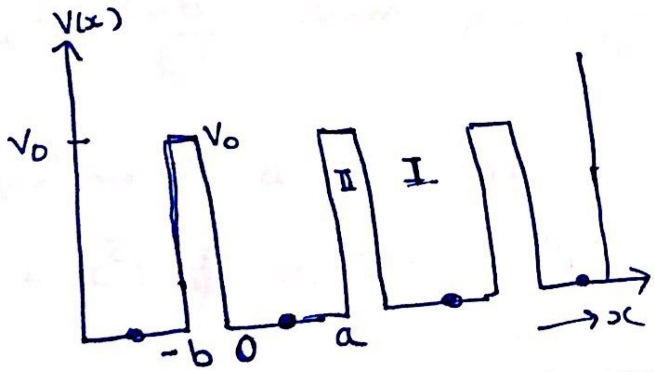
SEM - VI

B. SC. (H) - PHYSICS

Solid State Physics — C XIII

Kroning - Penny Model :— We have seen that the Bloch Theorem tells us about the periodicity of potential. This periodicity of the potential can be applied for distinguishing and classifying materials into conductors, insulators and semiconductors electrically. One such application of classifying the materials electrically was done by Kroning and Penny. and the model is known as Kroning - Penny Model. In this model in order to study the exact relationship between E and wave vector k. a well defined periodic potential was suggested by Kroning and Penny. This potential is in the form of square well potential as shown in the fig. ⓐ below, we can observe clearly two regions here, and we will write S.W.E. for two regions separately



In this model it was assumed that e^- is in periodic potential of square well type with a periodicity $(a+b)$.

Two regions are described as

Region I where P.E. of e^- is zero.

ie. $V = 0$ for $0 < x < a$.

and region II where P.E. of e^- is V_0

i.e. $V = V_0$ for $-b < x < 0$.

Each of the potential well (I) may be considered a rough approximation for the potential in the vicinity of an atom. Now we will write S.W.E. for these two regions and we will solve it for the wave functions associated with ~~the~~ e^-s in both the regions.

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} E\psi = 0 \quad \text{for } 0 < x < a \quad \text{—(1)}$$

and
$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E - V_0)\psi = 0 \quad \text{for } -b < x < 0 \quad \text{—(2)}$$

Since the expected solutions of the equations are similar to the Bloch functions, it is required that ψ and $\frac{d\psi}{dx}$ both sould be continuous through out the crystal. Assuming that the K.E. E of the electron is less than the Potential energy V_0, let us define two quantities as

$$\alpha^2 = \frac{2mE}{\hbar^2} \quad \text{and} \quad \beta^2 = \frac{2m}{\hbar^2}(V_0 - E) \quad \text{—(3)}$$

for region $-b < x < 0$

So that equations (1) and (2) are

$$\frac{d^2\psi}{dx^2} + \alpha^2 E \psi = 0 \quad \text{—(4)}$$

and
$$\frac{d^2\psi}{dx^2} + (-\beta^2)\psi = 0$$

or
$$\frac{d^2\psi}{dx^2} - \beta^2\psi = 0 \quad \text{—(5)}$$

Now making use of the fact that solution are similar to the Bloch functions of the form $e^{ikx} U_k(x)$, we write the possible solution of these differential equation as

$$\psi = e^{ikx} u_k(x) \quad \text{——} (6)$$

Differentiating equation (6) twice w.r.t. x, we get

$$\frac{d\psi}{dx} = e^{ikx}\frac{du_k(x)}{dx} + ik e^{ikx} u_k(x) \quad \text{——} (7)$$

and
$$\frac{d^2\psi}{dx^2} = -k^2 e^{ikx} u_k(x) + 2ik\, e^{ikx}\frac{du_k(x)}{dx} + e^{ikx}\frac{d^2u_k(x)}{dx^2} \quad \text{——} (8)$$

Substituting $\frac{d\psi}{dx}$ and $\frac{d^2\psi}{dx^2}$ in eq. (4) and (5) and rearranging the terms, we get.

$$\frac{d^2u_1}{dx^2} + 2ik\frac{du_1}{dx} + (\alpha^2 - k^2)u_1 = 0 \quad \text{——} (9)$$

and
$$\frac{d^2u_2}{dx^2} + 2ik\frac{du_2}{dx} + (\beta^2 + k^2)u_2 = 0 \quad \text{——} (10)$$

where u_1 is the value of $u_k(x)$ in the interval $0<x<a$.
and u_2 is the value of $u_k(x)$ in the interval $-b<x<0$.

