Lecture 4: 1D Diatomic Chain (M=m, K≠G)

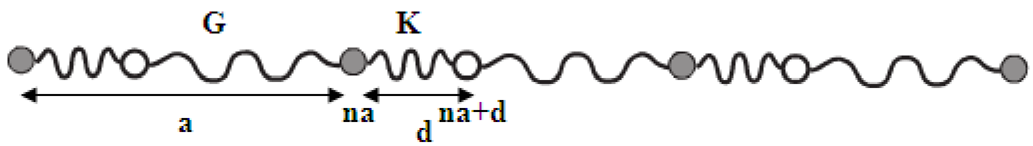
4-4 Introduction

In the previous lecture, we learned how to derive the dispersion relation for a Bravais lattice with a single-atom type.

In this lecture, using the same method, we will derive the **dispersion relation for a Bravais lattice with two different types of atoms (i.e., a two-atom basis**).

4-2 Model Description

As shown in the figure, there are two types of ions.
We assume (for simplicity here) that they have the **same mass M** in a one-dimensional primitive cell.



At temperature: T=0 K

- The first ion is located at: na
- The second ion is located at: na+d

Assumptions:

- $d \leq \frac{a}{2}$
- Only **nearest-neighbor interactions** are considered
- There are **two interaction constants between atoms**:
  - K
  - G
    where: G>K

- **Displacements**

- $u_1(na)$: displacement of atom at na
- $u_2(na)$: displacement of atom at na+d

This applies to all atoms in the lattice.

- **Harmonic Potential Energy**

From the previous lecture, the harmonic energy can be written as:

$$U_{harmonic} = \frac{K}{2}\sum_n[u_1\,(na) - u_2(na)]^2 + \frac{G}{2}\sum_n[u_2\,(na) - u_1((n+1)a)]^2 \quad (15)$$

- **Equations of Motion**

- For atom at na:

$$M\frac{\partial^2 u_1(na)}{\partial t^2} = -\frac{\partial U_{harmonic}}{\partial u_1(na)} \quad (16)$$

- For atom at na+d:

$$M\frac{\partial^2 u_2(na)}{\partial t^2} = -\frac{\partial U_{harmonic}}{\partial u_2(na)} \quad (17)$$

$$\frac{\partial U_{harmonic}}{\partial u_1(na)} = K[u_1(na) - u_2(na)](+1) + G[u_2((n-1)a) - u_1(na)](-1)$$
$$= K[u_1(na) - u_2(na)] + G[u_1(na) - u_2((n-1)a)] \quad (18)$$

Also,

$$M\frac{\partial^2 u_1(na)}{\partial t^2} = -K[u_1(na) - u_2(na)] - G[u_1(na) - u_2((n-1)a)] \quad (19)$$

We can do the same for the 2nd atom.

$$\frac{\partial U_{harmonic}}{\partial u_2(na)} = K[u_1(na) - u_2(na)](-1) + G[u_2((n)a) - u_1((n+1)a)](+1)$$
$$= K[u_2(na) - u_1(na)] + G[u_2(na) - u_1((n+1)a)]$$
$$M\frac{\partial^2 u_2(na)}{\partial t^2} = -K[u_2(na) - u_1(na)] - G[u_2(na) - u_1((n+1)a)] \quad (20)$$

- **Wave Solutions:**

Now we will, using the same previous method, seek two solutions to equations (19) and (20), as follows:

- $u_1(na) = A_1 e^{i(qna-\omega t)}$ and $u_2(na) = A_2 e^{i(qna-\omega t)}$

Remember that:

- q: wave vector
- ω: angular frequency
- A_1 and A_2: vibration amplitudes

- **Substitution into Equations**

After substitution, we obtain two homogeneous equations:

$$M(-A_1\omega^2)\, e^{i(qna-\omega t)} = -K[A_1 e^{i(qna-\omega t)} - A_2 e^{i(qna-\omega t)}] - G[A_1 e^{i(qna-\omega t)} - A_2 e^{i(q(n-1)a-\omega t)}]$$

$$MA_1\omega^2 = K[A_1 - A_2] + G[A_1 - A_2 e^{-iqa}]$$

$$A_1(M\omega^2 - (K+G)) + A_2(K + Ge^{-iqa}) = 0 \qquad (21)$$

For equations # (20): (2nd atom)

$$M(-A_2\omega^2)\, e^{i(qna-\omega t)} = -K[A_2 e^{i(qna-\omega t)} - A_1 e^{i(qna-\omega t)}] - G[A_2 e^{i(qna-\omega t)} - A_1 e^{i(q(n+1)a-\omega t)}]$$

