



Semiconductor Physics and Computational Methods (21PYB102J)

Course Instructor: Dr. Venkata Ravindra A

Assistant Professor

Department of Physics and Nanotechnology

SRM Institute of Science and Technology

Email: venkatar1@srmist.edu.in

Phone: 8019448666

Office: UB-709/A

The free electron theory of materials is to explain the structure and properties of solids through their electronic structure.

- It also gives information about bonding in solids, energy levels in metals and cohesive & repulsive forces in metals.

Development of Free Electron Theory

1. The classical free electron theory (Drude and Lorentz Model)
2. The quantum free electron theory (Sommerfeld Model)
3. Band Theory (Brillouin Zone Theory)



1. The Classical free electron theory [Drude and Lorentz]

It is a macroscopic theory, through which free electrons in lattice and it obeys the laws of classical mechanics. Here the electrons are assumed to move in a constant potential.

2. The Quantum free electron theory [Sommerfeld Theory]

It is a microscopic theory, according to this theory the electrons in lattice moves in a constant potential and it obeys law of quantum mechanics.

3. Brillouin Zone Theory [Band Theory]

Bloch developed this theory in which the electrons move in a periodic potential provided by periodicity of crystal lattice. It explains the mechanisms of conductivity, semiconductivity on the basis of energy bands.



Drude Theory

- According to kinetic theory of gases in a metal, Drude assumed free electrons are as a gas of electrons.
- This theory initially proposed by Drude in 1900
- It's the first theory to explain the electrical conduction in conducting materials and reveals that free electrons are responsible for the electrical conduction.

Free electrons

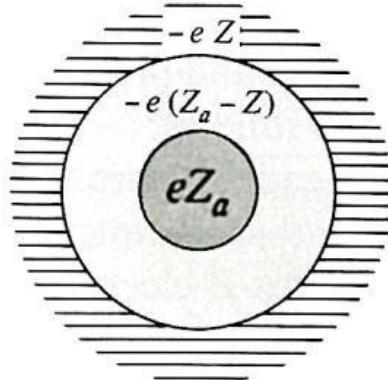
In certain metals especially in Cu, Ag and Al valence electrons are so weakly attached to the nuclei they can be easily removed or detached such electrons are called as free electrons.

But all the valence electrons in the metals are not free electrons.

Concept of Classical Free electron Theory

- According to this theory, metals consists of positive ions fixed in lattice and negative ions vander freely within the boundaries of the metal.
- As they are responsible for conductivity called as Conduction electrons
- This cloud of free electrons are called as electron gas
- They differ from ordinary gas in two aspects
 1. Free electron gas is charged while molecules of ordinary gases are neutral
 2. Concentration of electron is > ordinary gas concentration

Electron gas model in metals

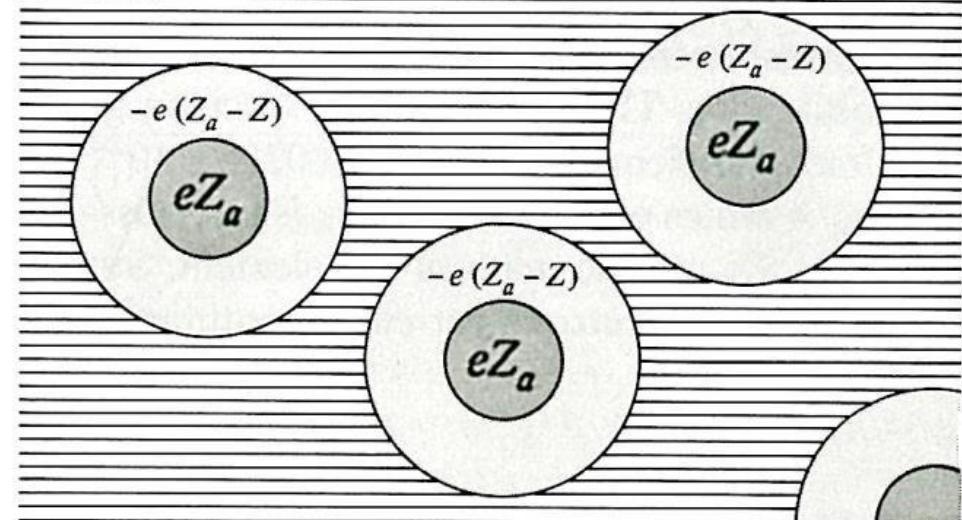


 Nucleus
 Core electrons
 Valence electrons

(a)

(a) Schematic picture of an isolated atom

Valence electrons form the electron gas



Ion {
 Nucleus
 Core
 Conduction electrons

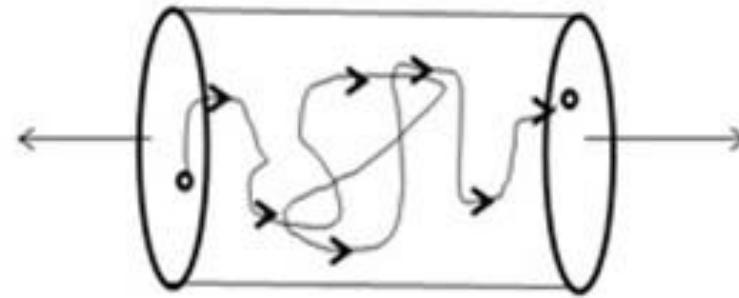
(b)

(b) In a metal the nucleus and ion core retain their configuration in the free atom, but the valence electrons leave the atom to form the electron gas.



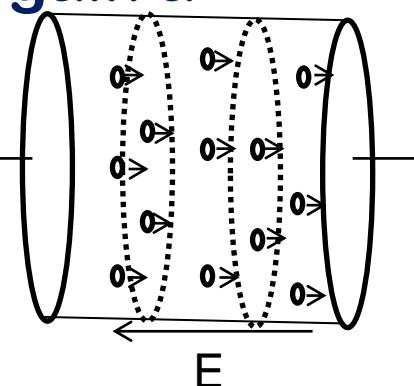
In absence of external field

- ✓ In the absence of external fields, random motion of electrons is observed.
- ✓ Net current is zero.



In presence of external field

- ✓ In the presence of external fields, electrons gain a constant velocity , DRIFT VELOCITY (v_d).
- ✓ Net current will not be zero.



Important characteristics

➤ **RELAXATION TIME (τ):**

Time taken for drift velocity to decay (1/e) of its initial value

➤ **MEAN COLLISION TIME (τ_c):**

- Mean or average time taken by an electron between two successive collisions
- It is also called mean free time [or] collision time

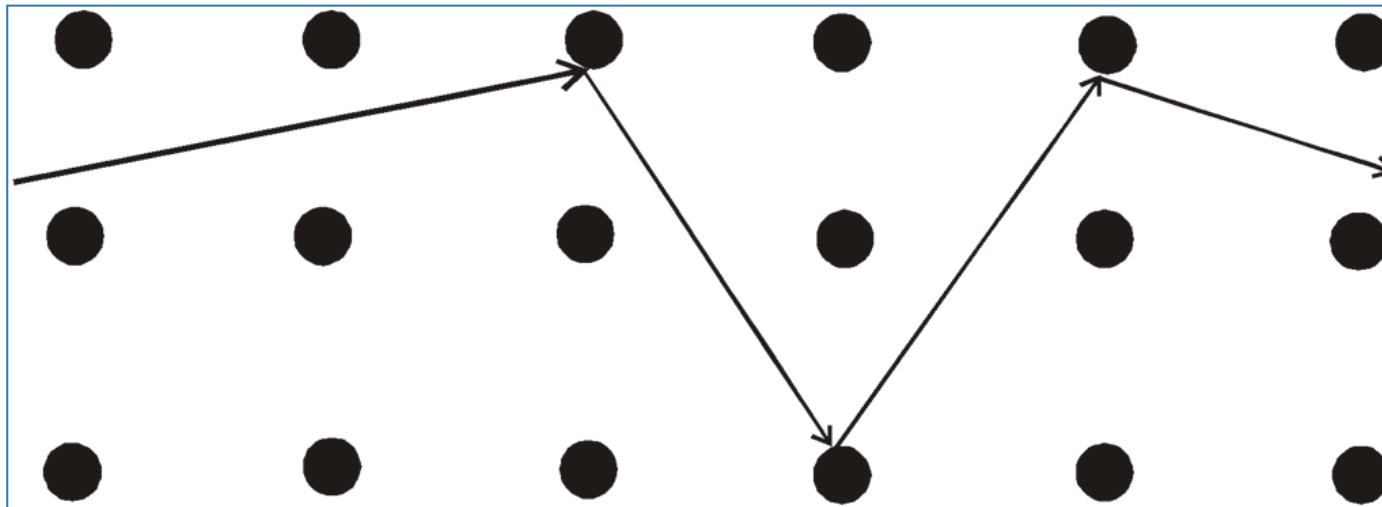
➤ **MEAN FREE PATH (λ):**

Average distance travelled by an electron between two successive collisions

$$\lambda = V_{\text{rms}} \cdot \tau_c$$



Electrons are assumed to achieve thermal equilibrium with their surroundings only through collision. These collisions are assumed to maintain local thermodynamic equilibrium in a particularly simple way.



Trajectory of a conduction electron



Success of classical free electron theory:

- (1) It verifies Ohm's law.
- (2) It explains the electrical and thermal conductivities of metals.
- (3) It derives Wiedemann – Franz law. (i.e.. the relation between electrical conductivity and thermal conductivity)
- (4) It explains optical properties of metals.



Drawbacks of classical free electron theory:

1. The phenomena such a photoelectric effect, Compton effect and the black body radiation couldn't be explained by classical free electron theory.
2. Cannot explain the electrical conductivity of semiconductors and Insulators.
3. Ferromagnetism cannot be explained by theory.



QUANTUM FREE ELECTRON THEORY

Classical free electron theory could not explain many physical properties.

In 1928, Sommerfield developed a new theory applying quantum mechanical concepts and Fermi-Dirac statistics to the free electrons in the metal.

This theory is called **quantum free electron theory**.

Classical free electron theory permits all electrons to gain energy. But quantum free electron theory permits only a fraction of electrons to gain energy.

According to Quantum mechanics moving particles has some sort of wave motion

Then wavelength $\lambda = h/p$ (De-Broglie wavelength)

To characterize moving particle having wave motion-(ψ)-wavefunction is introduced

According to quantum theory of free electrons energy of a free electron is given by

$$E_n = n^2 h^2 / 8mL^2$$

- According to quantum theory of free electrons the electrical conductivity is given by

$$\sigma = ne^2 T/m$$



MERITS OF QUANTUM FREE ELECTRON THEORY

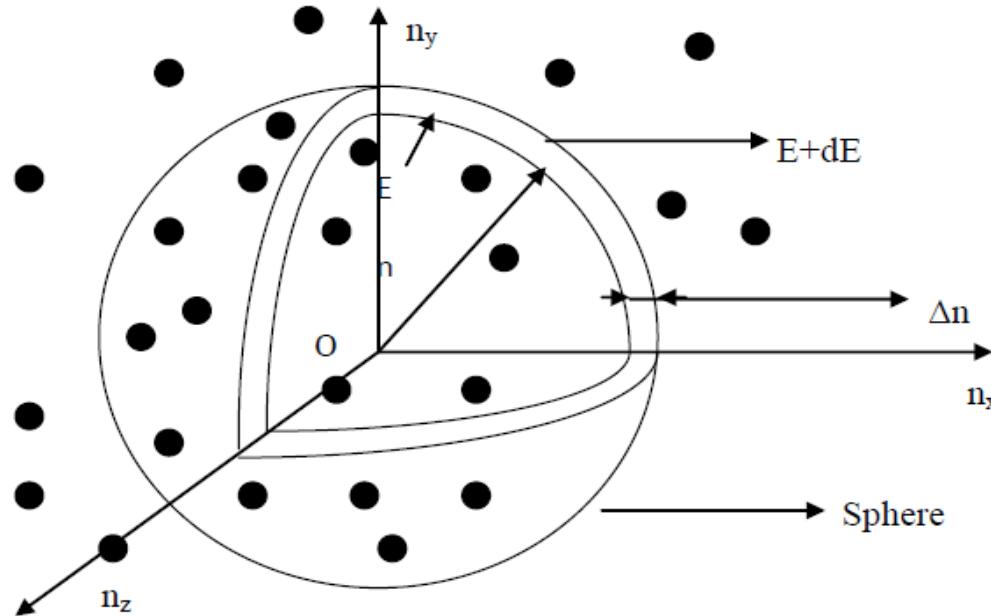
1. It successfully explains the electrical and thermal conductivity of metals.
2. It can explain the thermionic phenomenon.
3. Temperature dependence of conductivity of metals can be explained by this theory.
4. It can explain the specific heat of metals.
5. It explains magnetic susceptibility of metals.

DEMERITS OF QUANTUM FREE ELECTRON THEORY

1. It is unable to explain the metallic properties exhibited by only certain crystals
2. Failed to give difference of metals/semiconductors/ insulators
3. It is unable to explain why the atomic arrays in metallic crystals should prefer certain structures only

DENSITY OF STATES

Definition: Density of States $Z(E) dE$ is defined as the number of available electron states per unit volume in an energy interval (dE).



To find the number of energy levels in a cubical metal piece and to find number of electrons that can be filled in a given energy level, let us construct a sphere of radius ' n ' in the space.



The sphere is further divided in to many shells and each of this shell represents a particular combination of quantum numbers (n_x , n_y , and n_z) and therefore represents a particular energy value.

Let us consider two energy values E and $E + dE$. The number of energy states between E and $E + dE$ can be found by finding the number of energy states between the shells of the radius n and $n + \Delta n$, from the origin.

The number of energy states within the sphere of radius ‘ n ’ is $= 4/3 \pi n^3$

Since n_x , n_y , and n_z will have only positive values, we have to take only one octant of the sphere (i.e) $1/8$ th of the sphere volume.

The number of available energy states within the sphere of radius

$$n = 1/8 [4/3 \pi n^3]$$

Similarly the number of available energy states within the sphere of radius

$$n + dn = 1/8 [4/3 \pi (n+dn)^3]$$

The number of available energy states between the shells of radius n and $n + dn$ (or) between the energy levels

$$E \text{ and } E + dE = 1/8 [4/3 \pi (n+dn)^3 - 4/3 \pi n^3]$$

The number of available energy states between the energy interval

$$Z(E)dE = 1/8 \times 4/3 \pi [n^3 + dn^3 + 3n^2dn + 3dn^2n - n^3]$$

Since the higher powers of dn is very small, dn^2 and dn^3 terms can be neglected.

$$Z(E)dE = \pi / 6 (3n^2 dn)$$

$$Z(E)dE = \pi / 2(n^2 dn) \quad \longrightarrow \quad (1)$$

We know the energy of the electron in a cubical metal piece of sides ℓ

$$E = -\frac{n^2 h^2}{8m \ell^2}$$

$$n^2 = -\frac{8m \ell^2 E}{h^2} \quad \longrightarrow \quad (2)$$

$$n = \left[\frac{8m \ell^2 E}{h^2} \right]^{1/2} \quad \longrightarrow \quad (3)$$



Differentiating equation (2) we get

$$2ndn = \frac{8m \ell^2}{h^2} dE$$

(4)

$$ndn = \frac{8m \ell^2}{2 h^2} dE$$

Equation 1 can be written as

$$Z(E)dE = \pi / 2(n^2 dn)$$

$$Z(E)dE = \pi / 2 n (n dn)$$

Substituting equation (3) and (4) in the above equation we have

$$Z(E)dE = \pi / 2 \left[\frac{8m \ell^2 E}{h^2} \right]^{1/2} \left[\frac{8m \ell^2}{2 h^2} dE \right]$$



$$Z(E)dE = \pi / 4 \left[\frac{8m \ell^2}{h^2} \right]^{3/2} E^{1/2} dE$$



$$Z(E)dE = \pi / 4 \left[\frac{8m}{h^2} \right]^{3/2} \ell^3 \cdot E^{1/2} dE$$

Here ℓ^3 represents the volume of the metal piece. If $\ell^3 = 1$, then we can write that

The number of available energy states per unit volume (i.e) Density of states

$$Z(E)dE = \pi / 4 \left[\frac{8m}{h^2} \right]^{3/2} E^{1/2} dE \longrightarrow (5)$$

Since each energy level provides 2 electron states one with spin up and another spin down, we have

Density of states

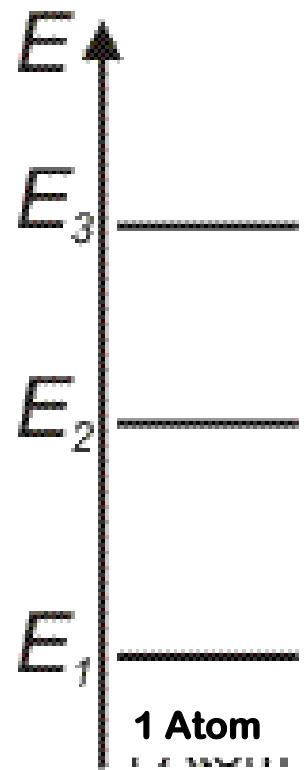
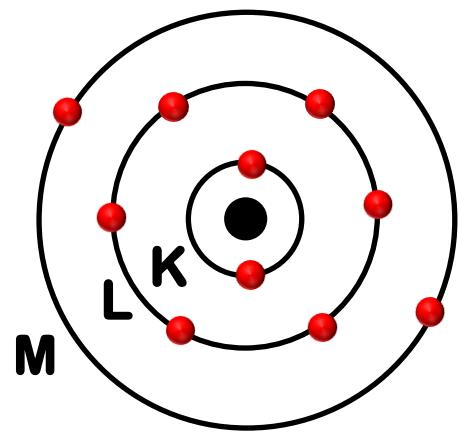
$$Z(E)dE = 2x \pi / 4 \left[\frac{8m}{h^2} \right]^{3/2} E^{1/2} dE$$

$$Z(E)dE = \pi / 2 \left[\frac{8m}{h^2} \right]^{3/2} E^{1/2} dE \longrightarrow (6)$$

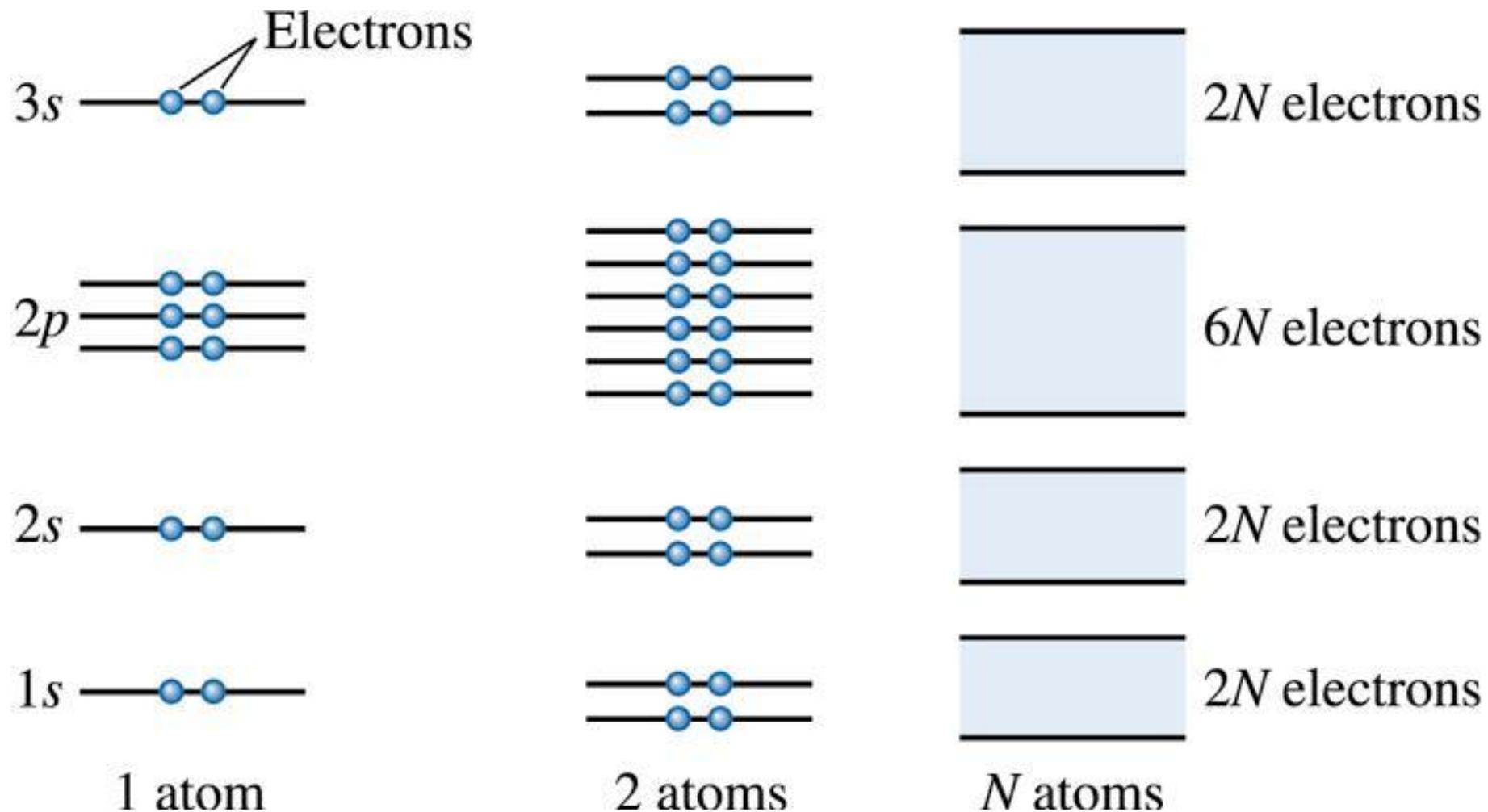
ENERGY BAND STRUCTURES IN SOLIDS

WHY ENERGY BANDS ARE FORMED?

