PHYSICS 210A : STATISTICAL PHYSICS
HW ASSIGNMENT #7

(1) Consider the ferromagnetic XY model, with

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

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 $\mathsf{H} > 0$, 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 $\cos(\phi_i - \phi_j) = \mathsf{Re}\,(z_i z_j^*)$.

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

(d) Find T_c.

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

Solution :

(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

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

The mean field free energy is then

$$\begin{aligned} F &= \tfrac{1}{2} N \hat{J}(0)\, m^2 - N k_B T \ln\left[\int\limits_0^{2\pi} \frac{d\phi}{2\pi}\, e^{(\hat{J}(0) m + \mathsf{H})\cos\phi / k_B T}\right] \\ &= \tfrac{1}{2} N \hat{J}(0)\, m^2 - N k_B T \ln I_0\!\left(\frac{\hat{J}(0)\, m + \mathsf{H}}{k_B T}\right) \ , \end{aligned}$$

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

(c) Differentiating, we find

$$\frac{\partial F}{\partial m} = 0 \qquad \Longrightarrow \qquad m = \frac{I_1\!\left(\frac{\hat{J}(0) m + \mathsf{H}}{k_B T}\right)}{I_0\!\left(\frac{\hat{J}(0) m + \mathsf{H}}{k_B T}\right)} \ ,$$

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 $h = \mathsf{H}/\hat{J}(0)$. 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

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

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 $d \leq 2$, 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.

(2) Consider a nearest neighbor two-state Ising *antiferromagnet* on a triangular lattice. The Hamiltonian is

$$\hat{H} = J \sum_{\langle ij \rangle} \sigma_i \sigma_j - \mathsf{H} \sum_i \sigma_i \ ,$$

with $J > 0$.

(a) Show graphically that the triangular lattice is *tripartite*, *i.e.* that it may be decomposed into three component sublattices A, B, and C such that every neighbor of A is either B or C, *etc.*

(b) Use a variational density matrix which is a product over single site factors, where

$$\begin{aligned} \rho(\sigma_i) &= \frac{1+m}{2}\, \delta_{\sigma_i,+1} + \frac{1-m}{2}\, \delta_{\sigma_i,-1} \qquad \text{if } i \in \mathrm{A} \text{ or } i \in \mathrm{B} \\ &= \frac{1+m_{\mathrm{C}}}{2}\, \delta_{\sigma_i,+1} + \frac{1-m_{\mathrm{C}}}{2}\, \delta_{\sigma_i,-1} \qquad \text{if } i \in \mathrm{C} \ . \end{aligned}$$

Compute the variational free energy $F(m, m_{\mathrm{C}}, T, \mathsf{H}, N)$.

(c) Find the mean field equations.

(d) Find the mean field phase diagram.

(e) While your mean field analysis predicts the existence of an ordered phase, it turns out that $T_{\mathrm{c}} = 0$ for this model because it is so highly frustrated for $h = 0$. The ground

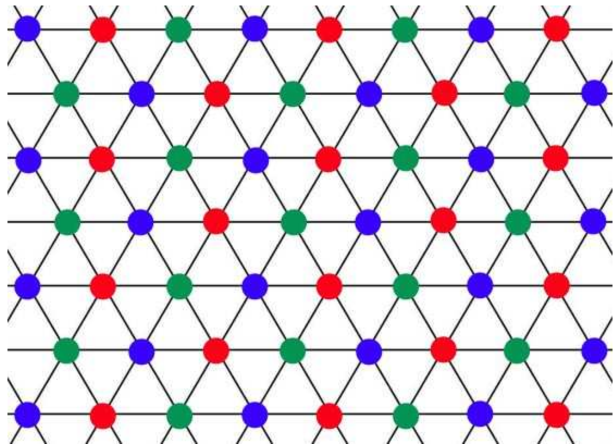

Figure 1: **(2)**(a) The three triangular sublattices of the (tripartite) triangular lattice.

state is highly degenerate. Show that for any ground state, no triangle can be completely ferromagnetically aligned. What is the ground state energy? Find a lower bound for the ground state entropy per spin.

Solution :

(a) See fig. 1.

