

21PYB102J – Semiconductor Physics and Computational Methods

Unit – 1 : Session – 1 : SLO - 1

Free Electron Theory

- The 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

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.

The Quantum free electron 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.

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 and hence It is called as Band theory

Classical free electron theory of metals

This theory was developed by Drude and Lorentz in 1900 and hence is also known as Drude-Lorentz theory.

it's the first theory to explain the electrical conduction in conducting materials and reveals that free electrons are responsible for the electrical conduction.

According to this theory, a metal consists of electrons which are free to move about in the crystal like molecules of a gas in a container.

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.

Mutual repulsion between electrons is ignored and hence potential energy is taken as zero.

Therefore the total energy of the electron is equal to its kinetic energy.

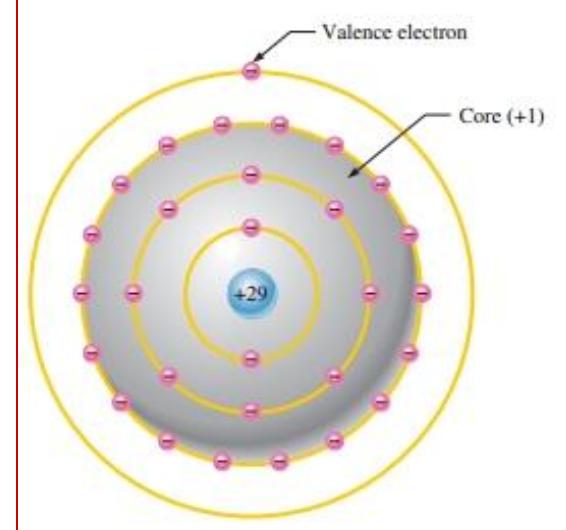
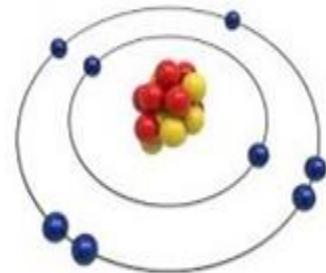
Assumptions

- Electrons travel with constant potential and confine to the boundaries of metal
- All the attractive and repulsive forces are neglected
- The energies of free electrons are not quantized
- The distribution of electrons is as per the Hund's rule and follows Pauli's exclusion principle

Postulates :

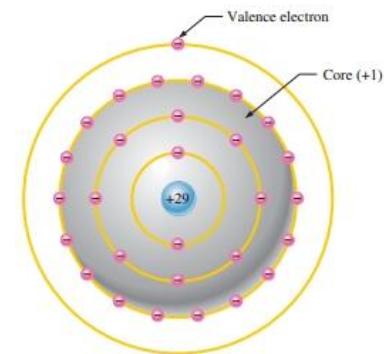
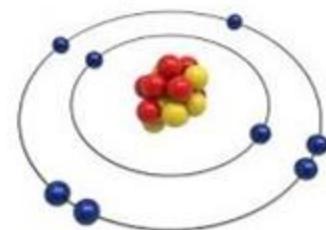
- (a) In an atom electrons revolve around the nucleus and a metal is composed of such atoms.
- (b). The valence electrons of atoms are free to move about the whole volume of the metals like the molecules of a perfect gas in a container. The collection of valence electrons from all the atoms in a given piece of metal forms electrons gas. It is free to move throughout the volume of the metal
- (c) These free electrons move in random directions and collide with either positive ions fixed to the lattice or other free electrons. All the collisions are elastic i.e., there is no loss of energy.

Assumptions of Classical Free Electron Theory



- (d). The movements of free electrons obey the laws of the classical kinetic theory of gases.
- (e). The *electron velocities in a metal obey the classical Maxwell – Boltzmann distribution of velocities.*
- (f). The electrons move in a completely uniform potential field due to ions fixed in the lattice.
- (g). When an electric field is applied to the metal, the free electrons are accelerated in the direction opposite to the direction of applied electric field.

Assumptions of Classical Free Electron Theory



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:

The phenomena such a photoelectric effect, Compton effect and the black body radiation couldn't be explained by classical free electron theory.

According to the classical free electron theory the value of specific heat of gas at constant volume is given by $3/2 R$, where R is universal gas constant, but experimentally it was observed that the specific heat of a metal by its conduction electron is given by $10^{-4} RT$.

Thus, the experimental value of C_v is very much lesser than the expected value of C_v . According to classical free electron theory C_v is independent of temperature, but the experimental value of C_v is directly proportional to temperature. Hence classical free electron theory fails to explain C_v .

Electrical conductivity of semiconductor or insulators couldn't be explained using this model.

Though $K/\sigma T$ is a constant (Wiedemann – Franz Law) according to the Classical free electron theory, it is not a constant at low temperature.

Ferromagnetism couldn't be explained by this theory. The theoretical value of paramagnetic susceptibility is greater than the experimental value.

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Unit – 1 : Session – 1 : SLO - 2

Quantum free electron theory

Classical free electron theory could not explain many physical properties. To overcome the drawbacks of Classical free electron theory, 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.

The following are the assumptions of quantum free electron theory:

- The free electrons in a metal can have only discrete energy values. Thus the energies are quantized.
- The electrons obey Pauli's Exclusion Principle, which states that there cannot be more than two electrons in any energy level.
- The distribution of electrons in various energy levels obey the Fermi-Dirac quantum statistics.
- Free electrons have the same potential energy everywhere within the metal, because the potential due to ionic cores is uniform throughout the metal.
- The force of attraction between electrons & lattice ions and the force of repulsion between electrons can be neglected.
- Electrons are treated as wave-like particles

Merits of quantum free electron theory

1. It successfully explains the electrical and thermal conductivity of metals.
2. We 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.

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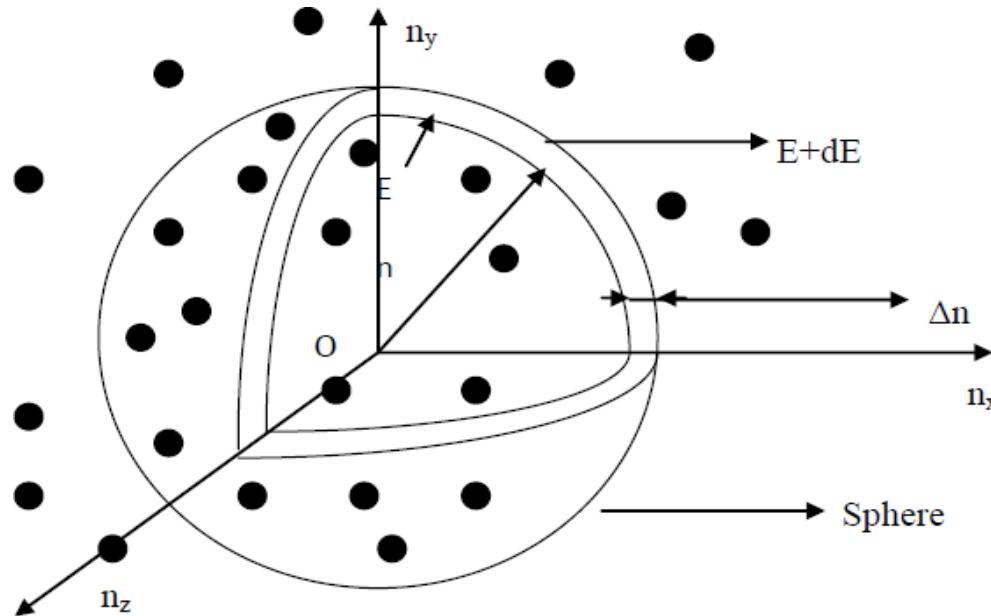
Unit – I: Session – 2: SLO - 1



Quantum Free Electron Theory – Density of States in 3D

DENSITY OF STATES

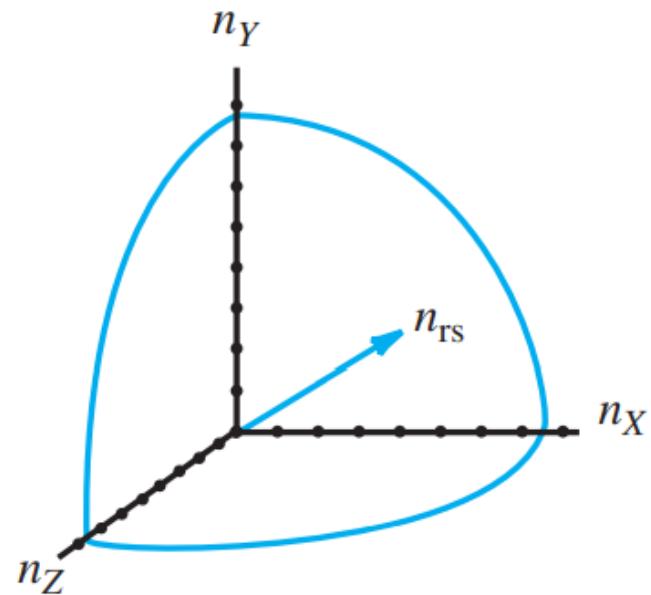
Definition: Density of States $Z(E) dE$ is defined as the number of available electron states per unit volume in an energy interval (dE).



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.

Expression for Density of States in 3D (1)

Consider a three-dimensional space with axes n_x , n_y and n_z . Each point in this space represents a quantum state of a particle trapped in a 3D box. In this space, the volume of a shell of some arbitrary radius n and thickness dn is given by difference between volumes of a sphere of radius n and $n + dn$.



$$dV = \frac{4\pi}{3} \{(n + dn)^3 - n^3\}$$

$$dV = \frac{4\pi}{3} \{n^3 + 3n^2dn + 3n(dn)^2 + (dn)^3 - n^3\}$$

Expression for Density of States in 3D (2)

Ignoring higher powers of dn , we get

$$dV = 4\pi n^2 dn$$

Considering only one octant of the sphere, the volume of the shell is

$$dV = \frac{1}{8} (4\pi n^2 dn)$$

Since the volume of each quantum state is one unit in the n space, the number of points (quantum states) dN in this volume is

$$dN = \frac{1}{8} (4\pi n^2 dn)$$

Expression for Density of States in 3D (3)

In each state, two electrons (one with spin up and other with spin down) can be accommodated. So total number of states (points) in the shell is

$$dN = 2 \left(\frac{1}{8} \right) (4\pi n^2 dn) = \pi n^2 dn$$
$$dN = \pi n(ndn)$$

Now consider the expression for energy of a particle trapped in a 3D box.

$$E = \frac{n^2 \pi^2 \hbar^2}{2mL^2}$$

If we take derivative on both sides of the energy equation keeping n as a variable,

$$dE = 2ndn \left(\frac{\pi^2 \hbar^2}{2mL^2} \right)$$

$$ndn = \left(\frac{mL^2}{\pi^2 \hbar^2} \right) dE$$

Expression for Density of States in 3D (4)

Taking square root of energy equation on both sides,

$$\sqrt{E} = n \left(\frac{\pi^2 \hbar^2}{2mL^2} \right)^{1/2}$$

Rearranging the above equation,

$$n = \left(\frac{2mL^2}{\pi^2 \hbar^2} \right)^{1/2} \sqrt{E}$$

Substituting expression for n and ndn in the expression for dN , we get

$$dN = \pi n(ndn)$$

$$dN = \pi \left(\frac{2mL^2}{\pi^2 \hbar^2} \right)^{1/2} \sqrt{E} \left(\frac{mL^2}{\pi^2 \hbar^2} \right) dE$$

Expression for Density of States in 3D (5)

$$g(E) = \frac{1}{V} \frac{dN}{dE} = \left(\frac{8\pi\sqrt{2}m^{3/2}}{h^3} \right) \sqrt{E}$$

The above is the expression for density of states. It gives the **number of electronic states available per unit volume in unit energy range**. The plot $g(E)$ of vs E is given below.



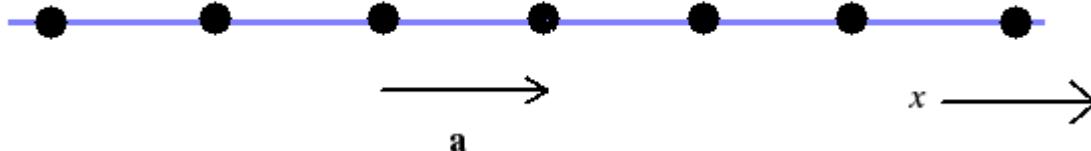
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Unit – I: Session – 2: SLO - 2



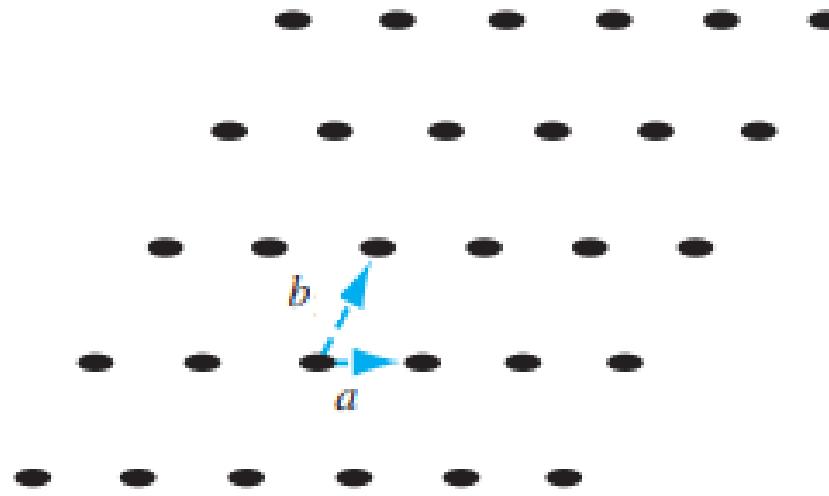
Band Theory of Solids - Lattice, Reciprocal Lattice, Concept of Energy Bands in Solids, Bloch Theorem

1D Lattice



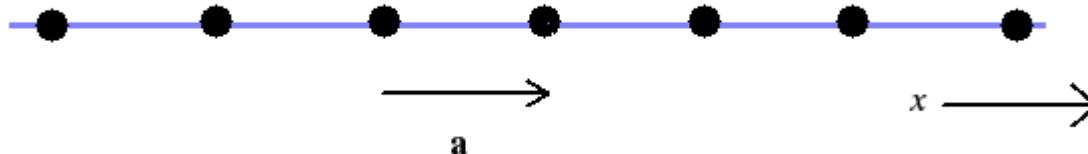
- Atoms (or ions) are arranged with equal spacing **a** called **lattice parameter**.

2D Lattice

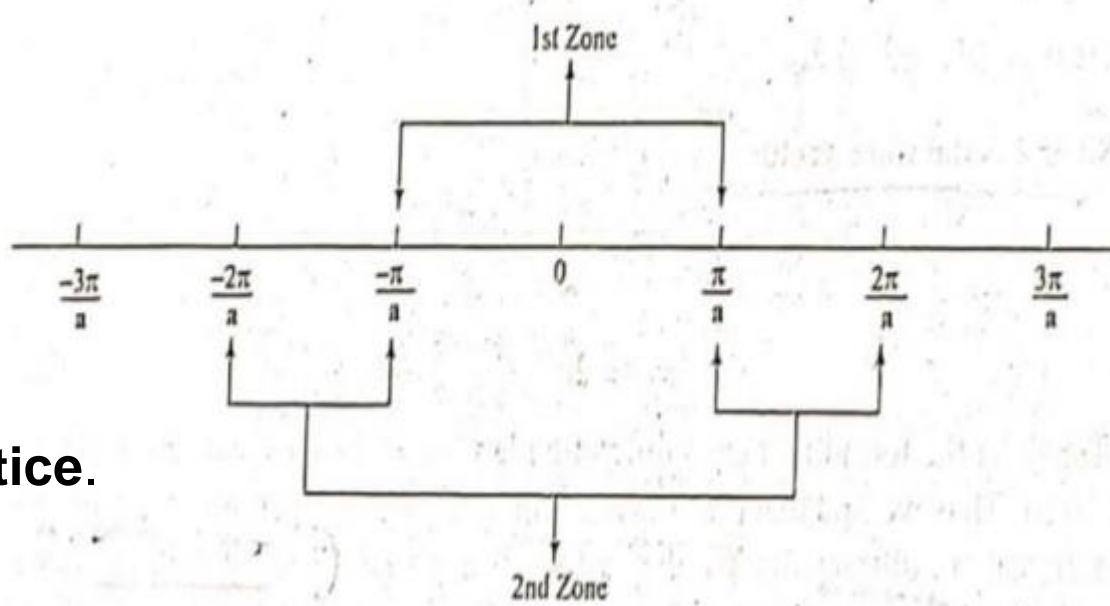


- Atoms (or ions) are periodically arranged in 2D space.
- Two lattice parameters \mathbf{a} and \mathbf{b} uniquely define the 2D lattice.

Reciprocal Lattice and Brillouin Zone in 1D

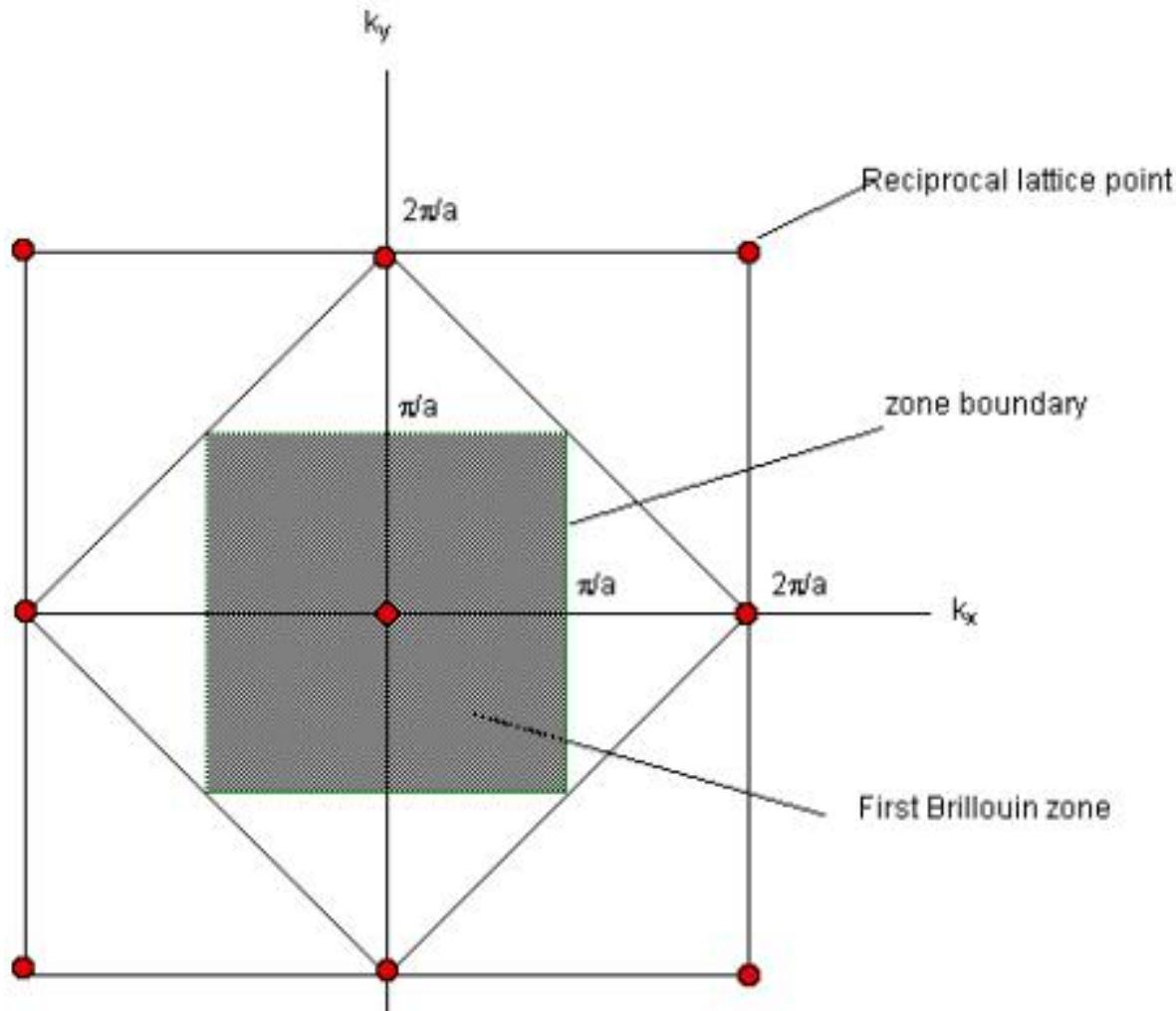


Direct lattice.