$$MA_2\omega^2 = K[A_2 - A_1] + G[A_2 - A_1 e^{iqa}]$$

$$A_1(K + Ge^{iqa}) + A_2(M\omega^2 - (K+G)) = 0 \qquad (22)$$

- **Dispersion Relation (Determinant Condition)**

We now have equations (21) and (22), which are homogeneous. To obtain a solution for them, we will use the determinant of the matrix:

$$\begin{bmatrix} M\omega^2 - (K+G) & K + Ge^{-iqa} \\ K + Ge^{iqa} & M\omega^2 - (K+G) \end{bmatrix} = 0$$

$$[M\omega^2 - (K+G)]^2 - [(K + Ge^{-iqa})(K + Ge^{iqa})] = 0$$

$$[M\omega^2 - (K+G)]^2 - [K^2 + G^2 + 2KG\cos_{(qa)}] = 0 \qquad (23)$$

$$[M\omega^2 - (K+G)]^2 - [K^2 + G^2 + 2KG\cos_{(qa)}] = 0$$

$$M\omega^2 = (K+G) \pm \sqrt{[K^2 + G^2 + 2KG\cos_{(qa)}]}$$

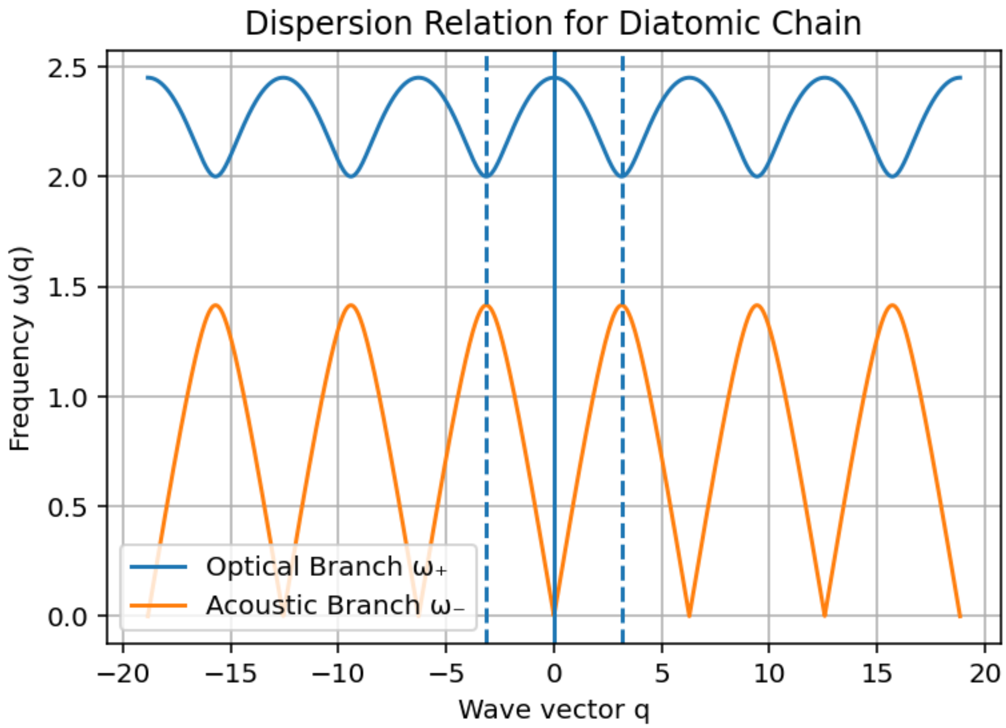
$$\omega^2 = \frac{(K+G)}{M} \pm \frac{1}{M}\sqrt{[K^2 + G^2 + 2KG\cos_{(qa)}]}$$

- **Two Branches of Solutions**

For each **q**, there are **two frequencies (ω)**:

$$\omega^2 = \frac{(K+G)}{M} + \frac{1}{M}\sqrt{[K^2 + G^2 + 2KG\cos_{(qa)}]} = \omega^2{}_{+}(q) \qquad (24)$$

$$\omega^2 = \frac{(K+G)}{M} - \frac{1}{M}\sqrt{[K^2 + G^2 + 2KG\cos_{(qa)}]} = \omega^2{}_{-}(q) \qquad (25)$$



◇ 1. Acoustic Branch ω_-

- Lower frequency
- Called the **acoustic branch**

Why? Because it behaves like sound waves at small **q**.

