5163, Exam 1
Monday, 02/28/2022, 2.5 hours (any time between noon and 10pm)

The exam consists of five problems. Please select four problems to work on (only four problems will be graded). If you are working on more than four problems, please state clearly which four problems you would like to be counted for your grade. All four problems carry equal weight.

If you are unclear about the wording of a problem, please indicate your questions and reasoning in your solutions.

Please upload your solutions and the first page to Canvas (the time it takes to upload the exam is not part of the 2.5 hours).

You are **not** allowed to search the internet while taking the exam, except for downloading the exam and uploading your solutions after you are done.
You are not allowed to refer to lecture notes, books, or other materials such as a calculator or computer software during the exam.
You are **not** allowed to discuss, by any means, with others while taking the exam. Also, please do not discuss the exam with anybody before 5pm on Tuesday, 03/01/2022.

After completing the exam, please sign—provided this is true—the following statements:

- *I spent no more than 2.5hours on the exam.*
- *I started working on the exam immediately after I downloaded it.*
- *I worked on the exam solutions by myself.*
- *I did not resort to any materials while taking the exam.*

Date, time, and signature

Problem 1:
A solid contains N non-interacting nuclei of spin 1. This means that each nucleus can have the projection quantum number $m_s = -1$, 0, or $+1$. Because of electric interactions with internal fields in the solid, a nucleus in the state $m_s = +1$ and in the state $m_s = -1$ has an energy ϵ, $\epsilon > 0$. A nucleus in the state $m_s = 0$ has energy 0.
Let the number of nuclei in states $m_s = -1$, 0, and $+1$ be N_-, N_0, and N_+, respectively.
(a) The number of microstates at energy E is given by

$$\Gamma(E, N) = \sum_{N_+=0,1,\cdots,E/\epsilon; N_+ + N_- = E/\epsilon} \frac{N!}{(N_0)!(N_+)!(N_-)!}. \tag{1}$$

Carefully explain this expression (you do not have to derive it). Your explanation should demonstrate an understanding of the concept of a microstate in the context of this concrete example.
(b) What is the entropy of the system? Can you write it as a function of only N and the energy E?
(c) What is the entropy at zero temperature? Please provide a physical and a mathematical explanation.

Problem 2:
(a) How do you interpret $\Delta S \geq 0$? Be as concise as you can and include a discussion of what S depends on.
(b) How do you interpret $\Delta A \leq 0$? Be as concise as you can and include a discussion of what A depends on.
(c) What is the equation that establishes the connection between statistical mechanics and thermodynamics for the microcanonical ensemble, the canonical ensemble, and the grand-canonical ensemble?
(d) What is the probability to find the system in a given allowed microstate for the micro-canonical ensemble, the canonical ensemble, and the grandcanonical ensemble?

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Problem 3 [parts (a), (b), (c), and (d) carry weights 0.2, 0.35, 0.1, and 0.35]:
This problem treats the internal energy U as a state function: $U = U(S, V, N)$; in this context, the variables S, V, and N are referred to as an "assembly". Consider

$$dU = TdS - PdV + \mu dN. \tag{2}$$

(a) Carefully comment on which quantities in Eq. (2) are extensive and which ones are intensive. Explain and, along the way, define "extensive" and "intensive".
(b) Using $A = U - TS$, $G = A + PV$, and $H = G + TS$, determine the assemblies for the state functions A, G, and H.
(c) Why does one not simply always work with U, i.e., why does one care about the thermodynamic potentials A, G, and H as well?
(d) Use the previous parts of the problem to provide as many expressions for μ, P, V, T, and S in terms of partial derivatives of state functions as possible.

Problem 4:
A collection of N particles of spin 1/2 are lined up on a straight line. Only nearest neighbors interact. When the spins of the neighbors are both up or both down, their interaction energy is J. When one spin is up and the other down, the interaction energy is $-J$.
(a) What are the possible values of the system energy? To address this question, it might be useful to start with all spins down (or all spins up), and to then "cut" the straight line once so that all spins are up to the left of the cut and all spins are down to the right of the cut (think about how many different positions for the cut there are), and to then "cut" the line twice so that all spins are up to the left of the first cut and to the right of the second cut and down between the two cuts, etc.
(b) Determine the number of microstates for each possible energy.
(c) Determine the canonical partition function $Q_N(T)$.

Problem 5:
A simple model of the DNA double helix molecule is analogous to a zipper: a chain of N links, each of which can be open or closed. A closed link has an energy ϵ_0 and an open link has an energy ϵ_1 ($\epsilon_1 > \epsilon_0$). Replication of the DNA starts with the opening of the "zipper". Assume that it can only open from one end (say the left), i.e., a link can only be open if all links left of it are also open.
(a) What is the probability of the first link from the left to be open?
(b) What is the probability of the second link from the left to be open?
(c) Find the average number of open links n as a function of N and temperature T.
(d) Calculate the partition function for this DNA model.