Band Theory of solid

Bloch theorem

An electron moves through + ve ions, it experiences varying potential. The potential of the electron at the +ve ions site is zero and is maximum in between two +ve ions sites.

The potential experienced by an e^- in this condition is regarded as real periodic potential variation.

Suppose an electron passes along X-direction in a one-dimensional crystal having periodic potentials:

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

where '*a*' is the periodicity of the potential. The Schrödinger wave equation for the moving electron is:

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

The solution for this Equation is of the form:

$\psi(x) = e^{iKx} u_k(x)$

where $u_k(x) = u_k(x + a)$ represents periodic function and

e^{ikx} represents plane wave.

The above statement is known as Bloch theorem.

The Bloch function has the property:

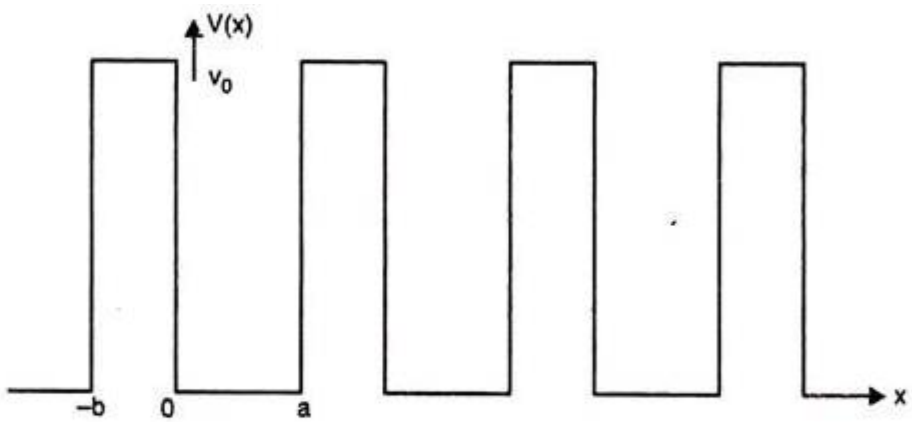
$\psi(x + a) = \exp[ik(x + a)]\, u_k(x + a) = \psi(x) \exp ika$

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

The Kronig-Penney model

The Kronig-Penney model demonstrates that a simple one-dimensional periodic potential yields energy bands as well as energy band gaps. While it is an oversimplification of the three-dimensional potential and band structure in an actual crystal, it is an instructive tool to demonstrate how the band structure can be calculated for a periodic potential, and how allowed and forbidden energies are obtained when solving the Schrodinger equation.

The Kronig-Penney model is represented by the one-dimensional periodic potential as :



The potential is defined as $V(x) = V_0 \quad -b < x < 0$

$\qquad\qquad\qquad\qquad\qquad\quad = 0 \qquad 0 < x < a$

The potential has a period of c = a + b.

The Schrodinger equation for this model is

$$\frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2}\psi = 0 \qquad 0 < x < a$$

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

Let

$$\alpha = \frac{(2mE)^{1/2}}{\hbar}$$

$$\beta = \frac{[2m(V_0 - E)]^{1/2}}{\hbar}$$

$\therefore$ The solutions of schrodinger Equations are

$$\psi_1 = Ae^{i\alpha x} + Be^{-i\alpha x} \qquad 0 < x < a$$

and

$$\psi_2 = Ce^{\beta x} + De^{-\beta x} \qquad -b < x < 0$$

Since the wave function has periodicity c

$$\therefore \psi(x + c) = e^{ik}c\psi(x)$$

Let $\psi_1(x) = \psi(x)$ for $-b < x < 0$

and $\psi_2(x) = \psi(x)$ for $0 < x < a$,

then following two boundary conditions are used

$\psi_1(0) = \psi_2(0)$ and $\frac{d\psi 1(0)}{dx} = \frac{d\psi 2(0)}{dx}$

Again , from Bloch's theorem, $u(x) = u(x + a)$ therefore $u(x)$ and its first derivative must also be periodic.

