# Band Theory of Solids. (1-D)

Band theory deals with the determination of eigenvalue and wave function (of an electron) for time independent schrödinger operator admitting periodic potential $V(x)$.

*Definition-1*: A potential $V(x)$ is said to be periodic with period $a$ (lattice constant) if $V(x+a) = V(x)$.

*Definition-2*: An operator $T_a$ is called lattice translation operator if
$$T_a f(x) = f(x+a)$$

*Theorem-1*: If $\psi(x)$ is an eigenfunction of
$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x),$$ with eigen value $E$
then $T_a\psi(x)$ is also an eigenfunction of $H$ corresponding to the same eigenvalue.

*Proof*: $T_a V(x) = V(x+a) = V(x)$ by def$^n$-1.

$$T_a \frac{d}{dx} = \frac{d}{d(x+a)} = \frac{d}{dx}$$

Let $H\psi = E\psi$

$$T H\psi = T E\psi$$

$$\Rightarrow H(x+a)\,\psi(x+a) = E(T\psi)$$

$$\Rightarrow H(T\psi) = E(T\psi)$$

*Remark*: 1. As $T\psi$ is an eigenfunction of $H$

$T\psi = \lambda\psi$. & there-fore $\psi(x+a) = \lambda\psi(x)$

2. As the probability density at $(x+a)$
$$\rho(x+a) = \psi^*(x+a)\,\psi(x+a)$$
$$= |\lambda|^2 \psi^* \psi(x) = |\lambda|^2 \rho(x)$$
This requires $|\lambda|^2 = 1 \Rightarrow \lambda = e^{\pm i\theta}$.

3. $\psi(x+a) = e^{\pm i\theta}\psi(x) \Rightarrow$ that the wave function is modified but the probability density remains to be the same.

Choosing $\theta = Ka$

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

*Theorem-2:* The wave function that satisfies the relation $\psi(x+a) = e^{iKa}\psi(x)$ can be given by

$$\psi(x) = e^{iKx}\varphi(x) \quad \text{where } \varphi(x+a) = \varphi(x)$$

*Proof:*
$$\psi(x+a) = e^{iK(x+a)}\varphi(x+a)$$
$$= e^{iKa}e^{iKx}\varphi(x) = e^{iKa}\psi(x)$$

*Remark:* Th-2. is known as Bloch Theorem.

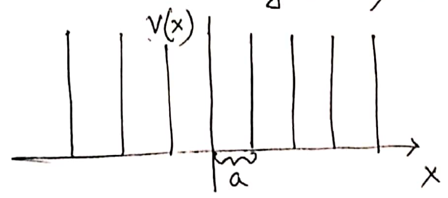
*Theorem-3:* To every periodic potential there exist a function $f(x)$ such that

$$\cos Ka = f(x)$$

*Proof:* Beyond our scope.

*Remark:* 1. $|f(K)| < 1$ for obvious reason. So $K$-values are restricted.

## Krönig-Penney Model (Qualitative)




The Dirac comb potential.

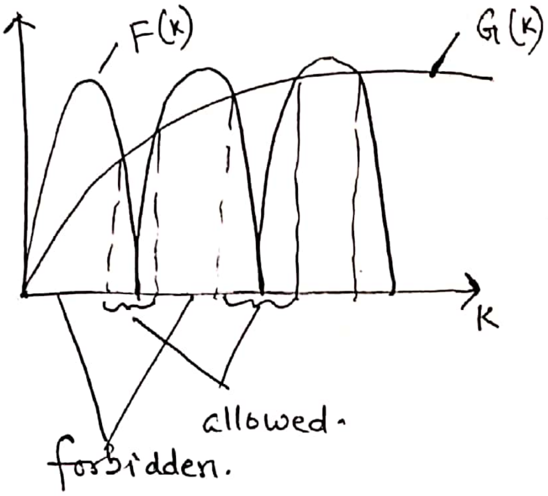
$f(k) = \cos ka + \frac{\Omega}{k} \sin ka$ , $\Omega$ = strength of the potential.

Now the condition $|f(k)| \leq 1$ gives.

$$\frac{1}{\sqrt{1+\Omega^2/k^2}} \cos ka + \frac{\Omega/k}{\sqrt{1+\Omega^2/k^2}} \sin ka \leq \frac{1}{\sqrt{1+\Omega^2/k^2}}$$

$$\Rightarrow \quad \cos\left(ka - \tan^{-1} \Omega/k\right) \leq \frac{k}{\sqrt{\Omega^2+k^2}}$$

$$\Rightarrow \quad F(k) \leq G(k)$$




Effective mass : $m^* = \hbar^2 / \left(d^2E/dk^2\right)$

$$E(k) = E(-k)$$

$$m^*(k) = m^*(-k)$$

Now $p$ (momentum) $= m^* v_g$

$\Rightarrow \quad p(k) = m^*(k)\, v_g(k)$ where $v_g = \frac{d\omega}{dk}$

$\Rightarrow \quad p(-k) = m^*(-k)\, v_g(-k)$ $\qquad = \frac{1}{\hbar}\frac{dE}{dk}$

$\Rightarrow$ odd function.

$$\Rightarrow \quad p(-k) = m^*(k)\left[-v_g(k)\right]$$

$$\Rightarrow \quad p(-k) = \underbrace{\left(-m^*(k)\right)}_{\text{hole.}} v_g(k)$$

Current density $j = nev_g$

$$j(k) = nev_g(k)$$

$$j(-k) = nev_g(-k) = ne[-v_g(k)]$$

$$= n(-e)v_g(k)$$

charge of hole $= (-e)$

Problem : 1. The band energy of a crystal is given by

$$E(k) = \alpha + \beta \cos ka$$

Calculate (i) Group velocity

(ii) Effective mass.

(iii) Band gap.

Ans. (i) $v_g = \frac{1}{\hbar}\frac{dE}{dk} = \frac{1}{\hbar}(-\beta a \sin ka)$

(ii) Effective mass $m^* = \dfrac{\hbar^2}{d^2E/dk^2} = \dfrac{\hbar^2}{(-\beta a^2 \cos ka)}$

(iii) $E_{max} = \alpha + \beta \quad E_{min} = \alpha - \beta$

$$\Delta E = E_{max} - E_{min} = 2\alpha.$$

Problem : 2 : The band energy of band is given by

$$E = a - bk^2, \quad a, b > 0$$

Show that the band is filled with holes.

Ans. $m^* = \dfrac{\hbar^2}{d^2E/dk^2} = \dfrac{\hbar^2}{-2b} = -\dfrac{\hbar^2}{2b} < 0$