(b) Of the $3N$ links of the lattice, N are between A and B sites, N are between A and C sites, and N are between B and C sites. Thus the mean field energy is

$$E = NJm^2 + 2NJmm_{\rm C} - \tfrac{2}{3}N\mathsf{H}m - \tfrac{1}{3}N\mathsf{H}m_{\rm C} \ .$$

The entropy of the A and B sublattices is $S_{\rm A} = S_{\rm B} = \frac{2}{3}Ns(m)$, while that for the C sublattice is $S_{\rm C} = \frac{1}{3}Ns(m_{\rm C})$, where

$$s(m) = -\bigg[\bigg(\frac{1+m}{2}\bigg)\ln\bigg(\frac{1+m}{2}\bigg) + \bigg(\frac{1-m}{2}\bigg)\ln\bigg(\frac{1-m}{2}\bigg)\bigg] \ .$$

The free energy is $F = E - TS$. We define $f \equiv F/2JN$, $\theta \equiv k_{\rm B}T/6J$, and $h \equiv \mathsf{H}/6J$. Then

$$f(m, m_{\rm C}, \theta, h) = \tfrac{1}{2}m^2 + mm_{\rm C} - 2hm - hm_{\rm C} - 2\theta s(m) - \theta s(m_{\rm C}) \ .$$

(c) The mean field equations are

$$\frac{\partial f}{\partial m} = 0 = m + m_{\rm C} - 2h + \theta\ln\bigg(\frac{1+m}{1-m}\bigg)$$

$$\frac{\partial f}{\partial m_{\rm C}} = 0 = m - h + \tfrac{1}{2}\theta\ln\bigg(\frac{1+m_{\rm C}}{1-m_{\rm C}}\bigg) \ .$$

Equivalently,

$$m = \tanh\left(\frac{2h - m - m_{\rm C}}{2\theta}\right) \qquad , \qquad m_{\rm C} = \tanh\left(\frac{h-m}{\theta}\right) .$$

(d) The order parameter for our model is the difference in sublattice magnetizations, $\varepsilon \equiv m_{\rm C} - m$. Let us first consider the zero temperature limit, $\theta \to 0$, for which the entropy term makes no contribution in the free energy. We compare two competing states: the ferromagnetic state with $m = m_{\rm C} = 1$, and the antiferromagnetic state with $m = 1$ and $m_{\rm C} = -1$. The energies of these two states are

$$e_0(1,1,h) = \tfrac{3}{2} - 3h$$

$$e_0(1,-1,h) = -\tfrac{1}{2} - h \ .$$

We see that for $h < 1$ the AF configuration wins (*i.e.* has lower energy per site e_0), while for $h > 1$ the F configuration wins. Thus, at $\theta = 0$ there is a first order transition from AF to F at $h_{\rm c} = 1$.

Next, let us examine the behavior with θ when $h = 0$. We can combine the two mean field equations to give

$$m + \theta \, \ln\left(\frac{1+m}{1-m}\right) = \tanh\big(m/\theta\big) \ .$$

Expanding in powers of m, we equate the coefficient of the linear term on either side to identify $\theta_{\rm c}$ and thus we obtain the equation $2\theta^2 + \theta - 1 = (2\theta - 1)(\theta + 1) = 0$, hence $\theta_{\rm c}(h = 0) = 1$.

We identify the order parameter as $\varepsilon = m_{\rm C} - m$, the difference in the sublattice magnetizations. We now seek the phase boundary $h(\theta)$ along which the order parameter vanishes in the (θ, h) plane. To this end, we write the two mean field equations in terms of m and ε, rather than m and $m_{\rm C}$. We find

$$\begin{aligned} m + \tfrac{1}{2}\varepsilon &= h - \frac{\theta}{2}\ln\left(\frac{1+m}{1-m}\right) \\ m &= h - \frac{\theta}{2}\ln\left(\frac{1+m+\varepsilon}{1-m-\varepsilon}\right) . \end{aligned}$$

Taking the difference, we obtain

$$\varepsilon = \theta \ln\left(\frac{1 + \frac{\varepsilon}{1+m}}{1 - \frac{\varepsilon}{1-m}}\right) = \frac{2\varepsilon\theta}{1-m^2} + \mathcal{O}\big(\varepsilon^2\big) \ .$$

