Chapter 3. Lattice Waves

Lattice waves

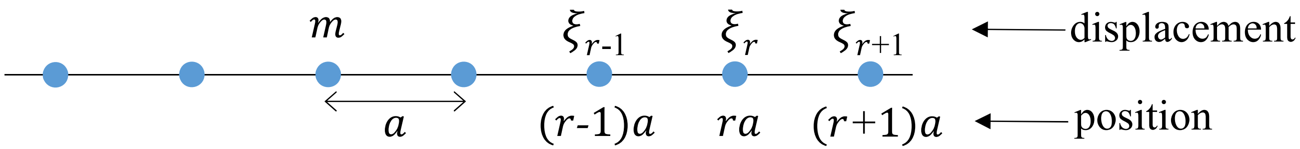
- Lattice waves

  : Vibrational motion of the atoms in a crystalline solid in terms of a wave passing through the atoms of the crystal as they are displaced by their thermal energy from their rest positions.

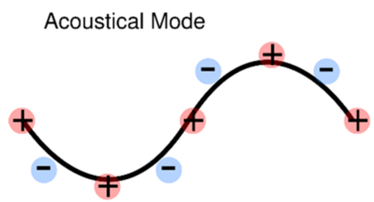
  - The thermal properties of solids are strongly related to the lattice waves
  - The movement of electrons (mobility) are hindered due to scattering by lattice waves.
  - Lattice waves have their particle-like counterpart, called phonons: quanta of energy $\hbar\omega_n$, ω_n: normal vibrational modes
  - Energy exchanging interactions with lattice waves occur in integral multiple of $\hbar\omega_n$.

Lattice waves

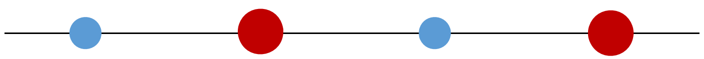
- Two examples:
  1. Vibrations associated with a one-dimensional crystal in which all the atoms have the same mass and the same atomic spacing.



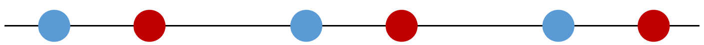
"Acoustic modes" : long wavelength longitudinal vibration corresponds to the sound wave.

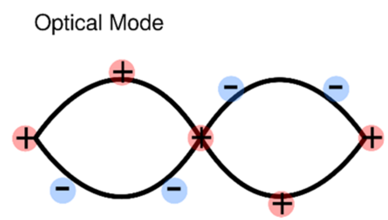


  2. Vibrations with two or more different kinds of atoms in a one-dimensional crystals.
     ① Two different masses with a common atomic spacing



     ② Two different atomic spacings for atoms with the same mass

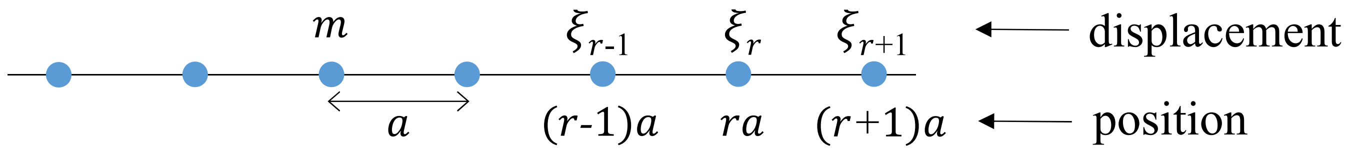




"Optical modes" : long wavelength transverse vibrations characterized by neighboring atoms being displaced in opposite directions. The long wavelength vibration can be excited by interaction with light if the material is at least partially ionic.

Transverse waves in a 1-D infinite lattice

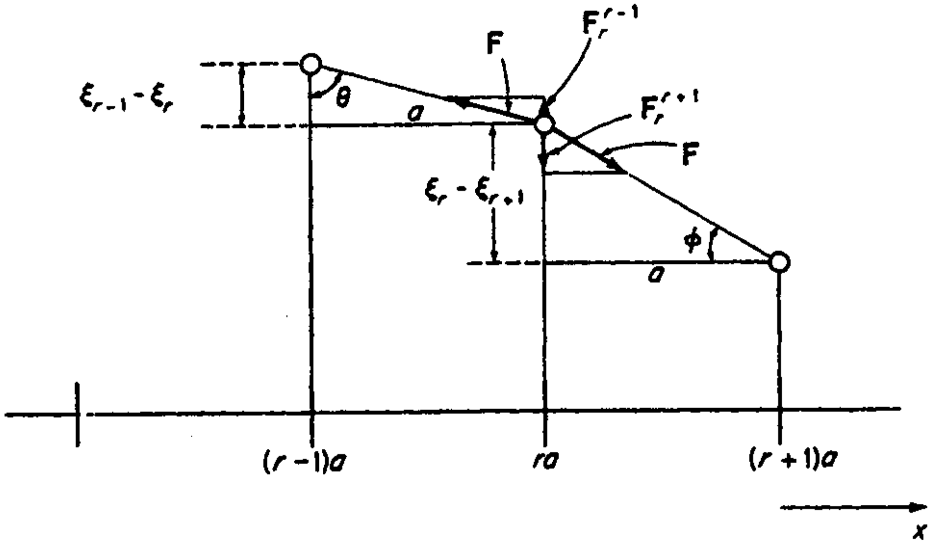
- Transverse waves in a one dimensional infinite string



