Kronig-Penney Model

Explained By

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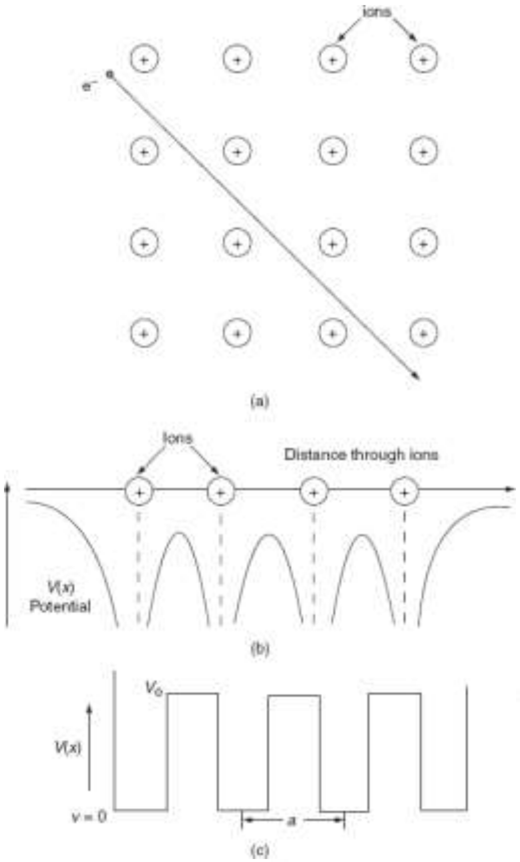
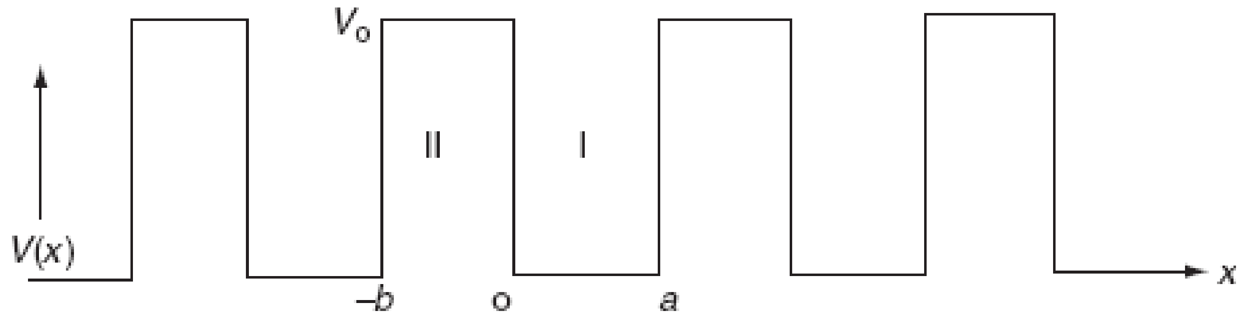
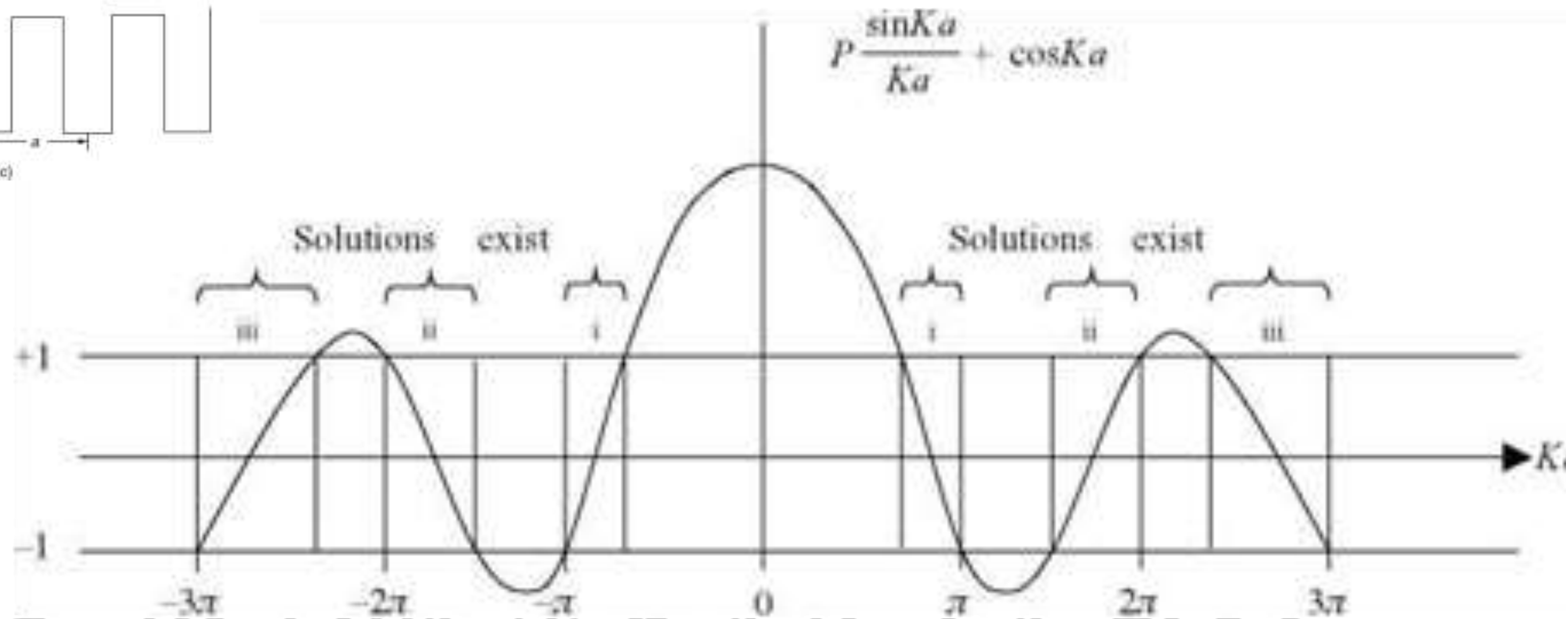
Kronig-Penney Model

