Free Electron Theory

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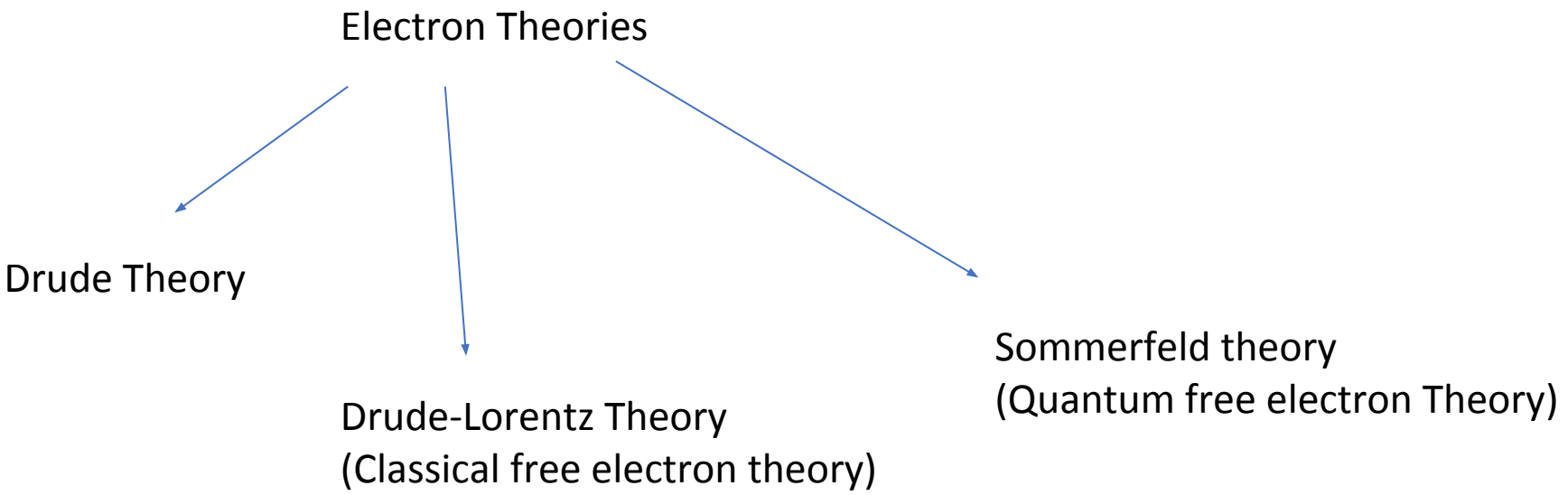
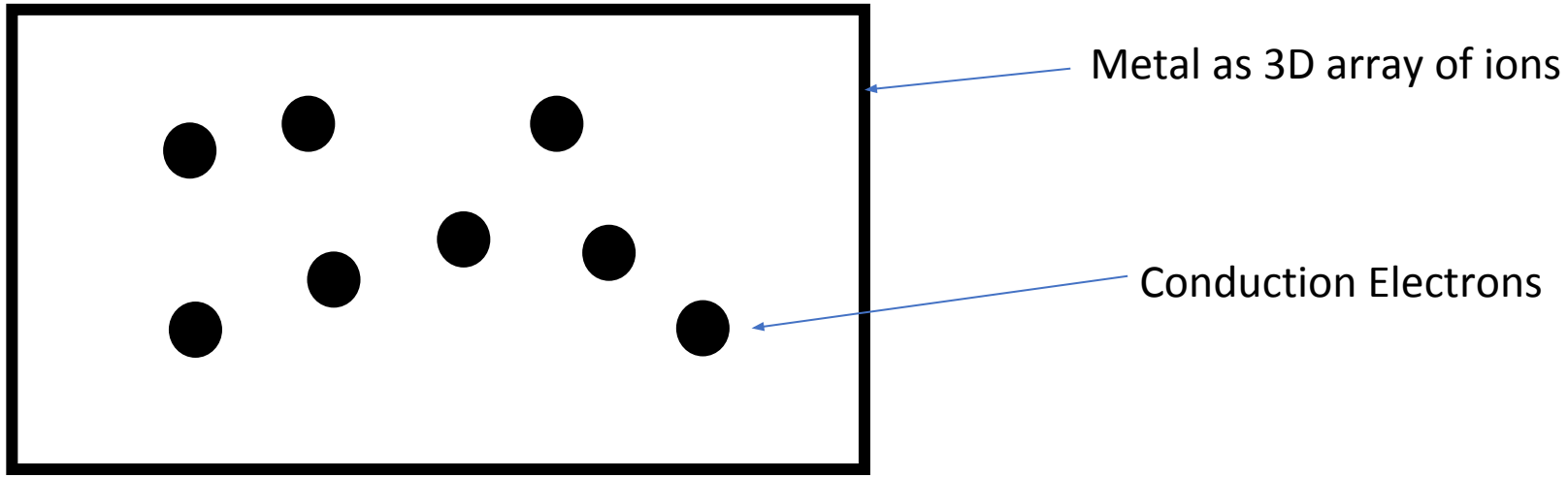
Introduction



Free Electron Theory

- Electrons are free to move anywhere in the metal in the same way as gas molecules. Therefore it can be terms as free electron gas model .



