Statistical Physics: Tutorial 6

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Oscillators and phonons

A: Core problems

1. **Einstein oscillator model**

   Given that the energy of a single 1D harmonic oscillator is $E = (n + 1/2)\hbar\omega$, calculate its mean energy in thermal equilibrium via the partition function. A set of N atoms is modelled as each independently inhabiting a spherically symmetric potential $V \propto r^2$; explain why this is equivalent to 3N 1D oscillators.

2. **Debye cutoff frequency**

   In the Debye model, atomic dynamics is modelled as elastic waves in a uniform solid of volume V. Show that the density of modes in terms of angular frequency is

   $$g(\omega) = \frac{3V\omega^2}{2\pi^2 c_s^3},$$

   where c_s is the speed of sound. Since there can be only $3N$ modes in total, what is the maximum frequency if we assume an isotropic cutoff to the frequency spectrum? If the solid is actually in the form of a cubic lattice, the maximum frequency will now depend on direction. What is the maximum frequency in this case, and what is the corresponding direction of wave propagation?

3. **Debye model with a different density of states**

   Consider a 3D solid consisting of N atoms where the density of modes is

   $$g(\omega) = b\omega^4,$$

   where b is a constant. The frequencies range from zero to some cut-off ω_{max}. Find an expression for ω_{max}. Use ω_{max} to define a characteristic temperature and identify high T and low T regimes.

   Calculate the total energy $\overline{E}$ and the heat capacity in the low and high temperature limits, which you should define. Express your results purely in terms of N, h, k, T and b (and a dimensionless integral where required).

B: Further problems

1. **High temperature limit and corrections to Debye model**

   First think about the density of states for a particle in a box in d dimensions and show that it should behave as $g(\omega) \propto \omega^{d-1}$.

   (a) Using this form of the density of states for the Debye model of phonons in a d-dimensional isotropic solid containing N atoms, show that

   $$\overline{E} = \frac{Nd^2\hbar\omega_D}{\alpha^{(1+d)}} f(\alpha)$$

where $\alpha = \dfrac{\hbar\omega_D}{kT}$ and

$$f(\alpha) = \int_0^\alpha \mathrm{d}x \frac{x^d}{\mathrm{e}^x - 1} \, .$$

(b) In the high temperature limit $kT \gg \hbar\omega_D$ calculate the leading behaviour of C_V and the first correction to this behaviour.

2. **Perturbation theory for interacting oscillators**

   A system of two oscillators with frequencies ω_i interact in such a way that (neglecting zero-point energies) the energy of the whole system is given by

$$E = \epsilon_1 n_1 + \epsilon_2 n_2 + \lambda n_1 n_2,$$

   where $\epsilon_i = \hbar\omega_i$ and λ is a small perturbation.

   Show that the canonical partition function to order λ is given by

$$Z_C(\lambda) = Z_C(0)\left[1 - \lambda\beta \frac{\exp[-\beta\epsilon_1]}{1 - \exp[-\beta\epsilon_1]} \frac{\exp[-\beta\epsilon_2]}{1 - \exp[-\beta\epsilon_2]}\right] \, .$$

3. **Renormalisation of energy levels**

   Show that the result of the previous problem is equivalent to a system of non-interacting oscillators with effective temperature-dependent energy-level spacings $\epsilon_i + \epsilon_i^{(1)}(T)$, where

$$\epsilon_1^{(1)}(T) = (\lambda/2)\, \frac{e^{-\beta\epsilon_2}}{1 - e^{-\beta\epsilon_2}}$$

   and vice-versa.