PHYSICS 140B : STATISTICAL PHYSICS
HW ASSIGNMENT #6 SOLUTIONS

(1) Consider a spin-2 Ising model with Hamiltonian

$$\hat{H} = -\tfrac{1}{2}\sum_{i,j} J_{ij}\, S_i\, S_j - H\sum_i S_i$$

where $S_i \in \{-2,-1,0,1,2\}$. The system is on a simple cubic lattice, with nearest neighbor coupling $J_1/k_B = 40\,\mathrm{K}$ and next-nearest neighbor coupling $J_2/k_B = 10\,\mathrm{K}$.

(a) Find the mean field free energy per site $f(\theta, h, m)$, where $\theta = k_B T/\hat{J}(0)$, $h = H/\hat{J}(0)$, $m = \langle S_i \rangle$, and $f = F/N\hat{J}(0)$.

(b) Find the mean field equation for m.

(c) Setting $h = 0$, find θ_c. What is T_c?

(d) Find the linear magnetic susceptibility $\chi(\theta)$ for $\theta > \theta_c$.

(e) For $0 < \theta_c - \theta \ll 1$ and $h = 0$, the magnetization is of the form $m = A(\theta_c - \theta)^{1/2}$. Find the coefficient A.

(a) he mean field Hamiltonian is

$$\hat{H}^{\mathrm{MF}} = \tfrac{1}{2} N \hat{J}(0)\, m^2 - \big(H + \hat{J}(0)\, m\big) \sum_i S_i \quad .$$

Here

$$\hat{J}(0)/k_B = z_1\, J_1/k_B + z_2\, J_2/k_B = 360\,\mathrm{K} \quad ,$$

since $z_1 = 6$ and $z_2 = 12$ on the simple cubic lattice. We'll need this number in part (c). Computing the partition function $Z_{\mathrm{MF}} = \mathtt{r}\, \exp(-\beta \hat{H}^{\mathrm{MF}})$, taking the logarithm, and dividing by $N\hat{J}(0)$, we find

$$f = \tfrac{1}{2} m^2 - \theta \ln\left(1 + 2\cosh\left(\frac{m+h}{\theta}\right) + 2\,\cosh\left(\frac{2m+2h}{\theta}\right)\right) \quad .$$

(b) The mean field equation is obtained by setting $\partial f/\partial m = 0$. Thus,

$$m = \frac{2\sinh\left(\frac{m+h}{\theta}\right) + 4\sinh\left(\frac{2m+2h}{\theta}\right)}{1 + 2\cosh\left(\frac{m+h}{\theta}\right) + 2\cosh\left(\frac{2m+2h}{\theta}\right)} \quad .$$

(c) To find θ_c, we set $h = 0$ and equate the slopes of the LHS and RHS of the above equation. This yields

$$\theta_c = 2 \quad \Rightarrow \quad T_c = \hat{J}(0)\, \theta_c = 720\,\mathrm{K} \quad .$$

(d) To find the zero field susceptibility, we assume that m and h are both small and expand the RHS of the self-consistency equation, yielding

$$m(h,\theta) = \frac{2h}{\theta - 2} \quad \Rightarrow \quad \chi(\theta) = \frac{2}{\theta - 2}$$

(e) When $\theta < \theta_{\rm c}$, we need to expand the RHS of the self-consistency equation to order m^3. Equivalently, we can work from f, and using $\cosh x = 1 + \frac{x^2}{2} + \frac{x^4}{24} + \ldots$, we have

$$\begin{aligned} f &= \tfrac{1}{2}m^2 - \theta \ln\!\bigg(5 + \frac{m^2}{\theta^2} + \frac{m^4}{12\theta^4} + \ldots + \frac{4m^2}{\theta^2} + \frac{4m^4}{3\theta^4} + \ldots\bigg) \\ &= -\theta \ln 5 + \tfrac{1}{2}m^2 - \theta \ln\!\bigg(1 + \frac{m^2}{\theta^2} + \frac{17\,m^4}{60\,\theta^4} + \ldots\bigg) \\ &= -\theta \ln 5 + \frac{\theta - 2}{2\theta}\,m^2 + \frac{13\,m^4}{60\,\theta^3} + \ldots \quad , \end{aligned}$$

since $\ln(1+x) = x - \frac{1}{2}x^2 + \frac{1}{3}x^3 - \ldots$. We can directly differentiate this with respect to m^2 and obtain

$$m^2 = \tfrac{15}{13}\,\theta^2\,(2-\theta) \simeq \tfrac{60}{13}\,(2-\theta) \quad \Rightarrow \quad A = 2\sqrt{\tfrac{15}{13}} \quad .$$

In deriving the above result we have assumed $\theta \approx \theta_{\rm c} = 2$ and worked only to lowest order in the difference $\theta_{\rm c} - \theta$.

