Kronig - Penny model

We know that the electrons in a crystalline are acted upon by periodically varying potential field. To understand the origin of the energy bands in solids it is necessary to solve the Schrödinger equation in the presence of such potential. Solving the Schrödinger equations for the three-dimensional motion of an electron considering the actual periodic potential in a solid is an extremely difficult problem. If instead of this we consider a one-dimensional lattice (i.e chain of atoms along a line), then assuming a rectangular periodic potential, it is possible to solve exactly the one-dimensional Schrödinger equation which was first done by R. de L. Kronig and W. G. Penny in 1930.

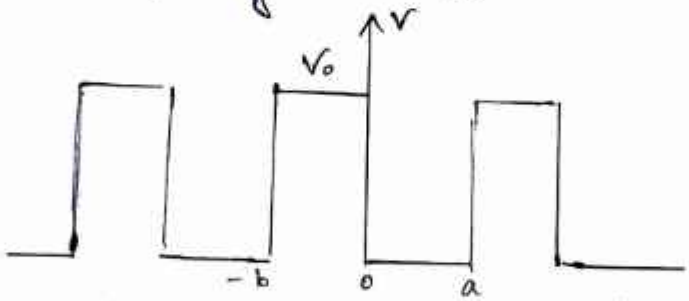

fig:1- Periodic rectangular potential

The one-dimensional rectangular periodic potential shown in fig 1 can be mathematically represented as follows:

$V = V_0 =$ constant for $-b < x < 0$

$V = 0$ for $0 < x < 0$

$V(x+L) = V(x)$ where $L = a+b$ is the period of the potential.

Each of the potential energy wells may be considered a rough expression for the potential in the vicinity of an atom. The Schrödinger equations for the two regions are

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

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

We shall assume $E < V_0$. Defining two real quantity α and β by

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

and making use of the fact that the solution must be Bloch functions of the form $e^{ikx} u_k(x)$, one obtains upon substitution into (1) and (2) the following eqns for $u_k(x)$:

$$\frac{d^2u}{dx^2} + 2ik\frac{du}{dx} + (\alpha^2 - k^2)u = 0 \qquad \text{— (4)}$$

$$\frac{d^2u}{dx^2} + 2ik\frac{du}{dx} - (\beta^2 + k^2)u = 0 \qquad \text{— (5)}$$

The solutions of these eqns are

$$u_1 = Ae^{i(\alpha - k)x} + Be^{-i(\alpha + k)x} \qquad 0 < x < a \quad \text{— (6)}$$

$$u_2 = Ce^{(\beta - ik)x} + De^{-(\beta + ik)x} \qquad -b < x < 0 \quad \text{— (7)}$$

where A, B, C and D are constants. These constants must be choosen in such a manner to satisfy the following conditions which are based on continuity of wave func, and their derivatives and the periodicity of $u_k(x)$

$$u_1(0) = u_2(0) \qquad u_1(a) = u_2(a)$$

$$\left(\frac{du_1}{dx}\right)_{x=0} = \left(\frac{du_2}{dx}\right)_{x=0} \qquad \left(\frac{du_1}{dx}\right)_{x=a} = \left(\frac{du_2}{dx}\right)_{x=a} \qquad \text{— (8)}$$

It is evident that application of (6), (7) and (8) leads to four linear homogeneous equations in the constants A, B, C, D; thus the wave function may be calculated. However for our purpose we are more interested in determining the values of the energy for which satisfactory solutions are obtained. The four equations just mentioned have a solutions only if the determinant of the coefficients of A, B, C, D vanishes. It can be shown that this leads to the following condition:

$$\frac{\beta^2 - \alpha^2}{2\alpha\beta} \sinh\beta b \sin\alpha a + \cosh\beta b \cos\alpha a = \cos k(a+b) \qquad \text{— (9)}$$

To obtain more convenient equation, Kronig and Penny consider the case for which potential barriers become delta functions i.e V_0 tends to infinity and b approaches zero, but the product $V_0 b$ remains finite. So, the equn (9) reduces to $(mV_0 b/\hbar^2\alpha)\sin\alpha a + \cos\alpha a = \cos ka$ ——— (10)

Let us now define the quantity, $(mV_0 b/\hbar^2\alpha) = P$ ——— (11)

which is evidently a measure for the area of potential barrier. So, increasing P has the physical meaning of binding a given electron more strongly to a particular potential well. So, the equation becomes.

$$P\frac{\sin\alpha a}{\alpha a} + \cos\alpha a = \cos ka \quad \text{---} \quad (12)$$

As an example we have represented in fig 2. the left hand side of equn as function of αa for the value $P = \frac{3\pi}{2}$. As α^2 is proportional to E i.e abcissa is a measure for the energy. The right hand side of the equn can accept only values between -1 and +1 as indicated by horizontal line in fig 2. Therefore the condition (12) can be satisfied only for values of αa for which left hand side lies between ± 1.

