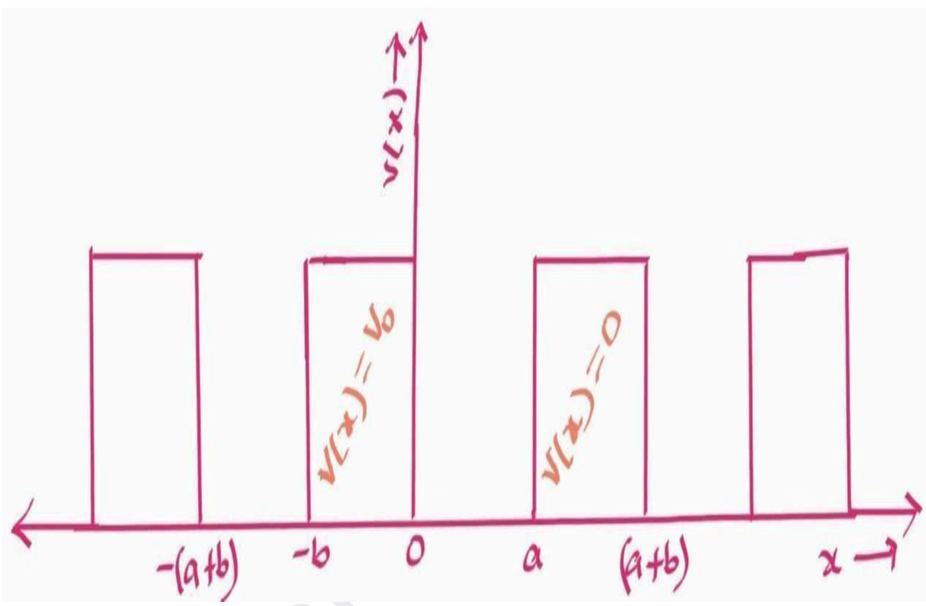
1.14.KRONIG-PENNEY MODEL

Introduction:

The Kronig - Penney model was introduced in 1931 by L. Kronig and WG. Penney.

- The Kronig-Penney model is a simplified quantum mechanical model that describes an electron in a 1-D periodic potential, yields energy bands as well as energy gaps.
- The free e's in a metal move under a periodic potential due to regularly arranged +vely ions.
- The nature of energies of the e's is determined by solving Schrodinger wave equation.
- The Kronig-Penney model represents the periodic potential (a+b) in the form of regular arrays of square well potentials as shown in figure.



- In a region where $0<x<a$, the Potential energy is assumed to be zero.

  $V=0$ -----------(1)
- In region where $-b<x<0$, the Potential energy is assumed to be V_0.

  $V=V_0$ ------------(2)
- The Schrodinger wave equation $\partial^2\psi/\partial x^2 + 8\pi^2 m(E-V)\psi/h^2$ for the above two regions are

  $\partial^2\psi/\partial x^2 + 8\pi^2 mE\psi/h^2 = 0$ ------------------(3)

  $\partial^2\psi/\partial x^2 + 8\pi^2 m(E-V_0)\psi/h^2 = 0$ -------------- (4)
- **Let** $8\pi^2 mE/h^2 = \alpha^2$ ------------------(5)

  $8\pi^2 m(E-V_0)/h^2 = \beta^2$ -----------------(6)
- **Then the (3) & (4) becomes**

  $\partial^2\psi/\partial x^2 + \alpha^2\psi = 0$ --- ---------- (7)

$$\partial^2\psi/\partial x^2 + \beta^2\psi = 0 \text{ --- ----------- } (8)$$

- **On solving (7) & (8)** by applying the Bloch function: $\psi(x) = e^{ikx}. U_k(x)$, we get

$$P \sin(\alpha a)/\alpha a + \cos(\alpha a) = \cos(ka) \text{ -------- ---}(6)$$

- ***where:*** P is scattering power of Barrier Potential
- **From (5)** => $8\pi^2 mE/h^2 = \alpha^2$

$$E = h^2\alpha^2/8\pi^2 m \text{ ------------ } (10)$$

- To derive the relationship for the allowed values of electron **energies** during the motion of an electron within a crystal lattice, Kronig and Penney made the following assumptions:

  (i)The energy of the electron (E) is less than the potential barrier height (V_0).

  (ii)The solutions to the Schrodinger wave equation are Bloch functions.

  (iii)The wave functions and their first derivatives are continuous throughout the crystal lattice.

Special Cases:

If P → ∞:

- $P \sin(\alpha a)/\alpha a + \cos(\alpha a) = \cos(ka)$

$$\Rightarrow \sin(\alpha a)/\alpha a + \cos(\alpha a)/P = \cos(ka)/P \text{ --------- ---- } (11)$$

- But $P = \infty \Rightarrow \sin(\alpha a)/\alpha a = 0$

$$\sin(\alpha a) = 0$$

$$\sin(\alpha a) = \sin n\pi \text{ (since } \sin n\pi = 0)$$

$$\alpha a = n\pi$$

$$\alpha = n\pi/a \quad \text{and}$$

$$\alpha^2 = n^2\pi^2/a^2 \text{ ----------- } (12)$$

- **But from (5) & (12**) => $8\pi^2 mE/h^2 = n^2\pi^2/a^2$

$$E = n^2h^2/8ma^2$$

- **when** P →∞ => $E = n^2h^2/8ma^2$ -------------- (13)
- This equation (13) is the special case of electrons trapped.

ii) If P → 0:

- **From (6)**: $\cos(\alpha a) = \cos(ka)$

$$\alpha a = ka \quad \text{and}$$

$$\alpha^2 = k^2 \text{ --------------}(14)$$

- **From (10) & (14):** $E = h^2k^2/8\pi^2m$ -----------(15)
- **Since** $k = 2\pi/\lambda \Rightarrow k^2 = 4\pi^2/\lambda^2$

$$E = h^2/8\cancel{\pi^2}m \times 4\cancel{\pi^2}/\lambda^2$$

$$E = h^2/2m \times 1/\lambda^2$$

$$E = h^2/2m \times 1/(h^2/p^2) \quad (\because \lambda = h/P \Rightarrow \lambda^2 = h^2/P^2)$$

$$E = \cancel{h^2}/2\cancel{m} \times \cancel{m}v^2/\cancel{h^2} \quad (\because P = mv \Rightarrow Pm = mv^2)$$

$$E = 1/2\ mv^2 \quad \text{-----------------(16)}$$

- Total energy E = K.E + P.E

$$E = 1/2\ mv^2 \quad (\because P.E = V = 0)$$

- When $P \to 0 \Rightarrow E = 1/2\ mv^2$ ------------------ (17)
- This is a special case of free electrons moving throughout the lattice.

<u>Conclusion:</u> Finally, we conclude that:

- Electrons in solids are permitted to be allowed energy bands separated by forbidden energy gaps.
- Allowed energy band widths increases with increase in Energy
- P ->→ ∞ is the case of electron trapped and
- P ->→ 0 is the case of free electron moves throughout the lattice.

<u>Applications of Kronig-Penney Model:</u>

- It is used in the development of semiconductor chips.
- It is used to select the correct material according to the need in the manufacturing of different electronic devices.
- It is used to understand the behavior of material.
- It is used to Identify the nature of material.