

Lecture 2.3

Last time, found the dispersion relation $\omega(k)$ for a diatomic 1D lattice:

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

This has two allowed frequencies for each wavenumber, corresponding to different types of wave.

The **Optical Branch** is so named because modes can be excited by **light** with an appropriate frequency in solids which are (at least partly) **ionic**. If there is a difference in charge associated with each type of atom, then an electric field can couple to a wave in which neighbouring atoms are moving in opposite directions: the optical branch.

How much do atoms move? This is straightforward in the long-wavelength limit i.e. $k \rightarrow 0$.

Starting with

$$\begin{aligned} A [2\mu - m\omega^2] &= 2\mu B \cos(ka/2) \\ B [2\mu - M\omega^2] &= 2\mu A \cos(ka/2) \end{aligned}$$

and letting $k \rightarrow 0$, we find

$$\frac{B}{A} = \frac{2\mu - m\omega^2}{2\mu} = \frac{2\mu}{2\mu - M\omega^2}$$

and

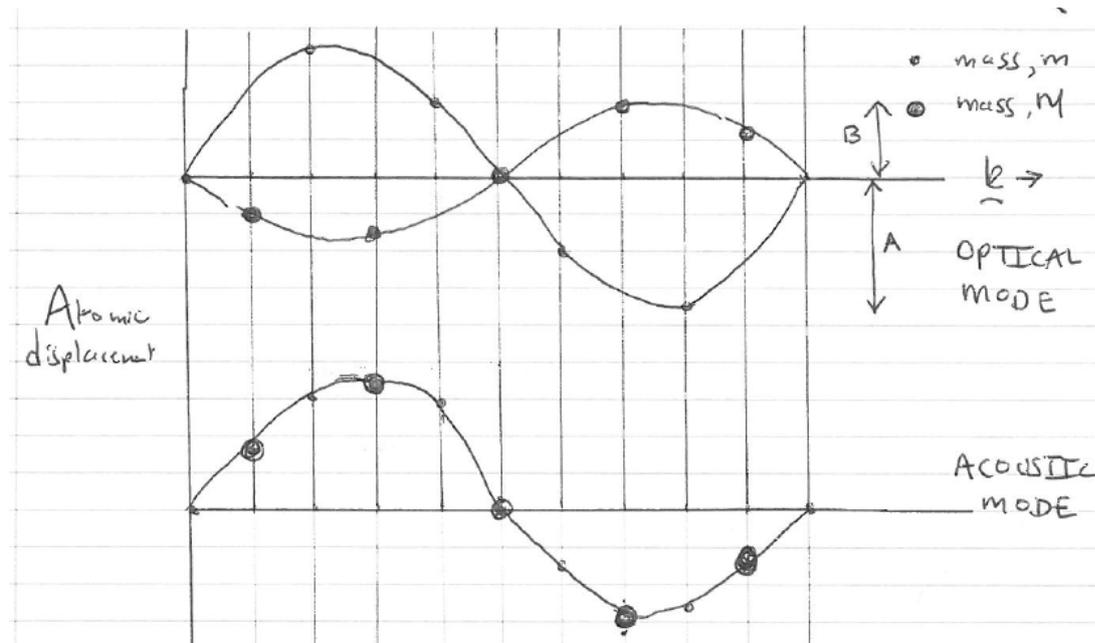
$$\omega = \omega_3 = \sqrt{2\mu \left(\frac{1}{m} + \frac{1}{M} \right)}$$

so we have

$$\frac{B}{A} = -\frac{m}{M}$$

valid at long wavelength. Thus, the heavy and light atoms move out of phase such that the centre of mass for neighbours does not move.

We have derive this for **longitudinal vibrations**, but all we really did was make the approximation that restoring force was linear with displacement. The treatment applies to **transverse vibrations** also.



(See also the Mathematica sheet.)

Infrared light

Let's take a (non-rigorous) look at the propagation of infra-red electromagnetic radiation through our idealised lattice.

Let $k = 0$ with $u = u_0 e^{-i\omega t}$ and $v = v_0 e^{-i\omega t}$.

Starting with the equations of motion for the atoms of different mass, and imagining them to also have *opposite charge* (i.e. a polar crystal) then we can write

$$-m\omega^2 u = 2\mu(v - u) + qE \quad (11)$$

$$-M\omega^2 v = 2\mu(u - v) - qE \quad (12)$$

with $u_{r+1} = u_{r-1}$ and $v_{r+1} = v_{r-1}$.

