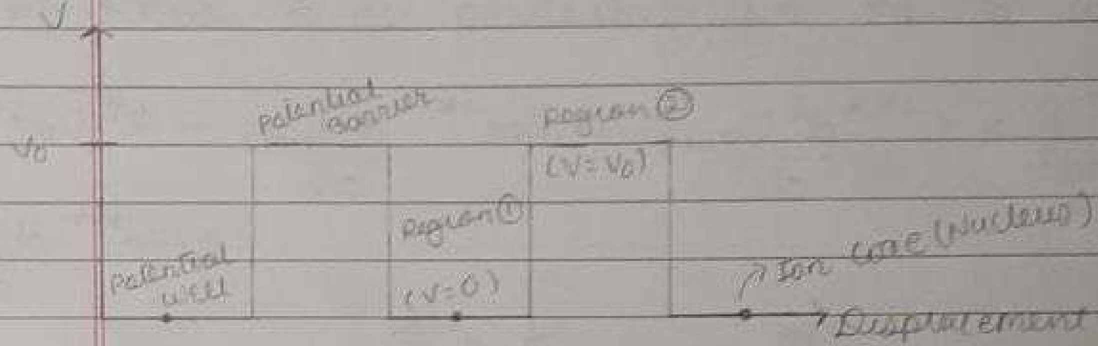
# Kronig - Penney Model

Theory: The potential of electron varies periodically with periodicity of Ion Core (Nucleus) and the potential energy of electron is zero near nucleus and maximum when it is lying between the adjacent nuclei which are separated by the inter-atomic spacing 'a'.




From Schrödinger Time Independent wave equation,

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

Now for region ①, $V=0$

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

For region ②, $V=V_0$

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

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

③

$\therefore$ Now eq ① and ② are,

$$\frac{d^2\psi}{dx^2} + \alpha^2\psi = 0 \quad \text{—— (4)}$$

$$\frac{d^2\psi}{dx^2} - \beta^2\psi = 0 \quad \text{—— (5)}$$

Now solving eq ④ and ⑤ we get,

$$\psi = e^{ikx} \cdot U_{k(x)} \quad \text{—— (6)}$$

Now double differentiating eq ⑥, w.r.t 'x'.

$$\frac{d^2\psi}{dx^2} = e^{ikx} \cdot \frac{d^2 U_{k(x)}}{dx^2} + ike^{ikx} \cdot \frac{dU_{k(x)}}{dx} - k^2 . U_k e^{ikx} + ike^{ikx} \frac{dU_{k(x)}}{dx} \quad \text{—— (7)}$$

Now put eq ⑦ in eq ④ & ⑤ and also divide throughout by $e^{ikx}$ we get,

$$\frac{d^2 U_{k(x)}}{dx^2} + 2ik\frac{dU_{k(x)}}{dx} + (\alpha^2 - k^2)\, U_{k(x)} = 0 \quad \text{—— (8)}$$

$$\frac{d^2 U_{k(x)}}{dx^2} + 2ik\frac{dU_{k(x)}}{dx} - (\beta^2 + k^2)\, U_{k(x)} = 0 \quad \text{—— (9)}$$

Solving eq ⑧ and ⑨ we get,

$$U_1 = Ae^{i(\alpha - k)x} + Be^{-i(\alpha + k)x} \quad \text{—— (10)}$$

$$U_2 = Ce^{(\beta - ik)x} + De^{-(\beta + ik)x} \quad \text{—— (11)}$$

Finally on solving eq ⑩ & ⑪ we get,

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

P = power of potential

a = interatomic distance

→ case - 1 : $P \to 0$

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

$\therefore \alpha = k$

$\therefore \alpha^2 = k^2$

But from eq 3 , $\alpha^2 = \frac{2m}{\hbar^2}(E)$

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

$\therefore \frac{4\pi^2}{\lambda^2} = \frac{2mE}{\hbar^2}$ $\left(\because k = \frac{2\pi}{\lambda}\right)$

$\therefore E = \frac{\hbar^2}{2m\lambda^2}$ $\left(\because \hbar = \frac{h}{2\pi}\right)$

$\therefore E = \frac{1}{2m} \cdot \frac{\hbar^2}{\lambda^2}$ $\left(\because p = \frac{h}{\lambda}\right)$

$\therefore \boxed{E = \frac{p^2}{2m}}$ → conductare

→ case - 2 : $P \to \infty$

Divide 'P' throughout the eq$^n$,

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

Now, $P \to \infty$

$\sin \alpha a = 0$

$\alpha a = n\pi$

$\alpha = \frac{n\pi}{a}$

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

But from eq 3 , $\alpha^2 = \frac{2m}{\hbar^2}(E)$

$$\therefore \frac{n^2 \pi^2}{a^2} = \frac{2mE}{\hbar^2} \qquad \left(\because \hbar = \frac{h}{2\pi}\right)$$

$$\therefore \boxed{E = \frac{n^2 h^2}{8ma^2}}$$ → Insulator.

n = order
m = mass of electron.
a = interatomic distance.