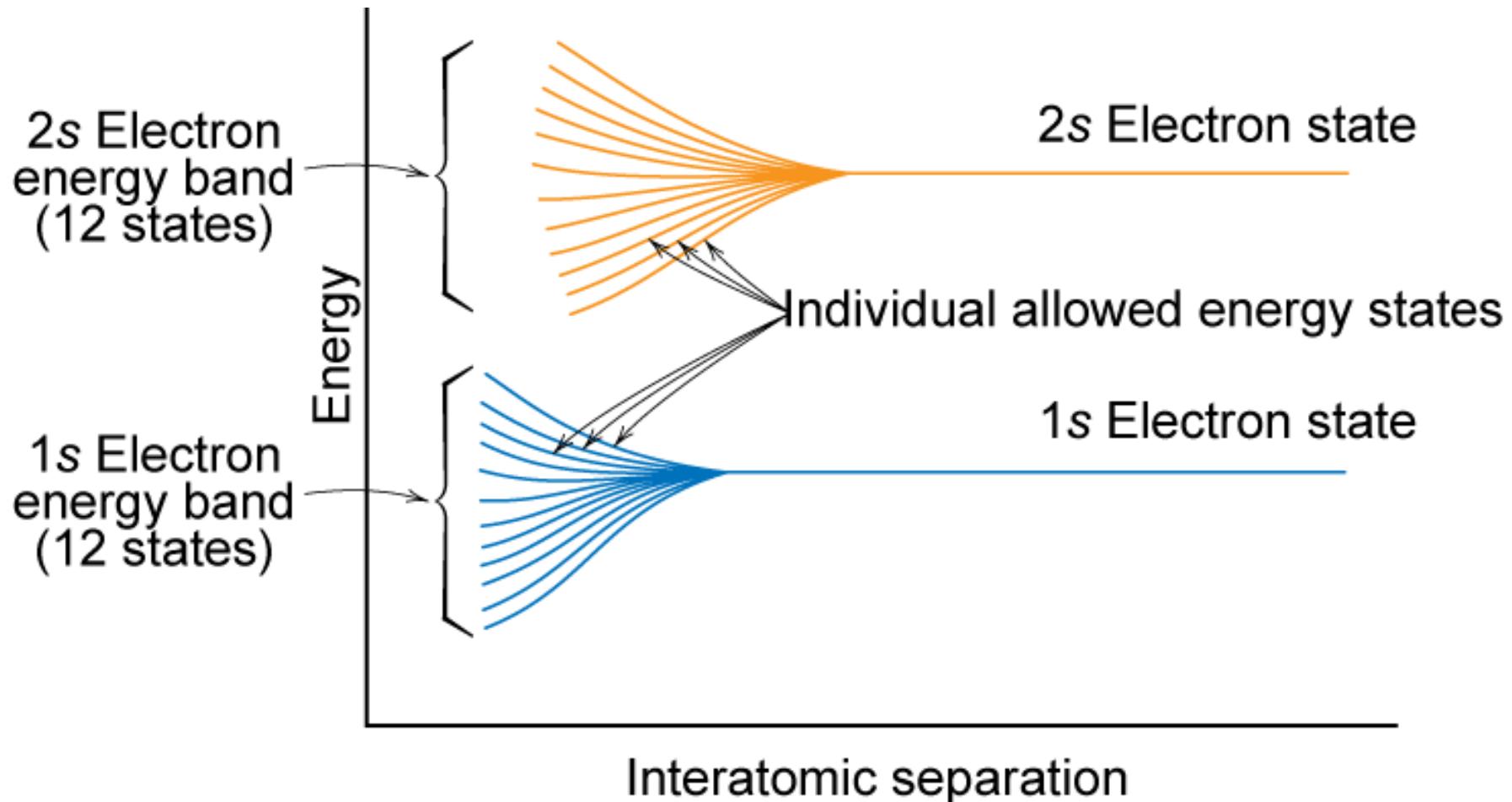
- Electrons of one atom are perturbed by the electrons and nuclei of the adjacent atoms.
 - Results in splitting of atomic states into a series of closely spaced electron states to form what are called **ELECTRON ENERGY BAND**.
 - Extent of splitting depends on **interatomic separation**.
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ENERGY BAND STRUCTURES IN SOLIDS



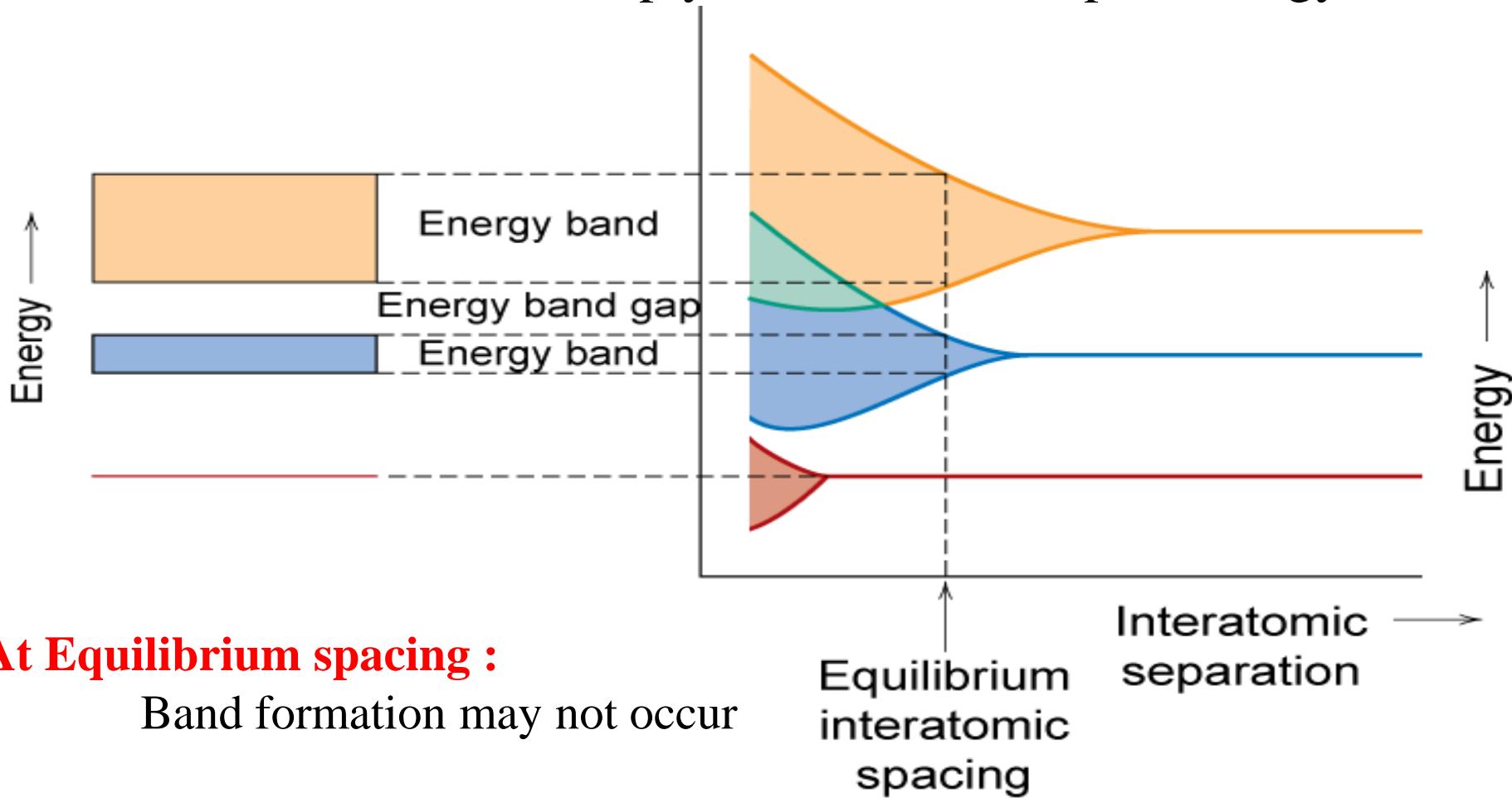
ENERGY BAND STRUCTURES IN SOLIDS



- For 12 atoms, each of the 1s and 2s atomic states splits to form an electron energy band consisting of 12 states.

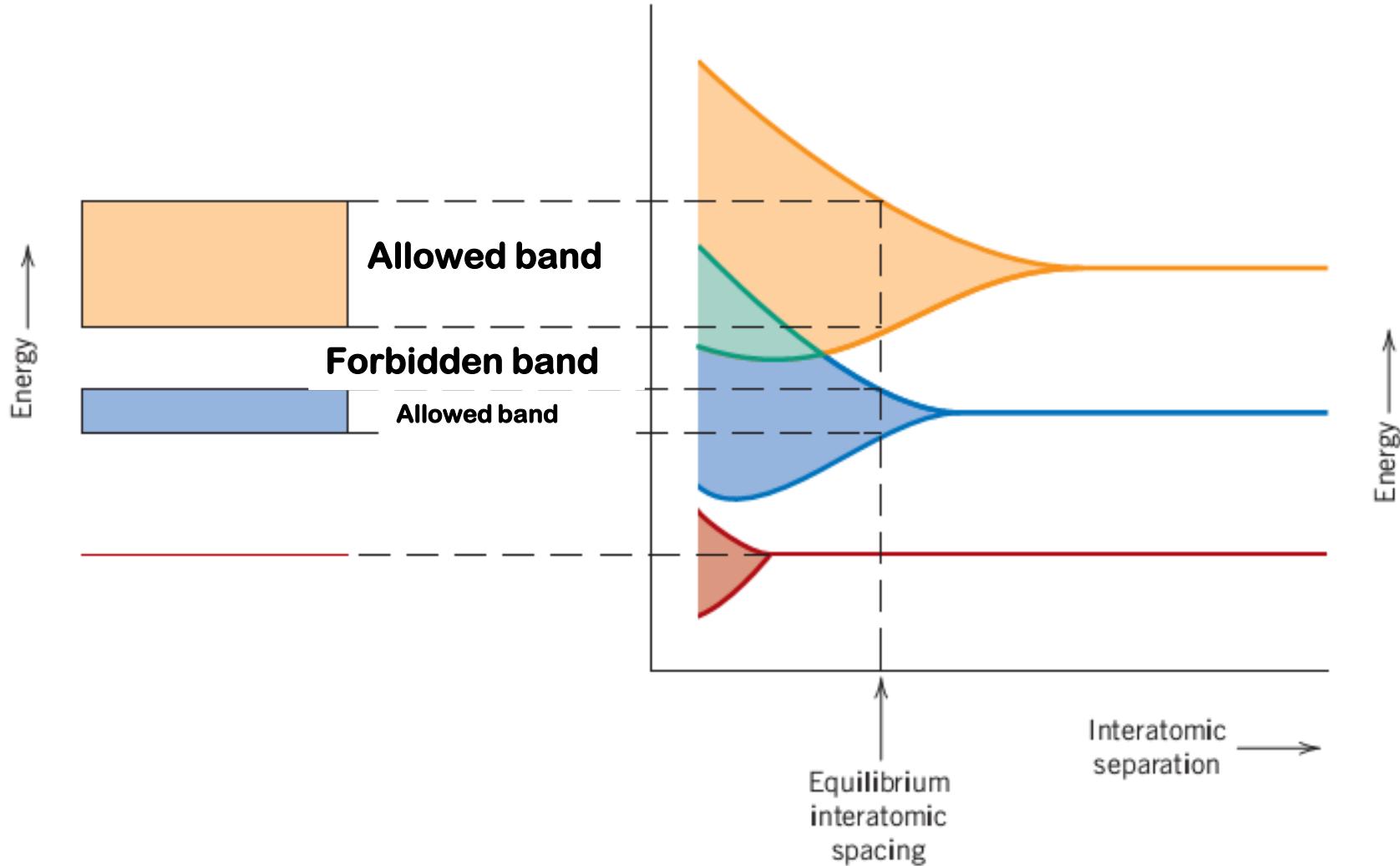
ENERGY BAND STRUCTURES IN SOLIDS

- **Valence band** – filled – highest occupied energy levels
- **Conduction band** – empty – lowest unoccupied energy levels



Formation of Bands in Solids

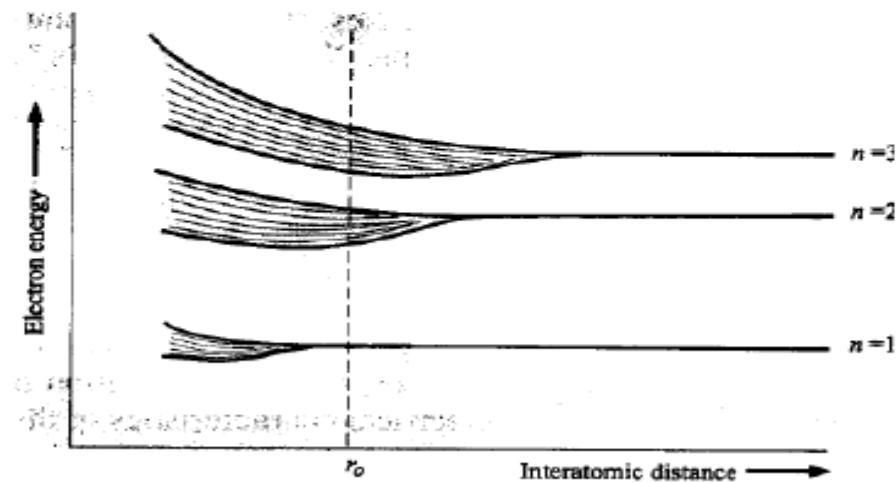
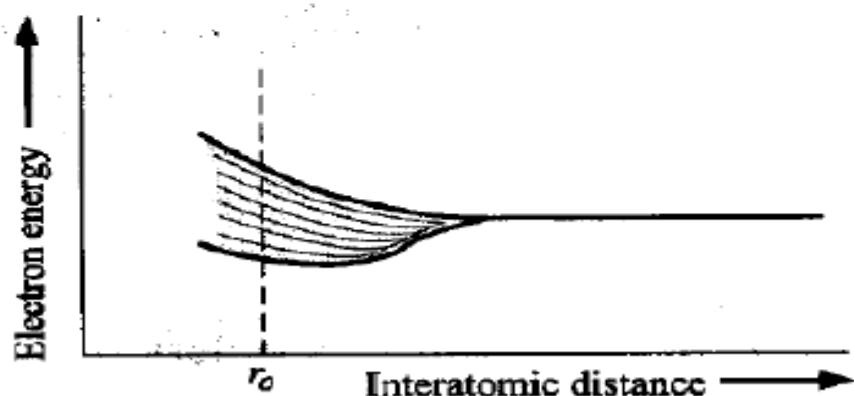
- ✓ In solids the outer electron energy levels split into a series of closely packed electron states to form bands



Energy bands in solids



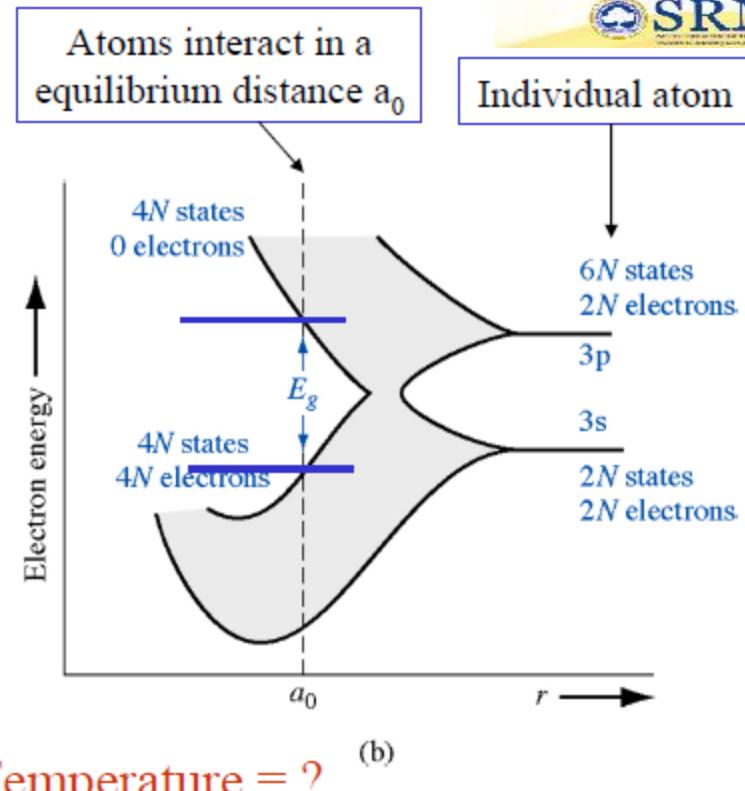
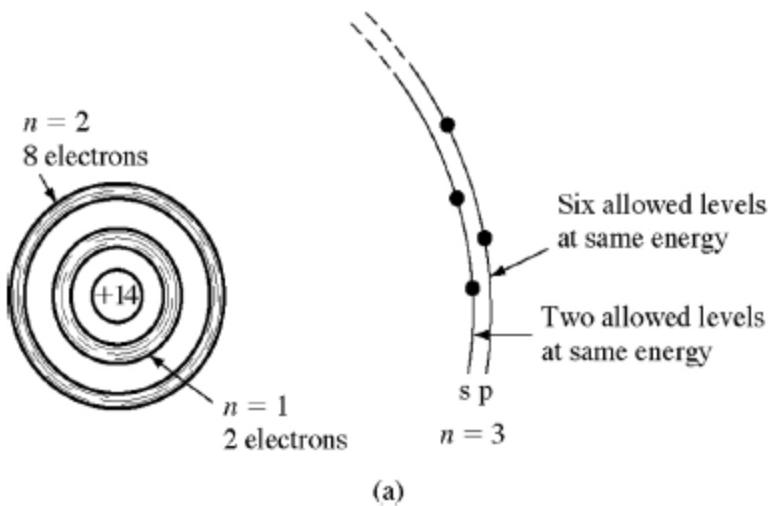
- Consider a regular periodic arrangement of atoms in which each atom contains more than one electron. If the atoms are initially far apart, the electrons in adjacent atoms will not interact and will occupy the discrete energy levels.
- If the atoms are brought closer enough, the outmost electrons will interact and the energy levels will split into a band of allowed energies.



The splitting of an energy state into a band of allowed energies.



$1s^2 2s^2 2p^6 3s^2 3p^{2+4}$



- (a) Schematic of an isolated Si atom. (b) The splitting of the 3s and 3p states of silicon into allowed and forbidden energy bands.



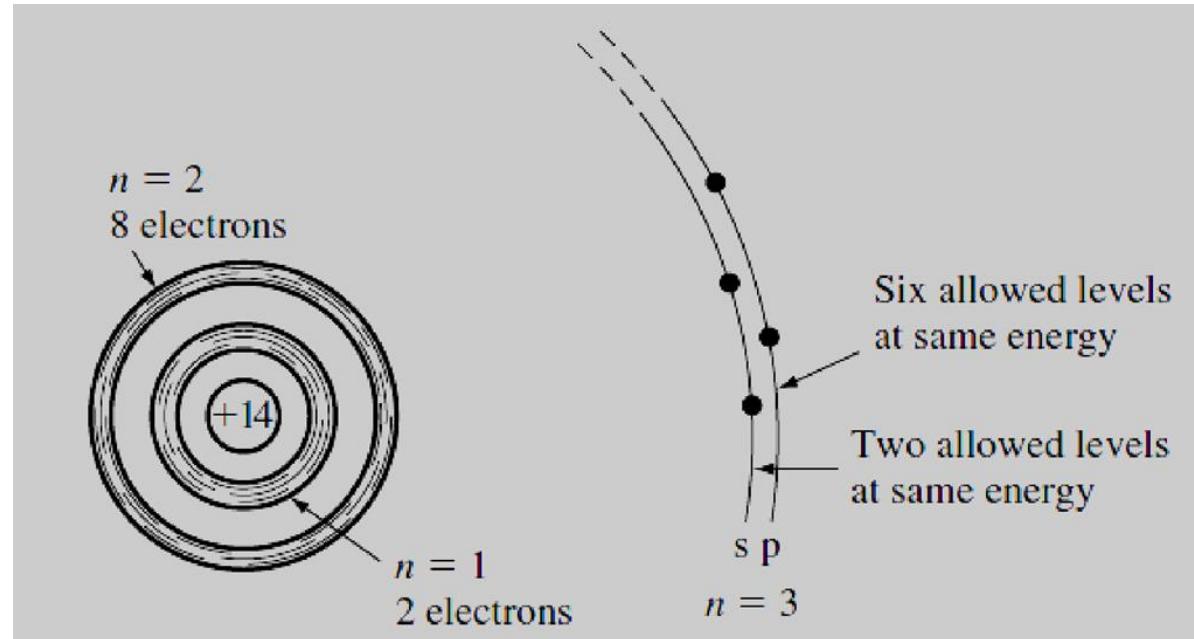
Energy Band Structure of Semiconductor Brillouin zone



To understand the Energy band structure, consider silicon atom.

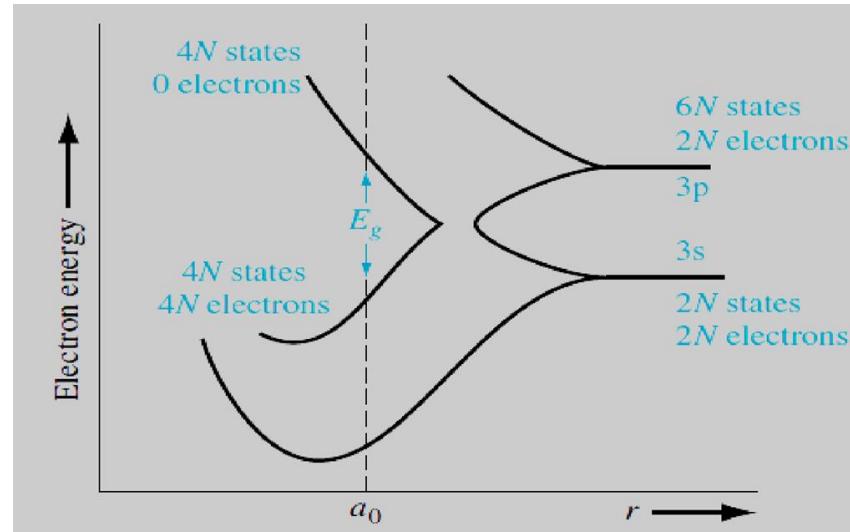
A schematic representation of an isolated silicon atom is shown in Figure.

