

Ex. 5

(a)

## Krönig - Penney Model ①

Particle is moving in a periodic potential.

For e.g., in case of a metal or semiconductor, where the crystal structure is periodic, the electrons experience a periodic potential.



Thus for discussing the conduction or insulation properties of solids, we should have the knowledge of what are energy eigenvalues and eigenstates of electrons in the periodic potential of these solids.

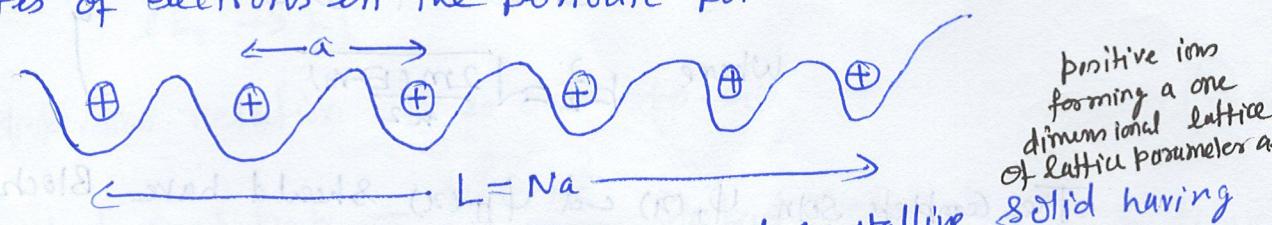


Fig: Periodic potential in a one-dimensional crystalline solid having  $N$  sites.

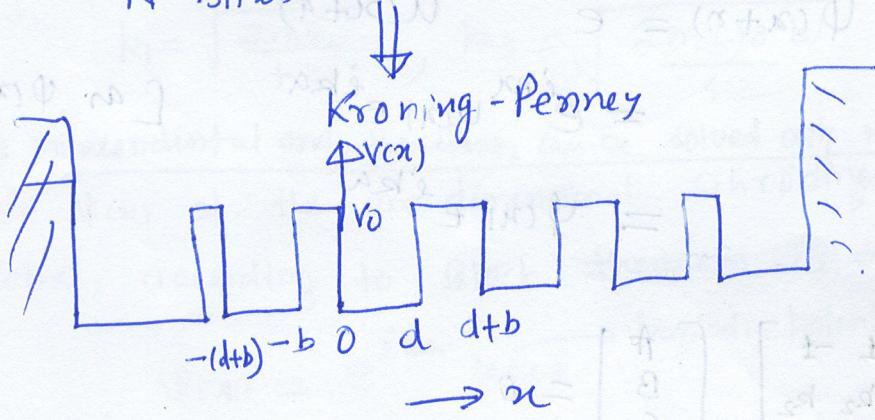


Fig:- Kroning - Penney Potential with periodicity  $a (= d+b)$

If we ignore the potential size at two boundaries the potential is periodic throughout and has the property

$$V(x) = V(x + na) \quad n \rightarrow \text{integer}$$

To find out energy eigenvalues and eigenstates of a particle in the periodic potential, we shall have to solve Schrödinger eqn.

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

with  $V(x) = 0$  for  $-a < x < a$

$V(x) = V_0$  for  $a < x < d$

and  $V(x) = V(x+a)$

The possible states that the electron can occupy are determined by the Schrödinger eqn, in case of Kroning - Penney Model

Case :- E > V<sub>0</sub>

The general soln of Schrödinger eq<sup>n</sup> in the potential well region ( $0 \leq x \leq d$ ) is

$$\Psi_I(x) = A e^{ik_1 x} + B e^{-ik_1 x}$$

where  $\frac{2mE}{\hbar^2} = k_1^2$

The wave function in the barrier region ( $-b \leq x \leq 0$ ) is

$$\Psi_{II}(x) = C e^{ik_2 x} + D e^{-ik_2 x}$$

where  $b_2^2 = \frac{2m(E-V_0)}{\hbar^2}$

The complete soln  $\Psi_I(x)$  and  $\Psi_{II}(x)$  should have Bloch form.

