Bloch theorem and Energy band

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Felix Bloch entered the Federal Institute of Technology (Eidgenössische Technische Hochschule) in Zürich. After one year's study of engineering he decided instead to study physics, and changed therefore over to the Division of Mathematics and Physics at the same institution. After Schrödinger left Zürich in the fall of 1927 he continued his studies with Heisenberg at the University of Leipzig, where he received his degree of Doctor of Philosophy in the summer of 1928 with a dissertation dealing with the quantum mechanics of electrons in crystals and developing the theory of metallic conduction.

By straight Fourier analysis I found to my delight that the wave differed from the plane wave of free electrons only by a periodic modulation. This was so simple that I did not think it could be much of a discovery, but when I showed it to Heisenberg, he said right away; "That's it!! (F. Bloch, July, 1928) (from the book edited by Hoddeson et al.[2]).

His paper was published in 1928 [F. Bloch, Zeitschrift für Physik 52, 555 (1928)]. There are many standard textbooks[3-10] which discuss the properties of the Bloch electrons in a periodic potential.

1. Derivation of the Bloch theorem

We consider the motion of an electron in a periodic potential (the lattice constant a). The system is one-dimensional and consists of N unit cells (the size $L = Na$, N: integer).

$$V(\hat{x} + a\hat{1}) = V(\hat{x}),$$

$$\hat{T}_x^{+}(\ell)\hat{x}\hat{T}_x(\ell) = \hat{x} + \ell\hat{1},$$

$$\hat{T}_x(\ell)|x\rangle = |x + \ell\rangle,$$

$$\hat{T}_x(\delta x) = \hat{1} - \frac{i}{\hbar}\hat{p}_x\delta x,$$

where l is any finite translation (one dimensional) and δx is the infinitesimal translation. a is the lattice constant. The commutation relations hold

$$[\hat{T}_x(\delta x), \hat{p}_x] = \hat{0},$$

and

$$[\hat{T}_x(\delta x), \hat{p}_x{}^2] = \hat{0}.$$

Therefore the kinetic energy part of the Hamiltonian is invariant under the translation. When $\ell = a$ (a is a period of potential $V(x)$),

$$\hat{T}_x^{+}(a)\hat{x}\hat{T}_x(a) = \hat{x} + a\hat{1},$$

$$\hat{T}_x^{+}(a)V(\hat{x})\hat{T}_x(a) = V(\hat{x} + a\hat{1}) = V(\hat{x}).$$

Thus we have

$$[\hat{H}, \hat{T}_x(a)] = \hat{0},$$

or

$$\hat{T}_x^{+}(a)\hat{H}\hat{T}_x(a) = \hat{H}. \tag{44}$$

The Hamiltonian is invariant under the translation with a.
Since $\hat{T}_x(a)|x\rangle = |x + a\rangle$ and $\hat{T}^{+}{}_x(a)|x\rangle = |x - a\rangle$ or $\hat{T}_x^{+}(-a)|x\rangle = |x + a\rangle$,
we have

$$\hat{T}_x^{+}(a) = \hat{T}_x(-a). \tag{45}$$

So $\hat{T}_x^{+}(a)$ is not a Hermite operator.

We consider the simultaneous eigenket of $\hat{H}$ and $\hat{T}_x(a)$ for the system with a periodicity of $L = Na$ (there are N unit cells), since $[\hat{H}, \hat{T}_x(a)] = \hat{0}$.

$$\hat{H}|\psi_k\rangle = E_k|\psi_k\rangle, \tag{46}$$

and

$$\hat{T}_x(a)|\psi_k\rangle = \frac{1}{p}|\psi_k\rangle, \tag{47}$$

or

$$[\hat{T}(a)]^n|\psi_k\rangle = p^{-n}|\psi_k\rangle \qquad (n = 1, 2, ..., N)$$