The solutions of these equations are

$$u_1 = Ae^{i(\alpha-k)x} + Be^{-i(\alpha+k)x} \quad \text{for } 0<x<a \quad \text{——} (11)$$

and
$$u_2 = Ce^{(\beta - ik)x} + De^{-(\beta+ik)x} \quad \text{for } -b<x<a \quad \text{——} (12)$$

Since the wave function ψ and $\frac{d\psi}{dx}$ or u & $\frac{d\psi}{dx}$ should be continous we have chosen constants A, B, C, D in such a way that the following conditions are satisfied

$$u_1(0) = u_2(0), \quad \left(\frac{du_1}{dx}\right)_{x=0} = \left(\frac{du_2}{dx}\right)_{x=0} \quad \text{——} (13)$$

$$u_1(a) = u_2(-b), \quad \left(\frac{du_1}{dx}\right)_{x=a} = \left(\frac{du_2}{dx}\right)_{x=-b} \quad \text{——} (14)$$

The first two conditions, given by eq. 13, are required for the continuity of the wave functions and their derivatives across the boundary. The other two conditions, given by eq. 14 are required because of the periodicity of $U_k(x)$. Applying first two conditions we get.

$$A+B = C+D \quad \text{—— (15)}$$

and $$Ai(\alpha-k) - Bi(\alpha+k) = C(\beta-ik) - D(\beta+ik)$$

$$\text{—— (16)}$$

and from last two conditions, we have

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

$$\text{—— (17)}$$

$$Ai(\alpha-k)e^{i(\alpha-k)a} - Bi(\alpha+k)e^{-i(\alpha+k)}$$
$$= C(\beta-ik)e^{-(\beta-ik)b} - D(\beta+ik)e^{(\beta+ik)b}$$

$$\text{—— (18)}$$

These four equations 15, 16, 17 and 18 will have a non vanishing solution only if the determinant of their coefficients vanishes, i.e.

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

On simplifying we get,

$$\frac{\beta^2-\alpha^2}{2\alpha\beta}\sinh\beta b\cdot\sin\alpha a+\cosh\beta b\cdot\cos\alpha a=\cos k(a+b) \quad \text{— (19)}$$

Equation (19) can further be simplified by assuming $b\to 0$ when $V\to\infty$ ie. as we increase height of the potential barrier the width b will decrease. Under this condition,

$$\sinh\beta b\longrightarrow\beta b,\quad \cosh\beta b\longrightarrow 1,\quad (\beta^2-\alpha^2)\simeq\beta^2$$

So that equation (19) reduces to

$$\frac{\beta^2}{2\alpha\beta}\cdot\beta b\sin\alpha a+\cos\alpha a=\cos ka$$

or

$$\frac{\beta^2 b}{2\alpha}\sin\alpha a+\cos\alpha a=\cos ka$$

$$\Rightarrow\quad P\left(\frac{\sin\alpha a}{\alpha a}\right)+\cos\alpha a=\cos ka \quad \text{—— (20)}$$

where $P=\frac{\beta^2 ab}{2}=\frac{2mV_0}{2\hbar^2}ab$ (as $V_0>>E$) from eq (3)

$$P=\frac{mV_0ab}{\hbar^2} \quad \text{— (21)}$$

here P is the measure of the area V_0b of the Potential barrier. Physically as P is increased an electron is more confined or ~~bound~~ restricted in to a particular Potential well. Equation (21) and $P=\frac{mV_0ab}{\hbar^2}$ can also be referred as the scattering power of the potential barrier.