ξ: displacement away from the x-axis

Assumption

1. Restrict the forces between nearest neighbor atoms
2. The force is an attractive force $\underset{\sim}{F}$
3. $\underset{\sim}{F}$ is constant and in the direction of the nearest neighbor atoms



Force at $x = ra$

$$F_{\text{up}} : F_r^{\,r-1} \sim \frac{\xi_{r\text{-}1} - \xi_r}{a} \cdot F$$

$$F_{\text{downward}} : F_r^{\,r+1} \sim -\frac{\xi_r - \xi_{r+1}}{a} \cdot F$$

(Assumption: $\xi \ll a$)

Transverse waves in a 1-D infinite lattice

$\therefore$ The net upward force on the atom at $x = ra$

$$F_r^{r-1} - F_r^{r+1} = m\frac{d^2\xi_r}{dt^2} \quad \Rightarrow \quad \boxed{\frac{d^2\xi_r}{dt^2} = \eta\xi_{r-1} - 2\eta\xi_r + \eta\xi_{r+1}} \text{ where } \eta = F/ma$$

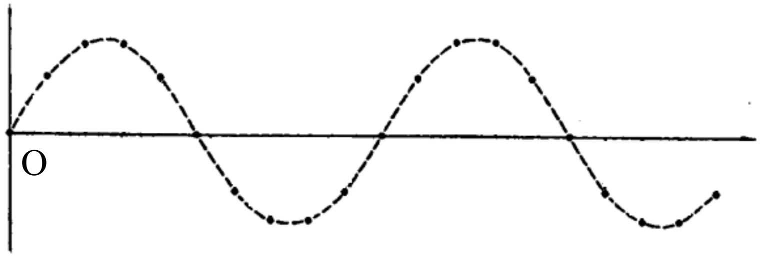
$$F_r^{r-1} \sim \frac{\xi_{r-1} - \xi_r}{a} \cdot F$$

$$F_r^{r+1} \sim -\frac{\xi_r - \xi_{r+1}}{a} \cdot F$$

- The harmonic solution

$$\xi(x,t) = A\exp\{i(kx - \omega t)\}$$

: mathematical wave passing through the displaced atoms.



Such a wave has physical reality only at the locations of atoms, i.e., only at x=ra. Then,

$$\xi_r(ra,t) = A\exp\{i(kra - \omega t)\}$$

$$\xi_{r-1} = Ae^{-ika}\xi_r$$

$$\xi_{r+1} = Ae^{ika}\xi_r$$

Transverse waves in a 1-D infinite lattice

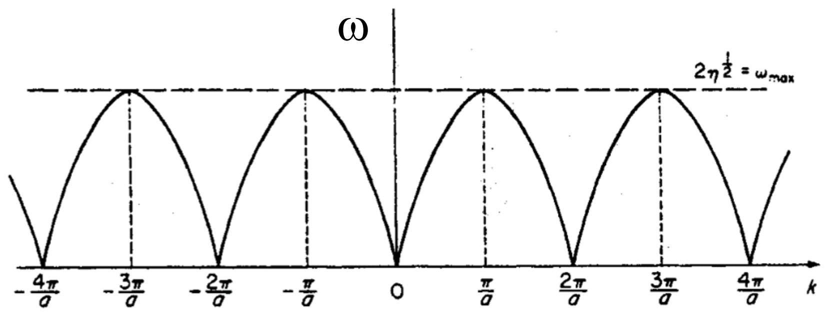
- Dispersion relationship

$$\omega^2 = 2\eta - \eta\{e^{ika} + e^{-ika}\}$$
$$= 2\eta(1 - \cos k\,a)$$

$$cf, \quad (1 - \cos 2\theta) = 2\sin^2\theta$$

$$\omega^2 = 4\eta\sin^2(k\,a/2) \;\Rightarrow\; \boxed{\omega = 2\eta^{1/2}|\sin(k\,a/2)|} \qquad \eta = F/ma$$

