UNIT – 1

ELECTRICAL PROPERTIES OF MATERIALS

CONTENTS

1.6. Quantum Free Electron Theory

The drawbacks of classical free electron theories were removed by **Sommerfeld in 1928**. Quantum concepts are used in classical theory and hence it is known as quantum free electron theory.

He applied Schrodinger's wave equation and De-Broglie's concept of matter waves to obtain the expression for electron energies. He substituted the quantum statistics of Fermi-Dirac in place of the classical statistics and hence, it is known as the quantum free electron theory.

1.6.1. Basic assumptions of Quantum free electron theory

- The electrons are considered as free electron gas.
- The electrons possess wave nature.
- Free electrons obey Fermi-Dirac statistics and Pauli's exclusion principle.
- The free electron is fully responsible for electrical conduction.
- The allowed energy levels of an electron are quantized.
- The correct values of electrical conductivity, thermal conductivity, specific heat, optical absorption, ferromagnetic susceptibility are determined by quantum free electron theory of solids.

1.6.2. Merits of Quantum theory

- ❖ In this theory, the electrons are treated quantum mechanically rather than classically.
- ❖ Quantum theory successfully explains the ohm's law.
- ❖ It explains the electrical conductivity, thermal conductivity, photoelectric effect, Compton effect and specific heat capacity of metals.

1.6.3. Demerits of Quantum theory

- It fails to explain the classification between metals, semiconductors and insulators.
- It fails to give the reason for positive value of Hall coefficient.
- It can't be able to explain the transport properties of metals.

1.7.1.Particle in a Three dimension box:

The solution of one dimension potential well is extended for a three dimensional potential box.

In a three dimensional potential box the particle can move in any direction .so we use three quantum numbers $n_{x,}n_y \; and \; n_z \;\; to \; the$ three coordinate axes namely x,y and z respectively.

If a,b,c are the lengths of the box along x,y and z axes then,

$$E_{n_{x,}n_y,n_z} = \frac{n_x^2}{8m}\frac{h^2}{a^2}$$

If a= b = c as for a cubical box then

$$E_{n_{x,}n_y,n_z} = \frac{h^2}{8ma^2}\left[\, n_x^2 + n_y^2 + n_z^2 \,\right] \text{------------(1)}$$

The corresponding normalized wave function is

$$\Psi_{n_{x,}n_y,n_z} = \sqrt{(\tfrac{2}{a})}\sqrt{(\tfrac{2}{a})}\sqrt{(\tfrac{2}{a})}\, sin\frac{n_{x,}\pi x}{a} \sin\frac{n_y \pi y}{a} \sin\frac{n_z \pi z}{a}$$

$$= \sqrt{(\tfrac{8}{a^3})}\, sin\frac{n_{x,}\pi x}{a} \sin\frac{n_y \pi y}{a} \sin\frac{n_z \pi z}{a} \text{-----------------(2)}$$

From the equations (1), (2)we understand that several combinations of the three quantum numbers($n_{x,}n_y$,nz) lead to different energy eigen values and eigen function.

1.7.2.Degenerate states:

For several combinations of quantum numbers,we have the same energy eigen value but different eigen function.Such a state of energy levels is called degenerate state.

The three combinations of quantum numbers (1,1,2),(1,2,1) and (2,1,1) which give the same Eigen value but different Eigen functions are called 3- fold degenerate state.

Example:

If ($n_{x,}n_y$, n_z) is (1,1,2) ,(1,2,1) and (2,1,1)

Then

$$E_{112} = \frac{h^2}{8ma^2}\left(1^2 + 1^2 + 2^2 \right) = \frac{6h^2}{8ma^2}$$

$$E_{121} = \frac{6h^2}{8ma^2}$$

$$E_{211} = \frac{6h^2}{8ma^2}$$

The corresponding wave functions are

$$\psi_{112} = \sqrt{\left(\frac{8}{a^3}\right)} \sin\frac{\pi x}{a} \sin\frac{\pi y}{a} \sin\frac{2\pi z}{a} \text{---}$$

$$\psi_{121} = \sqrt{\left(\frac{8}{a^3}\right)} \sin\frac{\pi x}{a} \sin\frac{2\pi y}{a} \sin\frac{\pi z}{a} \text{---}$$

$$\psi_{211} = \sqrt{\left(\frac{8}{a^3}\right)} \sin\frac{2\pi x}{a} \sin\frac{\pi y}{a} \sin\frac{\pi z}{a} \text{---}$$