7 Mean Field Theory of Phase Transitions : Worked Examples

(7.1) Find v_c, T_c, and p_c for the equation of state,

$$p = \frac{RT}{v-b} - \frac{\alpha}{v^3} \quad .$$

Solution :

We find $p'(v)$:

$$\frac{\partial p}{\partial v} = -\frac{RT}{(v-b)^2} + \frac{3\alpha}{v^4} \quad .$$

Setting this to zero yields the equation

$$f(u) \equiv \frac{u^4}{(u-1)^2} = \frac{3\alpha}{RTb^2} \quad ,$$

where $u \equiv v/b$ is dimensionless. The function $f(u)$ on the interval $[1,\infty]$ has a minimum at $u = 2$, where $f_{\rm min} = f(2) = 16$. This determines the critical temperature, by setting the RHS of the above equation to $f_{\rm min}$. Then evaluate $p_c = p(v_c, T_c)$. One finds

$$v_c = 2b \quad , \quad T_c = \frac{3\alpha}{16Rb^2} \quad , \quad p_c = \frac{\alpha}{16b^3} \quad .$$

(7.2) The Dieterici equation of state is

$$p\,(v-b) = RT\,\exp\!\bigg(-\frac{a}{vRT}\bigg) \quad .$$

(a) Find the critical point (p_c, v_c, T_c) for this equation of state

(b) Writing $\bar{p} = p/p_c$, $\bar{v} = v/v_c$, and $\bar{T} = T/T_c$, rewrite the equation of state in the form $\bar{p} = \bar{p}(\bar{v}, \bar{T})$.

(c) *For the brave only!* Writing $\bar{p} = 1 + \pi$, $\bar{T} = 1 + t$, and $\bar{v} = 1 + \epsilon$, find $\epsilon_{\rm liq}(t)$ and $\epsilon_{\rm gas}(t)$ for $0 < (-t) \ll 1$, working to lowest nontrivial order in $(-t)$.

Solution :

(a) We have

$$p = \frac{RT}{v-b}\,e^{-a/vRT} \quad ,$$

hence

$$\bigg(\frac{\partial p}{\partial v}\bigg)_{\!T} = p \cdot \bigg\{ -\frac{1}{v-b} + \frac{a}{v^2 RT} \bigg\} \quad .$$

Setting the LHS of the above equation to zero, we then have

$$\frac{v^2}{v-b} = \frac{a}{RT} \quad \Rightarrow \quad f(u) \equiv \frac{u^2}{u-1} = \frac{a}{bRT} \quad ,$$

where $u = v/b$ is dimensionless. Setting $f'(u^*) = 0$ yields $u^* = 2$, hence $f(u)$ on the interval $u \in (1,\infty)$ has a unique global minimum at $u = 2$, where $f(2) = 4$. Thus,

$$v_c = 2b \quad , \quad T_c = \frac{a}{4bR} \quad , \quad p_c = \frac{a}{4b^2}\,e^{-2} \quad .$$

(b) In terms of the dimensionless variables $\bar{p}$, $\bar{v}$, and $\bar{T}$, the equation of state takes the form

$$\bar{p} = \frac{\bar{T}}{2\bar{v}-1}\,\exp\!\bigg(2 - \frac{2}{\bar{v}\bar{T}}\bigg) \quad .$$

When written in terms of the dimensionless deviations π, ϵ, and t, this becomes

$$\pi = \bigg(\frac{1+t}{1+2\epsilon}\bigg)\exp\bigg(\frac{2(\epsilon+t+\epsilon t)}{1+\epsilon+t+\epsilon t}\bigg) - 1 \quad .$$

Expanding via Taylor's theorem, one finds

$$\pi(\epsilon,t) = 3t - 2t\epsilon + 2t^2 - \tfrac{2}{3}\epsilon^3 + 2\epsilon^2 t - 4\epsilon t^2 - \tfrac{2}{3}t^3 + \ldots \quad .$$

