

STATISTICAL PHYSICS

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 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 \bar{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 High and low temperature limits and corrections to Debye model [s/c]

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

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

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

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

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

c) Show that

$$f(\infty) = \zeta(d+1)\Gamma(d+1)$$

where the Riemann zeta function is defined as

$$\zeta(s) = \sum_{n=1}^{\infty} \frac{1}{n^s}$$

and the Gamma function is defined by

$$\Gamma(z) = \int_0^{\infty} u^{z-1} e^{-u} du$$

.

d) By expressing $f(\alpha) = f(\infty) - \Delta f(\alpha)$, calculate the leading behaviour of C_V and the first correction to this.

4.3 Second Virial Coefficient [S]

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

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

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

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

4.4 Simple form of 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.

4.5 Failure of Perturbation Theory for Coulomb Interaction [S]

Consider a system of particles whose interaction potential falls off like r^{-y} as $r \rightarrow \infty$. Show that B_2 is infinite if $y \leq 3$. What is the physical implication of this?