Therefore they obey law of kinetic theory of gases

Force of repulsion between electrons is considered insignificant

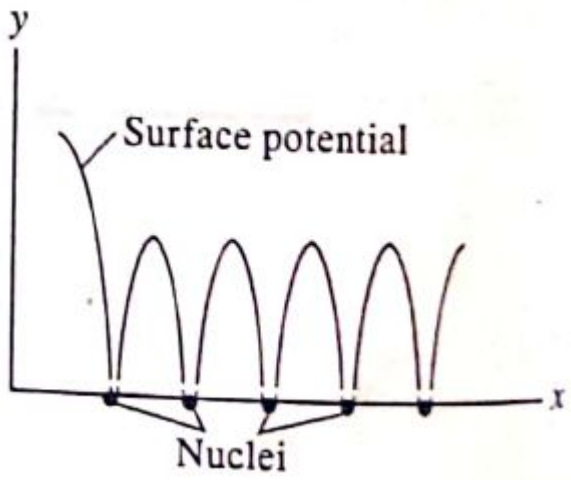
Potential = Constant

Force = 0

Failures

- Never explain the difference between metal, semiconductor, insulators.
- It tells that F=0 which is not actually true. When an electron passes near an ion , a force acts on it.
- V= constant (by theory) , but actually a periodic change in potential occurs when electron pass from one place to the other.

$$V \propto \frac{1}{r}$$



- It does not explain the concept of specific heat, temperature dependence of electrical conductivity and dependence of electrical conductivity on concentration of electrons.

Sommerfeld Theory- Quantum Free Electron theory

1. The energy values of the conduction electrons are quantized. The allowed energy values are realized in terms of a set of energy values.
2. The distribution of electrons in the various allowed energy levels occur as per Pauli's exclusion principle.
3. The electrons travel with a constant potential inside the metal but confined within its boundaries.
4. The attraction between the electrons and the lattice ions and the repulsion between the electrons themselves are ignored.
5. With the increase of temperature the energy levels below E_F are vacated and above E_F are occupied.
6. The distribution electrons among the different energy levels at any temperature is given by Fermi-Dirac distribution function f(E). It is defined as $f(E) = \frac{1}{1+\exp\left(\frac{E-E_F}{KT}\right)}$.
7. Electrons are treated as wave-like particles.

*The **wave function Ψ** is a mathematical expression. It carries crucial **information about the electron** it is associated with: from the **wave function** we obtain the electron's energy, angular momentum, and orbital orientation in the shape of the quantum numbers n, l, and m_l.*

*The **square of the wave function, ψ^2** , represents the **probability of finding** an **electron** in a given region within the atom.*

Q: Discuss the physical significance of the wave function Ψ ?

Bloch Theorem

Why do u study?

*Bloch's theorem (1928) applies to **wave functions** of electrons inside a crystal and rests in the fact that the Coulomb **potential in a crystalline solid is periodic**.*

*As a consequence, the **potential energy function**, $V(\vec{r})$, in Schrödinger's equation should be of the form:*

$$V\left(\vec{r}\right) = V\left(\vec{r} + \vec{R}_n\right)$$

*where $R_n^{\rightarrow}$ represents an arbitrary **translation vector** of the crystallographic lattice,*

The Bloch theorem enables us to calculate the electronic wave functions and electron energies

*The **translation vector** is the distance through which an atom must be moved (translated) in order to be in the next unit cell.*

$$\vec{R}_n = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3$$

a1,a2,a3 are the unit lattice vectors

Postulates of Bloch Theorem

Bloch's theorem establishes that

1) The wave function $\psi_k^{\rightarrow}(\vec{r})$ in a crystal can be expressed as the **product of a plane wave and a function $u_k^{\rightarrow}(\vec{r})$** which has the same periodicity as the lattice, i.e.

$$\psi_{\vec{k}}\left(\vec{r}\right) = e^{i\vec{k}\cdot\vec{r}}\, u_{\vec{k}}\left(\vec{r}\right) \qquad \text{.....(1)}$$

where

$$u_{\vec{k}}\left(\vec{r}\right) = u_{\vec{k}}\left(\vec{r} + \vec{R}_n\right)$$