Now, eq. 20 $P\left(\frac{\sin \alpha a}{\alpha a}\right) + \cos \alpha a = \cos ka$, with $P = \frac{m V_0 a b}{\hbar^2}$ can be solved graphically, as we see that $\cos ka$ can take values between -1 and $+1$ i.e. $-1 \leq \cos ka \leq +1$, L.H.S. of eq. 20 is valued between -1 and $+1$, now if equation 20 is plotted by taking its L.H.S. against αa, we can determine those values of α (and hence energy as $\alpha^2 = \frac{2mE}{\hbar^2}$) which are permissible, and other values of αa will not be allowed.

Ploting left hand side of eq. 20 against αa for a value $P = 3\pi/2$ (say) we get a plot as shown in fig (b) below. Since $\cos ka$ is between -1 and $+1$ ($-1 \leq \cos ka \leq +1$) as shown in fig by dotted lines, only those values of L.H.S. of eq. 20 are allowed which lie between -1 and $+1$,

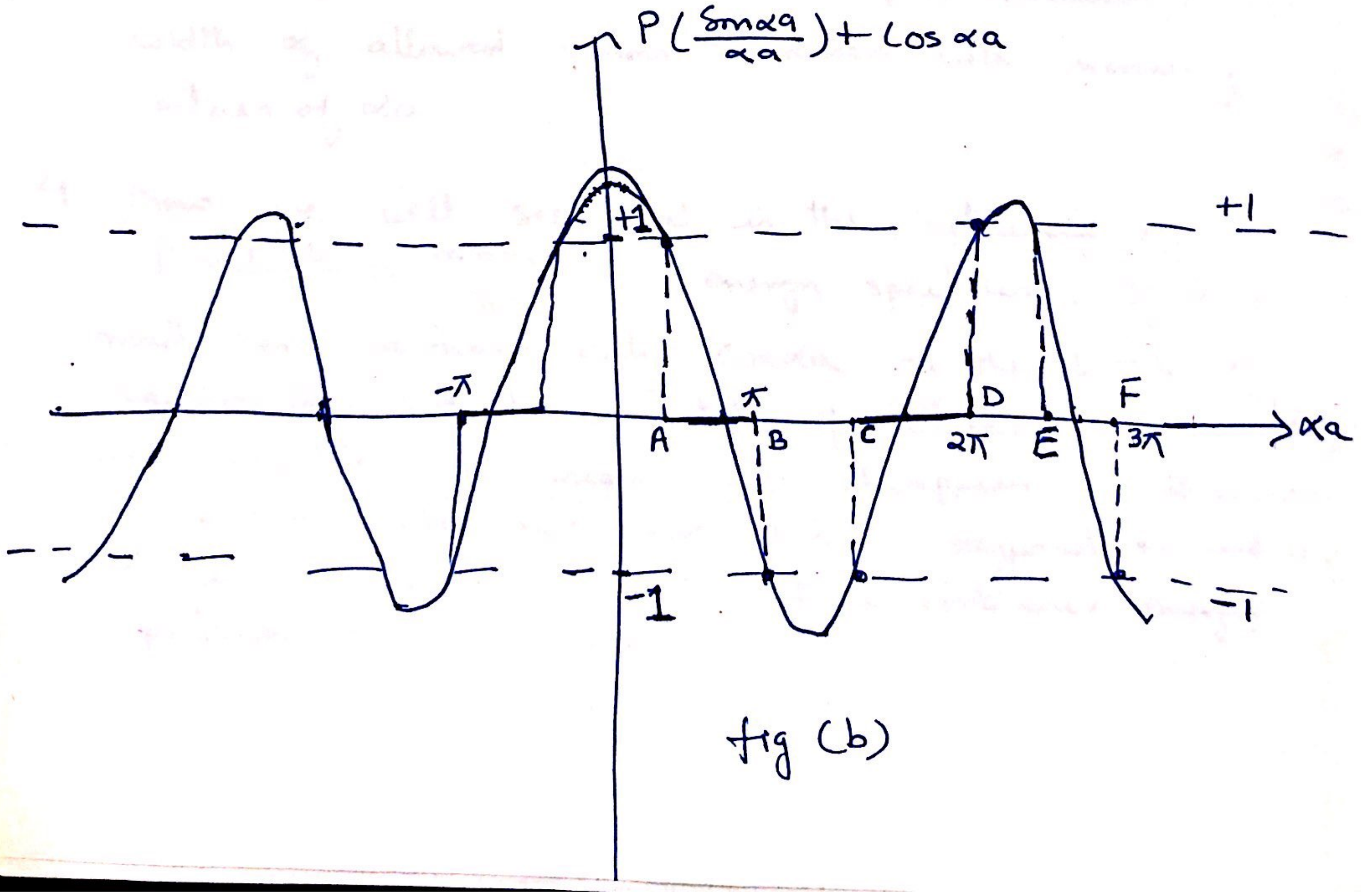


fig (b)

From the fig. following conclusions may be drawn

1. The part of the vertical axis lying between the horizontal lines (+1 and −1) represent the range acceptable to left hand side of eq. (20), since α^2 is proportional to energy E, abscissa (X-axis) will be a measure of energy.

2. The energy spectrum of electrons consists of a number of allowed energy bands viz. AB, CD, ... for which $\cos ka$ lies between ± 1, separated by forbidden regions; viz, BC, DE for which ~~cos~~ L.H.S. of equation has values beyond −1 and +1.

3. For a given value of P, as αa increases, the first term on the L.H.S. of eq. (20) decreases (since max. value of $\sin \alpha a = 1$, hence as αa increases, $1/\alpha a$ decreases). The width of allowed bands increases with increasing values of αa.