Along the phase boundary, *i.e.* in the $\varepsilon \to 0$ limit, we therefore have

$$\frac{2\theta}{1-m^2} = 1 \ .$$

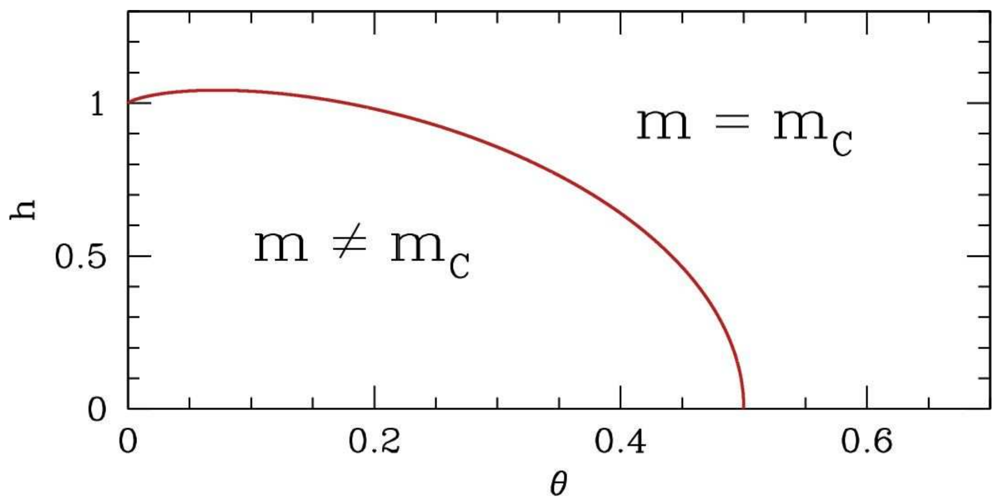

Figure 2: **(2)**(d) Phase diagram for the mean field theory of problem 2.

We also have the mean field equation for m,

$$m = \tanh\left(\frac{h - m}{\theta}\right) .$$

Putting these together, we obtain the curve

$$h^*(\theta) = \sqrt{1 - 2\theta} + \frac{\theta}{2} \ln\left(\frac{1 + \sqrt{1 - 2\theta}}{1 - \sqrt{1 - 2\theta}}\right) .$$

The phase boundary is shown in Fig. 2.

If we eliminate $m_{\rm C}$ through the second mean field equation, we can generate the Landau expansion

$$\begin{aligned} f(m, \theta, h) = -3\ln(2)\,\theta + \big(\theta - \tfrac{1}{2}\big)\big(\theta^{-1} + 1\big)\, m^2 + \tfrac{1}{6}\big(\theta + \tfrac{1}{2}\theta^{-3}\big)\, m^4 \\ - 2\theta^{-1}\big(\theta - \tfrac{1}{2}\big)\, hm - \tfrac{1}{3}\theta^{-3} h m^3 + \mathcal{O}\big(m^6, hm^5, h^3\big) \end{aligned}$$

The full expression $f(m, m_{\rm C}(m), \theta, h)$ is shown as a function of m for various values of θ and h in fig. 3. Thus, we obtain a Landau theory with a second order transition at $\theta_{\rm c} = \frac{1}{2}$. We retain the $\mathcal{O}\big(hm^3\big)$ term because the coefficient of hm vanishes at $\theta = \theta_{\rm c}$. Differentiating with respect to m, we obtain

$$\frac{\partial f}{\partial m} = 0 = 2\theta^{-1}\big(\theta + 1\big)\big(\theta - \tfrac{1}{2}\big)\, m + \tfrac{1}{3}\theta^{-3}\big(1 + 2\theta^4\big)\, m^3 - 2\theta^{-1}\big(\theta - \tfrac{1}{2}\big)\, h - \theta^{-2} h m^2$$