From Bloch theorem

$$\Psi(x+a) = e^{i(a+u)} \Psi(x+a)$$

$$= e^{ika} u(x) e^{ika}$$

$$[ \text{as } \Psi(x+a) = u(x) ]$$

Boundary Conditions:

$\Psi, \frac{d\Psi}{dx}$  at  $x=0$  &  $x=d$  to determine A, B, C & D.

$$\begin{bmatrix} 1 & 1 & -1 & -1 \\ k_1 & -k_1 & -k_2 & k_2 \\ e^{ik_1 d} & e^{ik_1 d} & e^{-ik_2 b} & e^{ik_2 b} \end{bmatrix} \begin{bmatrix} A \\ B \\ C \\ D \end{bmatrix} = 0$$

$$= \Psi(x) e^{ika}$$

dispersion relation

$$\cos k_1 d \cos k_2 b = \frac{k_1^2 + k_2^2}{2k_1 k_2} \sin k_1 d \sin k_2 b = \cos(k_1 d + b) \rightarrow (A)$$

$$\text{with } k_1 = \sqrt{\frac{2mE}{\hbar^2}} \quad \& \quad k_2 = \sqrt{\frac{2m(V_0-E)}{\hbar^2}}$$

$$k_1^2 - k_2^2 = \frac{2mV_0}{\hbar^2}$$

$$\begin{aligned} A+B &= c+d \\ \Rightarrow k_1(A-B) &= k_2(c-d) \end{aligned}$$

$$\begin{bmatrix} 1 & 1 & -1 & -1 \\ k_1 & -k_1 & -k_2 & k_2 \\ e^{ik_1 d} & e^{ik_1 d} & e^{-ik_2 b} e^{-ik_2 b} & e^{-ik_2 b} e^{ik_2 b} \\ k_1 e^{ik_1 d} & -k_1 e^{-ik_1 d} & -k_2 e^{ik_2 b} e^{-ik_2 b} & k_2 e^{ik_2 b} e^{ik_2 b} \end{bmatrix} \begin{bmatrix} A \\ B \\ C \\ D \end{bmatrix} = 0$$

(2)

Case 2:-

E < V<sub>0</sub>

$$\Psi_{\pm}(x) = A e^{ik_1 x} + B e^{-ik_1 x}$$

$$\Psi_{\mp}(x) = C e^{k_3 x} + D e^{-k_3 x}$$

where  $k_3 = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$

So, the dispersion relation for  $E < V_0$  case can be easily obtained from Eqn(A) simply by the replacement

$$ik_2 \rightarrow k_3$$

The dispersion relation comes out to be

$$\cos k_1 d \cosh k_3 b - \frac{k_1^2 - k_3^2}{2k_1 k_3} \sin k_1 d \sinh k_3 b = \cos k(d+b)$$

with

$$k_1 = \sqrt{\frac{2mE}{\hbar^2}}, \quad k_3 = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}, \quad k_1^2 + k_3^2 = \frac{2mV_0}{\hbar^2}$$

Eqn(A) & (B), are transcendental and, therefore, can be solved only numerically to find dispersion relation (Eqn C)

The soln  $\Psi(x)$  of the one-dimensional Schrödinger eqn for a periodic potential, according to Bloch theorem is of the form.

$$\Psi(x) = e^{ikx} u(x) \xrightarrow{\text{periodic potential}}$$

$$u(x+a) = u(x)$$

$$\begin{aligned} \Psi(x+L) &= \Psi(x+Na) = e^{ik(x+Na)} u(x+Na) \\ &= e^{ikNa} e^{ikx} u(x) \end{aligned}$$

