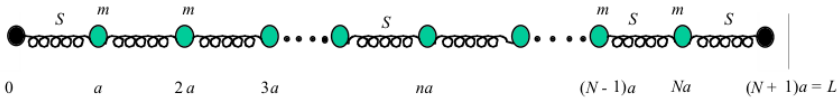
Theoretical Question 1 (vibrations of a linear crystal lattice)

A very large number N of movable identical point particles ($N >> 1$), each with mass m, are set in a straight chain with $N + 1$ identical massless springs, each with stiffness (spring constant) S, linking them to each other and the ends attached to two additional immovable particles. See figure. This chain will serve as a model of the vibration modes of a one-dimensional crystal. When the chain is set in motion, the longitudinal vibrations of the chain can be looked upon as a superposition of simple oscillations (called modes) each with its own characteristic mode frequency.



(a) Write down the equation of motion of the n^{th} particle. [0.7 marks]

(b) To attempt to solve the equation of motion of part (a) use the trial solution

$$X_n(\omega) = A \sin nka \cos(\omega t + \alpha),$$

where $X_n(\omega)$ is the displacement of the n^{th} particle from equilibrium, ω the angular frequency of the vibration mode and A, k and α are constants; k and ω are the wave numbers and mode frequencies respectively. For each k, there will be a corresponding frequency ω. Find the dependence of ω on k, the allowed values of k, and the maximum value of ω. The chain's vibration is thus a superposition of all these vibration modes. Useful formulas:

$$\frac{\mathrm{d}}{\mathrm{d}x}\cos \alpha x = -\alpha \sin \alpha x, \qquad \frac{\mathrm{d}}{\mathrm{d}x}\sin \alpha x = \alpha \cos \alpha x, \qquad \alpha = \text{constant}.$$

$$\sin(A + B) = \sin A \cos B + \cos A \sin B, \qquad \cos(A + B) = \cos A \cos B - \sin A \sin B$$

[2.2 marks]

According to Planck the energy of a photon with a frequency of ω is $\hbar\omega$, where $\hbar$ is the Planck constant divided by 2π. Einstein made a leap from this by assuming that a given crystal vibration mode with frequency ω also has this energy. Note that a vibration mode is not a particle, but a simple oscillation configuration of the entire chain. This vibration mode is analogous to the photon and is called a *phonon*. We will follow up the consequences of this idea in the rest of the problem. Suppose a crystal is made up of a very large ($\sim 10^{23}$) number of particles in a straight chain.

(c) For a given allowed ω (or k) there may be no phonons; or there may be one; or two; or any number of phonons. Hence it makes sense to try to calculate the *average energy* $\langle E(\omega)\rangle$ of a *particular* mode with a frequency ω. Let $P_p(\omega)$ represent the probability that there are p phonons with this frequency ω. Then the required average is

$$\langle E(\omega)\rangle = \frac{\sum_{p=0}^{\infty} p\hbar\omega\, P_p(\omega)}{\sum_{p=0}^{\infty} P_p(\omega)}.$$

Although the phonons are discrete, the fact that there are so many of them (and the P_p becomes tiny for large p) allows us to extend the sum to $p = \infty$, with negligible error. Now the probability P_p is given by Boltzmann's formula

$$P_p(\omega) \propto \exp(-p\hbar\omega/k_{\mathrm{B}}T),$$

where k_{B} is Boltzmann's constant and T is the absolute temperature of the crystal, assumed constant. The constant of proportionality does not depend on p. Calculate the average energy for phonons of frequency ω. Possibly useful formula: $(\mathrm{d}/\mathrm{d}x)\, e^{f(x)} = (\mathrm{d}f/\mathrm{d}x)\, e^{f(x)}$. [2 marks]

(d) We would like next to compute the *total* energy E_{T} of the crystal. In part (c) we found the average energy $\langle E(\omega)\rangle$ for the vibration mode ω. To find E_{T} we must

multiply $\langle E(\omega)\rangle$ by the number of modes of the crystal per unit of frequency ω and then sum up all these for the entire range from $\omega = 0$ to $\omega_{\max}$. Take an interval Δk in the range of wave numbers. For very large N and for Δk much larger than the spacing between successive (allowed) k values, how many modes can be found in the interval Δk? [1 mark]

(e) To make use of the results of (a) and (b), approximate Δk by $(\mathrm{d}k/\mathrm{d}\omega)\,\mathrm{d}\omega$ and replace any sum by an integral over ω. (It is more convenient to use the variable ω in place of k at this point.) State the total number of modes of the crystal in this approximation. Also derive an expression E_{T} but do not evaluate it. The following integral may be useful: $\int_0^1 dx\,/\sqrt{1-x^2} = \pi/2$. [2.2 marks]

(f) The molar heat capacity C_V of a crystal at constant volume is experimentally accessible: $C_V = \mathrm{d}E_{\mathrm{T}}/\mathrm{d}T$ (T = absolute temperature). For the crystal under discussion determine the dependence of C_V on T for very large and very low temperatures (i.e., is it constant, linear or power dependent for an interval of the temperature?). Sketch a qualitative graph of C_V versus T, indicating the trends predicted for very low and very high T. [1.9 marks]