CHAPTER III

BLOCH FUNCTION

F. Bloch[6] has given the important theorem that the solution of the Schrodinger equation for a periodic lattice must have the form*

$$\Psi(r) = u_k(r)\, exp(ikr) \quad , \qquad (3.1)$$

where $u_k(r)$ has the periodic of the lattice, $u_k(r) = u_k(r+R)$ for all R in a lattice and R is a lattice vector connecting the two cells. Eq.(3.1) is called as Bloch function which is the form of a plane wave times a function with the periodic of the lattice

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*See APPENDIX C.

Many problems of physics have been solved successfully by Bloch function, obviously in Quantum Mechanics and in Solid State Physics. We have reviewed some problems which relate to our work as follows.

Bloch Function in Solid State Physics

3.1 The Vibration of Monatomic Lattice[7]

When the elastic wave propagates into the lattice, the atoms move. The motions are called longitudinal if they are parallel to the propagation of elastic wave and they are called transverse if they are perpendicular to the propagation. In this Chapter, the longitudinal case is reviewed breifly ;as follows. Consider the monatomic chain as shown in Fig. 3.1.1.

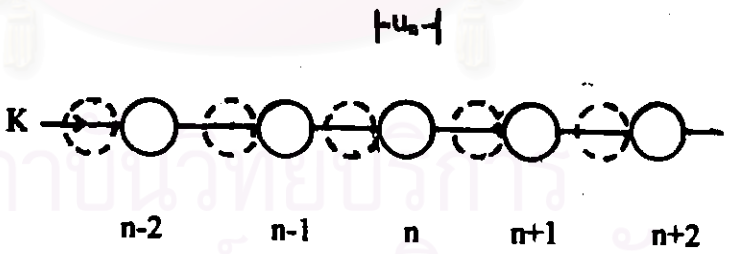

Fig. 3.1.1 The Vibration of Monatomic Lattice

When the line of atoms is displaced parallel to the wave vector K, we can describe the displacement of atoms from equilibrium by a single coordinate,u_n. We assume that the force F, due to the displacement of these atoms on the line , is, from the Hook's law,

$$F_k = \sum_n C_n (u_{n+k} - u_k) \quad , \qquad (3.1.2)$$

where C_n is the spring constant between atoms n steps apart and n is an integer.

From Newton's second law of motion;

$$F_k = m\frac{d^2u_k}{dt^2} \quad . \qquad (3.1.3)$$

With Eq.(3.1.2) and Eq.(3.1.3) we can write down the equation of motion of the k th atom as

$$m\frac{d^2u_k}{dt^2} = \sum_n C_n (u_{n+k} - u_k) \quad . \qquad (3.1.4)$$

The form of the solution in Eq.(3.1.4) is the form of traveling wave, Bloch function,

$$u_n = u\, exp(inKd)\, exp(iax) \quad , \qquad (3.1.5)$$

where d is the distance between nearest atoms and K is the elastic wave vector

Inserting Eq.(3.1.5) into Eq.(3.1.4) yields

$$\omega^2 m = -\sum_n C_n (exp[inKd] - 1) .$$

If $C_n = C_{-n}$ (translational symmetry),then

$$\omega^2 m = -\sum_{n>0} C_n (exp[inKd] + exp[-inKd] - 2) . \quad (3.1.6)$$

Thus $$\omega^2 = \frac{2}{m}\sum_{n>0} C_n (1 - cos[nKd]) . \quad (3.1.7)$$

If the interaction is due to the nearest neighbor atoms only,n=1, Eq.(3.1.7) becomes

$$\omega^2 = \frac{2}{m} C_1 (1 - cos[Kd]) ,$$

or $$\omega^2 = \frac{4C_1}{m} sin^2 \frac{Kd}{2} .$$

Thus $$\omega = \pm \left[\frac{4C_1}{m}\right]^{1/2} sin \frac{Kd}{2} . \quad (3.1.8)$$

The Eq.(3.1.8) is called the dispersion relation (between the frequency and the wave vector).

3.2 The Vibration of Diatomic Lattice[8]

We consider the lattice with two atoms per primitive cell. This is shown in Fig. 3.2.1

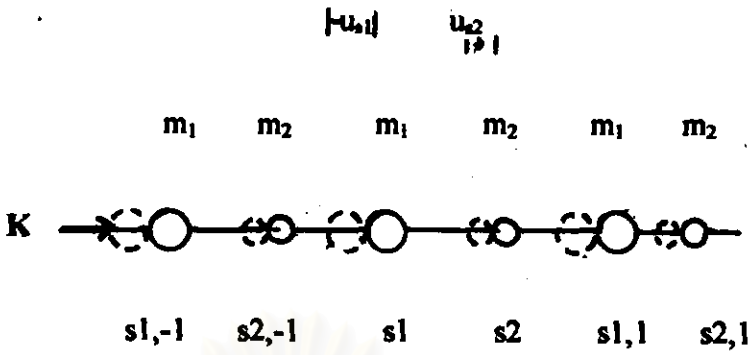

Fig. 3.2.1 The Vibration of Diatomic Lattice

and again assume that only nearest neighbor interacts and a spring constant C is identical for all pairs.