Noting that

$$\langle x - a| = \langle x|\hat{T}(a),$$

$$\langle x - Na| = \langle x|[\hat{T}(a)]^N$$

we get

$$\langle x|[\hat{T}(a)]^n|\psi_k\rangle = p^{-n}\langle x|\psi_k\rangle$$

or

$$\langle x - na|\psi_k\rangle = p^{-n}\langle x|\psi_k\rangle$$

When $n = N$,

$$\langle x - Na|\psi_k\rangle = p^{-N}\langle x|\psi_k\rangle$$

From the periodicity of the wave function

$$\langle x - Na|\psi_k\rangle = \langle x|\psi_k\rangle$$

we have

$$p^N = 1.$$

or

$$p = \exp(i\frac{2\pi s}{N}) = \exp(i\frac{2\pi as}{Na}) = \exp(ika), \tag{49}$$

with

$$k = \frac{2\pi}{Na}s = \frac{2\pi}{L}s \ \ (s\text{: integer}). \tag{50}$$

Therefore, we have

$$\hat{T}_x(a)|\psi_k\rangle = e^{-ika}|\psi_k\rangle. \tag{51}$$

The state $|\psi_k\rangle$ is the eigenket of $\hat{T}_x(a)$ with the eigenvalue e^{-ika}.
or

$$\langle x|\hat{T}_x(a)|\psi_k\rangle = \exp(-ika)\langle x|\psi_k\rangle,$$

$$\langle x|\hat{T}_x(a) = \langle x - a|,$$

$$\langle x-a|\psi_k\rangle = e^{-ika}\langle x|\psi_k\rangle ,$$

$$\psi_k(x-a) = e^{-ika}\psi_k(x) .$$

By changing for a to $-a$, we have

$$\psi_k(x+a) = e^{ika}\psi_k(x) .$$

This is called as the Bloch theorem.

2. Brillouin zone in one dimensional system

We know that the reciprocal lattice G is defined by

$$G = \frac{2\pi}{a}n \text{, } (n\text{: integer}).$$

When k is replaced by $k + G$,

$$\psi_{k+G}(x+a) = e^{i(k+G)a}\psi_{k+G}(x) = e^{ika}\psi_{k+G}(x) ,$$

since $e^{iGa} = e^{i2\pi n} = 1$. This implies that $\psi_{k+G}(x)$ is the same as $\psi_k(x)$.

$$\psi_{k+G}(x) = \psi_k(x) .$$

or the energy eigenvalue of $\psi_{k+G}(x)$ is the same as that of $\psi_k(x)$,

$$E_{k+G} = E_k .$$

Note that the restriction for the value of s arises from the fact that $\psi_{k+G}(x) = \psi_k(x)$.

$$k = \frac{2\pi s}{L} = \frac{2\pi s}{Na} = \frac{\pi}{a}(\frac{2s}{N}),$$

where

$$-\frac{N}{2} \le s \le \frac{N}{2} .$$

The first Brillouin zone is defined as $|k| \le \frac{\pi}{a}$. There are N states in the first Brillouin zone. When the spin of electron is taken into account, there are $2N$ states in the first Brilloiun

zone. Suppose that the number of electrons per unit cell is n_c (= 1, 2, 3, …). Then the number of the total electrons is n_cN.
(a) $n_c = 1$. So there are N electrons. $N/2N = 1/2$ (band-1: half-filled).
(b) $n_c = 2$. $2N/2N = 1$ (band-1: filled).
(c) $n_c = 3$. $3N/2N = 1.5$ (band-1: filled, band-2: half-filled).
(d) $n_c = 4$. $4N/2N = 2$ (band-1: filled, band-2: filled).
When there are even electrons per unit cell, bands are filled. Then the system is an insulator. When there are odd electrons per unit cell, bands are not filled. Then the system is a conductor.

3. Bloch wavefunction

Here we assume that

$$\psi_k(x) = e^{ikx}u_k(x),$$

$$\psi_k(x-a) = e^{ikx}e^{-ika}u_k(x-a) = e^{-ika}e^{ikx}u_k(x-a),$$

which should be equal to

$$e^{-ika}\psi_k(x) = e^{-ika}e^{ikx}u_k(x),$$

or

$$u_k(x-a) = u_k(x),$$

which is a periodic function of x with a period a.

