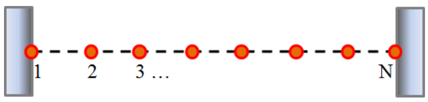
LATTICE VIBRATION

Overview: Lecture 4

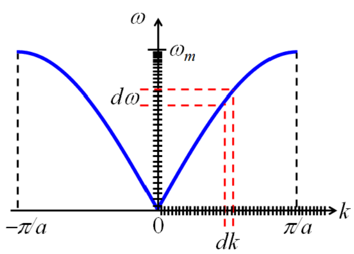
- Boundary conditions → allowed states, quantization



- Density of states

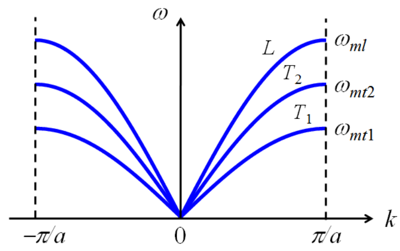
$$g(k)dk = \frac{Na}{2\pi}dk$$

$$g(\omega)d\omega = \frac{N}{\pi}\frac{d\omega}{\omega_m \cos(ka/2)}$$

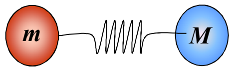


- Transverse vibration

$$\omega_l = \sqrt{\frac{4C_l}{m}}\left|\sin\frac{ka}{2}\right|,\ \omega_t = \sqrt{\frac{4C_t}{m}}\left|\sin\frac{ka}{2}\right|$$



Overview: This Lecture

- Diatomic lattice: 

- Equations of motions → Solutions → Dispersion relations
- Acoustic and optical modes

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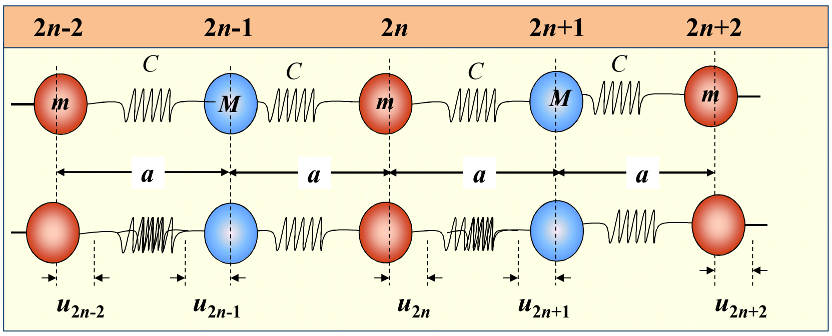
Linear Diatomic Lattice

- The atoms can have masses m and M → Ionic Crystals.
- In a chain of $2N$ atoms, N have mass m, and N have mass M.



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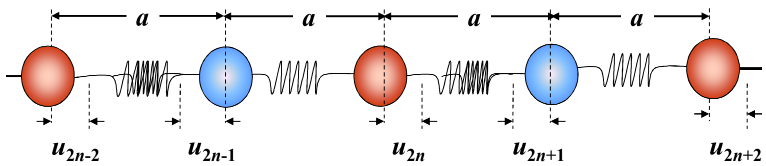
Interactions

- Equations of motions:

$$F_{2n} = m\frac{\partial^2 u_{2n}}{\partial t^2}$$
$$= C\left(u_{2n+1} + u_{2n-1} - 2u_{2n}\right)$$
$$F_{2n+1} = M\frac{\partial^2 u_{2n+1}}{\partial t^2}$$
$$= C\left(u_{2n+2} + u_{2n} - 2u_{2n+1}\right)$$

- Vibrations:

$$u_{2n} = Ae^{i(2kna-\omega t)}$$
$$u_{2n+1} = Be^{i[k(2n+1)a-\omega t]}$$
$$u_{2n+2} = Ae^{i[k(2n+2)a-\omega t]} = u_{2n}e^{i2ka}$$
$$u_{2n-1} = Be^{i[k(2n-1)a-\omega t]} = u_{2n+1}e^{-i2ka}$$



Solutions

- Replacing the solutions in the equations of motion

$$\left(m\omega^2 - 2C\right)u_{2n} + C\left(1 + e^{-i2ka}\right)u_{2n+1} = 0$$
$$C\left(1 + e^{i2ka}\right)u_{2n} + \left(M\omega^2 - 2C\right)u_{2n+1} = 0$$

- Determinant must be zero →

$$\begin{vmatrix} m\omega^2 - 2C & C\left(1 + e^{-i2ka}\right) \\ C\left(1 + e^{i2ka}\right) & M\omega^2 - 2C \end{vmatrix} = 0$$

Solutions

$$\begin{vmatrix} m\omega^2 - 2C & C\left(1+e^{-i2ka}\right) \\ C\left(1+e^{i2ka}\right) & M\omega^2 - 2C \end{vmatrix} = 0$$

$$\left(2C - m\omega^2\right)\left(2C - M\omega^2\right) - 4C^2\cos^2 ka = 0$$

$$\omega^4 - \frac{2C(m+M)}{mM}\omega^2 + \frac{4C^2\sin^2 ka}{mM} = 0$$

$$\omega^2 = \frac{C(m+M)}{mM}\left[1 \pm \sqrt{1 - \frac{4mM\sin^2 ka}{(m+M)^2}}\right]$$

- **Two separate branches of the dispersion relation:**
  - acoustical branch
  - optical branch.

