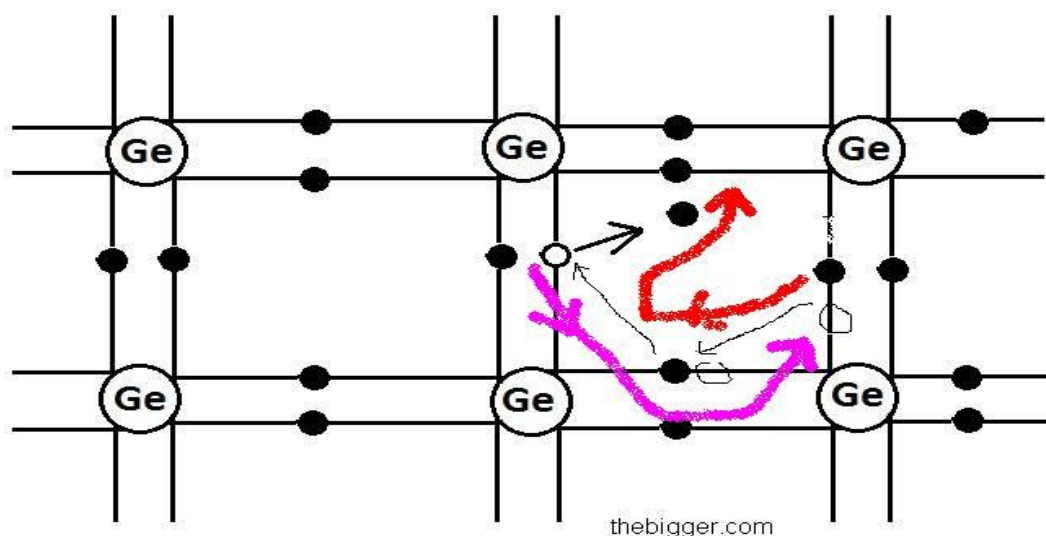
The pure semiconductors (elements of 14 (or IV) Group of periodic table) are called Intrinsic Semiconductor.

Practically pure semiconductors free from impurities are not possible. However if the impurities is less than 1 in part of semiconductor it can be treated as intrinsic.

Si and Ge are two common example of intrinsic type of semiconductor. The valency of these atoms is four. Thus, in a crystal each atom shares its four electrons with its immediate neighbors on a one to one basis, so that each atom is involved in four covalent bonds.

At 0 K, all the electrons are bound in covalent bonding and so the crystal is a perfect insulator. As the temperature of the crystal increases, electrons will get free due to thermal energy. When an electron escapes from a bond it leaves behind a vacancy in the lattice. This vacancy is termed as a 'hole'. Thus when covalent bond is broken due to thermal energy, an electron-hole pair is created. A bond where Hole created is now becomes unstable and hence an electron will occupy this vacancy from another neighboring bond. But again this bond becomes unstable due to vacancy of electron. So the process of escaping electron and creation of Hole will spread throughout the whole crystal. In short, electrons and Holes are appeared as they are moving in an opposite direction. This free movement of electron and Holes within the crystal gives rise to

Conductivity of the intrinsic semiconductor



Red curve: Path of movement of electron

Pink curve: Path of movement of Hole

Extrinsic Semiconductor :

The conductivity of the intrinsic semiconductor is very low. To increase the conductivity of an intrinsic semiconductor, a suitable impurity atom is added with the intrinsic semiconductor. The process of mixing suitable impurity with an intrinsic semiconductor is done by doping method.

Thus the extrinsic semiconductor is defined as a.....