T = ***translation vector***

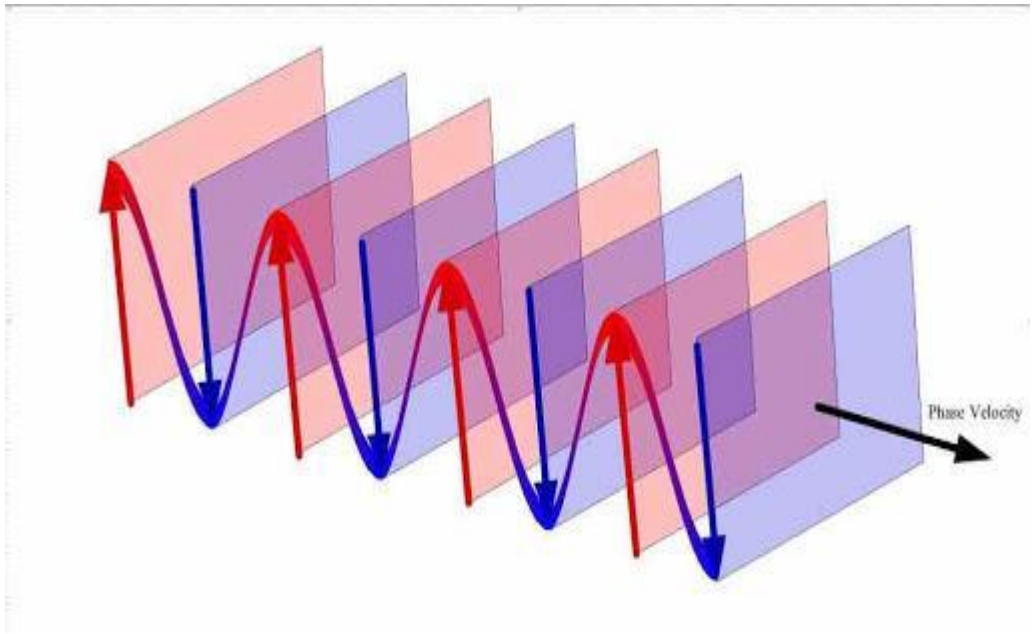
The electron wave functions, of the form of Eq. (1), are called ***Bloch functions***.

2) We can describe the Bloch wave function in terms of translational vector as -

$$\psi_{\vec{k}}\left(\vec{r}+\vec{R}_n\right)=e^{i\vec{k}\cdot\vec{R}_n}\psi_{\vec{k}}\left(\vec{r}\right)$$

Q: State Bloch's theorem for a periodic system
(2 Marks)

A **plane wave** is a special case of wave or field: a physical quantity ***whose value, at a given moment***, is constant for all points of any plane that is perpendicular to a fixed direction in space



Basic Concept

Wave nature of electrons [Sommerfeld (Quantum Free electron) theory]

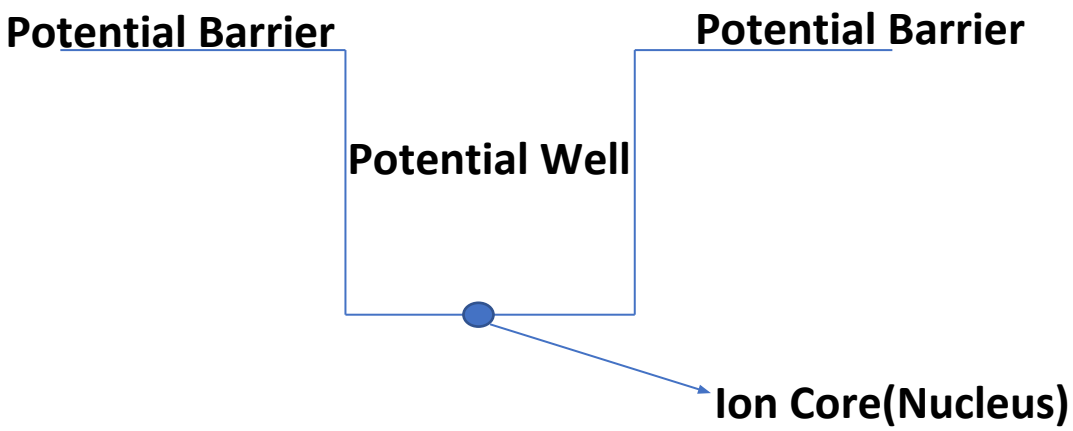
Assign a wave function to the electrons (Consider V is periodic) [Bloch Theory]

To study the effect of periodic potential on the energy of electrons [Kronig-Penny Model]

Kronig Penny model

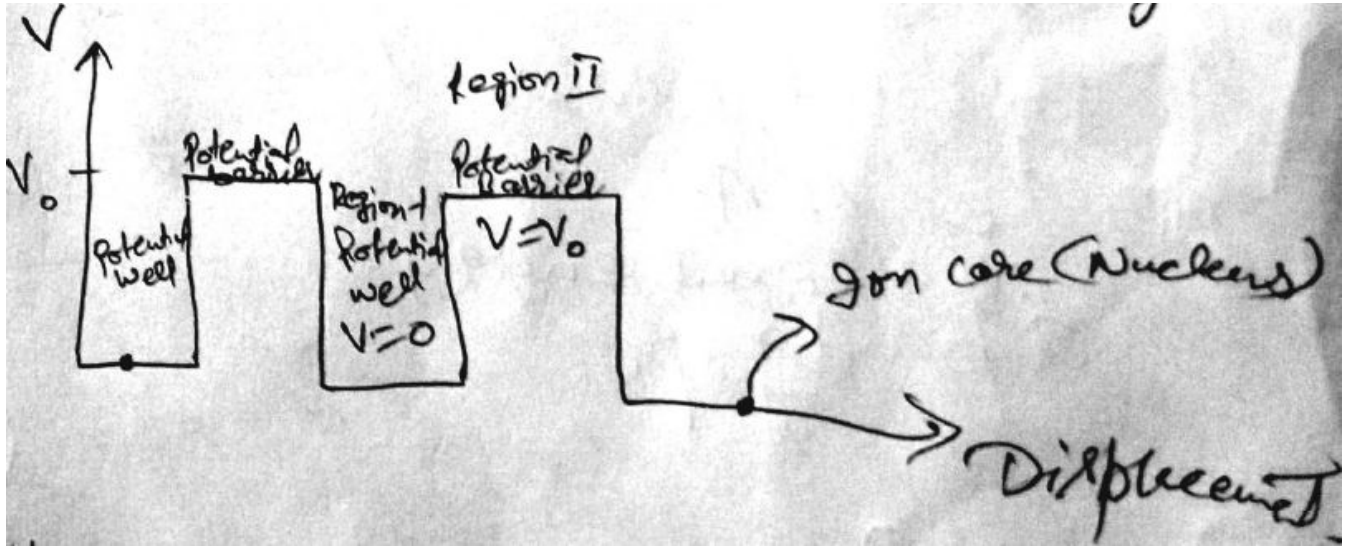
It tells us the effect of periodic potential on the energy of electrons in a metal.

