STATISTICAL PHYSICS 06/07

Phonons; Virial Expansion **Tutorial Sheet 4**

The questions that follow on this and succeeding sheets are an integral part of this course. The code beside each question has the following significance:

- **K**: key question – explores core material
- **R**: review question – an invitation to consolidate
- **C**: challenge question – going beyond the basic framework of the course
- **S**: standard question – general fitness training!

4.1 **Debye Model with a different density of states [S]**

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 $\omega_{\max}$.

Find an expression for $\omega_{\max}$.

Use $\omega_{\max}$ 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).

4.2 **Perturbation Theory for Interacting Oscillators [S]**

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

$$E = \sum_{i=1}^{N} \epsilon_i n_i + \frac{\lambda}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} A_{ij}\, n_i n_j,$$

where $\epsilon_i = \hbar\omega_i,\ A_{ij} = A_{ji},\ A_{ii} = 0,\ n_i = 0,\ 1, ...\infty$ is the occupation number for the i^{th} oscillator and λ is a small parameter.

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

$$Z_C(\lambda) = Z_C(0) \left[1 - \frac{\lambda\beta}{2} \sum_{ij=1}^{N} A_{ij} \frac{\exp -\beta\epsilon_i}{1 - \exp -\beta\epsilon_i} \, \frac{\exp -\beta\epsilon_j}{1 - \exp -\beta\epsilon_j} \right]$$

4.3 **Renormalisation of energy levels [C]**

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

$$\epsilon_i^{(1)}(T) = \frac{1}{2} \sum_{j=1}^{N} A_{ij} \, \frac{e^{-\beta\epsilon_j}}{1 - e^{-\beta\epsilon_j}} \, .$$

4.4 Second Virial Coefficient [S]

Show that for a spherically symmetric potential $\phi(r)$, the expression for the second virial coefficient may be written as

$$B_2 = 2\pi \int r^2 \left[1 - e^{-\phi(r)/kT}\right] dr\,.$$

If a gas of interacting particles is modelled as hard spheres of radius $a/2$, show that the second virial coefficient takes the form:

$$B_2 = \frac{2\pi a^3}{3}\,.$$

4.5 Simple form Second Virial Coefficient [S]

Assuming that $\phi(r)$ is large (on the scale of kT) and positive for $r < r_0$ and small for $r > r_0$, show that the second virial coefficient may be written as

$$B_2(T) = b_0 - \frac{a_0}{kT}$$

where you should obtain expressions for a_0 and b_0.

Compare this form of B_2 with that implied by the Van der Waals equation of state.

Calculate the entropy and show that

$$S = S_{\text{Ideal}} - Nkb_0\rho$$

Comment on why the entropy is reduced from the standpoint of information theory.

4.6 Failure of Perturbation Theory for Coulomb Interaction [S]

Consider a system of particles whose interaction potential falls off like r^{-y} as $r \to \infty$. Show that B_2 is infinite if $y \leq 3$. Comment.