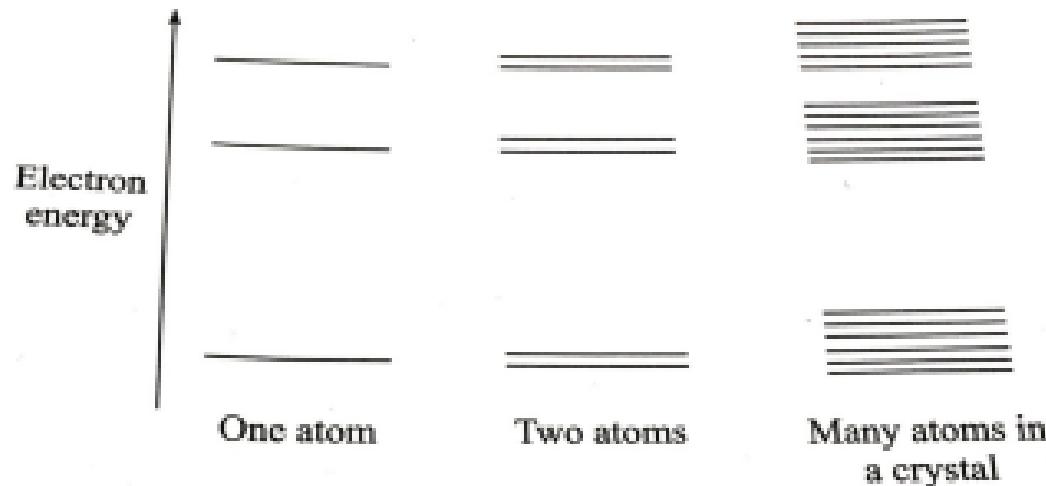
Reciprocal lattice.

Brillouin Zone in 2D



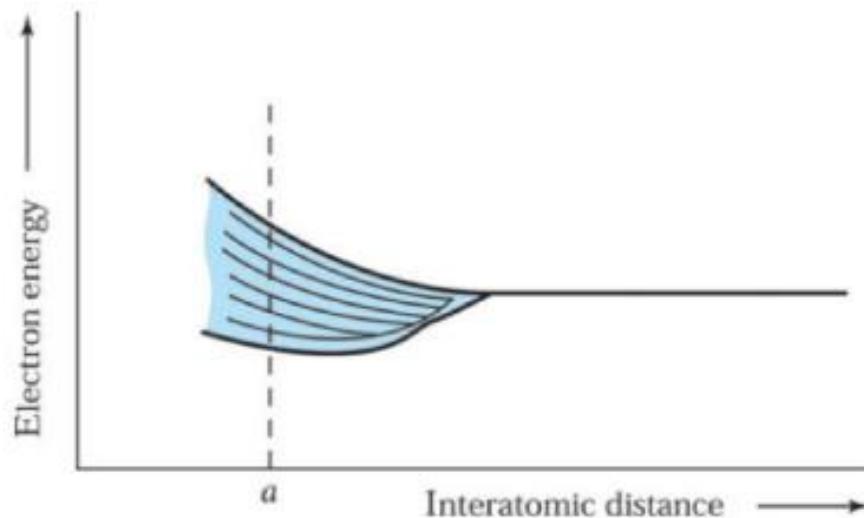
- Also called **Wigner-Seitz primitive cell** in the reciprocal lattice.

Concept of Energy Bands in Solids (1)



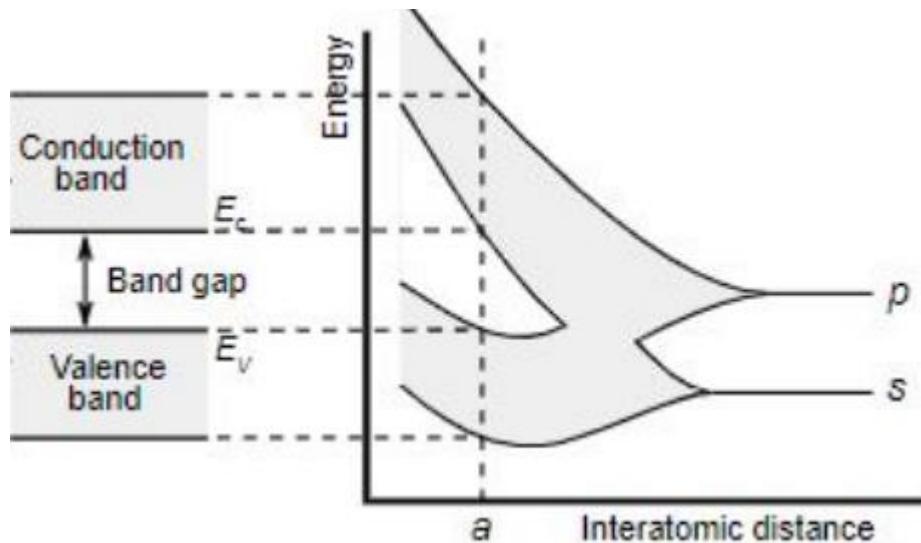
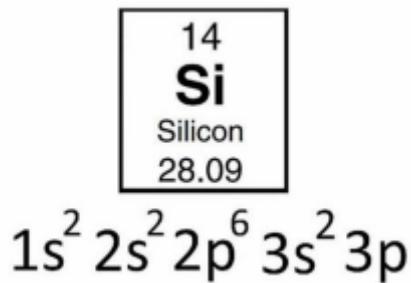
- When two identical atoms are far apart, the allowed energy levels for a given principal quantum number (for example $n = 1$) consist of one double degenerate level. That is, both atoms have exactly the same energy.
- When they are brought closer, the doubly degenerate energy levels will split into two levels by the interaction between atoms. This splitting occurs due to the Pauli's exclusion principle.

Concept of Energy Bands in Solids (2)



- As N isolated atoms are brought together to form a solid, it causes a shift in the energy levels of all N atoms, as in the case of two atoms.
- However, instead of two levels, N separate but closely spaced levels are formed. When N is very large, the result is essentially a continuous band of energy. This band of N levels can extend over a few eV at the inter-atomic distance of the crystal.

An Example: Energy Bands in Silicon



- When many Si atoms are brought together, the energy bands are formed in such a way it divides into two and in between there are no energy levels present. The gap between these bands are called **band gap**.
- The band lying below is called **valence band** owing to the presence of valence electrons which are tightly bound to the parent atoms. The band lying higher than the valence band is called **conduction band** which is responsible for conducting current in the material.

Band Theory of Solids

- Developed by **Felix Bloch** in 1928. (PhD thesis)
- **Free-electron approximation** is abandoned.
- Coulombic interaction between valence electrons and positively charged metal ions is included.
- **Independent-electron approximation** is retained.
- Explains band structure in solids.



Felix Bloch (1905 - 1983)
Nobel Prize in Physics, 1952

Bloch's Theorem

- A fundamental theorem in the quantum theory of crystalline solids.
- **Statement:** The wave function of an electron moving in a periodic 1D lattice is of the form

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

- $u(x)$ has the same periodicity as the lattice.

$$u(x + a) = u(x)$$

- **Alternate statement** of Bloch's theorem:

$$\psi(x + a) = e^{ika}\psi(x)$$



Band Theory of Solids - Kronig-Penney Model

de-Broglie's Wavelength:

A particle of mass 'm' moving with velocity 'c' possess energy given by

$$E = mc^2 \rightarrow (\text{Einstein's Equation}) \quad (1)$$

According to Planck's quantum theory the energy of quantum of frequency

'v' is

$$E = hv \rightarrow (2)$$

From (1) & (2)

$$mc^2 = hv = hc / \lambda \text{ since } v = c/\lambda$$

$$\lambda = hc / mc^2 = h/mc$$

$$\lambda = h/p$$

$$2\pi/k = h/p$$

$$p = (h/2\pi)k$$



Derivation of Time-Independent Schrodinger Equation

Schrodinger wave equation - (1926)

(12)

If particle exhibits wave property - some sort of wave equation associated with the particle describing the behaviour of wave nature in addition to particle nature.

It is mathematical equation derived by connecting de-Broglie wavelength into classical mechanical equation for moving particle.

This equation is applicable to both macro & microscopic particles.

(i) Schrodinger Time independent wave equation

$$\text{We know that total Energy of particle } (E) = k \cdot E + p \cdot E \\ E = \frac{p^2}{2m} + V$$

If momentum of particle is $p = mv$, we write $V = p/m$ then,

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

If ψ is wavefunction associated to particle we write

$$E\psi = \left[\frac{p^2}{2m} + V \right] \psi \rightarrow (1) \quad e^{i(kx-\omega t)}$$

$$\psi = e^{i(kx-\omega t)} \rightarrow (2)$$

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

$$\frac{\partial \psi}{\partial x} = ik \psi \quad (\text{using eq-2})$$

Again differentiate above eq. w.r.t. x

$$\frac{\partial^2 \psi}{\partial x^2} = i^2 k^2 \psi$$

$$\frac{\partial^2 \psi}{\partial x^2} = (-1) k^2 \psi \quad (\because i^2 = -1)$$

$$\frac{\partial^2 \psi}{\partial x^2} = -k^2 \psi \rightarrow (3)$$

In the above equation 'k' is called propagation constant is given by $k = 2\pi/\lambda$ where λ is de-Broglie wavelength ($\lambda = h/p$)

Then $k = \frac{2\pi p}{h}$, we know $h = \frac{p}{2\pi}$ then $k = \frac{p}{\hbar}$ $\rightarrow (4)$

$$\text{Sub (4) in (3) we get } \frac{\partial^2 \psi}{\partial x^2} = -\left(\frac{p^2}{\hbar^2}\right) \psi \rightarrow (5)$$

$$\text{If } p = mv \text{ then } p^2 = m^2 v^2$$

$$\text{Also } E = \frac{1}{2} mv^2 + V$$

$$2E = mv^2 + V$$

$$\times \text{ by } m \Rightarrow 2mE = m^2 v^2 + mV \\ 2m(E-V) = m^2 v^2 \rightarrow (6)$$

Sub (6) in eq (5) then

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

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

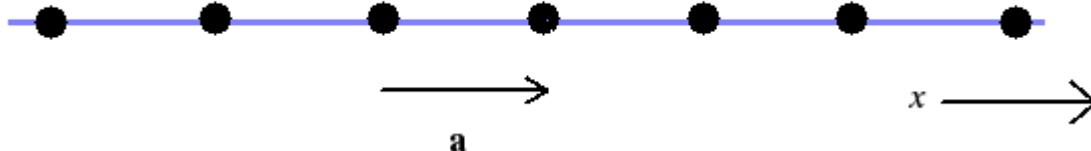
The above equation is called Schrodinger time independent wave equation



Time-Independent Schrodinger Wave Equation

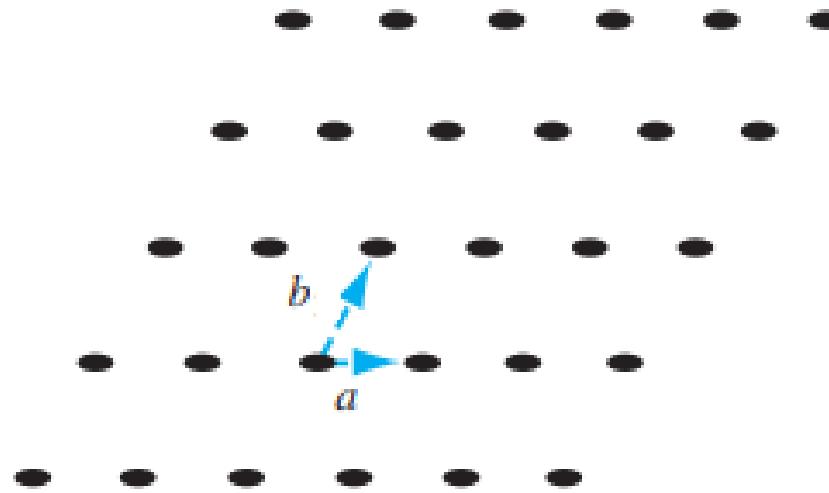
$$E\psi(x) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x) + V(x)\psi(x)$$

1D Lattice



- Atoms (or ions) are arranged with equal spacing **a** called **lattice parameter**.

2D Lattice



- Atoms (or ions) are periodically arranged in 2D space.
- Two lattice parameters \mathbf{a} and \mathbf{b} uniquely define the 2D lattice.

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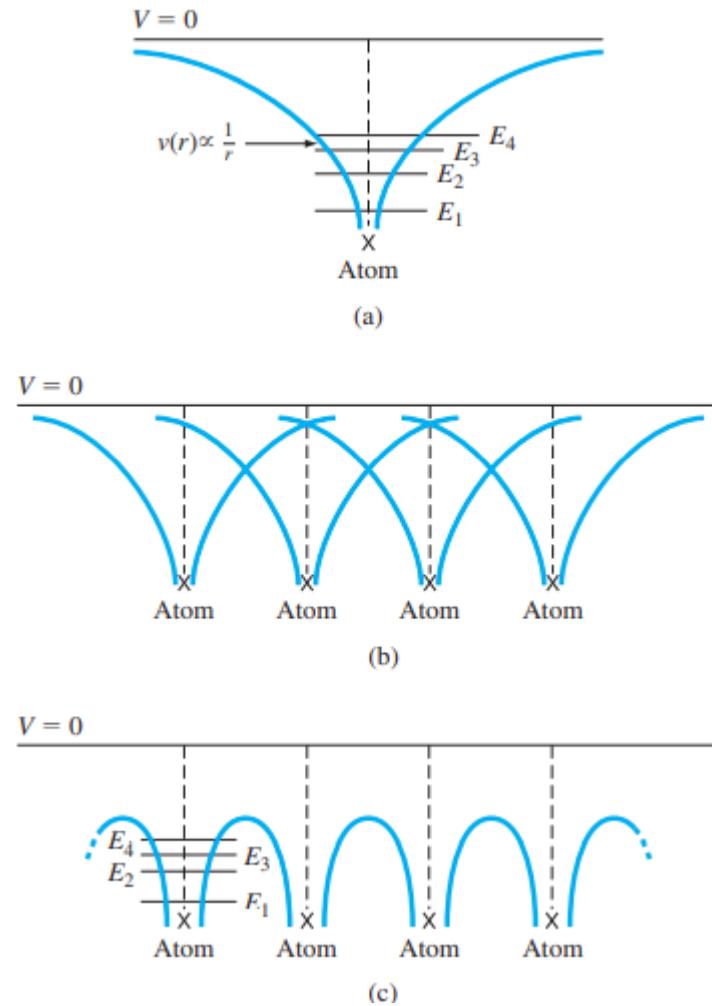
$$u(x + a) = u(x)$$

- **Alternate statement** of Bloch's theorem:

$$\psi(x + a) = e^{ika}\psi(x)$$

Periodic Ionic Potential in a 1D crystal

Figure 3.5 | (a) Potential function of a single isolated atom. (b) Overlapping potential functions of adjacent atoms. (c) Net potential function of a one-dimensional single crystal.



Kronig-Penney Model of Ionic Potential in a 1D crystal

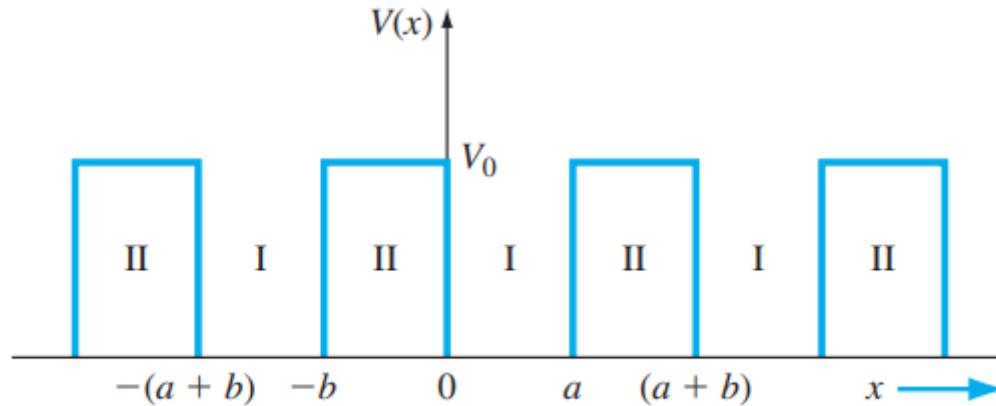


Figure 3.6 | The one-dimensional periodic potential function of the Kronig–Penney model.

- K-P model is an idealized periodic potential representing 1D crystalline solid.
- Schrodinger's equation needs to be solved in region I and II.
- Solution of Schrodinger's equation yields allowed values of energies of the electron in the 1D crystal.