◇ 2. Optical Branch ω_+

- Higher frequency
- Called the **optical branch**

▧ General Result

If there are **p** atoms per unit cell in 3D:

Number of branches=3p

- 3 acoustic branches
- 3(p−1) optical branches

- **Amplitude Ratios**

By substituting equation (24) into equation (22), the amplitude of oscillations in the optical branch can be obtained:

$$A_{1,+}\left(M\left(\frac{(K+G)}{M}+\frac{1}{M}\sqrt{\left[K^2+G^2+2KG\,cos_{(qa)}\right]}\right)-(K+G)\right)+A_{2,+}(K+Ge^{-iqa})=0$$

$$A_{1,+}\left(\sqrt{\left[K^2+G^2+2KG\,cos_{(qa)}\right]}\right)+A_{2,+}\left(K+Ge^{-iqa}\right)=0$$

$$\frac{A_{2,+}}{A_{1,+}}=-\frac{\sqrt{\left[K^2+G^2+2KG\,cos_{(qa)}\right]}}{(K+Ge^{-iqa})}=-\frac{|K+Ge^{iqa}|}{(K+Ge^{-iqa})} \qquad (26)$$

Where we use:

$$\sqrt{zz^*}=|z|$$

$$|K+Ge^{iqa}|=\sqrt{(K+Ge^{iqa})(K+Ge^{-iqa})}=\sqrt{(K^2+G^2+2K\cos_{qa})}$$

z is an imaginary number.

Similarly, for the acoustic branch:

$$A_{1,-}(M\left(\frac{(K+G)}{M}-\frac{1}{M}\sqrt{\left[K^2+G^2+2KG\,cos_{(qa)}\right]}\right)-(K+G))+A_{2,-}(K+Ge^{-iqa})=0$$

$$A_{1,-}\left(-\sqrt{\left[K^2+G^2+2KG\,cos_{(qa)}\right]}\right)+A_{2,-}(K+Ge^{-iqa})=0$$

$$\frac{A_{2,-}}{A_{1,-}}=\frac{\sqrt{\left[K^2+G^2+2KG\,cos_{(qa)}\right]}}{(K+Ge^{-iqa})}=\frac{|K+Ge^{iqa}|}{(K+Ge^{-iqa})} \qquad (27)$$

- Now we will study the vibrational behavior of atoms in the following special cases that help us to analyze the physical meaning of the two solutions:

- **Case 1:** q=0 **(Long Wavelength)**

$q=\frac{2\pi}{\lambda} \qquad \lambda=\infty$

- **Acoustic Branch**

$$\omega^2{}_{-}(q)=\frac{(K+G)}{M}-\frac{1}{M}\sqrt{\left[K^2+G^2+2KG\,cos_{(qa)}\right]}$$

$$\because qa<<1$$

$$\therefore cos_{(qa)}\approx 1-\frac{(qa)^2}{2!}$$

$$\omega^2{}_{-}(q)=\frac{(K+G)}{M}-\frac{1}{M}\sqrt{\left[K^2+G^2+2KG\left(1-\frac{(qa)^2}{2!}\right)\right]}$$

$$= \frac{(K+G)}{M} - \frac{1}{M}\sqrt{[K^2 + G^2 + 2KG - KG(qa)^2]}$$
$$= \frac{(K+G)}{M} - \frac{1}{M}\sqrt{[(K\ + G\ )^2 - KG(qa)^2]}$$
$$= \frac{(K+G)}{M} - \frac{1}{M}(K+G)\sqrt{\left[1 - \frac{KG(qa)^2}{(K\ + G\ )^2}\right]}$$
$$= \frac{(K+G)}{M} - \frac{1}{M}(K+G)\left(1 - \frac{1}{2}\left[\frac{KG(qa)^2}{(K\ + G\ )^2}\right]\right)$$

Where we use: $(1+X)^n \approx 1 + \frac{1}{2}x$

$$\omega^2{}_-(q) = +\frac{1}{2M}\left[\frac{KG(qa)^2}{(K\ + G\ )}\right]$$

When q=0, $\omega^2{}_-(0) = 0$

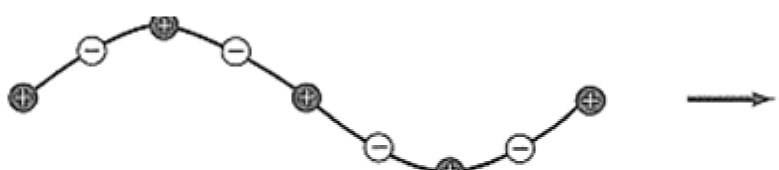
As for the amplitude of the vibrations, we will find that:

$$\frac{A_{2,-}}{A_{1,-}} = \frac{\left|K + Ge^{iqa}\right|}{(K + Ge^{-iqa})} = \frac{|K+G|}{(K+G)} = +1$$

