Statistical Physics: Tutorial 2

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A: Core problems

1. **Grand Potential** Define the grand potential, Φ, from the grand canonical partition function and its associated bridge equation. Using the expression for the Gibbs entropy, prove that Φ satisfies

$$\Phi = \langle E \rangle - TS_{\rm Gibbs} - \mu \langle N \rangle \, .$$

Now use the Gibbs-Duhem relation to show that a single species 'PVT' system obeys the relation

$$\Phi = -PV \, .$$

2. **Thermodynamics of a model magnet** When a particle with spin $^1/_2$ is placed in a magnetic field B, its energy level is split into $\pm \mu B$, corresponding to a magnetic moment μ or $-\mu$ along the direction of the magnetic field. Suppose that a system of N such particles on a lattice is placed in a magnetic field B and is kept at temperature T. In the limit that the individual spins are weakly interacting, find the internal energy, the entropy, the heat capacity and the total magnetic moment M of this system.

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

3. **Quantum rotor: classical and quantum limits**

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

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: $C_{V,{\rm rot}} = 3\hbar^4 I^{-2} k_B^{-1} T^{-2} \exp[-\beta\hbar^2/I] \simeq 0$ for $k_B T \ll \epsilon_1$; $C_{V,{\rm rot}} = k_B$ for large T.]

B: Further problems

1. **Canonical Distribution of two-state system: heat capacity**
(a) A system can be in one of two states, with energy $0, \epsilon$. Find its mean energy as a function of temperature and sketch the result. Sketch also the heat capacity $C_V = (\partial E/\partial T)_V$ and show that it peaks at a given critical temperature. Use dimensional arguments to estimate this temperature and C_V at that point.
(b) A similar system can be in one of four states, with energy $0, \delta, \epsilon, \epsilon + \delta$. By writing the partition function as a product of two factors, show that this can be viewed as two independent subsystems whose heat capacities are additive.

2. **Equivalence of ensembles**
   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?

3. **Magnetisation fluctuations in general magnetic system**
   A system of spin 1/2 constituents (e.g. atoms) at a fixed temperature T is subject to an applied magnetic field B. If the net magnetic moment of the system in state i is M_i, in the direction of the field, then the associated total energy is given by

   $$E_i = E_i(B = 0) - M_i B\,,$$

   where $E_i(B = 0)$ 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

   $$\langle \Delta M^2 \rangle \equiv \langle M^2 \rangle - \langle M \rangle^2 = kT\chi$$

   where χ is the isothermal magnetic susceptibility defined by

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

4. **Correlation of energy and pressure fluctuations** 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 $\langle P \rangle$.]