LATTICE VIBRATIONS

Lecture 8

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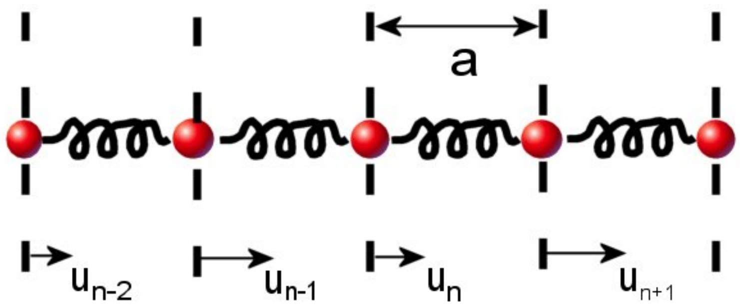
4 Dynamics of Crystals

- **Even in their ground states, the atoms have some kinetic energy (zero-point motion)**
- **Changes in temperature change the occupancy of the energy levels – heat capacity**
- **Motion affects the entropy, and hence the free energy – can affect the equilibrium structure**
- **Atomic motion affects the strength of diffraction patterns**
- **Vibrational energy can move through the structure**
  - **– sound waves**
  - **– heat transport**
- **Atoms away from regular sites alter the way electrons move through solids – electrical resistance**

4.1 Chains of Atoms

We shall start by assuming that every atom's interactions with its neighbours may be represented by a spring, so that the force in each 'spring' is proportional to the change in length of the spring.
This is called the *harmonic approximation*. We'll talk about it more later. Also assume that only forces between nearest neighbours are significant

4.1.1 Longitudinal Waves on Linear Chain



Atom n should be at a position na, but is displaced by an amount u_n. The 'unstretched string' corresponds to an interatomic spacing a. So

the force on atom n is

$$F_n = \alpha(u_{n+1} - u_n) - \alpha(u_n - u_{n-1}),$$

where α is the spring constant. Thus the equation of motion is

$$m\ddot{u}_n = \alpha(u_{n+1} + u_{n-1} - 2u_n),$$

for atoms of mass m. Now look for wave-like solutions,

$$u_n(t) = A\exp(ikna - i\omega t),$$

and substitute to find

$$\begin{aligned} -m\omega^2 &= \alpha\left(e^{ika} + e^{-ika} - 2\right) \\ \omega^2 &= \frac{\alpha}{m}(2 - 2\cos(ka)) \\ &= \frac{4\alpha}{m}\sin^2(ka/2). \end{aligned}$$

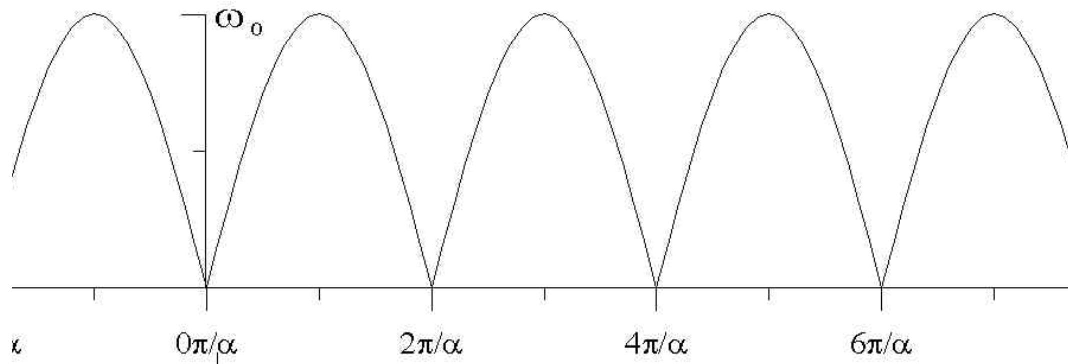
This gives us the *dispersion relation*

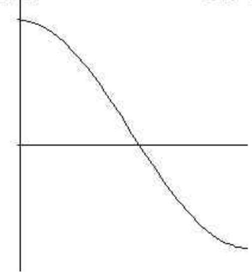
$$\omega = \omega_0\left|\sin\left(\frac{ka}{2}\right)\right|,$$

with a maximum cut-off frequency

$$\omega_0 = \sqrt{\frac{4\alpha}{m}}.$$

Dispersion relation in extended zone





Group Velocity

Group velocity $v_g = \frac{\omega_0 a}{2}\cos\left(\frac{ka}{2}\right)$ ***Limit of long wavelength,*** $k \to 0$**,**

$$\omega \to \frac{\omega_0 ka}{2},$$

and so in this limit

$$v_p = v_g = \frac{\omega_0 a}{2}.$$

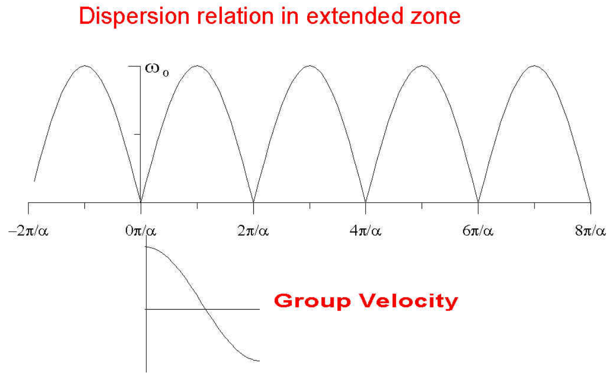
This is the normal sound velocity. Knowing $v_p \approx 10^3$ m s^{-1} and $a \approx 10^{-10}$ m, we find

