1. **Wait, are we talking about magnets or fluids? Or both?!** In class we introduced the Ising model. We considered a lattice of $M$ spins, each pointing either up ($s = 1$) or down ($s = -1$). The spins interact with an external magnetic field and with their neighboring spins such that the total energy is given by

$$E_{\text{Ising}} = -h \sum_i s_i - J \sum_{i,j}' s_i s_j, \tag{1}$$

where the prime on the summation sign is shorthand to indicate that we are only including spins for which $i$ and $j$ are at neighboring sites. Unlike our models with independent (decoupled) degrees of freedom, $J$ causes the various spins to be coupled together. A consequence is that the partition function no longer factorizes into a product of single-particle terms. Rather,

$$Q(\beta, M, h) = \sum_{s_1 = \pm 1} \sum_{s_2 = \pm 1} \cdots \sum_{s_M = \pm 1} e^{\beta h \sum_i s_i + \beta J \sum_{i,j}' s_i s_j}. \tag{2}$$

The Ising model is a lattice model, and in this class we have also talked about lattice models for gases. In particular, we have split up space into cells which are so small that they house zero or one particle. Unlike the Ising spins which take values $\pm 1$, each of our lattice gas cells took the value $n = 0$ or $n = 1$. You have always thought it was crazy that we acted like neighboring cells wouldn't influence each other. After all, if there is a van der Waals attraction between our gas molecules, then the presence of a molecule in one cell would decrease the energy if another molecule is in the neighboring cell. Let us model that attraction as an attractive energy

$$E_{\text{lattice gas}} = -\epsilon \sum_{i,j}' n_i n_j. \tag{3}$$

(i) Show that this form of $E_{\text{lattice gas}}$ corresponds to a decrease in energy of $\epsilon$ when two neighboring cells $i$ and $j$ are occupied, but that it contributes nothing to the energy in the other three cases—when neither cell is occupied, only cell $i$ is occupied, or only cell $j$ is occupied.

(ii) A microstate $\nu$ of the lattice gas corresponds to a vector $(n_1, n_2, \ldots, n_M) = (1, 0, \ldots, 1)$ that specifies the state of every cell. Let us assume that the gas can exchange energy and particles with the outside world but that the volume is fixed. In that case the possible microstates can have a fluctuating value of $E_{\text{lattice gas}}$ and a fluctuating value of $N = \sum_i n_i$. In terms of the grand canonical partition function $\Xi(\beta, M, \mu)$ for this lattice gas, what is the probability of microstate $\nu$?

(iii) Develop an explicit mapping between the Ising problem and the lattice gas problem to relate $Q$ and $\Xi$. In particular, derive the precise relationship between the Ising paramters $h$, and $J$ and the lattice gas parameters $\mu$ and $\epsilon$. Assume the spins/cells are in $d$-dimensional space.

2. **The Ising model in one dimension.** One of the core predictions of the theory of phase transitions is that the ordering of microscopic degrees of freedom changes dramatically as a function of temperature. In the Ising picture, this dramatic change corresponds to a transition from aligned spins at low temperature to disordered spins at high temperature. In the lattice gas picture, it is a change from a liquid with $\langle n \rangle \approx 1$ to a gas with $\langle n \rangle \approx 1$. Here we will focus on the Ising magnet in one dimension (you could map these results over to the liquid/vapor context using problem 1).

(i) First imagine that you already know how to compute $Q(\beta, M, h)$. Express $\langle s \rangle = M^{-1} \langle \sum_i s_i \rangle$ as a derivative of $\ln Q$.

(ii) For the one-dimensional Ising model it is possible to perform that computation of $Q$ via an accounting trick with the so-called transfer matrix

$$T = \begin{pmatrix} e^{\beta(J-h)} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J+h)} \end{pmatrix} \tag{4}$$

Take, as a simple example, an Ising model with periodic boundary conditions and with $M = 3$ sites. Then $Q$ is a sum over eight possible microstates: $(1, 1, 1), (1, 1, -1), \ldots, (-1, -1, -1)$. Explicitly show that $Q$ computed from Eq. (2) is equal to $\text{Tr}(T^3)$, where Tr is the trace of the matrix.

(iii) Determine $Q(\beta, M, h)$ in the limit of large $M$. [Hint: You will first want to generalize (ii) to $M$ spins. The trace is most easily computed if you first diagonalize $T$ and use the fact that the trace is unaffected by diagonalization.]

(iv) Combine your answers to (i) and (iii) to determine $\langle s \rangle$ as a function of $\beta$ in the absence of an external magnetic field ($h = 0$). If possible, identify the temperature of the phase transition between ordered and disordered states. Otherwise, explain why it is not possible to find such a temperature.

3. **Mean field theory.** Computing the exact partition function in more than one dimension is very hard (Lars Onsager famously did this in the 1940s for the two-dimensional $H = 0$ Ising model). But there are various ways to approximate $Q$. One strategy for approximating $Q$ is to use a computer to sample many possible microstates, the focus of next week's problem set. The advantage of a computational approach is that it can be made arbitrarily accurate, meaning you could systematically improve your estimate for $Q$ by spending more computer time. In contrast, there is an uncontrolled approximation scheme called mean field theory that has the benefit of being tractable with pen and paper.

The idea behind mean field theory is simple. Spin $i$ has four neighbors, each of which can either be $+1$ or $-1$. Assume instead that these neighbors all equal their average value $\langle s \rangle$. Then the effect of the neighboring spins is replaced by their average effect (the mean field that they impose on spin $i$). As a consequence, we approximate spin $i$ as being decoupled from the other spins but in the presence of an augmented external field of strength $h + 4J\langle s \rangle$.

(i) Express $\langle s \rangle$ in terms of a derivative of $\ln Q$.

(ii) Find the canonical partition function for $M$ independent spins, each in a field of strength $h+4J\langle s \rangle$.

(iii) Combine your results to (i) and (ii) to get a self-consistent expression for $\langle s \rangle$. In other words, obtain an equation of the form

$$\langle s \rangle = f(\langle s \rangle) \tag{5}$$

for some function $f$ which you will find.

(iv) Numerically solve your equation in (iii) for a variety of temperatures to generate a plot of $\langle s \rangle$ versus temperature. Does this plot display a phase transition? If so, at what temperature?