ENGINEERING PHYSICS

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

➢ ***Suggested Reading***

1. ***Concepts of Modern Physics, Arthur Beiser, Chapters 9 &10***
2. ***Learning material prepared by the department-Unit III***

➢ ***Reference Videos***

1. *Physics Of Materials-IIT-Madras/lecture-26.html*

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

Class #30

Motion of electron in periodic potential (one dimensional treatment), Bloch theorem

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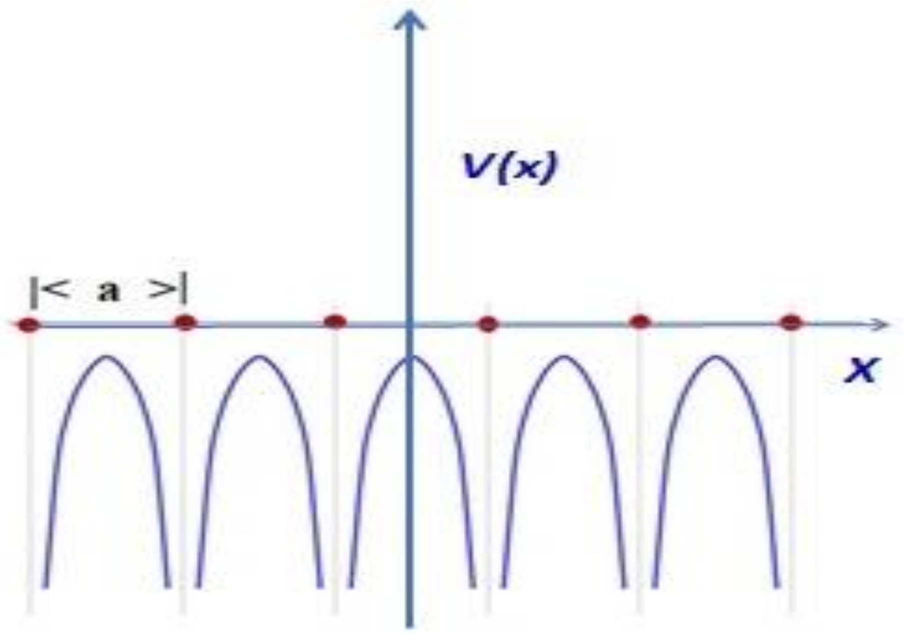
Motion of electron in periodic potential (1D)



The potential in a 1D lattice is shown to be periodic with a period "a"

Then if $V(x)$ is the potential at x then we can express mathematically this property as $V(x) = V(x + a)$

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Motion of electron in 1D-periodic lattice

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Consider wave function associated with free electron

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

If electrons move through a periodic lattice then

$$\psi(x+a) = e^{ik(x+a)}$$

$$= e^{ikx} * e^{ika}$$

We know that $k = \dfrac{n\pi}{a}$

$$= e^{ikx} * e^{in\pi}$$

Motion of electron in 1D-periodic potential

When the electrons moves through the periodic potential

$$V(x) = V(x+a) = V(x+2a)\cdots$$

According Bloch the free electron wave function is modulated

by the term $V_k(x)$ *which has the periodicity of the lattice*

So the wave function is $\psi_k(x) = V_k(x)e^{ikx}$

This is known as Bloch Theorem

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Motion of electron in 1D-periodic potential

In a periodic potential at any identical points (separated by a or na remains invariant

$$V_k(x) = V_k(x+a) = V_k(x+na)$$

Therefore the free electron wavefunction also remains invariant at points separated by a or na except for a phase factor

$$\psi(x+a) = e^{ik(x+a)} = e^{ikx}e^{ika} = \psi(x)e^{ika}$$

This shows that the wave function is got a phase factor added and the probability density is also invariant