Apply Schrodinger's time independent wave eq.
for the two regions

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

for $0 < x < a$ in diagram $V=0$ then

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} (E) \psi = 0 \rightarrow (1)$$

for $-b < x < 0$ in diagram $V=V_0$ then

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

$$\text{Put } \alpha^2 = \frac{2m}{\hbar^2} (E) \psi \text{ & } \beta^2 = \frac{2m}{\hbar^2} (V_0 - E) \psi \text{ then } (\because V_0 > E)$$

$$\frac{d^2\psi}{dx^2} + \alpha^2 \psi = 0 \rightarrow (3) \quad \& \quad \frac{d^2\psi}{dx^2} - \beta^2 \psi = 0 \rightarrow (4)$$

$$\text{According to zone theory we know } \psi = A_k(x) e^{ikx} \rightarrow (7)$$

Diff. eq (5) w.r.t. x

$$\frac{\partial \psi}{\partial x} = \frac{\partial}{\partial x} [U_k(x) e^{ikx}] \quad \left[\frac{\partial}{\partial x} \cdot UV \right]$$

$$\frac{\partial \psi}{\partial x} = -e^{ikx} \frac{\partial U_k}{\partial x} + U_k i k e^{ikx}$$

Again diff. w.r.t. x

$$\frac{\partial^2 \psi}{\partial x^2} = \left[e^{ikx} \frac{\partial^2 U_k}{\partial x^2} + \frac{\partial U_k}{\partial x} (i k e^{ikx}) \right] + i k \left[U_k i k e^{ikx} + e^{ikx} \frac{\partial U_k}{\partial x} \right]$$

$$\frac{\partial^2 \psi}{\partial x^2} = e^{ikx} \frac{\partial^2 U_k}{\partial x^2} + i k e^{ikx} \frac{\partial U_k}{\partial x} - k^2 U_k e^{ikx} + i k e^{ikx} \frac{\partial U_k}{\partial x} \quad (8)$$

Substituting (8) in (5)

$$e^{ikx} \frac{\partial^2 U_k}{\partial x^2} + i k e^{ikx} \frac{\partial U_k}{\partial x} - k^2 U_k e^{ikx} + i k e^{ikx} \frac{\partial U_k}{\partial x} + \alpha^2 e^{ikx} U_k = 0$$

÷ by e^{ikx}

$$\frac{\partial^2 U_k}{\partial x^2} + i k \frac{\partial U_k}{\partial x} - k^2 U_k + i k \frac{\partial U_k}{\partial x} + \alpha^2 U_k = 0$$

$$\frac{\partial^2 U_k}{\partial x^2} + 2 i k \frac{\partial U_k}{\partial x} + (\alpha^2 - k^2) U_k = 0 \rightarrow (9)$$

similarly for (8) in (6)

$$\frac{\partial^2 U_k}{\partial x^2} + 2 i k \frac{\partial U_k}{\partial x} - (\beta^2 + k^2) U_k = 0 \rightarrow (10)$$

Solutions for eq (7) & (8) is

$$U_1 = A e^{i(\alpha-k)x} + B e^{-i(\alpha+k)x} \rightarrow (11)$$

$$U_2 = C e^{i(\beta-k)x} + D e^{-i(\beta+k)x} \rightarrow (12)$$

Kronig-Penney Model in a 1D crystal

Properties of well-behaved wave functions

- ψ is continuous
- First derivative of ψ is also continuous

Kronig-Penney Model in a 1D crystal

Boundary conditions at $x = 0$:

$$(\psi \text{ is continuous}) \quad u_1(0) = u_2(0)$$

$$A + B - C - D = 0 \quad (1)$$

$$(\text{derivative of } \psi \text{ is continuous}) \quad \frac{du_1}{dx} \Big|_{x=0} = \frac{du_2}{dx} \Big|_{x=0}$$

$$Ai(\alpha - k) - Bi(\alpha + k) = C(\beta - ik) - D(\beta + ik) \quad (2)$$

Kronig-Penney Model in a 1D crystal

Periodic boundary conditions at $x = +a$ and $x = -b$:

$$(\psi \text{ is continuous}) \quad u_1(a) = u_2(-b)$$

$$Ae^{i(\alpha-k)a} + Be^{-i(\alpha+k)a} = Ce^{-(\beta-ik)b} + De^{(\beta+ik)b} \quad (3)$$

$$(\text{derivative of } \psi \text{ is continuous}) \quad \frac{du_1}{dx} \Big|_{x=a} = \frac{du_2}{dx} \Big|_{x=-b}$$

$$Ai(\alpha - k)e^{i(\alpha-k)a} - Bi(\alpha + k)e^{-i(\alpha+k)a} = C(\beta - ik)e^{-(\beta-ik)b} - D(\beta + ik)e^{(\beta+ik)b} \quad (4)$$

Four equations we got with four unknown A, B, C, D

$$A+B=C+D \quad (1)$$

$$Ai(\alpha - k) - Bi(\alpha + k) = C(\beta - ik) - D(\beta + ik) \quad (2)$$

$$Ae^{i(\alpha-k)a} + Be^{-i(\alpha+k)a} = Ce^{-(\beta-ik)b} + De^{(\beta+ik)b} \quad (3)$$

$$Ai(\alpha - k)e^{i(\alpha-k)a} - Bi(\alpha + k)e^{-i(\alpha+k)a} = C(\beta - ik)e^{-(\beta-ik)b} - D(\beta + ik)e^{(\beta+ik)b} \quad (4)$$

- The determinant of coefficients of A, B, C and D must be equal to zero for nontrivial solutions of A, B, C, and D.

After equating determinant to zero, we will get

$$\cos k(a+b) = \left[\frac{\beta^2 - \alpha^2}{2\alpha\beta} \right] \sin \alpha a \sinh \beta b + \cos \alpha a \cosh \beta b$$

This equation is quite complicated; however we must draw some conclusions

To solve above equation, Kronig Penney supposed that the potential energy is zero at lattice sites and equal V_0 inside. Also assumed that, as the height of the potential barrier V_0 tends to infinity and the width of the barrier b tends to zero so that the product $V_0 b$ remains finite. Under these assumptions

$$\sinh \beta b \rightarrow \beta b$$

$$\cosh \beta b \rightarrow 1 \text{ as } b \rightarrow 0$$

Therefore

$$\cos ka = \left[\frac{\beta^2 - \alpha^2}{2\alpha\beta} \right] \beta b \sin \alpha a + \cos \alpha a$$

$$\cos ka = \left[\frac{mV_0}{\alpha\beta h^2} \right] \beta b \sin \alpha a + \cos \alpha a$$

$$\cos ka = \left[\frac{mV_0 b}{\alpha h^2} \right] \sin \alpha a + \cos \alpha a$$

Or, $\cos ka = \left[\frac{mV_0 ba}{\alpha ah^2} \right] \sin \alpha a + \cos \alpha a$

Or, $\cos ka = \left[\frac{mV_0 ba}{h^2} \right] \frac{\sin \alpha a}{\alpha a} + \cos \alpha a$

Kronig-Penney Model in a 1D crystal

Value of the determinant:

$$\left(\frac{mV_0ba}{\hbar^2} \right) \frac{\sin \alpha a}{\alpha a} + \cos \alpha a = \cos ka$$

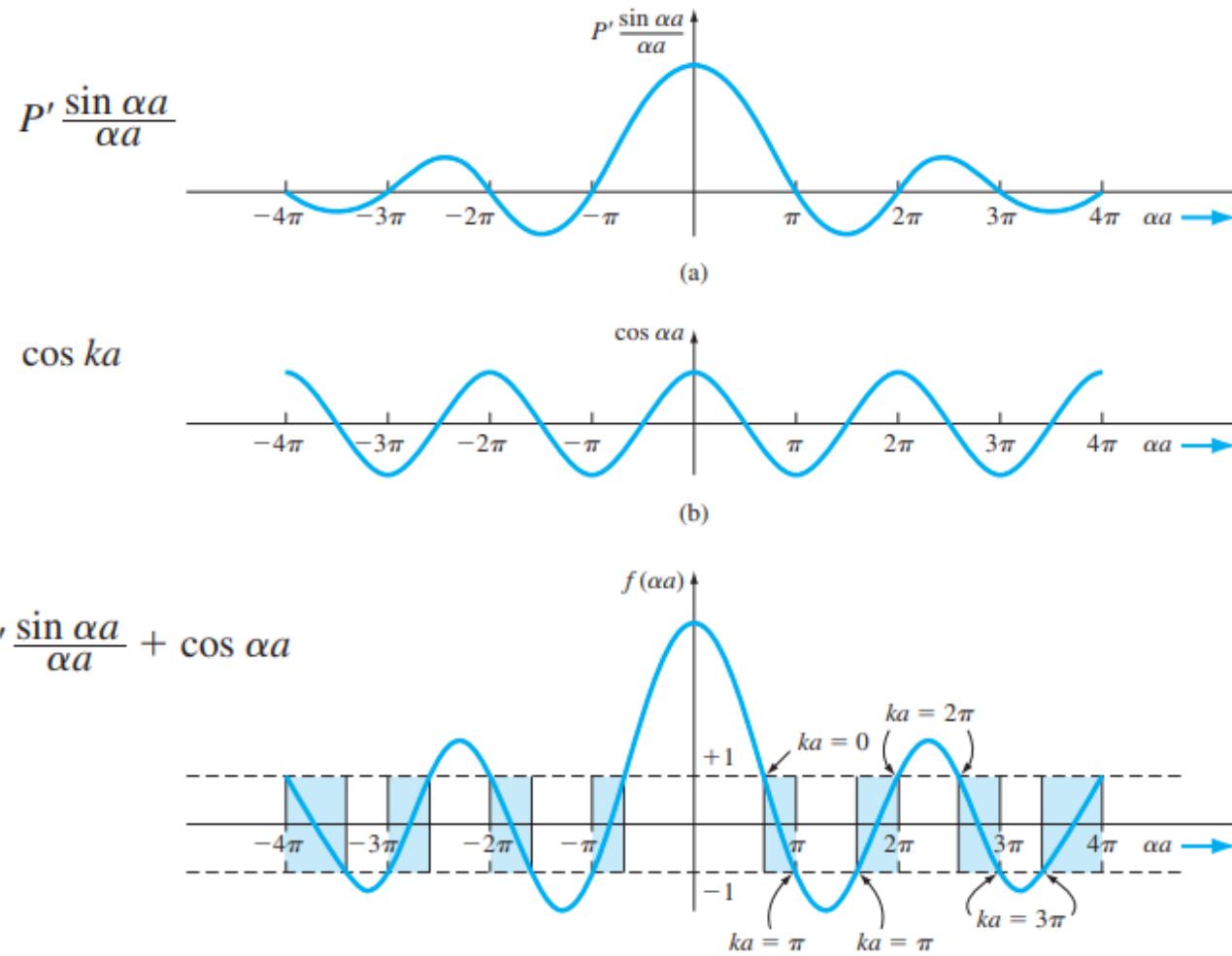
define a parameter P' as

$$P' = \frac{mV_0ba}{\hbar^2}$$

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

- The above equation is a **transcendental** equation. No analytical solutions are possible. Only graphical solutions can be obtained.

Case 2: Electron in a Periodic Potential



- Only values of αa for which f lies between $+1$ and -1 are allowed.

To find Energy of particles

Consider $p = \infty$ then eq (18) becomes

$\sin 2\alpha = 0$ and we know $\sin n\pi = 0$

$$\therefore 2\alpha = n\pi \Rightarrow \alpha = \frac{n\pi}{a} \Rightarrow \alpha^2 = \frac{n^2\pi^2}{a^2}$$

From eq (3) $\alpha^2 = \frac{2mE}{\hbar^2}$

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

$$\frac{n^2\pi^2\hbar^2}{a^2 2m} = E \Rightarrow \frac{\hbar^2\pi^2 h^2}{a^2 2m 4\pi^2} = E \quad [\because \hbar = h/2\pi]$$

$$E = \frac{\hbar^2 h^2}{8ma^2}$$

Consider $P=0$ then eq (18) becomes

$$\cos \alpha = \cos k a \Rightarrow \alpha = k \Rightarrow \lambda^2 = k^2$$

$$\text{we know } k = \frac{2\pi}{\lambda} \Rightarrow k^2 = \frac{4\pi^2}{\lambda^2}$$

Also $\lambda^2 = \frac{h^2}{m^2 v^2}$ (According to de-Broglie wave equation)

$$\text{then } k^2 = \frac{4\pi^2 m^2 v^2}{h^2} \quad \text{and} \quad \alpha^2 = \frac{2mE}{h^2} \quad (\text{from eq 8})$$

Then $\frac{2mE}{h^2} = \frac{4\pi^2 m^2 v^2}{h^2}$

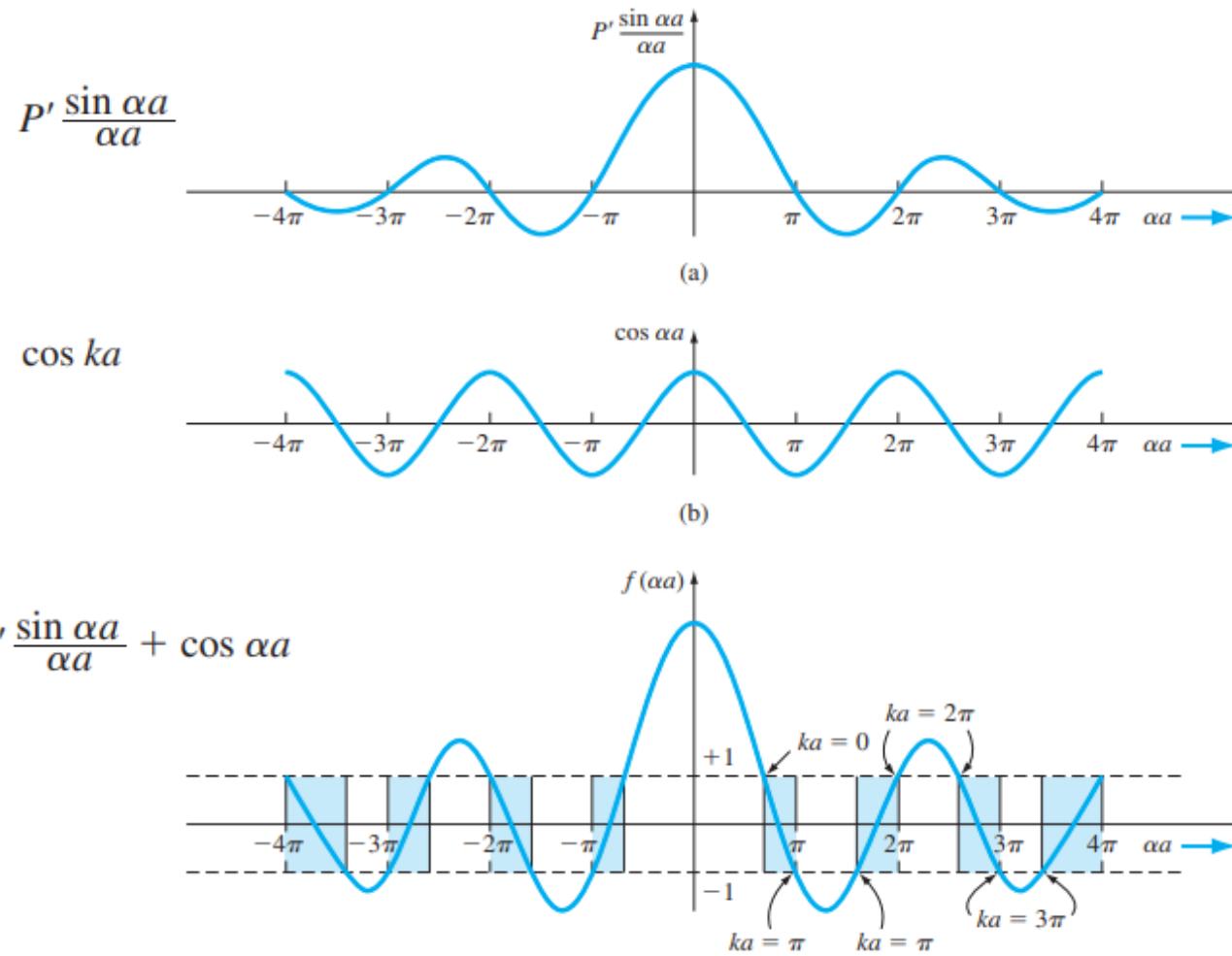
$$E = \frac{4\pi^2 m^2 v^2 h^2}{2m h^2}$$

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

$$[\because h = \hbar/2\pi]$$

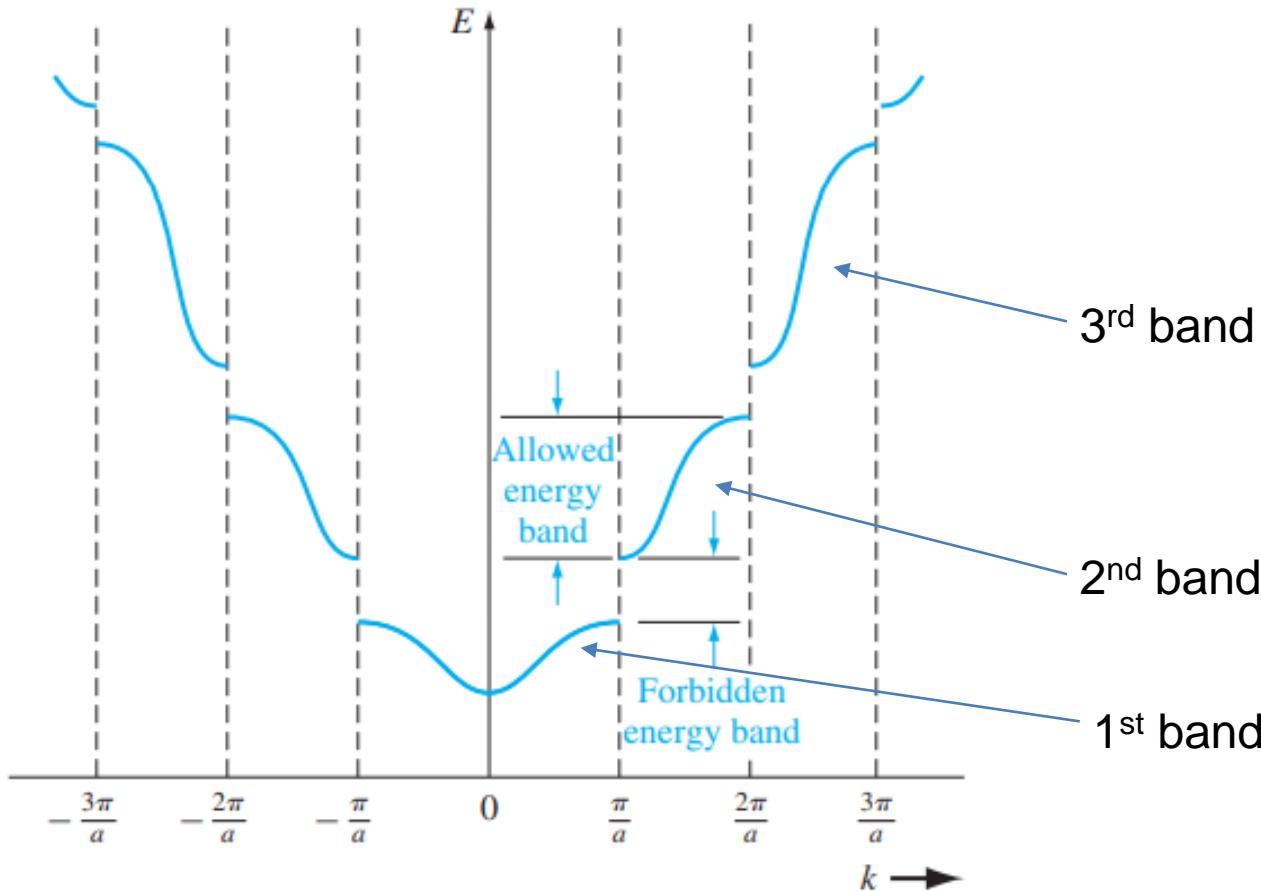
$$E = \frac{1}{2}mv^2$$

Case 2: Electron in a Periodic Potential



- Only values of αa for which f lies between +1 and -1 are allowed.

E-k Diagram for an Electron in a Periodic Potential



- Discontinuities in E indicate forbidden energies of the electron.