Dispersion relation between ω and k



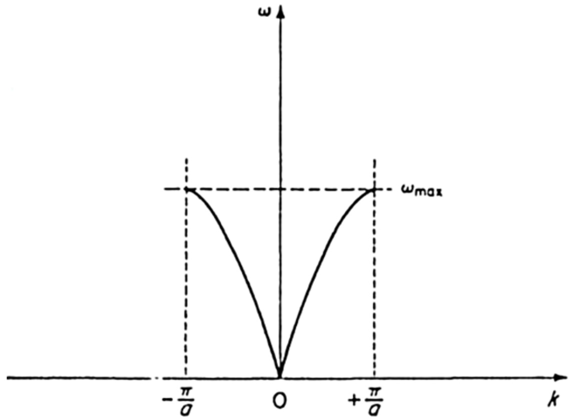
- Lattice wave has a dispersive system: The velocity varies with frequency and wave length
- Reducible to $0 \le k \le \pi/a$ (*The first Brillouin zone*)

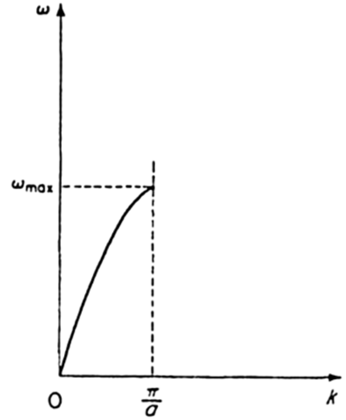
↑ The shortest wavelength

Transverse waves in a 1-D infinite lattice

cf) Displacement is identical for any k and $k' = k + \frac{2\pi n}{a}$

$$\begin{aligned} \xi' &= Ae^{i(k'x - wt)} \\ &= Ae^{i\left[\left(k + \frac{2\pi n}{a}\right)x - wt\right]} \\ &= Ae^{i2\pi n/a \cdot x} e^{i(kx - wt)} \\ &= \xi e^{in \cdot 2\pi/a \cdot ra} = \xi \exp(in2\pi r) = \xi \end{aligned}$$





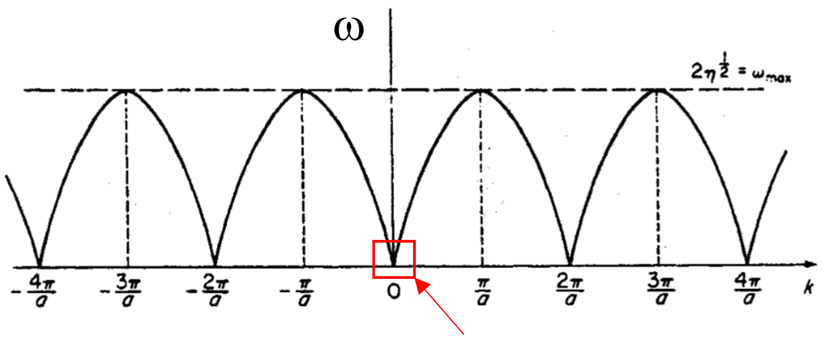
For small k (long wavelength)

$$\omega = 2\eta^{1/2} |\sin(k\,a/2)|$$

$$\sin(k\,a/2) \;\rightarrow\; ka/2$$

$$v\Big|_{k\sim 0} = v_g\Big|_{k\sim 0} = \frac{\omega}{k} = \eta^{1/2} a = (Fa/m)^{1/2}$$

