Due ~~June 13, Friday~~ June 10 or 11 (for problems 1–4)

Problem 1 (40 points) *The Ising model with an AFM interaction, mean field theory.* Consider the following Ising model where $\sigma_i \pm 1$ and $J > 0$.

$$\mathcal{H} = J \sum_{\langle i,j \rangle} \sigma_i \sigma_j - \mu_B H \sum_i \sigma_i .$$

The symbol $\langle i, j \rangle$ means the nearest-neighbor (hitherto referred to as "nn") pairs. Note that $J > 0$ means that the first term in the Hamiltonian is an *anti-ferromagnetic* (AFM) interaction term, preferring two oppositely directed spins if $H = 0$.

The solution to this AFM model depends on the lattice structure. Here, we assume *a two dimensional (2D) square lattice.* We shall refer to the spin at origin by the index $i = 0$, corresponding to the center of the crystal. The 2D square lattice means that (1) the number of nn's is 4 and (2) the mean field solution has the following "bipartite" lattice of spins:

$$\overline{\langle \sigma_i \rangle} = \begin{cases} m_A & i = 0 \\ m_B & i = \text{ a nn of } i = 0 \\ m_A & i = \text{ a nn of a nn of } i = 0 \\ m_B & i = \text{ a nn of a nn of a nn of } i = 0 \\ \cdots & \cdots \end{cases}$$

Within the mean field approximation, answer the following questions.

(a) Find the solutions for m_A and m_B of this problem. [Hint: As in the ferro-magnetic case, an explicit solution is not possible. Only an implicit solution is possible. Different from the ferro-magnetic case, an implicit solution requires *two* coupled equations for m_A and m_B, not a single equation.]

(b) Find the critical temperature (T_c) for $H = 0$, assuming that $m_A = -m_B$ in zero field. [Hint: The two coupled equations must become identical for $H = 0$ and $m_A = -m_B$.]

(c) Show that the non-zero "staggered magnetization order parameter" $m_A = -m_B$ is determined by $m_A^2 = -3t$, just below T_c, where $t \equiv \frac{T}{T_c} - 1$.

(d) Find the weak field ($H \approx 0$) magnetic susceptibility

$$\chi = \frac{\partial m}{\partial H}, \qquad \text{where } m = \frac{m_A + m_B}{2},$$

for $t \approx 0$.

(e) Do you expect the last expression for χ for small $t > 0$ to be valid at very high temperatures ($t \to \infty$)? Explain.

[Potentially useful formula: $\tanh\delta \approx \delta - \frac{1}{3}\delta^3$.]

Problem 2 (40 points) *The Landau theory (Potts model).* In the Landau mean field theory of a certain Potts model, the Landau free energy per particle is given by

$$\frac{G}{N} \approx a(T) + (k_B T - J)m^2 - \frac{k_B T}{3}m^3 + \frac{k_B T}{2}m^4,$$

where $a(T)$ is an analytic function of T, $J > 0$ represents a ferro-magnetic interaction, and m is the order parameter.

(a) Find the transition temperature T_c, and the values of m above T_c and just below T_c. [Hints: $T_c > J/k_B$. $\frac{\partial G}{\partial m} = 0$ *and* $\frac{G}{N} - a(T) = 0$ at $T = T_c$.]

(b) Find the entropy, $S(t)$, just above T_c and just below T_c, ignoring the smooth part of $S(t)$ that arises from $a(T)$.

(c) From the results of the previous two parts, what is the nature of the phase transition, first order or second order? [Here is a short guide. A first order phase transition is a *discontinuous* transition involving a sudden change of the order parameter and a latent heat ($T\Delta S$), as in the evaporation/condensation of a liquid. This means a phase separation at the phase boundary. A second order phase transition is a *continuous* transition, where the order parameter changes continuously through the transition. This means a critical state at the phase boundary.]

Problem 3 (40 points) For the given Landau free energy of Eq. 16.34, calculate the magnetization per spin, the magnetic susceptibility, and the specific heat, below and above T_c, in terms of a, b_0, and c. Assuming that $a(T)$ and $c(T)$ are smooth and finite at T_c. Also, note the conditions stated in Eqs. 16.32, 16.33. The calculated results must be verified to reproduce the results of Lecture 16 (Eqs. 16.18, 16.19, 16.23, 16.24, 16.30, all for $T \approx T_c$), by appropriately identifying a, b_0 and c for the Ising model case. [Note: In this problem, you are being asked to reproduce the core results of Lecture 16, using only the Landau free energy. This means that the physical quantities are calculated in terms of abstract parameters a, b_0 and c, and only for T near T_c.]

Problem 4 (40 points) A three-state Potts Hamiltonian in one dimension is given by

$$\mathcal{H} \;=\; -J\sum_{i=1}^{N}\delta_{n_i,n_{i+1}},$$

where $n_i = 0, 1, 2$ denotes one of the three states possible at each site. Calculate the free energy using the transfer matrix technique (see LN 18) and discuss the energy and the entropy at high temperature and low temperature for both the ferro-magnetic model ($J > 0$) and the anti-ferromagnetic model ($J < 0$).

Problem 5 (Optional; ____ points) Construct a Metropolis Monte Carlo code for a two dimensional Ising magnet with the periodic boundary condition. (A partial python example is provided on the homework page of the course web site: it should be enough for part (a), and should be easily extensible for parts (b,c).) In the following, assume a ferromagnetic model, except in (b).

(a) Pick at least three temperatures, including one well above T_c, one near T_c, and one well below T_c. Start from the initial configuration where the system is magnetized up on the left half and down on the right half. Run the same number of runs (suggestion: ~ 2000 for 40×40 lattice). Compare the final configurations for different temperatures and discuss the results.

(b) Do the same for the anti-ferromagnetic model ($J < 0$). Discuss the results.

(c) Measure the magnetization and the spin correlation function

$$\Gamma_{ij} \equiv \overline{\langle \sigma_i \sigma_j \rangle} - \overline{\langle \sigma_i \rangle}\,\overline{\langle \sigma_j \rangle}$$

Examine these quantities at least for three temperatures. Try to demonstrate the existence of long range correlations near the critical point, and the spontaneous symmetry breaking below T_c.

Problem 6 (Optional; ____ points) The renormalization group (RG) equation that we set up for the one dimensional Ising model, in Section 19.2, can be improved so that the equation applies to the anti-ferromagnetic case ($J < 0$) as well as the ferromagnetic case ($J > 0$).

(a) By constructing such an improved RG equation (hint: e.g., sum over two spins for every three spins), show that $K = J\beta = \pm\infty, 0$ are all fixed points, now.

(b) Calculate, numerically, about 20 RG iterations, starting from $K = \pm 10$, $K = \pm 5$. At each iteration, print out the value of the running constant K as well as the quantity g (Eq. 19.11), which can be compared with the exact result (which can be deduced directly from Eq. 18.7). For the initial value of g, an approximate form of the partition function for $T \approx 0$ (corresponding to the energy minimum) can be used.

(c) Do similar numerical calculations, but this time, starting from $K = \pm 0.001$, and applying the RG equation *backwards*. For the initial value of g, an approximate form of the partition function for $T \approx \infty$ (corresponding to the entropy maximum) can be used.

(d) Discuss your results in terms of how error for g propagates in case (c) or (d). Make a subsequent observation as to which scheme, (c) or (d), is more viable for calculating the free energy using the renormalization group technique.