Review on statistical physics & ensembles

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Problem 1

- Consider a system consisting of N spin$-\frac{1}{2}$ particles, each of which can be in one of two quantum states, namely $\uparrow$ and $\downarrow$. In presence of a magnetic field B, the energy of a spin in a $\uparrow$ / $\downarrow$ state is $\pm\mu_m B/2$ where μ_m is the magnetic moment. Show that the partition function is

$$Z = 2^N \cosh^N \left(\frac{\beta \mu_m B}{2} \right), \tag{1}$$

with $1/\beta = k_B T$ in the canonical ensemble. Find the average energy E and entropy S. Compute both quantities at zero temperature and $T \to \infty$.

Problem 2

- Compute the partition function of a quantum harmonic oscillator at frequency ω in the canonical ensemble. *Hint:* the energy levels are given by

$$E_n = \hbar\omega \left(n + \frac{1}{2} \right), \tag{2}$$

with $n \in \mathbb{Z}$.

- A simple model of a solid can be made considering N atoms that vibrates all of them at the same frequency ω. Consider these vibrations as a harmonic oscillator. Show that at high temperatures, $k_B T \gg \hbar\omega$ one has a heat capacity

$$C_V = N k_B. \tag{3}$$

Derive the limit also for low temperatures.

Problem 3

Consider the Gibbs entropy for a probability distribution $p(n)$,

$$S = -k_B \sum_n p(n) \ln p(n). \tag{4}$$

- Through the use of a Lagrange multiplier, show that when restricted to states of fixed energy E, the entropy is maximized by the microcanonical ensemble, in which all such states are equally likely. Further show that in this case, the Gibbs entropy coincides with the Boltzmann entropy. *Hint:* recall that probabilities are positive and are constrained to sum up to 1.

- Show that at fixed average energy, i.e.: $\langle E \rangle = \sum_n p(n) E_n$, the entropy is maximized by canonical ensemble. Moreover, show that the Lagrange multiplier imposing the constraint is proportional to the inverse of temperature, β. Check that maximizing the entropy is equivalent to minimize the free energy.

- Show that at fixed average energy and average particle number, the entropy is maximized by the grand canonical ensemble. What is the interpretation of the Lagrange multiplier in this case?