

## Summary of Results: 1D Diatomic Chain ( $M = m, K \neq G$ )

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### 1. Periodicity of the Dispersion Relation

The dispersion relation is periodic:

$$\omega(q) = \omega(q + 2\pi/a)$$

### 2. Existence of Two Branches

- Upper branch: Optical
- Lower branch: Acoustic

### 3. Acoustic Branch Behavior

$$\omega_- \propto q$$

Represents sound-like propagation.

### 4. Optical Branch Behavior

$$\omega_+ \neq 0 \text{ at } q = 0$$

Represents internal vibration of atoms in the unit cell.

### 5. Forbidden Frequency Band

A frequency gap exists between the acoustic and optical branches due to different force constants.

A forbidden frequency range means that **no vibrational wave can exist in the crystal at those frequencies.**

### 6. Width of the Gap

$$\Delta\omega \propto |K - G|$$

Larger difference  $\rightarrow$  wider gap.

## 7. First Brillouin Zone

$$-\pi/a < q < \pi/a$$

## 8. Frequency Range

$$0 \leq \omega \leq \sqrt{2(K + G)/M}$$

## 9. Effect of Interaction Strengths

Increasing  $|K - G|$  increases the frequency gap and modifies the dispersion curves.

## 10. Amplitude Ratio

At  $q = 0$ :

- Acoustic:  $A_2/A_1 = +1$  (in phase)
- Optical:  $A_2/A_1 = -1$  (out of phase)

At  $q = \pi/a$ :

- Acoustic:  $A_2/A_1 = +1$
- Optical:  $A_2/A_1 = -1$

**Note:** Since  $M = m$ , both atoms always move equally (no atom at rest).

## Final Insight

Even with identical masses, different bond strengths result in two vibrational modes and a frequency gap.

| Case              | Origin of Gap          |
|-------------------|------------------------|
| $M \neq m$        | Mass difference        |
| $M = m, K \neq G$ | Interaction difference |