

BLOCH-THEOREM - Dr. Namita Singh

In this topic we will discuss an very interesting theorem of solid-state physics namely the Bloch's Theorem. The existing theory before Bloch's theorem which came into picture was the Free-Electron Theory. Main assumption of this theory was that it was assumed that there is a three dimensional potential well of constant potential in every solid and the electrons move inside this constant potential well. This theory was very successful in explaining many phenomenon viz. Electrical Conductivity, Thermionic Emission but it failed to explain many other properties as -

- ① why some materials are good conductors?
- ② why some materials are good insulators?
- ③ why some materials are semiconductor?

OR we can say free Electron Theory failed to explain classification of material on the basis of their conductivity:

Thus the fundamental assumption of free electron theory that the potential well inside the crystal is constant is wrong and it is varying. But how this potential is not constant can be explained with the help of the figure below.

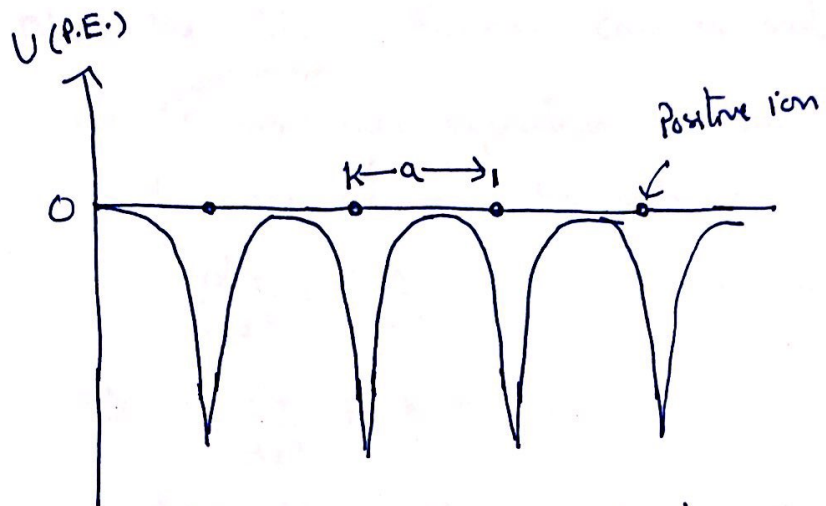


fig (a)
Varying P.E. of electron in periodic array of positive charge

When an electron approaches a positive ion, the e^- has a $-ve$ charge and ion has a positive charge, automatically potential near positive ion decreases. Thus we need to introduce a varying potential inside the crystal. Let us assume that the potential is periodic with the periodicity of the lattice as in fig (a).

$$V(x) = V(x+a) \quad \text{--- (1)}$$

Here a is the lattice constant or parameter. This equation explains that potential at any point x will be same as that at other point $(x+a)$, where a is the distance between two consecutive $+ve$ ions.

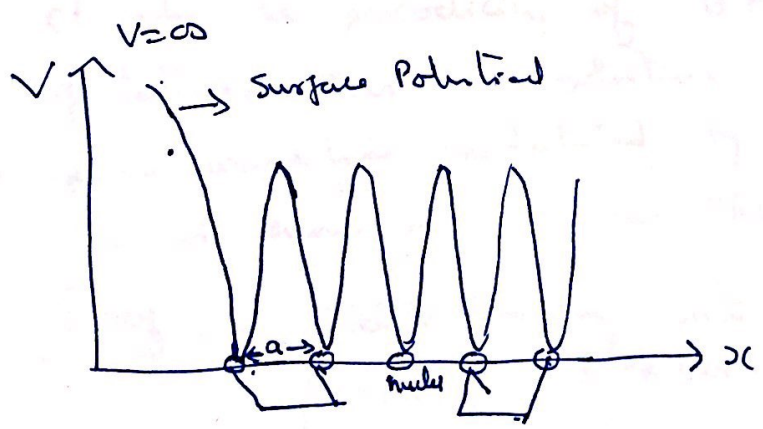


fig (b)

fig (b) further explains the fall of potential at ion sites.