The solution of the Schrodinger equation for a periodic potential must be of a special form such that $\psi_k(x) = e^{ikx}u_k(x)$, where $u_k(x+a) = u_k(x)$. In other words, the wave function is a product of a plane wave and a periodic function which has the same periodicity as a potential

Here we consider the 3D case. The solutions of the Schrödinger equation for a periodic potential must be of a special form:

$$\psi_{\boldsymbol{k}}(\boldsymbol{r}) = u_{\boldsymbol{k}}(\boldsymbol{r})e^{i\boldsymbol{k}\cdot\boldsymbol{r}} \quad \text{(Bloch function)},$$

where

$$u_{\boldsymbol{k}}(\boldsymbol{r}) = u_{\boldsymbol{k}}(\boldsymbol{r}+\boldsymbol{T}).$$

Bloch functions can be assembled into localized wave packets to represent electrons that propagate freely through the potential of the ion cores. $\boldsymbol{T}$ is any translation vectors which is expressed by $\boldsymbol{T} = n_1\boldsymbol{a}_1+n_2\boldsymbol{a}_2+n_3\boldsymbol{a}_3$ (n_1, n_2, n_3 are integers, $\boldsymbol{a}_1$, $\boldsymbol{a}_2$, $\boldsymbol{a}_3$ are fundamental lattice vectors). From Eq.(67), $u_{\boldsymbol{k}}(\boldsymbol{r})$ can be expanded as follows. (Fourier transform)

$$u_{\mathbf{k}}(\mathbf{r}) = \sum_{\mathbf{G}} C_{\mathbf{k}-\mathbf{G}} e^{-i\mathbf{G}\cdot\mathbf{r}} \,. \tag{68}$$

where $\boldsymbol{G}$ is the reciprocal lattice vector. We use the same discussion for the periodic charge density in the x-ray scattering. Then the wave function in a periodic potential is given by

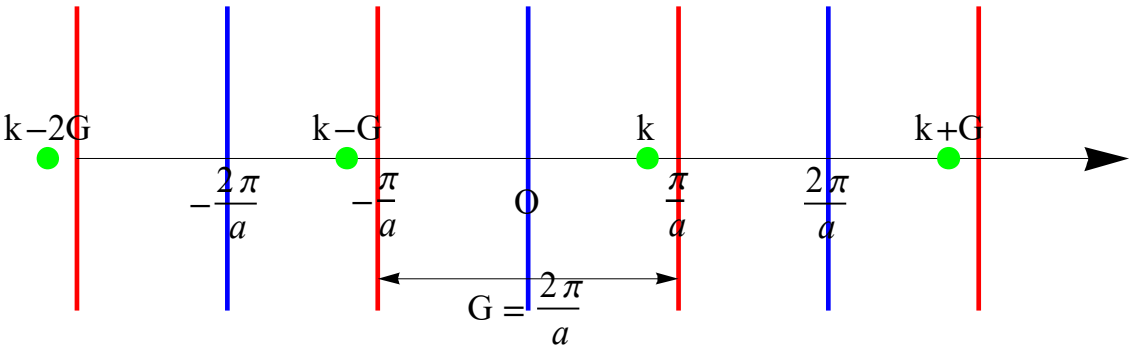
$$\psi_k(\boldsymbol{r}) = \sum_{\boldsymbol{G}} C_{k-\boldsymbol{G}} e^{i(k-\boldsymbol{G})\cdot r} = C_k e^{i\boldsymbol{k}\cdot r} + C_{k-\boldsymbol{G}} e^{i(k-\boldsymbol{G})\cdot r} + \ldots$$

or

$$\psi_k(\boldsymbol{r}) = \ldots + C_{k-2\boldsymbol{G}} e^{i(k-2\boldsymbol{G})\cdot r} + C_{k-\boldsymbol{G}} e^{i(k-\boldsymbol{G})\cdot r} + C_k e^{ik\cdot r} + C_{k+\boldsymbol{G}} e^{i(k+\boldsymbol{G})\cdot r} + C_{k+2\boldsymbol{G}} e^{i(k+2\boldsymbol{G})\cdot r} + \ldots.$$

or

$$|\psi_k\rangle = \ldots. + C_{k-2\boldsymbol{G}}|\boldsymbol{k}-2\boldsymbol{G}\rangle + C_{k-\boldsymbol{G}}|\boldsymbol{k}-\boldsymbol{G}\rangle + C_k|\boldsymbol{k}\rangle + C_{k+\boldsymbol{G}}|\boldsymbol{k}+\boldsymbol{G}\rangle + C_{k+2\boldsymbol{G}}|\boldsymbol{k}+2\boldsymbol{G}\rangle + \ldots$$



The eigenvalue-problem

$$\hat{H}|\psi_{\mathbf{k}}\rangle = E_{\mathbf{k}}|\psi_{\mathbf{k}}\rangle, \qquad \text{or} \qquad H\psi_k(x) = E_k\psi_k(x)\,.$$

E_{k} is the eigenvalue of the Hamiltonian and has the following properties.