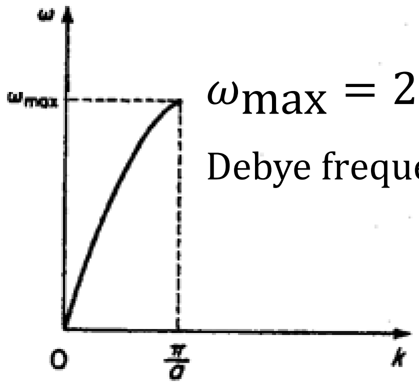
velocity becomes constant



small k region

Transverse waves in a 1-D infinite lattice

- Note:
  - ① k space is the reciprocal lattice
  - ② Acoustical Branch

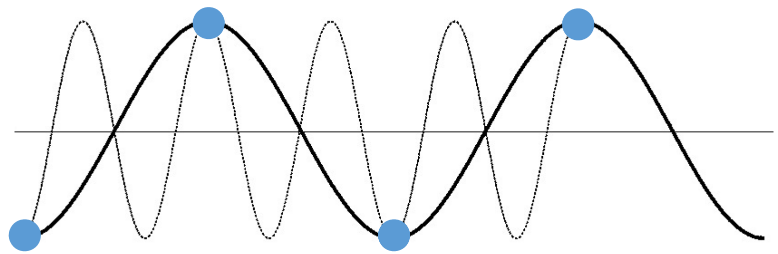


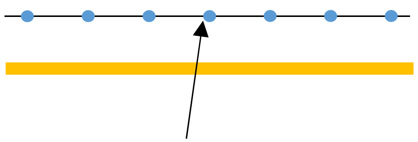
$\omega_{\max} = 2\sqrt{F/ma}$ $\quad (\because \omega = 2\eta^{1/2}|\sin(k\,a/2)|\,)$

Debye frequency

$\lambda \to \infty$ $\qquad \lambda = 2a$

Infinite wavelength





All atoms displaced by the same amount in the same direction.

- Neighboring atoms are displaced by the same distance in opposite directions.
- The shortest wavelength; $\lambda_{min} = 2a$
- The dashed wave (n>2) has shorter wavelength. However it does not give any new information on the position of atoms.
- Equivalent to the Bragg reflection condition
  $n\lambda = 2d\sin\theta\ (\lambda = 2a, n = 1, d = a)$
- Cannot propagate: group velocity at $k=\pi/a$ is equivalent to zero

Transverse waves in a 1-D finite lattice

- General solution for transverse waves

$$\xi(x,t) = A\exp\{i(kx-\omega t)\} + B\exp\{-i(kx+\omega t)\}$$

$$\xi(0) = \xi(L) = 0 \quad \text{(boundary conditions)}$$

$$\therefore\ k = \frac{m\pi}{L} \qquad m = 1,\ 2,\ \cdots,(n+1)$$

$$\omega = \omega_{max}\sin\left(\frac{m\pi a}{2L}\right)$$

$$= \omega_{max}\sin\left(\frac{m\pi a}{2(n+1)a}\right)$$

n: # of moving atoms
$n+2$: total number of atoms

$$\therefore\ \omega_{\mathrm{m}} = \omega_{max}\sin\left[\frac{m\pi}{2(n+1)}\right]$$: normal modes (allowed frequencies)

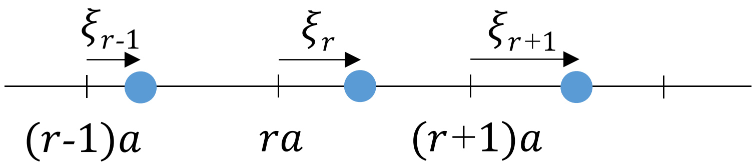
$$\xi_{rm} = A_m \sin(m\pi r/(n+1))e^{-i\omega t}$$ (displacement at $x = ra$ and for ω_{m})

The general solution for the atom at $x = ra$ is

$$\xi_r = \sum_m A_m \xi_{rm}$$

Finite set of discrete (ω, k) values

Longitudinal waves in a 1-D infinite lattice



- The restoring force for longitudinal displacement depends on the spatial variation of the force (F) between atoms
- Let $F(a)$ represent the force between atoms when separated by a normal lattice spacing (a), then the net force on the r^{th} atom is

$$F = F(a + \xi_{r+1} - \xi_r) - F(a + \xi_r - \xi_{r-1})$$

For very small displacement

$$F(a + \xi_{r+1} - \xi_r) \approx F(a) + (\xi_{r+1} - \xi_r)\left.\frac{dF}{d\xi}\right|_a + \cdots$$

$$F(a + \xi_r - \xi_{r-1}) \approx F(a) + (\xi_r - \xi_{r-1})\left.\frac{dF}{d\xi}\right|_a + \cdots$$

$$\therefore\ F = (\xi_{r+1} - 2\xi_r + \xi_r - 1)\left.\frac{dF}{d\xi}\right|_a = m\frac{d^2\xi}{dt^2}$$

Longitudinal waves in a 1-D infinite lattice

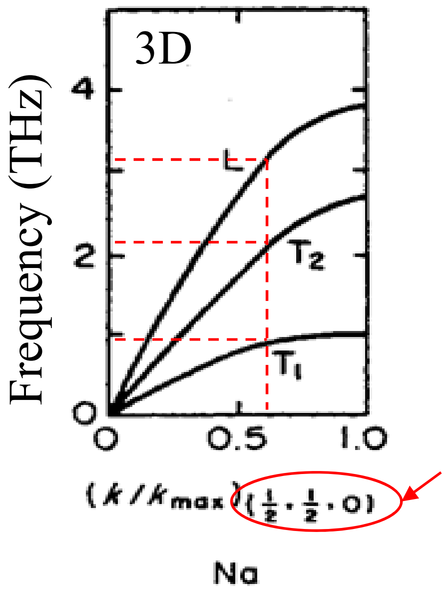
$$F = (\xi_{r+1} - 2\xi_r + \xi_{r-1}) \left.\frac{dF}{d\xi}\right|_a = m\frac{d^2\xi}{dt^2}$$

