DEPARTMENT OF PHYSICS AND NANOTECHNOLOGY
SRM INSTITUTE OF SCIENCE AND TECHNOLOGY

Lecture 3

KRONIG PENNEY MODEL

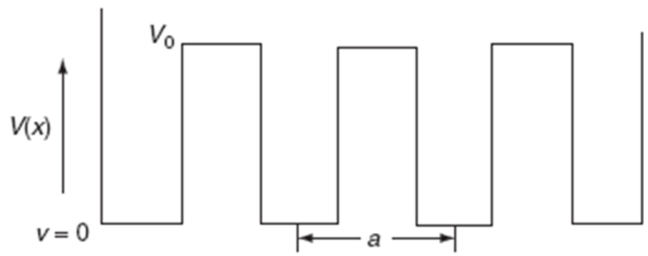
Kronig Penney model :

- According to Kronig and Penney the electrons move in a periodic square well potential.

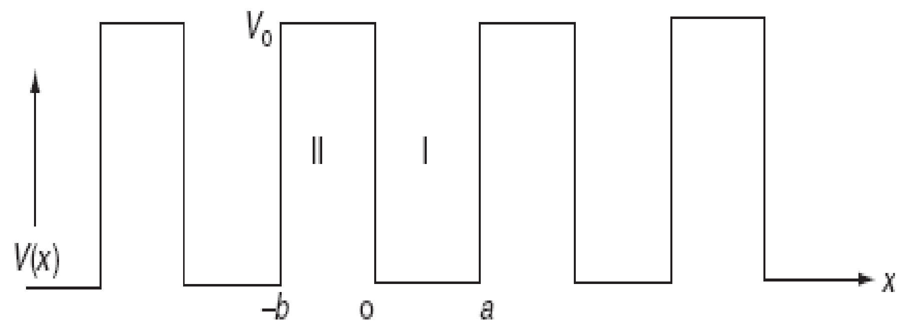
- This potential is produced by the positive ions (ionized atoms) in the lattice.

- The potential is zero near to the nucleus of positive ions and maximum between the adjacent nuclei. The variation of potential is shown in figure.

It is not easy to solve Schrödinger's equation with these potentials. So, Kronig and Penney approximated these potentials inside the crystal to the shape of rectangular steps as shown in Fig. (c). This model is called Kronig-Penney model of potentials.



(c)



The energies of electrons can be known by solving Schrödinger's wave equation in such a lattice. The Schrödinger time-independent wave equation for the motion of an electron along X-direction is given by:

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

The energies and wave functions of electrons associated with this model can be calculated by solving time-independent one-dimensional Schrödinger's wave equations for the **two regions I and II as shown in Fig.**

The Schrödinger's equations are:

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

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}[E - V_o]\psi = 0$$ for -b<x<0............(2)

We define two real quantities (say) α and β such that:

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

$$\frac{d^2\psi}{dx^2} + \alpha^2\psi = 0$$ for 0<x<a ---------------(4)

$$\frac{d^2\psi}{dx^2} - \beta^2\psi = 0$$ for -b<x<0 ---------------(5

As the potential is periodic, the wave functions must have the Bloch form

$$\Psi(x) = e^{ikx}\, u(x)$$ -----------------(6)

If $u_1(x)$ and $u_2(x)$ represent the values of $u(x)$ in two regions $(0 < x < a)$ and $(-b < x < 0)$ of potential functions respectively, then eqautions (4) and (5) give

$$\frac{d^2 u_1}{dx^2} + 2ik\frac{du_1}{dx} - (k^2 - \alpha^2)\, u_1 = 0 \; (0 < x < a). \qquad \text{...(7)}$$

$$\frac{d^2 u_2}{dx^2} + 2ik\frac{du_2}{dx} - (\beta^2 + k^2)\, u_2 = 0 \; (-b < x < 0) \qquad \text{...(8)}$$

The solution of these equations may be written as

$$u_1 = Ae^{i(\alpha - k)x} + Be^{-i(\alpha + k)x} \; (0 < x < a) \qquad \text{...(9)}$$

$$u_2 = C\, e^{(\beta - ik)x} + De^{-(\beta + ik)x} \; (-b < x < 0) \qquad \text{...(10)}$$