Thus,

$$m\big(\theta, h_{\rm c}\big) = \sqrt{2}\, \big(\theta_{\rm c} - \theta\big)_{+}^{1/2} + \mathcal{O}\big(|\theta - \theta_{\rm c}|^{3/2}\big)$$

$$m\big(\theta, h\big) = \tfrac{2}{3} h + \mathcal{O}\big(h^3\big)$$

$$m\big(\theta_{\rm c}, h\big) = \tfrac{4}{3} h + \mathcal{O}\big(h^3\big) .$$

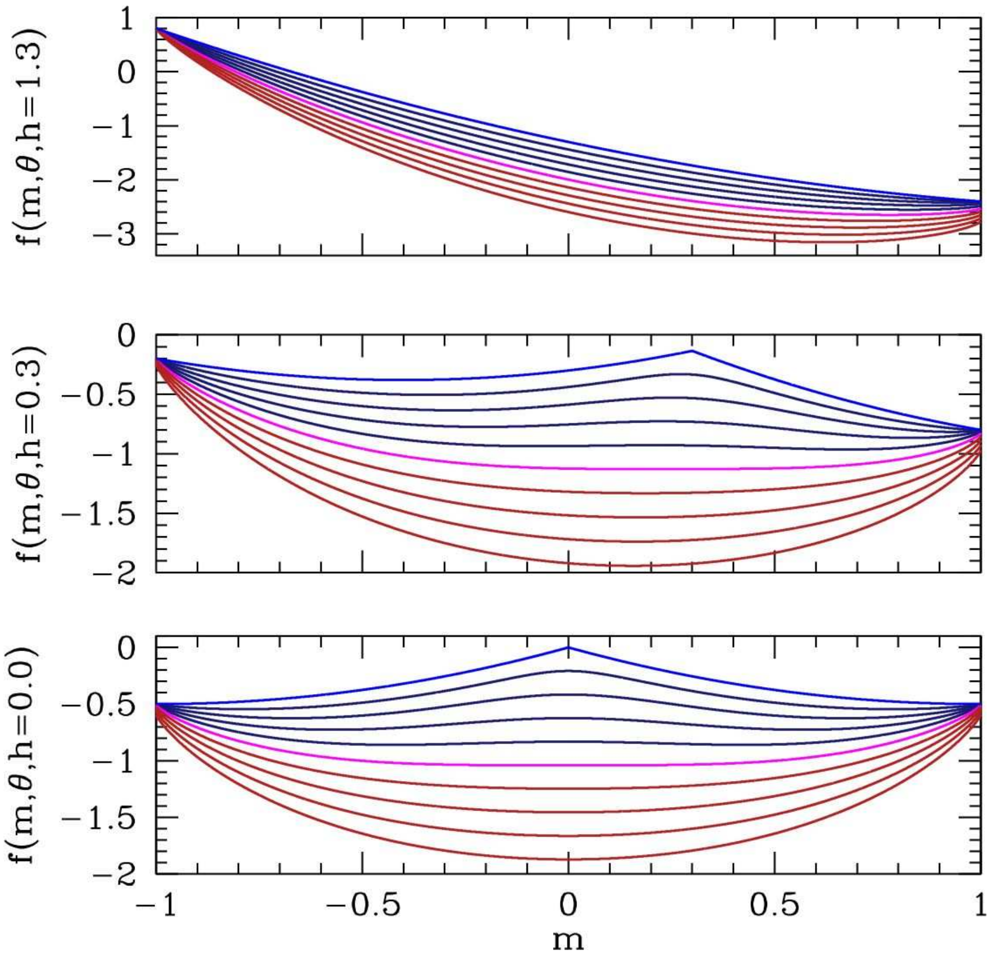

Figure 3: **(2)**(d) Free energy for the mean field theory of problem (2) at ten equally spaced dimensionless temperatures between $\theta = 0.0$ and $\theta = 0.9$. Bottom panel: $h = 0$; middle panel: $h = 0.3$; top panel: $h = 1.3$.

Note that $h_{\mathrm{c}} = 0$. In the second equation, we have $\epsilon \equiv \theta - \theta_{\mathrm{c}} \to 0$ with $\epsilon \gg h$, while in the third equation we have $h \to 0$ with $\epsilon \equiv 0$, so the two equations represent two different limits. We obtain the exponents $\alpha = 0$, $\beta = \frac{1}{2}$, $\gamma = 0$, $\delta = 1$. This seemingly violates the Rushbrooke scaling law $\alpha + 2\beta + \gamma = 2$, but satisfies the Griffiths relation $\beta + \gamma = \beta\delta$. However, this is because we are using the wrong field. Rather than defining the exponents γ and δ with respect to a uniform field h, we should instead consider a *staggered* field h_{s} such that $h_{\mathrm{A}} = h_{\mathrm{B}} = h_{\mathrm{s}}$ but $h_{\mathrm{C}} = -h_{\mathrm{s}}$.

