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B.Sc (PS) Computer Science VI Sem

Kronig Penney model

# Kronig-Penney Model

classmate

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## Band theory of solids

The free electron theory of metal assumed that a conduction electron in a metal undergoes a constant zero potential and is completely free to move about in the crystal and restricted only by the surface of the crystal. The model explained successfully several properties like thermal conductivity, electrical conductivity, thermionic emission and specific heat of metals, ~~yet~~ yet there are other electronic properties of solids for which the free electron model provide no help. The model failed to explain why some chemical elements crystallize to form good conductors of electricity while other form insulators and semi-conductors. Explanation of these properties require a detail knowledge of the energy levels of the electrons in solids. In particular, the interaction of the electrons with ions, which gives rise to energy bands. The energy bands arise in solids because of the change of the atomic energy levels of the isolated atoms when a large number of atoms are brought close together.

Free electron model considers that the conduction electron in the crystal moves in a region of constant potential is too drastic. It is suggested that the crystal is an infinite array of lattice points and boundary conditions are periodic boundary conditions, first schrodinger <sup>wave</sup> equation will be solved for the electron under the periodic lattice.

## Wave function in a periodic lattice: Bloch theorem

To discuss the motion of the electron in a solid, Schrodinger equation ~~we~~ have to be solved under periodic boundary condition. Bloch solved the Schrodinger equation by introducing the symmetry properties of the potential in which the electrons move in a solid. Bloch's analysis points that the boundary condition satisfied by the wavefunction in a periodic potential is different from the boundary condition for obtaining a bound state.

The Schrodinger equation for an electron moving in one dimensional periodic potential is

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} (E - V(x)) \psi = 0 \quad (1)$$

where  $V(x)$  is the potential at a distance  $x$  from the origin which is assumed to vary periodically such that

$$V(x) = V(x+a) \quad (2)$$

where  $a$  is the period i.e. potential at  $x$  and  $x+a$  is the same. With reference to the solutions of eq. (1) there is an important theorem which states that there exist solutions of the form

$$\psi(x) = e^{\pm ikx} U_k(x) \quad (3)$$

$$\text{where } U_k(x) = U_k(x+a) \quad (4)$$

i.e. the solutions are plane waves ( $e^{\pm ikx}$ ) modulated by a function  $U_k(x)$ , which has the same ~~periodicity~~ periodicity as the lattice. The result eq. (3) is known as Bloch theorem.

It states that the eigenfunctions of the wave equation for a periodic potential are of the form of the product of a plane wave  $e^{\pm ikx}$

times a function  $u_k(x)$  with the periodicity of the crystal lattice,

$$\psi_k(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} u_k(\vec{r}) \quad (5)$$

This function is called Bloch function. These solutions are composed of travelling waves, and they can be assembled into wave packets to represent electrons that propagate through the potential field of the ion cores.

The wave vector  $\vec{k}$  used to label the Bloch function has the properties

(a) under the crystal translation which carries  $\vec{r}$  to  $\vec{r} + \vec{T}$  ( $\vec{T}$  is translation vector), we have

$$\psi_k(\vec{r} + \vec{T}) = e^{i\vec{k}\cdot\vec{T}} e^{i\vec{k}\cdot\vec{r}} u_k(\vec{r} + \vec{T})$$

$$\text{or } \psi_k(\vec{r} + \vec{T}) = e^{i\vec{k}\cdot\vec{T}} \psi_k(\vec{r}) \quad (6)$$

$$\text{because } u_k(\vec{r} + \vec{T}) = u_k(\vec{r})$$

(b) if the lattice potential vanishes,  $u_k(\vec{r})$  is constant. Thus  $\psi_k(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}$  just as for free e<sup>-</sup>.

### Kronig - Penney Model:-

It is assumed that potential energy of an electron has the form of a periodic array of rectangular wells and it is possible to obtain an exact solution of the Schrodinger's eq<sup>n</sup>. The period of the potential is  $(a+b)$ . For  $0 < x < a$ ,  $V(x) = 0$  &  $-b < x < 0$ ,  $V(x) = V_0$ .