Ten of the 14 silicon atom electrons occupy deep-lying energy levels close to the nucleus. The four remaining valence electrons are relatively weakly bound and are the electrons involved in chemical reactions.





Energy Band Structure of Semiconductor Brillouin zone



Above Figure shows the band splitting of silicon. We need only to consider the $n=3$ level for the valence electrons, since the first two energy shells are completely full and are tightly bound to the nucleus.

The $3s$ state corresponds to $n=3$ and $l=0$ and contains two quantum states per atom. This state will contain two electrons at $T= 0$ K. The $3p$ state corresponds to $n= 3$ and $l=1$ and contains six quantum states per atom. This state will contain the remaining two electrons in the individual silicon atom.



As the interatomic distance decreases, the 3s and 3p states interact and overlap (*covalent bonding and crystal formation*).

At the equilibrium interatomic distance, the bands have again split, but now four quantum states per atom are in the lower band and four quantum states per atom are in the upper band.

At absolute zero degrees, electrons are in the lowest energy state, so that all states in the lower band (the valence band) will be full and all states in the upper band (the conduction band) will be empty.

The **bandgap energy** E_g between the top of the valence band and the bottom of the conduction band is the width of the forbidden energy band.



Energy Band Structure of Semiconductor Brillouin zone



At $T = 0 \text{ K}$, the $4N$ states in the lower band, the valence band, are filled with the valence electrons. All of the valence electrons are in the valence band. The upper energy band, the conduction band, is completely empty at $T = 0 \text{ K}$.

As the temperature increases above 0 K , a few valence band electrons may gain enough thermal energy to break the covalent bond and jump into the conduction band.

This means that, as the negatively charged electron breaks away from its covalent bonding position, a positively charged “empty state” is created in the original covalent bonding position in the valence band.

As the temperature further increases, more covalent bonds are broken, more electrons jump to the conduction band, and more positive “empty states” are created in the valence band.

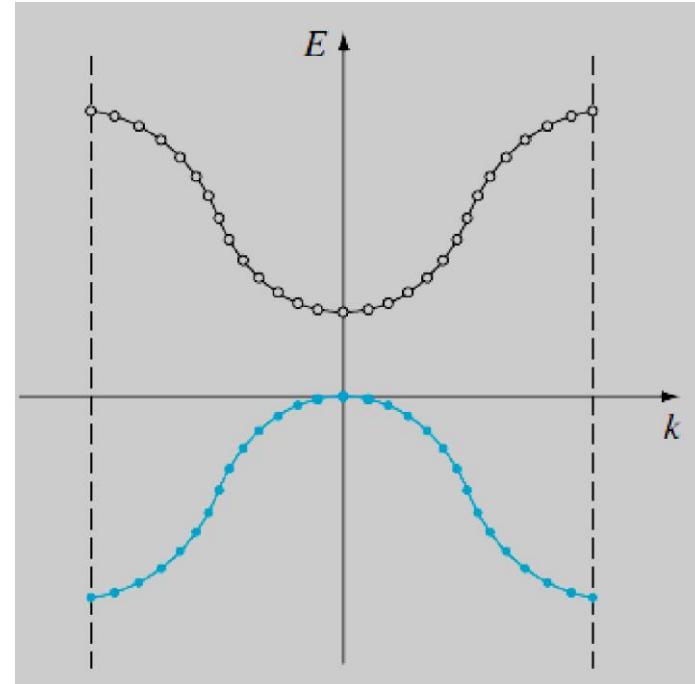


Energy Band Structure of Semiconductor Brillouin zone



This bond breaking can be related to the E versus k energy bands(first brillouin zone).

Figure shows the E versus k diagram of the conduction and valence bands at $T=0$ K. The energy states in the valence band are completely full and the states in the conduction band are empty.

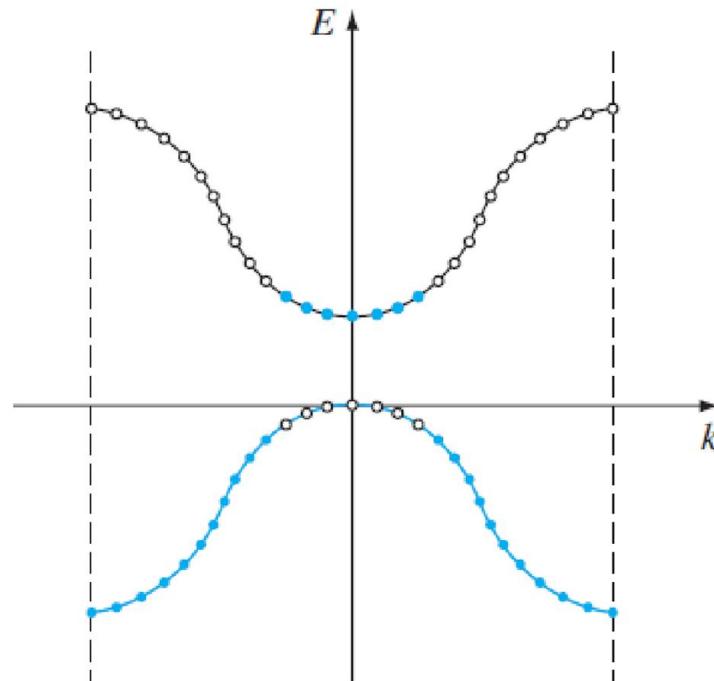




Energy Band Structure of Semiconductor Brillouin zone



Below Figure shows these same bands for $T > 0$ K, in which some electrons have gained enough energy to jump to the conduction band and have left empty states in the valence band.

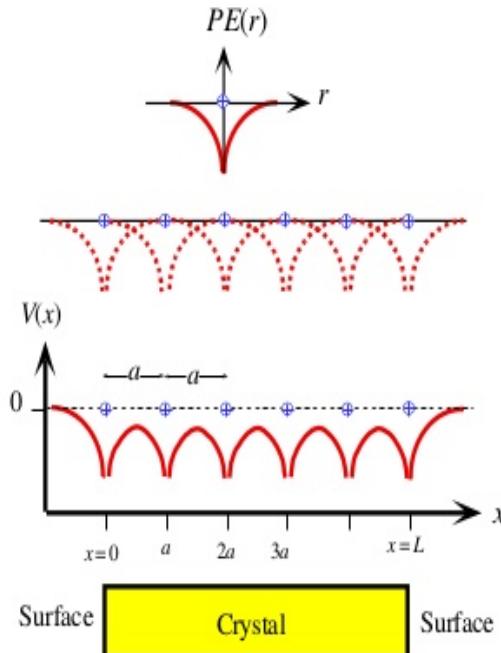


Kroning Penney model :

- According to Kroning and Penney the electrons move in a periodic square well potential.
- This potential is produced by the positive ions (ionized atoms) in the lattice.
- The potential is zero near to the nucleus of positive ions and maximum between the adjacent nuclei. The variation of potential is shown in figure.

Bloch Theorem

- Most of the semiconductors are in crystalline form, i.e the atoms are arranged in periodic manner.
- The motion of electron in a crystal is governed by the laws of quantum mechanics.
- If we have one electron and one proton system like hydrogen atom it is easy to solve Schrodinger equation.
- But in solid there are large number of atoms and electrons present, so its very difficult to solve the Schrodinger equation.
- If we consider a one dimensional periodic lattice and the potential energy (PE) of a moving electron depends on its position inside the lattice, but the PE is said to be periodic in nature by F. Bloch, and the probability of finding a electron is also periodic, the wave-function associated with electron is also periodic in nature.
- Since the probability of finding electron is equal to $|\Psi|^2$



PE of the electron around an isolated atom

When N atoms are arranged to form the crystal then there is an overlap of individual electron PE functions.

PE of the electron, $V(x)$, inside the crystal is periodic with a period a .

The electron potential energy (PE), $V(x)$, inside the crystal is periodic with the same periodicity as that of the crystal, a . Far away outside the crystal, by choice, $V = 0$ (the electron is free and $PE = 0$).

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Schrödinger's one-Dimensional time independent wave equation

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} (E - V) \psi = 0 \quad \dots\dots(1)$$

Bloch postulated that the potential (V) inside the crystal is periodic, so V can be written as $V(x)$ for one dimensional lattice.

Again the periodic potential $V(x)$ can be written as by means of lattice constant $V(x+a)$
i.e $V(x) = V(x+a)$ $\dots\dots(2)$

Bloch also postulated that the wave function of an electron moving in a periodic lattice is periodic and which is given as

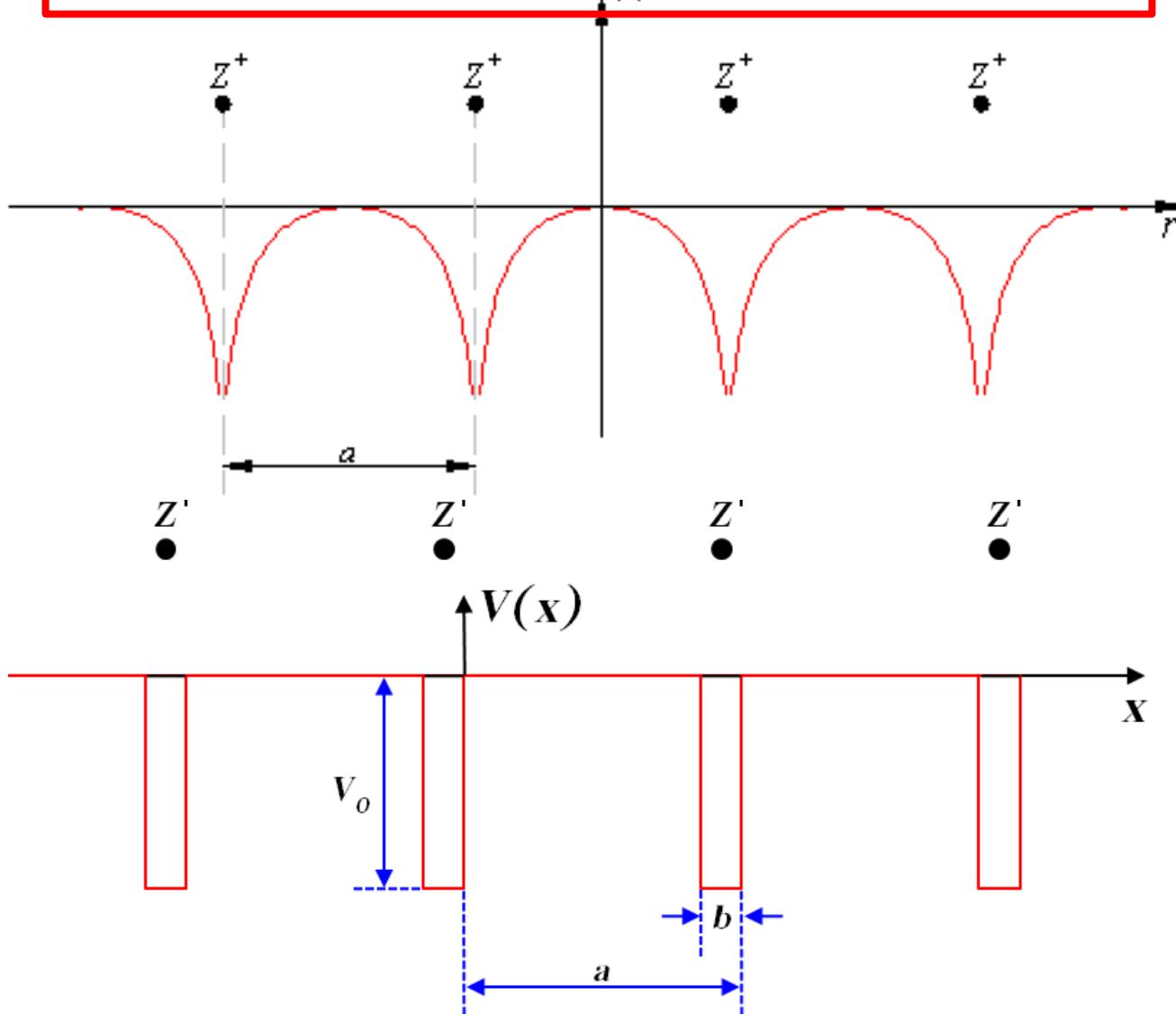
$$\psi_k(x) = e^{ikx} u_k(x) \quad \dots\dots(3), \text{ where } u_k(x) = u_k(x+a) \text{ (periodicity of crystal)}$$

If we substitute the eqs 2 & 3 in eq 1 one can get the solution for the Schrödinger's time independent equation by Numerical and analytical methods

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

From the above equation if we plot energy Eigen values vs wave vector K will give the E-K diagram
So the energy Eigen values are periodic in k space

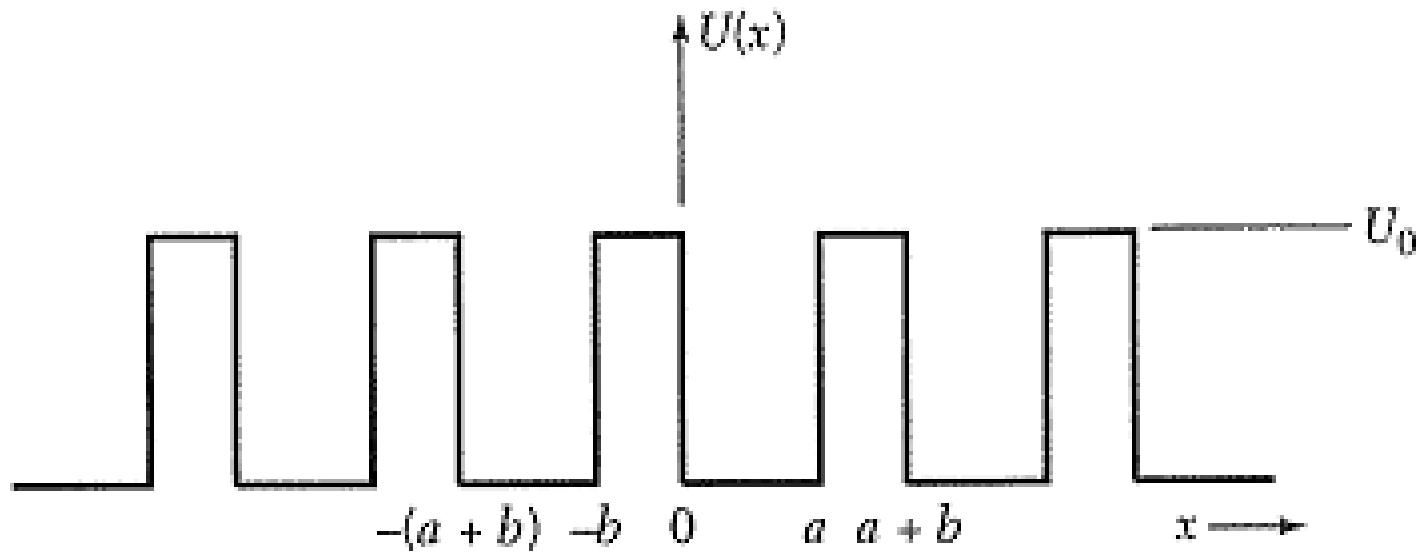
variation of potential with distance in real solid



variation of potential with distance by Kronig-Penny

Kronig-Penney Model

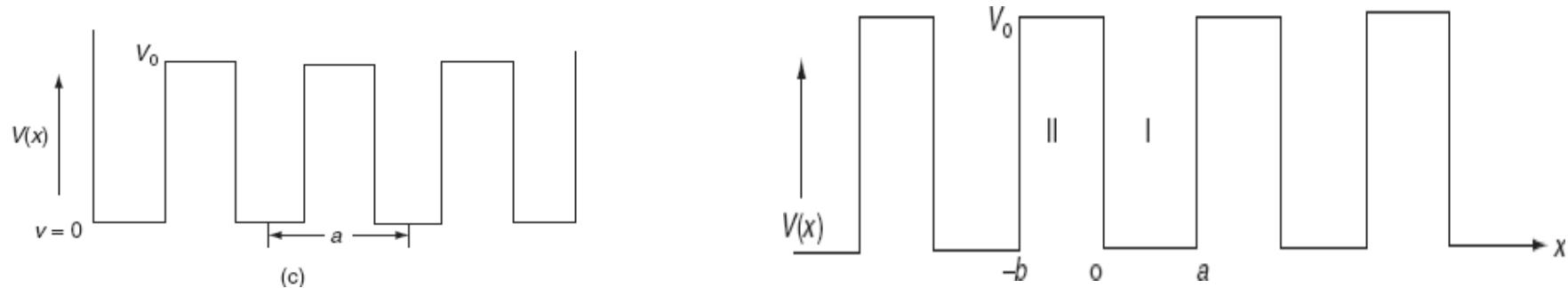
✓ Uniform potential is replaced by periodic potential



$V(x) = 0$, for $0 < x < a$ (potential well)

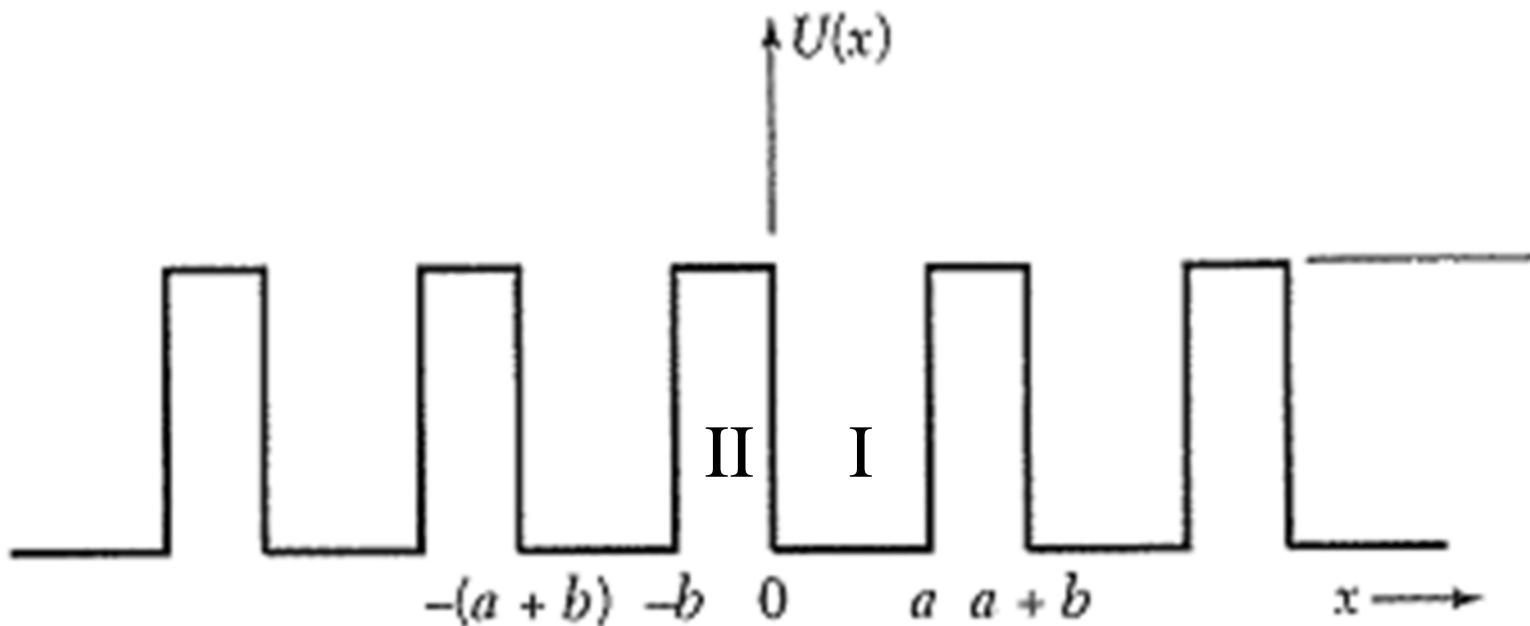
$V(x) = U_0$, for $-b < x < 0$ (potential barrier)

It is not easy to solve Schrödinger's equation with these potentials. So, Kroning and Penney approximated these potentials inside the crystal to the shape of rectangular steps as shown in Fig. (c). This model is called Kroning-Penney model of potentials.



