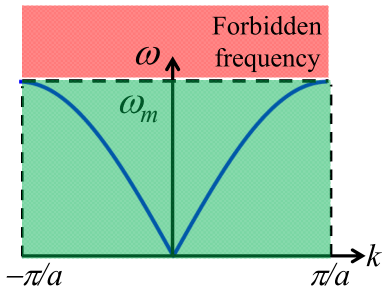
LATTICE VIBRATION

Overview

Lecture 2:

- Mathematical model of vibration in 1D monatomic lattice.
- Dispersion relation:

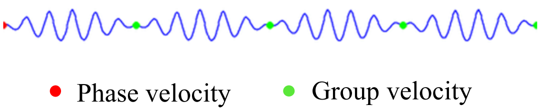
$$\omega = \omega_m \left| \sin \frac{ka}{2} \right|$$

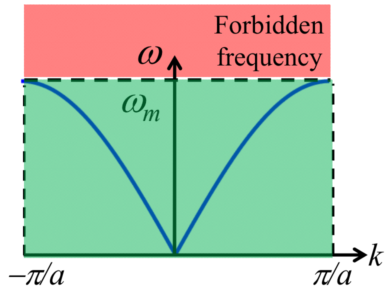


This lecture:

- Velocity of propagation through crystals.
- Brillouin zones → many solutions.
- What happens if $\omega > \omega_m$?

Velocity





$$\omega = \omega_m \left| \sin \frac{ka}{2} \right|$$

- **Phase velocity:**

$$v_p = \frac{\omega}{k} = a\sqrt{\frac{C}{m}} \left| \frac{\sin \frac{1}{2} ka}{\frac{1}{2} ka} \right| = v_0 \left| \frac{\sin \frac{1}{2} ka}{\frac{1}{2} ka} \right|$$

- **Group velocity:**

$$v_g = \frac{d\omega}{dk} = v_0 \left| \cos \frac{1}{2} ka \right|$$

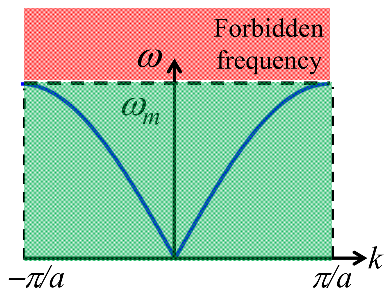
Long Wavelength Limits

$$\omega = \sqrt{\frac{4C}{m}} \left| \sin \frac{ka}{2} \right| = \omega_m \left| \sin \frac{ka}{2} \right|$$

$$k \approx 0$$

$$\sin \frac{ka}{2} \approx \frac{ka}{2}$$

$$\omega = ka\sqrt{\frac{C}{m}} = v_0 k$$



$v_p = v_g = v_0$ → Dispersionless propagation

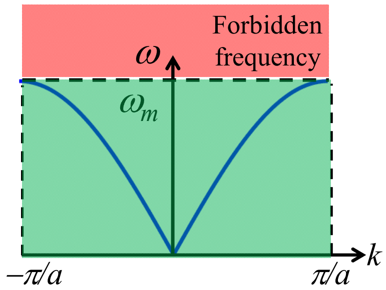
Cutoff Frequency

Long wavelength limit:

$$\omega = ka\sqrt{\frac{C}{m}} = v_0 k$$

$$v_0 = a\sqrt{\frac{C}{m}}$$

$$\omega_m = \sqrt{\frac{4C}{m}} = \frac{2v_0}{a}$$

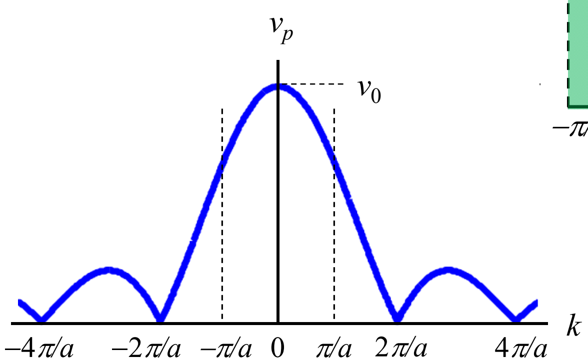


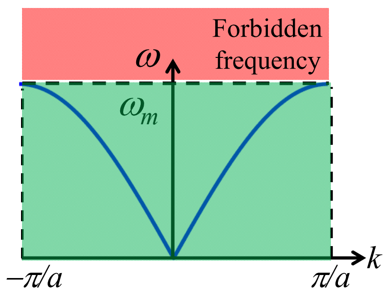
Typically: $\omega_m \approx 10^{13}$ rad/s

5

Phase Velocity

$$v_p = \frac{\omega}{k} = v_0 \left| \frac{\sin \frac{1}{2}ka}{\frac{1}{2}ka} \right|$$