Case 1: Free Electron

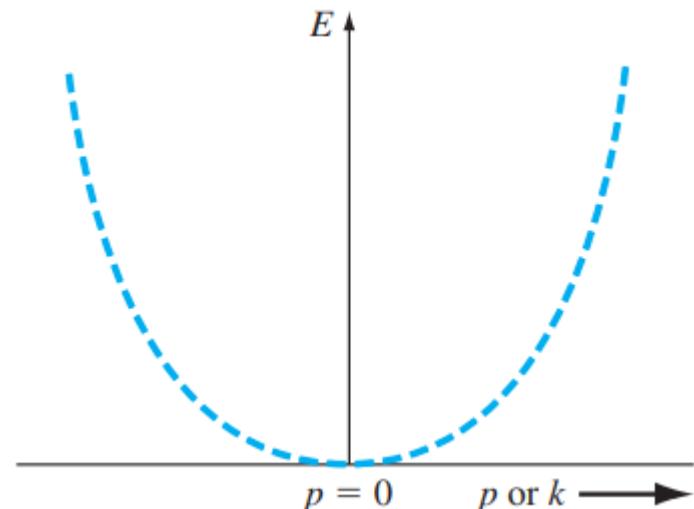
To begin to understand the nature of the solution, initially consider the special case for which $V_0 = 0$. In this case $P' = 0$, which corresponds to a free particle

$$\cos \alpha a = \cos ka$$

$$\alpha = k$$

$$\alpha = \sqrt{\frac{2mE}{\hbar^2}} = \sqrt{\frac{2m(\frac{1}{2}mv^2)}{\hbar^2}} = \frac{p}{\hbar} = k$$

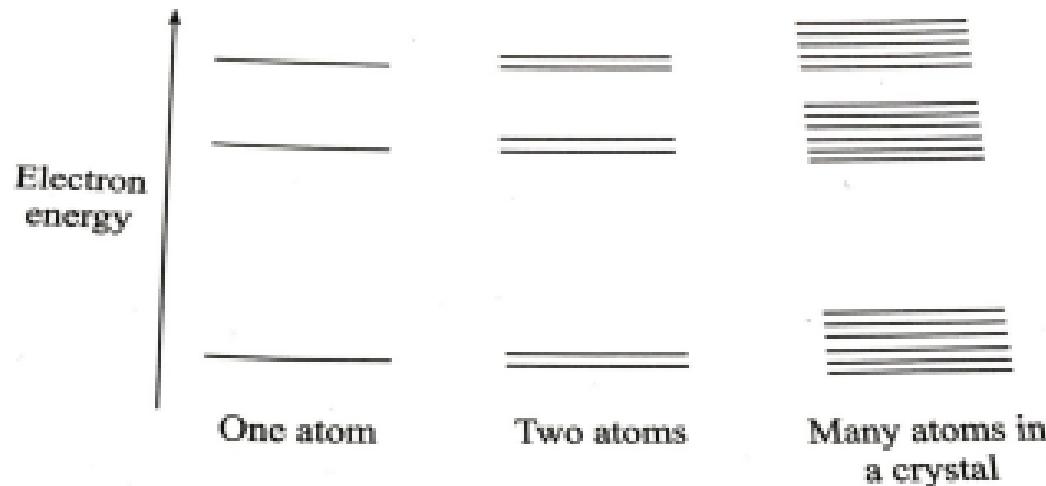
$$E = \frac{p^2}{2m} = \frac{k^2\hbar^2}{2m}$$



Kronig-Penney Model: Conclusion

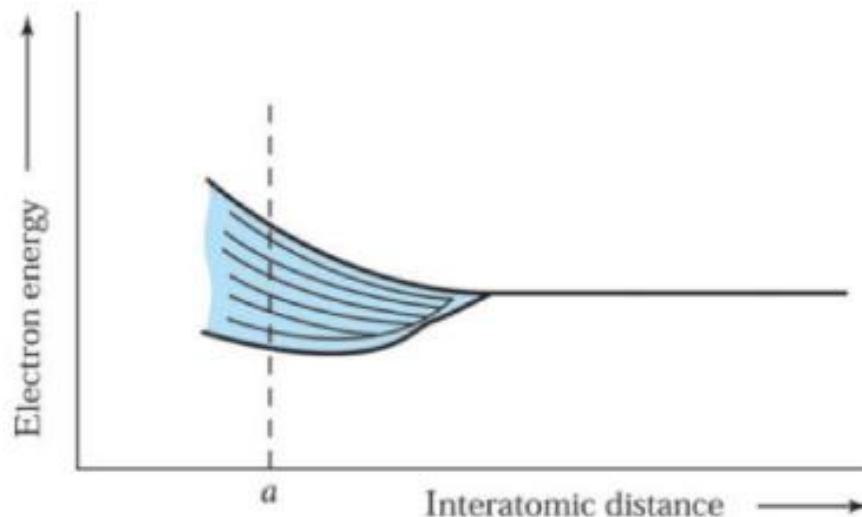
We have been considering the Kronig–Penney model, which is a one-dimensional periodic potential function used to model a single-crystal lattice. The principal result of this analysis, so far, is that electrons in the crystal occupy certain allowed energy bands and are excluded from the forbidden energy bands.

Concept of Energy Bands in Solids (1)



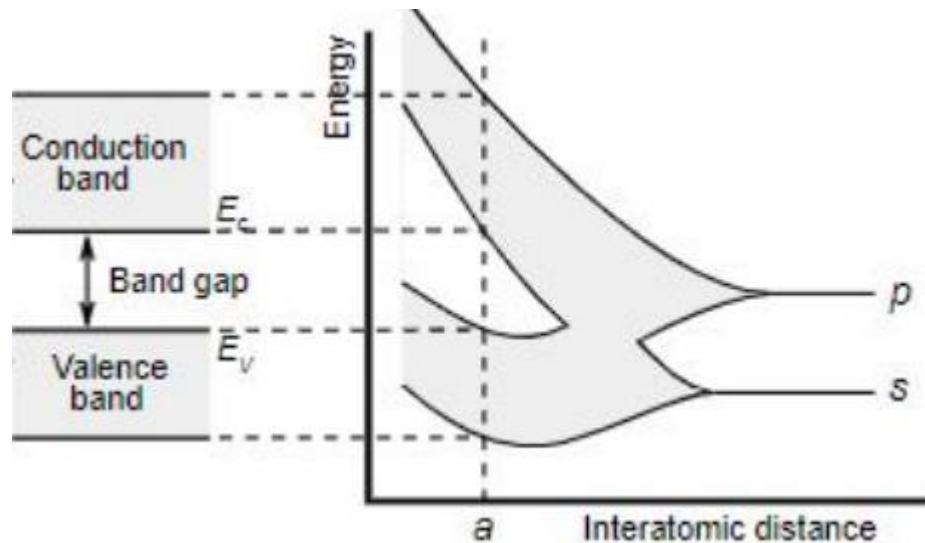
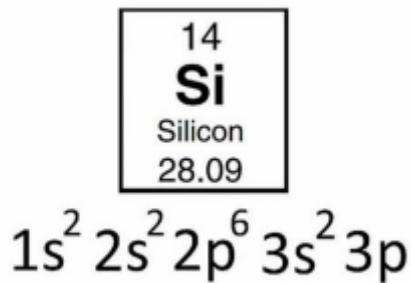
- When two identical atoms are far apart, the allowed energy levels for a given principal quantum number (for example $n = 1$) consist of one double degenerate level. That is, both atoms have exactly the same energy.
- When they are brought closer, the doubly degenerate energy levels will split into two levels by the interaction between atoms. This splitting occurs due to the Pauli's exclusion principle.

Concept of Energy Bands in Solids (2)



- As N isolated atoms are brought together to form a solid, it causes a shift in the energy levels of all N atoms, as in the case of two atoms.
- However, instead of two levels, N separate but closely spaced levels are formed. When N is very large, the result is essentially a continuous band of energy. This band of N levels can extend over a few eV at the inter-atomic distance of the crystal.

An Example: Energy Bands in Silicon



- When many Si atoms are brought together, the energy bands are formed in such a way it divides into two and in between there are no energy levels present. The gap between these bands are called **band gap**.
- The band lying below is called **valence band** owing to the presence of valence electrons which are tightly bound to the parent atoms. The band lying higher than the valence band is called **conduction band** which is responsible for conducting current in the material.

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Unit – I : Session – 4: SLO - 1

Problem Solving

Calculate the density of states per unit volume with energies between 0 and 1 eV.

Solution

$$\begin{aligned} \int_0^{1eV} g(E) dE &= \frac{4\pi(2m)^{\frac{3}{2}}}{h^3} \int_0^{1eV} \sqrt{E} dE \\ &= \frac{4\pi(2m)^{3/2}}{h^3} \left[\frac{2}{3} E^{\frac{3}{2}} \right]_0^1 \\ &= 4.5 \times 10^{21} \text{ states/cm}^3 \end{aligned}$$

Problem Solving

Find the Variation of $P' \frac{\sin \alpha a}{\alpha a} + \cos \alpha a = \cos ka$ with αa for $P' = \infty$

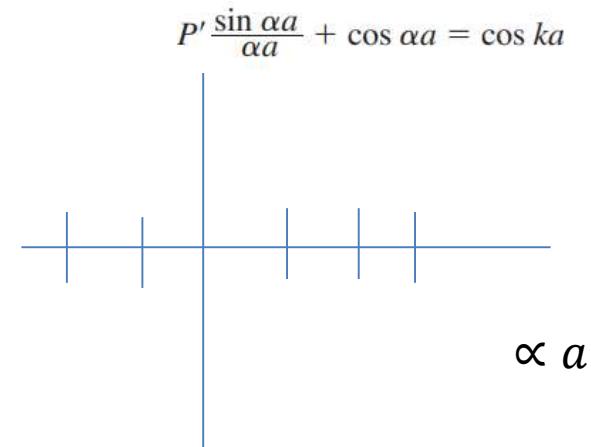
For $P' \rightarrow \infty$, spectrum becomes a line.

$$\sin \alpha a = 0$$

$$\alpha a = \pm n\pi$$

$$\alpha^2 = \frac{n^2 \pi^2}{a^2} = \frac{8\pi^2 m E}{h^2}$$

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



This expression shows that the energy of the particle is discrete. Width of the allowed band Decreases with increase in P' , i.e., with more binding energy of electrons

if $P = 0$, then

$$\cos \alpha = \cos ka$$

$$\alpha = k \rightarrow k^2 = \alpha^2 = \frac{8\pi^2 m E}{h^2}$$

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

Using de-Broglie's formula for wave-particle duality

$$E = \frac{h^2}{2m} \left(\frac{p}{h}\right)^2 = \frac{p^2}{2m}$$

This is just equivalent to the case of free particle.

For $P=0$ the free electron model and energy spectrum is (quasi) continuous

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Unit – I : Session – 4: SLO - 2

Problem Solving

Introduce Time Independent Schroedinger Equation in 1D

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{8\pi^2 m}{h^2} (E - V) \psi = 0$$

Diagram illustrating the components of the 1D Schrödinger Equation:

- Second derivative with respect to X: $\frac{\partial^2 \psi}{\partial x^2}$
- Shrodinger Wave Function: ψ
- Position: x
- Energy: E
- Potential Energy: V

For 3D

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

Problem Solving

Time-Dependent Schrodinger Wave Equation

$$i\hbar \frac{\partial}{\partial t} \Psi(x, t) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \Psi(x, t) + V(x) \Psi(x, t)$$



$$\Psi(x, t) = e^{-iEt/\hbar} \psi(x)$$

Further simplification and re-arrangement lead to
Hamiltonian form Time-Dependent Schroedinger Equation

$$\left(-\frac{\hbar^2}{2m} \nabla^2 + V \right) \Psi = i\hbar \frac{\partial \Psi}{\partial t}$$

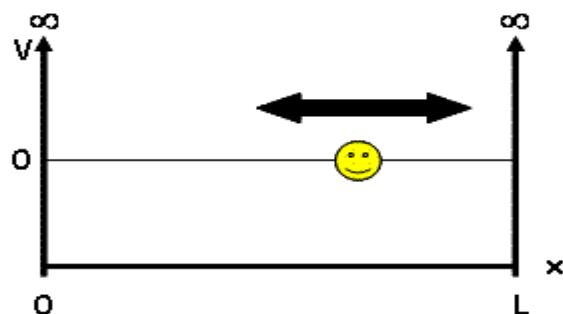
$$\text{where } H = \frac{-\hbar^2}{2m} \nabla^2 + V$$

Problem Solving

To solve the problem for a particle in a 1-dimensional box

- Step 1. Define the Potential Energy, V
- Step 2. Solve the Schrödinger Equation
- Step 3. Define the wavefunction
- Step 4. Define the allowed energies

Step 1. Define the Potential Energy, V



A particle in a 1D infinite potential well of dimension L .

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.

Problem Solving

Step 2. Solve the Schrödinger Equation

Introduce Schrödinger Time independent wave Equation and apply $V = 0$

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

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

$$\frac{d^2\psi}{dx^2} + k^2 \psi = 0$$

Solution of the above Schrödinger equation becomes

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

where A and B are called as arbitrary constants which can be determined uniquely using **BOUNDARY CONDITIONS**

Problem Solving

Step 3. Define the wavefunction

Apply Boundary condition $x = 0$, then the above equation becomes

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

$\sin 0 = 0 \longrightarrow$ hence $B = 0$, then the wave function

$$\Psi(x) = A \sin kx$$

Apply Boundary condition $x = L$, then the above equation becomes

$$0 = A \sin kL \quad \text{sine } A \neq 0; \sin kL = 0$$

$$\sin n\pi = 0 \longrightarrow kL = n\pi \longrightarrow k = n\pi/L$$

Solution of the equation becomes $\psi_n(x) = A \sin \frac{n\pi x}{l}$

Problem Solving

Step 4. Find the allowed energy levels

We know that

$$k^2 = \frac{2mE}{\hbar^2} \quad \text{and} \quad k^2 = \frac{n^2\pi^2}{L^2}$$

Solving for E results in the allowed energies for a particle in a box:

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

Problem Solving

Step 5. Normalization of wavefunction

To determine A, 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 wavefunction.

$$P = \int_0^l |\psi|^2 dx = 1$$

$$P = \int_0^l A^2 \sin^2 \frac{n\pi x}{l} dx = 1$$

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

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

$$A^2 \left[\frac{l}{2} - \frac{1}{2} \frac{\sin 2n\pi / l}{2n\pi / l} \right] = 1$$

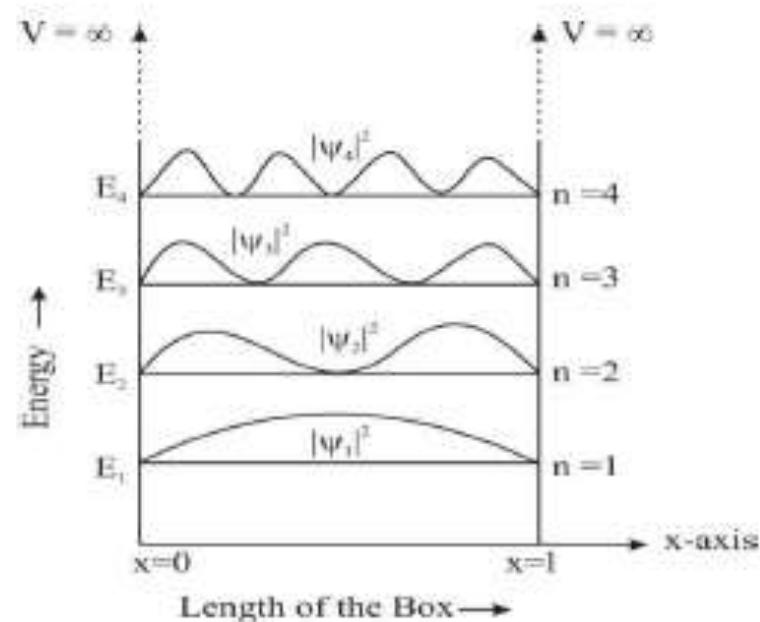
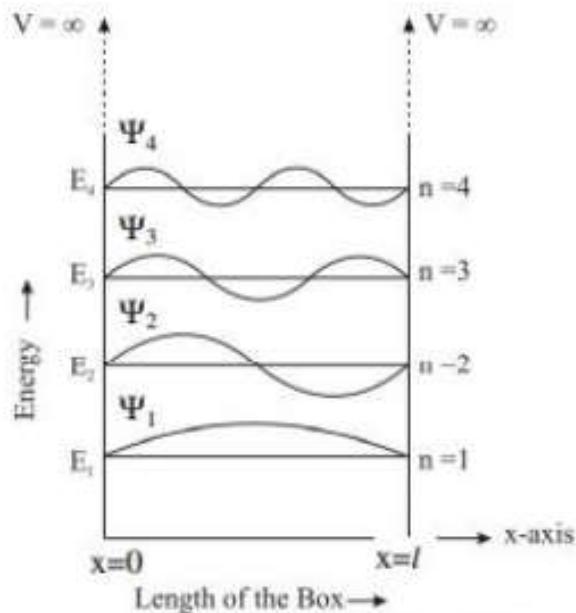
$$A^2 \left[\frac{l}{2} - \frac{1}{2} \frac{\sin 2n\pi}{2n\pi / l} \right] = 1$$

$$\frac{A^2 l}{2} = 1$$
$$A = \sqrt{\frac{2}{l}}$$

Problem Solving

normalized wavefunction for a particle in a 1-dimensional box

$$\Psi_n = \sqrt{\frac{2}{l}} \sin \frac{n\pi x}{l}$$



Wavefunction of the particle in different energy levels looks like

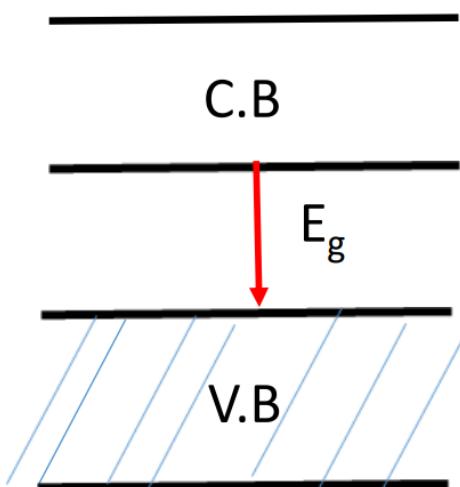
Probability of the particle in different energy levels looks like

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Unit- I : Session 7 : SLO 1

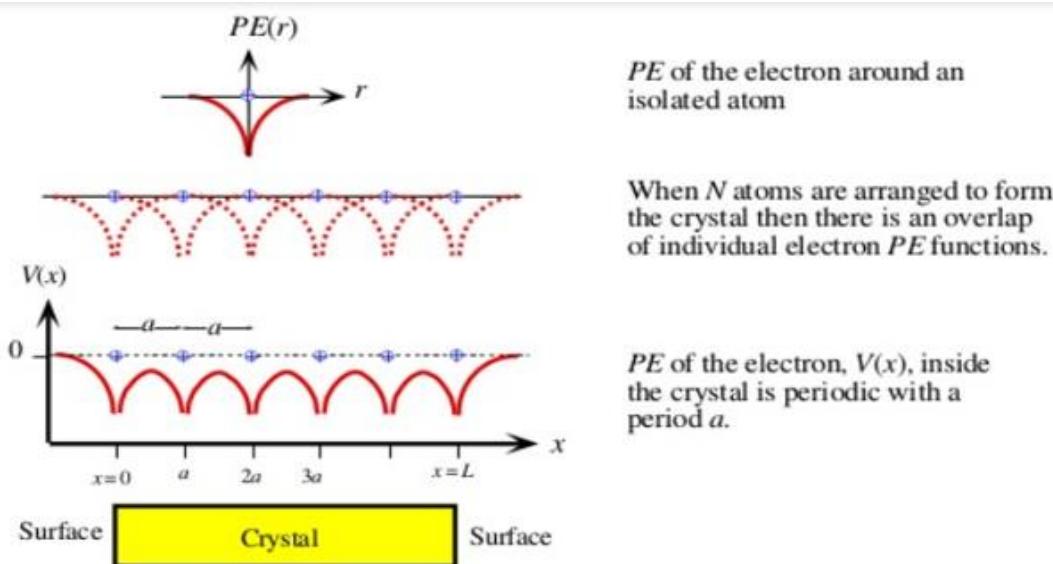
E-K Diagram

- The conventional band diagram shows the band gap energy only.
- To know more electrical and optical properties of semiconductor material we need to know 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.



