Bloch Theorem. In the free electron theory, the electron is supposed to move in a constant potential V_0 and Schrodinger's wave equation for a one dimensional case is

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

The solution of this equation is

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

where $$k^2 = \frac{2m}{\hbar^2}(E - V_0)$$

$\therefore$ $$E - V_0 = \frac{\hbar^2 k^2}{2m} = \frac{h^2}{4\pi^2}\cdot\frac{4\pi^2}{\lambda^2}\frac{1}{2m} = \frac{h^2}{\lambda^2}\frac{1}{2m} = \frac{p^2}{2m} = E_{kinetic}$$

The physical meaning of k is that it represents the momentum of the electron divided by $\hbar$ as shown:

The magnitude of $$\vec{k} = |\vec{k}| = \frac{2\pi}{\lambda} = 2\pi\frac{mv}{h} = \frac{mv}{\hbar} = \frac{p}{\hbar}$$

Each electron will have its own $\vec{k}$ and its own energy.

For an electron moving in a one dimensional periodic potential the potential energy is given by the relation

$$V(x) = V(x + a)$$

where a is the period equal to lattice constant. In this case Schrödinger's equation becomes

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}[E - V(x)]\psi = 0 \quad ...(ii)$$

With reference to the solution of this equation there is an important theorem known as *Bloch theorem* or *Floquet's theorem* which states that there exist solutions of the form

$$\psi(x) = e^{\pm ikx}\mu_k(x) \quad ...(iii)$$

where $$\mu_k(x) = \mu_k(x + a) \quad ...(iv)$$

Thus the solutions are plane waves of the type $e^{\pm ikx}$ modulated by the function $\mu_k(x)$ which has the same periodicity as the lattice constant.

Bloch function. The wave function of the type $\psi(x) = e^{\pm ikx}\mu_k(x)$ is called *Bloch function*. The wave vector $\vec{k}$ gives the direction of Bloch wave.

Proof. Suppose $f(x)$ and $g(x)$ are two real and independent solutions of equation (*ii*). Then the general solution is

$$\psi(x) = A f(x) + B g(x) \quad ...(v)$$

where A and B are arbitrary constants. As the potential is periodic, *i.e.*, $V(x) = V(x + a)$, therefore the functions $f(x + a)$ and $g(x + a)$ must also be the solutions of equation (*ii*). Since a differential equation of the second order can have only two independent solutions, the functions $f(x + a)$ and $g(x + a)$ must be able to be expressed in terms of functions $f(x)$ and $g(x)$, *i.e.*,

$$f(x + a) = \alpha_1 f(x) + \alpha_2 g(x) \quad ...(vi)$$

and $$g(x + a) = \beta_1 f(x) + \beta_2 g(x) \quad ...(vii)$$

where α_1, α_2, β_1 and β_2 are real functions of energy E.

According to Eq. (v), the general solution of Schrodinger's equation is

$$\psi(x) = A f(x) + B g(x)$$

and $$\psi(x + a) = A f(x + a) + B g(x + a)$$

According to Eq. (*vi*) and (*vii*), we have

$$\psi(x+a) = A\alpha_1 f(x) + A\alpha_2 g(x) + B\beta_1 f(x) + B\beta_2 g(x)$$
$$= (A\alpha_1 + B\beta_1) f(x) + (A\alpha_2 + B\beta_2) g(x) \quad \text{... (viii)}$$

Now select A and B such that

$$A\alpha_1 + B\beta_1 = \lambda A \quad \text{... (ix)}$$

and

$$A\alpha_2 + B\beta_2 = \lambda B \quad \text{... (x)}$$

where λ is a constant. Substituting in Eq. (*viii*), we get

$$\psi(x+a) = \lambda A f(x) + \lambda B g(x)$$
$$= \lambda (A f(x) + B g(x)) = \lambda \psi(x) \quad \text{... (xi)}$$

Equations (*ix*) and (*x*) will give non-zero values of A and B if the determinant of their coefficient vanishes, *i.e.*,

$$\begin{vmatrix} \alpha_1 - \lambda & \beta_1 \\ \alpha_2 & \beta_2 - \lambda \end{vmatrix} = 0$$

or

$$\lambda^2 - (\alpha_1 + \beta_2)\lambda + \alpha_1\beta_2 - \alpha_2\beta_1 = 0 \quad \text{... (xii)}$$

We shall first prove that $\alpha_1\beta_2 - \alpha_2\beta_1 = 1$ as given below.