4. Now we will see what is the influence of $P = \frac{\beta^2 ab}{2} = \frac{mV_0 ab}{\hbar^2}$ on energy spectrum. If P is made zero we have only $\cos \alpha a$ on the L.H.S. of equation (20) which can take of values between +1 & −1. and forbidden gap region will disappear as it comes into pictures when we have values beyond +1 and −1. The in this case we will get a continous energy spectrum of a free electron.

So for $P=0$, $\cos\alpha a = \cos ka$

i.e. $\alpha = k$ or $\alpha^2 = k^2$

or $\frac{2mE}{\hbar^2} = \left(\frac{2\pi}{\lambda}\right)^2$ $\quad (\because k = \frac{2\pi}{\lambda})$

or $E = \left[\frac{\hbar^2}{2m}\right]\left[\frac{1}{\lambda^2}\right] = \left[\frac{\hbar^2}{2m}\right]\left[\frac{p^2}{\hbar^2}\right]$

$E = \frac{p^2}{2m} = \frac{1}{2}mv^2$

This is appropriate for free $\bar{e}$s. So no energy ~~bdc~~ levels exist and all energies are allowed to electrons.

Further,

$\cos\alpha a = \cos ka \Rightarrow \alpha a = ka$

$\Rightarrow \alpha^2 = k^2 \Rightarrow \frac{2mE}{\hbar^2} = k^2$

$\Rightarrow E = \frac{\hbar^2 k^2}{2m} \Rightarrow E \propto k^2$

This shows E-k curve is a parabola. As P is gradually increased, the forbidden regions appear, the width of the allowed regions decrease and that of the forbidden regions increases. In the extreme case, when $P \to \infty$, the allowed regions become extremely narrow and energy spectrum becomes a line spectrum. In this case eq. 20 has a solution only if, $\sin\alpha a = 0 = \sin n\pi$, where $n = \pm 1, \pm 2$ ----