k → wave vector

$$= e^{ikNa} \Psi(x) \quad \text{--- (C)}$$

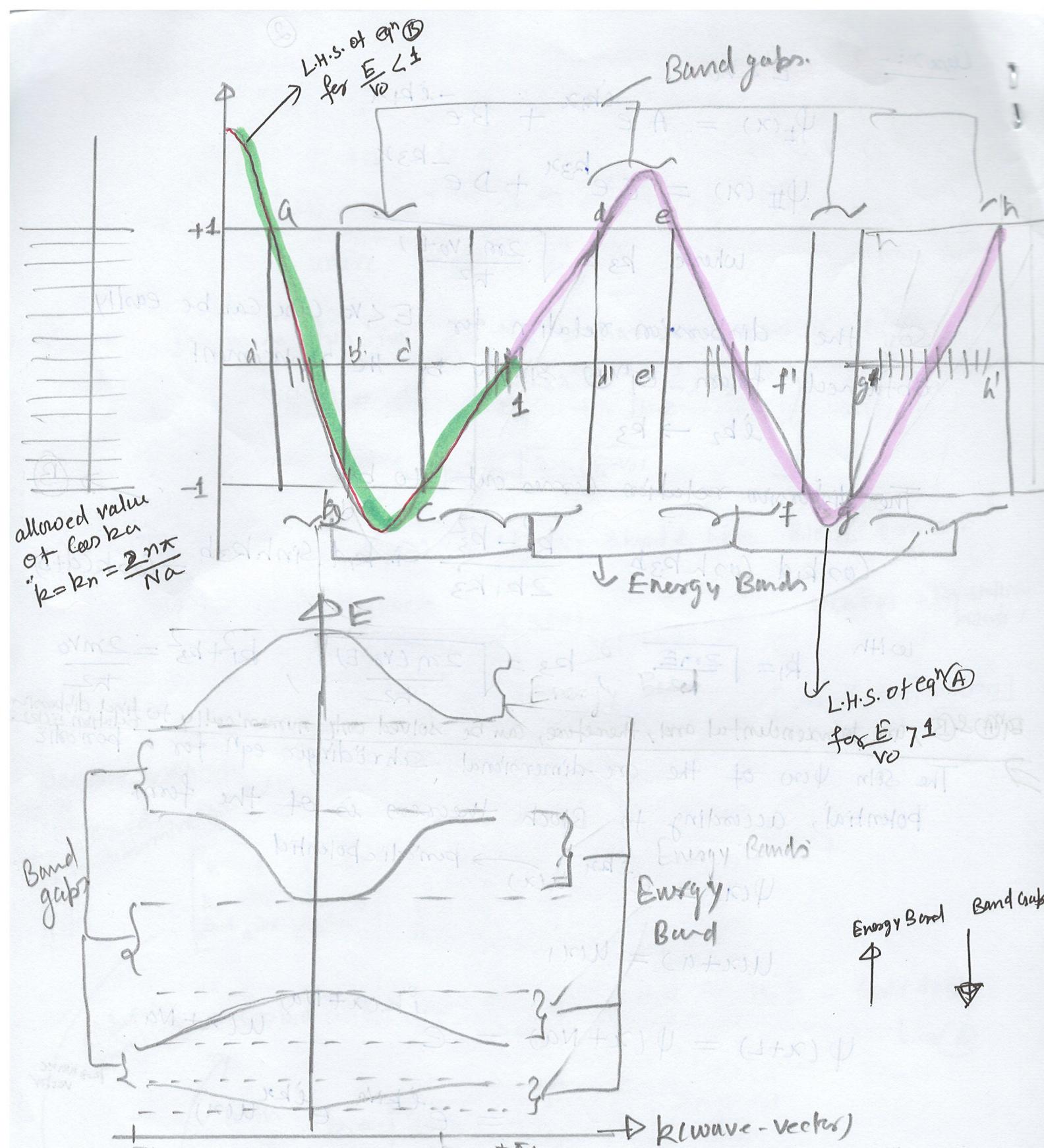
Also we know that

$$\Psi(x+L) = \Psi(x) \quad \text{--- (D)}$$

Comparing (C) & (D), we get

$$e^{ikNa} = 1$$

$$k = (\text{say}) k_n = \frac{2n\pi}{Na} = \frac{2n\pi}{L}$$



- (N) The horizontal lines (in the left part of the figure) may be imagined to be extending towards right side and whenever these cut the curve, we get allowed energy eigenvalues.

$[a', b'] ; [c', d'] ; [e', f']$  and  $[g', h'] \rightarrow$  allowed energy

$[b', c'] ; [d', e'] ; [f', g'] \rightarrow$  Band gaps