The energies of electrons can be known by solving Schrödinger's wave equation in such a lattice. The Schrödinger time-independent wave equation for the motion of an electron along X-direction is given by:

The energies and wave functions of electrons associated with this model can be calculated by solving time-independent one-dimensional Schrödinger's wave equations for the two regions I and II as shown in Fig



$$\frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2}\psi = 0 \quad 0 < x < a$$

$$\frac{d^2\psi}{dx^2} + \frac{2m(E - V_0)}{\hbar^2}\psi = 0 \quad -b < x < 0$$

The Schrödinger's equations are:

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} E \psi = 0 \quad \text{for } 0 < x < a \dots \dots \dots (2)$$

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} [E - V_0] \psi = 0 \quad \text{for } -b < x < 0 \dots \dots \dots (3)$$

We define two real quantities (say) α and β such that:

$$\alpha^2 = \frac{2mE}{\hbar^2} \quad \text{and} \quad \beta^2 = \frac{2m}{\hbar^2} (V_0 - E) \quad \dots \dots \dots (5.43)$$

$$\frac{d^2\psi}{dx^2} + \alpha^2 \psi = 0 \quad \text{for } 0 < x < a$$

$$\frac{d^2\psi}{dx^2} - \beta^2 \psi = 0 \quad \text{for } -b < x < 0$$

The total wave function is therefore of the form

where $u(x)$ is the periodic function as defined by $u(x) = u(x + a)$, and $k(x)$ is the wave number. Rewriting the wave function in such form allows the simplification of the Schrödinger equation, which we now apply to region I, between the barriers where $V(x) = 0$ and region II, the barrier region where $V(x) = V_0$:

In region I, Schrödinger's equation becomes:

$$\frac{d^2u_I(x)}{dx^2} + 2ik \frac{du_I(x)}{dx} + (\beta^2 - k^2)u_I(x) = 0 \text{ for } 0 < x < a-b$$

$$\beta = \frac{2\pi}{h} \sqrt{2mE}$$

While in region II, it becomes:

$$\frac{d^2u_{II}(x)}{dx^2} + 2ik \frac{du_{II}(x)}{dx} - (k^2 + \alpha^2)u_{II}(x) = 0 \text{ for } a-b < x < a$$

$$\alpha = \frac{2\pi}{h} \sqrt{2m(V_0 - E)}$$

$$u_I(x) = (A \cos \beta x + B \sin \beta x) e^{-ikx} \text{ for } 0 < x < a-b$$

$$u_{II}(x) = (C \cosh \alpha x + D \sinh \alpha x) e^{-ikx} \text{ for } a-b < x < a$$

Since the potential, $V(x)$, is finite everywhere, the solutions for $u_I(x)$ and $u_{II}(x)$ must be continuous as well as their first derivatives. Continuity at $x = 0$ results in:

$$u_I(0) = u_{II}(0) \text{ so that } A = C$$

and continuity at $x = a-b$ combined with the requirement that $u(x)$ be periodic results in:

$$u_I(a-b) = u_{II}(-b)$$

so that

$$(A \cos \beta(a-b) + B \sin \beta(a-b)) e^{-ik(a-b)} = (C \cosh \alpha b - D \sinh \alpha b) e^{ikb}$$

Continuity of the first derivative at $x = 0$ requires that:

$$\left. \frac{du_I(x)}{dx} \right|_{x=0} = \left. \frac{du_{II}(x)}{dx} \right|_{x=0}$$

The first derivatives of $u_I(x)$ and $u_{II}(x)$ are:

$$\frac{du_I(x)}{dx} = (A\beta \sin \beta x - B\beta \cos \beta x) e^{-ikx} - ik(A \cos \beta x + B \sin \beta x) e^{-ikx}$$

$$\frac{du_{II}(x)}{dx} = (C\alpha \sinh \alpha x + D\alpha \cosh \alpha x) e^{-ikx} - ik(C \cosh \alpha x + D \sinh \alpha x) e^{-ikx}$$

so that (2.3.15) becomes:

$$-B\beta - ikA = D\alpha - ikC$$

Finally, continuity of the first derivative at $x = a - b$, again combined with the requirement that $u(x)$ is periodic, results in:

$$\left. \frac{du_I(x)}{dx} \right|_{x=a-b} = \left. \frac{du_{II}(x)}{dx} \right|_{x=-b}$$

so that

$$\begin{aligned} & (A\beta \sin \beta(a-b) - B\beta \cos \beta(a-b))e^{-ik(a-b)} \\ & - ik(A \cos \beta(a-b) + B \sin \beta(a-b))e^{-ik(a-b)} \\ & = (-C\alpha \sinh \alpha b + D\alpha \cosh \alpha b)e^{ikb} - ik(C \cosh \alpha b - D \sinh \alpha b)e^{ikb} \end{aligned}$$

This equation can be simplified using equation (2.3.14) as:

$$(A\beta \sin \beta(a-b) - B\beta \cos \beta(a-b)) = (-C\alpha \sinh \alpha b + D\alpha \cosh \alpha b)e^{ika}$$

$$\begin{vmatrix} 1 & 0 & -1 & 0 \\ 0 & \beta & 0 & \alpha \\ \cos \beta(a-b) & \sin \beta(a-b) & -\cosh \alpha b \exp ika & \sinh \alpha b \exp ika \\ \beta \sin \beta(a-b) & -\beta \cos \beta(a-b) & \alpha \sin \alpha b \exp ika & -\alpha \cosh \alpha b \exp ika \end{vmatrix} = 0$$



three rows and column, while replacing $\cos\beta(a-b)$ by β_c , $\sin\beta(a-b)$ by β_s , $\cosh ab e^{ika}$ by α_c and $\sinh ab e^{ika}$ by α_s , which results in:

$$\begin{vmatrix} \beta & 0 & \alpha \\ \beta_s & -\alpha_c & \alpha_s \\ -\beta\beta_c & \alpha\alpha_s & -\alpha\alpha_c \end{vmatrix} = \begin{vmatrix} 0 & \beta & \alpha \\ \beta_c & \beta_s & \alpha_s \\ \beta\beta_s & -\beta\beta_c & -\alpha\alpha_c \end{vmatrix}$$

Working out the determinants and using $\beta_c^2 + \beta_s^2 = 1$, and $\alpha_c^2 - \alpha_s^2 = e^{2ika}$, one finds:

$$(\alpha^2 - \beta^2) \sinh ab \sin \beta(a-b) \exp ika + 2\alpha\beta \cosh ab \cos \beta(a-b) \exp ika = \alpha\beta$$

And finally, substituting β_c , β_s , α_c and α_s :

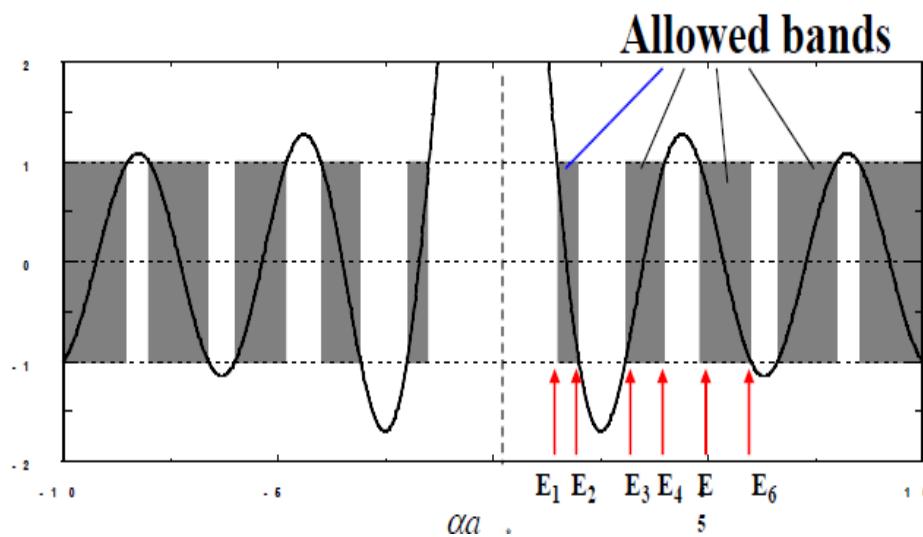
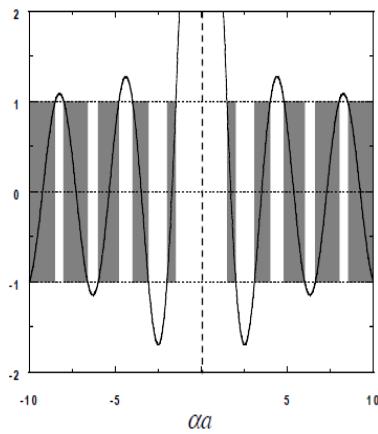
$$\cos ka = F = \frac{\alpha^2 - \beta^2}{2\alpha\beta} \sinh ab \sin \beta(a-b) + \cosh ab \cos \beta(a-b)$$

By solving the determinant we get

$$\frac{\beta^2 + \alpha^2}{2\alpha\beta} \sin h\beta a \sin \alpha a + \cosh h\beta a \cos \alpha a = \cos k(a + b) \rightarrow (17)$$

Again solving the above eq, $\frac{P}{\alpha a} \sin \alpha a + \cos \alpha a = \cos ka \rightarrow (18)$

Here P - power of potential well & $\cos ka$ takes value between $+1$ and -1 .



$$P \frac{\sin \alpha a}{\alpha a} + \cos \alpha a = \cos ka$$

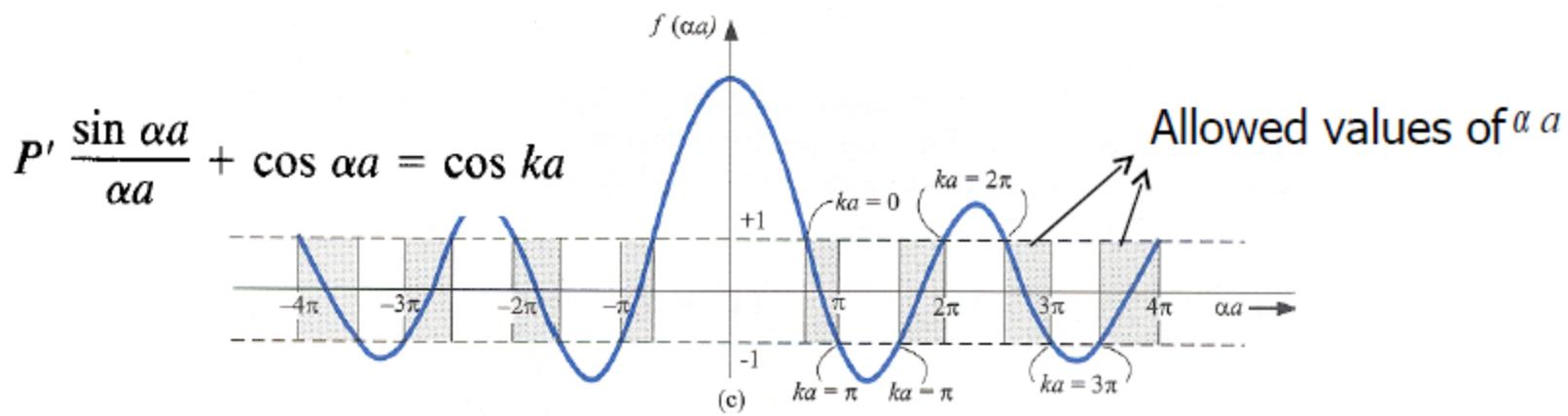
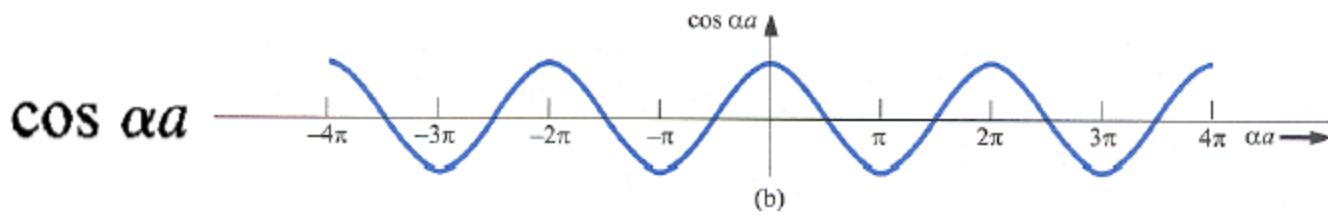
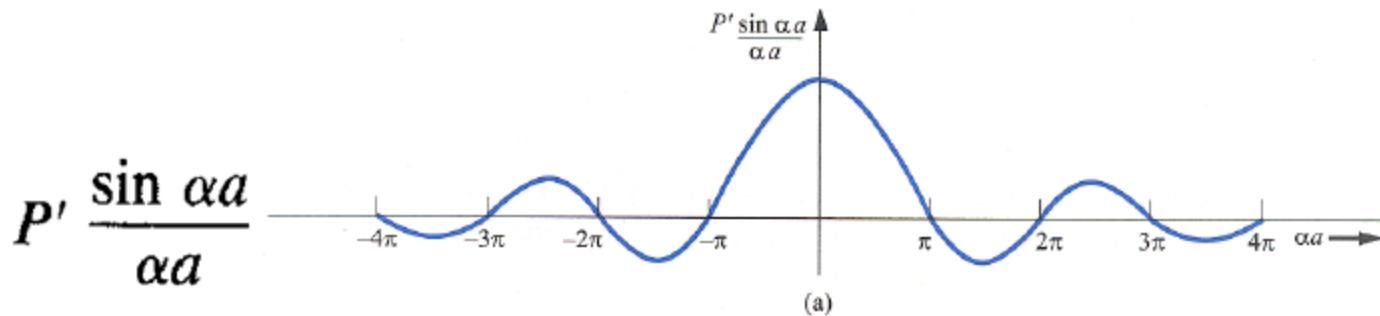
$$P = \frac{mV_o ba}{\hbar^2}$$

$V_o b$ is potential barrier or barrier strength, P is height of potential barrier or it is a measure of the strength with which electrons are bound to the positive ions.

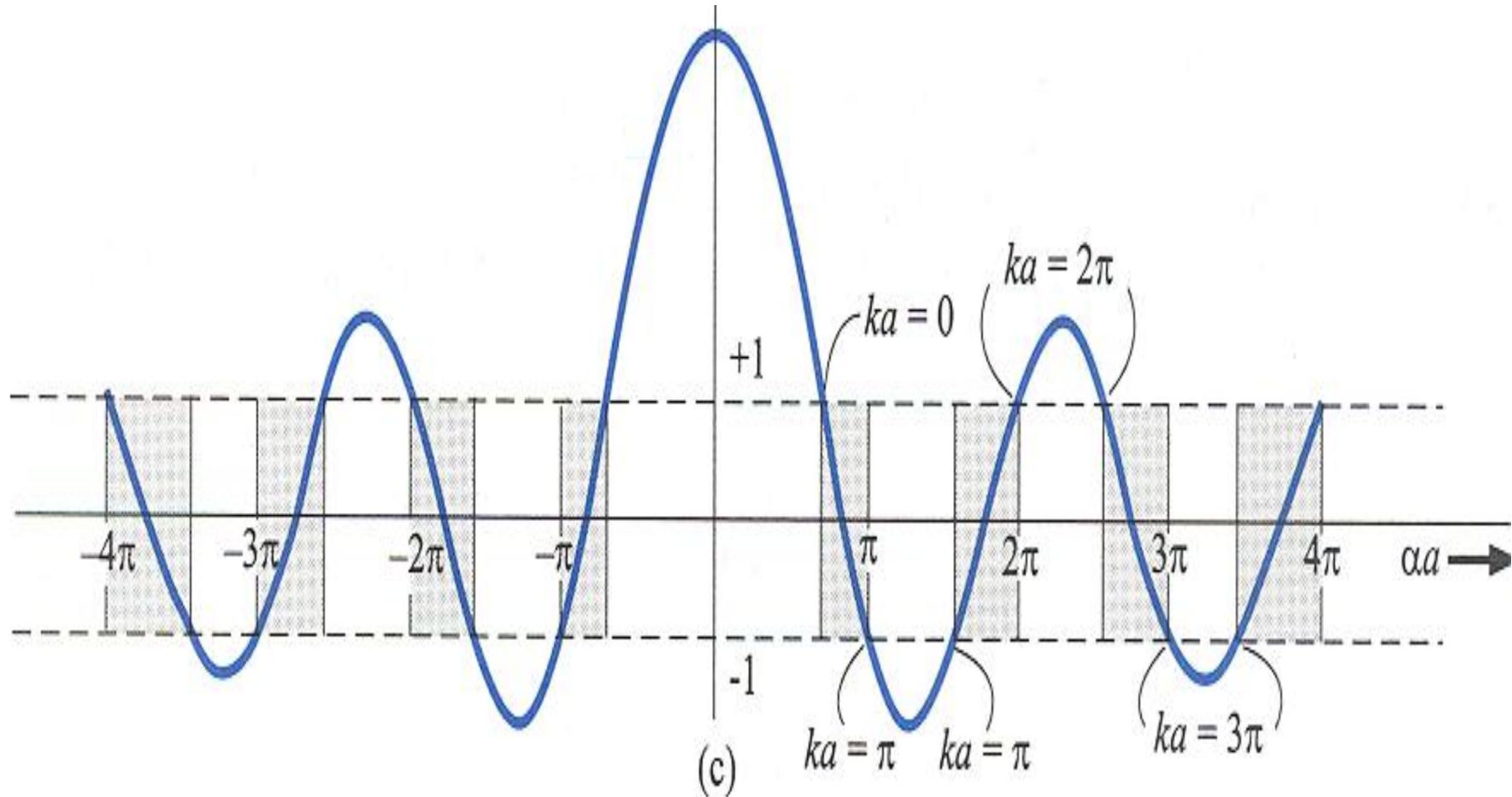
This is a relation between parameter k , total Energy E (through parameter α) and potential barrier bV_o .

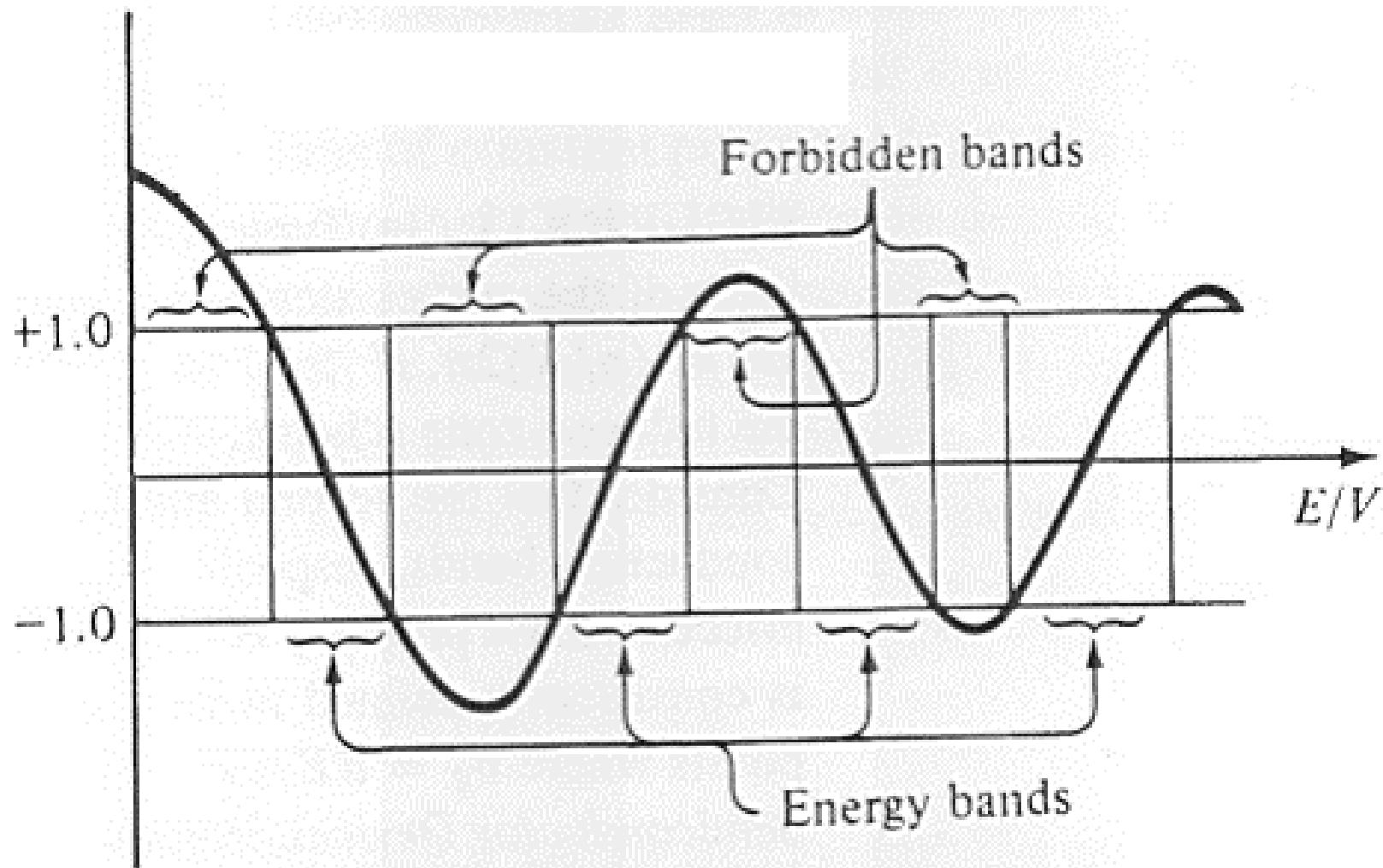
$$\alpha^2 = \frac{2mE}{\hbar^2}$$

This is not a solution to Schrodinger's equation but a condition for a solution to exist.



$$P \frac{\sin \alpha a}{\alpha a} + \cos \alpha a = \cos ka$$





Conclusions from the above graph

- ✓ There exists a number of energy bands separated by forbidden energy ranges called energy gaps.
- ✓ The width of the allowed energy bands increases with increasing value of α i.e. with increase in energy values.
- ✓ The width of a particular band decreases with increasing value of P , i.e. with increasing binding energy of the electron.