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 $|\Psi|^2$



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 $PE = 0$).

Schrödinger's one-Dimensional time independent wave equation

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

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 $V(x+a)$

$$\text{i.e } V(x) = V(x+a) \quad \text{---(2)}$$

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

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

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

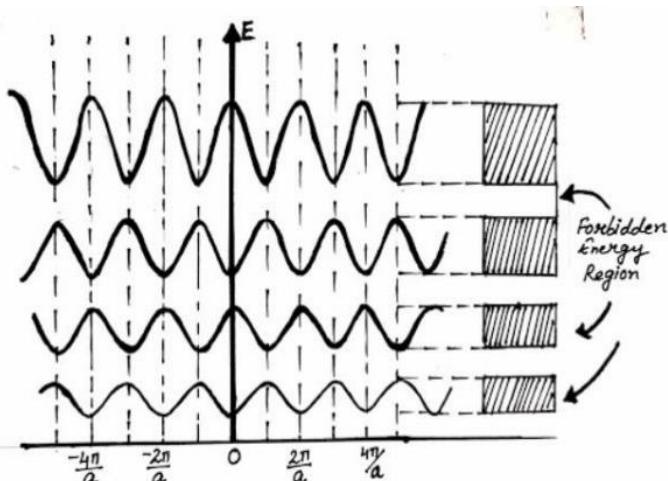


There are three types of E-K diagram

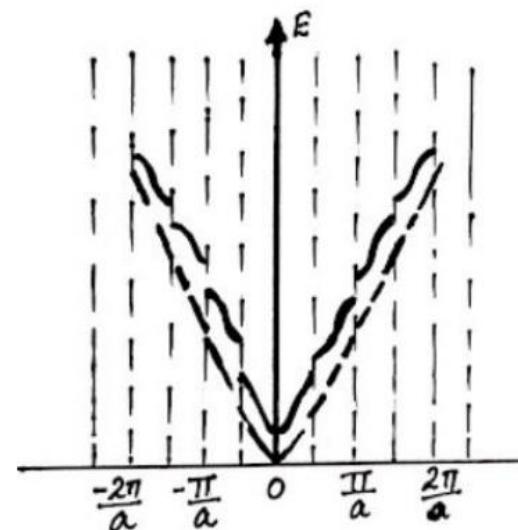
- Periodic zone
- Extended zone
- Reduced zone

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



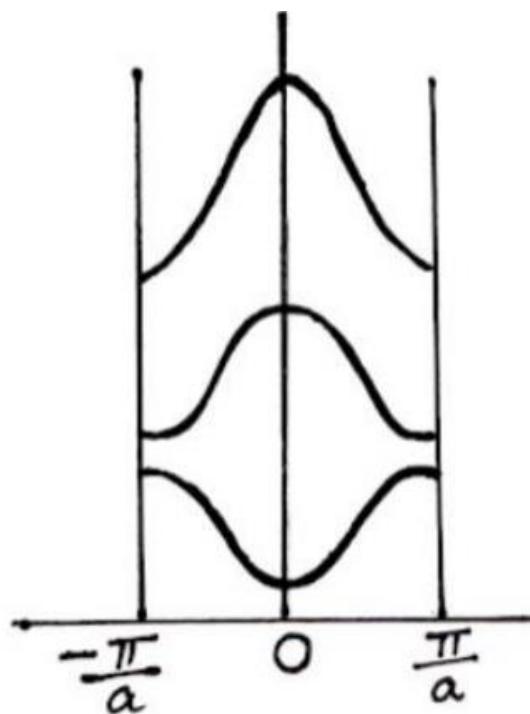
Extended Zone

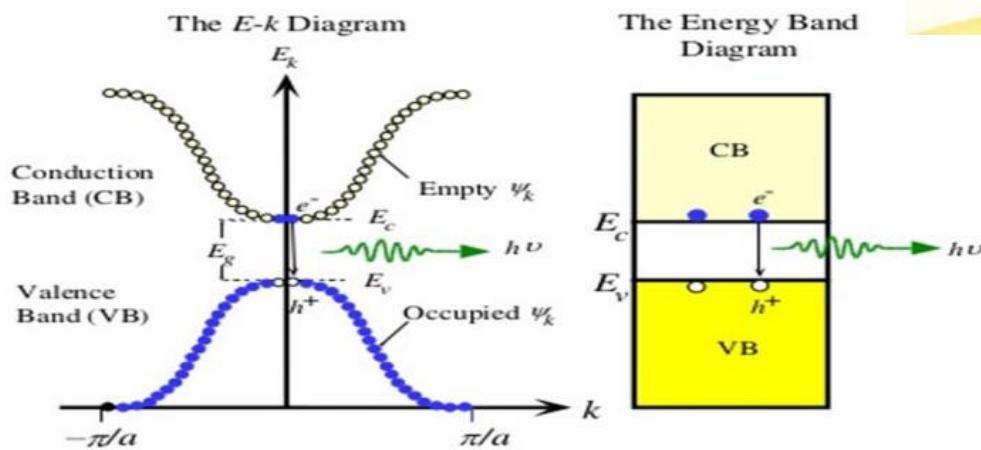
Extended Zone Scheme:

In this scheme, different bands are drawn in different zones. In k - space. A discontinuities is obtained at $\mathbf{K} = \pm \frac{n\pi}{a}$ where $n = \pm 1, \pm 2, \dots$ For $k = -\frac{\pi}{a}$ to $\frac{\pi}{a}$ is first Brillouin zone For $k = -\pi a$ to $-2\pi a$ and πa to $2\pi a$ is second Brillouin zone The discontinuities in the curve is due to Braggs law of reflection at the edges of allowed bands (i.e) $\mathbf{K} = \pm \frac{n\pi}{a}$

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.





The $E\text{-}k$ diagram of a direct bandgap semiconductor such as GaAs. The $E\text{-}k$ 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 $E\text{-}k$ relationship as a continuous curve. In the energy range E_v to E_c there are no points ($\psi_k(x)$ solutions).

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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.



We know

$$P = \hbar k$$

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

Momentum (p) = mv

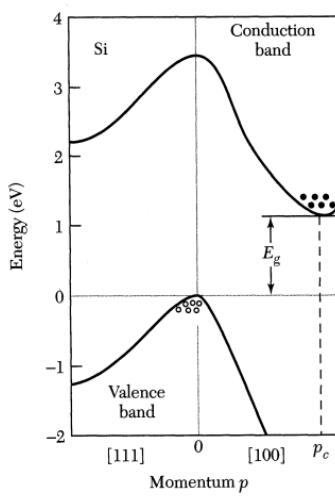
Where, symbols have usual meaning.

Now,

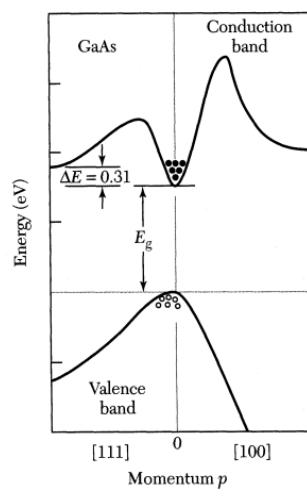
$$K = \frac{1}{2}mv^2 = \frac{1}{2}mv^2 \times \frac{m}{m} = \frac{1}{2} \frac{m^2v^2}{m} = \frac{(mv)^2}{2m} = \frac{p^2}{m}$$

therefore,

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



Indirect BG



Direct BG

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

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.

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*.
- 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.

Direct Band-gap Semiconductor	Indirect Band-gap Semiconductor
<ol style="list-style-type: none"> 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. 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. 3. The efficiency factor of a DBG semiconductor is higher. 4. Example of DBG semiconductor material is Gallium Arsenide (GaAs). 5. DBG semiconductors are always preferred over IBG for making optical sources. 6. The probability of a radiative recombination is high. 	<ol style="list-style-type: none"> 1. An 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. 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 IBC semiconductor is lower. 4. Examples of IBG semiconductors are Silicon and Germanium. 5. The IBG semiconductors cannot be used to manufacture optical sources. 6. The probability of a radiative recombination is comparatively low.

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Unit- I : Session 7 : SLO 2

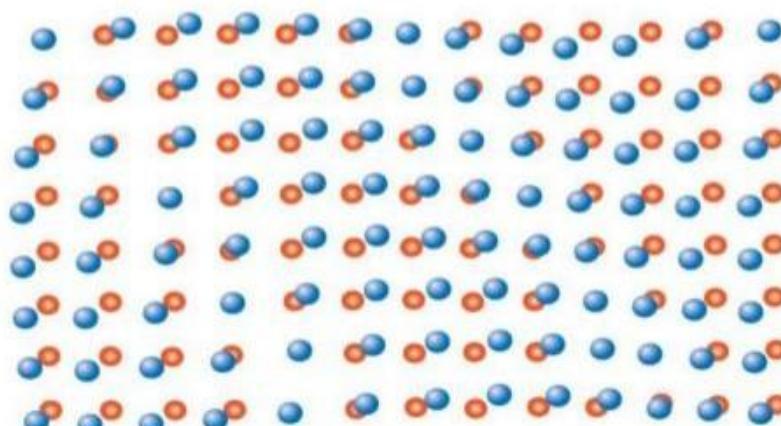


CONCEPT OF PHONONS

- 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



Normal lattice positions for atoms
Positions displaced because of vibrations

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

$$E_{phonon} = \frac{hv_s}{\lambda}$$

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

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):

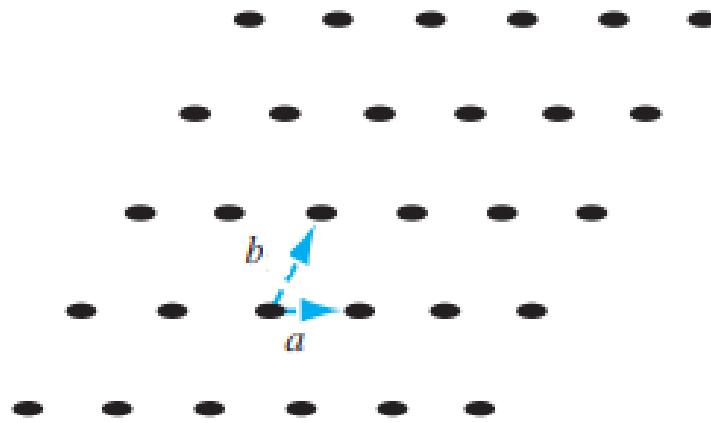
$$\lambda_{photon} \approx 10^{-6} \text{ m}$$

Concept of 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:
 - Draw lines to connect a given lattice points to all nearby lattice points.
 - Draw lines to connect a given lattice points to all nearby lattice points.
 - Draw new lines or plane at the mid point and normal to the lines in(i).
 - The smallest volume enclosed in this way is the WS primitive cell.



2D Lattice

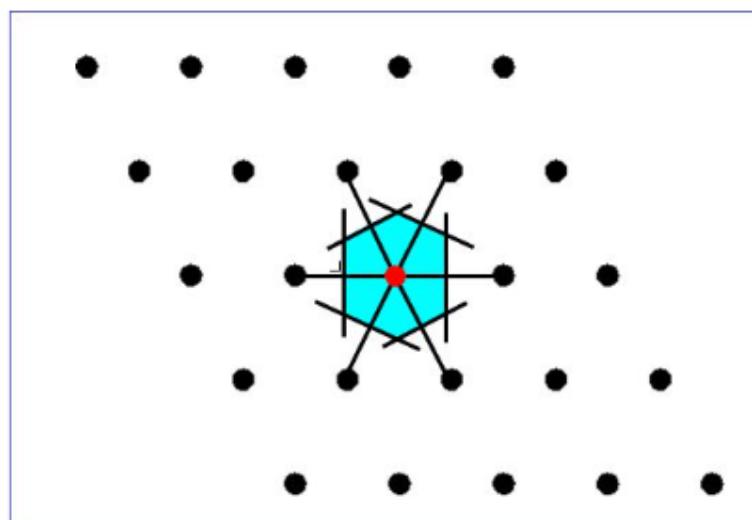


- Atoms (or ions) are periodically arranged in 2D space.
- Two lattice parameters \mathbf{a} and \mathbf{b} uniquely define the 2D lattice.



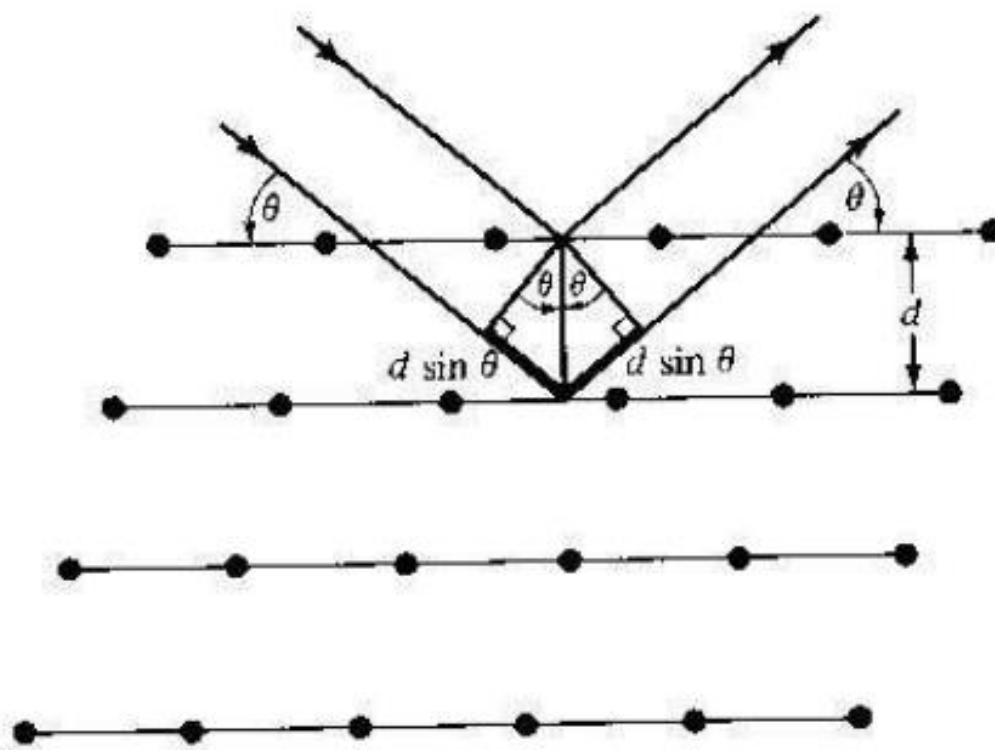
Wigner-Seitz Cell

The Wigner–Seitz cell around a lattice point is defined as the locus of points in space that are closer to that lattice point than to any of the other lattice points.



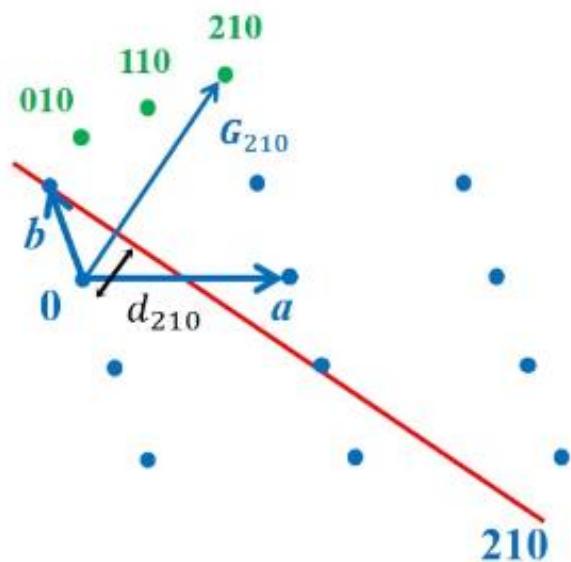


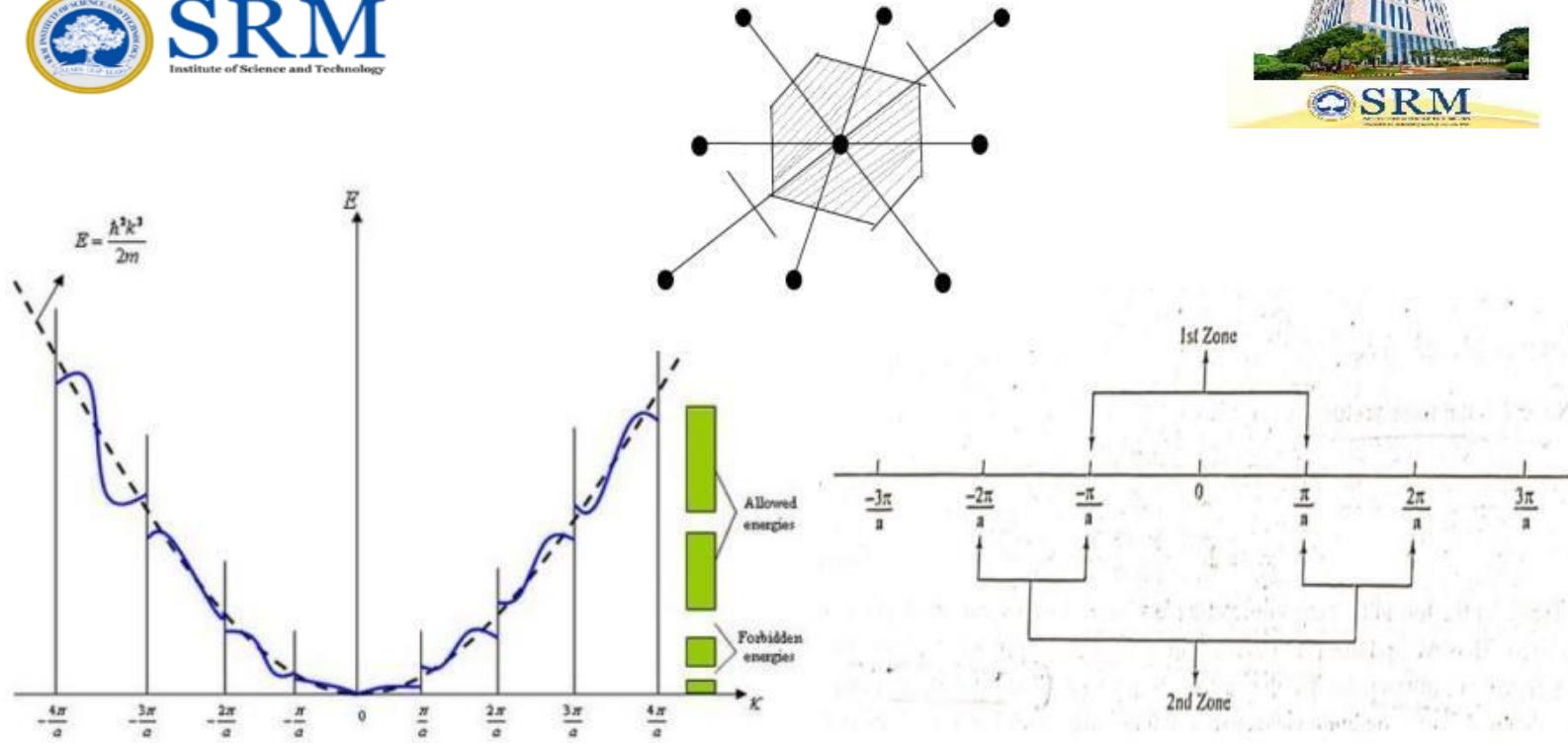
X-Ray Diffraction Bragg's Law





Reciprocal 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 link 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

[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 latter relation].