(2) Consider an Ising model on a square lattice with Hamiltonian

$$\hat{H} = -J \sum_{i \in {\rm A}} \sum_{j \in {\rm B}}{}' S_i\,\sigma_j \;,$$

where the sum is over all nearest-neighbor pairs, such that i is on the A sublattice and j is on the B sublattice (this is the meaning of the prime on the j sum), as depicted in Fig. 1. The A sublattice spins take values $S_i \in \{-1, 0, +1\}$, while the B sublattice spins take values $\sigma_j \in \{-1, +1\}$.

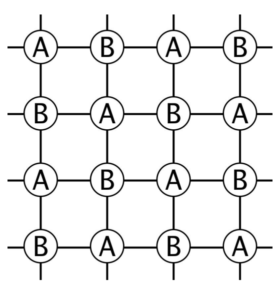

Figure 1: The square lattice and its A and B sublattices.

(a) Make the mean field assumptions $\langle S_i \rangle = m_{\rm A}$ for $i \in$ A and $\langle \sigma_j \rangle = m_{\rm B}$ for $j \in$ B. Find the mean field free energy $F(T, N, m_{\rm A}, m_{\rm B})$. Adimensionalize as usual, writing $\theta \equiv k_{\rm B}T/zJ$ (with $z = 4$ for the square lattice) and $f = F/zJN$. Then write $f(\theta, m_{\rm A}, m_{\rm B})$.

(b) Write down the two mean field equations (one for m_{A} and one for m_{B}).

(c) Expand the free energy $f(\theta, m_{\mathrm{A}}, m_{\mathrm{B}})$ up to fourth order in the order parameters m_{A} and m_{B}. You may find the following useful:

$$\ln\big(2\cosh x\big) = \ln 2 + \frac{x^2}{2} - \frac{x^4}{12} + \mathcal{O}(x^6) \quad , \quad \ln\big(1 + 2\cosh x\big) = \ln 3 + \frac{x^2}{3} - \frac{x^4}{36} + \mathcal{O}(x^6) \, .$$

(d) Show that the part of $f(\theta, m_{\mathrm{A}}, m_{\mathrm{B}})$ which is quadratic in m_{A} and m_{B} may be written as a quadratic form, *i.e.*

$$f(\theta, m_{\mathrm{A}}, m_{\mathrm{B}}) = f_0 + \tfrac{1}{2} \begin{pmatrix} m_{\mathrm{A}} & m_{\mathrm{B}} \end{pmatrix} \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \begin{pmatrix} m_{\mathrm{A}} \\ m_{\mathrm{B}} \end{pmatrix} + \mathcal{O}\big(m_{\mathrm{A}}^4, m_{\mathrm{B}}^4\big) \, ,$$

where the matrix M is symmetric, with components $M_{aa'}$ which depend on θ. The critical temperature θ_{c} is identified as the largest value of θ for which $\det M(\theta) = 0$. Find θ_{c} and explain why this is the correct protocol to determine it.

(a) Writing $S_i = m_{\mathrm{A}} + \delta S_i$ and $\sigma_j = m_{\mathrm{B}} + \delta\sigma_j$ and dropping the terms proportional to $\delta S_i \, \delta\sigma_j$, which are quadratic in fluctuations, one obtains the mean field Hamiltonian

$$\hat{H}_{\mathrm{MF}} = \tfrac{1}{2} N z J m_{\mathrm{A}} m_{\mathrm{B}} - z J m_{\mathrm{B}} \sum_{i \in A} S_i - z J m_{\mathrm{A}} \sum_{j \in B} \sigma_j \, ,$$