Intrinsic Semiconductor + Impurity atom

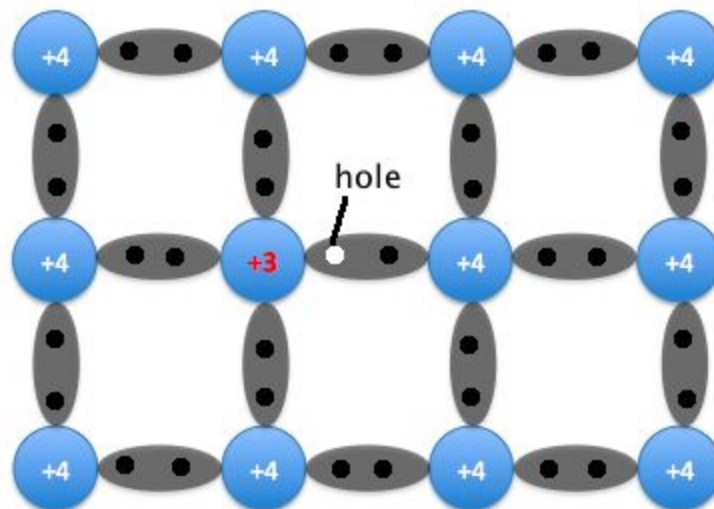
Type of the extrinsic semiconductor

1. P-Type Extrinsic semiconductor
2. N-Type Extrinsic semiconductor

1. P-Type Extrinsic semiconductor

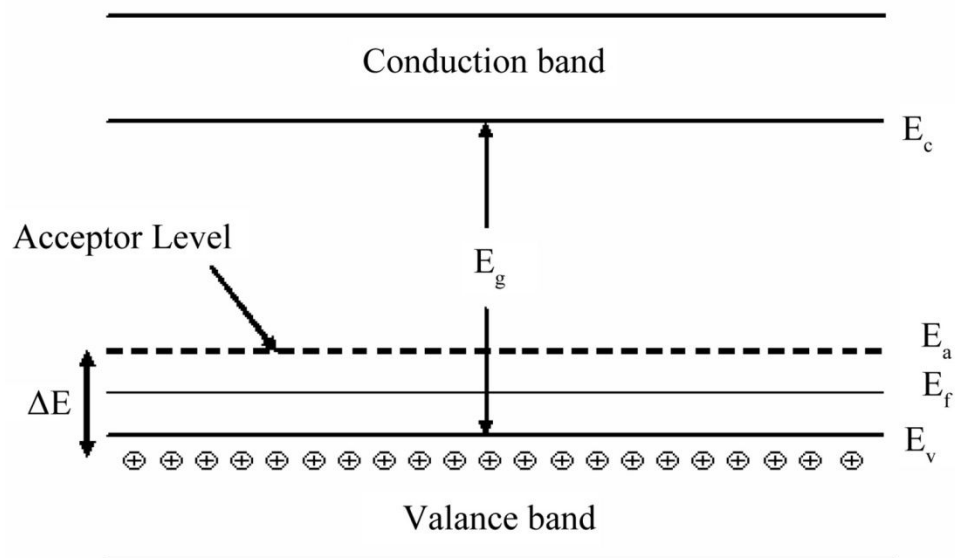
Intrinsic Semiconductor + Impurity trivalent atom of III Group of periodic table (e.g. Al, Ga, In, B etc)

Conductivity in P-Type Extrinsic semiconductor



In P-Type semiconductor, a trivalent atom has three electrons to share in covalent bond whereas semiconductor atom Si/Ge has four electrons to

share. In above figure, it can be seen that the three electrons of B atom combine with three electrons of Si atom to form covalent bonds. But for the fourth electron of Si, B has no electron to share. This means impurity atom (B) has one vacancy of electron i.e. hole. At room temperature, lattice vibrations readily provide sufficient energy to electron in a nearby Si-Si bond to move across and fill the vacancy on the B atom. Here again a hole is created in Si-Si atom. Because the trivalent impurity atom B accept electron from the Si-Si bond, they are called accepters. Note that, by accepting the additional electron the impurity atom becomes a negative ion. At this stage there are total two holes (one with B atom and other due to the escaping electron from Si-Si bond) one electron (escaped from Si-Si bond) and one negative ion. So in general crystal maintain the total charge zero (two hole, one electron and one negative ion = two plus, two minus). It is also notable that the number of holes are greater than the number of electrons hence in P-type semiconductor, holes are majority charge carriers whereas electrons are minority charge carriers.