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

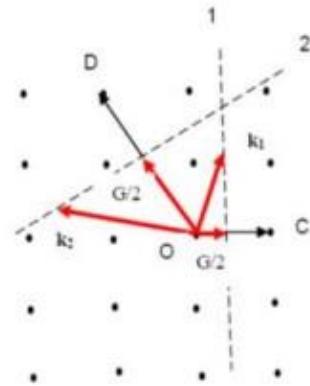


Thus the procedure to build up the first Brillouin zone is as follows (see figure 30):

- 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.

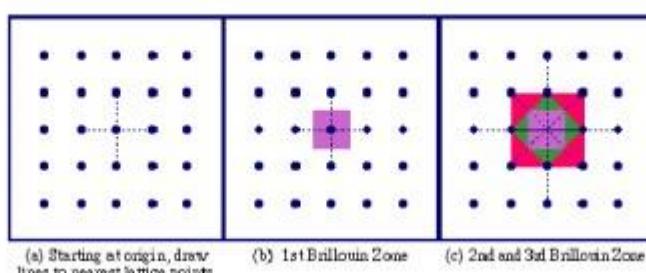
Important note:

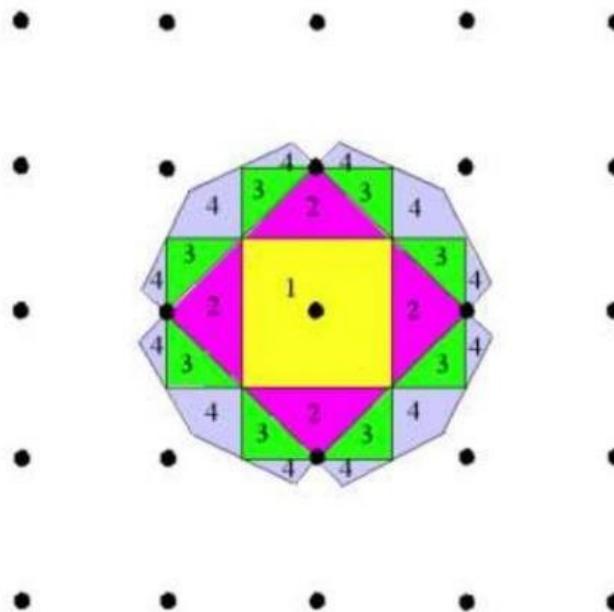
A wave whose wave vector drawn from the origin terminates on any of the planes will satisfy the condition of diffraction. Such planes are the perpendicular bisectors of the reciprocal vectors.



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.



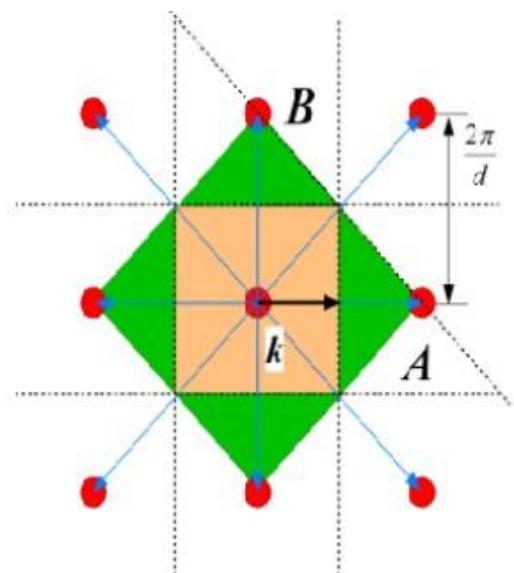


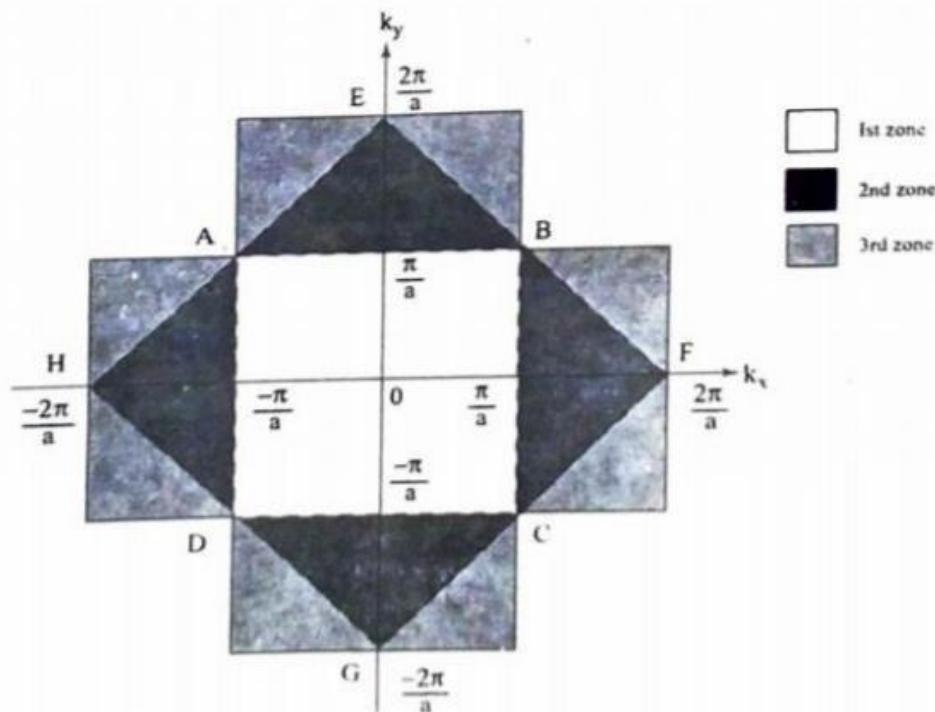
BZ construction

- reciprocal lattice
- bisect vectors to the nearest neighbors
- area defined by bisecting lines represents 1BZ.

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 1. Brillouin zone (orange).
- The next area (going over one line only) is 2. Brillouin zone (green).





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

Conclusion:

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)

The importance of Brillouin zone:

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

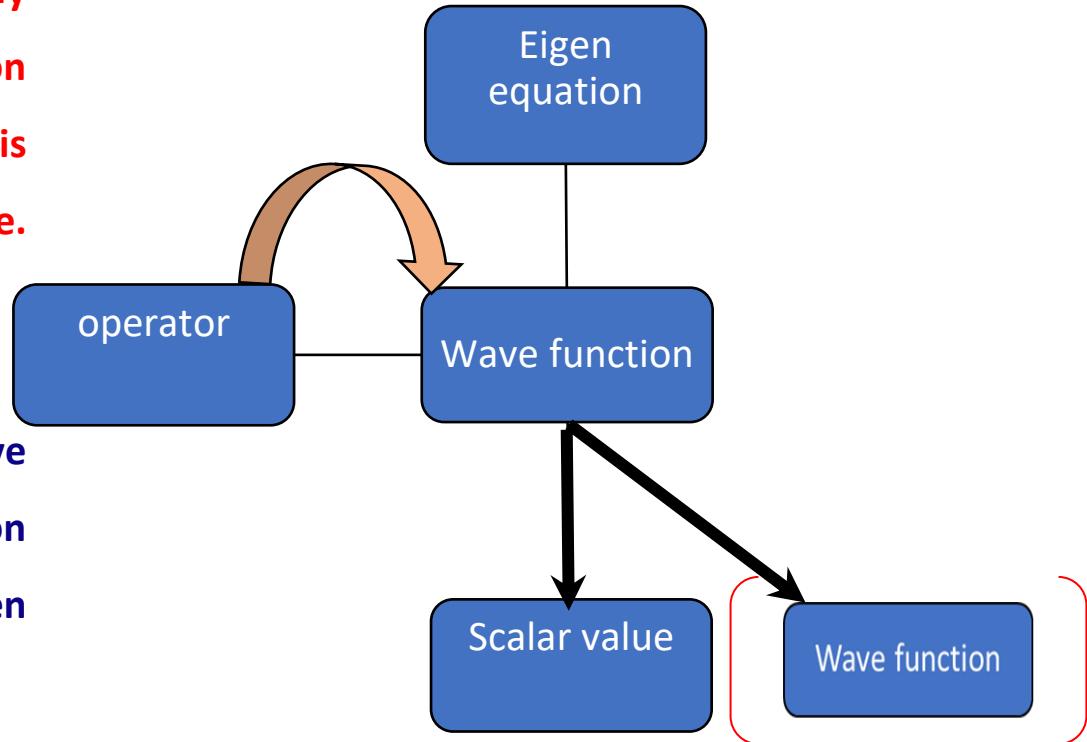
21PYB102J – Semiconductor Physics and Computational Methods

Unit – I: Session – 8: SLO - 1

Computational determination of Band Structure – Concepts , Eigenvalue equation

Eigen function and equations

- In quantum mechanics, If we apply an operator on wave function then the same wave function is achieved back with a scalar value. (see pictorial illustration)



- In that scenarios, the Wave function is called Eigen function and the scalar value is called Eigen value.
- Equation which includes Eigen function, operator and Eigen value is called Eigen equation.

Mathematical Examples

$$\frac{d}{dx} \sin(x) = \cos(x)$$

No same function is achieved back after applying differential operator , (i.e. Sin and Cos functions are different).

$$\frac{d}{dx} e^{3x} = 3e^{3x}$$

↓
Eigenvalue

Same function is achieved back with a multiple of '3' after applying differential operator.

Conclusion: Sin (X) is not an Eigenfunction of d/dx , however, exponential function e^{3x} is an Eigenfunction of d/dx .



Examples

- Show that the Sin (X) is an Eigenfunction of d^2/dx^2

$$\frac{d^2}{dx^2} \sin(x) = -\sin(x)$$

Same function is achieved back with a multiple of '-1' after applying 2nd order differential operator.

-

Sin(KX) is an Eigenfunction with double order derivative

- Now we must take the derivative of the sin function and also the function kx inside the parentheses.

$$-\frac{d}{dx} \sin(kx) = -k \cos(kx)$$

$$-\frac{d^2}{dx^2} \sin(kx) = k^2 \sin(kx)$$

Here K^2 is the Eigen value.



Quantum Physics Eigen function example

The Schrödinger equation

Based on these considerations we can write a compact form for the Schrödinger equation.

$$H\Psi = E\Psi$$

$$H = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2}$$

Energy operator, Hamiltonian

$$E = \frac{\hbar^2 k^2}{2m}$$

Energy eigenvalue, Energy

$$\Psi = \sin(kx)$$

Wavefunction

Sin(kx) is an eigenfunction of the Schrödinger equation

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \sin(kx) = \frac{\hbar^2 k^2}{2m} \sin(kx)$$

In this equation, \hbar is Planck's constant divided by 2π and m is the mass of the particle that is traveling through space.

Computational Band structure methods



Difference between localized and delocalized wave functions

Localized function

- A localized wave function is one that is confined to a **specific region of space**.
- Herein, an electron bound to an atom is localized within a **certain distance from the nucleus**.
- The probability density of finding the electron is concentrated in a **small region** and the wave function decreases rapidly as we move away from the nucleus.

Delocalized function

- A delocalized wave function, on the other hand, is one that is **spread out over a large region of space**.
- Herein, an **electron in a metal is delocalized over the entire metal**, as the electron can be found anywhere in the metal with some probability.
- The probability density of finding the electron **is not confined to a specific region**, but is distributed over a large region of space.

The tight binding method

- The tight binding approximation method (**TBA**), we don't calculate the general band structure directly, instead, we specifically calculate the bands formed by some atomic orbital.
- For example, for graphene, We calculate the energy band of 2Pz orbital of C atoms.

- It uses a set of **matrix equations** to determine the **energy levels of the localized wave functions** and the **band structure of the solid is computed**.

- It is not always accurate method for materials with a complex crystal structure or electronic behavior.

How to solve matrix equation using localized wave function?

- Write down the Hamiltonian operator for the system in the form of a matrix in a particular basis set.
- Form the Hamiltonian matrix, calculate the matrix elements of the Hamiltonian operator in the chosen basis set.

$$\hat{H} \Psi = E \Psi$$

↓ ↓
 Hamiltonian Operator (Energy operator) Energy eigenvalue

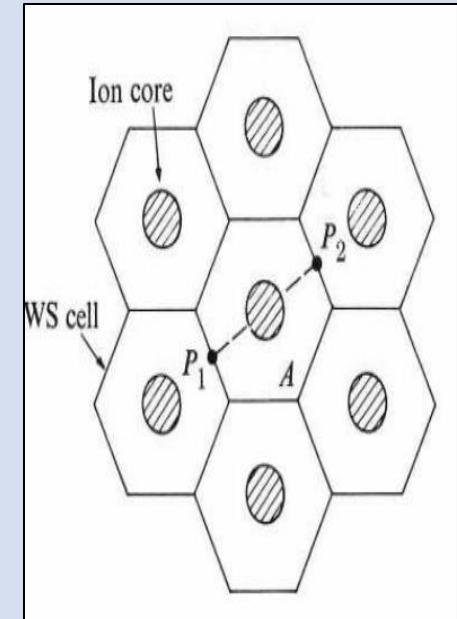
- Once the eigenvalues and eigenvectors are determined, they can be used to calculate various properties of the system such as the probability density, energy levels, and transition probabilities.

Cellular method for computing band structures (cell means Unit cell oriented method)

- Conceptually, the most simple method for solving the energy band problem **is the cellular method** in which one solves the Schrodinger equation within the **unit cell**.
- Unit cell:** It is based on the idea of dividing the solid into a periodic array of identical cells.
- The earliest method employed in the band structure calculations by **Wigner and Seitz cell (WS cell)**. An attempt to solve the Schrödinger equation in a single cell, using for $V(r)$ the potential of a free ion.
- Schrodinger equation** solved to find out eigen values is given below:

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}) \right] \psi_{\mathbf{k}}(\mathbf{r}) = E(\mathbf{k}) \psi_{\mathbf{k}}(\mathbf{r}).$$

where $V(\mathbf{r})$ is the crystal potential and $\psi_{\mathbf{k}}(\mathbf{r})$ the Bloch function.



To ensure that the function satisfies the Bloch form.

$$\psi_{\mathbf{k}} = e^{i\mathbf{k}\mathbf{r}} u_{\mathbf{k}}$$

it is necessary that $u_{\mathbf{k}}$ be periodic, i.e. $u_{\mathbf{k}}$ be the same on opposite faces of the cell, e.g., points P1 and P2

Augmented plane wave method for computing band structures

- The Augmented Plane Wave (APW) method is a computational approach used in electronic structure calculations in solid-state physics.
- It is used to solve the Schrödinger equation for the electron wave function in a crystal lattice.
- APW begins with the assumption that the effective crystal potential is constant between the cores (**muffin-tin like potential**).
- Outside the core the wave function is a plane wave as the potential is constant, and inside the core the function is atom-like to be solved by the free-atom Schrödinger equation.

Pseudopotential Method for computing band structures

1. In the calculation of the electronic structure using pseudopotentials, the interaction between the electrons and ions is modeled by the pseudopotential rather than the full Coulomb interaction. **The term "pseudo" indicates that the model is not the real interaction, but rather a simplification used for computational convenience.**
2. **The Schrödinger equation is then solved for the electrons in the presence of the pseudopotential, which represents the electron-ion interaction.**
3. The solution of the Schrödinger equation gives the Eigenvalues, which correspond to the allowed energy levels for the electrons in the solid, and the eigenvectors, which correspond to the wave functions of the electrons.
4. The Eigen values and eigenvectors are used to calculate various electronic properties of the material, such as the band structures.

Density functional theory (DFT)

- The DFT method is a computational approach for calculating the band structure of a solid.
- In DFT, the solutions of the Kohn-Sham equations give the electronic eigenvalues and eigenfunctions, which are used to calculate the band structure of the solid.

The band structure of a solid can be calculated using different exchange-correlation functionals in DFT

- Local Density Approximation (LDA)
- LDA is a simple functional that is computationally efficient but not always accurate
- Generalized Gradient Approximation (GGA)
- GGA is more accurate but computationally expensive

Kohn –Sham equations

In the Hartree-Fock term:

$$\left(-\frac{1}{2} \nabla^2 + V_{ext}(\vec{r}) + \int \frac{n(\vec{r}')}{|\vec{r} - \vec{r}'|} d\vec{r}' \right) \Psi_i = \epsilon_i \Psi_i$$

- V_{ext} is the nuclear potential or external potential
- ϵ_i is the eigen value
- Small problem in above HF equation : This equation neglects electron correlations and the Pauli exclusion principle is not obeyed.
- Thus, Kohn-sham equation is introduced as per below to find out correct eigen values using electron exchange and corelation term.

$$\left(-\frac{1}{2} \nabla^2 + V_{ext}(\vec{r}) + \int \frac{n(\vec{r}')}{|\vec{r} - \vec{r}'|} d\vec{r}' + V_{xc}(\vec{r}) \right) \Psi_i = \epsilon_i \Psi_i$$

- Kohn-Sham orbitals and eigenvalues are calculated with LDA and GGA functionals for a set of systems by varying basis.

MCqs

Which of the following method uses ‘atomic orbital approach’ to compute electronic band structure computationally?

- (a) cellular method
- (b) APW method
- (c) Pseudopotential method
- (d) Tight binding method

Which is Eigen function of d/dx ?

- I. X^2
- II. $2\sin(X)$
- III. e^{2x}
- IV. $\sin(2X)$

Which is Eigen function of d^2/dx^2 ?

- I. X^2
- II. $\sin(X)$
- III. $\ln(X)$
- IV. $\tan(X)$

Which of the following method uses ‘primitive cell approach’ to compute electronic band structure computationally?

- (a) Wigner-seitz method
- (b) APW method
- (c) Pseudopotential method
- (d) Tight binding method

1. Which of the following is an Eigen function of Schrodinger equation?

- I. $\sin(kx)$
- II. $\tan(kx)$
- III. $\ln(x)$
- IV. $\text{Cosec}(x)$

Important Questions

- What is Tight binding method? Similarly what are other methods?
- Show that the $\sin(kx)$ is an Eigenfunction of Schrodinger equation.
- Differentiate between localised and delocalized wave functions.
- Explain the concept of Eigen function, Eigen value and Eigen equation through an example of function.



21PYB102J – Semiconductor Physics and Computational Methods

Unit – 1 : Session – 10 : SLO - 1

Classification of Electronic Materials



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. It having infinite conductivity. **Example :** copper , silver etc.

Resistivity on the order of 10^{-8} to 10^{-4} cm

Semiconductors

Semiconductors are materials which have the conductivity between conductors and insulators. Semiconductors are the elements of group-III, group-IV and group-V elements. At normal temperature the conductivity of semiconductor is very low. With increase in temperature the conductivity of semiconductors increases exponentially. **Example:** Germanium, Silicon, Gallium Arsenic etc.

