CHAPTER VI

DISCUSSIONS AND CONCLUSIONS

From Chapter V, when the sinusoidally varying force is applied into the semi-infinite diatomic linear chain, it yields two coupled response functions, χ_1 and χ_2. When we have plotted the graphs(these have been shown in Fig. 5.2.3, 5.2.4) in the last Chapter. The graphs are plotted together as Fig. 6.1.

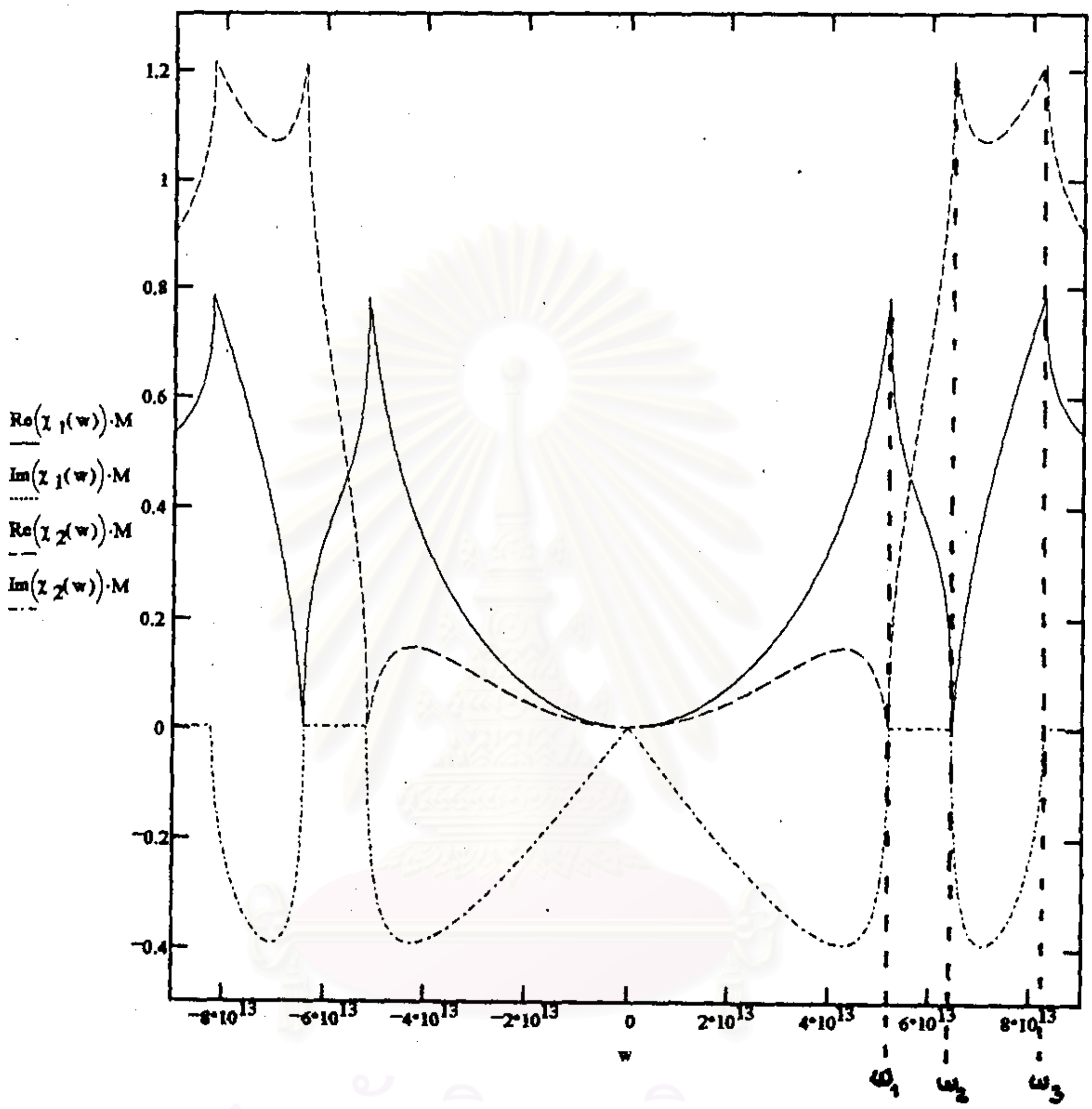

Fig. 6.1 The Real and the Imaginary parts of χ_1 and χ_2

In Figure 6.1, the imaginary parts of χ_1 and χ_2 are equal. They have two ranges for the imaginary part equal to zero. When the response functions are maximum, they mean that the chain has a maximum response. Similarly, the response functions are minimum, they mean that the chain has a minimum response.