(e) With antiferromagnetic interactions and $h = 0$, it is impossible for every link on an odd-membered ring (*e.g.* a triangle) to be satisfied. This is because on a k-site ring (with $(k+1) \equiv 1$), taking the product of $\sigma_j \sigma_{j+1}$ over all links on the ring gives

$$\big(\sigma_1 \sigma_2\big)\big(\sigma_2 \sigma_3\big) \cdots \big(\sigma_k \sigma_1\big) = 1 \ ,$$

If we assume, however, that each link satisfies the antiferromagnetic interaction, then

$\sigma_j \sigma_{j+1} = -1$ and the product would be $(-1)^k = -1$ since k is odd. So not all odd-membered rings can be completely satisfied. Clearly the best we can do on any odd-membered ring is to have $k-1$ of the bonds antiferromagnetically aligned and the remaining bond ferromagnetically aligned.

Now let us decompose the triangular lattice into A, B, and C sublattices. If we place all spins on the A and B sublattices are up ($\sigma = +1$) and all spins on the C sublattice are down ($\sigma = -1$), then each elementary triangle has two AF bonds and one F bond, which is the best we can do for the nearest neighbor triangular lattice Ising antiferromagnet. The energy of this configuration is given in part (b) above: $E = NJm^2 + 2NJmm_{\mathrm{C}} = -NJ$, since $m = 1$ and $m_{\mathrm{C}} = -1$. However, it is clear that at each site of the B sublattice, the choice of σ_i is arbitrary. This is because one third of all the links on the lattice are AC links, and they are already antiferromagnetically aligned. Now there are $\frac{1}{3}N$ sites on each of the sublattices, hence we have identified $2^{N/3}$ degenerate ground states. This set of ground state configurations is not complete, however. We could immediately double it simply by choosing to reverse spins on the A sublattice instead, leaving the B sublattice with $m_{\mathrm{B}} = 1$. But even this enumeration is not complete – we have simply identified a lower bound to the number of degenerate ground states. The ground state entropy per spin is then

$$\frac{S_0}{N} \geq \tfrac{1}{3} \ln 2 \approx 0.23105 \ .$$

The exact value, obtained by Wannier and by Houtappel in 1950, is $s_0 \approx 0.3231$ per spin. So there are exponentially (in the system size!) many more ground states than we have identified here.

(3) A system is described by the Hamiltonian

$$\hat{H} = -J \sum_{\langle ij \rangle} \mathcal{I}(\mu_i, \mu_j) - \mathsf{H} \sum_i \delta_{\mu_i, \mathrm{A}} \ , \tag{1}$$

where on each site i there are four possible choices for μ_i: $\mu_i \in \{\mathrm{A}, \mathrm{B}, \mathrm{C}, \mathrm{D}\}$. The interaction matrix $\mathcal{I}(\mu, \mu')$ is given in the following table:

$\mathcal{I}$	A	B	C	D
A	$+1$	-1	-1	0
B	-1	$+1$	0	-1
C	-1	0	$+1$	-1
D	0	-1	-1	$+1$

(a) Write a trial density matrix

$$\varrho(\mu_1, \ldots, \mu_N) = \prod_{i=1}^{N} \varrho_1(\mu_i)$$
$$\varrho_1(\mu) = x\, \delta_{\mu,\mathrm{A}} + y(\delta_{\mu,\mathrm{B}} + \delta_{\mu,\mathrm{C}} + \delta_{\mu,\mathrm{D}}) \ .$$

What is the relationship between x and y? Henceforth use this relationship to eliminate y in terms of x.

(b) What is the variational energy per site, $E(x, T, \mathsf{H})/N$?

(c) What is the variational entropy per site, $S(x, T, \mathsf{H})/N$?

(d) What is the mean field equation for x?

(e) What value x^* does x take when the system is disordered?

(f) Write $x = x^* + \frac{3}{4}\varepsilon$ and expand the free energy to fourth order in ε. (The factor $\frac{3}{4}$ should generate manageable coefficients in the Taylor series expansion.)

(g) Sketch ε as a function of T for $\mathsf{H} = 0$ and find T_c. Is the transition first order or second order?