Let $\eta' = \frac{1}{m} \left.\frac{dF}{d\xi}\right|_a$

Then $\frac{d^2\xi}{dt^2} = \eta'\xi_{r-1} - 2\eta'\xi_r + \eta'\xi_{r+1}$

simiar to transverse waves except for $\eta \rightarrow \eta'$

$$\frac{d^2\xi_r}{dt^2} = \eta\xi_{r-1} - 2\eta\xi_r + \eta\xi_{r+1}$$



L: longitudinal acoustic wave

T_1, T_2: transverse acoustic waves

T_1=T_2 for isotropic crystal structure

long λ longitudinal wave ≡ sound waves

Q: Why are the frequencies for L greater than T?

Longitudinal waves in a 1-D infinite lattice

- Long wavelength longitudinal wave ≡ sound waves
- Velocity is given by the slope at k=0

$$v_{longitudinal} = \frac{\omega}{k}\bigg]_{k\sim 0} = (\eta')^{1/2}a$$

$$v_{transverse} = \frac{\omega}{k}\bigg]_{k\sim 0} = (\eta)^{1/2}a$$

$$\eta' = \frac{1}{m}\frac{dF}{d\xi}\bigg|_a , \quad \eta = \frac{F}{ma} , \quad F \propto r^{-n} \quad \Rightarrow \quad \eta' = n\eta$$

$$v_{longitudinal} = (n\eta)^{\frac{1}{2}}a = (n)^{\frac{1}{2}}v_{transverse}$$

➡ The longitudinal waves are $(n)^{\frac{1}{2}}$ times faster than transverse waves.

Density of states for lattice waves

- Density of states: # of allowed vibrational modes, $N(\nu)$, per unit frequency interval, $d\nu$.

$$\nu = \nu_{\max} \sin\left[\frac{m\pi}{2(n+1)}\right] \qquad \text{From } \omega = 2\eta^{1/2} \sin\left(\frac{m\pi}{2(n+1)}\right)$$

$$\Delta\nu = \frac{d\nu}{dm} = \frac{\pi}{2(n+1)} \nu_{\max} \cos\left[\frac{m\pi}{2(n+1)}\right] \qquad \text{cf) } \cos\theta = (1 - \sin^2\theta)^{\frac{1}{2}}$$

$$\Delta\nu = \frac{\pi\nu_{\max}}{2(n+1)}\left[1 - \left(\frac{\nu}{\nu_{\max}}\right)^2\right]^{1/2} \quad : \text{ frequency spacing between allowed modes}$$

In a frequency interval dν, there are dν/Δν states. Therefore,

$$N(\nu)d\nu \cong \frac{2(n+1)}{\pi\nu_{\max}}\left[1 - \left(\frac{\nu}{\nu_{\max}}\right)^2\right]^{-1/2} d\nu$$

$N(\nu)$ starts with a value of $[2(n+1)/\pi\nu_{max}]$ at $\nu=0$ and then increases with increasing ν to a large value as ν approaches ν_{max}.

Lattice waves for two kinds of atoms

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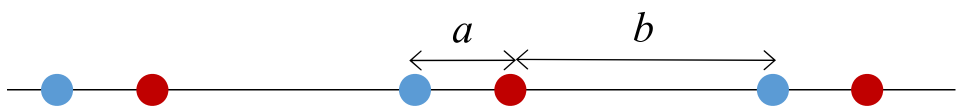
  ① Lattice parameter is the same (a)
  ② Masses are different (m and M)

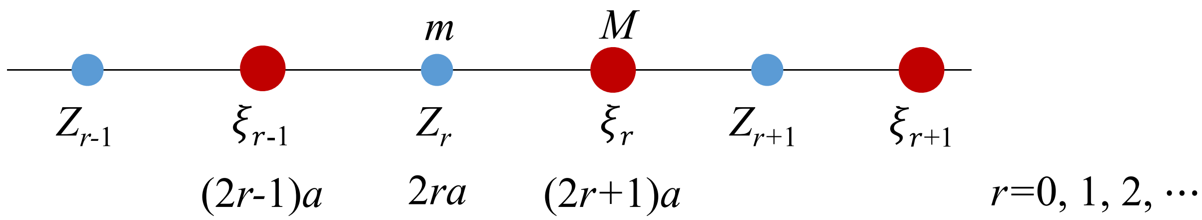
  ex) compound

- 

  ① Lattice parameters are different (a and b)
  ② Mass is the same (m)

  ex) more atoms in a unit cell

The first case (different masses & same spacing)