(3)

Now the Bloch Theorem can be stated as:

The ^{Corresponding} Schrödinger equation for an electron moving in one-dimensional periodic potential is

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

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

where $V(x) = V(x+a)$, a is the lattice constant

$$\text{and } k^2 = \frac{2m}{\hbar^2} [E - V(x)] \quad \text{--- (2)}$$

The according to the Bloch theorem the solutions of the S.W.E. (1) will be given as. (as given by Bloch)

$$\psi(x) = e^{\pm ikx} u_k(x) \quad \text{--- (3)}$$

$$\text{where } u_k(x) = u_k(x+a) \quad \text{--- (4)}$$

functions of the type given by equation (3) are known as Bloch functions. The Bloch functions represent the free electron wave modulated by a periodic function given by eq (4). This is our Bloch's Theorem. Clearly the periodicity of B.F. is same as periodicity of lattice. Thus the solutions are similar to the plane wave type modulated by a periodic wave function. This is known as Bloch's Theorem.

Proof :- ~~Take~~ Taking into account periodicity

$$\psi(x+a) = e^{\pm ik(x+a)} u_k(x+a)$$

$$= e^{\pm ikx} \cdot e^{\pm ika} \cdot u_k(x) \quad (\because u_k(x+a) = u_k(x))$$

$$\therefore \psi(x+a) = e^{\pm ika} \psi(x) \quad \text{--- from eq (3)}$$

$$\Rightarrow \psi(x+a) = Q\psi(x) \quad \text{--- (5)}$$

$$\text{where } Q = e^{\pm ika} = \text{a const.} \quad \text{--- (6)}$$

If it is proved that eq. (1) satisfies the property given by equation (5) Bloch Theorem will be proved.

Equation (1) is a differential equation of second degree and has two independent linear solutions say $f(x)$ and $g(x)$. The general solution of eq. (1) will be

$$\psi(x) = Af(x) + Bg(x) \quad \text{--- (7)}$$

where A and B are const.

Since $f(x)$ and $g(x)$ are the solutions of S.W. E. $f(x+a)$ and $g(x+a)$ are too solutions of eq. (1) according to Bloch's assumption. And since they represent differential equation of the second order as before, $f(x+a)$ and $g(x+a)$ have two solutions; thus they too should be expressed as a linear combination of the independent one. Let

$$f(x+a) = \alpha_1 f(x) + \alpha_2 g(x) \quad \text{--- (8)}$$

$$\text{and } g(x+a) = \beta_1 f(x) + \beta_2 g(x) \quad \text{--- (9)}$$

where $\alpha_1, \alpha_2, \beta_1, \beta_2$ are real functions of energy E . According to these equations the general solution in the latter case is (from (7))

$$\begin{aligned} \psi(x+a) &= Af(x+a) + Bg(x+a) \\ &= A[\alpha_1 f(x) + \alpha_2 g(x)] + B[\beta_1 f(x) + \beta_2 g(x)] \\ &= (A\alpha_1 + B\beta_1)f(x) + (A\alpha_2 + B\beta_2)g(x) \\ &= \underbrace{A\alpha_1 + B\beta_1}_Q f(x) + BQ g(x) \\ &= [Af(x) + Bg(x)]Q \end{aligned}$$

here Q is a constant, then $\psi(x+a)$ shows that. (5)

$$\Rightarrow \psi(x+a) = Q\psi(x) \quad \text{--- (10) from (7)}$$

where $A\alpha_1 + B\beta_1 = AQ$

$$\Rightarrow A(\alpha_1 - Q) + B\beta_1 = 0 \quad \text{--- (11)}$$

and $A\alpha_2 + B\beta_2 = BQ$

$$A\alpha_2 + B(\beta_2 - Q) = 0 \quad \text{--- (12)}$$

Equations (11) and (12) will have non vanishing solution for A and B only if the determinant of their coefficients vanishes,

$$\begin{vmatrix} \alpha_1 - Q & \beta_1 \\ \alpha_2 & \beta_2 - Q \end{vmatrix} = 0$$

$$\Rightarrow (\alpha_1 - Q)(\beta_2 - Q) - \alpha_2\beta_1 = 0 \quad \text{--- (13)}$$

$$Q^2 - (\alpha_1 + \beta_2)Q + \alpha_1\beta_2 - \alpha_2\beta_1 = 0$$

Since $f(x)$ and $g(x)$ are two independent solutions of S.W.E. (Schrodinger eq), we have