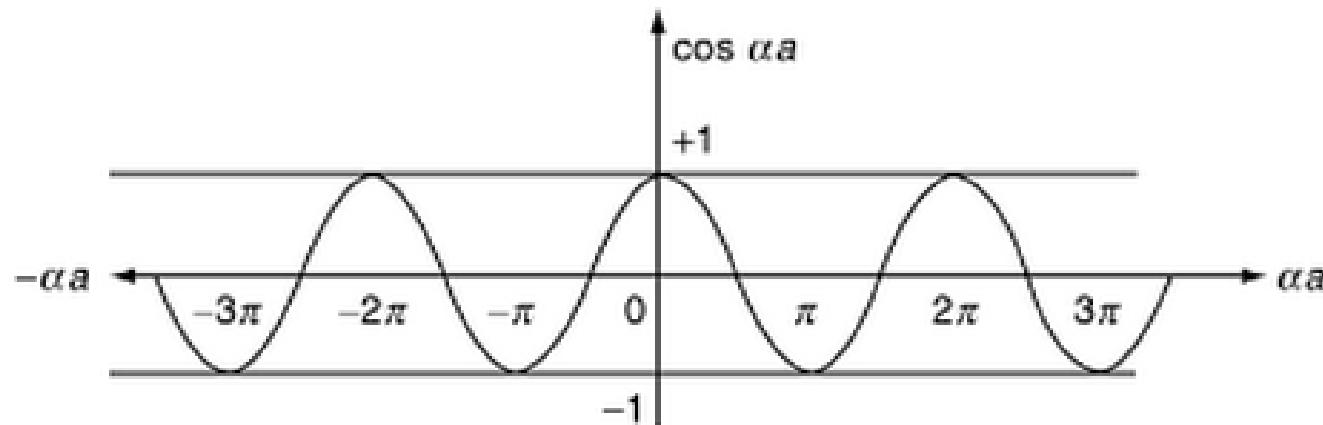
1st case, free electron: $P \rightarrow 0$

$V_0=0$ hence:

$$\cos \alpha a = \cos ka \implies \alpha = k$$

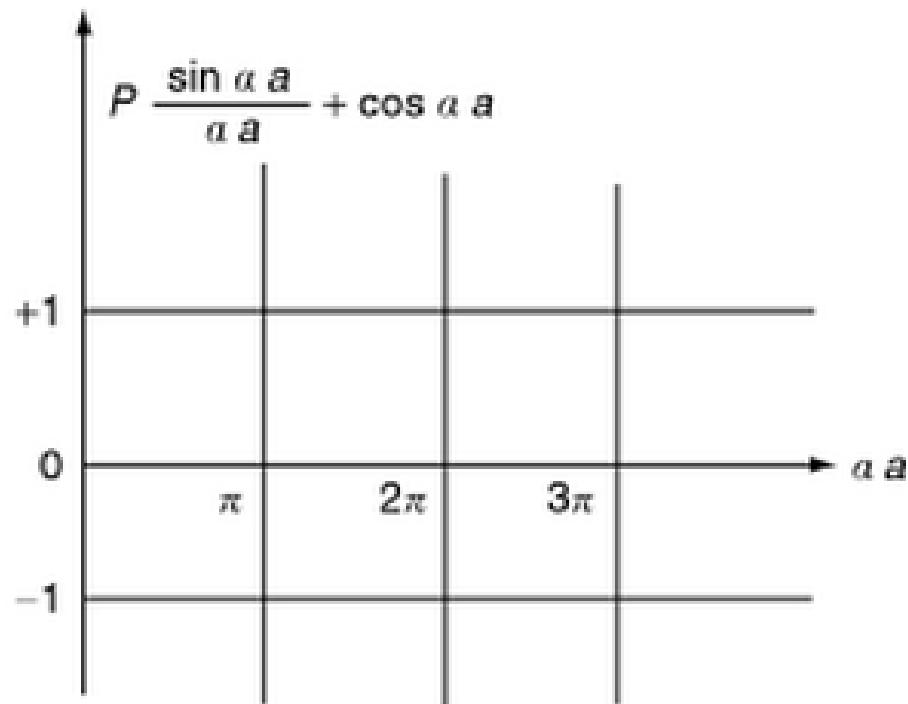
$$\alpha^2 = \frac{2mE}{\hbar^2} \quad \text{and} \quad E = \frac{p^2}{2m} = \frac{k^2 \hbar^2}{2m}$$

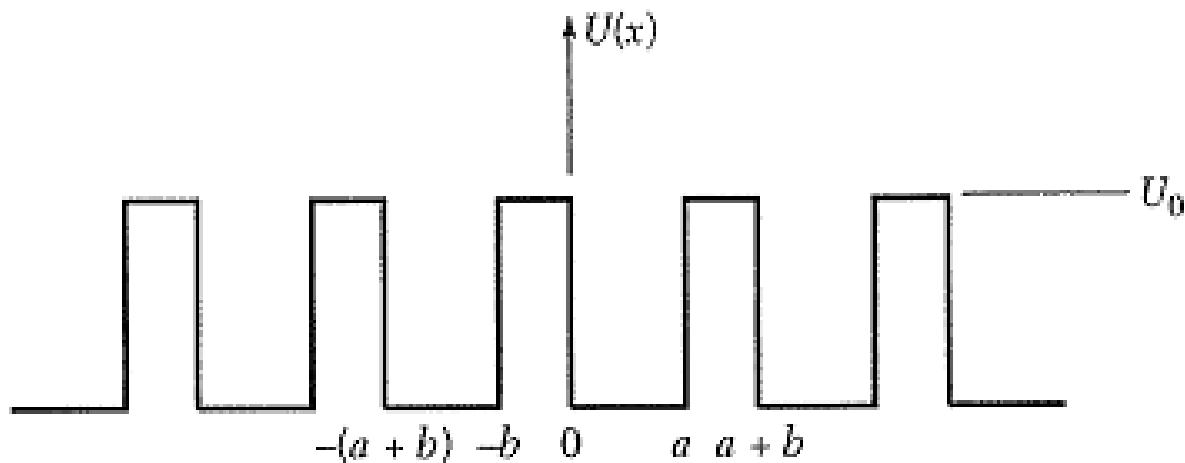
Shows that all energies are allowed to the electrons as $P \rightarrow 0$



$P \rightarrow \text{infinity}$

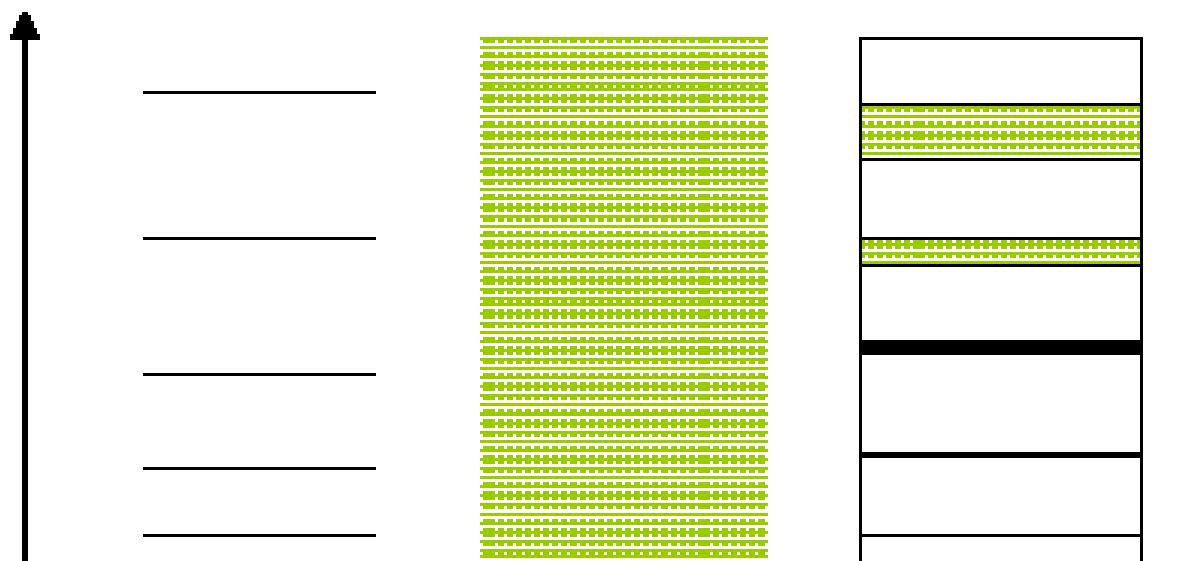
Shows that the allowed energy bands reduces to single energy levels as $P \rightarrow \infty$





Strength of the barrier P $= \frac{mV_o ba}{\hbar^2}$

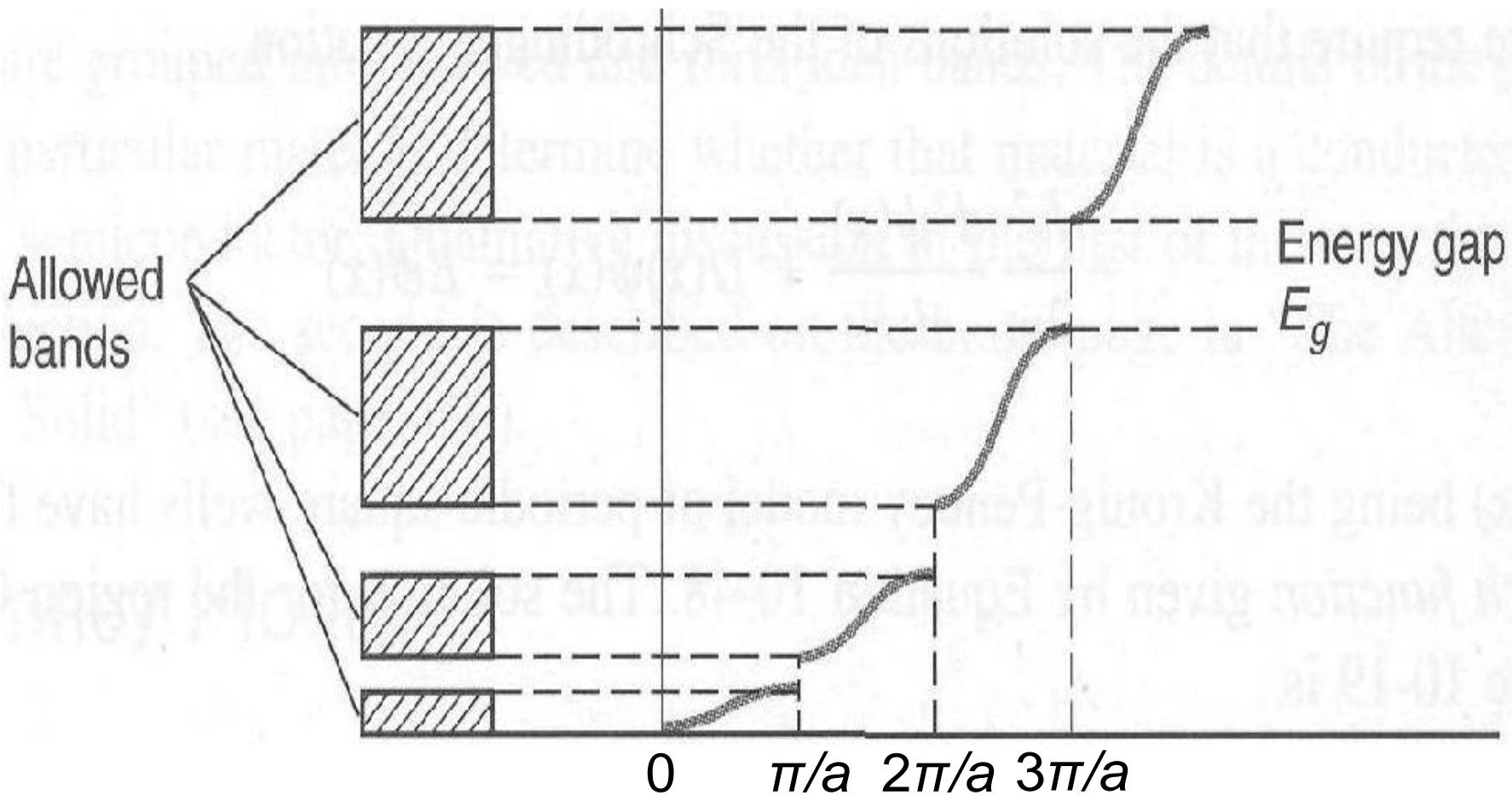
Energy

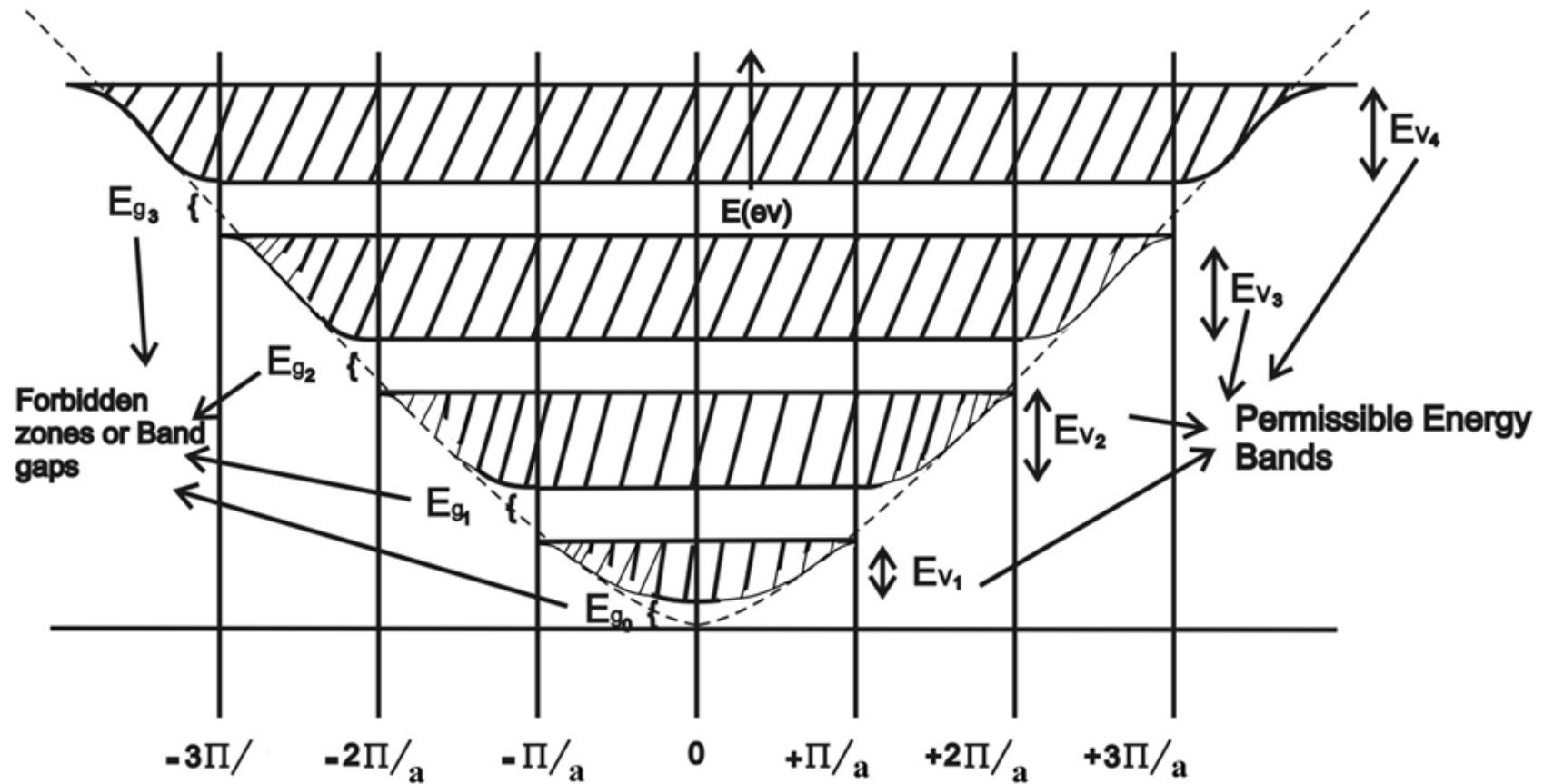


$P \rightarrow \infty$

$P \rightarrow 0$

$P \rightarrow \text{Intermediate}$

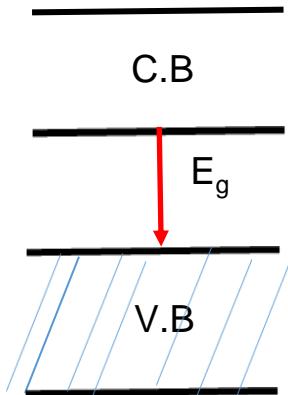






E-K Diagram

- The conventional band diagram shows the band gap energy only
- To know more about electrical and optical properties of semiconductor material, we need to know about the E-K diagram.
- An E-K diagram shows characteristics of particular semiconductor material
- *It shows the relationship between energy and momentum of available states for electron in the crystal*
- K being the momentum and E as the energy. From a mathematical point of view K is the wave vector
- The E-K diagram of semiconductor is obtained by solving the Schrodinger's equation.

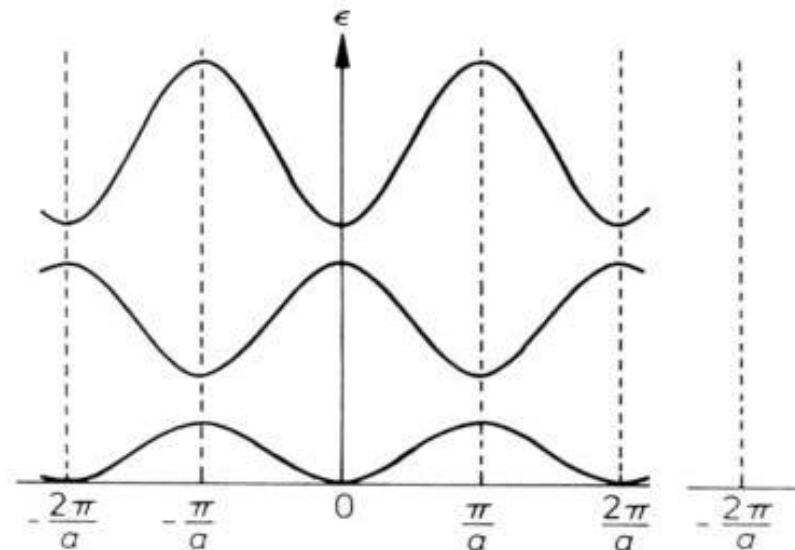


There are three types of E-K diagram

- Periodic zone scheme
- Extended zone scheme
- Reduced zone scheme

Periodic zone scheme:

The periodic repetition of allowed energy values corresponding to each allowed band, which is obtained by the periodic repetition of the region of $-\frac{\pi}{a} < k < \frac{\pi}{a}$ through whole k-space.



Periodic Zone



Extended Zone Scheme:

In this scheme, different bands are drawn in different zones. In k-space.

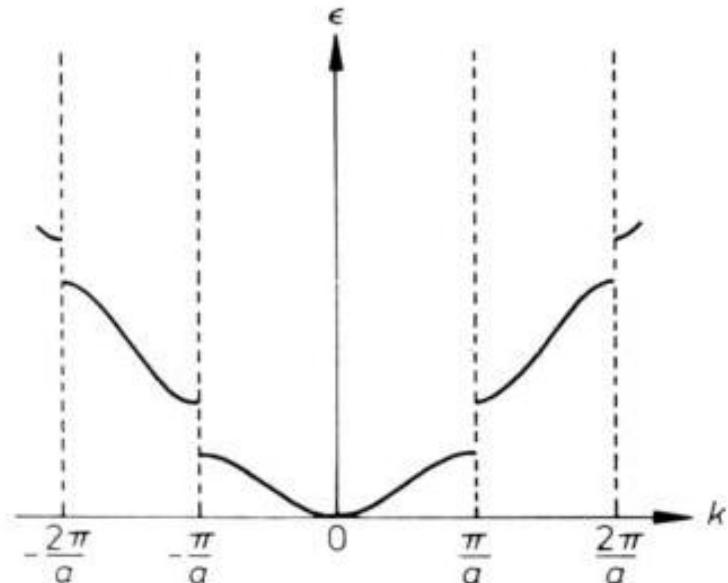
A discontinuity is obtained at $K = \pm \frac{n\pi}{a}$ where $n = \pm 1, \pm 2, \dots$

For $k = -\frac{\pi}{a}$ to $\frac{\pi}{a}$ is first Brillouin zone

For $k = -\frac{\pi}{a}$ to $-\frac{2\pi}{a}$ and $\frac{\pi}{a}$ to $\frac{2\pi}{a}$ is second Brillouin zone

The discontinuity in the curve is due to Bragg's law of reflection

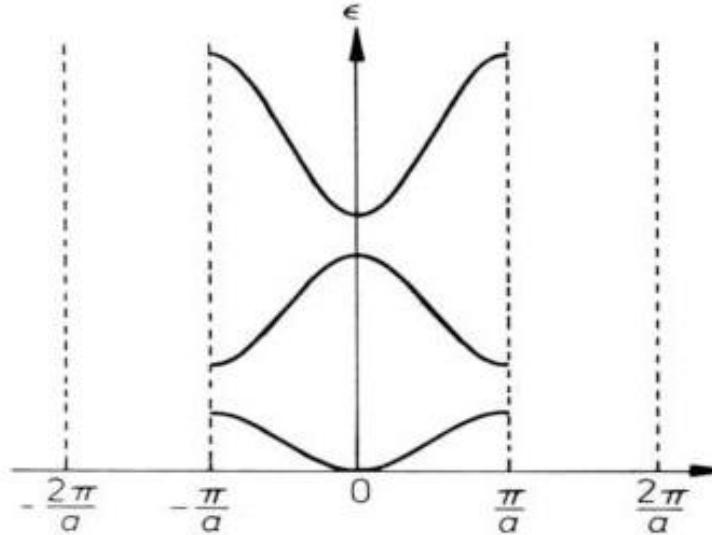
at the edges of allowed bands (i.e) $K = \pm \frac{n\pi}{a}$



Extended Zone

Reduced zone scheme :

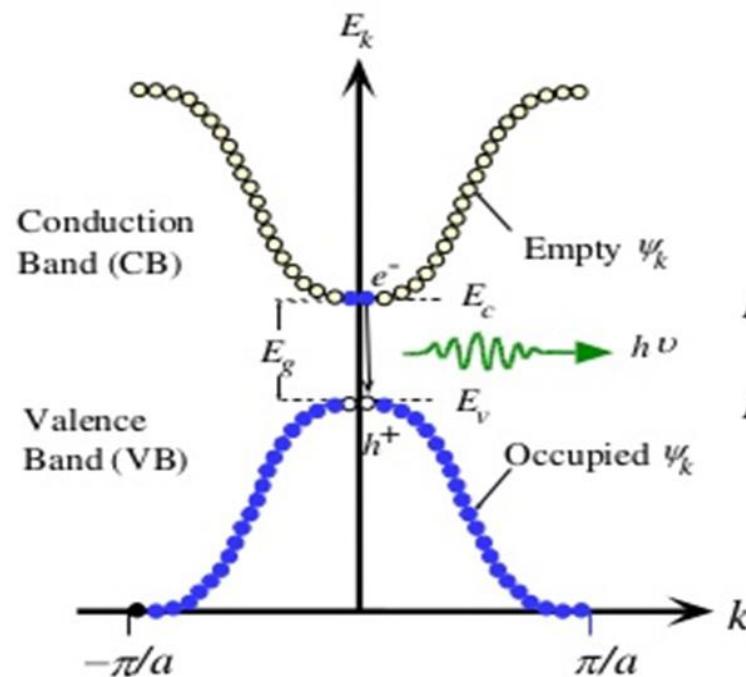
- In this scheme the first Brillouin zone is shown, since the E-K diagram is periodic, it is sufficient to restrict to first zone in the reduced scheme.
- If we know the energy values of first zone with respect to K then we know every where because
energy Eigen values are periodic
- In many of optoelectronic text books the reduce zone scheme is shown



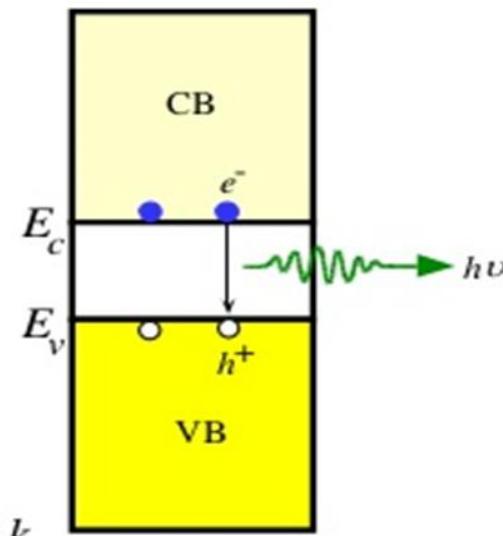
Reduced Zone



The E - k Diagram



The Energy Band Diagram



The E - k diagram of a direct bandgap semiconductor such as GaAs. The E - k curve consists of many discrete points with each point corresponding to a possible state, wavefunction $\psi_k(x)$, that is allowed to exist in the crystal. The points are so close that we normally draw the E - k relationship as a continuous curve. In the energy range E_v to E_c there are no points ($\psi_k(x)$ solutions).