The displacement of the mass m_1 is defined as u_{s1} and the displacement of the mass m_2 is defined as u_{s2}. Then, the equations of motion for these atoms are

$$m_1 \frac{d^2 u_{s1}}{dt^2} = C(u_{s2} + u_{s2-1} - 2u_{s1}) \quad , \tag{3.2.1}$$

$$m_2 \frac{d^2 u_{s2}}{dt^2} = C(u_{s1} + u_{s1+1} - 2u_{s2}) \quad , \tag{3.2.2}$$

where the general solutions are

$$u_{s1} = u_1 \exp(iKds1) \exp(-i\omega t)) \quad , \tag{3.2.3}$$

and

$$u_{s2} = u_2 \exp(iKds2) \exp(-i\omega t) \quad . \tag{3.2.4}$$

Inserting Eq.(3.2.3) and Eq.(3.2.4) into Eq.(3.2.1) and Eq.(3.2.2) respectively yields

$$-\omega^2 m_1 u_1 = C u_2 [1 - exp(-iKd)] - 2C u_1 \quad , \qquad (3.2.5)$$

and $$-\omega^2 m_2 u_2 = C u_1 [1 + exp(iKd)] - 2C u_2 \quad . \qquad (3.2.6)$$

To get nonzero solutions u_{n1} and u_{n2} from these coupled equations, the determinant must be equal to zero,

$$\begin{vmatrix} 2C - \omega^2 m_1 & -C[1 + exp(-iKd)] \\ -C[1 + exp(iKd)] & 2C - \omega^2 m_2 \end{vmatrix} = 0 \quad ,$$

$$(2C - \omega^2 m_1)(2C - \omega^2 m_2) - (C[1 + exp(-iKd)])(C[1 + exp(iKd)]) = 0 \quad .$$

Thus

$$m_1 m_2 \omega^4 - 2C(m_1 + m_2)\omega^2 + 2C^2(1 - cos(Kd)) = 0 \quad . \qquad (3.2.7)$$

$$\omega^2 = \frac{2C(m_1 + m_2) \pm \sqrt{[2C(m_1 + m_2)]^2 - 8m_1 m_2 C^2 (1 - cos(Kd))}}{2m_1 m_2} \quad ,$$

$$= \frac{2C(m_1 + m_2) \pm 2C(m_1 + m_2)\sqrt{1 - 2m_1 m_2 (1 - cos(Kd)) / (m_1 + m_2)^2}}{2m_1 m_2} \quad ,$$

$$\omega^2 = \frac{2C(m_1+m_2) \pm 2C(m_1+m_2)(1-2m_1m_2(1-\cos(Kd))/(m_1+m_2)^2)^{1/2}}{2m_1m_2} .$$

As $K \to 0$, $\cos(Kd) \to 1$, and the two roots are given by

$$\omega^2_+ = \frac{2C(m_1+m_2)}{m_1m_2} = \omega^2_{max} , \qquad (3.2.8a)$$

and

$$\omega^2_- = 0 = \omega^2_{min} . \qquad (3.2.8b)$$

At $K = \pi/d$, Eq.(3.2.7) yields

$$\omega^2_+ = 2C/m_2 , \qquad (3.2.9a)$$

and

$$\omega^2_- = 2C/m_1 . \qquad (3.2.9b)$$

When we have plotted the graph of Eq.(3.2.7) between the frequency ω and the wave vector K, as shown in Fig. 3.2.2

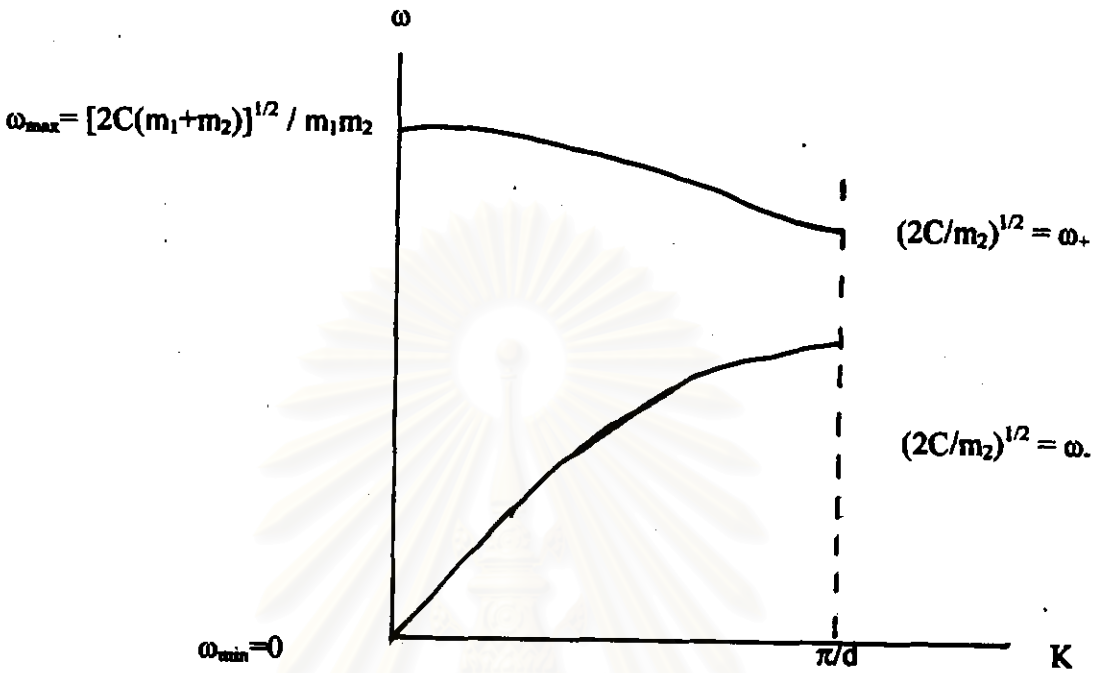

Fig. 3.2.2 The Dispersion Relation for The Diatomic Chain

From this figure,there is the forbidden gap($\omega_- < \omega < \omega_+$ and $\omega_{max} > \omega$). The forbidden gap means if the waves incident on the crystal in the frequency region between ω_- and ω_+, the waves will be reflected. Hence the region between $\omega_- < \omega < \omega_+$ and $\omega_{max} > \omega$ are outside the band.