Substitute in for u, v from above

$$-m\omega^2 u_0 = 2\mu(v_0 - u_0) + qE \quad (13)$$

$$-M\omega^2 v_0 = 2\mu(u_0 - v_0) - qE \quad (14)$$

And it can be shown, after a little algebra (see Mathematica sheet 1d-diatomic-infrared.nb), that

$$u_0 = \frac{qE/m}{\omega_T^2 - \omega^2} \quad \text{and} \quad v_0 = -\frac{u_0 m}{M} \quad (15)$$

where

$$\omega_T = \sqrt{\frac{2\mu}{m^*}}$$

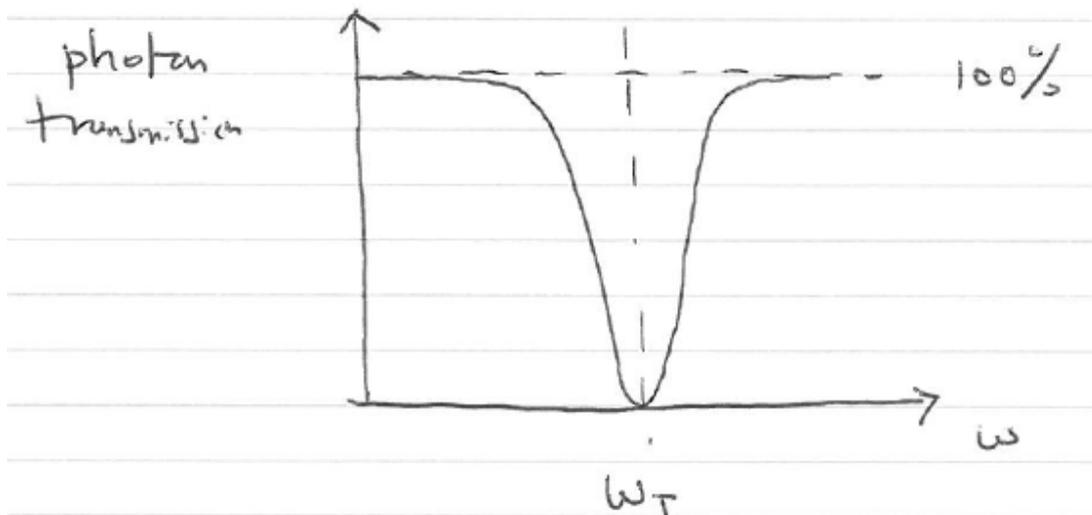
and

$$m^* = \frac{mM}{m + M}$$

is the reduced mass.

ω_T is called the "Reststrahlen" frequency.

At $\omega = \omega_T$, $u_0 \rightarrow \infty$, $v_0 \rightarrow \infty$ and we get strong absorption of light. (Of course, there is some *dissipation* which damps the oscillations, and keeps u_0 and v_0 finite.)



This can be thought of as the *generation of a phonon* of energy $\hbar\omega_T$ by a photon.

This leads us to think of the quantum nature of phonons.

We need this approach when looking at the Thermal Properties of the lattice, since it is possible to excite phonons, in general, with thermal energy. This suggests that phonons will make a contribution to the crystal/lattice specific heat capacity.

Look ahead. . .

- Phonons are *quantized*
- They obey quantum statistics: Bosons or Fermions
- Phonons can be excited by *heat*
- Therefore, phonons contribute to **specific heat capacity**
- We can build simple models and see whether they agree with experiment
 - Equipartition
 - * Fully classical
 - * Doesn't work at low temperature
 - Einstein model
 - * Bose statistics
 - * Considers only single phonon energy
 - * Sort of works. . .
 - Debye model
 - * Bose statistics still
 - * Considers range of phonon energies
 - * Works really well!
 - * (As simple as possible, and no simpler)

Problem Sheet 1 - Hints

- 1. Lattices and vectors
 1. Try moving integer multiples of the given vectors; does the lattice look the same when you do?
- 2. Lattice vectors and primitive cells
 1. Volume of the primitive unit cell is the volume associated with one lattice point
 - The volume associated with n lattice points is a^3
 - For cubic crystals, can often work out volume of primitive *without* brute-force cross-product calculation
 2. Go through mechanically and find lattice vectors for FCC.
 3. Don't need to prove these are lattice vectors for FCC; just identify from bookwork.
 4. $4\pi/a$ refers to the length of the conventional unit cell
 - Note the factor of a half: $(a/2)(0, 1, 1) = a(0, 1/2, 1/2)$ is a lattice vector for an FCC with conventional (cubic) cell of side a
- 3. X-ray powder diffraction
 1. (Our use of the) Geometric structure factor means we're describing some cubic crystal (SC, FCC, BCC, . . .) using **conventional** SC lattice vectors
 2. Hence, the **reciprocal** lattice vectors are also SC
 3. The GSF arises from interference between the > 1 points in the conventional unit cell.
- 4. Hexagonal lattice
 1. Use general cross-product form for \mathbf{b}_i .
 2. To find the angle between two vectors, use $\mathbf{u} \cdot \mathbf{v} = uv \cos \theta$.