2. N-Type Extrinsic semiconductor

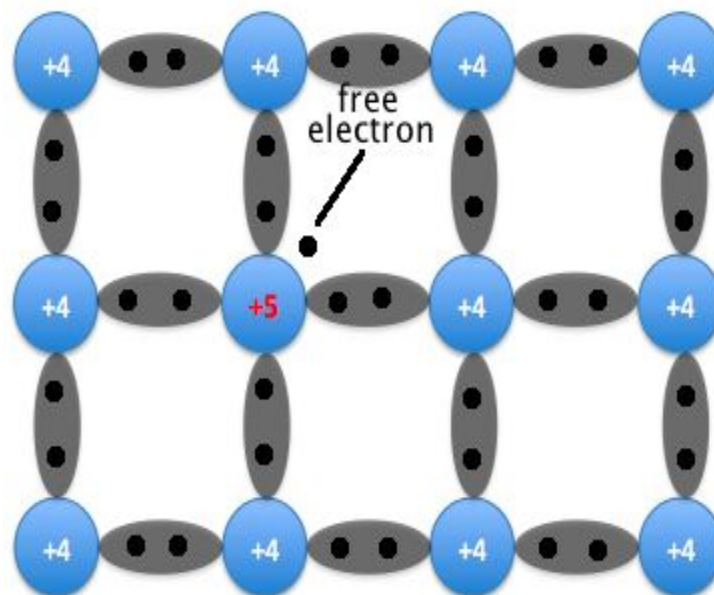
Intrinsic Semiconductor + Impurity pentavalent atoms of IV Group of periodic table (e.g. As, Sb, Petc)

Conductivity in N-Type Extrinsic semiconductor

In N-Type semiconductor, a pentavalent atom has five electrons to share in covalent bond whereas semiconductor atom Si/Ge has four electrons to

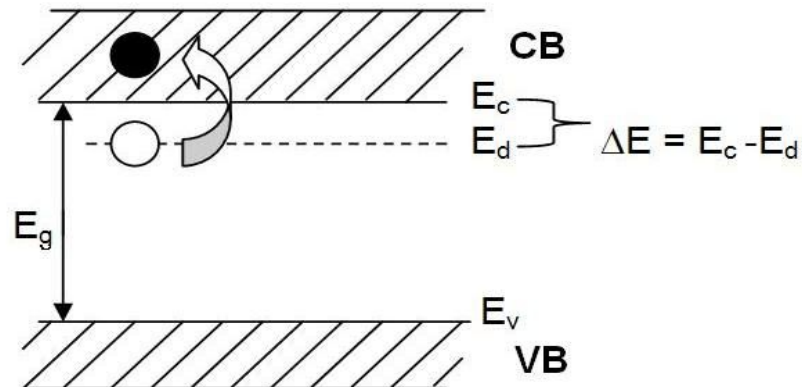
share. In above figure, it can be seen that the four electrons of As atom combine with four electrons of Ge atom to form covalent bonds. But for the fifth's electron of As, Si has no electron to share. This means impurity atom (As) has one extra electron.

The fifth electron of As is not involved in covalent bonding and it is loosely bound to As atom and needs only about 0.05 eV energy to become free. This energy can be easily achieved from thermal excitations of the crystals. In other words impurity atom donates one electron to the crystal. Such atom/impurity is therefore termed as donor atom/impurity and on donating electron it becomes positive ion.