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

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

Multiplying both sides by $g(x)$, the above equation gives

$$g(x) \frac{d^2 f(x)}{dx^2} - \frac{2m}{\hbar^2} V f(x) g(x) = -\frac{2m}{\hbar^2} E f(x) g(x) \quad \text{--- (14)}$$

Similarly for $g(x)$

$$f(x) \frac{d^2 g(x)}{dx^2} - \frac{2m}{\hbar^2} V f(x) g(x) = -\frac{2m}{\hbar^2} E f(x) g(x) \quad \text{--- (15)}$$

(6)

Subtracting Eq (14) from (15)

$$f(x) \frac{d^2 g(x)}{dx^2} - g(x) \frac{d^2 f(x)}{dx^2} = 0$$

$$f g'' - g f'' = 0$$

$$\Rightarrow \frac{d}{dx} [f g' - g f'] = 0$$

$\Rightarrow \therefore \begin{vmatrix} f & g \\ f' & g' \end{vmatrix}$ is a const, let this is represented by $W(x)$ the Wronskian.

$$\therefore W(x) = f g' - g f' \leftarrow (16)$$

Now $w(x+a)$ will be

$$W(x+a) = f(x+a) \cdot \frac{dg(x+a)}{dx} - g(x+a) \cdot \frac{df(x+a)}{dx}$$

$$= [\alpha_1 f(x) + \alpha_2 g(x)] \frac{d}{dx} [\beta_1 f(x) + \beta_2 g(x)] -$$

~~$$W(x+a) = [\alpha_1 f(x) + \alpha_2 g(x)] \frac{d}{dx} [\beta_1 f(x) + \beta_2 g(x)]$$~~

$$[\beta_1 f(x) + \beta_2 g(x)] \frac{d}{dx} [\alpha_1 f(x) + \alpha_2 g(x)]$$

$$W(x+a) = [\alpha_1 f(x) + \alpha_2 g(x)] [\beta_1 f'(x) + \beta_2 g'(x)]$$

$$- [\beta_1 f(x) + \beta_2 g(x)] [\alpha_1 f'(x) + \alpha_2 g'(x)]$$

$$W(x+a) = (\alpha_1 \beta_2 - \alpha_2 \beta_1) \{ f(x) g'(x) - g(x) f'(x) \}$$

$$W(x+a) = (\alpha_1 \beta_2 - \alpha_2 \beta_1) W(x) \text{ from (16)}$$

Since the wave function is periodic

$$W(x+a) = W(x)$$

$$\Rightarrow \alpha_1 \beta_2 - \alpha_2 \beta_1 = 1$$

Eq. (13) therefore reduces to

$$Q^2 - (\alpha_1 + \beta_2)Q + 1 = 0 \quad \text{--- (17)}$$

Equation (17) is a quadratic equation in Q. two roots are

$$Q_1 = \frac{(\alpha_1 + \beta_2) + \sqrt{(\alpha_1 + \beta_2)^2 - 4}}{2} \quad \text{--- (18)}$$

$$Q_2 = \frac{(\alpha_1 + \beta_2) - \sqrt{(\alpha_1 + \beta_2)^2 - 4}}{2} \quad \text{--- (19)}$$

Two different cases resulting are

- (1) For certain range of energy E if $(\alpha_1 + \beta_2)^2 < 4$ the roots will be complex and since $Q_1 Q_2 = 1$, Q_1 and Q_2 will be conjugate of each other.

In this case we may write

$$Q_1 = e^{ika} \text{ and } Q_2 = e^{-ika}$$

$$\text{and } \psi_1(x+a) = e^{ika} \psi_1(x) \text{ and } \psi_2(x+a) = e^{-ika} \psi_2(x)$$

And the solution can be written as Bloch function

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

- (2) In this case of range of energy $(\alpha_1 + \beta_2)^2 > 4$ the two roots Q_1 and Q_2 are real and reciprocal of each other. The solution do not represent a wave function and thus there are not electronic states in energy region corresponding to Q_1 & Q_2

This leads to concept of periodic potential consisting of allowed and forbidden energy regions in bands. The Kronig - Penney Model will further explain this.