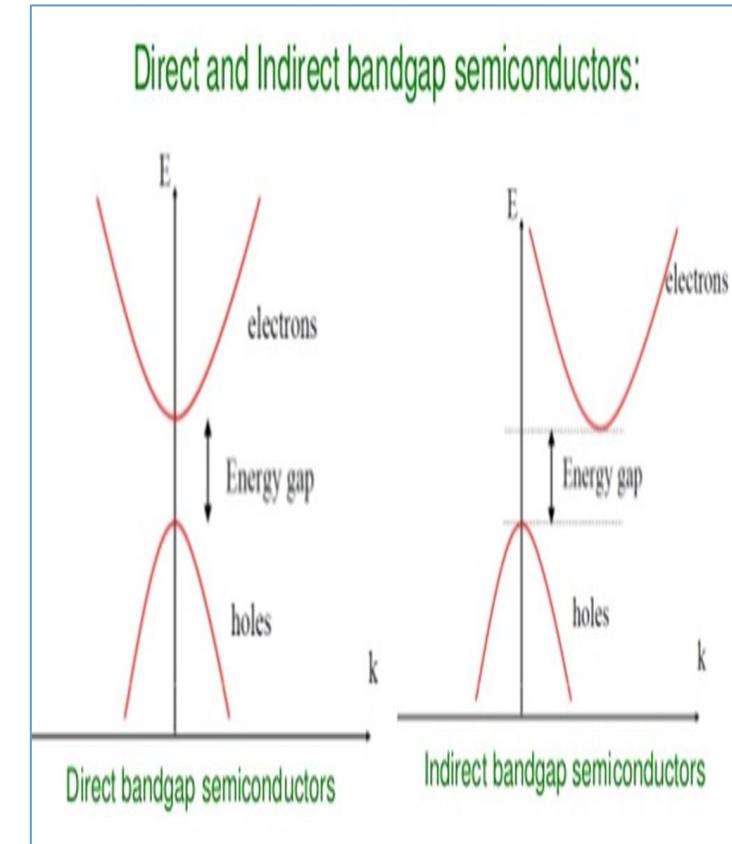
What are the significance of E-K diagram

- No theoretical study, experimentation and technological application can take place without E-K diagram.
- This diagram indicates the band gap E_g which is the difference in energy between top of the valance band and bottom of the conduction band
- This diagram demonstrate electron (hole) mobility
- This diagram explains electron (hole) effective mass
- This diagram indicate how the electron states are equally spaced in K-Space
- This diagram clearly shows direct vs indirect band gap

Direct and Indirect band gap semiconductors



- We know the relation between energy and wave number for an one dimensional lattice. In real crystals the E – K relationship is much more complicated.
- In crystals the interatomic distances and internal potential energy distribution vary with direction of the crystal.
- Hence the E – K relationship and energy band formation depends on the orientation of the electron wave vector to the crystallographic axes.
- In few crystals like GaAs, the maximum of the valence band occurs at the same value of K as the minimum of the conduction band.
- This is called *direct band gap semiconductor*.



Direct and Indirect band gap semiconductors



- In few semiconductors like Si the maximum of the valence band does not always occur at the same K values the maximum of the conduction band. This we call *indirect band gap semiconductor*.
- In direct band gap semiconductors the direction of motion of an electron during a transition across the energy gap, remains unchanged.
- Hence the efficiency of transition of charge carriers across the band gap is more in direct band gap than in indirect band gap semiconductors.



We know
 $P=\hbar k$

$$\text{Kinetic energy (K)} = \frac{1}{2}mv^2, \text{ and}$$

$$\text{Momentum (p)} = mv$$

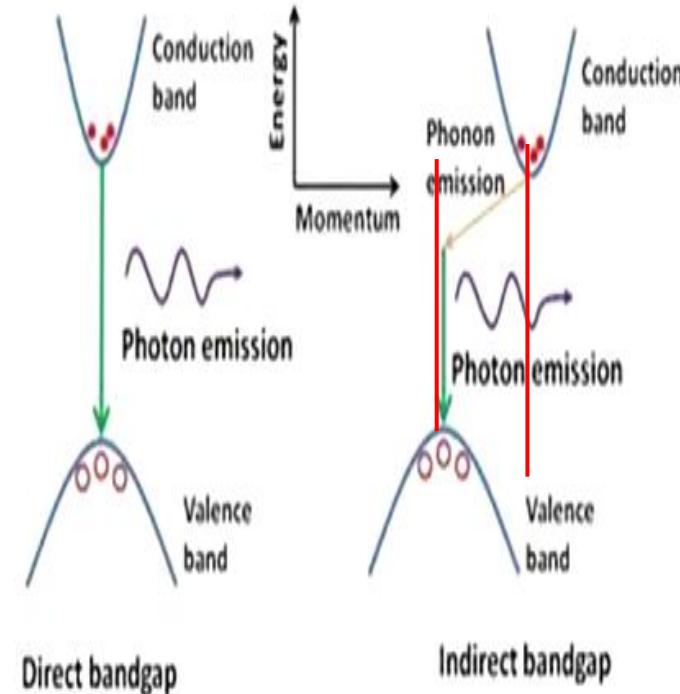
Where, symbols have usual meaning.

Now,

$$K = \frac{1}{2}mv^2 = \frac{1}{2}mv^2 \times \frac{m}{m} = \frac{1}{2} \frac{m^2v^2}{m} = \frac{(mv)^2}{2m} = \frac{p^2}{m}$$

therefore,

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



Indirect bandgap semiconductors:

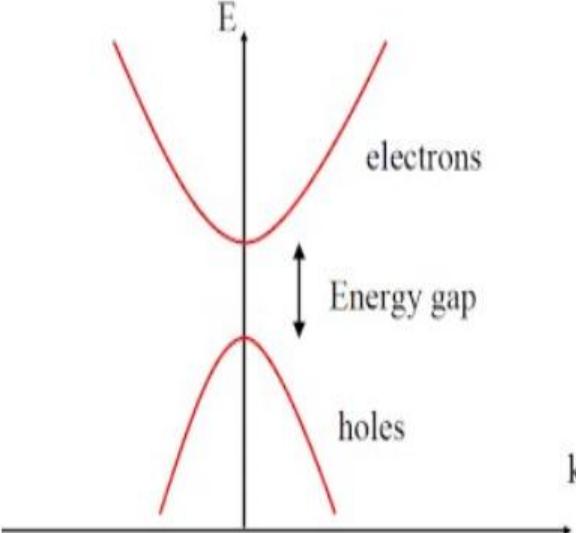
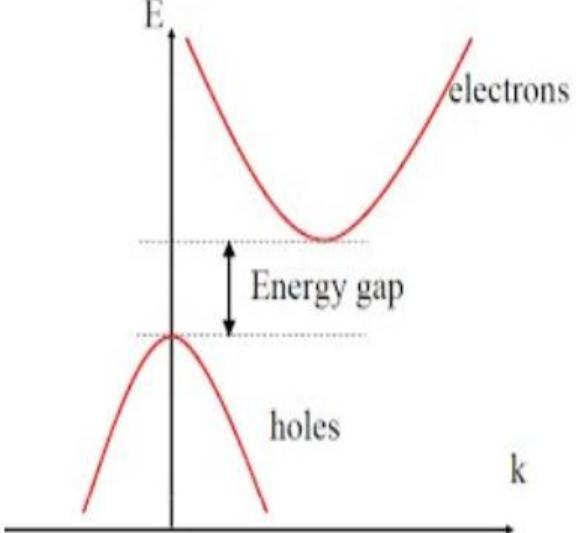
- A direct recombination occurs with the release of energy equals to energy difference between two levels such as E_g .
- The probability of radiative recombination is high and hence direct bandgap semiconductors are used in optical sources

Indirect bandgap semiconductors:

Due to relative difference in momentum, first the momentum is conserved by release of energy only after both the momentum align themselves. The probability of radiative recombination is comparatively low.



No	Direct Band gap semiconductor	Indirect band gap semiconductor
1	A direct band-gap (DBG) semiconductor is one in which the maximum energy level of the valence band aligns with the minimum energy level of the conduction band with respect to momentum.	A indirect band-gap (DBG) semiconductor is one in which the maximum energy level of the valence band are misaligned with the minimum energy level of the conduction band with respect to momentum.
2	In a DBG semiconductor, a direct recombination takes place with the release of the energy equal to the energy difference between the recombining particles.	Due to a relative difference in the momentum, first, momenta align themselves, a recombination occurs accompanied with the release of energy.
3	The efficiency factor of a DBG semiconductor is higher.	The efficiency factor of a IBG semiconductor is lower.
4	Example of DBG semiconductor material is Gallium Arsenide (GaAs).	Examples of IBG semiconductors are Silicon and Germanium.
5	DBG semiconductors are always preferred over IBG for making optical sources.	The IBG semiconductors cannot be used to manufacture optical sources.

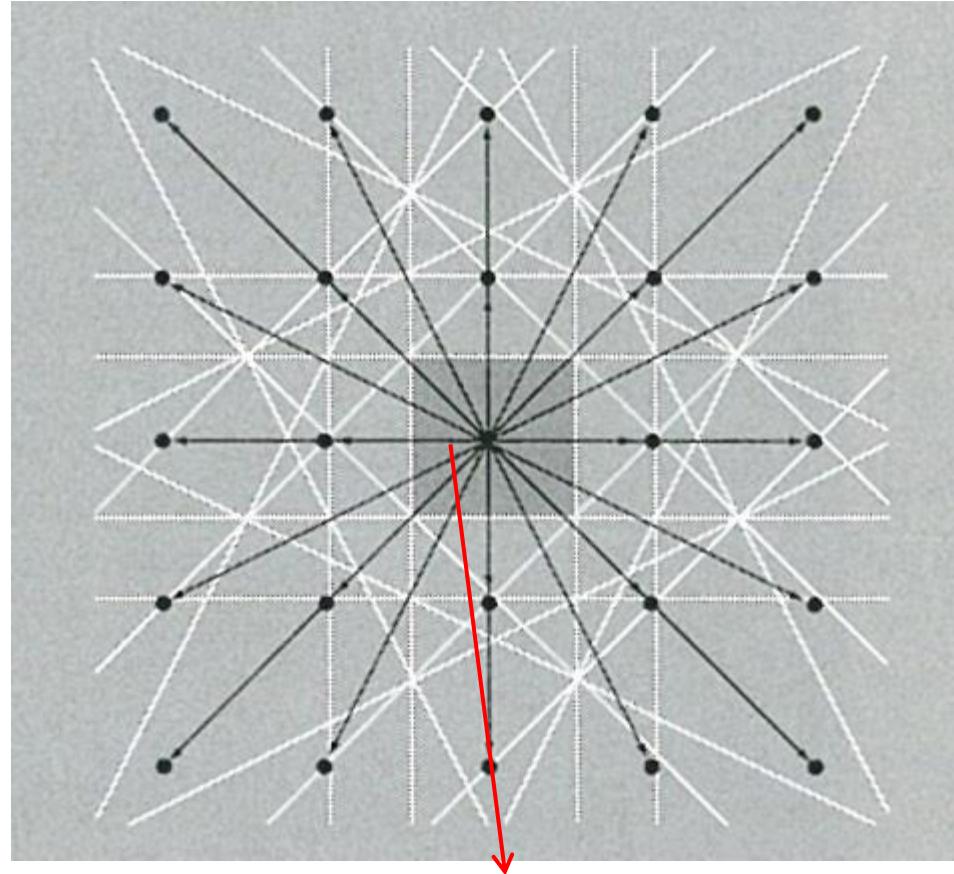
No	Direct Band gap semiconductor	Indirect band gap semiconductor
6	The probability of a radiative recombination is high.	The probability of a radiative recombination is comparatively low.
7		

Brillouin Zone

Brillouin zone is defined as the Wigner-Seitz primitive cell in the reciprocal lattice

Reciprocal Lattice

It is easy to think a set of parallel crystal planes in terms of their normals, since as the planes are two dimensional, their normals will be one dimensional in nature.



First Brillouin Zone of Square Lattice

- Wigner-Seitz cell: smallest possible primitive cell, which consist of one lattice point and all the surrounding space closer to it than to any other point.
- The construction of the W-S cell in the reciprocal lattice delivers the first Brillouin zone (important for diffraction)

Importance of Brillouin zone:

The Brillouin zones are used to describe and analyze the electron energy in the band energy structure of crystals.

Brillouin Zones

- Electrons in solids are permitted to be in allowed energy bands separated by forbidden energy gaps.
- The allowed energy band width increases with $k\alpha$.
- The electron has allowed energy values in the region or zone extending from $k = (-\pi/a)$ to (π/a) , called the first Brillouin zone.
- Similarly, second Brillouin zone extends from
$$k = (-\pi/a) \text{ to } (-2\pi/a) \text{ and}$$
$$k = (\pi/a) \text{ to } (2\pi/a).$$

Brillouin zone

- The different Brillouin zones correspond to primitive cells of a different type that come up in the theory of electronic levels in a periodic potential.
- The first Brillouin zone is considered as the Wigner-Seitz (WS) primitive cell in the reciprocal lattice. In other words, the first Brillouin zone is a geometrical construction to the WS primitive cell in the k-space.
- In a direct lattice, **the procedure of drawing a WS cell is as follows:**
 1. Draw lines to connect a given lattice points to all nearby lattice points.
 2. Draw new lines or plane at the mid point and normal to the lines in (i)
 3. The smallest volume enclosed in this way is the WS primitive cell.

First Brillouin Zone of linear lattice

Crystal and reciprocal lattices in one dimension

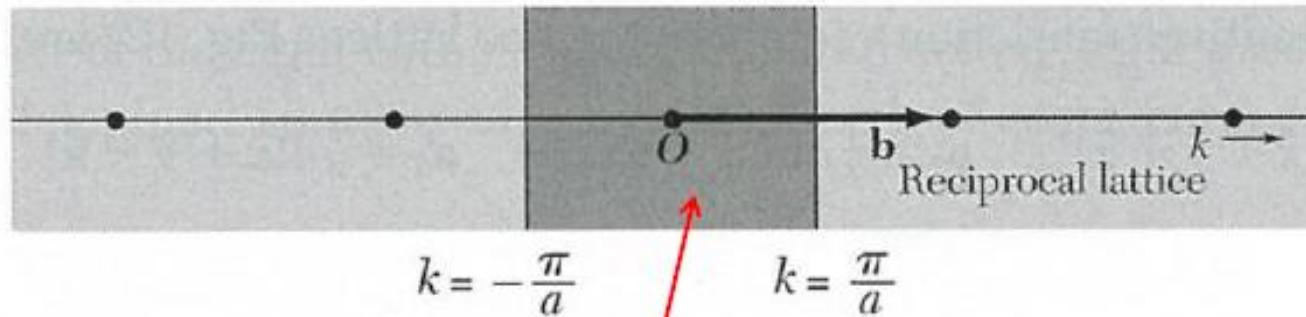
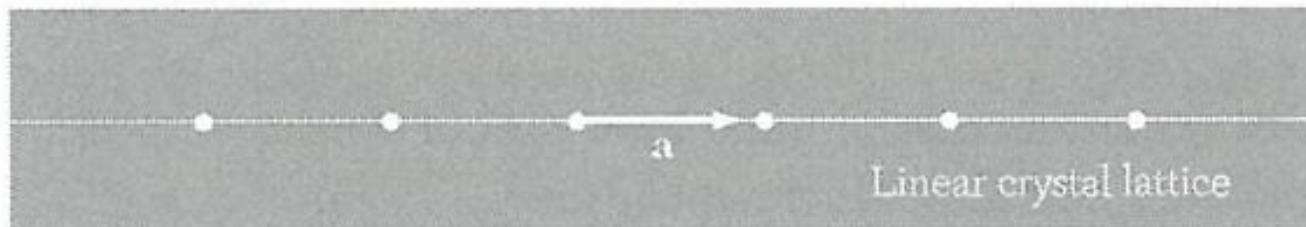
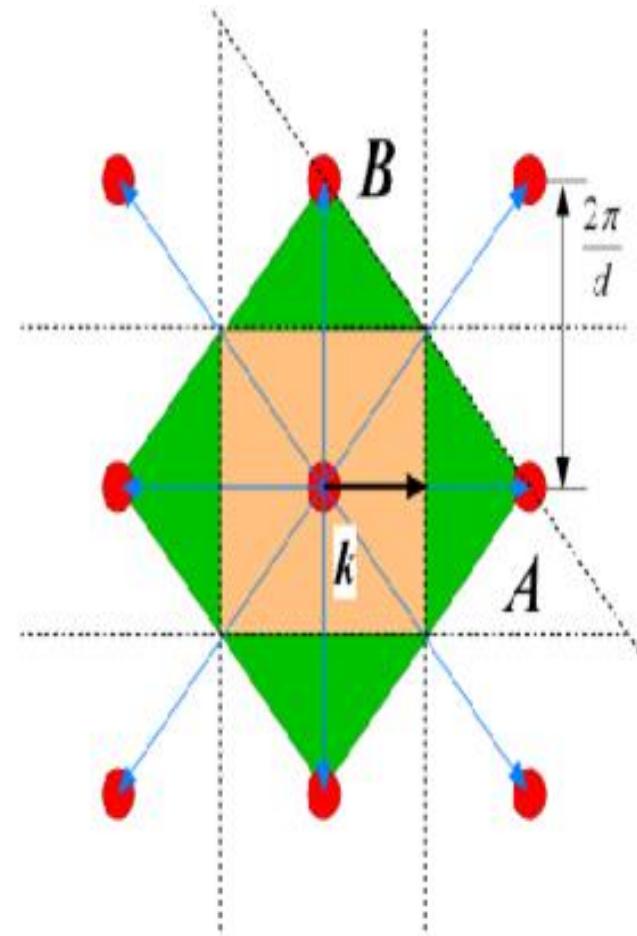


Figure 11 Crystal and reciprocal lattices in one dimension. The basis vector in the reciprocal lattice is b, of length equal to $2\pi/a$. The shortest reciprocal lattice vectors from the origin are **b** and $-\mathbf{b}$. The perpendicular bisectors of these vectors form the boundaries of the first Brillouin zone. The boundaries are at $k = \pm\pi/a$.

First Brillouin zone

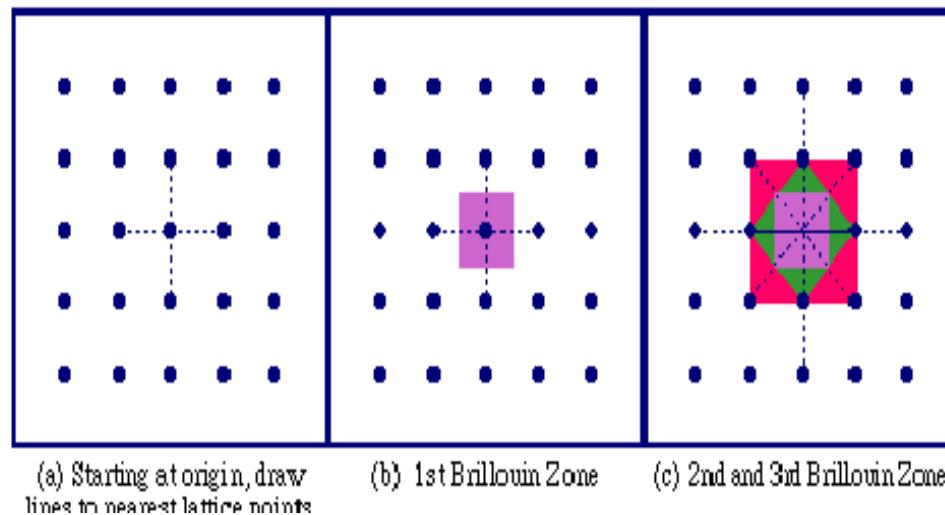
First Brillouin zone is determined by:

- Select lattice point and draw a line segment to all neighbouring lattice points (blue).
- Draw center normal planes (black, dotted). In 2D they are lines.
- The bounded area closest to the selected point is Brillouin zone (orange).
- The next area (going over one line only) is 2. Brillouin zone (green).