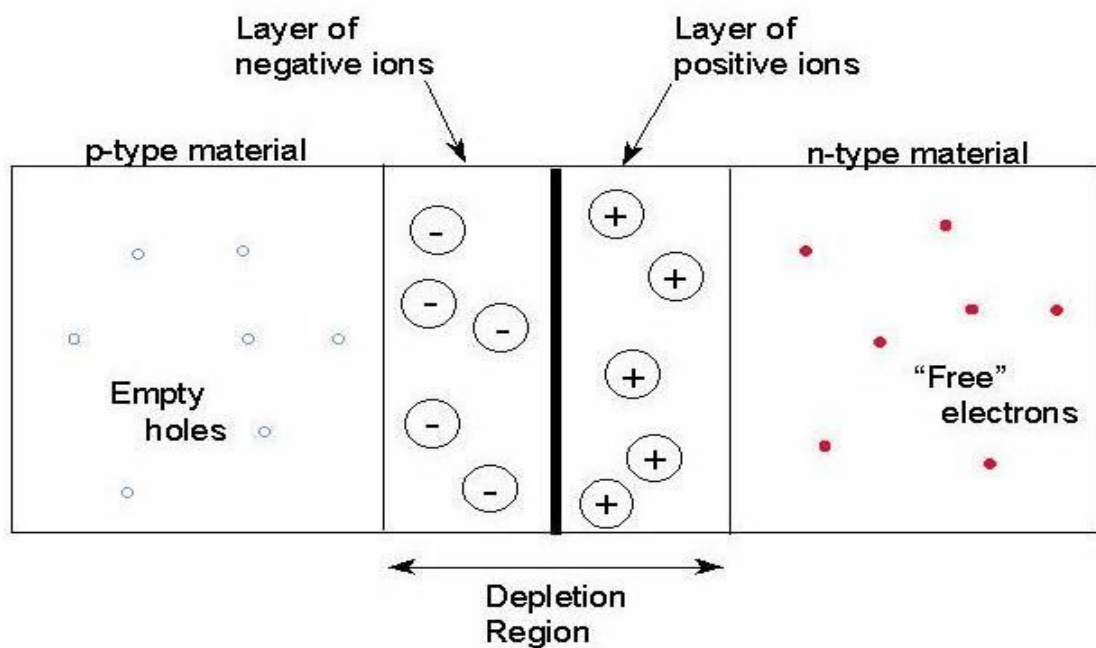
Now if more thermal energy supplied through the crystal, Ge-Ge covalent bond will break and hence electron will get free in the lattice. So, at this stage there are total two electrons (one with As atom and other due to the breaking of Ge-Ge bond) one hole (In Ge-Ge bond due to removal of extra electron due to thermal excitation) and one positive ion.

So in general crystal maintain the total charge zero (two electron, one hole and one positive ion= two plus, two minus). It is also notable that the number of electrons are greater than the number of holes hence in N-type semiconductor, electrons are majority charge carriers whereas holes are minority charge carriers.



PN JUNCTION DIODE :

PN Junction are semiconductor device which is formed by special fabrication technique where a single crystal of Silicon or Germanium is doped in such a way that one half of its becomes P-type and the other is N-type. The technique should be in such a manner that the crystal structure remains continuous at the boundary of P and N part.