Schrodinger eq<sup>n</sup> for the two regions are

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} E\psi = 0 \quad \text{for } 0 < x < a \quad (7)$$

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} (E - V_0)\psi = 0 \quad \text{for } -b < x < 0 \quad (8)$$

$$\text{Assume } \alpha^2 = \frac{2mE}{\hbar^2} \quad \& \quad \beta^2 = \frac{2m(V_0 - E)}{\hbar^2} \quad (9)$$

When  $a$  &  $b$  are real quantities,  
 Eq. 7 & 8 then becomes

$$\frac{d^2\psi}{dx^2} + \alpha^2\psi = 0 \quad \text{for } 0 < x < a \quad (10)$$

$$\frac{d^2\psi}{dx^2} + \beta^2\psi = 0 \quad \text{for } -b < x < 0 \quad (11)$$

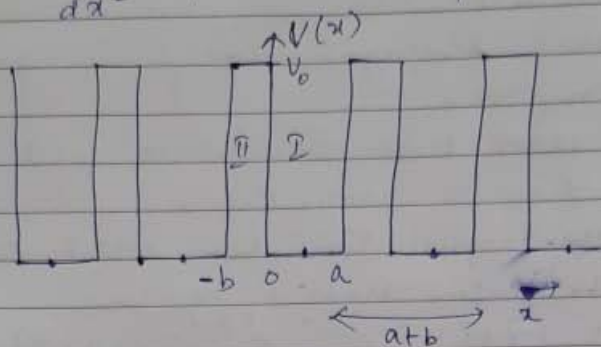


Fig: Kronig and Penney one-dim periodic potential

Using the fact that the solution of a wave equation for a periodic potential must be Bloch function of the form

$$\psi(x) = e^{ikx} u_k(x) \quad (12)$$

Where  $u_k(x)$  is the periodic function in  $x$  with period  $(a+b)$ . From eq. (12) we have

$$\left. \begin{aligned} \frac{d^2\psi}{dx^2} &= ik e^{ikx} u_k(x) + e^{ikx} \frac{d^2u_k}{dx^2} \\ \frac{d^2\psi}{dx^2} &= -k^2 e^{ikx} u_k(x) + 2ik e^{ikx} \frac{du_k}{dx} + e^{ikx} \frac{d^2u_k}{dx^2} \end{aligned} \right\} (13)$$

Putting (12) & (13) in (10) & (11) we get

$$\frac{d^2u_1}{dx^2} + 2ik \frac{d^2u_1}{dx^2} + (\alpha^2 - k^2) u_1 = 0 \quad 0 < x < a \quad (14)$$

$$\frac{d^2u_2}{dx^2} + 2ik \frac{d^2u_2}{dx^2} - (\beta^2 + k^2) u_2 = 0 \quad -b < x < 0 \quad (15)$$

Where  $u_1$  represents the value of  $u_k(x)$  in the

interval  $0 < x < a$  and  $u_2$  in the interval  $-b < x < 0$ .

The general solutions of eq. (14) and (15) are

$$u_1 = A e^{i(\alpha-k)x} + B e^{-i(\alpha+k)x} \quad 0 < x < a \quad (16)$$

$$u_2 = C e^{(\beta-ik)x} + D e^{-(\beta+ik)x} \quad -b < x < 0 \quad (17)$$

$A, B, C$  &  $D$  are const., const. must be chosen such that the boundary conditions are satisfied:

$$\left. \begin{aligned} (u_1)_{x=0} &= (u_2)_{x=0} & \left( \frac{du_1}{dx} \right)_{x=0} &= \left( \frac{du_2}{dx} \right)_{x=0} \\ (u_1)_{x=a} &= (u_2)_{x=-b} & \left( \frac{du_1}{dx} \right)_{x=a} &= \left( \frac{du_2}{dx} \right)_{x=-b} \end{aligned} \right\} \quad (18)$$

Application of bdy. condition to eq. (16) & (17) leads to four linear homogeneous equations for  $A, B, C, D$

$$A + B = C + D$$

$$\left. \begin{aligned} A i(\alpha-k) - B i(\alpha+k) &= C(\beta-ik) - D(\beta+ik) \\ A e^{i(\alpha-k)a} + B e^{-i(\alpha+k)a} &= C e^{-(\beta-ik)b} + D e^{(\beta+ik)b} \\ A i(\alpha-k) e^{i(\alpha-k)a} - B i(\alpha+k) e^{-i(\alpha+k)a} &= C(\beta-ik) e^{-(\beta-ik)b} + D(\beta+ik) e^{(\beta+ik)b} \end{aligned} \right\} \quad (19)$$

The four equations have solutions only if the determinants of the co-efficient of  $A, B, C$  &  $D$  vanishes, which requires that

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

Solving the determinant leads to

$$\frac{\alpha^2 - \beta^2}{2\beta} \sinh \beta b \sin \alpha a + \cos \beta b \cos \alpha a = \cos k(a+b) \quad (20)$$

In order to obtain simplified form of this relation, Kronig and Penney considered the case when  $V_0$  tends

to infinity and  $b$  approaches zero, but the product  $V_0 b$  remains finite i.e., the potential barriers become delta functions. Under these conditions the model is modified to one of a series of wells separated by infinitesimally thin potential barriers, the quantity  $\lim_{\substack{V_0 \rightarrow \infty \\ b \rightarrow 0}} (V_0 b)$  rep. the barrier strength.

