Statistical Mechanics

August 19, 2023

Work 2 (and only 2) of the 3 problems. Please put each problem solution on a separate sheet of paper and your name on each sheet.

Problem 1

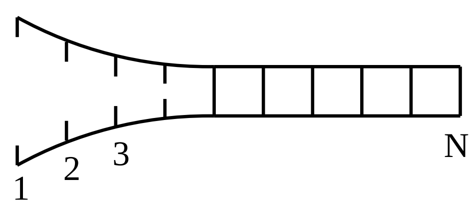
Consider a simple model of a DNA molecule in which it is treated as a zipper with N links, as depicted in the figure below. Assume that the zipper can only be opened from its left end. The last link on the right end always remains closed. A closed link has zero energy, whereas an open link has energy $\varepsilon > 0$. The closed link state is not degenerate, but the open link state is g-fold degenerate, $g \geq 2$.

a.) Find the canonical partition function of this system.

b.) Calculate the total energy of the DNA molecule as a function of temperature.

c.) Find the average number of open links at temperature T.

d.) Explain what happens to the DNA in the limits $T \to 0$ and $T \to \infty$.



Problem 2

A system consists of three spin-1/2 particles arranged along a line, coupled by nearest-neighbor interactions. This system is placed in an external magnetic field H in the z-direction and equilibrated at temperature T ($\beta = 1/(k_B T)$). The Hamiltonian for this equilibrated system can be approximated by a classical Ising model:

$$\mathcal{H} = J \cdot S_z(1) \cdot S_z(2) + J \cdot S_z(2) \cdot S_z(3) - 2\mu_B H \cdot (S_z(1) + S_z(2) + S_z(3))$$

where J and μ_B are positive constants, and $S_z(i)$ is the z-component of the spin at site i. In the following, neglect any quantum effects.

a.) List all possible microscopic states of the system, their energy, degeneracies, and total spin.

b.) For each of the following cases write down the limiting values of internal energy $U(T, H)$, entropy $S(T, H)$, and magnetization $M(T, H)$:

  i.) $T = 0$ and $H = 0$.

  ii.) $J \ll k_B T$ and $H = 0$.

c.) Does the specific heat at constant H, $C_H(T, H = 0)$, for this model Hamiltonian have a maximum? Explain.

d.) Find a closed form expression for the canonical partition function $Z(T, H)$. Derive the limiting value of $Z(T \to \infty, H)$.

e.) Find the magnetization $M = (1/\beta)\partial(\ln Z)/\partial H$ and find an approximate expression for this quantity that is valid at high temperatures, $k_B T \gg \mu_B H$ or J.

Hint: For small x, $\sinh x \sim x$.

Problem 3

Thermodynamics of a Three-Level System: You design a quantum dot to have three energy levels,

$$E \in \{+2\epsilon\,,\ +\epsilon\,,\ -\epsilon\}$$

and need to predict the thermodynamic properties of a collection of many quantum dots.

a.) *(2 pts.)* Calculate the (properly-normalized) **occupation probabilities** P of each of the three quantum levels and the **average energy** $\langle E \rangle$ of the quantum dot when it is brought in contact with a heat bath at temperature T.

b.) *(2 pts.)* **Evaluate the average energy** $\langle E \rangle$ quantitatively for the four values

$$k_B T = 0 \ \ , \quad k_B T = \left(\frac{1}{\ln 2}\right)\epsilon \ \ , \quad k_B T = \left(\frac{1}{\ln(4/3)}\right)\epsilon \ \ , \quad k_B T = \infty \ \ .$$

Sketch the plot of $\langle E \rangle/\epsilon$ versus $k_B T/\epsilon$ and **describe the behavior** of the plot in terms of the occupation probabilities. *(Note that* $1/\ln 2 \approx 1.44$ *and* $1/\ln(4/3) \approx 3.48$*).*

c.) *(2 pts.)* Calculate the **heat capacity at constant volume** C_V of a system of N non-interacting quantum dots.

d.) *(2 pts.)* **Expand the exact result** for the heat capacity C_V in a power series in the high temperature limit, **keeping terms up to an accuracy of** $\mathcal{O}\left((\epsilon/k_B T)^3\right)$.

e.) *(2 pts.)* Using the high-temperature approximation from Part d.), **calculate the total heat** Q required to raise a system of N non-interacting quantum dots from temperature $k_B T = 2\epsilon$ to $k_B T = 3\epsilon$.