- The **Kronig** - **Penney model** is a simplified **model** for an electron in a one-dimensional periodic potential.
- The possible states that the electron can occupy are determined by the Schrödinger equation, In the case of the Kroning-**Penney model**, the potential V(x) is a periodic square wave.

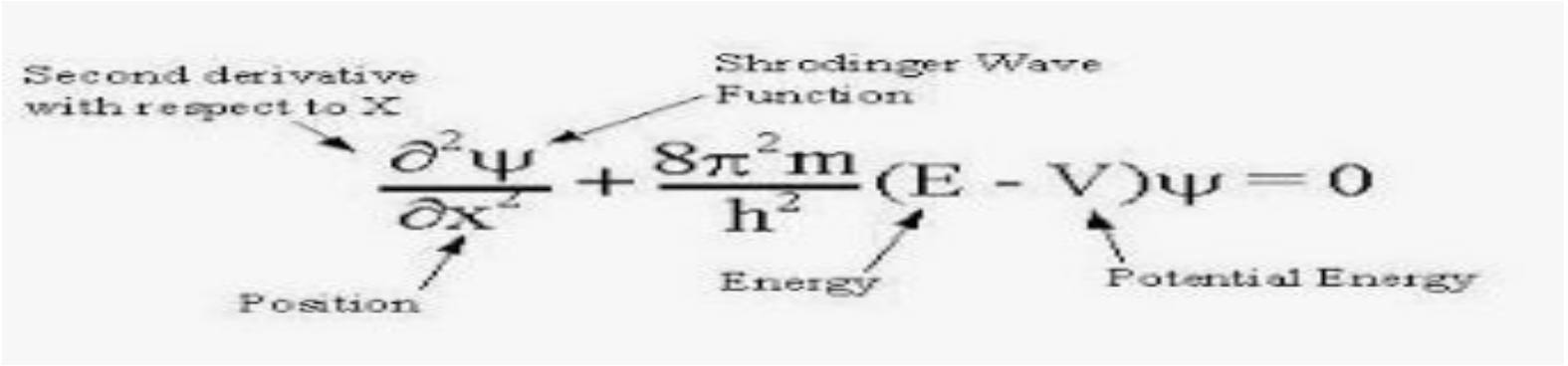


Theory :

1. **Potential of electrons varied periodically with periodicity of ion core (nucleus).**
2. **Potential energy of electrons is zero near nucleus V= 0 (Region I)**
3. **Potential energy is maximum when it is lying between the adjacent nuclei which are separated by the interatomic spacing ''a'' => V = Vo (Region II)**



Applying Schrodinger time independent equation (for region I and II)



$\hbar = h/2\pi$

h is Planck's constant

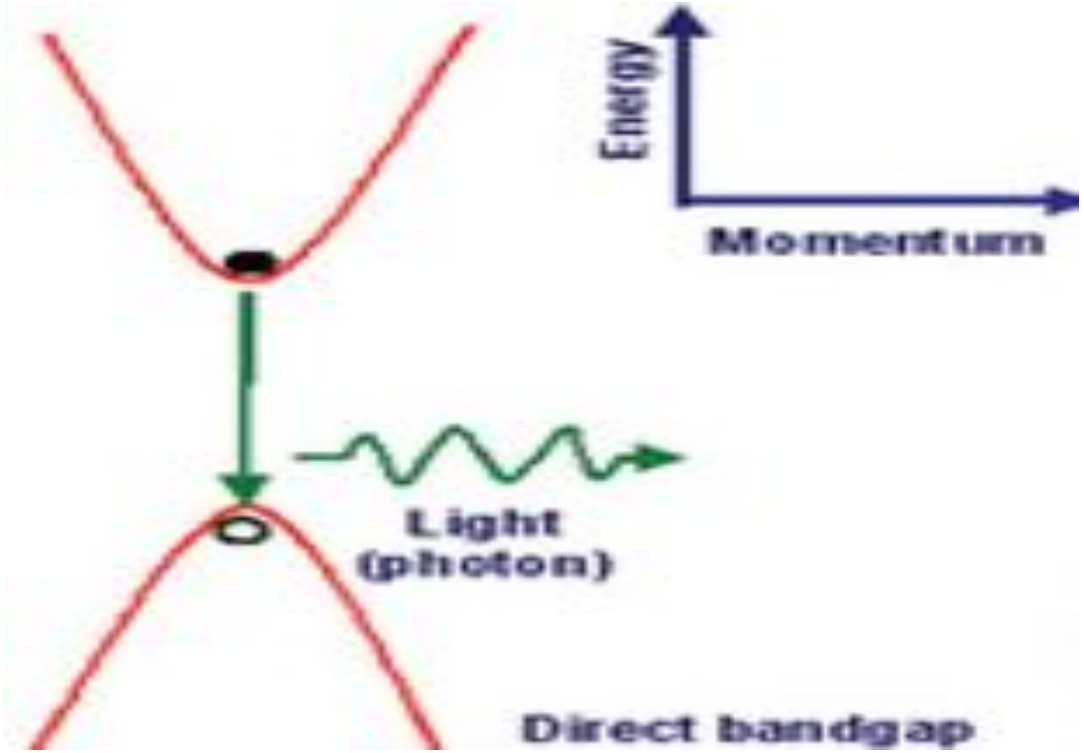
By solving all parameters we get..(see in notes)