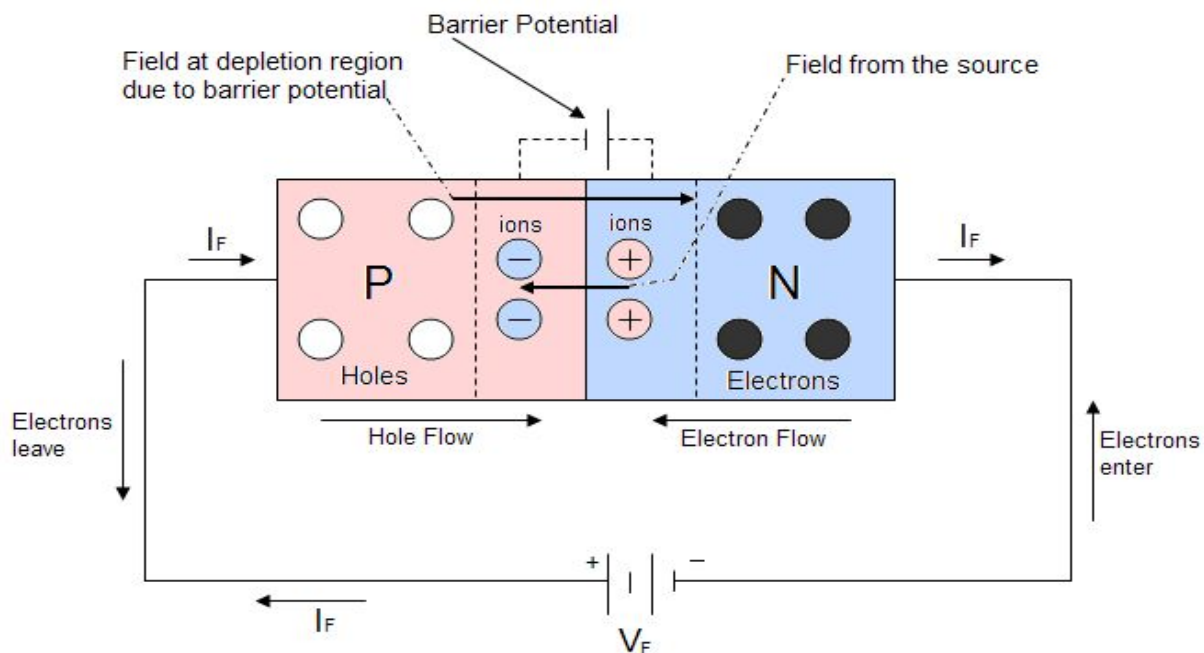


In an unbiased PN junction, the holes of P type and electron of N type diffuse towards the junction. At junction electrons and holes recombine themselves and hence a lack of free carriers in a narrow region near the junction is created. This region is called as depletion region. In depletion region, the electron negative ion on p side and positive ion on n side are immobile as these remain bounded to their respective lattice sites. This presence of ions in depletion layer create an electric field directed from N to P. The negative layer opposes further diffusion of electrons from N to P and positive layer opposes further diffusion of holes from P to N. Thus the developed electric field at junction which opposes further diffusion of majority charge carrier through junction is called Barrier electric field and voltage associated with this field is called Barrier potential. If d is the width of depletion layer then barrier electric field is given by,

BIASING OF PN- JUNCTION DIODE :

Forward biasing

A forward biasing can be applied to a p-n junction by connecting the positive terminal of the battery to the p-type semiconductor and the negative terminal of the battery to the n-type semiconductor.