$$\psi(x+a)^2 = \psi(x)^2$$

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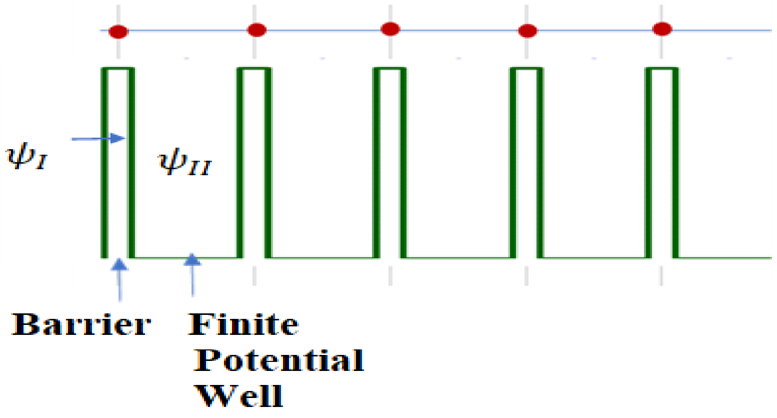
Motion of electron in 1D-periodic potential

Potentials in real crystals - approximated as series rectangular potentials wells and barriers



Kronig Penny model, Allowed energy bands

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Schrodinger equations in region I and II

$$\frac{d^2\psi_I}{dx^2} + \frac{2mE}{\hbar^2}\psi_I = 0$$

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

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

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

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Kronig Penny model, Allowed energy bands

$$\frac{d^2\psi_I}{dx^2} + K^2\psi_I = 0$$

$$\frac{d^2\psi_{II}}{dx^2} - \alpha^2\psi_{II} = 0$$

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 $V_k(x + a) = V_k(x)$

Kronig Penny model, Allowed energy bands

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Solving SWE equation for the wave functions and applying the boundary conditions with the Bloch theorem applied results in the transcendental equation

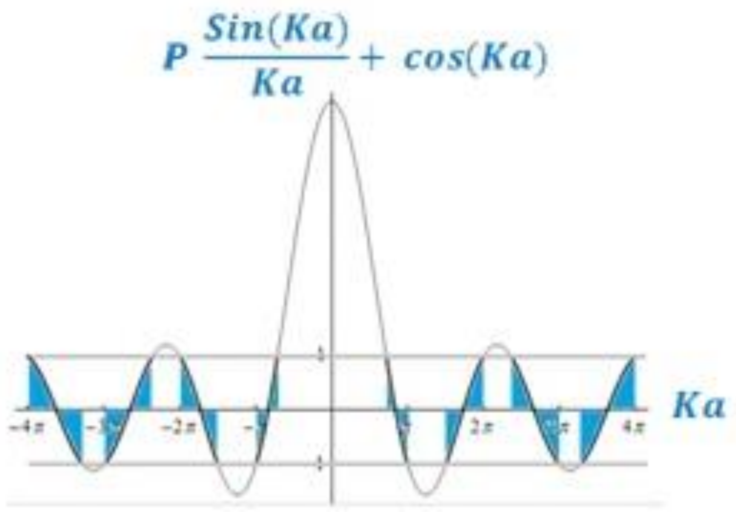
$$P\frac{sin(Ka)}{Ka} + cos(Ka) = sin(ka)$$

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

P *is the scattering power of the potential barrier &* $V_o * c$ *gives the barrier strength.*

The solutions to the transcendental equation can be obtained by numerical methods of graphical solutions of plotting the LHS and RHS in an overlapping graph

Plot LHS of the equation as a function of Ka is as shown



The solution to the equation exists only when the values of LHS lies in the interval ± 1 (which are the limits of the RHS).

It can be seen that only certain values of Ka results in allowed energies of the electrons as shown by the shaded regions.

This is the origin of the allowed and forbidden energies of electrons in a material – the band theory of solids

Quiz ...

Identify the concepts which are correct ....

1. *Electrons move in a periodic potential due to the regular arrangement of ionic cores.*
2. *The potential of the electron at the positive ionic site is maximum and zero between the site .*
3. *The wave function of the electrons is not affected by the periodic potential*
4. *The potential in the real crystal is approximated by rectangular potentials.*
5. *Electrons cannot occupy all energy states*

THANK YOU

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