(i) $E_{\mathbf{k}} = E_{\mathbf{k}+\mathbf{G}}$.
(ii) $E_{\mathbf{k}} = E_{-\mathbf{k}}$.

The first property means that any reciprocal lattice point can serve as the origin of E_{k}. The relation $E_{\mathbf{k}} = E_{-\mathbf{k}}$ is always valid, whether or not the system is centro-symmetric. The proof of this is already given using the time-reversal operator. The proof can be also made analytically as follows.

$$H\psi_k(x) = E_k\psi_k(x),$$

$$H\psi_k^*(x) = E_k\psi_k^*(x) \qquad (\hat{H} \text{ is Hermitian}),$$

or

$$H\psi_{-k}^*(x) = E_{-k}\psi_{-k}^*(x).$$

From the Bloch theorem given by

$$\psi_k(x-a) = e^{-ika}\psi_k(x),$$

or

$$\psi_k(x) = e^{ikx}u_k(x), \text{ and } \psi_k^*(x) = e^{-ikx}u_k^*(x),$$

we have

$$\psi_k^*(x-a) = e^{-ik(x-a)}u_k^*(x-a) = e^{-ik(x-a)}u_k^*(x) = e^{ika}\psi_k^*(x),$$

or

$$\psi_{-k}^*(x-a) = e^{-ika}\psi_{-k}^*(x).$$

Thus the wave functions $\psi_k(x)$ and $\psi_{-k}^*(x)$ are the same eigenfunctions of $\hat{T}_x(a)$ with the same eigenvalue e^{-ika}. Thus we have

$$\psi_{-k}^*(x) = \psi_k(x), \tag{71}$$

with

$$E_{\mathbf{k}} = E_{-\mathbf{k}}.$$

What does this relation mean?

$$\psi_{\mathbf{k}}(\mathbf{r}) = \sum_{\mathbf{G}} C_{\mathbf{k}-\mathbf{G}}e^{i(\mathbf{k}-\mathbf{G})\cdot\mathbf{r}} = C_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{r}} + C_{\mathbf{k}-\mathbf{G}}e^{i(\mathbf{k}-\mathbf{G})\cdot\mathbf{r}} + \ldots$$
$$\psi_{\mathbf{k}}^*(\mathbf{r}) = \sum_{\mathbf{G}} C_{\mathbf{k}-\mathbf{G}}^* e^{-i(\mathbf{k}-\mathbf{G})\cdot\mathbf{r}},$$