Semiconductors have an electrical resistivity value between those of conductors and insulators 10^{-4} to 10^8 cm

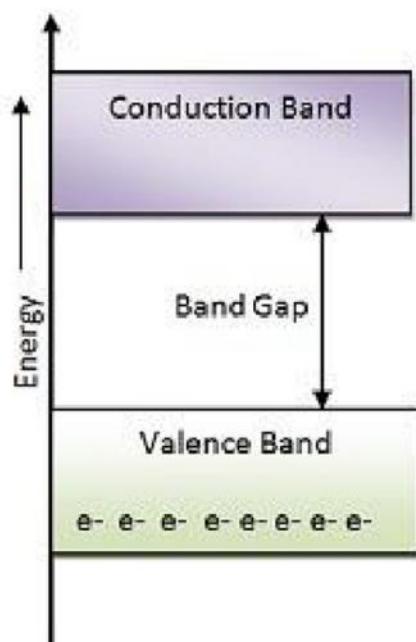
Insulators Insulators are very poor conductor of electricity. The forbidden gap value is 3eV

Example: wood ,oil, mica.

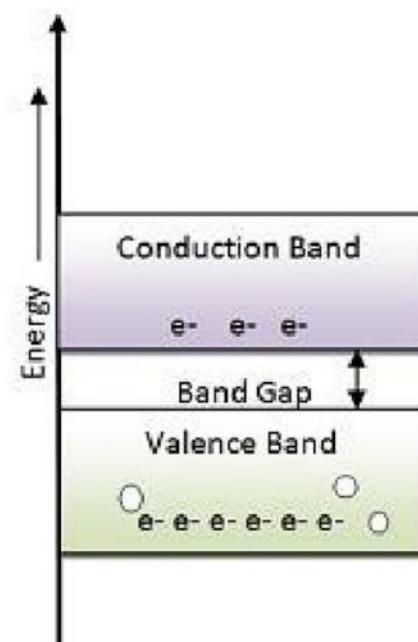
electrical resistivity on the order of 10^8 to 10^{18} Ω cm



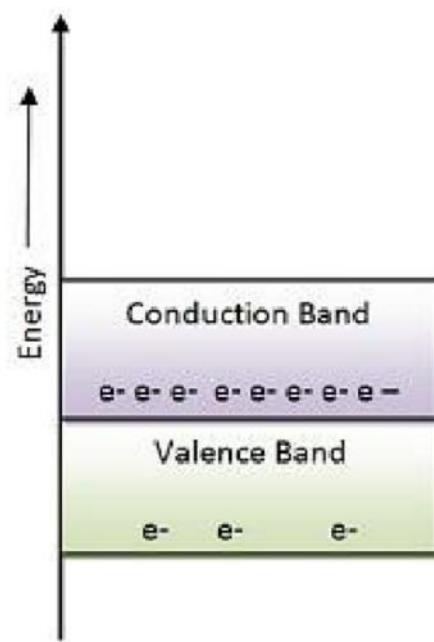
Classification Of Electronic Materials



Insulators



Semiconductors



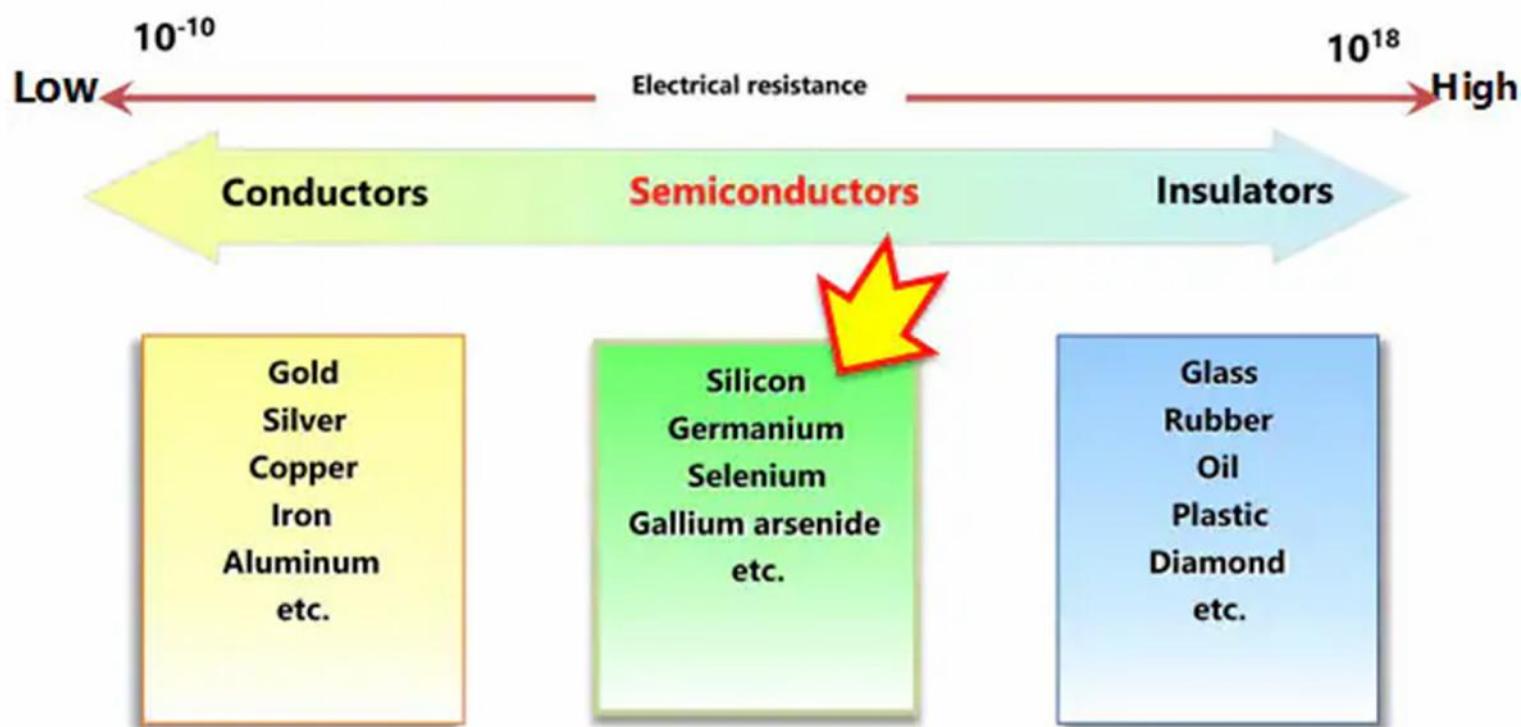
Conductors

e- →

electrons

○ →

Holes





21PYB102J – Semiconductor Physics and Computational Methods

Unit – 1 : Session – 9 : SLO - 2

Fermi level- Probability of occupation

Comparison between Maxwell- Boltzmann, Bose-Einstein and Fermi- Dirac statistics

There are three different statistics:

- These three statistics concern when how particles occupy a system which consists of several energy levels (and each energy level could also have several energy states).
- A particle in this system can be in one of those energy levels depending on the energy particle has.
- It's impossible to have just one particle in a system since in real life it needs various particles to constitute a system.
- They occupy the levels under a statistics rule.

- Particles which are regulated by **Maxwell-Boltzmann Statistics** have to be **distinguishable** each other and one energy state can be occupied by two or more particles. Distinguishable means that if we have 2 particles, let say A and B, also two states, 1 and 2, and we put A to state 1 and B to state 2, it will be different with the distribution A to state 2 and B to state 1. It means that A and B are distinct.
- Particles which are regulated by **Bose-Einstein Statistics** have to be **indistinguishable** each other and one energy state can be occupied by two or more particles. So instead of saying it as particle A or B, we call it as just “particle” since they are the same thing
- Particles which are regulated by **Fermi-Dirac Statistics** have to be **indistinguishable** each other and one energy state can be occupied by only one particle. So we have to fill it to another state when a state has just been occupied by another particle.

- **Maxwell Boltzmann** statistics is applicable to identical, *distinguishable* particle of any type spin. The molecules of gas are particle of this type.
Eg. : Gaseous particles
- **Bose Einstein** statistics is applicable to the identical, *indistinguishable* particles of zero or integral spin. These particles are called Bosons.
Eg: Photons. Gluons, ${}^4\text{He}$ atoms,
- **Fermi Dirac** statistics is applicable to the identical, indistinguishable particles of half integral spin. These particles obey **Pauli Exclusion Principle** .
Eg: Electrons, Protons, Neutrons,
Quarks, Neutrinos etc.,

The expressions for three statistics are following

1. Maxwell-Boltzmann Statistics:

$$f(E) = \frac{1}{e^{\frac{(hv)}{KT}}}$$

2. Bose-Einstein Statistics

$$f(E) = \frac{1}{e^{\frac{(hv)}{KT}} - 1}$$

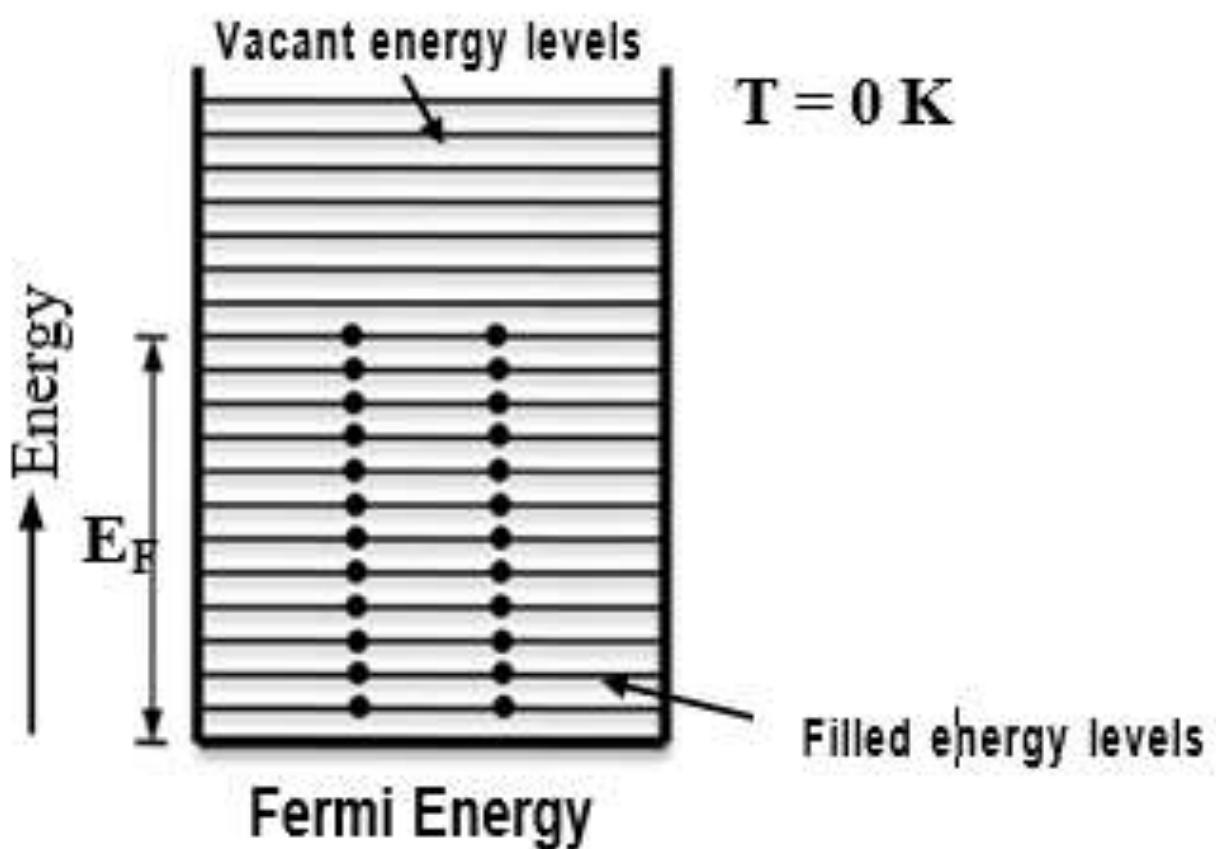
3. Fermi-Dirac Statistics

$$f(E) = \frac{1}{1 + e^{\frac{(hv)}{KT}}}$$

Fermi - level, Fermi - energy and Fermi - factor

- As we know that for a metal containing N atoms, there will be N number of energy levels in each band.
- According to Pauli's exclusion principle, each energy level can accommodate a maximum of two electrons, one with spin up ($+1/2$) and the other with spin down ($-1/2$).
- At absolute zero temperature, two electrons with opposite spins will occupy the lowest available energy level.
- The next two electrons with opposite spins will occupy the next energy level and so on.
- Thus, the top most energy level occupied by electrons at absolute zero temperature is called **Fermi-energy level**. The energy corresponding to that energy level is called **Fermi- energy**.

- The energy of the highest occupied level at zero degree absolute is called Fermi energy, and the energy level is referred to as the Fermi level. The Fermi energy is denoted as E_F .
- All energy levels below Fermi level are completely filled and above which all energy levels are completely empty.



The Fermi-Dirac Distribution Function

- The **Fermi-Dirac distribution function**, which provides the probability of occupancy of energy levels by electrons, is based on following premises:
 - Particles (electrons) are indistinguishable, and only one particle is allowed in each quantum state.
 - At absolute zero temperature ($T = 0 \text{ K}$), the energy levels are all filled up to a maximum level, called the **Fermi level**. Beyond the Fermi level, all states are empty.
 - At higher temperature, there is a gradual transition between the completely filled states and the completely empty states.
- Mathematically, Fermi-Dirac distribution function is given by,

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

and gives the probability that an available state at energy E will be occupied by an electron at absolute temperature T . The quantity E_F is called the **Fermi level**, and k is **Boltzmann's constant** ($k = 1.38 \times 10^{-23} \text{ J/K} = 8.62 \times 10^{-5} \text{ eV/K}$)

- Consider the situation where $T = 0 \text{ K}$.

$$\text{For } E < E_F, \quad f(E) = \frac{1}{1 + e^{(E-E_F)/kT}} = \frac{1}{1 + e^{-\Delta E/(kT \rightarrow 0)}} = \frac{1}{1 + e^{-\infty}} = 1$$

$$\text{For } E > E_F, \quad f(E) = \frac{1}{1 + e^{(E-E_F)/kT}} = \frac{1}{1 + e^{\Delta E/(kT \rightarrow 0)}} = \frac{1}{1 + e^{\infty}} = 0$$

- Thus for $T = 0 \text{ K}$, For energies $E < E_F$, all states are filled. For energies $E > E_F$, all states are empty.

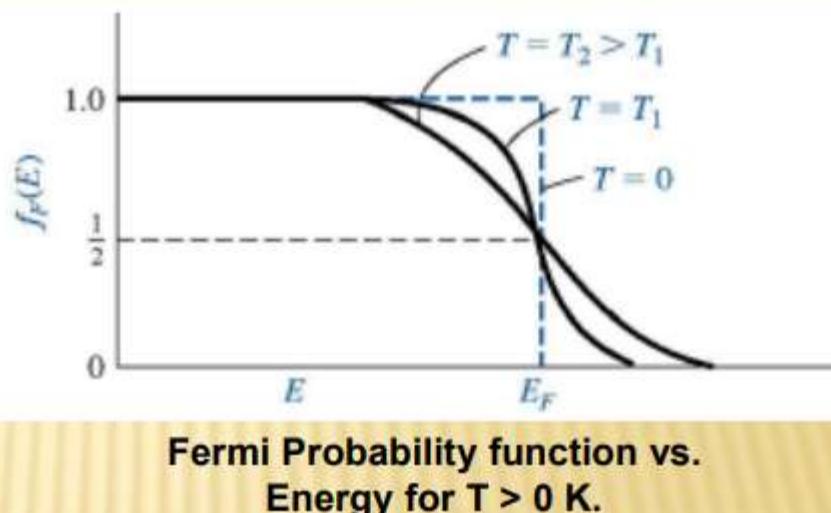
- Consider the situation where $T > 0$ K. For $E = E_F$,

$$f(E) = \frac{1}{1 + e^{(E-E_F)/kT}} = \frac{1}{1 + e^{0/kT}} = \frac{1}{2}$$

thus an energy state at the Fermi level has a probability of $\frac{1}{2}$ of being occupied by an electron.

In general, for temperatures $T > 0$ K, there is a nonzero probability that some energy states above E_F will be occupied by electrons and some energy states below E_F will be empty.

As the temperature climbs, we notice that more states below E_F are empty and more states above E_F are filled.



- For $E - E_F \gg kT$, Fermi-Dirac distribution function can be approximated to,

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



**DEPARTMENT OF PHYSICS AND NANOTECHNOLOGY
SRM INSTITUTE OF SCIENCE AND TECHNOLOGY**

21PYB102J – Semiconductor Physics and Computational Methods

Unit – 1 : Session – 10 : SLO - 1

Solving Problems

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

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

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 $F(E) = 0.2689$

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

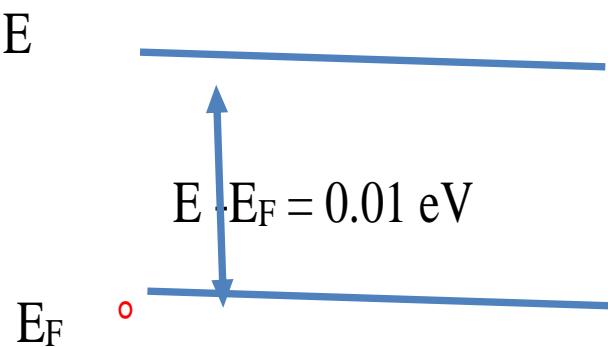
Given: T = 27 °C = 300K, k = $8.625 \times 10^{-5} \frac{e}{^{\circ}k}$

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

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

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

$$= 0.595$$



3. Use the Fermi distribution function to obtain the value of F (E) for E - E_F = 0.01 eV at 200 K.

Given data:

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

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

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

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

$$\begin{aligned} F(E) &= \frac{1}{1+e^{(1.6 \times 10^{-21})/(1.38 \times 10^{-23} \times 200))}} \\ &= \frac{1}{1+e^{0.5797}} \\ &= \frac{1}{1+1.7855} = \frac{1}{2.7855} \end{aligned}$$

$$\text{Fermi function } F(E) = 0.3589$$

4. 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,

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

Probability of occupying an energy level 0.11 eV above Fermi level

$$F(E) = \frac{1}{1+e^{(0.11\text{ eV})/k}} = \frac{1}{1+e^{-4.2307}} = 0.0126$$

Probability of occupying an energy level 0.11 eV below Fermi level

$$F(E) = \frac{1}{1+e^{(-0.11\text{ eV})/k}} = \frac{1}{1+e^{-4.2307}} = 0.987$$

21PYB102J – Semiconductor Physics and Computational Methods

Unit – 1 : Session – 10 : SLO - 2

Solving Problems

5. (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 occupied at $E = E_v - kT$

$$\text{Ans: (a)} f_F(E) = \frac{1}{1 + e^{-\left[\frac{E-E_v}{k}\right]}} = \frac{1}{1 + e^{-\left[\frac{E_c+k - E_c}{k}\right]}} = \frac{1}{1 + e^x} [1] = 0.269$$

$$\text{(b)} 1 - f_F(E) = 1 - \frac{1}{1 + e^{-\left[\frac{E-E_v}{k}\right]}} = 1 - \frac{1}{1 + e^{-\left[\frac{E_v-k - E_v}{k}\right]}} = 1 - \frac{1}{1 + e^x} [-1] = 0.269$$

6. Calculate the temperature at which there is 1% probability that a state of 0.3 eV below the Fermi energy level will not contain electron

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

$$0.01 = 1 - \frac{1}{1 + e^{\frac{0.3}{K}}}$$

$$KT = 0.06259 \text{ eV}$$

$$T = 0.06259 \text{ eV} / 8.62 \times 10^{-5} \text{ eV}$$

$$T = 756 \text{ K}$$

7. Determine the probability that an energy level $4KT$ above the Fermi energy is occupied by an electron at 300K

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

$$= \frac{1}{1+e^{\frac{(4K)}{K}}}$$

$$= \frac{1}{1+54.6}$$

$$= 0.1798$$

$$\sim 18\%$$

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Numerical determination of probability of occupation and carrier concentration

The Fermi-Dirac Distribution Function

- The **Fermi-Dirac distribution function**, which provides the probability of occupancy of energy levels by electrons, is based on following premises:
 - Particles (electrons) are indistinguishable, and only one particle is allowed in each quantum state.
 - At absolute zero temperature ($T = 0 \text{ K}$), the energy levels are all filled up to a maximum level, called the **Fermi level**. Beyond the Fermi level, all states are empty.
 - At higher temperature, there is a gradual transition between the completely filled states and the completely empty states.
- Mathematically, Fermi-Dirac distribution function is given by,

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

and gives the probability that an available state at energy E will be occupied by an electron at absolute temperature T . The quantity E_F is called the **Fermi level**, and k is **Boltzmann's constant** ($k = 1.38 \times 10^{-23} \text{ J/K} = 8.62 \times 10^{-5} \text{ eV/K}$)

- Consider the situation where $T = 0 \text{ K}$.

$$\text{For } E < E_F, \quad f(E) = \frac{1}{1 + e^{(E-E_F)/kT}} = \frac{1}{1 + e^{-\Delta E/(kT \rightarrow 0)}} = \frac{1}{1 + e^{-\infty}} = 1$$

$$\text{For } E > E_F, \quad f(E) = \frac{1}{1 + e^{(E-E_F)/kT}} = \frac{1}{1 + e^{\Delta E/(kT \rightarrow 0)}} = \frac{1}{1 + e^{\infty}} = 0$$

- Thus for $T = 0 \text{ K}$, For energies $E < E_F$, all states are filled. For energies $E > E_F$, all states are empty.