$$\omega_0 \approx 10^{13}\ \mathrm{rad\ s}^{-1},$$

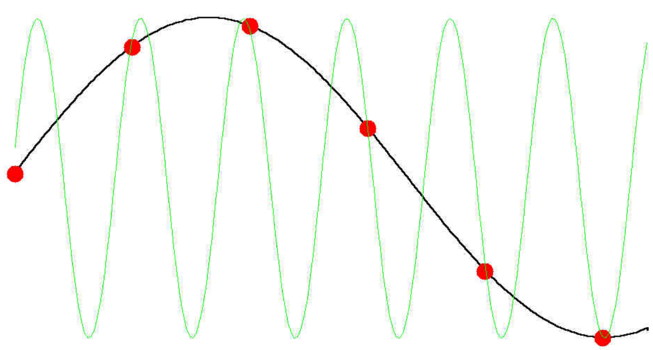
so that maximum frequencies of lattice vibrations are THz (10^{12} Hz). In the infrared range.

4.1.2 The Brillouin Zone

The dispersion is periodic in k. The frequency at k is the same as at $k + 2\pi/a$.

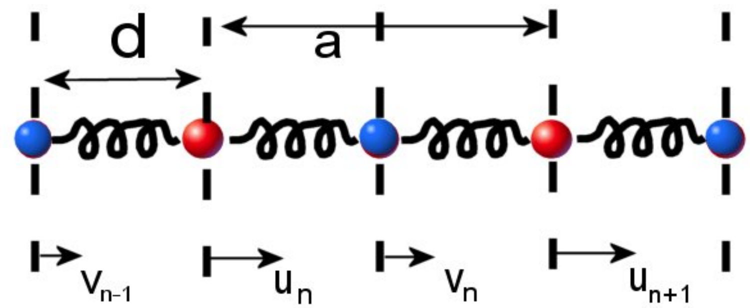


We only sample the wave at the atomic positions, so we cannot tell the waves k and $k + 2\pi/a$ apart.



Conventionally, we only consider the wavevectors between $-\pi/a$ and π/a. This region corresponds to a *unit cell in reciprocal space*. Symmetrical treatment of waves travelling to right or left. Just as the physics is determined by the contents of a unit cell in real space, it is also determined by the behaviour of a unit cell in reciprocal space.

4.1.3 More than one atom per cell



Assume atoms of mass m are at u_n, atoms of mass M at v_n. Let the atoms be d apart, with the unit cell side still a. If the force constant is

again α we get coupled equations:

$$m\ddot{u}_n = \alpha(v_n + v_{n-1} - 2u_n)$$
$$M\ddot{v}_n = \alpha(u_n + u_{n+1} - 2v_n).$$

Again look for travelling waves,

$$u_n(t) = A\exp(ikna - i\omega t) \qquad v_n(t) = B\exp(ik(na+d) - i\omega t).$$

Substitute, and for simplicity take $a = 2d$,

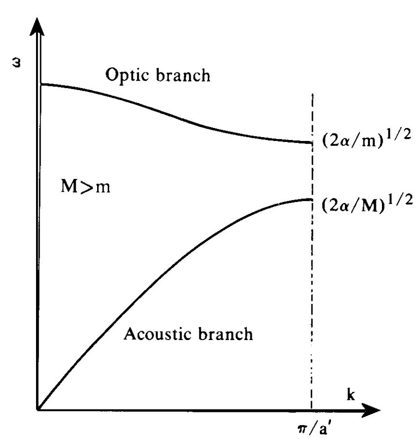
$$m\omega^2 A = 2\alpha(A - B\cos(kd))$$
$$M\omega^2 B = 2\alpha(B - A\cos(kd)).$$

This is a pair of linear homogeneous equations in A and B, which only has a non-trivial solution if the determinant of the coefficients is zero, that is

$$\begin{vmatrix} 2\alpha - m\omega^2 & -2\alpha\cos(kd) \\ -2\alpha\cos(kd) & 2\alpha - M\omega^2 \end{vmatrix} = 0,$$

which has solutions

$$\omega^2 = \alpha\left(\frac{1}{m} + \frac{1}{M}\right) \pm \alpha\sqrt{\left(\frac{1}{m} + \frac{1}{M}\right)^2 - \frac{4\sin^2(kd)}{mM}}.$$



Summary

- **Lattice vibrations - linear chain**
- **Periodic nature of dispersion curve**
- **Unit cell in k-space (Brillouin zone)**
- **Lattice vibrations in non-monatomic systems**

Next:

- **Phonons**
- **Thermal energy**