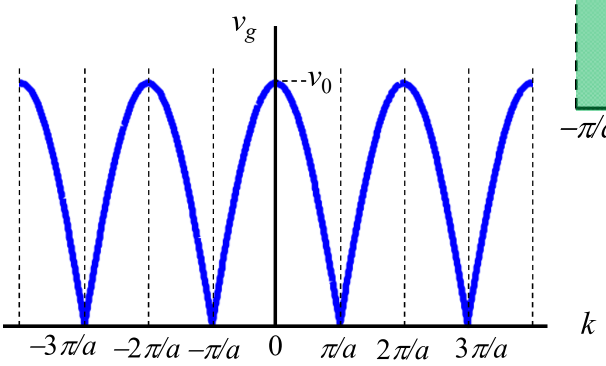


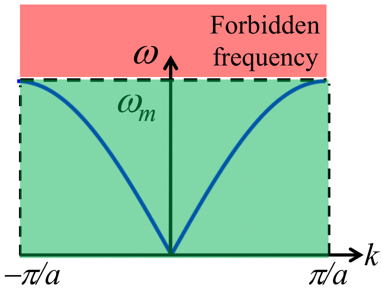


6

Group Velocity

$$v_g = \frac{d\omega}{dk} = v_0 \left| \cos \frac{1}{2} ka \right|$$





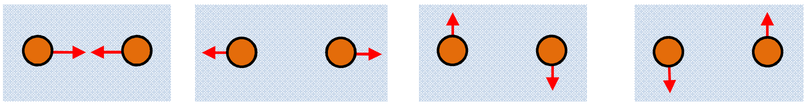
Phase

$$u_n = Ae^{i(kx_n - \omega t)} = Ae^{i(kna - \omega t)}$$

$$u_{n+1} = Ae^{i[k(n+1)a - \omega t]} = e^{ika} u_n$$

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

- Phase between nearest neighbors differs by *ka*.
- At $k = \pi/a$, adjacent atoms have a phase difference of π, and oscillate in opposite directions.



$k = \pi/a$

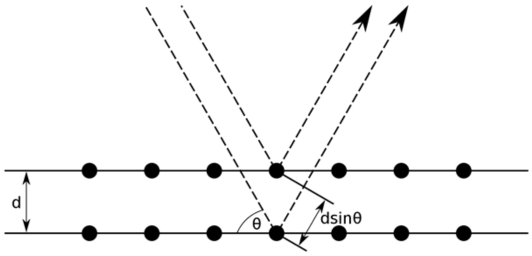
- π phase difference between adjacent atoms → standing waves → zero group velocity.
- This can also be explained from Bragg diffraction:

$$n\lambda = 2d\sin\theta$$

$$d = a, \quad \theta = \frac{\pi}{2}$$

- Bragg condition:

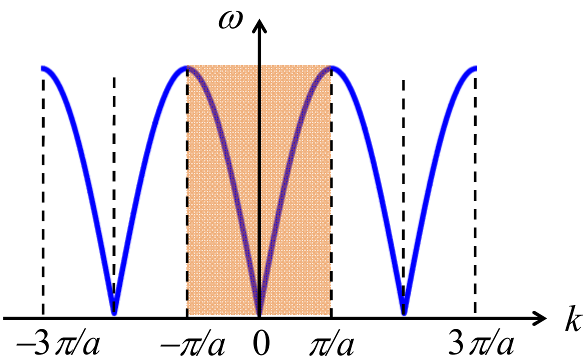
$$\lambda = 2a$$



9

First Brillouin Zone

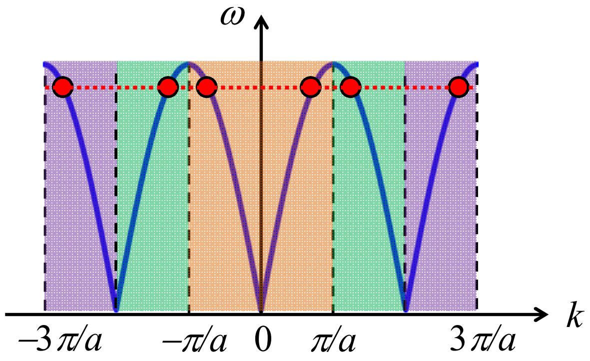
- The dispersion is periodic in k with a periodicity of $2\pi/a$.



10

Many Zones

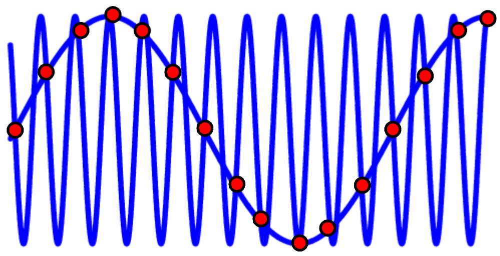
- For $\omega < \omega_m$, there are many possible values for k.
- Many possible solutions with many possible wavelengths.