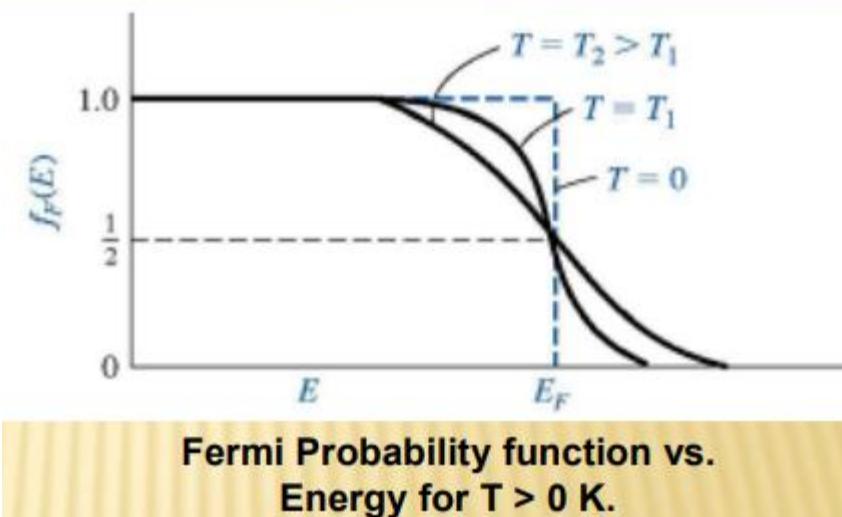
- Consider the situation where $T > 0$ K. For $E = E_F$,

$$f(E) = \frac{1}{1 + e^{(E-E_F)/kT}} = \frac{1}{1 + e^{0/kT}} = \frac{1}{2}$$

thus an energy state at the Fermi level has a probability of $\frac{1}{2}$ of being occupied by an electron.

In general, for temperatures $T > 0$ K, there is a nonzero probability that some energy states above E_F will be occupied by electrons and some energy states below E_F will be empty.

As the temperature climbs, we notice that more states below E_F are empty and more states above E_F are filled.



- For $E - E_F \gg kT$, Fermi-Dirac distribution function can be approximated to,

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

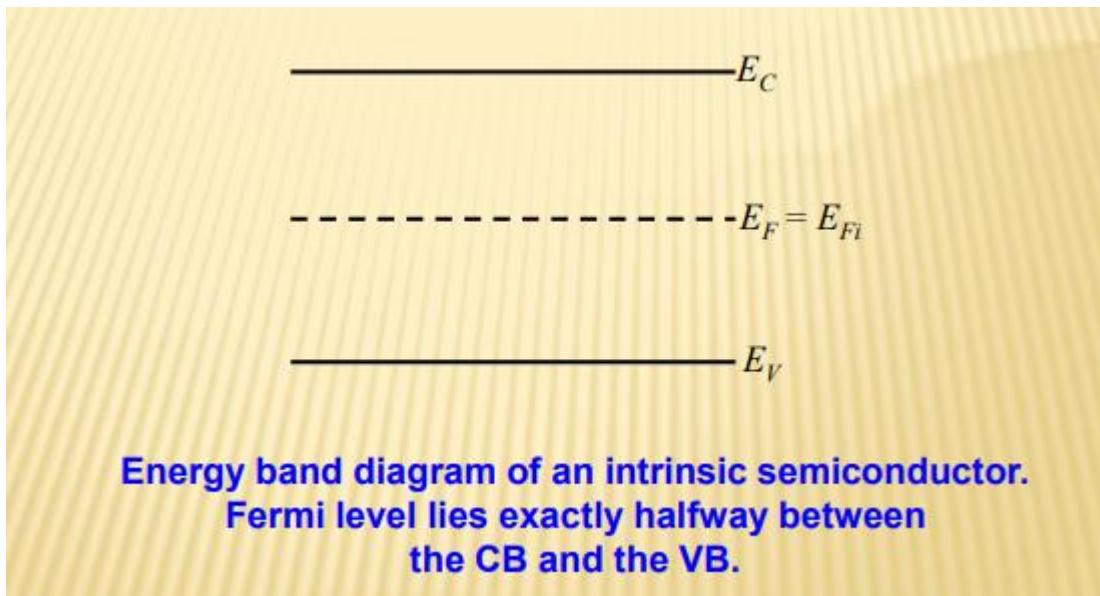
The Fermi Level – Intrinsic Semiconductor

For intrinsic semiconductor, since electrons and holes are generated in pairs, $n_0 = p_0$ for all temperature. This leads to,

$$\begin{aligned}
 f(E_C) &= 1 - f(E_V) \\
 \Rightarrow \frac{1}{1+e^{(E_C-E_F)/kT}} &= 1 - \frac{1}{1+e^{(E_V-E_F)/kT}} = \frac{e^{(E_V-E_F)/kT}}{1+e^{(E_V-E_F)/kT}} = \frac{1}{1+e^{-(E_V-E_F)/kT}} \\
 \Rightarrow e^{(E_C-E_F)/kT} &= e^{-(E_V-E_F)/kT} \Rightarrow E_C - E_F = -(E_V - E_F) \\
 \Rightarrow \boxed{E_F = \frac{1}{2}(E_C + E_V) = E_{Fi}}
 \end{aligned}$$

i stands for intrinsic, and E_{Fi} is the Fermi level for intrinsic semiconductor.

This shows that for *intrinsic semiconductor*, Fermi level lies exactly halfway between the CB and the VB.





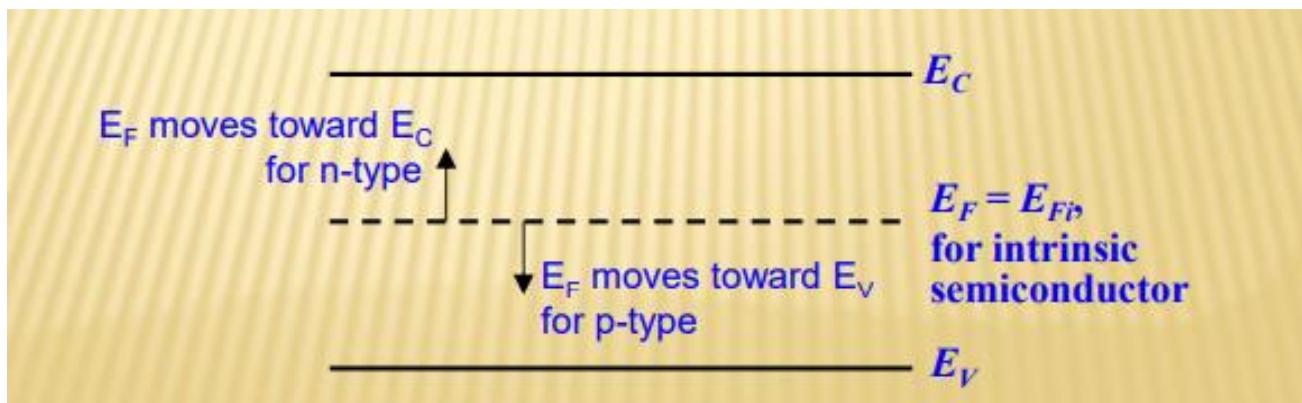
It can be concluded that

for n-type material E_F is closer to E_C

and as $(E_C - E_F) \downarrow \quad n \uparrow \quad p \downarrow$

Similarly for p-type material, E_F is closer to E_V

and as $(E_F - E_V) \downarrow \quad p \uparrow \quad n \downarrow$



We can now determine the position of the Fermi energy level as a function of the doping concentrations.

For n-type semiconductor

$$n_0 = N_C e^{-(E_C - E_F)/kT} \approx N_D$$
$$\Rightarrow E_C - E_F = kT \ln\left(\frac{N_C}{N_D}\right)$$

For p-type semiconductor

$$E_F - E_V = kT \ln\left(\frac{N_V}{N_A}\right)$$

Numerical determination of probability of occupation

Exercise: Assume the Fermi energy level is 0.30 eV below the conduction band energy and $T = 300$ K. Determine the probability of a state being occupied by an electron at E_c .

$$f(E) = \frac{1}{1 + e^{(E - E_F)/kT}} = \frac{1}{1 + e^{(E_c - E_F)/kT}} = \frac{1}{1 + e^{0.03\text{eV}/0.0259\text{eV}}} = 9.323 \times 10^{-6}$$

Exercise: Assume the Fermi energy level is exactly in the center of the bandgap energy of a semiconductor at $T = 300$ K.. Calculate the probability that an energy state in the bottom of the conduction band (at E_c) is occupied by an electron for Si

For Si, $E_g = 1.12$ eV. Since, $E - E_F = E_C - E_F = 0.56 \gg kT$, we can use the Boltzmann approximation:

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

$$\text{Hence, } f(E) = e^{-(E - E_F)/kT} = e^{-(E_c - E_F)/kT} = e^{\frac{-0.56\text{eV}}{0.02586\text{eV}}} = 3.938 \times 10^{-10}$$

CARRIER CONCENTRATION

- Current is the rate at which charge flows. The charge carriers in a semiconductor are electrons and holes. To determine the electrical properties and analyze device behavior, we often need to know the carrier concentration i.e., number of electrons and holes per cm^3 of the material.
- For heavily doped extrinsic semiconductor,

$$n_0 \approx N_D \gg p_0 \quad (\text{for n-type}) \text{ and}$$

$$p_0 \approx N_a \gg n_0 \quad (\text{for p-type})$$

However, we don't know anything about the minority carrier concentration. Nor do we know about the temperature dependence of the carriers.

- In this section, we wish to determine the concentration of electrons and holes in the conduction and valence bands.
- Electrons and holes are distributed over the empty conduction band and valence band states, respectively, as function of energy. The distribution depends upon the temperature. So it is important to find the electron and hole distribution over the required energy range, in order to determine the carrier concentration.

Equilibrium Electron and Hole Concentrations

To calculate the number of electrons in the CB and holes in the VB we must know

- 1) How many states are available
- 2) What is the probability of occupancy We thus introduce $g(E)dE$, DENSITY OF STATES (cm^{-3}), available for occupancy in the energy range dE .

Electron Distribution

- The distribution (with respect to energy) of electrons in the conduction band is given by the density of allowed quantum states, $g_c(E)$, times the probability, $f(E)$, that an electron occupies a state.

$$n(E) = g_c(E)f(E)$$

where $f(E)$ is the Fermi-Dirac probability function and $g_c(E)$ is the density of quantum states in the conduction band.

Hole Distribution

- The distribution (with respect to energy) of holes in the band is given by the density of allowed quantum states, $g_v(E)$, times the probability, $1-f(E)$, that a state is Not occupied by an electron.

$$p(E) = g_v(E)[1 - f(E)]$$

- Both $g(E)$ and $f(E)$ are in terms of per unit volume per unit energy

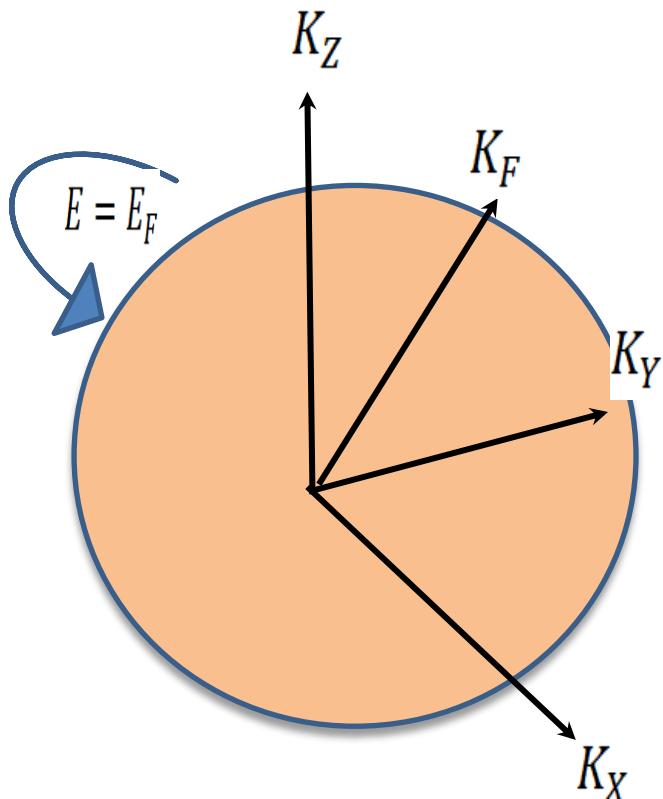
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Concept of Fermi surface of a metal

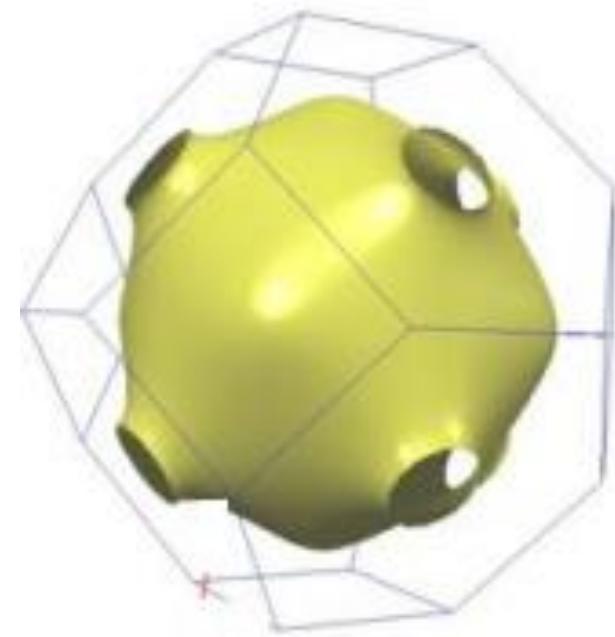
Fermi surface



- The Fermi surface: It is the distribution of the electrons in momentum space. It is the surface in reciprocal space which separates occupied from unoccupied electron states at zero temperature.
- In other words, it is the boundary in momentum space beyond which no electrons can exist. The surface of this sphere is called the Fermi surface.
- It is a plot of constant energy with $E = E_F$.
- All the free electron states within a Fermi sphere in k -space are filled up to a Fermi wavevector, \mathbf{k}_F .

Fermi Surface of Copper

- Cu electronic configuration is [Ar] $3d^{10} 4s^1$, The electron concentration in a monovalent (i.e. single electron delocalized in S orbital) metal atom is found to be $n=4/a^3$ {i.e. 4es are in cube of volume $a^3\}$
- The shape of the Fermi surface is an important factor in determining the electrical and thermal conductivity of the metal, as well as other properties like magnetism.
- It is nonspherical with 8necks, they are in contact with the first BZ of FCC lattice.





Calculation of Fermi Sphere radius and diameter

The radius of a free e Fermi sphere is

$$K_F = (3\pi^2 n)^{1/3}$$

$$n = \frac{4}{a^3}$$

$$\begin{aligned} K_F &= (12\pi^2/a^3)^{1/3} \\ &= (12 \times 3.14^2/a^3)^{1/3} \\ &= 4.90/a \end{aligned}$$

I. Concentration of the electrons in a monovalent (i.e. single electron delocalized in S orbital) metal such as Copper atom is found to be $n=4/a^3$ {i.e. 4es are in cube of volume a^3 }

Thus, Diameter of sphere is $9.80/a$

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Computational determination of Fermi Surface



Compute Fermi Surface :

- It is possible to compute the Fermi surface and use it to forecast a variety of material properties.
- These properties include thermal, electrical, magnetic, and optical properties.
- The shape is generated from the crystal lattice's periodicity and symmetry, as well as the energy bands.

Computational approach and Fermi surface

- Computational determination of the Fermi surface involves several steps and relies on quantum mechanical calculations. The most commonly used method for electronic structure calculations is Density Functional Theory (DFT).

Density Functional Theory (DFT) Calculations:

- This is a widely used first-principles approach that calculates the electronic structure of a material by modeling of the solid crystal in periodic manner using varieties of the software.
- DFT: On Brillouin zone calculation using high symmetry K-Points, and of the Fermi surface is computed.



Steps are followings:

Brillouin Zone and k-point Sampling:

- **Reciprocal Space:** Transform the crystal structure to reciprocal space to define the Brillouin zone. This zone represents the periodicity of the crystal structure in reciprocal lattice space.
- **k-point Sampling:** Discretize the Brillouin zone into a set of special k-points. The number and distribution of k-points influence the accuracy of the calculations. High symmetry points are often used in the k-point sampling.



Band Structure Calculation:

- Calculate the electronic band structure by solving the Kohn-Sham equations at each k-point.
- Get the energy eigenvalues and corresponding eigenvectors for each k-point, representing the electronic bands.

Fermi Surface Construction:

- Construct the Fermi surface by connecting the points in the Brillouin zone where the electronic bands cross the Fermi level.
- The Fermi surface represents the boundary between occupied and unoccupied electronic states.