Remarks:

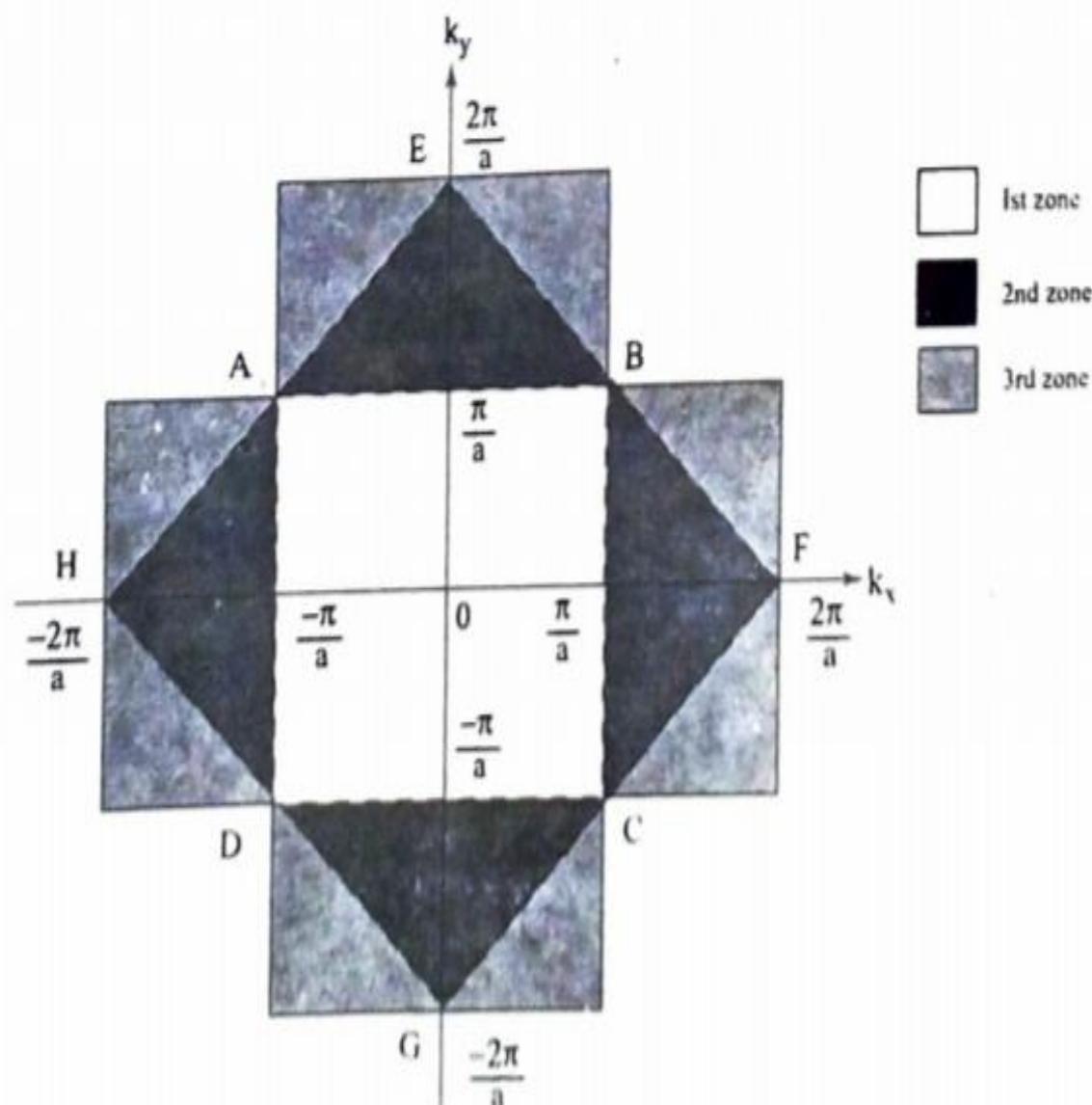
- The planes divide the Fourier space of the crystal into fragments as shown for a square lattice.
- The central square is a primitive cell of the reciprocal lattice. It is a Wigner-Seitz cell of the reciprocal lattice (called the first Brillouin zone).
- The first Brillouin zone is the smallest volume entirely enclosed by the planes.



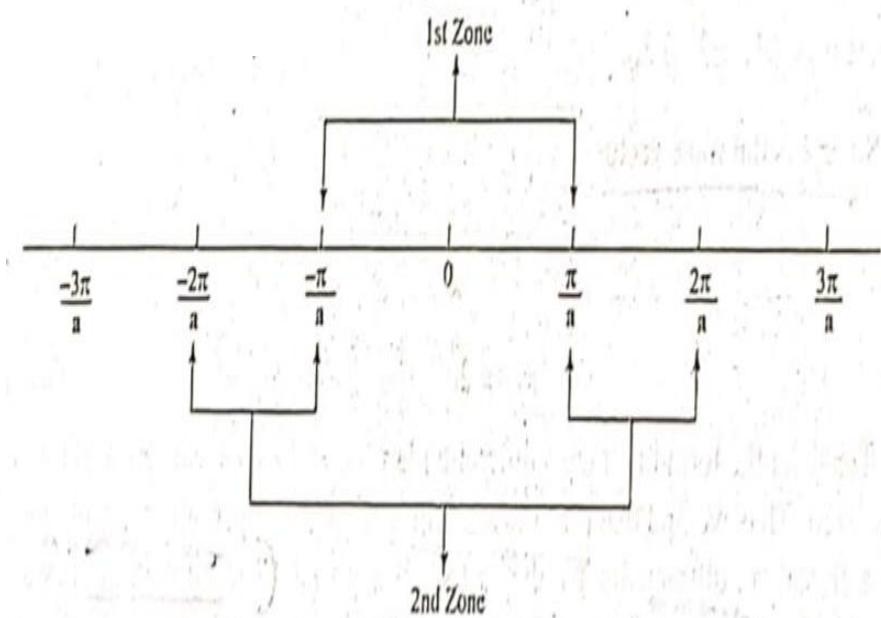
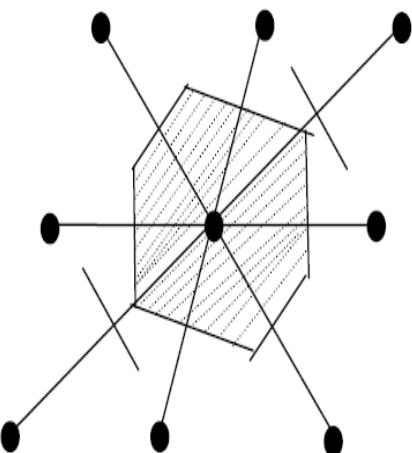
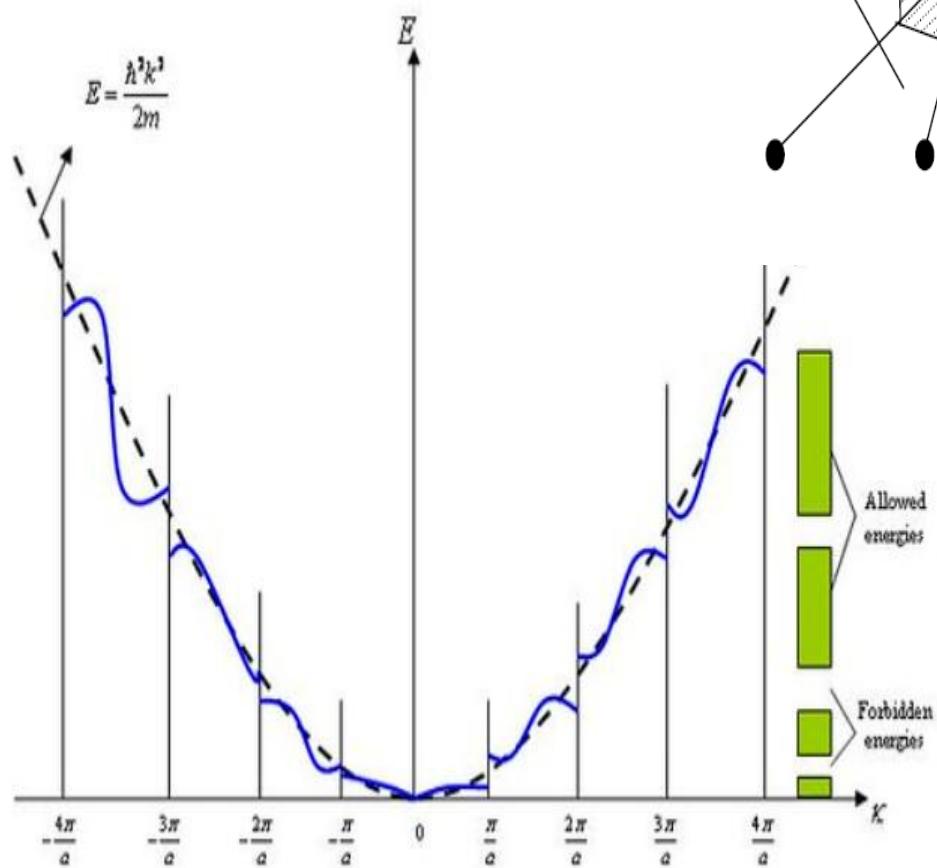


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The first three Brillouin Zones for a two dimensional square lattice.



Construction of a Wigner-Seitz cell in the reciprocal lattice (called first Brillouin zone):

- To construct the first Brillouin zone, we need to find the relation between the incident beam (like electron or neutron or phonon beam) of wave vector k and the reciprocal lattice vector G .
- This relation may be found as

$$\vec{k} \cdot \left(\frac{\vec{G}}{2}\right) = \left(\frac{G}{2}\right)^2$$

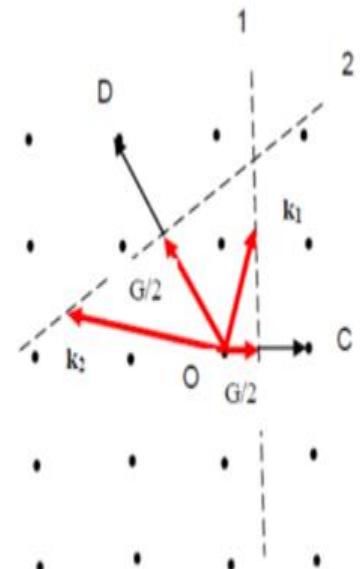
- For example, an x-ray beam in the crystal will be diffracted if its wave vector k has the magnitude and direction required by this relation.

Thus the procedure to build up the first Brillouin zone is as follows:

- i) Select a vector \mathbf{G} from the origin to a reciprocal lattice point.
- ii) Construct a plane normal to the vector \mathbf{G} at its mid point. This plane forms a part of the zone boundary.
- iii) The diffracted beam will be in the direction $\mathbf{k} - \mathbf{G}$.
- iv) Thus the Brillouin construction exhibits all the wave vectors \mathbf{k} which can be Bragg-reflected by the crystal.

Important note:

A wave whose wave vector drawn from the origin terminates on any of the planes will satisfy the condition of diffraction. Such planes are the perpendicular bisectors of the reciprocal vectors.



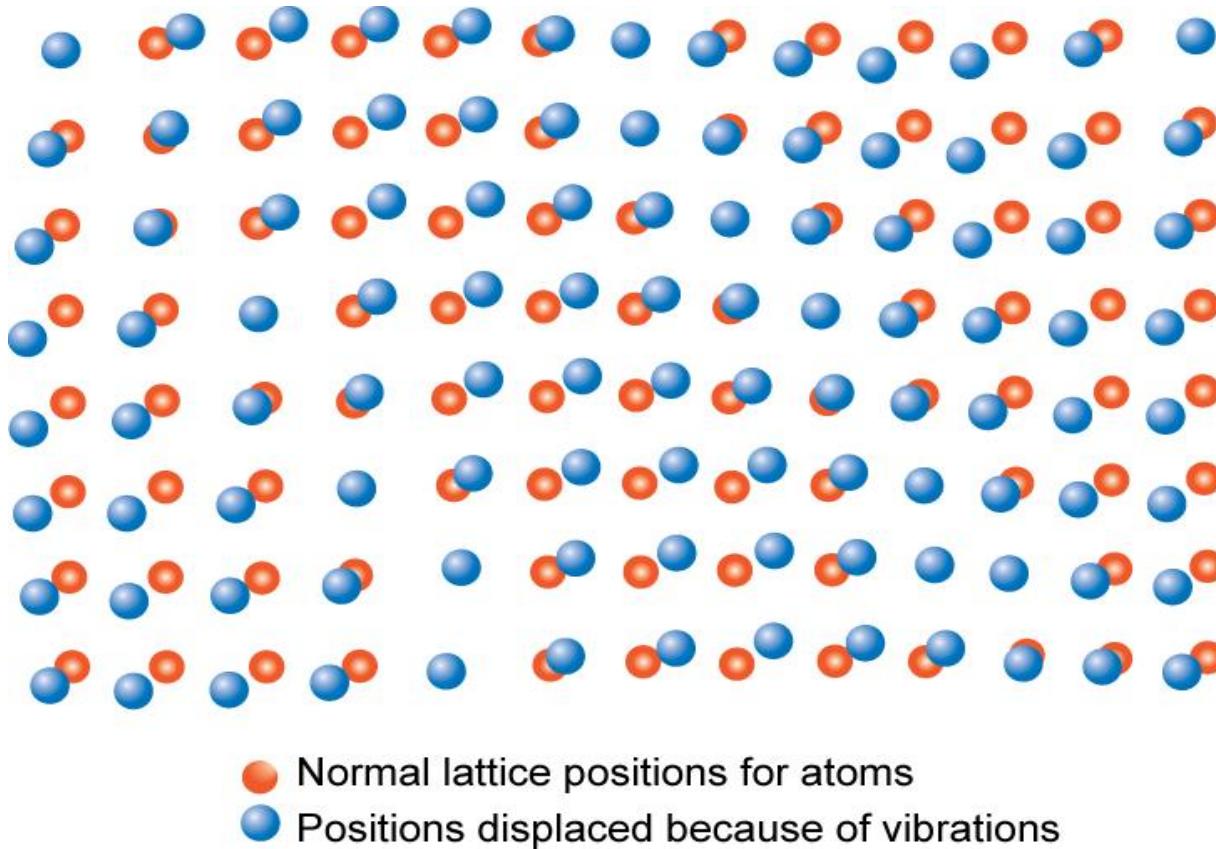
CONCEPT OF PHONONS



- Any solid crystal consists of atoms bound into a specific repeating three-dimensional spatial pattern called a lattice.
- Here the atoms behave as if they are connected by tiny springs, their own thermal energy or outside forces make the lattice vibrate.
- This generates mechanical waves that carry heat and sound through the material.
- *A packet of these waves can travel throughout the crystal with a definite energy and momentum, so in quantum mechanical terms the waves can be treated as a particle, called a phonon.*
- A phonon is a definite discrete unit or *quantum* of vibrational mechanical energy, just as a photon is a quantum of electromagnetic or light energy.

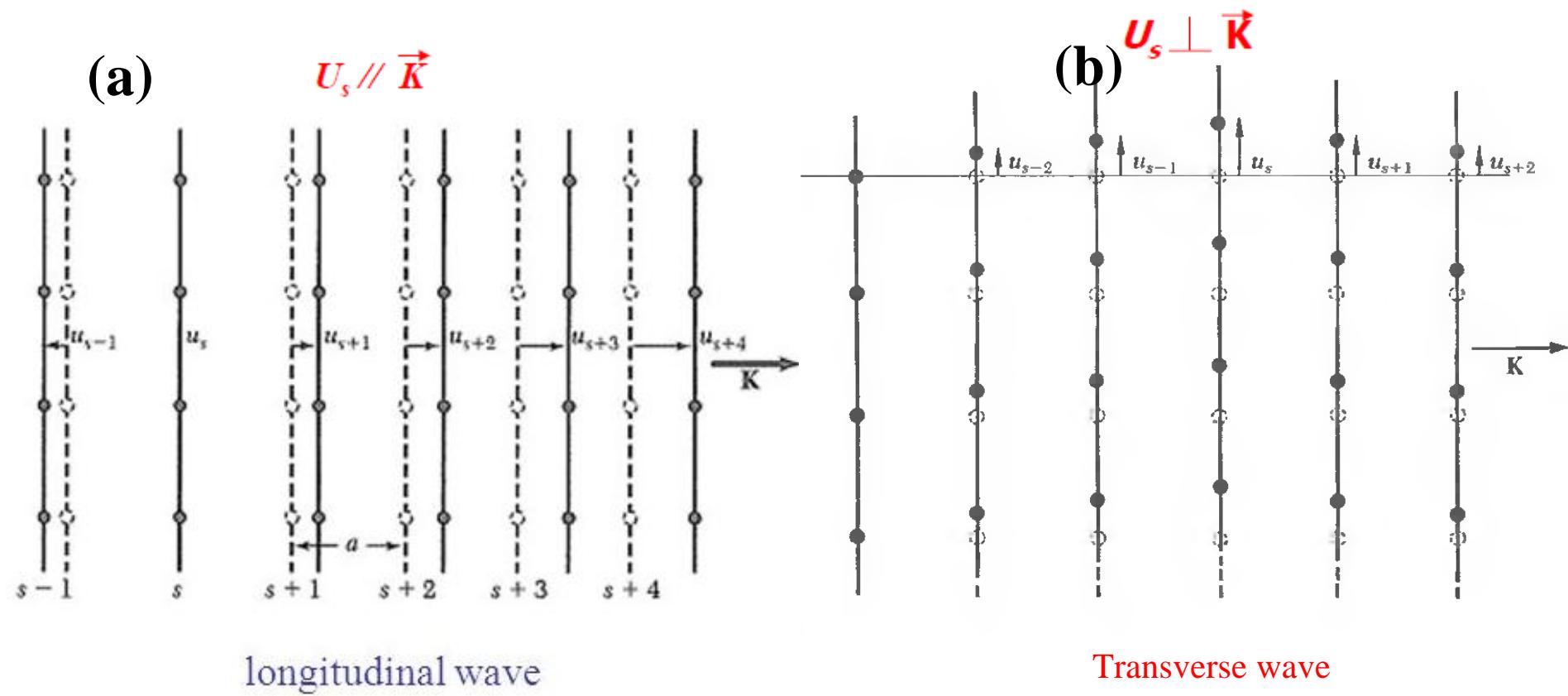
Atomic Vibrations

- Atomic vibrations are in the form of lattice waves or phonons.



- The energy of a lattice vibration is quantized
- The quantum of energy is called a phonon
- Analogous to photon-quantum of electromagnetic radiation

Vibrations of crystal with monatomic basis



Schematic illustration of displacements of planes along one spatial direction.

Phonon:

- ❖ A photon is the smallest unit of light. Similarly, for sound, the smallest unit is called phonon. In a lattice structure, vibrations are created by atoms. The quantized, lowest state energy of vibration is called phonon.
- ❖ Atoms were considered as rigid, with atoms stuck in their lattice. In reality, atoms can be considered as simple harmonic oscillators. The harmonic oscillator has a ground state energy and an associated vibrational mode even at 0 K.
- ❖ It is named phonons because at high energy levels long wavelength phonons give rise to sound. According to quantum mechanics, similar particles have wave nature, waves must also have particle nature. So, phonon is also treated as quasi particle. Similar to particles, these waves can carry throughout the crystal, heat, energy and momentum.

- ❖ In solid state physics, the elementary particles are electrons and phonons. The arrangement of the electrons will help determine material's electrical properties whereas the speed of sound through material and heat required to change its temperature is given by phonons.
- ❖ Another important application of phonons is in the field of superconductivity, where the electrical resistance of certain materials become zero near absolute zero. In ordinary crystals, there is a loss of energy as heat as the electrons collide with impurities. But in superconductors, at low temperatures, they tend to attract slightly because of phonons. Now the movement occur as a coherent group thus minimizing energy loss.
- ❖ Phonons also have important application in detectors like Cryogenic Dark Matter Search, which aim to detect even the slightest vibration in a crystal lattice caused by even a single phonon.



Comparison between Phonons and Photons

PHONONS

- Quantized normal modes of lattice vibrations. The energies & momenta of phonons are quantized

$$E_{phonon} = \frac{h\nu_s}{\lambda}$$

$$p_{phonon} = \frac{h}{\lambda}$$

Phonon wavelength:

$$\lambda_{phonon} \approx a_0 \approx 10^{-10} \text{ m}$$

PHOTONS

- Quantized normal modes of electromagnetic waves. The energies & momenta of photons are quantized

$$E_{photon} = \frac{hc}{\lambda}$$

$$p_{photon} = \frac{h}{\lambda}$$

Photon wavelength (visible):

$$\lambda_{photon} \approx 10^{-6} \text{ m}$$



This statistics applicable to the identical, indistinguishable particles of half spin.

These particles obey Pauli's exclusion principle and are called fermions (e.g.) Electrons, protons, neutrons,

In such system of particles, not more than one particle can be in one quantum state.

Fermi Dirac Distribution Law is

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

Fermi Energy



Fermi Energy (E_F)

Fermi Energy is the energy of the state at which the probability of electron occupation is $\frac{1}{2}$ at any temperature above 0 K.

It is also the maximum kinetic energy that a free electron can have at 0 K.

The energy of the highest occupied level at absolute zero temperature is called the *Fermi Energy or Fermi Level*.

Fermi Energy



The Fermi energy at 0 K for metals is given by

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

When temperature increases, the Fermi level or Fermi energy also slightly decreases.