- Follow the same procedure of transverse wave except that near atoms are different kinds.

$$\text{I}.\ \frac{d^2\xi_r}{dt^2} = \eta_M Z_r - 2\eta_M \xi_r + \eta_M Z_{r+1} \qquad \text{where } \eta_M = \frac{F}{Ma}$$

$$\text{II}.\ \frac{d^2 Z_r}{dt^2} = \eta_m \xi_r - 2\eta_m Z_r + \eta_m \xi_{r-1} \qquad \text{where } \eta_m = \frac{F}{ma}$$

- Assume that harmonic waves with the same values of k and ω for both types of atoms

$$\xi_r = Ae^{i(kx-\omega t)} \qquad \text{for } x = (2r+1)a$$

$$Z_r = Be^{i(kx-\omega t)} \qquad \text{for } x = 2ra$$

The first case (different masses & same spacing)

$$\xi_r = Ae^{i(k(2r+1)a-\omega t)} = e^{ika}Ae^{i(k2ra-\omega t)} \quad \text{for } x = (2r+1)a$$

$$Z_r = Be^{i(k2ra-\omega t)} \quad \text{for } x = 2ra$$

$$\Rightarrow \quad \xi_r = \left(\frac{A}{B}\right)e^{ika}Z_r$$

$$\begin{cases} \dfrac{d^2\xi_r}{dt^2} = \eta_M Z_r - 2\eta_M\xi_r + \eta_M Z_{r+1} \\ \dfrac{d^2 Z_r}{dt^2} = \eta_m\xi_r - 2\eta_m Z_r + \eta_m\xi_{r-1} \end{cases}$$

$$\begin{cases} -\omega^2 e^{ika}A + 2\eta_M e^{ika}A - \eta_M B - \eta_M e^{2ika}B = 0 \\ -\omega^2 A + 2\eta_M A - \eta_M e^{-ika}B - \eta_M e^{ika}B = 0 \end{cases}$$

$$\frac{A}{B} = -\frac{2\eta_M \cos k\,a}{\omega^2 - 2\eta_M}$$

$$\begin{cases} (\omega^2 - 2\eta_M)A + 2\eta_M B\cos ka = 0 \\ 2\eta_m A\cos ka + (\omega^2 - 2\eta_m)B = 0 \end{cases} \quad \Rightarrow \quad \begin{vmatrix} \omega^2 - 2\eta_M & 2\eta_M\cos ka \\ 2\eta_m\cos ka & \omega^2 - 2\eta_m \end{vmatrix} = 0$$

$$\omega^4 - (2\eta_M + 2\eta_m)\omega^2 + 4\eta_M\eta_m - 4\eta_M\eta_m\cos^2 ka = 0$$

$$\omega^4 - 2(\eta_M + \eta_m)\omega^2 + 4\eta_M\eta_m\sin^2 ka = 0$$

$$\omega_\pm^2 = (\eta_M + \eta_m) \pm \sqrt{(\eta_M + \eta_m)^2 - 4\eta_M\eta_m\sin^2 k\,a} \quad \text{(dispersion relations)}$$

±: two separate branches in the vibration spectrum

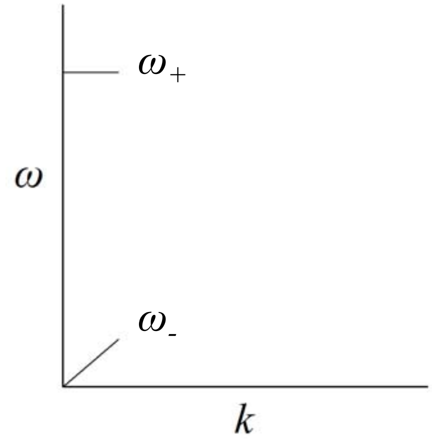
The first case (different masses & same spacing)

1) For $k = 0$

From previous solution,

$$\omega_{\pm}^2 = (\eta_M + \eta_m) \pm (\eta_M + \eta_m) \times \left(1 - \underbrace{\frac{4\eta_M \eta_m k^2 a^2}{(\eta_M + \eta_m)^2}}_{<<1}\right)^{1/2}$$