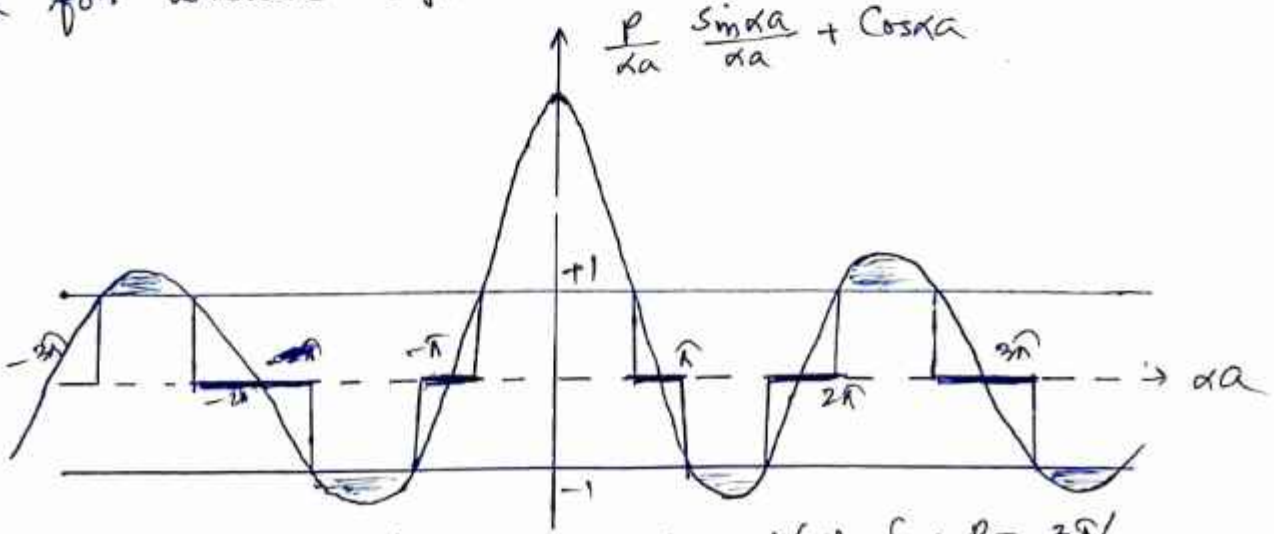

fig 2. The left hand side of equn (12) for $P = 3\pi/2$. plotted as function of αa. Allowed regions are bearing drawn lines.

☐ The following important conclusions of the theory are to be noted:

1) Since the energy varies continuously within finite limits in both the permitted and forbidden energy regions, we get a series of allowed energy bands intervened by forbidden gaps.

2) The width of the allowed energy bands increases with the increasing value of αa ie. with increasing energy. This is due to the fact that the first term on R.H.S of (12) decreases with increasing αa.

3) The width of an allowed band decreases with increasing P. ie with increasing energy of binding of the electron. On the limit of $P \to \infty$, the allowed bands become infinitely narrow and we get a line spectrum. On this case $\alpha a = \pm n\pi$ with n = integer so that the energy becomes $E_n = \frac{n\pi^2\hbar^2}{2ma^2}$

This is equal to the energy of the levels in a potential box with rigid walls.

4) The plot of E vs K shows discontinuities at $K = \frac{n\pi}{a}$ where $n = 1, 2, 3 \ldots$ These discontinuities define the boundaries between successive Brillouin Zones.

5) Within a given energy band, E is periodic func. of K so that if we replace K by $K + 2n\pi/a$, the R.H.S of eqn (12) remain the same. The K in is not uniquely determined. The reduced wave vector K is defined by the relation

$$-\frac{\pi}{a} \leq K \leq \frac{\pi}{a}$$

The plot of E ~~against~~ against wave vector is shown in below fig (3). It will be seen that $\frac{dE}{dk} = 0$ at the boundaries of the Brillouin Zones.

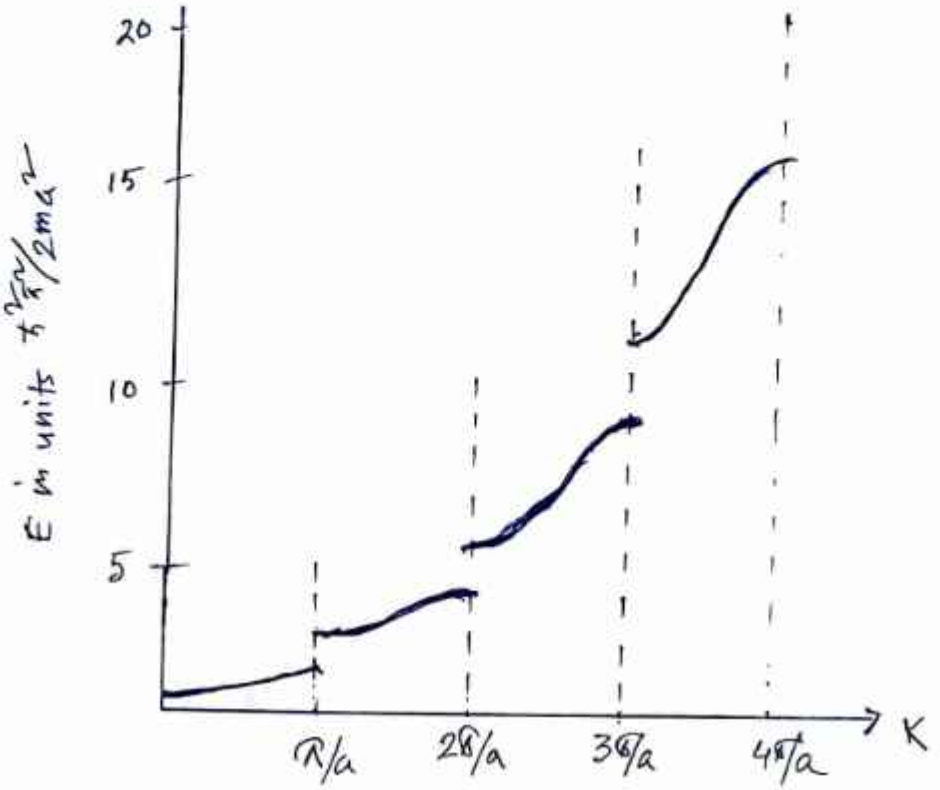

fig 3. The energy is represented as function of K for $\rho = \frac{3\pi}{2}$; the Brillouin zones are indicated (note this is only half the picture)