Here A, B, C, D are constants to be determined by the following boundary conditions

$$\left.\begin{aligned} (u_1)_{x=0} &= (u_2)_{x=0}; \; \left(\frac{du_1}{dx}\right)_{x=0} = \left(\frac{du_2}{dx}\right)_{x=0} \\ (u_1)_{x=a} &= (u_2)_{x=-b}; \; \left(\frac{du_1}{dx}\right)_{x=a} = \left(\frac{du_2}{dx}\right)_{x=-b} \end{aligned}\right\} \qquad \text{...(11)}$$

The first two conditions are due to requirement of continuity of wave function ψ and its derivative $(d\psi/dx)$; while the last two conditions are due to periodicity of $u(x)$. The application of these boundary conditions to (9) and (10) yields

$$\left.\begin{aligned} &A + B = C + D \\ &Ai\,(\alpha - k) - Bi\,(\alpha + k) = C\,(\beta - ik) - D\,(\beta + ik) \\ &Ae^{i(\alpha - k)a} + Be^{-i(\alpha + k)a} = Ce^{-(\beta - ik)b} + De^{(\beta + ik)b} \\ &Ai\,(\alpha - k)\,e^{i(\alpha - k)a} - Bi\,(\alpha + k)\,e^{-i(\alpha + k)a} \\ &= C\,(\beta - ik)\,e^{-(\beta - ik)b} - D\,(\beta + ik)\,e^{(\beta + ik)b} \end{aligned}\right\} \quad \ldots(12)$$

The coefficients A, B, C and D may be evaluated by solving these equations. However we are interested in evaluation of energy-values. Equations (12) give non-vanisihing solutions if the determinant coefficients vanishes. This leads to the following equation

$$\frac{\beta^2 - \alpha^2}{2\alpha\beta} \sinh \beta b \sin \alpha a + \cosh \beta b \cos \alpha a = \cos k\,(a + b) \quad \ldots(13)$$

This equation is quite complicated, however we may draw important conclusions. Kronig and Penny considered the possibility that $V_0 \to \infty$ and $b \to 0$ such that $V_0 b$ remains finite. Under these circumstances this model is modified to one of a series of wells separated by infinitely thin potential barriers, the quantity $V_0 b$ (under the limits $V_0 \to \infty$ and $b \to 0$) representing the barrier strength. Under this possibility equation (13) becomes

$$\left(\frac{mV_0 b}{\hbar^2 \alpha}\right) \sin \alpha a + \cos \alpha a = \cos ka \qquad ...(14)$$

Introducting the quantity such that

$$P = \frac{mV_0 ba}{\hbar^2} \qquad ...(15)$$

Then (14) reduces to

$$\boxed{P\left(\frac{\sin \alpha a}{\alpha a}\right) + \cos \alpha a = \cos ka.} \qquad ...(16)$$

This *is the condition for the solutions of the wave equation to exist.* We see that this is satisfied only for those value of αa for which its left-hand side lies between + 1 and – 1; this is because its right-hand side must lie in range. Such values of αa will, therefore, represent the wave-like solutions (6) and are accessible.

The other values of αa will be inaccessible. The consequence of this can be understood with reference to fig. 2·6 which represents the left-hand side $\left(\frac{P \sin \alpha a}{\alpha a} + \cos \alpha a\right)$ of (16) as a function of αa for the value $P = \frac{3\pi}{2}$. The part

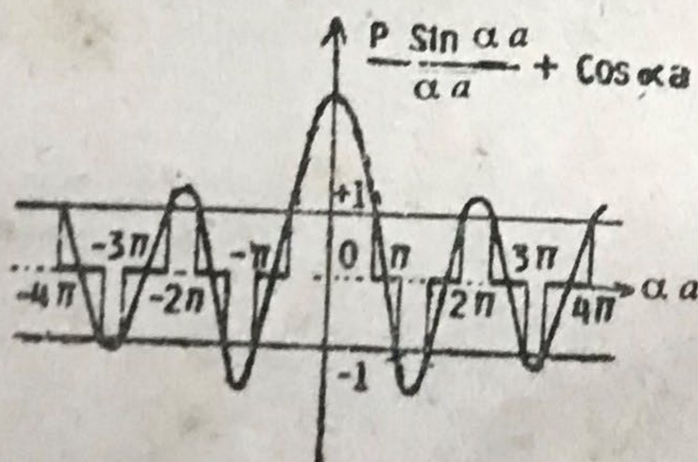


Fig. 2.6

of the vertical axis lying between the horizontal lines represents the range acceptable to the left-hand side $\left(\frac{P \sin \alpha a}{\alpha a} + \cos \alpha a\right)$. Remembering that α^2 is proportional to the energy E, the abscissa (αa) will be a measure for the energy.