That means:

👉 Atoms move in phase
- Same direction
- Same motion

👉 Entire unit cell moves together



q

Acoustical mode

◆ **Optical Branch**

$$\omega^2{}_+(q) = \frac{(K+G)}{M} + \frac{1}{M}\sqrt{\left[K^2 + G^2 + 2KG\ cos_{(qa)}\ \right]}$$
$$\because qa << 1$$
$$\therefore cos_{(qa)} \approx 1 - \frac{(qa)^2}{2!}$$

$$\omega^2{}_+(q) = \frac{(K+G)}{M} + \frac{1}{M}\sqrt{\left[K^2 + G^2 + 2KG\left(1 - \frac{(qa)^2}{2!}\right)\right]}$$

$$= \frac{(K+G)}{M} + \frac{1}{M}\sqrt{[K^2 + G^2 + 2KG - KG(qa)^2]}$$

$$= \frac{(K+G)}{M} + \frac{1}{M}\sqrt{[(K\ + G\ )^2 - KG(qa)^2]}$$

$$= \frac{(K+G)}{M} + \frac{1}{M}(K+G)\sqrt{\left[1 - \frac{KG(qa)^2}{(K\ + G\ )^2}\right]}$$

$$= \frac{(K+G)}{M} + \frac{1}{M}(K+G)\left(1 - \frac{1}{2}\left[\frac{KG(qa)^2}{(K\ + G\ )^2}\right]\right)$$

$$\omega^2{}_+(q) = +\frac{2(K+G)}{M} - \frac{1}{2M}\frac{KG(qa)^2}{(K\ + G\ )}$$

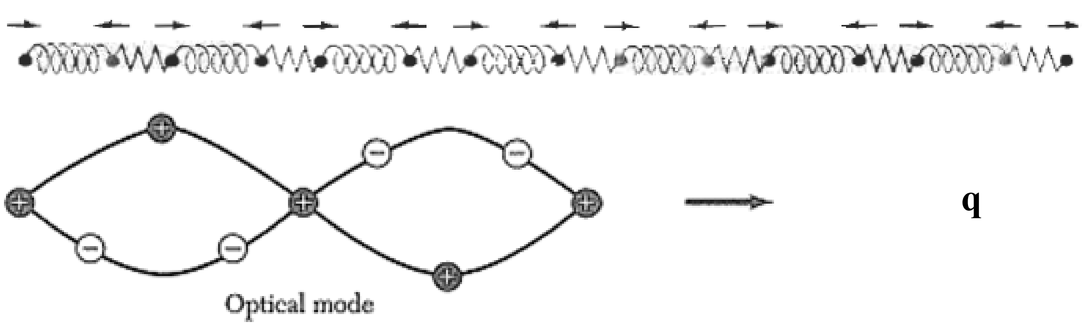
When q=0, we obtain:

$$\omega^2{}_+(q) = +\frac{2(K+G)}{M}$$

Similarly, for the amplitude of the vibrations:

$$\frac{A_{2,+}}{A_{1,+}} = -\frac{\left|K + Ge^{iqa}\right|}{(K + Ge^{-iqa})} = -\frac{|K+G|}{(K+G)} = -1$$

This means that adjacent atoms oscillate in opposite directions when propagating in the optical branch.



👉 Atoms move **out of phase**

- Opposite directions

👉 Internal vibration within unit cell

- **Case 2:** $q = \frac{\pi}{a}$ (Brillouin zone)

◆ **Acoustic Branch**

$$\omega^2{}_{-}(q) = \frac{(K+G)}{M} - \frac{1}{M}\sqrt{\left[K^2 + G^2 + 2KG\cos_{(qa)}\right]}$$

$$\omega^2{}_{-}(q) = \frac{(K+G)}{M} - \frac{1}{M}\sqrt{(K-G)^2} = \frac{2G}{M}$$

$$\frac{A_{2,-}}{A_{1,-}} = +\frac{\left|K + Ge^{i\pi}\right|}{(K + Ge^{-i\pi})} = +\frac{|K-G|}{(K-G)} = +1$$

Also, we can investigate the amplitude:

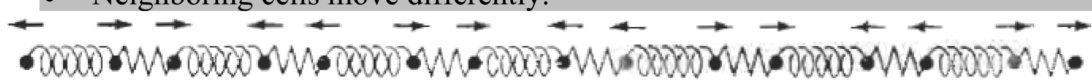
$$u_{1,-}(ma) = A_{1,-}e^{i(m\pi)} = A_{1,-}(-1)^m$$

$$u_{2,-}(ma) = A_{2,-}e^{i(m\pi)} = A_{2,-}(-1)^m = A_{1,-}(-1)^m$$

That means:

👉 Motion:

- Atoms in each unit cell move **in phase**.
- Neighboring cells move differently.