$\Rightarrow \alpha a = n\pi$

$\alpha^2 a^2 = n^2\pi^2$

$\Rightarrow \frac{2mE}{\hbar^2} \cdot a^2 = n^2\pi^2$

$\Rightarrow E = \frac{n^2 h^2}{8ma^2}$ — 23 $\quad (\hbar = \frac{h}{2\pi})$

Now eq. (20) gives the energy levels of a particle in a constant potential box of atomic dimensions. (9)

(5) From fig (b) and equation (20) it follows that energy discontinuities occur when

$$ka = n\pi,$$

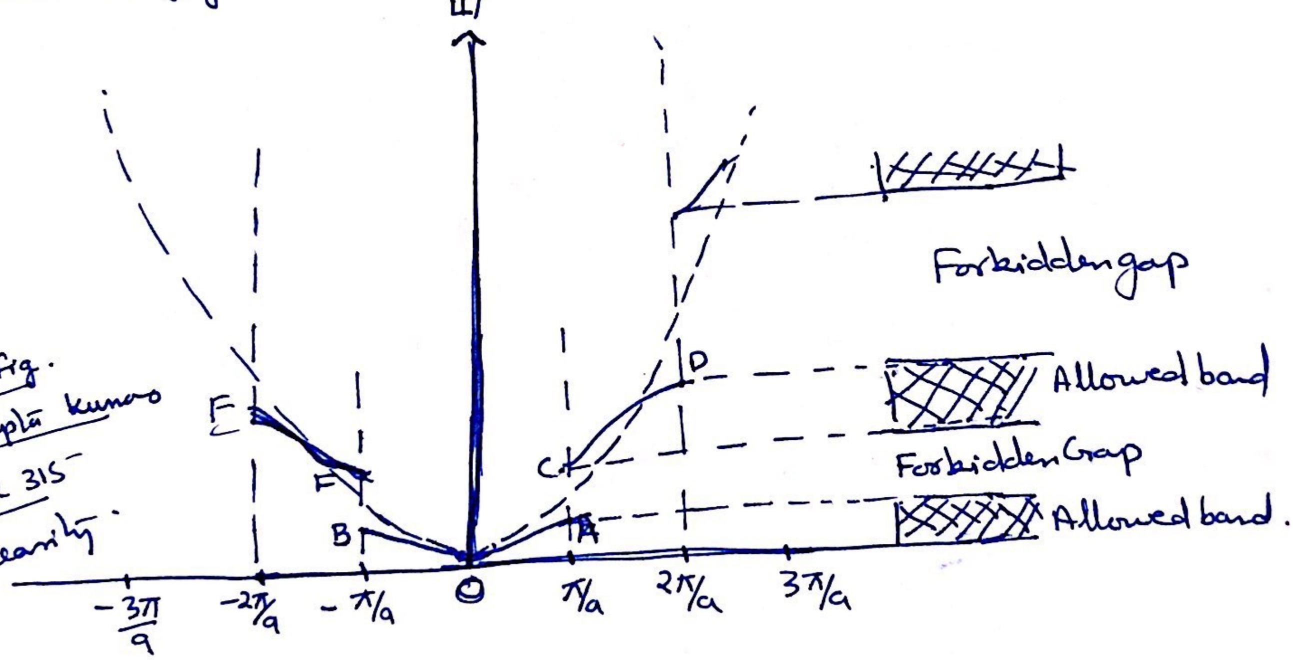
$$\Rightarrow k = \frac{n\pi}{a}, \text{ where } n = \pm 1, \pm 2, \ldots \quad (24)$$

where a is the periodicity of lattice.

$$\Rightarrow k = \pm\frac{\pi}{a}, \pm\frac{2\pi}{a}, \pm\frac{3\pi}{a} \pm \ldots \pm\frac{n\pi}{a}$$

Fig (c) below shows a relationship between energy E and wave number k for one dimensional lattice. The dashed curve is free-electron parabola. The origin of the allowed energy bands and forbidden gaps are also seen in fig below.

Refer fig. in Gupta kumar Page 315 for clearity.



In next lecture we will cover other topics related to Kroning-Penney Model..

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