with $z = 4$ for the square lattice. Thus, the internal field on each A site is $H_{\mathrm{int,A}} = zJm_{\mathrm{B}}$, and the internal field on each B site is $H_{\mathrm{int,B}} = zJm_{\mathrm{A}}$. The mean field free energy, $F_{\mathrm{MF}} = -k_{\mathrm{B}} T \ln Z_{\mathrm{MF}}$, is then

$$F_{\mathrm{MF}} = \tfrac{1}{2} N z J m_{\mathrm{A}} m_{\mathrm{B}} - \tfrac{1}{2} N k_{\mathrm{B}} T \ln\Big[1 + 2\cosh(zJm_{\mathrm{B}}/k_{\mathrm{B}}T)\Big] - \tfrac{1}{2} N k_{\mathrm{B}} T \ln\Big[2\cosh(zJm_{\mathrm{A}}/k_{\mathrm{B}}T)\Big] \, .$$

Adimensionalizing,

$$f(\theta, m_{\mathrm{A}}, m_{\mathrm{B}}) = \tfrac{1}{2} m_{\mathrm{A}} m_{\mathrm{B}} - \tfrac{1}{2}\theta \ln\Big[1 + 2\cosh(m_{\mathrm{B}}/\theta)\Big] - \tfrac{1}{2}\theta \ln\Big[2\cosh(m_{\mathrm{A}}/\theta)\Big] \, .$$

(b) The mean field equations are obtained from $\partial f / \partial m_{\mathrm{A}} = 0$ and $\partial f / \partial m_{\mathrm{B}} = 0$. Thus,

$$m_{\mathrm{A}} = \frac{2\sinh(m_{\mathrm{B}}/\theta)}{1 + 2\cosh(m_{\mathrm{B}}/\theta)}$$

$$m_{\mathrm{B}} = \tanh(m_{\mathrm{A}}/\theta) \, .$$

(c) We have

$$f(\theta, m_{\mathrm{A}}, m_{\mathrm{B}}) = f_0 + \tfrac{1}{2} m_{\mathrm{A}} m_{\mathrm{B}} - \frac{m_{\mathrm{A}}^2}{4\,\theta} - \frac{m_{\mathrm{B}}^2}{6\,\theta} + \frac{m_{\mathrm{A}}^4}{24\,\theta^3} + \frac{m_{\mathrm{B}}^4}{72\,\theta^3} + \ldots \, ,$$

with $f_0 = -\frac{1}{2}\theta \ln 6$.

(d) From the answer to part (c), we read off

$$M(\theta) = \begin{pmatrix} -\frac{1}{2\theta} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{3\theta} \end{pmatrix} ,$$

from which we obtain $\det M = \frac{1}{6}\theta^{-2} - \frac{1}{4}$. Setting $\det M = 0$ we obtain $\theta_c = \sqrt{\frac{2}{3}}$.

(3) Consider the ferromagnetic XY model, with

$$\hat{H} = -\sum_{i<j} J_{ij} \cos(\phi_i - \phi_j) - H \sum_i \cos\phi_i \, .$$

Defining $z_i \equiv \exp(i\phi_i)$, write $z_i = \langle z_i \rangle + \delta z_i$ with

$$\langle z_i \rangle = m \, e^{i\alpha} \, .$$

(a) Assuming $H > 0$, what should you take for α?

(b) Making this choice for α, find the mean field free energy using the 'neglect of fluctuations' method. *Hint*: Note that $\cos(\phi_i - \phi_j) = \text{Re}\,(z_i z_j^*)$.

(c) Find the self-consistency equation for m.

(d) Find T_c.

(e) Find the mean field critical behavior for $m(T, H = 0)$, $m(T = T_c, H)$, $C_V(T, H = 0)$, and $\chi(T, H = 0)$, and identify the critical exponents α, β, γ, and δ.

(a) To minimize the free energy we clearly must take $\alpha = 0$ so that the mean field is aligned with the external field.