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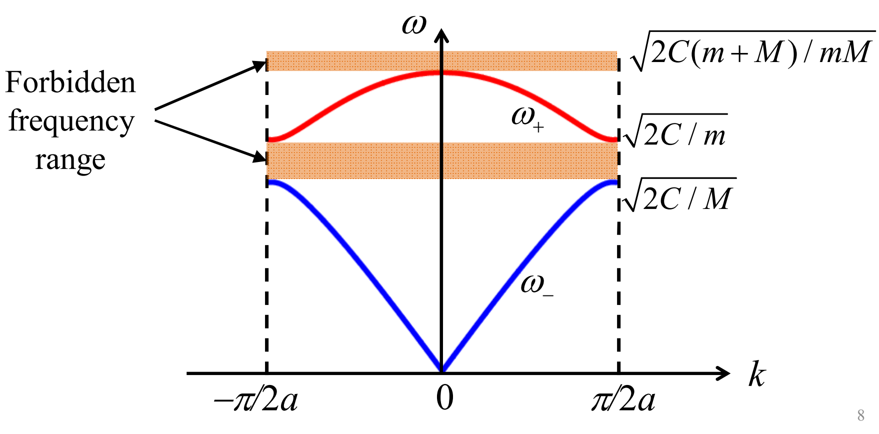
Dispersion Relation

$$\omega^2 = \frac{C(m+M)}{mM}\left[1 \pm \sqrt{1 - \frac{4mM\sin^2 ka}{(m+M)^2}}\right]$$



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Dispersion Relation

- The length of the cell is $2a$, therefore, the edges of the first Brillouin zone are at $k = \pm \pi/2a$.

$$\omega_-^2(\pi/2a) = \frac{C(m+M)}{mM}\left[1-\sqrt{1-\frac{4mM\sin^2(\pi a/2a)}{(m+M)^2}}\right]$$

$$= \frac{C(m+M)}{mM}\left[1-\sqrt{\frac{(m+M)^2-4mM}{(m+M)^2}}\right]$$

$$= \frac{C(m+M)}{mM}\left[1-\frac{M-m}{m+M}\right]$$

$$= \frac{C(m+M)}{mM}\frac{2m}{m+M}$$

$$\omega_-(\pi/2a) = \sqrt{\frac{2C}{M}}$$

- Similarly,

$$\omega_+(\pi/2a) = \sqrt{\frac{2C}{m}}$$

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Long Wavelength Limit

- $k = 0$

$$\omega_-^2(0) = \frac{C(m+M)}{mM}\left[1-\sqrt{1-\frac{4mM\sin^2(0)}{(m+M)^2}}\right]$$

$$= \frac{C(m+M)}{mM}[1-1] = 0$$

$$\omega_-(0) = 0$$

$$\omega_+^2(0) = \frac{C(m+M)}{mM}\left[1+\sqrt{1-\frac{4mM\sin^2(0)}{(m+M)^2}}\right]$$

$$= \frac{C(m+M)}{mM}[1+1] = \frac{2C(m+M)}{mM}$$

$$\omega_+(0) = \sqrt{\frac{2C(m+M)}{mM}}$$

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Long Wavelength Limit

- $k \approx 0$

$$\omega^4 - \frac{2C(m+M)}{mM}\omega^2 + \frac{4C^2 \sin^2 ka}{mM} = 0$$

$$\frac{2C(m+M)}{mM}\omega^2 = \frac{4C^2 k^2 a^2}{mM}$$

$$\omega_-(k) = ka\sqrt{\frac{2C}{m+M}}$$

- Phase velocity:

$$v_0 = \frac{\omega_-}{k} = a\sqrt{\frac{2C}{m+M}}$$

Acoustic Branch

$$\frac{u_{2n+1}}{u_{2n}} = \frac{C\left(1+e^{i2ka}\right)}{2C - M\omega^2} = \frac{B}{A}e^{ika}$$

$$\frac{B}{A} = \frac{C\left(e^{-ika}+e^{ika}\right)}{2C - M\omega^2} = \frac{\cos ka}{1 - \frac{M\omega^2}{2C}}$$

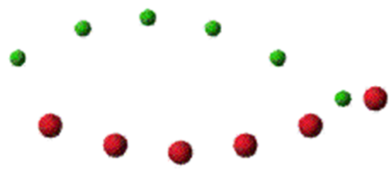
- $k \rightarrow 0$, $\omega \rightarrow 0$, $u_{2n+1}/u_{2n} \rightarrow 1$
- Neighboring atoms move in the same direction.

Optical Branch

$$\omega_+(0) = \sqrt{\frac{2C(m+M)}{mM}}$$

$$\frac{B}{A} = \frac{\cos ka}{1 - \frac{M\omega^2}{2C}} = \frac{1}{1 - \frac{M}{2C}\frac{2C(m+M)}{mM}}$$

$$= \frac{1}{1 - \frac{m+M}{m}} = -\frac{m}{M}$$



- Neighboring atoms move in opposite directions.
- Optical branch can be excited in ionic crystals.