11

Many Solutions

- More than one harmonic wave can be fitted to a given arrangements of atomic displacements.
- Any possible harmonic motion of the atoms can be described using a value of k within the first zone.



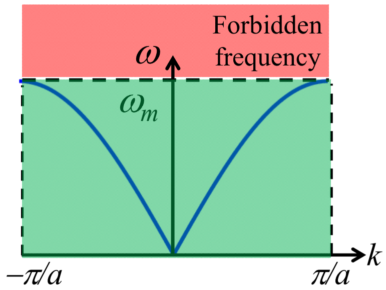
12

Frequencies above Cutoff

- $\omega > \omega_m$
- $\omega = \omega_m \left|\sin \dfrac{ka}{2}\right|$

  $\omega > \omega_m \rightarrow \sin \dfrac{ka}{2} > 1$
- ka must be a complex number

  $\rightarrow \; k = k_r + ik_i$
- $u_n = Ae^{i\left[(k_r + ik_i)na - \omega t\right]} = Ae^{i(k_r na - \omega t)}e^{-k_i na}$ $\rightarrow$ Solutions in this range of frequencies must be damped.



Frequencies above Cutoff

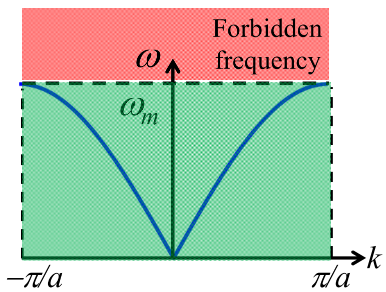
$$\omega = \omega_m \sin \frac{ka}{2}$$

$$\frac{\omega}{\omega_m} = \sin \frac{1}{2}(k_r + ik_i)a$$

$$= \sin \frac{1}{2}k_r a \cos \frac{1}{2}ik_i a + \cos \frac{1}{2}k_r a \sin \frac{1}{2}ik_i a$$

$$\cos ix = \frac{e^{i(ix)} + e^{-i(ix)}}{2} = \frac{e^x + e^{-x}}{2} = \cosh x$$

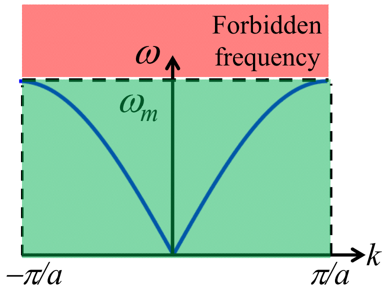
$$\sin ix = \frac{e^{i(ix)} - e^{-i(ix)}}{2i} = -\frac{1}{i}\frac{e^x - e^{-x}}{2} = i \sinh x$$



$$\sin \frac{1}{2}k_r a \cosh \frac{1}{2}k_i a + i \cos \frac{1}{2}k_r a \sinh \frac{1}{2}k_i a = \frac{\omega}{\omega_m} + i(0)$$

Frequencies above Cutoff

$$\sin\frac{1}{2}k_r a\cosh\frac{1}{2}k_i a + i\cos\frac{1}{2}k_r a\sinh\frac{1}{2}k_i a$$
$$= \frac{\omega}{\omega_m} + i(0)$$



- Equating real and imaginary terms

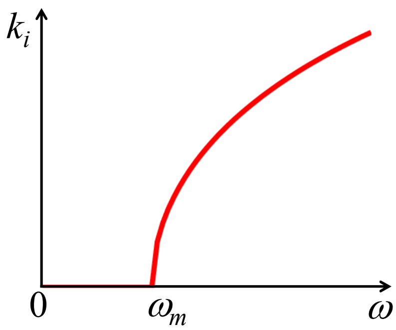
$$\sin\frac{1}{2}k_r a\ \cosh\frac{1}{2}k_i a = \frac{\omega}{\omega_m}$$
$$\cos\frac{1}{2}k_r a\ \sinh\frac{1}{2}k_i a = 0$$

$$k_i \neq 0 \rightarrow \cos\frac{1}{2}k_r a = 0 \Rightarrow k_r a = \pm\pi, \pm 3\pi, \pm 5\pi, \cdots$$
$$\frac{\omega}{\omega_m} = \cosh\frac{1}{2}k_i a \Rightarrow k_i = \frac{2}{a}\cosh^{-1}\left(\frac{\omega}{\omega_m}\right)$$

15

Frequencies above Cutoff

$$k_i = 0, \quad \omega \le \omega_m$$
$$= \frac{2}{a}\cosh^{-1}\left(\frac{\omega}{\omega_m}\right), \quad \omega > \omega_m$$



- Waves with $\omega > \omega_m$ are strongly attenuated.
- Example:
  ω/ω_m=1.01 $\Rightarrow \cosh^{-1}(1.01) = 0.1413$
  $k_i = 9.42 \times 10^8\ \mathrm{m}^{-1}$ → waves are attenuated by a factor $1/e$ in a distance corresponding to only about three times the atomic spacing.

16