Thus,

$$\pi_{\epsilon t} \equiv \frac{\partial^2\pi}{\partial\epsilon\,\partial t} = -2 \quad , \quad \pi_{\epsilon\epsilon\epsilon} \equiv \frac{\partial^3\pi}{\partial\epsilon^3} = -4 \quad ,$$

and according to the results in ch. 7 of the lecture notes, we have

$$\epsilon_{\mathsf{L,G}} = \mp\bigg(\frac{6\,\pi_{\epsilon t}}{\pi_{\epsilon\epsilon\epsilon}}\bigg)^{1/2} = \mp\big(-3t\big)^{1/2} \quad .$$

(7.3) Consider a ferromagnetic spin-1 triangular lattice Ising model . The Hamiltonian is

$$\hat{H} = -J \sum_{\langle ij \rangle} S_i^z \, S_j^z - H \sum_i S_i^z \quad ,$$

where $S_i^z \in \{-1\,,\,0\,,\,+1\}$ on each site i, H is a uniform magnetic field, and where the first sum is over all links of the lattice.

(a) Derive the mean field Hamiltonian $\hat{H}_{\rm MF}$ for this model.

(b) Derive the free energy per site F/N within the mean field approach.

(c) Derive the self consistent equation for the local moment $m = \langle S_i^z \rangle$.

(d) Find the critical temperature $T_{\rm c}(H=0)$.

(e) Assuming $|H| \ll k_{\rm B}|T - T_{\rm c}| \ll J$, expand the dimensionless free energy $f = F/6NJ$ in terms of $\theta = T/T_{\rm c}$, $h = H/k_{\rm B}T_{\rm c}$, and m. Minimizing with respect to m, find an expression for the dimensionless magnetic susceptibility $\chi = \partial m/\partial h$ close to the critical point.

Solution :

(a) Writing $S_i^z = m + \delta S_i^z$, where $m = \langle S_i^z \rangle$ and expanding $\hat{H}$ to linear order in the fluctuations δS_i^z, we find

$$\hat{H}_{\rm MF} = \tfrac{1}{2} N z J m^2 - (H + zJm) \sum_i S_i^z \quad ,$$

where $z = 6$ for the triangular lattice.

(b) The free energy per site is

$$\begin{aligned} F/N &= \tfrac{1}{2} z J m^2 - k_{\rm B} T \ln \text{Tr}\, e^{(H+zJm)S^z} \\ &= \tfrac{1}{2} z J m^2 - k_{\rm B} T \ln\left\{ 1 + 2\cosh\left(\frac{H + zJm}{k_{\rm B}T}\right) \right\} \quad . \end{aligned}$$

(c) The mean field equation is $\partial F/\partial m = 0$, which is equivalent to $m = \langle S_i^z \rangle$. We obtain

$$m = \frac{2\sinh\left(\frac{H+zJm}{k_{\rm B}T}\right)}{1 + 2\cosh\left(\frac{H+zJm}{k_{\rm B}T}\right)} \quad .$$

(d) To find $T_{\rm c}$, we set $H = 0$ in the mean field equation:

$$\begin{aligned} m &= \frac{2\sinh(\beta z J m)}{1 + 2\cosh(\beta z J m)} \\ &= \tfrac{2}{3} \beta z J m + \mathcal{O}(m^3) \quad . \end{aligned}$$

The critical temperature is obtained by setting the slope on the RHS of the above equation to unity. Thus,

$$T_{\rm c} = \frac{2zJ}{3k_{\rm B}} \quad .$$

So for the triangular lattice, where $z = 6$, one has $T_{\rm c} = 4J/k_{\rm B}$.

(e) Scaling T and H as indicated, the mean field equation becomes

$$m = \frac{2\sinh\big((m+h)/\theta\big)}{1+2\cosh\big((m+h)/\theta\big)} = \frac{m+h}{\theta/\theta_\mathrm{c}} + \ldots \quad ,$$

where $\theta_\mathrm{c} = \frac{2}{3}$, and where we assume $\theta > \theta_\mathrm{c}$. Solving for $m(h)$, we have

$$m = \frac{h}{1-\frac{\theta_\mathrm{c}}{\theta}} = \frac{\theta_\mathrm{c}\, h}{\theta - \theta_\mathrm{c}} + \mathcal{O}\big((\theta-\theta_\mathrm{c})^2\big) \quad .$$

Thus, $\chi = \theta_\mathrm{c}/(\theta - \theta_\mathrm{c})$, which reflects the usual mean field susceptibility exponent $\gamma = 1$.

