

1. The dispersion relation for the lattice vibrations of a one dimensional chain of identical atoms of mass M , where each atom is connected to its nearest neighbour by a spring constants K is

$$M\omega^2 = 2K [1 - \cos(ka)] ,$$

with displacements at each atom n given by

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

By sketching $\text{Re } u_n$ show that $k = 2\pi/\lambda$ with λ the wavelength of the wave. Let $M\omega^2 = K$. What is k ? Sketch such a wave for $n = 1, 2, \dots, 5$ at times $t = 0, \pi/(2\omega), \pi/\omega$.

2. Show that the dispersion relation for the lattice vibrations of a one dimensional chain of identical atoms of mass M , where each atom is connected to its nearest and next-nearest neighbour by spring constants K_1 and K_2 is

$$M\omega^2 = 2K_1 [1 - \cos(ka)] + 2K_2 [1 - \cos(2ka)] .$$

Show that

- (a) This dispersion relation reduces to the relation for sound waves when the wavelength λ is large enough. What is the velocity of the sound waves?
- (b) The group velocity, $v_g = \partial\omega/\partial k$, vanishes at $k = \pm\pi/a$.
- (c) ω is periodic in k with period $2\pi/a$.

Which of (a-c) would hold if we add longer range connections and why?

3. **To be handed in.** Obtain expressions for the heat capacity due to longitudinal vibrations of a chain of identical atoms:
- (a) in the Debye approximation;
 - (b) using the exact density of states.

Which gives the higher heat capacity? Show that for low temperatures they give the same value. Why should this be the case?

4. A polyethylene chain can be modelled as a series of bonds of alternating strengths given by spring constants K_1 and K_2 , with atoms of identical masses M . Show that the characteristic frequencies are given by

$$\omega^2 = \frac{K_1 + K_2}{M} \left[1 \pm \sqrt{1 - \frac{4K_1K_2 \sin^2\left(\frac{1}{2}ka\right)}{(K_1 + K_2)^2}} \right] .$$

Sketch the optical and acoustic branches of the dispersion curves. *Hint: Consider the limits $k \rightarrow 0$ and $k \rightarrow \pm\pi/a$.*

5. Starting from the average energy of a quantum harmonic oscillator at a temperature T , calculate an explicit form of the average energy and find the heat capacity. The average energy can be written as the sum of two terms, what are their physical interpretations? Sketch the average energy and heat capacity as functions of temperature.