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Unit III: Application of Quantum Mechanics to Electrical transport in Solids



- > Suggested Reading
 - 1. Concepts of Modern Physics, Arthur Beiser, Chapter 10
 - 2. Solid state Physics, S.O Pillai, Chapter 6
 - 3. Learning material prepared by the department-Unit III

- > Reference Videos
 - 1. https://nptel.ac.in/courses/115/104/115104109/

Unit III: Application of Quantum Mechanics to Electrical transport in Solids



Class #31

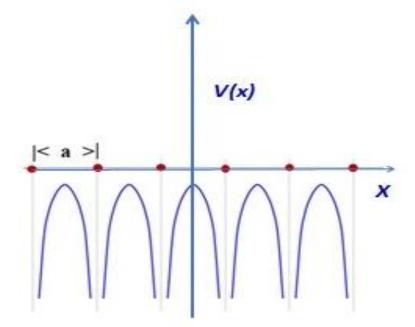
- Kronig Penny model,
- Allowed energy zones/energy bands

Kronig Penny model, Allowed energy bands

In real crystal, electrons move in a regularly arranged lattice of positive ions.

Observed potential is periodic – due to the periodicity of the

lattice



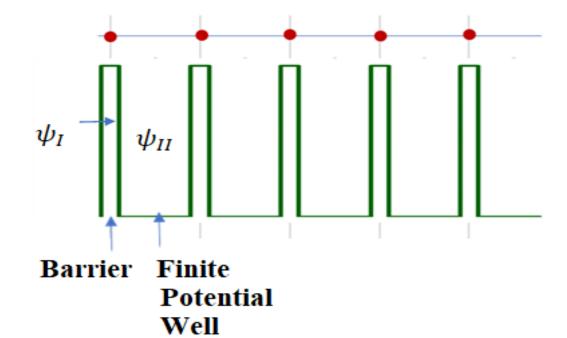
Potentials of electron at the positive ion site is zero and maximum in between two ions.



Kronig Penny model, Allowed energy bands

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Real potentials approximated as - long chain of coupled finite square wells and barrier with height V_o , period 'a' and barrier thickness b.



Kronig Penny model, Allowed energy bands



Schrodinger equations in region I and II

$$\frac{d^2\psi_I}{dx^2} + \frac{2mE}{\hbar^2}\psi_I = 0 \qquad for \ 0 < x < a$$

$$\frac{d^2\psi_{II}}{dx^2} - \frac{2m(V_o - E)}{\hbar^2}\psi_{II} = 0 \ for \ or - b < x < 0$$

Total energy (E < V) - define two real quantities K and α

$$K^2=rac{2mE}{\hbar^2}$$
 and $lpha^2=rac{2m(V_0-E)}{\hbar^2}$

Kronig Penny model, Allowed energy bands



$$\frac{d^2\psi_I}{dx^2} + K^2\psi_I = 0 \qquad \text{for } 0 < x < a$$

$$\frac{d^2\psi_{II}}{dx^2} - \alpha^2\psi_{II} = 0 \quad for \ or - b < x < 0$$

The wave function of the electron is a modulated wave given by Bloch function $\psi_k(x) = V_k(x)e^{ikx}$

 $V_k(x)$ is a periodic function, satisfies $V_k(x + a) = V_k(x)$

Applying the boundary conditions and solving SWE equation

Kronig Penny model, Allowed energy bands



$$P \frac{Sin(Ka)}{Ka} + cos(Ka) = coska$$

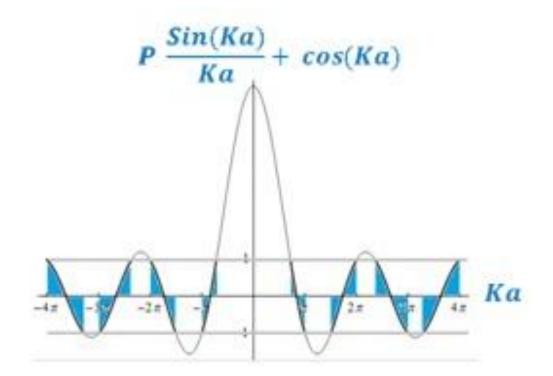
Where
$$P = \frac{ma}{\hbar^2} V_o$$
. c and $K = \sqrt{\frac{2m(E)}{\hbar^2}}$

 V_o c is the barrier strength and P is the scattering power of the potential barrier.

The values of k are obtained by solving this equation.

Kronig Penny model, Allowed energy bands

Plot LHS of the equation as a function of αa

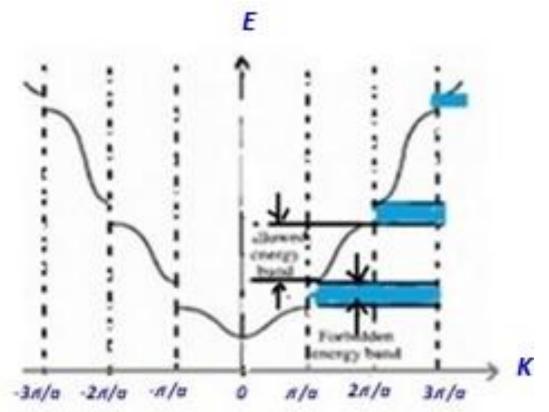


Whenever LHS goes beyond \pm 1, the equation has no solution as the RHS lies between \pm 1



Kronig Penny model, Allowed energy bands

E- k diagram

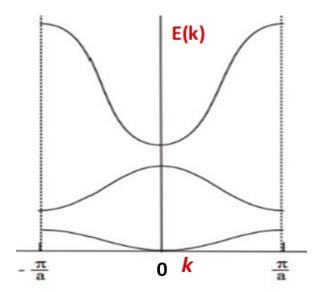






Kronig Penny model, Allowed energy bands

Classification of Material based on band structure:



Metal- partially filled conduction band

- ➤ Semiconductors-fully filled valence band and empty conduction band, energy gap 3 -5 eV
- > Insulators- energy band gap > 5 eV



Class 31. Quiz ...

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The concepts which are correct are....

- 1. In the Kronig-Penney model the periodic potential is approximated as a long chain of coupled infinite square wells
- 2. The potential of the electron at the positive ionic site is maximum and zero between the site.
- 3. Scattering power is the measure of the strength with which electrons in a crystal are attracted to the ions on the crystal lattice sites.
- 4. Metal are characterized by a fully filled conduction band.



THANK YOU

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