(b) Writing $z_i = m + \delta z_i$ we have

$$\begin{aligned} H &= -\tfrac{1}{2} \sum_{i,j} J_{ij} \, \text{Re}\,\big(m^2 + m\,\delta z_i + m\,\delta z_j + \delta z_i\,\delta z_j\big) - H \sum_i \text{Re}\,(z_i) \\ &= \tfrac{1}{2} N \hat{J}(0)\, m^2 - \big(\hat{J}(0)\, m + H\big) \sum_i \cos\phi_i + \mathcal{O}\big(\delta z_i\,\delta z_j\big) \end{aligned}$$

The mean field free energy is then

$$\begin{aligned} F &= \tfrac{1}{2} N \hat{J}(0)\, m^2 - N k_B T \ln \left[\int_0^{2\pi} \frac{d\phi}{2\pi} \, e^{(\hat{J}(0)\, m + H)\cos\phi / k_B T} \right] \\ &= \tfrac{1}{2} N \hat{J}(0)\, m^2 - N k_B T \ln I_0\!\left(\frac{\hat{J}(0)\, m + H}{k_B T} \right) , \end{aligned}$$

where $I_\alpha(x)$ is the modified Bessel function of order α.

(c) Differentiating, we find

$$\frac{\partial F}{\partial m} = 0 \quad \Longrightarrow \quad m = \frac{I_1\Big(\frac{\hat{J}(0)\,m+H}{k_\mathrm{B}T}\Big)}{I_0\Big(\frac{\hat{J}(0)\,m+H}{k_\mathrm{B}T}\Big)} \ ,$$

which is equivalent to eqn. 6.119 of the notes, which was obtained using the variational density matrix method.

(d) It is convenient to define $f = F/N\hat{J}(0)$, $\theta = k_\mathrm{B}T/\hat{J}(0)$, and $h = H/\hat{J}(0)$. Then

$$f(\theta,h) = \tfrac{1}{2}m^2 - \theta \ln I_0\bigg(\frac{m+h}{\theta}\bigg) \ .$$

We now expand in powers of m and h, keeping terms only to first order in the field h. This yields

$$f = \bigg(\frac{1}{2} - \frac{1}{4\theta}\bigg)\, m^2 + \frac{m^4}{64\theta^3} - \frac{hm}{2\,\theta} + \ldots \ ,$$

from which we read off $\theta_\mathrm{c} = \frac{1}{2}$, *i.e.* $T_\mathrm{c} = \hat{J}(0)/2k_\mathrm{B}$.

(e) The above free energy is of the standard Landau form for an Ising system, therefore $\alpha = 0$, $\beta = \frac{1}{2}$, $\gamma = 1$, and $\delta = 3$. The $\mathsf{O}(2)$ symmetry, which cannot be spontaneously broken in dimensions $d \le 2$, is not reflected in the mean field solution. In $d = 2$, the $\mathsf{O}(2)$ model *does* have a finite temperature phase transition, but one which is *not associated with a spontaneous breaking of the symmetry group*. The $\mathsf{O}(2)$ model in $d = 2$ undergoes a Kosterlitz-Thouless transition, which is associated with the unbinding of vortex-antivortex pairs as T exceeds T_c. The existence of vortex excitations in the $\mathsf{O}(2)$ model in $d = 2$ is a special feature of the topology of the group.

(4) Consider the free energy

$$f(\theta, m) = f_0 + \tfrac{1}{2}am^2 + \tfrac{1}{4}bm^4 + \tfrac{1}{8}dm^8$$

with $d > 0$. Note there is an octic term but no sextic term. Derive results corresponding to those in fig. 7.17 of the lecture notes. Find the equation of the first order line in the $(a/d, b/d)$ plane. Also identify the region in parameter space where there exist metastable local minima in the free energy (curve E in fig. 7.17).

Note that

$$\begin{aligned} f(m) &= f_0 + \tfrac{1}{2}am^2 + \tfrac{1}{4}bm^4 + \tfrac{1}{8}dm^8 \\ f'(m) &= am + bm^3 + dm^7 \\ f''(m) &= a + 3bm^2 + 7dm^6 \quad . \end{aligned}$$