$(\because\ (1-x)^{1/2} = 1 - x/2$ for $x<<1)$



a) $$\omega_-^2 = (\eta_M + \eta_m) - (\eta_M + \eta_m) \times \left(1 - \frac{2\eta_M \eta_m k^2 a^2}{(\eta_M + \eta_m)^2}\right)$$

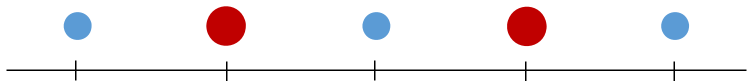
$$= (\eta_M + \eta_m) - (\eta_M + \eta_m) + \frac{2\eta_M \eta_m k^2 a^2}{(\eta_M + \eta_m)}$$

$$= \frac{2\eta_M \eta_m k^2 a^2}{(\eta_M + \eta_m)}$$

$\because\ \cos ka = 1$ and $\omega = 0$ at $k = 0$

$$\frac{A}{B} = -\frac{2\eta_M \cos k\, a}{\omega^2 - 2\eta_M} = \frac{2\eta_M}{2\eta_M} = 1$$

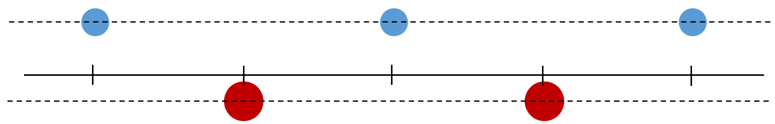
:Equal displacement of neighboring atoms



< acoustic mode >

b) $$\omega_+^2 = 2(\eta_M + \eta_m)$$

$$\frac{A}{B} = -\frac{\eta_M}{\eta_m}$$:Opposite displacement



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: In the long wavelength mode(k=0), neighboring atoms are displaced in opposite directions.

The first case (different masses & same spacing)

2) Near $k = \pi / 2a$, $\sin^2 ka \rightarrow 1$

$$\omega^2 = (\eta_M + \eta_m) \pm \sqrt{(\eta_M + \eta_m)^2 - 4\eta_M\eta_m \sin^2 k\,a}$$
$$= (\eta_M + \eta_m) \pm \sqrt{(\eta_M + \eta_m)^2 - 4\eta_M\eta_m}$$
$$= (\eta_M + \eta_m) \pm (\eta_m - \eta_M)$$

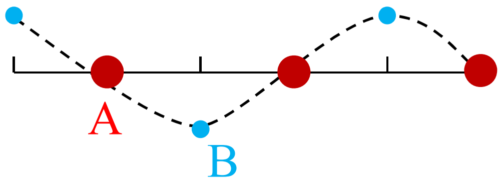
$$\frac{A}{B} = -\frac{2\eta_M \cos k\,a}{\omega^2 - 2\eta_M}$$

