



Bloch Theorem

- ▶ Presenter: Manpreet Saini, B.sc NM 3 (5614)

Introduction

BLOCH'S THEOREM (1928) APPLIES TO WAVE FUNCTIONS OF ELECTRONS INSIDE A CRYSTAL AND RESTS IN THE FACT THAT THE COULOMB POTENTIAL IN A CRYSTALLINE SOLID IS PERIODIC. AS A CONSEQUENCE, THE POTENTIAL ENERGY FUNCTION, $V(\vec{r} \rightarrow)$, IN SCHRÖDINGER'S EQUATION SHOULD BE OF THE FORM:

$$V(x) = V(x + a) \dots(1)$$

So the Schrodinger's equation for an electron moving in periodic potential $V(x)$ is written as

$$\frac{d^2\Psi}{dx^2} + \frac{2m}{\hbar^2} (E - V(x))\Psi = 0 \quad \dots(3)$$

The solution of Eq. (3) are of the type

$$\Psi(x) = \exp(\pm iKx) u_K(x) \quad \dots(4)$$

Where $u_K(x)$ is known as Bloch function and which is again periodic with the same periodicity of the lattice.

i.e.

$$u_K(x) = u_K(x + a) \quad \dots(5)$$

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i.e.,

$$\Psi(x + a) = \exp(iKx) \exp(iKa) u_K(x)$$

or

$$\Psi(x + a) = \Psi(x) \exp(iKa)$$

$$\Psi(x + a) = \gamma \Psi(x) \quad \dots(6)$$

Where

$$\gamma = \exp(iKa)$$

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Proof -

We know that Schrodinger wave eq. (3) is a second-order differential eq. and hence there exist only two real independent solutions for this equation.

Say $f(x)$ and $g(x)$ any other solution will be simply a linear combination of independent solutions.

Hence $f(x+a)$ and $g(x+a)$ are to be solutions of the eq. (3), there can

be written as $f(x + a) = \alpha_1 f(x) + \alpha_2 g(x) \dots(7)$

$$g(x + a) = \beta_1 f(x) + \beta_2 g(x) \dots(8)$$

Let $\Psi(x)$ be another solution of eq. (3), hence it must be represented as

$$\Psi(x) = Af(x) + Bg(x) \quad \dots(9)$$

$$\therefore \Psi(x+a) = Af(x+a) + Bg(x+a) \quad \dots(10)$$

By using eq. (7) and (8), above eq. become

$$\begin{aligned} \Psi(x+a) &= A[\alpha_1 f(x) + \alpha_2 g(x)] + B[\beta_1 f(x) + \beta_2 g(x)] \\ &= (A\alpha_1 + B\beta_1)f(x) + (A\alpha_2 + B\beta_2)g(x) \quad \dots(11) \end{aligned}$$

Now, by using eq. (6), we can write eq. (9) as

$$\Psi(x+a) = \gamma[Af(x) + Bg(x)] \quad \dots(12)$$

Now, by comparing eq. (11) and (12), we get

$$A\alpha_1 + B\beta_1 = \gamma A$$

$$A\alpha_2 + B\beta_2 = \gamma B$$

$$(\alpha_1 - \gamma)A + \beta_1 B = 0 \quad \dots(13a)$$

$$\alpha_2 A + (\beta_2 - \gamma)B = 0 \quad \dots(13b)$$

...(13b)

Now eq. (13) have non-vanishing solutions for A and B if and only if the determinant of the coefficient is zero, i.e.,

$$\begin{vmatrix} \alpha_1 - \gamma & \beta \\ \alpha_2 & \beta_2 - \gamma \end{vmatrix} = 0$$

$$\text{Or } \gamma^2 - (\alpha_1 + \beta_2)\gamma + (\alpha_1\beta_2 - \alpha_2\beta_1) = 0 \quad \dots(14)$$

$$\text{Or } \gamma^2 - (\alpha_1 + \beta_2)\gamma + 1 = 0 \quad \dots(15)$$

We have written $(\alpha_1\beta_2 - \alpha_2\beta_1) = 1$ in eq. (15) and this result is proved below this topic.

Now, eq. (15) gives two roots of γ , so there are two wave functions $\Psi_1(x)$ and $\Psi_2(x)$. It must be noted that $\gamma_1\gamma_2 = 1$ and $(\alpha_1 + \beta_2)$ is a real function of energy E.

Let us consider two cases for the energy ranges.

Case 1. For energy range $(\alpha_1 + \beta_2)^2 < 4$

In this case the two roots will be the complex conjugate of each other, we can write $\gamma_1 = \exp(iKa)$ and $\gamma_2 = \exp(-iKa)$ Where K is real and the corresponding wave functions $\Psi_1(x)$ and $\Psi_2(x)$ can be written as

$$\Psi_1(x + a) = \exp(iKa) \Psi_1(x)$$

$$\text{and } \Psi_2(x + a) = \exp(-iKa) \Psi_2(x)$$

i.e., in general

$$\Psi(x + a) = \exp(\pm iKa) \Psi(x) \dots(16)$$

Case 2. For energy range $(\alpha_1 + \beta_2)^2 > 4$

In this case the roots are real and will be reciprocals of each other these correspond to wave functions of the type

$$\Psi_1(x) = \exp(\mu a) \Psi_1(x)$$

And

$$\Psi_2(x) = \exp(-\mu a) \Psi_2(x)$$

Where μ is real. These are not acceptable wave functions since these are not bounded and approaches $\pm\infty$ when approaches infinity. Thus we find that the energy spectrum of an electron in a periodic potential consists of allowed and forbidden energy regions as bands. This will further be discussed in Kronig-Penney Model.