At $\omega = \omega_1 \approx 5.160 \times 10^{13}$ s^{-1} , the response function of mass m_2, χ_2 , is minimum but the response function of mass m_1, χ_1 , is maximum. They mean the masses m_1 are moving while the masses m_2 are almost at rest.

At $\omega = \omega_2 \approx 6.415 \times 10^{13}$ s^{-1} , the response function of mass m_1, χ_1 , is minimum but the response function of mass m_2, χ_2 , is maximum. They mean the masses m_2 are moving while the masses m_1 are almost at rest.

At $\omega = \omega_3 \approx 8.230 \times 10^{13}$ s^{-1} , the response function of mass m_2, χ_2 , and the response function of mass m_1, χ_1 , are maximum. They mean the masses m_1 and the masses m_2 are moving but the masses m_2 are moving more than and the vibrations are out of phase .

From Chapter III, Bloch Function, and Fig. 3.2.2 ,we get that we have two regions are inside the band ($\omega_+ < \omega < \omega_{max}$ and $0 < \omega < \omega_-$).

If $\omega_- < \omega < \omega_+$ and $\omega > \omega_{max}$, they are outside the band. From Eq.(3.2.8a),(3.2.9 a), and (3.2.9b)

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

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

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

We can calculated the values of that

$\omega_{max} = 8.2349\text{x}10^{13}\ s^{-1}$,

$\omega_{+} = 6.4138\text{x}10^{13}\ s^{-1}$,

$\omega_{-} = 5.1648\text{x}10^{13}\ s^{-1}$.

Hence the frequencies at the maximum and the minimum of the response function method in Fig. 6.1 are almost equal to the frequencies at the maximum and the minimum of the Bloch function method in Fig. 3.2.2. Hence, $\omega_{-} \approx \omega_1$, $\omega_{+} \approx \omega_2$, $\omega_{max} \approx \omega_3$. Hence the region between $\omega_1 < \omega < \omega_2$ and $\omega > \omega_3$ are outside the band.

($\text{Im}(\chi_1(\omega))$ and $\text{Im}(\chi_2(\omega))$ are equal to zero).

Then we can consider the forbidden gap in the response function method from the imaginary part of the response function. Hence if the imaginary part of the response function is equal to zero, it is a forbidden gap.

This is difference from the Bloch function method. The forbidden gap in the Bloch function method is considered from the frequency.

We have plotted the graphs between the recursion relations(Eq.(5.1.3) and Eq(5.1.6))and ω (these have been shown in Fig. 5.3.1) together as Fig. 6.2

$$\frac{u_{s1\theta,n}(\omega)}{u_{s2\theta,n-1}(\omega)} = \frac{\chi_1(\omega)C}{\chi_1(\omega)C-\omega^2} \quad . \tag{5.1.3}$$

$$\frac{u_{s2\theta,n}(\omega)}{u_{s1\theta,n}(\omega)} = \frac{\chi_2(\omega)C}{\chi_2(\omega)C-\omega^2} \quad . \tag{5.1.6}$$