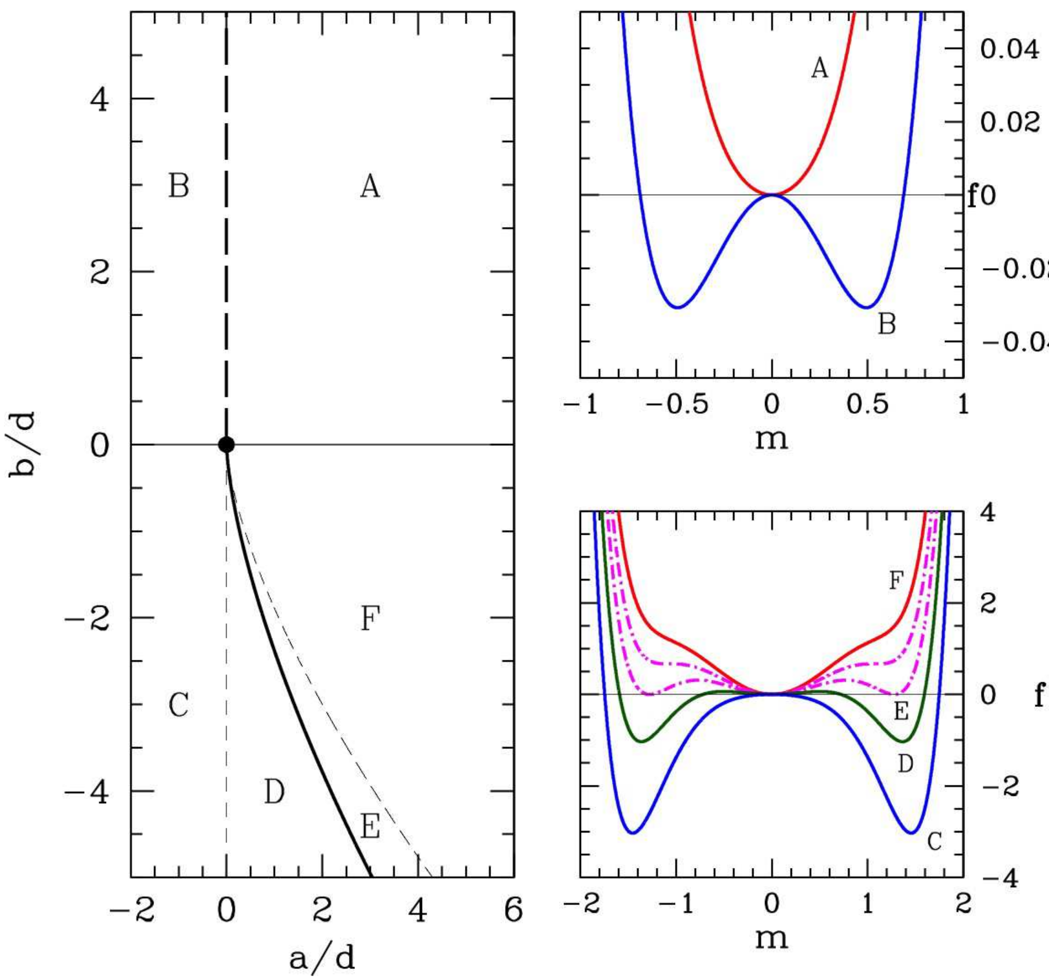

Figure 2: Regimes for the octic free energy in problem 5..

To find the first order line, we set $f(m) = f_0$ and $f'(m) = 0$ simultaneously. Dividing out by the root at $m = 0$ we obtain the simultaneous equations

$$\frac{1}{2}a + \frac{1}{4}bm^2 + \frac{1}{8}dm^6 = 0$$
$$a + bm^2 + dm^6 = 0 \quad .$$

Eliminating the m^6 terms, we obtain $m^2 = 3a/|b|$ (remember $a > 0$ and $b < 0$ for a first order transition). Inserting this back in either of the above equations yields the relation

$$a^* = \sqrt{\frac{2|b|^3}{27d}} \quad .$$

To obtain the condition for the saddle-node bifurcation, where the metastable $m \neq 0$ local minima in $f(m)$ first appear, we simultaneously solve $f'(m) = 0$ and $f''(m) = 0$, yielding the simultaneous equations

$$\begin{aligned} a + bm^2 + dm^6 &= 0 \\ a + 3bm^2 + 7dm^6 &= 0 \quad . \end{aligned}$$

Again we eliminate the m^6 term and solve for m^2, obtaining $m^2 = 3a/2|b|$. Inserting this back into either of the above equations yields the condition for the first order transition,

$$a_{\rm c} = \sqrt{\frac{4|b|^3}{27d}} \quad .$$

The results are plotted in fig. 2.