UNIT-2(BAND THEORY OF SOLIDS)

07 August 2025

CLASSICAL FREE ELECTRON THEORY (Qualitative)

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What is Classical Free Electron Theory?

This theory was proposed by **Drude and Lorentz** to explain the electrical and thermal properties of metals.

• It treats **electrons in a metal** as **free particles** that move like gas molecules.

• These free electrons can move in **any direction** inside the metal without being bound to atoms.

• When an electric field is applied, electrons **move and create electric current**.

Key Assumptions:

• Metals have **a large number of free electrons**.

• Electrons obey **classical laws (Newton's laws)**.

• **No interaction** between electrons.

• **Scattering** happens when electrons hit metal ions, causing resistance.

Limitations:

• Could **not explain** why some metals are good or bad conductors.

• Fails to explain **heat capacity, Hall effect,** and **temperature dependence of conductivity**.

• Does **not include quantum ideas** like wave nature of electrons.

14. KRONIG-PENNEY MODEL (Qualitative)

What is the Kronig-Penney Model?

The Kronig-Penney model is a **quantum mechanical model** that explains how **electrons behave in a crystal** (a periodic structure of atoms).

• It uses **periodic potential wells** to represent how electrons feel forces from **repeating atoms** in a crystal.

• Helps to understand the formation of **energy bands and band gaps** in solids.

• It is a better model than the free-electron model because it includes **quantum effects** and **periodic structure** of crystals.

What It Shows:

• Electrons are not completely free – they move through a **repeating potential** due to atoms.

• Electrons can exist in **allowed energy bands**, but there are also **forbidden energy gaps** (band gaps).

• Explains why **metals, semiconductors, and insulators** behave differently.

15. POSTULATES OF KRONIG-PENNEY MODEL

Basic Postulates:

1. **Periodic Potential**:

   The potential energy of an electron in a crystal is **periodic** (repeats at regular intervals), because atoms are arranged in a regular pattern.

2. **One-Dimensional Model**:

   The model considers electron motion in **one direction** (1D) for simplicity.

3. **Square Well Potential**:

   The potential is assumed to be a **series of square wells** (regions of low and high potential energy).

4. **Schrödinger Equation Used**:

   Electron behavior is studied using the **Schrödinger equation** with this periodic potential.

5. **Bloch's Theorem Applies**:

   The wave function of the electron follows **Bloch's theorem**, meaning it has a special form that reflects the periodic nature of the crystal.

   Here is a **clear and simple explanation** of the **Origin of Energy Bands in Solids** with a basic **derivation**, following your preferred structured format:

16. ORIGIN OF ENERGY BANDS IN SOLIDS

What are Energy Bands?

In solids, electrons do **not have individual, fixed energy levels** like in isolated atoms. Instead, their energy levels form **bands** — large groups of closely spaced energy levels.

• These are called **energy bands**, and the **forbidden gaps** between them are called **band gaps**.

• This concept explains why some materials are **conductors**, some are **semiconductors**, and others are insulators.

How do Energy Bands Form?

1. **In isolated atoms**, electrons have **discrete energy levels**.
2. When many atoms come close to form a **solid**, their energy levels **overlap**.
3. Due to **Pauli's exclusion principle**, no two electrons can have the same quantum state.
4. So, each energy level splits into **many closely spaced levels** — forming **bands**.
5. As the number of atoms (N) becomes very large (~10^{23}), these levels appear **continuous**, forming **energy bands**.

Two Important Bands:

- **Valence Band**: The highest range of electron energies that are normally filled.
- **Conduction Band**: The range of energies where electrons can move freely and conduct electricity.
- **Band Gap (Eg)**: The energy gap between the valence band and conduction band.

DERIVATION (Simple Model using Kronig-Penney)

Let's use the **Kronig-Penney Model** to derive the idea of **energy bands**.

Assumption:

The potential inside a crystal is **periodic**:

$$V(x) = V(x+a)$$

(Where **a** is the spacing between atoms)

Schrödinger's Equation:

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

Using **Bloch's theorem**:

$$\psi(a) = e^{iKa}\psi(0)$$

$$\psi'(a) = e^{iKa}\psi'(0)$$

Substitute and solve for allowed energy values → gives the condition:

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

Where:

- **k** = electron wave vector
- **a** = lattice constant
- **P** = constant depending on potential
- **$\alpha = \sqrt{2mE}/\hbar$**

Result:

- This equation is **not always solvable** for every value of E.
- Only certain **energy values** satisfy it → these are the **allowed energy bands**.
- The values of E that **don't satisfy** the equation form **band gaps**.

NOTE:• In a **crystal**, due to periodic atomic arrangement, the electron's wave nature leads to **splitting of energy levels** into **bands**.

• The **existence of allowed and forbidden energy regions** (bands and gaps) explains electrical properties:

– **Conductor** → overlapping bands

– **Semiconductor** → small band gap

– **Insulator** → large band gap

17. CLASSIFICATION OF CONDUCTORS, SEMICONDUCTORS, AND INSULATORS

Based on Energy Band Theory, materials are classified into three types depending on how electrons fill the energy bands and the size of the band gap (the energy difference between the valence band and the conduction band):

1. CONDUCTORS

What are Conductors?

Materials that allow **easy flow of electric current** because they have **free electrons** available for conduction.

Band Theory Explanation:

• **Valence band and conduction band overlap** (no band gap).

• Electrons can easily move to the conduction band without needing extra energy.

• Example: **Metals** like copper, silver, and aluminum.

2. SEMICONDUCTORS

What are Semiconductors?

Materials that **do not conduct electricity well at room temperature**, but can conduct under **certain conditions** (like heat or doping).

Band Theory Explanation:

• Small band gap, typically around **1 eV** (electron volt).

• At **absolute zero**, the conduction band is empty.

• At **room temperature**, some electrons gain enough energy to jump into the conduction band.

• Their conductivity increases with **temperature or light**.

• Example: **Silicon (Si)**, **Germanium (Ge)**

3. INSULATORS

What are Insulators?

Materials that **do not conduct electricity** under normal conditions.

Band Theory Explanation:

• Large band gap (typically **> 5 eV**).

• Electrons in the valence band **cannot jump** to the conduction band easily.

• Therefore, **no free electrons** are available for conduction.

• Example: **Wood, Glass, Rubber**