Thus for  $b \rightarrow 0$   $\sinh pb = pb$  &  $\cosh pb = 1$

Hence eq. (20) becomes

$$\left( \frac{\beta^2 - \alpha^2}{2\alpha\beta} \right) \beta b \sin \alpha a + \cos \alpha a = \cos \alpha a \quad (21)$$

$$\text{Now } (\beta^2 - \alpha^2) = \frac{2m(V_0 - E)}{\hbar^2} = \frac{2m}{\hbar^2} E = \frac{2m}{\hbar^2} (V_0 - 2E)$$

Since  $V_0 \gg E$ , therefore

$$(\beta^2 - \alpha^2) = \frac{2m}{\hbar^2} V_0$$

and  $\frac{\beta^2 - \alpha^2}{2\alpha\beta} = \frac{2mV_0}{\hbar^2} \cdot \frac{1}{2\alpha\beta}$ , thus eq. (20) becomes

$$\frac{mV_0 b}{\hbar^2 \alpha} \sin \alpha a + \cos \alpha a = \cos \alpha a \quad (22)$$

Let us now define a quantity

$$P = \frac{mV_0 b a}{\hbar^2} \quad (23)$$

then eq. (22) becomes

$$P \frac{\sin \alpha a}{\alpha a} + \cos \alpha a = \cos \alpha a \quad (24)$$

from eq. (23) since  $V_0$  tends to  $\infty$  i.e.  $P$  is a measure of the quantity  $V_0 b$ , which is the area of the potential barrier, called barrier strength. In other words the physical significance of this quantity is that if  $P$  is increased, the area of the potential barrier is increased and the given electron is

bound more strongly to a particular potential well. When  $P \rightarrow 0$ , the potential barrier becomes weak, which means that electrons are free electrons.

Further fig 2 shows the plot of left hand side of eq. 24 as a function of  $ka$  for the values of  $P = \frac{3\pi}{I}$ . As  $\alpha^2$  is proportional to energy, thus the  $x$ -axis  $z$  is proportional to energy.