The Fermi energy at non-zero temperatures,

$$E_F = E_{F_0} \left[1 - \frac{\pi^2}{12} \left(\frac{kT}{E_{F_0}} \right)^2 \right]$$

Here the subscript ‘0’ refers to the quantities at zero kelvin



The free electron gas in a solid obeys Fermi-Dirac statistics.

Suppose in an assemblage of fermions, there are $M(E)$ allowed quantum states in an energy range between E and $E+dE$ and $N(E)$ is the number of particles in the same range.

The Fermi-Dirac distribution function is defined as,

$$\frac{N(E)}{M(E)} = \frac{1}{1 + \exp((E - E_F)/kT)}$$

$N(E) / M(E)$ is the fraction of the possible quantum states which are occupied.



The distribution of electrons among the levels is described by function $f(E)$, *probability of an electron occupying an energy level ' E '.*

If the level is certainly empty, then $f(E) = 0$. Generally the $f(E)$ has a value in between zero and unity.

When $E < E_F$ (i.e.,) for energy levels lying below E_F , $(E - E_F)$ is a negative quantity and hence,

$$f(E) = \frac{1}{1 + e^{-\infty}} = \frac{1}{1 + 0} = 1$$

That means all the levels below E_F are occupied by the electrons.



When $E > E_F$ (i.e.) for energy levels lying above E_F , $(E - E_F)$ is a positive quantity

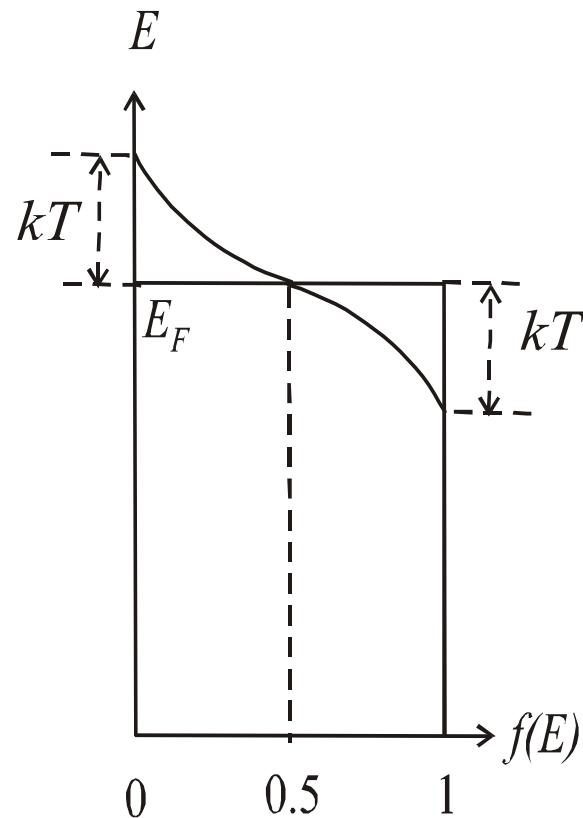
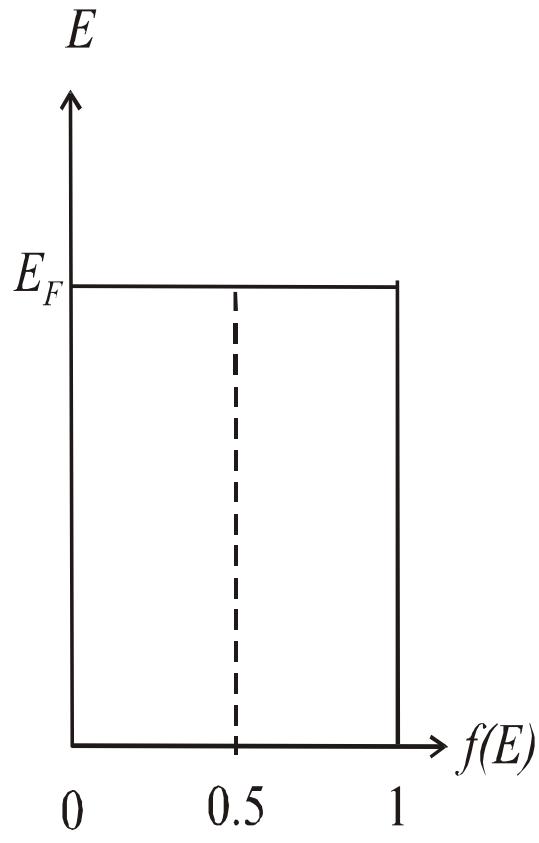
$$f(E) = \frac{1}{1 + e^{\infty}} = \frac{1}{1 + \infty} = 0$$

This equation indicates all the levels above E_F are vacant.

At absolute zero, all levels below E_F are completely filled and all levels above E_F are completely empty.

This level, which divides the filled and vacant states, is known as the Fermi energy level.

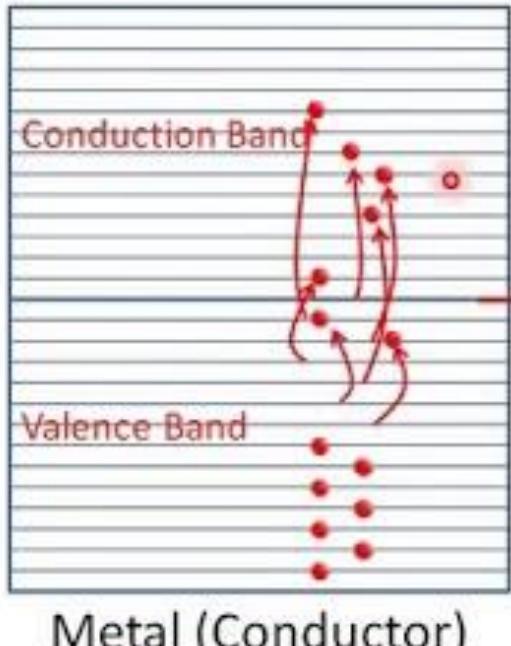
Fermi-Dirac Distribution Function $f(E)$



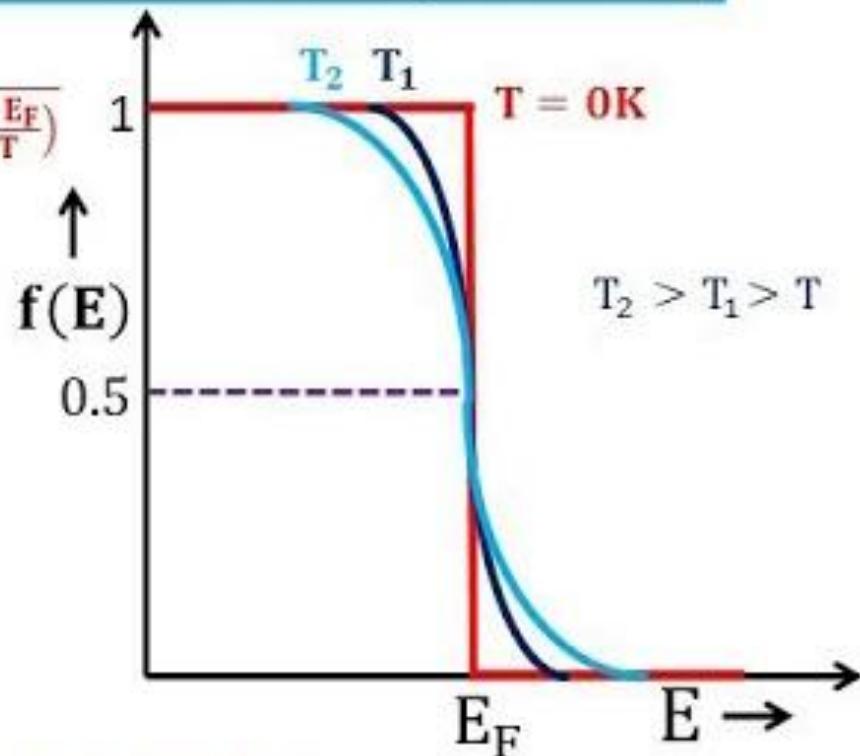
Fermi Dirac distribution function at different temperatures



Fermi-Dirac Distribution Function at various temperatures



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





When $E = E_F$,

$$f(E) = \frac{1}{1 + e^0} = \frac{1}{1+1} = \frac{1}{2} \quad \text{at all temperatures}$$

The probability of finding an electron with energy equal to the Fermi energy in a metal is $\frac{1}{2}$ at any temperature.

At $T = 0$ K all the energy level upto E_F are occupied and all the energy levels above E_F are empty .

When $T > 0$ K, some levels above E_F are partially filled while some levels below E_F are partially empty.



Classification of electronic materials

Conductors

Semiconductors

Insulators

Superconductor

Conductors

Conductors are substances which have free electrons, which can move under the action of an electric field. The electrons are free in the sense that they belong to the crystal as a whole and not tied down (bound) to a particular atom or a molecule.

Example : copper , silver etc.



Semiconductors

Semiconductors are materials which have the conductivity between conductors and insulators. Semiconductors are the elements of group-III, group-IV and group-V.

At normal temperature the conductivity of semiconductor is very low. With increase in temperature the conductivity of semiconductors increases exponentially.

Example: Germanium (Ge), Silicon (Si), Gallium Arsenide (GaAs) etc.

Insulators

Insulators are very poor conductor of electricity. The forbidden gap value is $3eV$

Example: wood, oil, mica.

Classification of materials

Conduction Band

Valence Band

Conduction Band

Valence Band

Conductors

- Overlapping of bands
- Fermi energy level lies in valance band
- Ex: Ag, Cu, Au...

Semiconductors

- Lower energy gap between the bands
- Fermi energy level lies at middle of the two bands
- Ex: Si, Ge etc...

Conduction Band

E_g

E_f

E_f

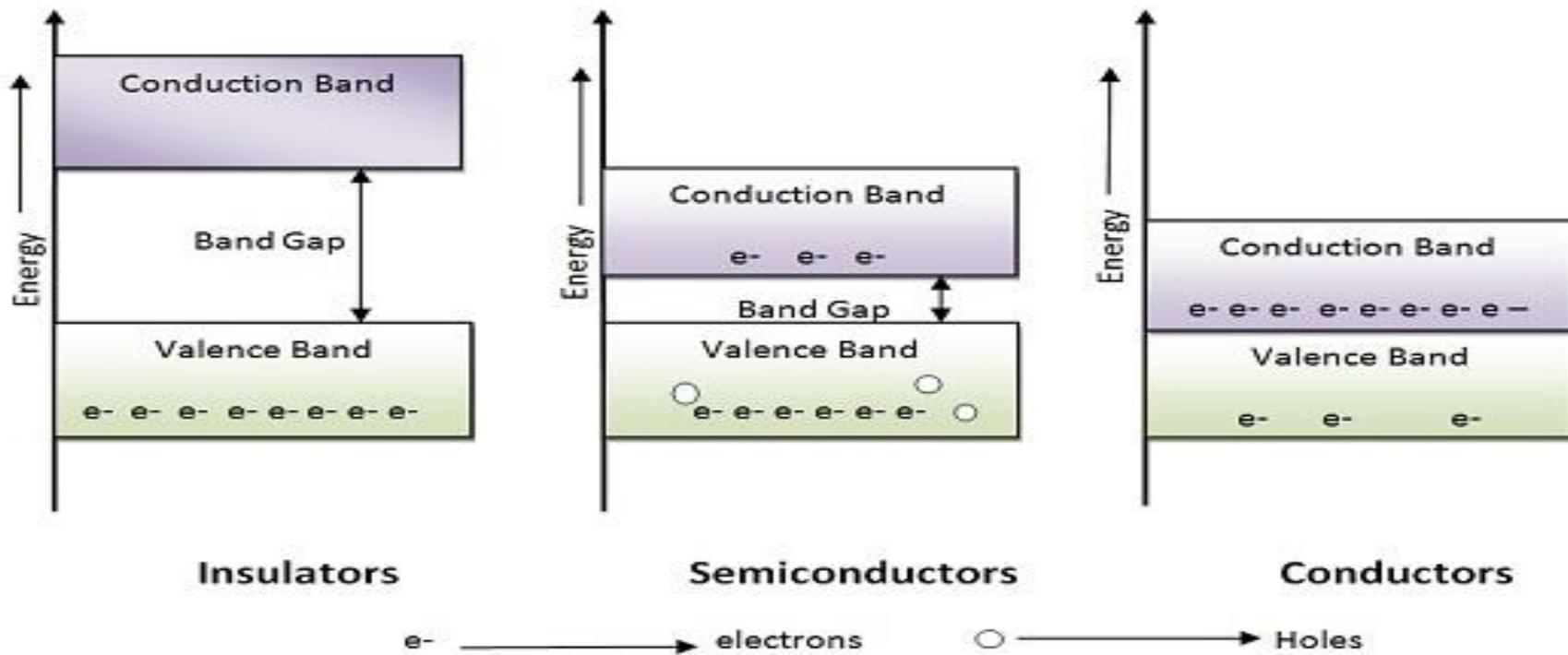
Valence Band

Insulators

- Large energy gap between the bands
- Fermi energy level lies at middle of the two bands
- Ex: Plastic, Paper...



Classification Of Electronic Materials





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18PYB103J –Semiconductor Physics

SOLVING PROBLEMS

1. The electrical resistivity of copper at 27°C is $1.72 \times 10^{-8} \text{ Ohm m}$. Compute its thermal conductivity if the Lorentz number is $2.26 \times 10^{-8} \text{ W Ohm K}^{-2}$

$$\text{Given } (\rho) = 1.72 \times 10^{-8} \text{ Ohm m}$$

$$T = 27^\circ\text{C} \Rightarrow 273 + 27 = 300 \text{ K}$$

$$L = 2.26 \times 10^{-8} \text{ W Ohm K}^{-2}$$

According to Wiedemann - Franz law using classical free electron theory

$$\frac{k}{\sigma} = LT$$

$$(\text{or}) \quad k = \sigma LT$$

$$k = \frac{LT}{\rho} \quad [\because \sigma = \frac{1}{\rho}]$$

$$\text{Therefore thermal Conductivity } k = \frac{2.26 \times 10^{-8} \times 300}{1.72 \times 10^{-8}}$$

$$k = 394.18 \text{ W m}^{-1} \text{ K}^{-1}$$

2. Calculate the drift velocity of electrons in copper and current density in wire of diameter 0.16 cm which carries a steady current of 10 A. Given $n = 8.46 \times 10^{28} \text{ m}^{-3}$.

Solution:

Given:

$$\begin{aligned}\text{Diameter of the wire } d &= 0.16 \text{ cm} \\ \text{Current flowing} &= 10 \text{ A}\end{aligned}$$

$$\begin{aligned}\text{Current density } J &= \frac{\text{Current}}{\text{Area of cross section (A}^2\text{)}} \\ &= \frac{10}{\pi r^2} = \frac{10}{\pi(d/2)^2} \quad \left[\because r = \frac{d}{2} \right] \\ &= \frac{10}{3.14 \times [0.16 \times 10^{-2}/2]^2} \\ J &= 4.976 \times 10^6 \text{ Am}^{-2} \\ J &= neV_d \\ V_d &= \frac{J}{ne} \\ &= \frac{4.97 \times 10^6}{8.46 \times 10^{28} \times 1.6 \times 10^{-19}} \\ \text{Drift velocity } V_d &= 3.67 \times 10^{-4} \text{ m s}^{-1}\end{aligned}$$

3. Find the lowest energy of an electron confined in one dimensional potential box separated by distance 0.1 nm.

Given $\lambda = 0.1 \text{ nm} \Rightarrow$ we know $\hbar = 6.62 \times 10^{-34}$

We know Energy of electron in 1-D Box is

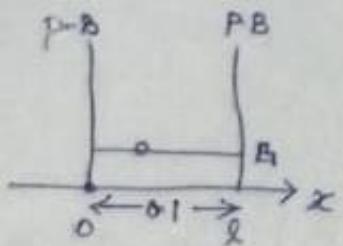
$$E_n = \frac{n^2 \hbar^2}{8 m l^2}$$

To find, Lowest energy of an electron ($n=1$)

$$E_1 = \frac{(1)^2 \times (6.62 \times 10^{-34})^2}{8 \times (9.1 \times 10^{-31}) \times (0.1 \times 10^{-9})^2}$$

$$E_1 = \frac{4.38244 \times 10^{-67}}{7.28 \times 10^{-31} \times 10^{-18}} = \frac{4.38244 \times 10^{-67}}{7.28 \times 10^{-49}}$$

$$E_1 = 6.0198 \times 10^{-19} \text{ J}$$





4. An electron is bound in one dimensional infinite well of width $1 \times 10^{-10}\text{m}$. Find the energy value in the ground state, first and second excited states.

We know $E_n = \frac{\hbar^2 n^2}{8m\ell^2}$

To find lowest energy of an electron ($n=1$)

$$E_1 = \frac{(1)^2 \times (6.62 \times 10^{-34})^2}{8 \times (9.1 \times 10^{-31}) \times (1 \times 10^{-10})^2}$$

$$E_1 = 0.6031 \times 10^{-17} \text{ J}$$

$$\begin{aligned} \text{Energy of first excited state} &= 4 \times 0.6031 \times 10^{-17} \\ &= 2.412 \times 10^{-17} \text{ J} \end{aligned}$$

$$\begin{aligned} \text{Energy of second excited state} &= 9 \times 0.6031 \times 10^{-17} \\ &= 5.428 \times 10^{-17} \text{ J} \end{aligned}$$

5. Find the least energy of an electron moving in one-dimensional potential box (infinite height) of width 0.05nm.

$$E_n = \frac{n^2 h^2}{8mL^2} \quad L = 0.05 \text{ nm} = 0.05 \times 10^{-9} \text{ m}$$

$$E_1 = \frac{h^2}{8mL^2} = \frac{(6.63 \times 10^{-34})^2}{8 \times 9.1 \times 10^{-31} \times 0.5 \times 10^{-10} \times 0.5 \times 10^{-10}} \text{ J}$$

$$= \frac{6.63 \times 6.63}{8 \times 9.1 \times 0.25} \times 10^{-17} \text{ J} = 2.4 \times 10^{-17} \text{ J}$$

$$= \frac{2.4 \times 10^{-17}}{1.6 \times 10^{-19}} = 150.95 \text{ eV}$$



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Numericals Based on Fermi Level and Fermi Distribution Function

Evaluate the Fermi function for energy $K_B T$ above the Fermi energy.

Solution:

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

We know Fermi Function $F(E) = \frac{1}{1 + e^{(E-E_F)K_B T}}$

For an energy $K_B T$ above Fermi energy

$$E - E_F = K_B T$$

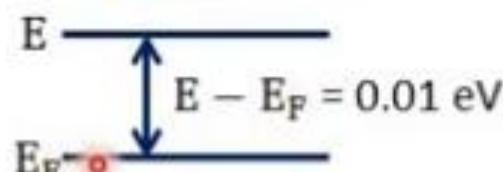
$$F(E) = \frac{1}{1 + e^1} = \frac{1}{1 + 2.7183}$$

Fermi distribution function $F(E) = 0.2689$

Calculate probability of non-occupancy for the energy level which lies 0.01 eV above the Fermi energy level at 27 °C.

Given : $T = 27 \text{ } ^\circ\text{C} = 300 \text{ } ^\circ\text{K}$, $k = 8.625 \times 10^{-5} \frac{\text{eV}}{\text{°K}}$

$$\text{Probability of occupancy } f(E) = \frac{1}{1 + e^{\left(\frac{E - E_F}{kT}\right)}}$$



$$\therefore \text{Probability of non-occupancy} = 1 - f(E) = 1 - \frac{1}{1 + e^{\left(\frac{E - E_F}{kT}\right)}}$$

$$= 1 - \frac{1}{1 + e^{\left(\frac{0.01}{8.625 \times 10^{-5} \times 300}\right)}}$$

$$= 0.595$$

3. (a) If $E_F = E_c$, find the probability of a state being occupied at $E = E_c + kT$
- (b) If $E_F = E_v$, find the probability of a state being empty at $E = E_v - kT$

Ans. (a) $f_F(E) = \frac{1}{1+\exp\left[\frac{E-E_F}{kT}\right]} = \frac{1}{1+\exp\left[\frac{E_c + kT - E_c}{kT}\right]} = \frac{1}{1+\exp[1]} = 0.269$

(b) $1 - f_F(E) = 1 - \frac{1}{1+\exp\left[\frac{E-E_F}{kT}\right]} = 1 - \frac{1}{1+\exp\left[\frac{E_v - kT - E_v}{kT}\right]} = 1 - \frac{1}{1+\exp[-1]} = 0.269$



4. Use the Fermi distribution function to obtain the value of $F(E)$ for $E - E_F = 0.01 \text{ eV}$ at 200K.

Given data:

$$\text{Fermi Function} \quad F(E) = \frac{1}{1 + e^{(E-E_F)/K_B T}}$$

$$\text{Boltzmann constant} \quad K_B = 1.38 \times 10^{-23} \text{ JK}^{-1}$$

$$E - E_F = 0.01 \text{ eV} = 0.01 \times 1.6 \times 10^{-19} = 1.6 \times 10^{-21} \text{ J}$$

$$T = 200 \text{ K}$$

$$F(E) = \frac{1}{1 + e^{1.6 \times 10^{-21} / (1.38 \times 10^{-23} \times 200)}}$$

$$= \frac{1}{1 + e^{0.5797}}$$

$$= \frac{1}{1 + 1.7855} = \frac{1}{2.7855}$$

Fermi function

$$F(E) = 0.3589$$

5. Calculate the probabilities for an electronic state to be occupied at 20°C, if the energy of these states lies 0.11 eV above and 0.11 eV below the fermi level.

Solution:- Probability of occupying an energy level E,

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

Probability of occupying an energy level 0.11eV above Fermi level

$$f(E) = \frac{1}{1 + e^{0.11eV/kT}} = \frac{1}{1 + e^{4.2307}} = 0.0126$$

Probability of occupying an energy level 0.11eV below Fermi level

$$f(E) = \frac{1}{1 + e^{-0.11eV/kT}} = \frac{1}{1 + e^{-4.2307}} = 0.987$$