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

This is Kronig Penny Model

Direct Band Gap

- *The **band gap** is called "**direct**" if the crystal momentum of electrons and holes is the same in both the conduction **band** and the valence **band***
- *An electron can **directly** emit a photon.*



Indirect Band Gap

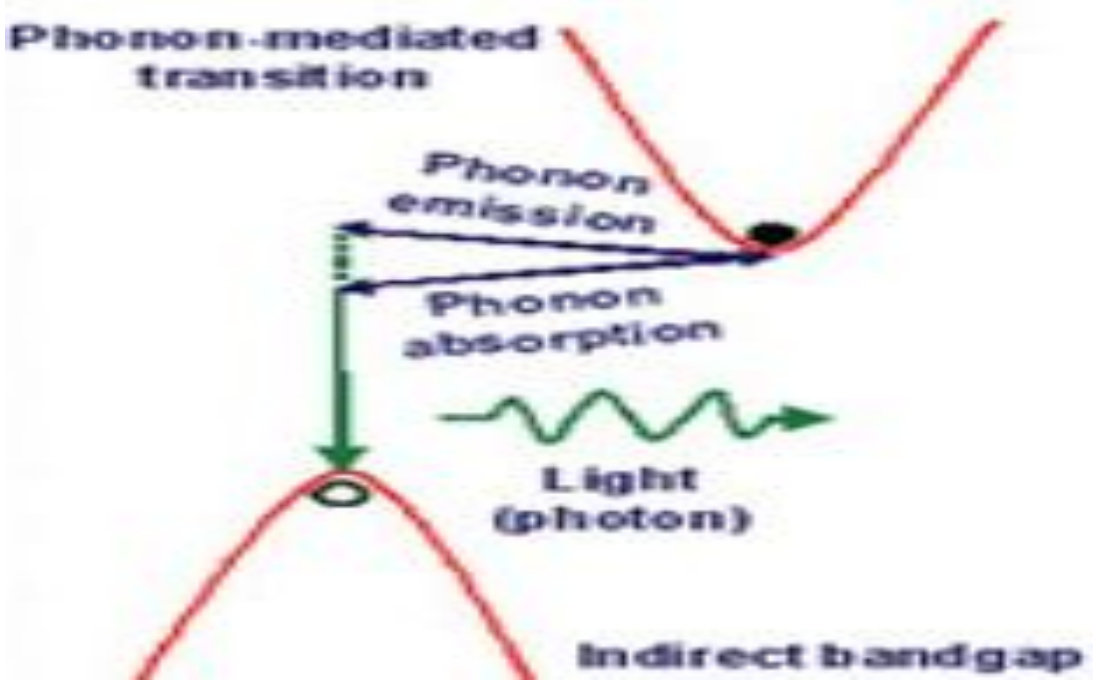
Upper and the lower electronic states (conduction and valence bands) do not occur at the same value of crystal momentum.

Mechanism:-

Because visible or infrared photons have negligible momentum (compared to that of the electron), the de-excitation of an electron (recombination) needs to be mediated by emitting or absorbing a phonon in order to conserve momentum.

The electron in the upper state has to sit and wait until a phonon with the right momentum shows up. While waiting, it becomes prone to non-radiative recombination with the energy being dissipated as heat.