- ✓ Free electron theory was given to explain the properties of solids. The fundamental assumption was electron moves in a constant potential well.
- ✓ The free electron theory was successfully explained the electric conductivity and thermionic emission of metals.
- ✓ But it failed to explain the classification of materials as solids, insulators and semiconductors.
- ✓ To solve this problem the basic assumption of free electron theory was modified by Bloch.
- ✓ Bloch proposed that the electron inside the material are not in constant potential but they are moving in periodic potential well as per the periodicity of lattice.
- ✓ Kronig and Penney define the periodic one dimensional square potential well (they gave the shape of square potential well).
- ✓ They explained mainly band in solids and classification of semiconductor and insulators.

Important diagrams

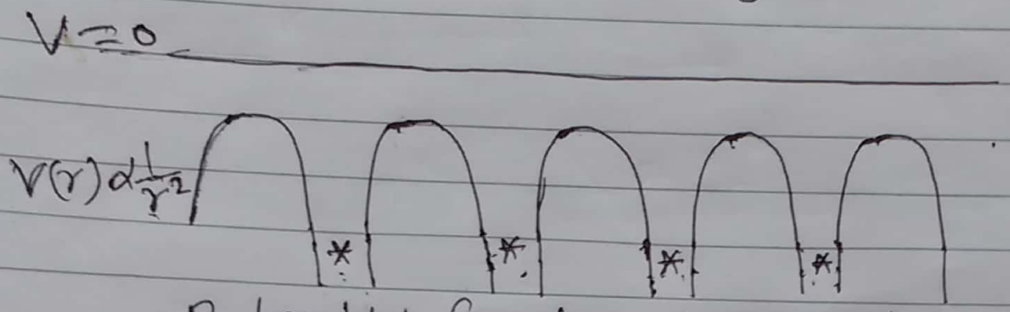




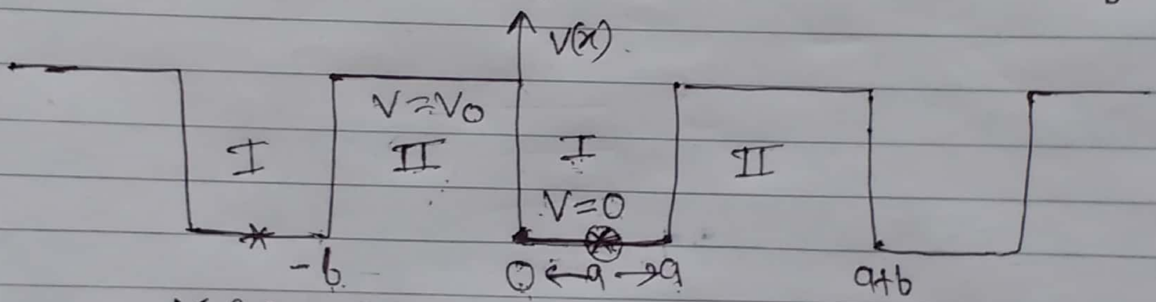


The KRONIG PENNEY MODEL

→ Why kronig Penney Model ?