(7.4) Consider a ferromagnetic spin-S Ising model on a lattice of coordination number z. The Hamiltonian is

$$\hat{H} = -J\sum_{\langle ij\rangle} \sigma_i\,\sigma_j - \mu_0 H \sum_i \sigma_i \quad ,$$

where $\sigma \in \{-S, -S+1, \ldots, +S\}$ with $2S \in \mathbb{Z}$.

(a) Find the mean field Hamiltonian $\hat{H}_{\rm MF}$.

(b) Adimensionalize by setting $\theta \equiv k_{\rm B}T/zJ$, $h \equiv \mu_0 H/zJ$, and $f \equiv F/NzJ$. Find the dimensionless free energy per site $f(m,h)$ for arbitrary S.

(c) Expand the free energy as

$$f(m,h) = f_0 + \tfrac{1}{2}am^2 + \tfrac{1}{4}bm^4 - chm + \mathcal{O}(h^2, hm^3, m^6)$$

and find the coefficients f_0, a, b, and c as functions of θ and S.

(d) Find the critical point $(\theta_{\rm c}, h_{\rm c})$.

(e) Find $m(\theta_{\rm c}, h)$ to leading order in h.

Solution :

(a) Writing $\sigma_i = m + \delta\sigma_i$, we find

$$\hat{H}_{\rm MF} = \tfrac{1}{2}NzJm^2 - (\mu_0 H + zJ)\sum_i \sigma_i \quad .$$

(b) Using the result

$$\sum_{\sigma=-S}^{S} e^{\beta\mu_0 H_{\rm eff}\sigma} = \frac{\sinh\big((S+\frac{1}{2})\beta\mu_0 H\big)}{\sinh\big(\frac{1}{2}\beta\mu_0 H\big)} \quad ,$$

we have

$$f = \tfrac{1}{2}m^2 - \theta\ln\sinh\big((2S+1)(m+h)/2\theta\big) + \theta\ln\sinh\big((m+h)/2\theta\big) \quad .$$

(c) Expanding the free energy, we obtain

$$\begin{aligned} f &= f_0 + \tfrac{1}{2}am^2 + \tfrac{1}{4}bm^4 - chm + \mathcal{O}(h^2, hm^3, m^6) \\ &= -\theta\ln(2S+1) + \left(\frac{3\theta - S(S+1)}{6\theta}\right)m^2 + \frac{S(S+1)(2S^2+2S+1)}{360\,\theta^3}\,m^4 - \tfrac{2}{3}\,S(S+1)\,hm + \ldots \quad . \end{aligned}$$

Thus,

$$f_0 = -\theta\ln(2S+1) \quad , \quad a = 1 - \tfrac{1}{3}S(S+1)\theta^{-1} \quad , \quad b = \frac{S(S+1)(2S^2+2S+1)}{90\,\theta^3} \quad , \quad c = \tfrac{2}{3}\,S(S+1) \quad .$$

(d) Set $a=0$ and $h=0$ to find the critical point: $\theta_{\rm c} = \frac{1}{3}S(S+1)$ and $h_{\rm c} = 0$.

(e) At $\theta = \theta_{\rm c}$, we have $f = f_0 + \frac{1}{4}bm^4 - chm + \mathcal{O}(m^6)$. Extremizing with respect to m, we obtain $m = (ch/b)^{1/3}$. Thus,

$$m(\theta_{\rm c}, h) = \left(\frac{60}{2S^2+2S+1}\right)^{1/3} \theta\, h^{1/3} \quad .$$

(7.5) Consider the O(2) model,

$$\hat{H} = -\tfrac{1}{2}\sum_{i,j} J_{ij}\,\hat{\boldsymbol{n}}_i\cdot\hat{\boldsymbol{n}}_j - \boldsymbol{H}\cdot\sum_i \hat{\boldsymbol{n}}_i \quad ,$$

where $\hat{\boldsymbol{n}}_i = \cos\phi_i\,\hat{\boldsymbol{x}} + \sin\phi_i\,\hat{\boldsymbol{y}}$. Consider the case of infinite range interactions, where $J_{ij} = J/N$ for all i, j, where N is the total number of sites.