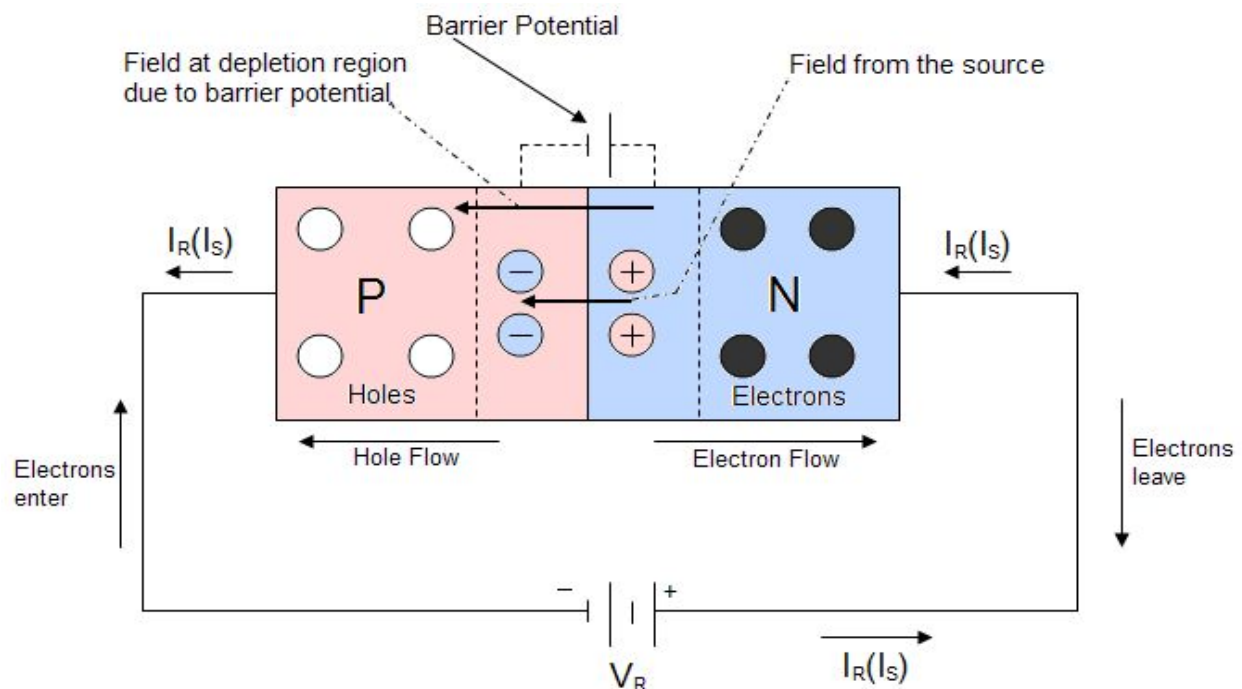


In forward bias, holes in P region are pushed towards junction by positive terminal of the battery and electrons are pushed towards junction by

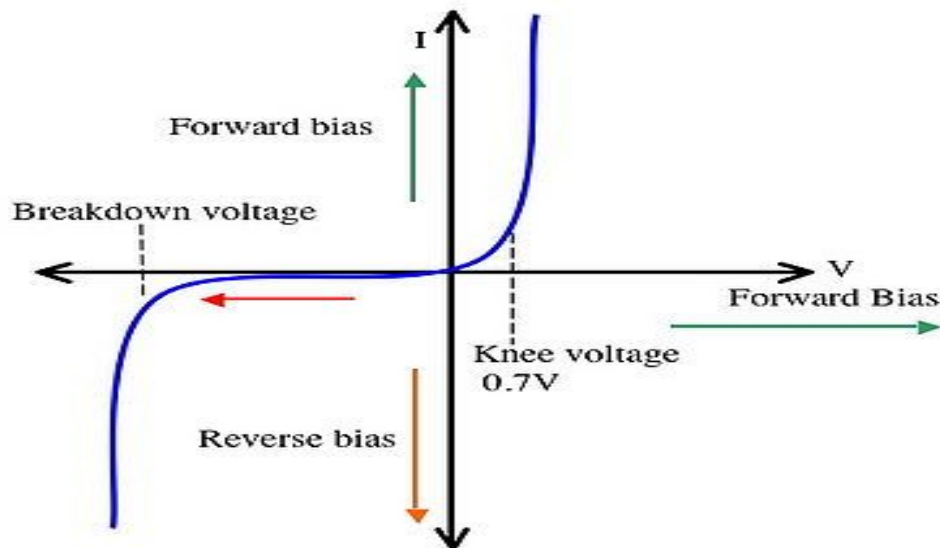
negative terminal of the battery due to opposite polarity. An internal electric field produced in opposite to the barrier electric field. Due to this, more and more charge carriers (holes and electrons) cross the junction. As a result thickness of depletion layer gets reduced. Initially, at lower input voltage, the probability of crossing the junction by charge particles is smaller because there is a chance to recombine electron and holes themselves. But as input voltage increases, the thermal excitation enhances and hence electrons are enabled to reach the P part from N part (towards positive terminal of battery). This flow of electrons gives rise to flow of current.

