

Consider a linear chain of N atoms, each with mass M . The atoms are arranged on a lattice with spacing d . The total length of the chain is $L = Nd$. The atoms are coupled to each other by elastic forces with spring constant K which couple only nearest neighbor atoms. The normal modes of this chain, with periodic boundary conditions, are labelled by a wave vector k in the range $|k| \leq \pi/d$ with spacing $\Delta k = 2\pi/Nd$. The normal modes of this chain are acoustic waves. To simplify the analysis we will use the following approximate frequencies:

$$\omega(k) = v_s |k|, \quad v_s = d \sqrt{\frac{K}{M}}$$

where v_s is the speed of sound in this chain. In Quantum Mechanics this system is described by a set of quanta, acoustic phonons of energy $E(k) = \hbar v_s |k|$. The total energy of a state $|\{n(k)\}\rangle$, with $n(k) = 0, \dots, \infty$ acoustic phonons, in the thermodynamic limit is

$$E[n] = Nd \int_{-\pi/d}^{\pi/d} \frac{dk}{2\pi} \hbar \omega(k) \left(n(k) + \frac{1}{2} \right)$$

- Use the methods of Statistical Mechanics to derive a formula for the internal energy of this linear chain, $U = \langle E \rangle$ at temperature T . Express your results in the form of integrals over the wave vector k . Find an expression for U in terms of this integral written in terms of a dimensionless variable, and of the physical parameters of the problem, and of the Debye temperature, defined by $k_B \theta_D = \pi \hbar v_s / d$. **(Do not compute the ground state energy!)**
- Consider the *classical limit* for this system. Use the classical Equipartition Theorem to compute the heat capacity of a linear chain. For what range of temperatures do you expect this result to apply?
- Derive a formula for the heat capacity C of this chain, at constant length.
- Use the result derived in (c) to calculate the heat capacity in the *high temperature* regime. Explain in physical terms the temperature dependence.
- Use the result derived in (c) to calculate the temperature dependence of the heat capacity at *low temperatures*. Using a dimensional argument, justify the power law with which T enters your answer. (Hint: it might be helpful to recall your answer to part a).

Useful integrals:

$$\int_0^{\infty} dx \frac{x}{e^x - 1} = - \int_0^{\infty} dx \ln(1 - e^{-x}) = \frac{\pi^2}{6}$$

$$\int_0^{\infty} dx x^2 \frac{e^x}{(e^x - 1)^2} = \frac{\pi^2}{3}$$