(a) Show that

$$\exp\left[\frac{\beta J}{2N}\sum_{i,j}\hat{\boldsymbol{n}}_i\cdot\hat{\boldsymbol{n}}_j\right] = \frac{N\beta J}{2\pi}\int\! d^2m\, e^{-N\beta J\boldsymbol{m}^2/2}\, e^{\beta J\boldsymbol{m}\cdot\sum_i\hat{\boldsymbol{n}}_i} \quad .$$

(b) Using the definition of the modified Bessel function $I_0(z)$,

$$I_0(z) = \int_0^{2\pi}\!\frac{d\phi}{2\pi}\, e^{z\cos\phi} \quad ,$$

show that

$$Z = \mathsf{Tr}\, e^{-\beta\hat{H}} = \int\! d^2m\, e^{-NA(\boldsymbol{m},\boldsymbol{h})/\theta} \quad ,$$

where $\theta = k_{\rm B}T/J$ and $\boldsymbol{h} = \boldsymbol{H}/J$. Find an expression for $A(\boldsymbol{m},\boldsymbol{h})$.

(c) Find the equation which extremizes $A(\boldsymbol{m},\boldsymbol{h})$ as a function of $\boldsymbol{m}$.

(d) Look up the properties of $I_0(z)$ and write down the first few terms in the Taylor expansion of $A(\boldsymbol{m},\boldsymbol{h})$ for small m and h. Solve for θ_c.

Solution :

(a) We have

$$\frac{\hat{H}}{k_{\rm B}T} = -\frac{J}{2Nk_{\rm B}T}\bigg(\sum_i\hat{\boldsymbol{n}}_i\bigg)^2 - \frac{\boldsymbol{H}}{k_{\rm B}T}\cdot\sum_i\hat{\boldsymbol{n}}_i \quad .$$

Therefore

$$\begin{aligned} e^{-\hat{H}/k_{\rm B}T} &= \exp\left[\frac{1}{2N\theta}\bigg(\sum_i\hat{\boldsymbol{n}}_i\bigg)^2 + \frac{\boldsymbol{h}}{\theta}\cdot\sum_i\hat{\boldsymbol{n}}_i\right] \\ &= \frac{N}{2\pi\theta}\int\! d^2m\,\exp\left[-\frac{N\boldsymbol{m}^2}{2\theta} + \bigg(\frac{\boldsymbol{m}+\boldsymbol{h}}{\theta}\bigg)\cdot\sum_i\hat{\boldsymbol{n}}_i\right] \quad . \end{aligned}$$

(b) Integrating the previous expression, we have

$$\begin{aligned} Z = \mathsf{Tr}\, e^{-\hat{H}/k_{\rm B}T} &= \prod_i\int\!\frac{d\hat{\boldsymbol{n}}_i}{2\pi}\, e^{-\hat{H}[\{\hat{\boldsymbol{n}}_i\}]/k_{\rm B}T} \\ &= \frac{N}{2\pi\theta}\int\! d^2m\, e^{-N\boldsymbol{m}^2/2\theta}\Big[I_0\big(|\boldsymbol{m}+\boldsymbol{h}|/\theta\big)\Big]^N \quad . \end{aligned}$$

Thus, we identify

$$A(\boldsymbol{m},\boldsymbol{h}) = \tfrac{1}{2}\boldsymbol{m}^2 - \theta\ln I_0\big(|\boldsymbol{m}+\boldsymbol{h}|/\theta\big) - \frac{\theta}{N}\ln(N/2\pi\theta) \quad .$$