Solution :

(a) Clearly we must have $y = \frac{1}{3}(1 - x)$ in order that $\mathsf{Tr}(\varrho_1) = x + 3y = 1$.

(b) We have

$$\frac{E}{N} = -\tfrac{1}{2} zJ\big(x^2 - 4\,xy + 3\,y^2 - 4\,y^2\big) - \mathsf{H}x \ ,$$

The first term in the bracket corresponds to AA links, which occur with probability x^2 and have energy $-J$. The second term arises from the four possibilities AB, AC, BA, CA, each of which occurs with probability xy and with energy $+J$. The third term is from the BB, CC, and DD configurations, each with probability y^2 and energy $-J$. The last term is from the BD, CD, DB, and DC configurations, each with probability y^2 and energy $+J$. Finally, there is the field term. Eliminating $y = \frac{1}{3}(1 - x)$ from this expression we have

$$\frac{E}{N} = \tfrac{1}{18} zJ\big(1 + 10\,x - 20\,x^2\big) - \mathsf{H}x$$

Note that with $x = 1$ we recover $E = -\frac{1}{2}NzJ - \mathsf{H}$, *i.e.* an interaction energy of $-J$ per link and a field energy of $-\mathsf{H}$ per site.

(c) The variational entropy per site is

$$\begin{aligned} s(x) &= -k_{\mathrm{B}}\, \mathsf{Tr}\,\big(\varrho_1 \ln \varrho_1\big) \\ &= -k_{\mathrm{B}}\Big(x \ln x + 3y \ln y\Big) \\ &= -k_{\mathrm{B}}\left[x \ln x + (1 - x) \ln\!\left(\frac{1 - x}{3}\right)\right] . \end{aligned}$$

(d) It is convenient to adimensionalize, writing $f = F/N\varepsilon_0$, $\theta = k_{\mathrm{B}}T/\varepsilon_0$, and $h = \mathsf{H}/\varepsilon_0$, with $\varepsilon_0 = \frac{5}{9} zJ$. Then

$$f(x,\theta,h) = \tfrac{1}{10} + x - 2x^2 - hx + \theta \left[x \ln x + (1-x) \ln\!\left(\frac{1-x}{3}\right) \right] .$$

Differentiating with respect to x, we obtain the mean field equation

$$\frac{\partial f}{\partial x} = 0 \qquad \Longrightarrow \qquad 1 - 4x - h + \theta \ln\!\left(\frac{3x}{1-x}\right) = 0 \ .$$

(e) When the system is disordered, there is no distinction between the different polarizations of μ_0. Thus, $x^* = \frac{1}{4}$. Note that $x = \frac{1}{4}$ is a solution of the mean field equation from part (d) when $h = 0$.

(f) Find

$$f\big(x = \tfrac{1}{4} + \tfrac{3}{4}\,\varepsilon, \theta, h\big) = f_0 + \tfrac{3}{2}\big(\theta - \tfrac{3}{4}\big)\,\varepsilon^2 - \theta\,\varepsilon^3 + \tfrac{7}{4}\,\theta\,\varepsilon^4 - \tfrac{3}{4}\,h\,\varepsilon$$

with $f_0 = \frac{9}{40} - \frac{1}{4}h - \theta \ln 4$.

(g) For $h = 0$, the cubic term in the mean field free energy leads to a first order transition which preempts the second order one which would occur at $\theta^* = \frac{3}{4}$, where the coefficient of the quadratic term vanishes. We learned in §6.7.1,2 of the notes that for a free energy $f = \frac{1}{2}am^2 - \frac{1}{3}ym^3 + \frac{1}{4}bm^4$ that the first order transition occurs for $a = \frac{2}{9}\,b^{-1}y^2$, where the magnetization changes discontinuously from $m = 0$ at $a = a_c^+$ to $m_0 = \frac{2}{3}\,b^{-1}y$ at $a = a_c^-$. For our problem here, we have $a = 3\big(\theta - \frac{3}{4}\big)$, $y = 3\theta$, and $b = 7\theta$. This gives

$$\theta_c = \tfrac{63}{76} \approx 0.829 \qquad , \qquad \varepsilon_0 = \tfrac{2}{7} \ .$$

As θ decreases further below θ_c to $\theta = 0$, ε increases to $\varepsilon(\theta = 0) = 1$. No sketch needed!