or

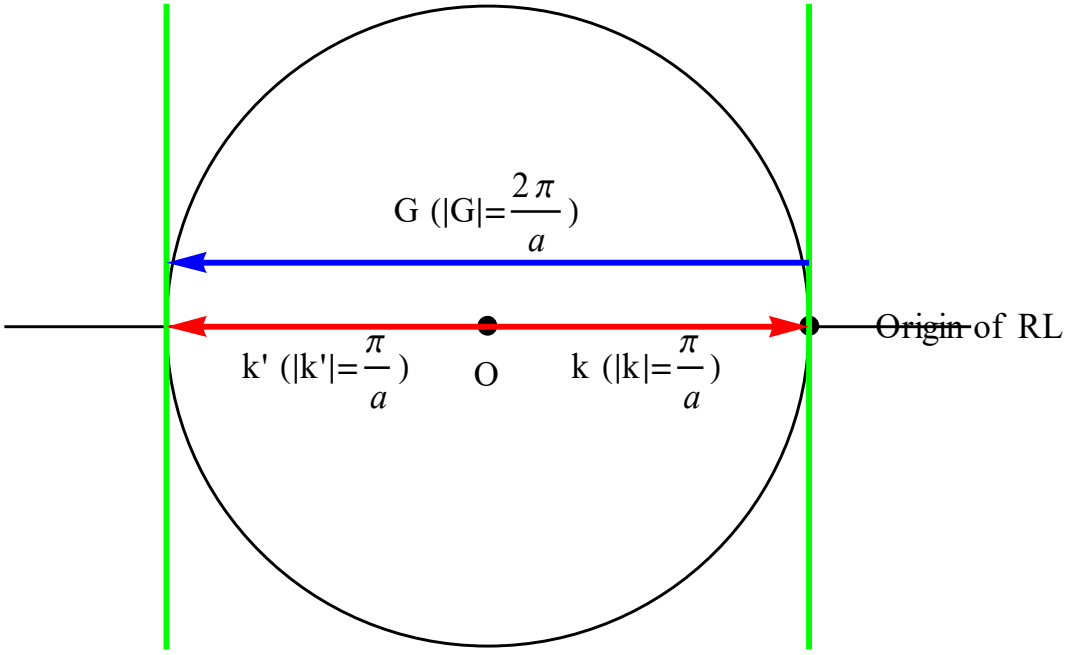
$$\psi_{-\mathbf{k}}{}^{*}(\mathbf{r}) = \sum_{\mathbf{G}} C_{-\mathbf{k}-\mathbf{G}}{}^{*} e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{r}} = \sum_{\mathbf{G}} C_{-\mathbf{k}+\mathbf{G}}{}^{*} e^{i(\mathbf{k}-\mathbf{G})\cdot\mathbf{r}} .$$

Then we have the relation

$$C_{-\mathbf{k}+\mathbf{G}}{}^{*} = C_{k-G} ,$$

or

$$C_{\mathbf{k}-\mathbf{G}}{}^{*} = C_{-\mathbf{k}+\mathbf{G}} .$$



APPENDIX
Properties of translation operator

(i)

$$\hat{T}(a)|x\rangle = |x+a\rangle$$

(ii)
From the property (i),

$$\hat{T}^{+}(a)\hat{T}(a)|x\rangle = \hat{T}^{+}(a)|x+a\rangle$$

or

$$\hat{T}^{+}(a)\left|x+a\right\rangle = \left|x\right\rangle$$

(iii)
When a is changed into -a,

$$\hat{T}^{+}(-a)\left|x-a\right\rangle = \left|x\right\rangle$$

When x is changed into $x+a$

$$\hat{T}^{+}(-a)\left|x\right\rangle = \left|x+a\right\rangle, \qquad \text{h.c.} \qquad \left\langle x\right|\hat{T}(-a) = \left\langle x+a\right|$$

or

$$\left|x+a\right\rangle = \hat{T}^{+}(-a)\left|x\right\rangle, \qquad \text{h.c.} \qquad \left\langle x+a\right| = \left\langle x\right|\hat{T}(-a)$$

or by changing a into -a

$$\left|x-a\right\rangle = \hat{T}^{+}(a)\left|x\right\rangle, \qquad \text{h.c.} \qquad \left\langle x-a\right| = \left\langle x\right|\hat{T}(a)$$

Then we have

$$\hat{T}^{+}(-a) = \hat{T}(a),$$

using the relation

$$\left|x+a\right\rangle = \hat{T}(a)\left|x\right\rangle$$

which means that $\hat{T}(a)$ is not a Hermitian operator.

(iv) Commutation relation I

$$\hat{T}^{+}(a)\hat{x}\hat{T}(a) = \hat{x} + a\hat{1}$$

and

$$\hat{T}^{+}(a)V(\hat{x})\hat{T}(a) = V(\hat{x} + a\hat{1})$$

When $V(\hat{x}+a\hat{1})=V(\hat{x})$ (periodic potential), we have

$$\hat{T}^{+}(a)V(\hat{x})\hat{T}(a)=V(\hat{x})$$

(v) Commutation relation II

$$\hat{T}^{+}(a)\hat{p}\hat{T}(a)=\hat{p}$$

and

$$\hat{T}^{+}(a)\hat{p}^{2}\hat{T}(a)=\hat{p}^{2}$$

or more generally

$$\hat{T}^{+}(a)f(\hat{p})\hat{T}(a)=f(\hat{p})$$

where $f(\hat{p})$ is a polynomial function of $\hat{p}$.