Potential function of One dimensional Single Crystal



KRONIG - PENNEY MODEL

According to Bloch thearam Periodically varying potential energy function will be

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

the schrodinger's wave equation

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

For I - Region (from 0 - a) $V = 0$

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}E\psi = 0 \quad \text{—} \; (1)$$

For II - Region $(-b < x < 0)$ $V = V_0$

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

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

$$\frac{d^2\psi}{dx^2} + \alpha^2\psi = 0 \quad - (3) \quad \& \quad \frac{d^2\psi}{dx^2} - \beta^2\psi = 0 \quad - (4)$$

Bloch thearam $\psi(x) = e^{ikx} u_k(x)$ — (5)

$$\frac{d\psi}{dx} = e^{ikx}\frac{d}{dx}u_k + u_k\, ik\, e^{ikx}$$

$$\frac{d^2\psi}{dx^2} = e^{ikx}\frac{d^2u_k}{dx^2} + \frac{du_k}{dx}(ik)e^{ikx} + \frac{du_k}{dx}(ik)e^{ikx} + u_k(ik)^2 e^{ikx}$$

$$\frac{d^2\psi}{dx^2} = e^{ikx}\left(\frac{d^2u_k}{dx^2} + 2ik\frac{du_k}{dx} - u_k k^2\right) \quad - (6)$$

on putting (5) and (6) in (3)

$$e^{ikx}\left(\frac{d^2u_k}{dx^2} + 2ik\frac{du_k}{dx} - u_k k^2\right) + \alpha^2 e^{ikx} u_k = 0$$

$$\frac{d^2u_k}{dx^2} + 2ik\frac{du_k}{dx} + (\alpha^2 - k^2)u_k = 0$$

$$\frac{d^2u_k}{dx^2} + 2ik\frac{du_k}{dx} + (\alpha^2 - k^2)u_k = 0 \quad - (7)$$

$$\frac{d^2 u_k}{dx^2} + 2ik\frac{du_k}{dx} - (\beta^2 + k^2)u_k = 0 \quad \text{— (8)}$$