(c) Extremizing with respect to the vector $\boldsymbol{m}$, we have

$$\frac{\partial A}{\partial \boldsymbol{m}} = \boldsymbol{m} - \frac{\boldsymbol{m}+\boldsymbol{h}}{|\boldsymbol{m}+\boldsymbol{h}|} \cdot \frac{I_1\big(|\boldsymbol{m}+\boldsymbol{h}|/\theta\big)}{I_0\big(|\boldsymbol{m}+\boldsymbol{h}|/\theta\big)} = 0 \quad ,$$

where $I_1(z) = I_0'(z)$. Clearly any solution requires that $\boldsymbol{m}$ and $\boldsymbol{h}$ be colinear, hence

$$m = \frac{I_1\big((m+h)/\theta\big)}{I_0\big((m+h)/\theta\big)} \quad .$$

(d) To find θ_c, we first set $h = 0$. We then must solve

$$m = \frac{I_1(m/\theta)}{I_0(m/\theta)} \quad .$$

The modified Bessel function $I_\nu(z)$ has the expansion

$$I_\nu(z) = \left(\tfrac{1}{2}z\right)^\nu \sum_{k=0}^{\infty} \frac{\left(\frac{1}{4}z^2\right)^k}{k!\,\Gamma(k+\nu+1)} \quad .$$

Thus,

$$\begin{aligned} I_0(z) &= 1 + \tfrac{1}{4}z^2 + \ldots \\ I_1(z) &= \tfrac{1}{2}z + \tfrac{1}{16}z^3 + \ldots \quad , \end{aligned}$$

and therefore $I_1(z)/I_0(z) = \frac{1}{2}z - \frac{1}{16}z^3 + \mathcal{O}(z^5)$, and we read off $\theta_c = \frac{1}{2}$.

(7.6) Consider the O(3) model,

$$\hat{H} = -J \sum_{\langle ij \rangle} \hat{\boldsymbol{n}}_i \cdot \hat{\boldsymbol{n}}_j - \boldsymbol{H} \cdot \sum_i \hat{\boldsymbol{n}}_i \quad ,$$

where each $\hat{\boldsymbol{n}}_i$ is a three-dimensional unit vector.

(a) Writing

$$\hat{\boldsymbol{n}}_i = \boldsymbol{m} + \delta\hat{\boldsymbol{n}}_i \quad ,$$

with $\boldsymbol{m} = \langle \hat{\boldsymbol{n}}_i \rangle$ and $\delta\hat{\boldsymbol{n}}_i = \hat{\boldsymbol{n}}_i - \boldsymbol{m}$, derive the mean field Hamiltonian.

(b) Compute the mean field free energy $f(m, \theta, \boldsymbol{h})$, where $\theta = k_{\rm B}T/zJ$ and $\boldsymbol{h} = \boldsymbol{H}/zJ$, with $f = F/NzJ$. Here z is the lattice coordination number and N the total number of lattice sites, as usual. You may assume that $\boldsymbol{m} \parallel \boldsymbol{h}$. Note that the trace over the local degree of freedom at each site i is given by

$$\mathop{\rm Tr}_i \rightarrow \int \frac{d\hat{\boldsymbol{n}}_i}{4\pi} \quad ,$$

where the integral is over all solid angle.

(c) Find the critical point $(\theta_{\rm c}, h_{\rm c})$.

(d) Find the behavior of the magnetic susceptibility $\chi = \partial m/\partial h$ as a function of temperature θ just above $\theta_{\rm c}$.

Solution :

(a) Making the mean field *Ansatz*, one obtains the effective field $\boldsymbol{H}_{\rm eff} = \boldsymbol{H} + zJ\boldsymbol{m}$, and the mean field Hamiltonian

$$\hat{H}_{\rm MF} = \tfrac{1}{2}NzJ\boldsymbol{m}^2 - (\boldsymbol{H} + zJ\boldsymbol{m}) \cdot \sum_i \hat{\boldsymbol{n}}_i \quad .$$

(b) We assume that $\boldsymbol{m} \parallel \boldsymbol{h}$, in which case

$$\begin{aligned} f(m, \theta, h) &= \tfrac{1}{2}m^2 - \theta \ln \int \frac{d\hat{\boldsymbol{n}}}{4\pi}\, e^{(m+h)\hat{\boldsymbol{z}}\cdot\hat{\boldsymbol{n}}/\theta} \\ &= \tfrac{1}{2}m^2 - \theta \ln\left(\frac{\sinh\big((m+h)/\theta\big)}{(m+h)/\theta}\right) \quad . \end{aligned}$$

Here we have without loss of generality taken $\boldsymbol{h}$ to lie in the $\hat{\boldsymbol{z}}$ direction.

