STATISTICAL PHYSICS

The Microcanonical, Canonical and Grand Canonical Distributions Tutorial Sheet 2

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!

2.1 **Revision of Model Magnet** [r] When a particle with spin $^1/_2$ is placed in a magnetic field H, its energy level is split into $\pm\mu H$ and it has a magnetic moment μ or $-\mu$ along the direction of the magnetic field, respectively. Suppose that an assembly of N such particles on a lattice is placed in a magnetic field H and is kept at temperature T. Find the internal energy, the entropy, the heat capacity and the total magnetic moment M of this assembly.

Sketch the internal energy and heat capacity, identifying and analysing the low temperature and high temperature regimes.

Hint: Note that the particles are *weakly interacting*. Think first about whether the particles are *distinguishable* or *indistinuguishable* then take advantage of the appropriate factorisation of the problem.

2.2 **Magnetisation Fluctuations in General Magnetic System** [s] An assembly of spin 1/2 constituents (e.g. atoms) at a fixed temperature T is subject to an applied magnetic field H. If the net magnetic moment of the assembly in state i is M_i, in the direction of the field, then the associated total energy is given by

$$E_i = E_i(H = 0) - \mu_0 M_i H \, ,$$

where $E_i(H = 0)$ represents the mutual interaction of the individual spins in the absence of an external field, and μ_0 is the permeability of free space.

Show that fluctuations of the magnetic moment about its mean value are given by

$$\langle \Delta M^2 \rangle \equiv \langle M^2 \rangle - \langle M \rangle^2 = \frac{kT\chi}{\mu_0}$$

where χ is the isothermal magnetic susceptibility defined by

$$\chi = [\partial \langle M \rangle / \partial H]_T \, .$$

2.3 **Quantum rotor: classical and quantum limits** [s]

$$\epsilon_r = \frac{\hbar^2}{2I} r(r+1) \quad , \quad r = 0, 1, 2...$$

where I is a constant and the level ϵ_r is $(2r+1)$-fold degenerate.
(a) Write down the canonical partition function of the rotational motion, and obtain manageable approximations for it (i) at low temperatures and (ii) at high ones.

[Hint: to decide on suitable approximations, consider in each limit how many terms matter in the sum. If only one or two terms matter, neglect the rest. If many matter, consider how a sum of many terms (if the summand is slowly varying) can be approximated by an integral.]
(b) Find the mean energy $E(T)$ in each limit and hence obtain expressions for the heat capacity at low and high temperatures.
[Answers: $c_{V,rot} = 3\hbar^4 I^{-2} k_B^{-1} T^{-2} \exp[-\beta\hbar^2/I] \simeq 0$ for $k_B T \ll \epsilon_1$; $c_{V,rot} = k_B$ for large T.]

2.4 **Stirling's formula and entropy [r]**

a) Starting from Stirling's formula

$$\ln(N!) \simeq N[\ln N - 1]$$

show using Boltzmann's formula for entropy that, for a lattice of $\mathcal{N}$ independent (weakly interacting) spins, each either up or down, the entropy is given by

$$S = -k\mathcal{N}[c \ln c + (1-c)\ln(1-c)]$$

where c is the fraction of up spins

Rederive this result from the Gibbs entropy, using the fact that for a weakly interacting system the Gibbs entropy reduces to $\mathcal{N}S_G(1)$, where $S_G(1)$ is the Gibbs entropy of a single spin.

(b) From Stirling's formula, show that if, instead of having spins, each lattice site can be either empty, or occupied by a particle of type 1 (concentration c_1) or occupied by a particle of type 2 (concentration c_2), then

$$S = -k\mathcal{N}[c_1 \ln c_1 + c_2 \ln c_2 + (1-c_1-c_2)\ln(1-c_1-c_2)]$$

Rederive this result using the Gibbs entropy.

2.5 **Grand Potential [r]** Prove from the grand canonical partition function and the associated bridge equation that the grand potential is given by

$$\Phi = \langle E \rangle - TS_{gibbs} - \mu\langle N \rangle$$

(Hint: Start from the expression for S_{gibbs}.)

Show also that for a single species 'PVT' systen

$$\Phi = -PV$$

2.6 **Equivalence of ensembles [k]** It is sometimes said that, in the limit of large N, the canonical ensemble becomes equivalent to the microcanonical ensemble. How can this statement be justified? [Hint consider energy fluctuations] Similarly, when does the grand canonical ensemble become equivalent to the canonical ensemble? When might we expect equivalences to break down?

2.7 **Correlation of energy and pressure fluctuations [s]** Show that the fluctuations in the pressure and total energy of a fluid in a container of fixed volume V, satisfy the relation

$$\langle \Delta E\, \Delta P \rangle = kT^2 \left(\frac{\partial \langle P \rangle}{\partial T} \right)_V ,$$

provided that the fluid is in thermal equilibrium.

[Hint: You will need to introduce the 'instantaneous pressure' of microstate i,

$$P_i = -\frac{\partial E_i}{\partial V}\,,$$

and use this to calculate $\langle P \rangle$.]