Large mass

Small mass

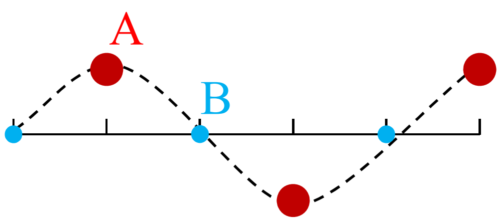
① $\omega_+{}^2 = 2\eta_m$

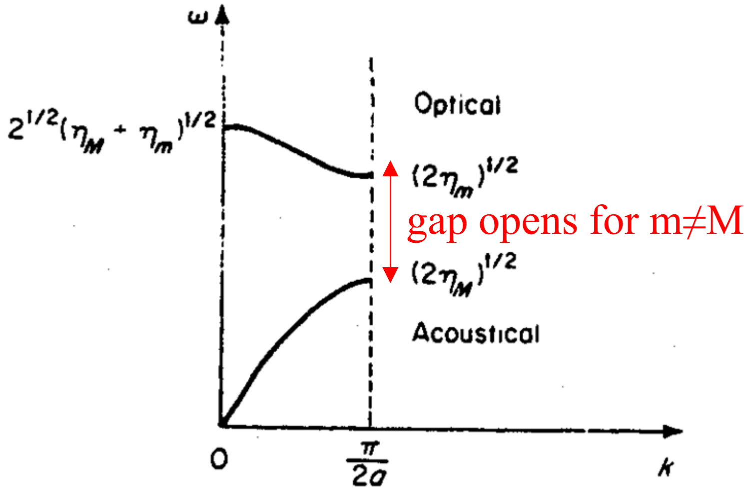
$\dfrac{A}{B} = 0$



② $\omega_-{}^2 = 2\eta_M$

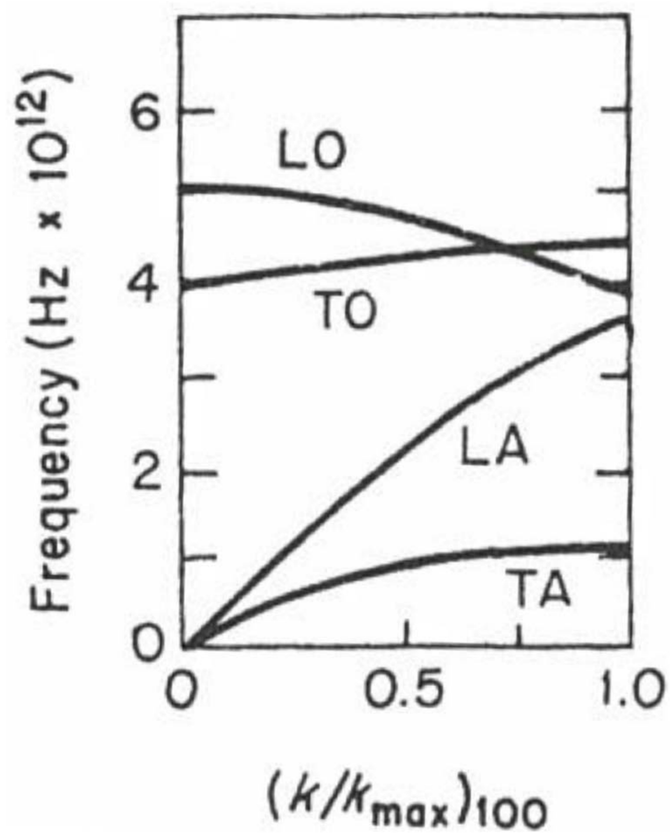
$\dfrac{A}{B} = \infty$





$k = 0$	$k = \pi / 2a$
$\omega_+^2 = 2(\eta_M + \eta_m)$	$\omega_+{}^2 = 2\eta_m$
$\omega_-^2 = \dfrac{2\eta_M\eta_m k^2 a^2}{(\eta_M + \eta_m)}$	$\omega_-{}^2 = 2\eta_M$

Vibration spectrum pf CdTe



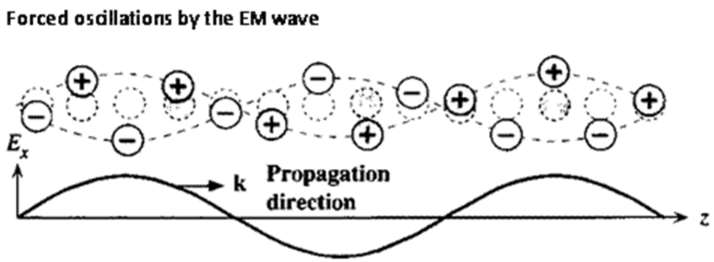
LO: Longitudinal optical vibration
TO: Transverse optical vibration

LA: Longitudinal acoustic vibration
TA: Transverse acoustic vibration

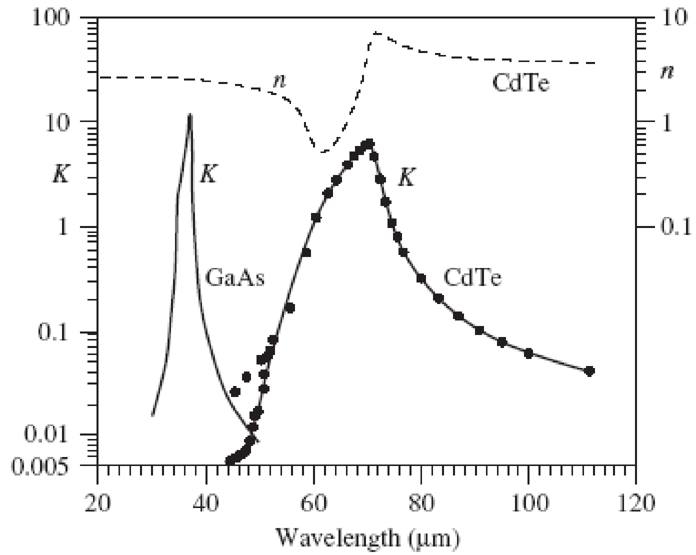
Reststrahlen absorption

: (German: residual rays)

- long wavelength transverse modes in partially ionic crystals could be directly excited by light of a suitable.
- Strong interaction between a light wave and a lattice wave under the unusual conditions for resonance.



extinction coefficient K versus wavelength



An EM wave that propagates the lattice displaces the oppositely charged ions in opposite directions and forces them to vibrate at the frequency of the wave. Most of the energy is then absorbed from the EM wave and converted to lattice vibrational energy (heat).