As $f(x)$ and $g(x)$ are two real and independent solutions of Eq. (*ii*), we have

$$\frac{d^2 f(x)}{dx^2} + \frac{2m}{\hbar^2}[E - V(x)] f(x) = 0 \quad \text{... (xiii)}$$

and

$$\frac{d^2 g(x)}{dx^2} + \frac{2m}{\hbar^2}[E - V(x)] g(x) = 0 \quad \text{... (xiv)}$$

Multiplying Eq. (*xiii*) by $g(x)$ and Eq. (*xiv*) by $f(x)$ and subtracting former from the latter, we get

$$f(x)\frac{d^2 g(x)}{dx^2} - g(x)\frac{d^2 f(x)}{dx^2} = 0$$

or

$$f(x)\frac{dg(x)}{dx} - g(x)\frac{df(x)}{dx} = \text{a constant}$$

The left hand side is called Wronskian, $W(x)$, of the solution and is constant in this case.

$$\therefore \quad W(x) = f(x)\frac{dg(x)}{dx} - g(x)\frac{df(x)}{dx}$$

Now from Eq. (*vi*) and (*vii*), we get

$$W(x+a) = f(x+a)\frac{dg(x+a)}{dx} - g(x+a)\frac{df(x+a)}{dx}$$

$$= f(x+a)\left[\beta_1\frac{df(x)}{dx} + \beta_2\frac{dg(x)}{dx}\right] - g(x+a)\left[\alpha_1\frac{df(x)}{dx} + \alpha_2\frac{dg(x)}{dx}\right]$$

$$= [\alpha_1 f(x) + \alpha_2 g(x)]\left[\beta_1\frac{df(x)}{dx} + \beta_2\frac{dg(x)}{dx}\right]$$
$$- [\beta_1 f(x) + \beta_2 g(x)]\left[\alpha_1\frac{df(x)}{dx} + \alpha_2\frac{dg(x)}{dx}\right]$$

$$= (\alpha_1\beta_2 - \alpha_2\beta_1)\left[f(x)\frac{dg(x)}{dx} - g(x)\frac{df(x)}{dx}\right]$$

$$= (\alpha_1\beta_2 - \alpha_2\beta_1) W(x) \quad \text{... (xv)}$$

Thus, $W(x+a) = (\alpha_1\beta_2 - \alpha_2\beta_1)\, W(x)$

But $W(x+a) = W(x) =$ a constant

$\therefore \quad \alpha_1\beta_2 - \alpha_2\beta_1 = 1$

Hence, Eq. (*xii*) becomes

$$\lambda^2 - (\alpha_1 + \beta_2)\,\lambda + 1 = 0 \quad \text{... (xvi)}$$

The quantity $(\alpha_1 + \beta_2)$ is a real function of energy E. There are two roots λ_1 and λ_2 of this quadratic equation, so there will be two functions $\psi_1(x)$ and $\psi_2(x)$ which have the property $\psi_1(x+a) = \lambda\psi(x)$. The product of the two roots $\lambda_1\lambda_2 = 1$.

We consider the following cases:

(*i*) *For energy ranges such that* $(\alpha_1 + \beta_2)^2 < 4$. In such a case Eq. (*xvi*), will have complex roots. Since $\lambda_1\lambda_2 = 1$ these roots will be *complex* conjugate of each other. Therefore, we write

$$\lambda_1 = e^{ika} \quad \text{and} \quad \lambda_2 = e^{-ika}$$

where k is real.

The corresponding functions $\psi_1(x)$ and $\psi_2(x)$ will then have the property

$$\psi_1(x+a) = e^{ika}\,\psi_1(x) \quad \text{... (xvii)}$$

and

$$\psi_2(x+a) = e^{-ika}\,\psi_2(x) \quad \text{... (xviii)}$$

Thus in general

$$\psi(x+a) = e^{\pm ika}\,\psi(x) \quad \text{... (xix)}$$

It can be seen that a function having the property given by Eq. (*xix*) is the Bloch function of the type given in Eq. (*iii*)

i.e., $\psi(x) = e^{\pm ikx}\,\mu_k(x)$

by replacing x by $(x + a)$, then we get

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

$$= e^{\pm ika}\,e^{\pm ikx}\,\mu_k(x)$$

because $\mu_k(x+a) = \mu_k(x)$ Also $e^{\pm ikx}\,\mu_k(x) = \psi(x)$

$$\therefore \quad \psi(x+a) = e^{\pm ika}\,\psi(x) = \lambda\psi(x) \quad \text{... (xx)}$$

where $\lambda = e^{\pm ika}$

We, therefore, find that Eq. (*xix*) and Eq. (*xx*) are the same. This proves Bloch theorem.

(*ii*) *For the energy range such that* $(\alpha_1 + \beta_2)^2 > 4$. In such a case Eq. (*xvi*) will have *real* roots λ_1 and λ_2, which may be taken as

$$\lambda_1 = e^{\mu a} \quad \text{and} \quad \lambda_2 = e^{-\mu a}$$

where μ is real. The corresponding solutions to the Schrödinger's equation are

$$\psi_1(x) = e^{\mu x}\,\mu(x) \text{ and } \psi_2(x) = e^{-\mu x}\,\mu(x) \quad \text{... (xxi)}$$

Though mathematically valid, these wave functions are not allowed because these functions become infinite at $+\infty$ or $-\infty$, *i.e.*, they are not bounded functions.

The roots $\lambda_1 = e^{ika}$ and $\lambda_2 = e^{-ika}$ (*allowed roots*) as well as the roots $\lambda_1 = e^{\mu a}$ and $\lambda_2 = e^{-\mu a}$ (forbidden roots) are functions of $(\alpha_1 + \beta_2)$, hence of energy E. The allowed roots correspond to the *allowed energy regions* and the forbidden (or disallowed) roots are associated with *forbidden energy regions*. This means that the energy spectrum of an electron moving in a periodic potential consists of allowed and forbidden energy regions or bands.

EC-⑨

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