Therefore, we have the two additional conditions

$$u(-b) = u(a) \quad \text{and} \quad \frac{du(-b)}{dx} = \frac{du(a)}{dx}$$

By using these four basic boundary condition

We get $A + B = C + D$ -------------------------(1)

$\beta C - \beta D = i\alpha A - i\alpha B$-------------------------(2)

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

$i(\alpha - k)Ae^{i(\alpha-k)a} - i(\alpha + k)Be^{-i(\alpha+k)a} =$

$(\beta - ik)Ce^{-(\beta-ik)b} - (\beta + ik)De^{(\beta+ik)b}$ -------(4)

For nontrivial solution of the above four equations

$$\begin{vmatrix} 1 & 1 & 1 & 1 \\ \beta & -\beta & i\alpha & -i\alpha \\ e^{(ik-\beta)b} & e^{(ik+\beta)b} & e^{i\alpha(\alpha-k)} & e^{i\alpha(\alpha+k)} \\ (\beta - ik)e^{(ik-\beta)b} & -(\beta + ik)e^{(ik+\beta)b} & i(\alpha - k)e^{ia(\alpha-k)} & -i(\alpha + k)e^{ia(\alpha+k)} \end{vmatrix} = 0$$

On solving the determinant ,we get

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

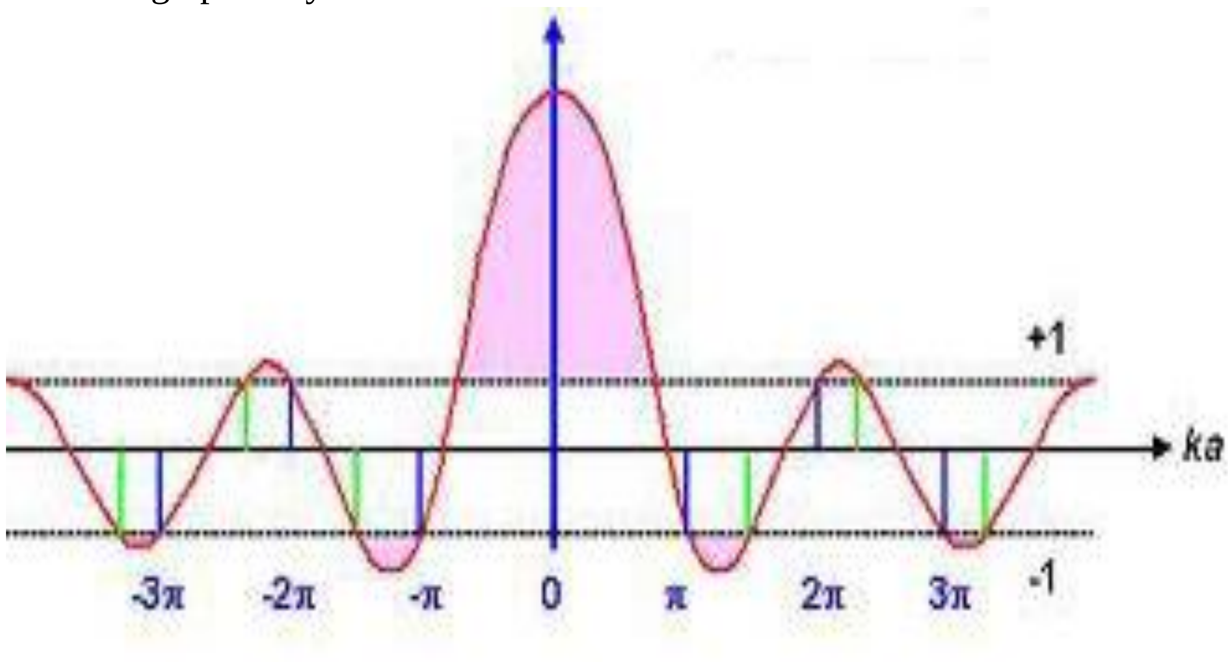
On substituting the value of α and β
We get

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

Here $p = \frac{m v_0 b a}{h^2}$ is scattering power

And 'v_0 b' is known as barrier strength.

It can be solved graphically.



We notice that the only allowed energies are those for which

$$-1 \leq f(\alpha a) \leq 1$$

Whenever f(αa) is outside the domain [−1, 1], there are no solutions.

Conclusion from Kronig –Penny Model:

1).The Energy spectrum of E consists of an infinite number of allowed energy bonds separated by intervals in which, there are no allowed energy levels. These are known as forbidden regions.
2). When α a increase, the first term of e on LHS decrease , so that the width of the allowed energy bonds is increased and forbidden energy regions become narrow.
3). The width of the allowed bond decrease with the increase of p value. When p → α, the allowed energy regions become infinity narrow and the energy spectrum becomes line spectrum.