◆ **Optical Branch**

$$\omega_{+}{}^2(q) = \frac{(K+G)}{M} + \frac{1}{M}\sqrt{(K-G)^2} = \frac{2K}{M}$$

$$\frac{A_{2,-}}{A_{1,-}} = -\frac{\left|K + Ge^{i\pi}\right|}{(K + Ge^{-i\pi})} = -\frac{|K-G|}{(K-G)} = -1$$

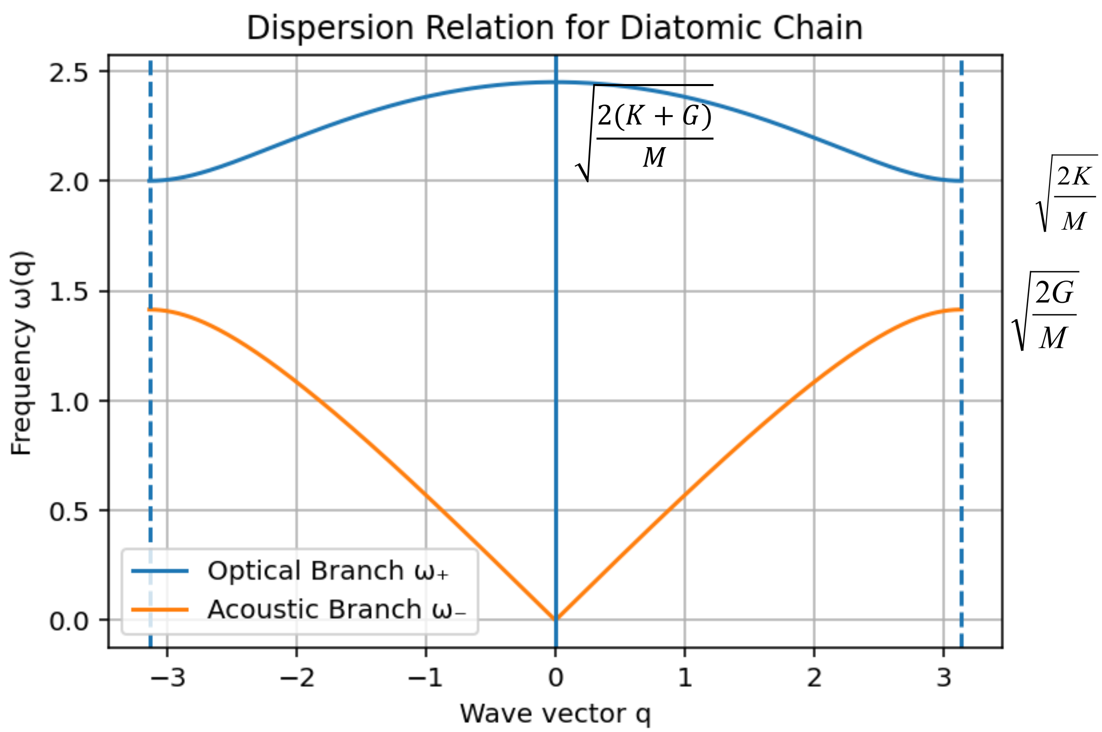
$$u_{1,+}(ma) = A_{1,+}e^{i(m\pi)} = A_{1,+}(-1)^m$$

$$u_{2,+}(ma) = A_{2,+}e^{i(m\pi)} = A_{2,+}(-1)^m = -A_{1,+}(-1)^m$$

👉 Motion:

- Atoms move **out of phase (180° phase difference)**.
- Even inside the same unit cell.

The results of the previous special cases can be summarized in the following figure:



- ✓ At q=0, the optical branch has a finite frequency, indicating a frequency gap between acoustic and optical modes.
- ✓ A forbidden frequency range means that no vibrational wave can exist in the crystal at those frequencies.
- ✓ If you try to excite the lattice at a frequency inside the gap, the energy is **not transmitted through the crystal.**
- ✓ This result shows that the presence of two atoms per unit cell leads to two distinct vibration modes.
- ✓ In contrast to the monoatomic chain (one branch), the diatomic chain exhibits two branches.

Simulation Link

You can simulate these vibrations here:

http://dept.kent.edu/projects/ksuviz/leeviz/phonon/phonon.html

Exercise:

Explain how the Brillouin zone boundary corresponds ($q = \pm\frac{\pi}{a}$) to **Bragg reflection from planes (100)**.