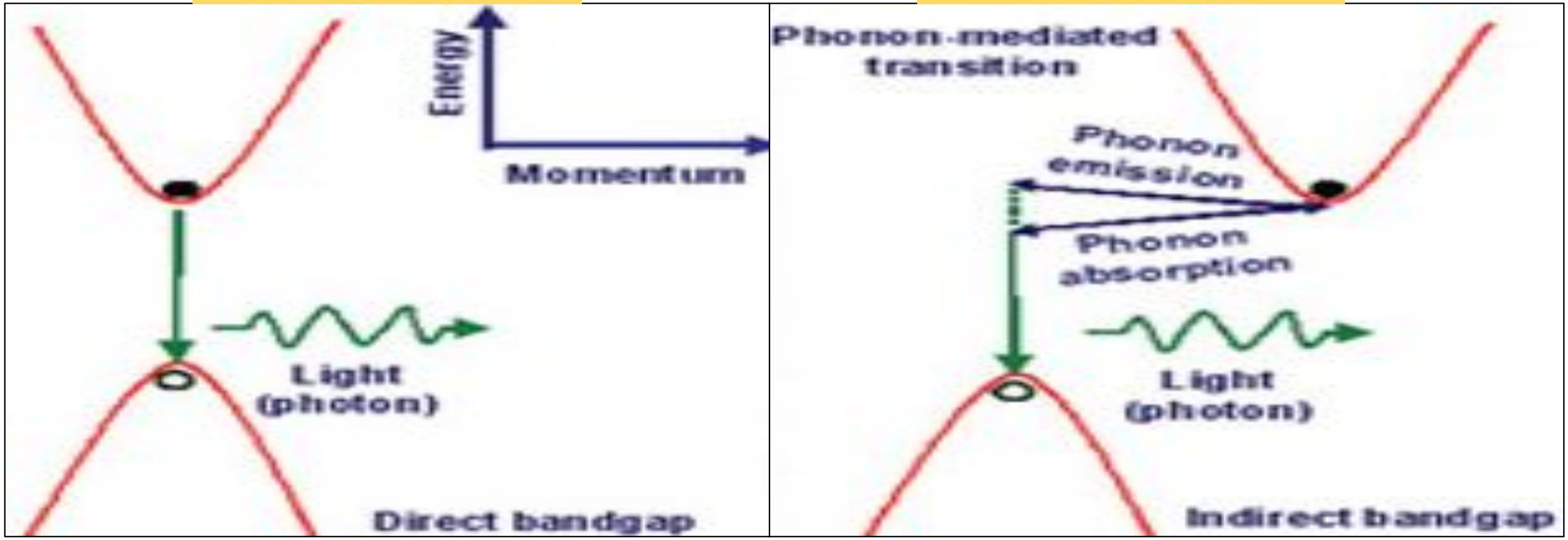
The desired radiative processes are insignificant compared to undesired nonradiative recombination.



Q:-Why do we use direct band gap semiconductors in LASER?

Direct Band Gap

Indirect Band Gap



Phonon

- **The quanta of energy of lattice vibration is called phonon.**
- **A quantum of energy or a quasiparticle associated with a compressional wave such as sound or a vibration of a crystal lattice.**
- **They are quantized sound waves.**
- **a phonon is a collective excitation in a periodic, elastic arrangement of atoms or molecules in condensed matter, specifically in solids and some liquids.**
- phonons have been treated with wavevector *k* as though it has a momentum *ħk and energy ħw.*

Phonon on lattice does not carry momentum but phonon of wave vector k interacts with other particles and fields as if its momentum were *ħk.*

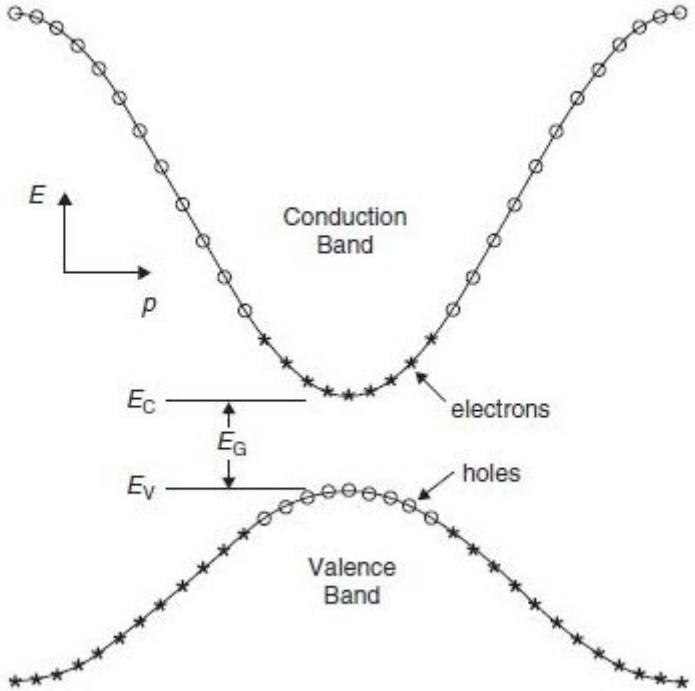
Photon

They are quantized light waves

E-k diagram

The E-k diagram (or band structure) converts the mathematical formalism of the wave vector into useful information about the allowed energy levels of an electron in a crystal.

According to E-K diagram, For a given k (which corresponds to motion in a certain direction in the crystal) only certain energy levels E are accessible to an elec



Effective mass

A particle's effective mass (m*) is the mass that it seems to have when responding to forces, or the mass that it seems to have when interacting with other identical particles in a thermal distribution.