from (7) & (8) The general Solution will be

$$u_1(x) = A e^{i(\alpha-k)x} + B e^{-i(\alpha+k)x} \quad \text{— (9) for I}$$

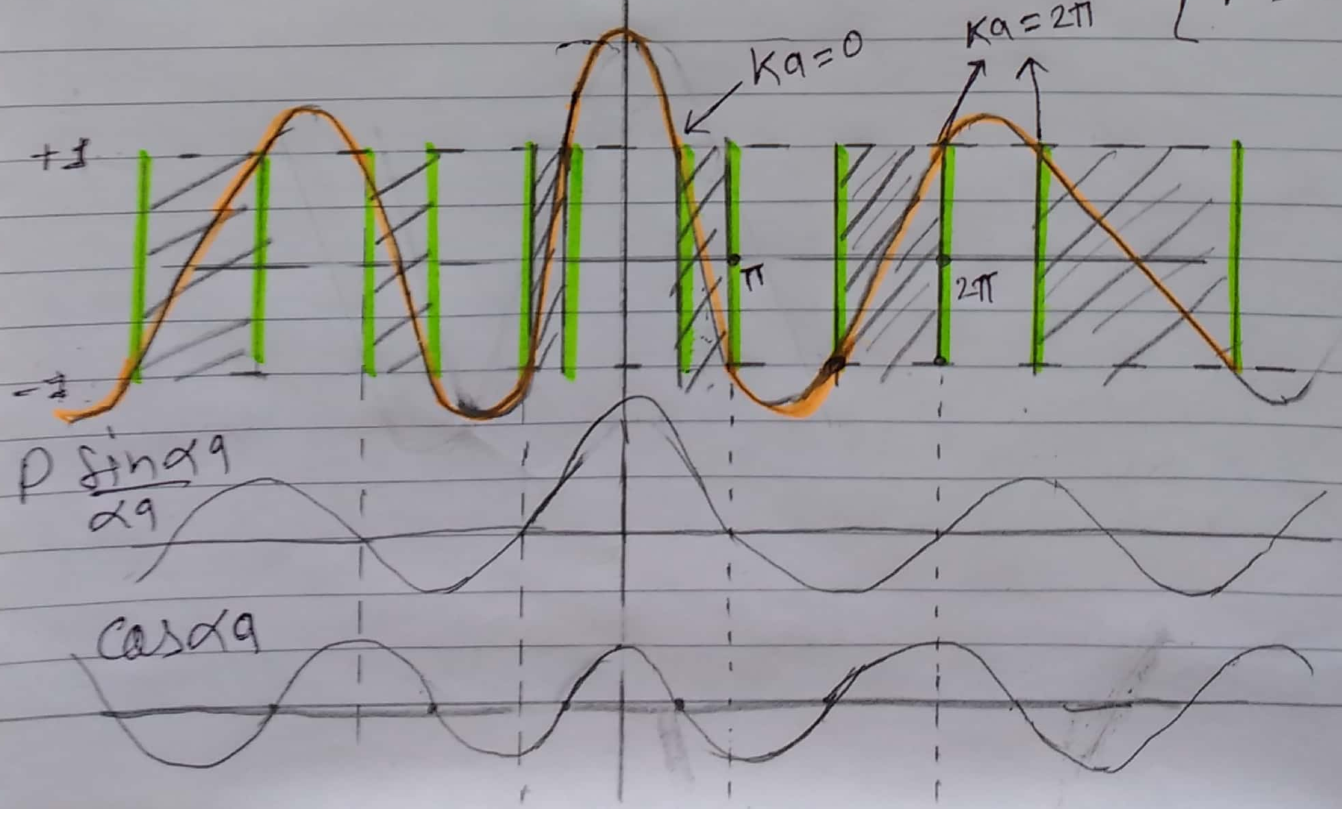
$$u_2(x) = C e^{i(\beta-k)x} + D e^{-i(\beta+k)x} \quad \text{— (10) for II}$$

Considering the boundary condition $x=0$

$$u_1(0) = u_2(0)$$

$$A+B = C+D$$

by Solving $P\frac{\sin\alpha a}{\alpha a} + \cos\alpha a = \cos ka$ $\left\{ P = \frac{mV_0 ba}{\hbar^2} \right.$



$$P \frac{\sin \alpha a}{\alpha a} + \cos \alpha a = \cos K a$$

where $P = \frac{m V_0 b a}{\hbar^2}$

Case 1:

$V_0 = 0$ then $P = 0$

$$\cos \alpha a = \cos K a$$

$$\alpha = K$$

$$\alpha^2 = K^2$$

$$\frac{2mE}{\hbar^2} = \frac{4\pi^2}{\lambda^2} \quad \left\{ \alpha^2 = \frac{2mE}{\hbar^2}, K^2 = \frac{4\pi^2}{\lambda^2} \right.$$

$$E = \frac{4\pi^2}{\lambda^2} \times \frac{h^2}{4\pi^2 2m} \Rightarrow E = \frac{h^2}{2m\lambda^2}$$

We know that

$$\lambda = h/mv$$

$$E = \frac{\cancel{h^2}}{2\cancel{m}} \times \frac{m^{\cancel{2}} v^2}{\cancel{h^2}}$$

$$E = \frac{1}{2} m v^2$$

$$E = \frac{p^2}{2m}$$

Here the energy of electron is KE only which shows that electrons are free

It indicates a nature of Conductor

Case - II $P \to \infty$ means $V_0 = \infty$

$$\sin \alpha a = 0$$
$$\alpha a = n\pi$$
$$\alpha = n\pi/a$$
$$\alpha^2 = \frac{n^2\pi^2}{a^2} \quad \left\{ \alpha^2 = \frac{2mE}{\hbar^2} \right.$$

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

$$E = \frac{n^2\pi^2}{a^2} \times \frac{\hbar^2}{2m}$$

$$E = \frac{n^2\pi^2}{a^2} \times \frac{h^2}{4\pi^2(2m)} \quad \left\{ \hbar = h/2\pi \right.$$

$$\boxed{E = \frac{n^2h^2}{8ma^2}}$$

→ Energy levels are discreate

→ Similar to Potential box

→ No KE energy