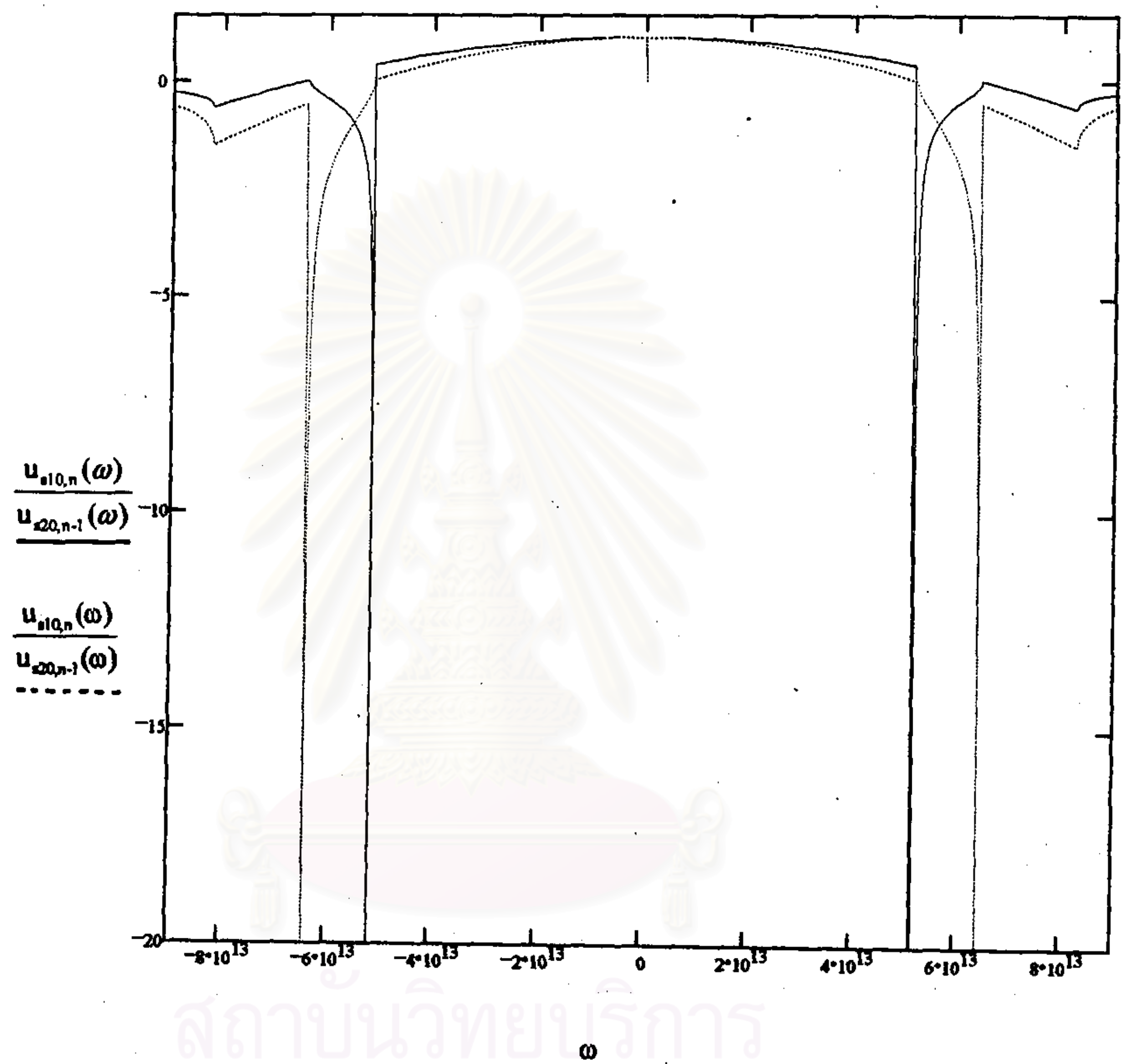

Fig. 6.2 The Recursion Relations of χ_1 and χ_2.

we can consider the motions of the chain and we get the reason to support the conclusion before. Hence, in Fig. 6.2 we can consider(only real part) in two cases (inside the band).

First; at $0<|\omega|<\omega_1$; $u_{s10,n}(\omega)/u_{s20,n-1}(\omega)$ and $u_{s20,n}(\omega)/u_{s10,n}(\omega)$ are larger than zero which they mean that the motions in neighboring masses have the same direction. This is shown in Fig. 6.3,

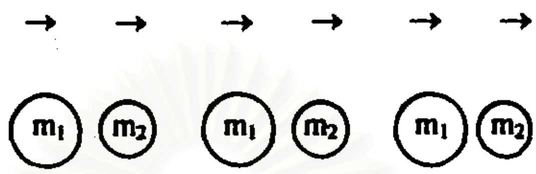

Fig. 6.3 The Motion at $0<|\omega|<\omega_1$.

Note that, when $|\omega| \to \omega_1$ then $u_{s10,n}(\omega)/u_{s20,n-1}(\omega) >> u_{s20,n}(\omega)/u_{s10,n}(\omega)$ It means that the motions of the masses m_2 are almost rest with respect to m_1. This is shown in Fig 6.4,

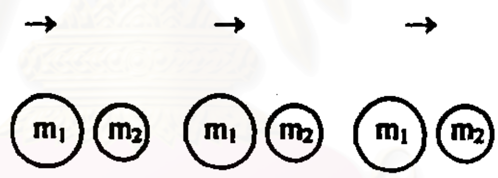

Fig. 6.4 The Motion when $|\omega| \to \omega_1$.