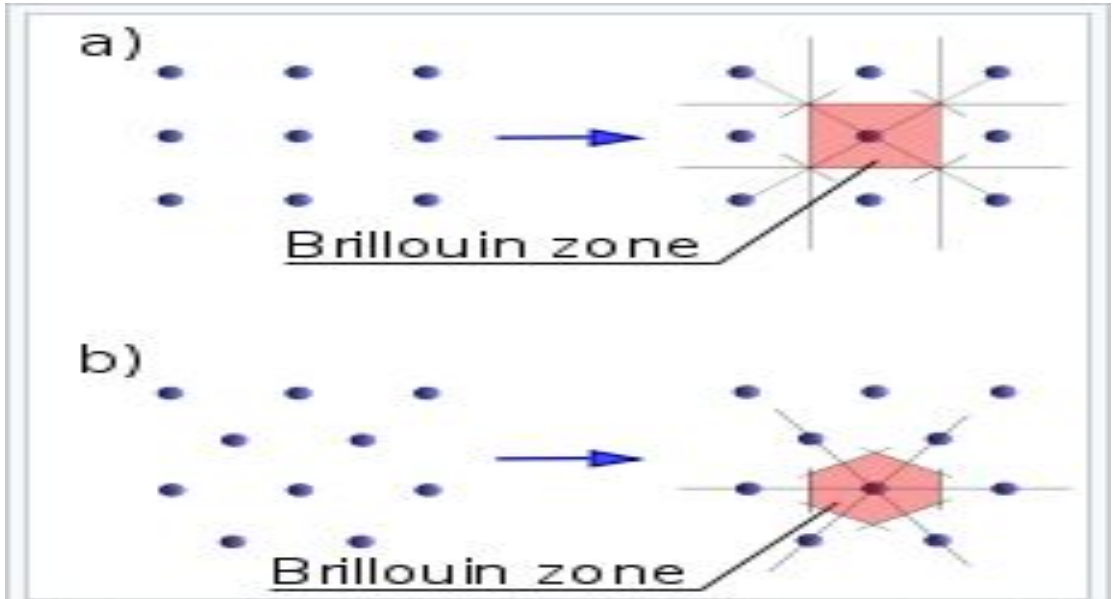
Application:-The electronic effective mass can be seen as an important basic parameter that influences measurable properties of a solid, including everything from the efficiency of a solar cell to the speed of an integrated circuit.

Brillion Zone

Set of points in *k*-space that can be reached from the origin without crossing any Bragg plane.

or

First **Brillouin zone** is a uniquely defined primitive cell in reciprocal space.

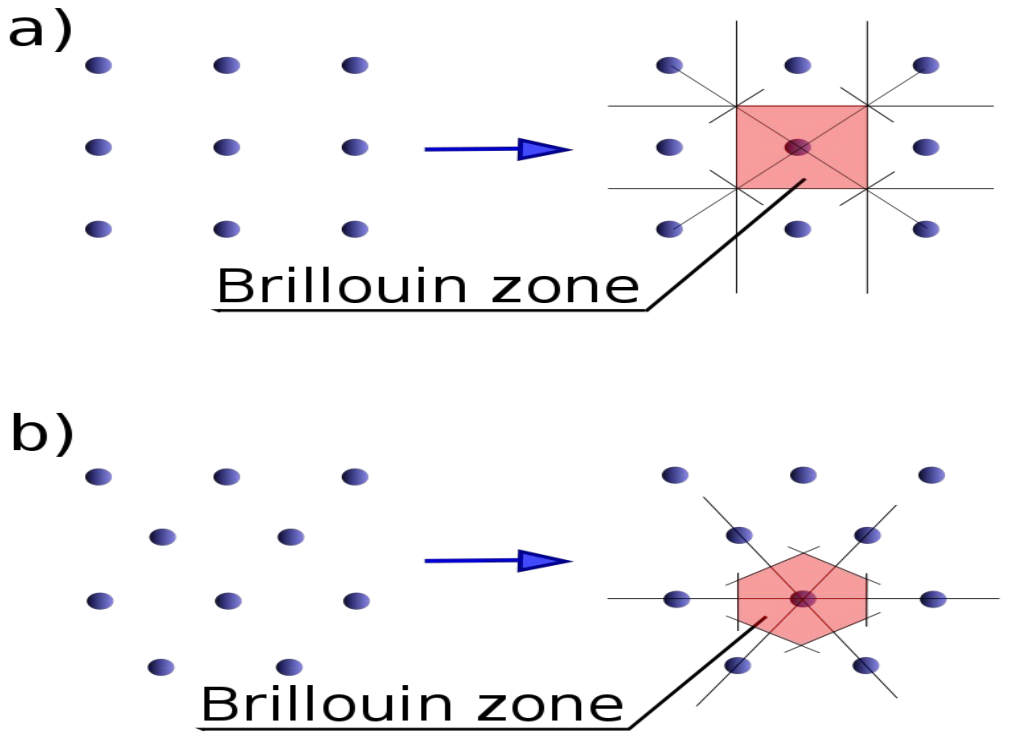


The reciprocal lattices (dots) and corresponding first Brillouin zones of (a) square lattice and (b) hexagonal lattice.

Brillouin zones are nothing but allowed energy regions in momentum space for electrons present in periodic crystals. The electrons present in periodic crystals are commonly referred as ‘Bloch electrons or Bloch waves’. The Brillouin zones are also referred as primitive cells in the reciprocal lattice or Wigner Seitz cell of the corresponding lattice.