Clearly there are regions for αa where the value of $\left[\frac{P \sin \alpha a}{\alpha a} + \cos \alpha a\right]$ does not lie between -1 and $+1$. For these values of αa and hence of energy E, no solutions exist. Such regions of energy are prohibited and are called *forbidden bands.*

1. *The energy spectrum of the electron consists of alternate regions of allowed energy* (continuous) and forbidden energy (dotted). These regions are usually referred as the allowed and forbidden energy bands.

2. *The width of the allowed energy bands increases as the* value of αa *(i.e. energy) increases.*

3. It is to be noted that P is a measure of the potential barrier strength. If P is large, the barriers are strong; and in the limit $P \rightarrow \infty$ (corresponding to infinitely deep wells), the electron can be considered as confined into a single potential well. This case applies to crystals where the electrons are very tightly bound with their nuclei. On the other hand, if P is small, the barrier strength is small; and in the limit $P \rightarrow 0$ (corresponding to no barrier), the electron can be considered to be moving freely through the potential wells. This case applies to crystals where the electrons are almost free of their nuclie. The effect of varying P on the band structure is shown in fig. 2·7. We conclude that.

The width of particular allowed band decreases as P increases. In one extreme case $P \to \infty$, the allowed energy bands are compressed into energy levels and the energy and the energy spectrum is thus a line spectrum. In the other extreme case $P \to 0$, we simply have the free electron model of energy spectrum ; it is quasi-continuous. Between these two limits, the position and the width of the allowed and forbidden bands for any value of P are obtained by drawing vertical lines ; the shaded areas correspond to allowed bands.

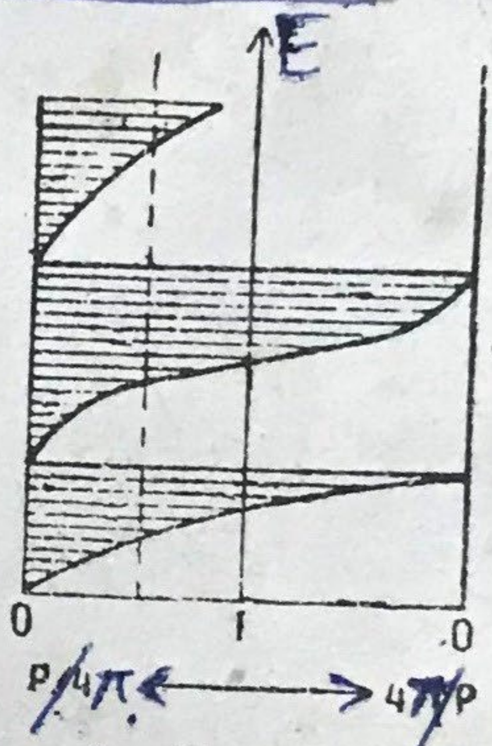


Fig. 2.7

Let us now calculate the energy spectrum in the two extreme cases by making use of (16). In one extreme case, when $P \to \infty$ it can easily be calculated by letting $P \to \infty$. We find (16) has solutions in this case only if $\sin \alpha a = 0$, or

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$$\alpha a = n\pi \quad \text{where } n \text{ is an integer}$$

i.e.

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

Using (3), we get

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

or

$$E = \frac{\pi^2 \hbar^2}{2ma^2} \cdot n^2 \qquad \text{...(17)}$$

One can easily recognise (17) as giving the energy levels of a particle in a constant potential box of atomic dimensions. This is a physically expected result because the large P makes the tunneling through the barrier almost improbable. In the other extreme case, when $P \to 0$, (16) leads to

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

or

$$\alpha = k \text{ i.e. } \alpha^2 = k^2 \text{ i.e. } \frac{2mE}{\hbar^2} = k^2$$

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

which is appropriate to the completely free particles.