Secondly;at $\omega_2<|\omega|<\omega_3$; $u_{s10,n}(\omega)/u_{s20,n-1}(\omega)$ and $u_{s20,n}(\omega)/u_{s10,n}(\omega)$ are smaller than zero which they mean that the motions in neighboring masses have the opposite direction. This is shown in Fig. 6.5,

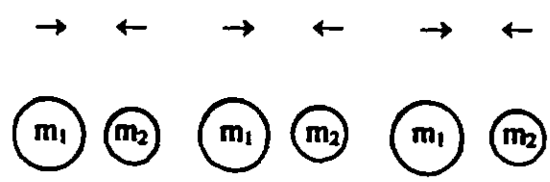

Fig. 6.5 The Motion at $\omega_2<|\omega|<\omega_3$.

Note that, when $|\omega| \rightarrow \omega_2$ then $u_{s10,n}(\omega)/u_{s20,n-1}(\omega) << u_{s20,n}(\omega)/u_{s10,n}(\omega)$ It means that the motions of the masses m_1 are almost rest with respect to m_2. This is shown in Fig 6.6,

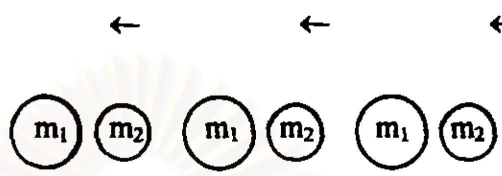

Fig. 6.6 The Motion when $|\omega| \rightarrow \omega_2$.

Then we can consider the motions of the semi-infinite diatomic linear chain by the response function method which we get the modes of vibrations as the same as the consideration by the Bloch function method.

The Bloch function method is difference from the response function method in such a way that we can solve the problems by the response function method when the sinusoidally varying force is applied. But if the force is not applied, we can solve the problems by the Bloch function method.

We can consider the energy transport in the chain from energy fluxes which is determined from the response functions.

The energy flux in s1,n th mass(Eq.(5.4.1.5)) is consisted of terms of the real part and the imaginary part of $\chi_1(\omega)$ and $\chi_2(\omega)$,

$$\dot{E}_{f(s1,n)}(t) = \frac{\omega^3 A^2 \exp(-2n\gamma)}{|\chi_1|^2}[\sin 2\beta \,\mathrm{Re}(\chi_1) - \cos 2\beta \,\mathrm{Im}(\chi_1)] - \frac{\omega^3 B^2 \exp(-2n\gamma)}{|\chi_2|^2}[\sin 2\beta \,\mathrm{Re}(\chi_2) - \cos 2\beta \,\mathrm{Im}(\chi_2)] \quad (5.4.1.5)$$

We find that if the energy flux is negative. It means that the motion does not transport energy. Then the energy transport is occurred when the energy flux is positive.

Similarly, The energy flux in s2,n th mass(Eq.(5.4.2.5)) is consisted of terms of the real part and the imaginary part of $\chi_1(\omega)$ and $\chi_2(\omega)$.

$$\dot{E}_{f(s2,n)}(t) = \frac{-\omega^3 A^2 \exp(-2[n+1]\gamma)}{|\chi_1|^2}[\sin 2\beta \operatorname{Re}(\chi_1) - \cos 2\beta \operatorname{Im}(\chi_1) + \frac{\omega^3 B^2 \exp(-2n\gamma)}{|\chi_2|^2}[\sin 2\beta \operatorname{Re}(\chi_2) - \cos 2\beta \operatorname{Im}(\chi_2)] \quad . \quad (5.4.2.5)$$

We find that if the energy flux is negative. It means that the motion does not transport energy. Then the energy transport is occurred when the energy flux is positive.

Finally, it can be concluded that the response function method can be determined the frequencies which are inside the band as same as the Bloch function method; and we can find the motions in the chain in the both cases. We can find the energy transport in the chain from the response function but in the Bloch function method, the energy transport is not mentioned.

Some part of this thesis (section 5.2) were presented in the 22 nd Congress on Science and Technology of Thailand , Bangkok Convention Center, The Central Plaza Ledprao, Bangkok.