Reverse biasing

In reverse bias, p part of diode connected to the negative terminal of the battery and n part of battery connected to the positive terminal of the battery. The holes in p part are pulled by negative terminal of the battery and electrons in n part are pulled by positive terminal of the battery. As a result the thickness of depletion layer increases. Only the minority charge carriers are enabled to cross the junction on applying external voltage. Hence, in reverse bias current flows only due to minority charge carriers. Initially at lower input voltage, the produced electric current due to the minority charge carriers is very less (micro ampere) and almost constant. This current is called saturation current. In general we can say that PN diode does not show conductivity in reverse bias.



Characteristics curve of PN Junction diode (V-I curve)



Carrier Transport : Drift and Diffusion

Carrier Drift:

Any motion of free carriers in a semiconductor leads to a current. This motion can be caused by an electric field due to an externally applied voltage, since the carriers are charged particles. We will refer to this transport mechanism as carrier drift. In addition, carriers also move from regions where the carrier density is high to regions where the carrier density is low. This carrier transport mechanism is due to the thermal energy and the associated random motion of the carriers. We will refer to this transport mechanism as carrier diffusion. The total current in a semiconductor equals the sum of the drift and the diffusion current.

As one applies an electric field to a semiconductor, the electrostatic force causes the carriers to first accelerate and then reach a constant average velocity, v , due to collisions with impurities and lattice vibrations. The ratio of the velocity to the applied field is called the mobility. The velocity saturates at high electric fields reaching the saturation velocity. Additional scattering occurs when carriers flow at the surface of a semiconductor, resulting in a lower mobility due to surface or interface scattering mechanisms.

Carrier Diffusion:

Carrier diffusion is due to the thermal energy, kT , which causes the carriers to move at random even when no field is applied. This random motion does not yield a net flow of carriers nor does it yield a net current in material with a uniform carrier density since any carrier which leaves a specific location is on average replaced by another one.

Diffusion of carriers is obtained by creating a carrier density gradient. Such gradient can be obtained by varying the doping density in a semiconductor or by applying a thermal gradient. However if a carrier gradient is present, the diffusion process will even out the carrier density variations: carriers diffuse from regions where the density is high to regions where the density is low.

Assignment (for practice) :-

Descriptive & Analytical Questions :

1. Write short notes on the following,
 - a. Intrinsic and Extrinsic semiconductors
 - b. Band theory of solids
 - c. Kronig Penney model
 - d. Density of states and Occupation probability
 - e. Fermi-Dirac probability distribution function
 - f. Conduction band and Valence band
2. Mention the major differences between metal, semiconductor and insulator on the basis of energy band-gap.
3. What do you mean by P-type and N-type semiconductors? How are these formed from pure semiconductors like Silicon?
4. Derive an expression of carrier (either electron or hole) concentration in intrinsic semiconductor.
5. Find the position of the Fermi-level in an intrinsic semiconductor. Draw the necessary diagram.

6. Discuss the effect of donor and acceptor impurities in semiconductor. Explain with suitable diagram how does the Fermi-level change due to doping.
7. What is a junction diode? Describe the forward and reverse biasing of the P-N junction diode with necessary diagram.
8. What is the effect of temperature on n-type or p-type semiconductor?

Numerical Problems :

1. Find the position of Fermi level E_F at room temperature ($=27^\circ\text{C}$) for Germanium crystal having 5×10^{22} atoms/ m^3 .
2. For an intrinsic semiconductor having band gap $E_g = 0.7$ eV, calculate the density of holes and electrons at room temperature ($=30^\circ\text{C}$).
3. Consider the Fermi level 0.3eV below the conduction band at room temperature ($=27^\circ\text{C}$) in an n-type semiconductor. If the temperature is raised to 55°C , what be the new position of Fermi level?