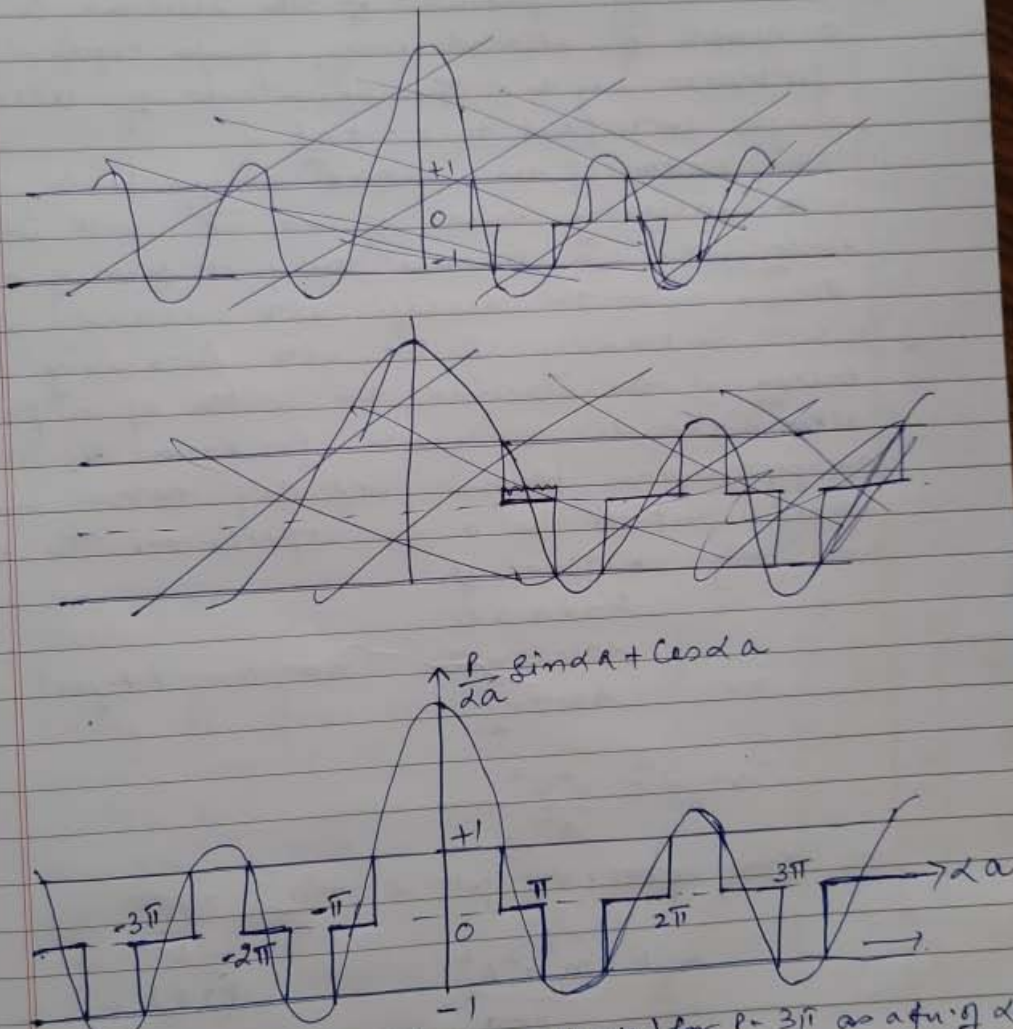


Fig 2: Plot of function  $\left(\frac{P}{2a} \sin ka + \cos ka\right)$  for  $P = \frac{3\pi}{I}$  as a fn. of  $ka$ .

The right hand side of eq. 24 can take values only between +1 and -1 as indicated by the horizontal lines in fig. 7.2. Therefore the condition eq. (21) can be satisfied only for values of  $\alpha a$  for which left hand side lies between  $\pm 1$ .  
Following conclusions can be drawn:

- (i) The energy spectrum of the electrons consist of a number of allowed energy bands separated by forbidden region. The boundaries of allowed ranges correspond to  $k = \pm n\pi/a$ .
- (ii) The width of the allowed energy bands increases with increasing values of  $\alpha a$ , i.e., with increasing energy. This is because the first term of eq. 24 decreases on the average with increasing  $\alpha a$ .
- (iii) With increasing  $P$  i.e., with increasing binding energy of the electrons, the width of a particular allowed band decreases. For  $P \rightarrow \infty$  the allowed energy region becomes infinitely narrow and the energy spectrum is a line spectrum. The eq. 24 has only solutions if

$$\sin \alpha a = 0$$

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

$$\text{or } \alpha = \pm \frac{n\pi}{a}$$

$$\text{or } \alpha^2 = \frac{n^2 \pi^2}{a^2}$$

from eq. (9), we get  $\alpha^2 = \frac{n^2 \pi^2}{a^2} = \frac{2mE}{\hbar^2}$

$$\text{or } E = \frac{n^2 \pi^2 \hbar^2}{2ma^2} \quad (2.5)$$

The energy levels in this case are discrete and result in similar to energy levels of a particle in a constant potential box of atomic dimension. Physically, this is expected because for large  $P$  tunnelling through the barrier becomes difficult.

(iv) Also if when  $P \rightarrow 0$ , eq. (24) leads to

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

$$\text{or } \alpha = k \quad \text{and} \quad \alpha^2 = k^2$$

from eq. 9, we get

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

$$\text{which gives } E = \frac{\hbar^2 k^2}{2m} \quad \text{--- (26)}$$

$$\text{where } k = \frac{2\pi}{a}, \text{ thus } E = \frac{\hbar^2}{2m} \cdot \frac{1}{a^2} = \frac{\hbar^2}{2m} \cdot \frac{P^2}{h^2}$$

$$= \frac{1}{2} m v^2 \quad \text{--- (27)}$$

This is appropriate for completely free particles. Hence no energy levels exist, all energies are allowed to the electrons.

The conclusions are summarised in fig. 3, where the energy spectrum is given as function of  $P$ .

When  $P = 0$  i.e.  $V_0$  is zero, the energy spectrum is continuous, simply the free electron model.

When  $P \rightarrow \infty$ , a line spectrum results. For a given value of  $P$  the position and width of the allowed and forbidden bands are obtained by drawing a vertical line, the shaded area correspond to allowed band.

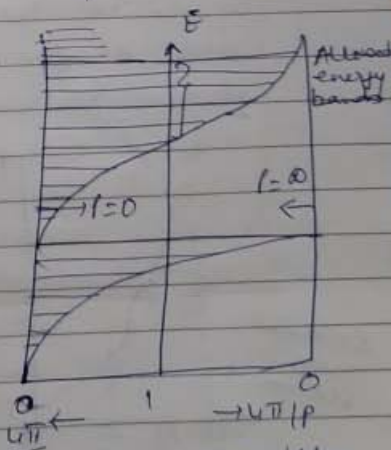


Fig. 3: Allowed and forbidden energy bands as a fun. of  $P$