The allowed energy regions (Brillouin zones) have certain boundaries in momentum space. For simple cubic structures , at the boundaries of Brillouin zone the group velocity of the Bloch waves tends to zero. Consequently, standing waves are formed at the boundaries. In contrast, within the Brillouin zone Bloch waves behave as traveling like waves. Such a change in the behavior of Bloch waves from traveling to standing wave formation, results in origin of energy gap at the boundaries. This is commonly called Bragg diffraction of Bloch electrons at the zone boundaries. The diffraction at the zone boundary depends on the crystal structure under investigation. Of course the magnitude of band gap and shapes of energy bands are ultimately determined by the periodic potentials involved. Brillouin zones play important role in understanding the electronic properties of crystals.

Thank You


a)
Brillouin zone
b)
Brillouin zone

Several Types of Differential Equations and their solution:

1) Solution of differential equation $\frac{dy}{dx} = f(x)$ is $y = \int f(x)\,dx + c$

2) Solution of differential equation $\frac{dy}{dx} = f(x)\,g(y)$ is $y = \int \frac{dy}{g(y)} = f(x)\,dx + c$

3) Solution of differential equation $\frac{dy}{dx} = f(ax + by + c)$ by putting

ax + by + c = v and $\frac{dy}{dx} = \frac{1}{b}\left(\frac{dv}{dx} - a\right)\frac{dv}{a + b\,f(x)} = dx$

Thus solution is by integrating $\int \frac{dv}{a + b\,f(v)} = \int dx$.

4) To solve the homogeneous differential equation $\frac{dy}{dx} = \frac{f(x,y)}{g(x,y)}$,

Substitute y = vx and so $\frac{dy}{dx} = v + x\frac{dv}{dx}$.

Thus $v + x\frac{dv}{dx} = f(v) \Rightarrow \frac{dx}{x} = \frac{dv}{f(v) - v}$

There solution is $\int \frac{dx}{x} = \int \frac{dv}{f(v) - v} + c$

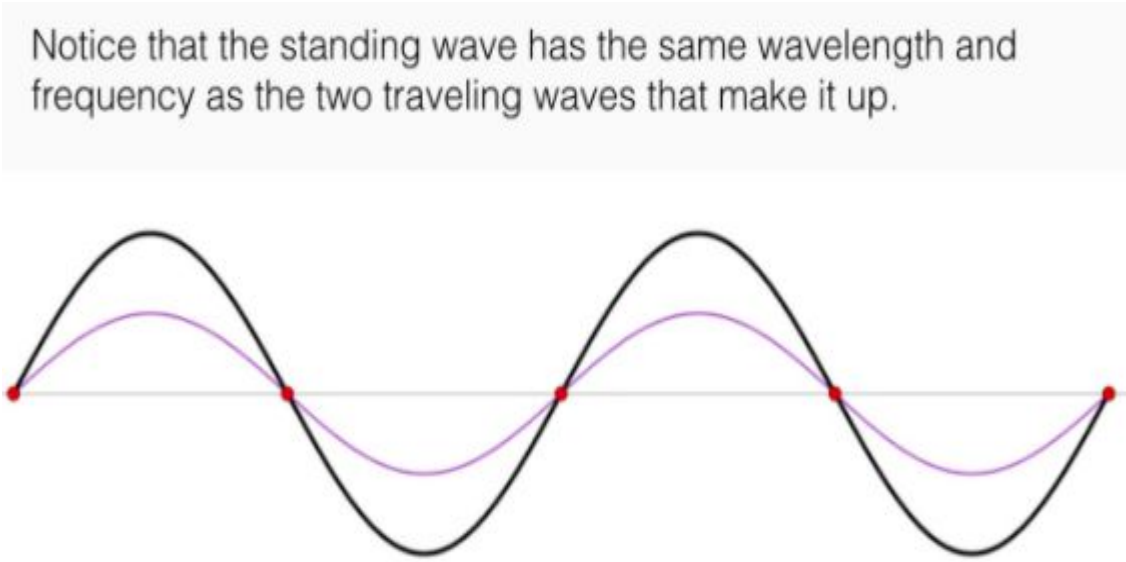
5) Solution of the linear differential equation $\frac{dy}{dx} + Py = Q$. where P and Q are either constants or functions of x, is $ye^{\int P\,dx} = \int \left(Qe^{\int P\,dx}\right)dx + c$ where $e^{\int P\,dx}$ is called the integrating factor.

6) Solution of the differential equation $\frac{d^2y}{dx^2} = f(x)$ is obtained by integrating if with respect to x twice.

- There is the **time dependent** Schrodinger equation used for describing progressive waves, applicable to the motion of free particles.

- The **time independent** form of this equation used for describing standing waves

Standing wave, also known as a stationary wave, is a wave which oscillates in time but whose peak amplitude profile does not move in space. The peak amplitude of the wave oscillations at any point in space is constant with time, and the oscillations at different points throughout the wave are in phase.



Crystal Momentum

phonons have been treated with wavevector k as though it has a momentum $\hbar k$, however, this is not strictly correct, because $\hbar k$ is not actually a physical momentum; it is called the *crystal momentum* or *pseudomomentum*.