5163, Exam 2
Friday, 04/08/2022, 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.

Some equations that may be useful:

$$\sum_{n=0}^{\infty} x^n = \frac{1}{1-x}. \tag{1}$$

$$\int_{-\infty}^{\infty} \exp(-ax^2)dx = \sqrt{\frac{\pi}{a}}. \tag{2}$$

Problem 1:
A single one-dimensional quantum harmonic oscillator has the eigen energies

$$E_n = (n + 1/2)\hbar\omega, \tag{3}$$

where $n = 0, 1, \cdots$.
(a) What is the probability of finding the oscillator in its nth quantum state at temperature T?
(b) Which ensemble did you work in when answering part (a)? Explain why you worked in this ensemble. Could you have used a different ensemble? If so, why and which one? If not, why not?

Problem 2:
Critical point behavior: The pressure P of a gas is related to its density n ($n = N/V$) and temperature T by the truncated expansion

$$P = k_B T n - \frac{b}{2} n^2 + \frac{c}{6} n^3, \tag{4}$$

where b and c are assumed to be positive temperature independent constants.
(a) Locate the critical temperature T_c below which this equation must be invalid, and the corresponding density n_c and pressure P_c.
Note: You do not have to solve for T_c, n_c, and P_c explicitly. You "only" have to set up the equations that will determine their values and explain the steps you would take. If you went through the calculation, you would find

$$k_B T_c = \frac{b^2}{2c}, \tag{5}$$

$$n_c = \frac{b}{c}, \tag{6}$$

and

$$P_c = \frac{b^3}{6c^2}. \tag{7}$$

(b) Show that the units of the expressions given in part (a) for T_c, n_c, and P_c are correct.
(c) Provide an interpretation of T_c and sketch the pressure as a function of the density n for three different temperatures: $T > T_c$, $T = T_c$, and $T < T_c$.

Problem 3:

This problem considers the classical Ising model Hamiltonian

$$\mathcal{H} = -J \sum_{(i,j)} s_i s_j, \tag{8}$$

where s_i takes the value $+1$ when the ith spin points up and the value -1 when the ith spin points down (no other orientations of the spins are allowed). The notation (i, j) indicates that only nearest neighbor interactions are being considered. We assume that the spins are fixed on a (two-dimensional) square lattice and we consider a 2×2 lattice with periodic boundary conditions.

(a) What is implied by "2×2 square lattice with periodic boundary conditions"? Draw pictures and be specific.

(b) Enumerate the possible microstates and their energy and magnetization. The magnetization is defined through

$$M = \sum_{i=1}^{N} s_i. \tag{9}$$

(c) Using the canonical ensemble, calculate $U = \langle \mathcal{H} \rangle$, $U^2 = \langle \mathcal{H}^2 \rangle$, and $\langle M \rangle$.

Problem 4:

The Hamiltonian $\hat{\mathcal{H}}$ for an electron in a magnetic field $\vec{B}$ reads

$$\hat{\mathcal{H}} = -\mu_B \hat{\vec{\sigma}} \cdot \vec{B}, \tag{10}$$

where μ_B denotes the Bohr magneton. In the spin-up/spin-down basis, the Pauli operators $\hat{\sigma}_x$, $\hat{\sigma}_y$, and $\hat{\sigma}_z$ take the form

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \tag{11}$$

$$\sigma_y = \begin{pmatrix} 0 & -\imath \\ \imath & 0 \end{pmatrix}. \tag{12}$$

and

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{13}$$

(a) Using the quantum canonical ensemble, evaluate the density matrix operator $\hat{\rho}_{can}$ for the case where the magnetic field lies along the z-axis. You can either keep $\hat{\rho}_{can}$ as an operator or you can express it in matrix form.

(b) Repeat the calculation assuming that the magnetic field points along the x-direction.

(c) Calculate the thermal energy for the cases considered in parts (a) and (b).

Problem 5:

Consider a quantum rotor in two dimensions with Hamiltonian $\hat{\mathcal{H}}$,

$$\hat{\mathcal{H}} = -\frac{\hbar^2}{2I}\frac{d^2}{d\theta^2}, \tag{14}$$

where $0 \leq \theta < 2\pi$ and I denotes the moment of inertia.

(a) Find the eigenstates and energy levels of this rotor.

(b) Find an expression for the density matrix operator $\hat{\rho}_{can}$ in the canonical ensemble.

(c) Simplify the partition function in the high-temperature limit. How is the high-temperature limit defined, i.e., what does $k_B T$ need to be compared to?

(d) Simplify the density matrix operator $\hat{\rho}_{can}$ in the $T \to 0$ limit.