(c) We expand $f(m, \theta, h)$ for small m and θ, obtaining

$$\begin{aligned} f(m, \theta, h) &= \tfrac{1}{2}m^2 - \frac{(m+h)^2}{6\,\theta} + \frac{(m+h)^4}{180\,\theta^3} + \ldots \\ &= \tfrac{1}{2}\left(1 - \frac{1}{3\theta}\right)m^2 - \frac{hm}{3\,\theta} + \frac{m^4}{180\,\theta^4} + \ldots \end{aligned}$$

We now read off $h_{\rm c} = 0$ and $\theta_{\rm c} = \frac{1}{3}$.

(d) Setting $\partial f/\partial m = 0$, we obtain

$$\left(1 - \frac{\theta_{\rm c}}{\theta}\right) m = \frac{\theta_{\rm c}}{\theta}\, hm + \mathcal{O}(m^3) \quad .$$

We therefore have

$$m(h, \theta > \theta_{\rm c}) = \frac{\theta_{\rm c}\, h}{\theta - \theta_{\rm c}} + \mathcal{O}(h^3) \qquad , \qquad \chi(\theta > \theta_{\rm c}) = \frac{\partial m}{\partial h}\bigg|_{h=0} = \frac{\theta_{\rm c}}{\theta - \theta_{\rm c}} \quad .$$

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

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

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 $\sigma_j \in \{-1, +1\}$.

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

(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}.

(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.*

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

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.

Solution :

(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

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

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

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

Adimensionalizing,

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

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

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

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

(c) Using

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

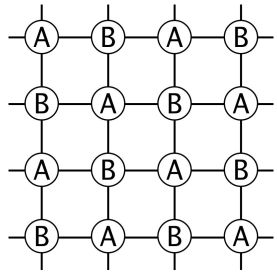

Figure 1: The square lattice and its A and B sublattices.

we have

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

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

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

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

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

(7.8) The spin lattice Hamiltonian for the three state ($\mathbb{Z}_3$) clock model is written

$$\hat{H} = -J \sum_{\langle ij \rangle} \hat{\boldsymbol{n}}_i \cdot \hat{\boldsymbol{n}}_j \quad ,$$

where each local unit vector $\hat{\boldsymbol{n}}_i$ is a planar spin which can take one of three possible values:

$$\hat{\boldsymbol{n}} = \hat{\mathbf{e}}_1 \quad , \quad \hat{\boldsymbol{n}} = -\tfrac{1}{2}\,\hat{\mathbf{e}}_1 + \tfrac{\sqrt{3}}{2}\,\hat{\mathbf{e}}_2 \quad , \quad \hat{\boldsymbol{n}} = -\tfrac{1}{2}\,\hat{\mathbf{e}}_1 - \tfrac{\sqrt{3}}{2}\,\hat{\mathbf{e}}_2 \quad .$$

Note that the *internal space* in which each unit vector $\hat{\boldsymbol{n}}_i$ exists is distinct from the physical Euclidean space in which the lattice points reside.

(a) Consider the clock model on a lattice of coordination number z. Make the mean field assumption $\langle \hat{\boldsymbol{n}}_i \rangle = m\,\hat{\mathbf{e}}_1$. Expanding the Hamiltonian to linear order in the fluctuations, derive the mean field Hamiltonian for this model $\hat{H}_{\text{MF}}$.

(b) Rescaling $\theta = k_{\text{B}}T/zJ$ and $f = F/NzJ$, where F is the Helmholtz free energy and N is the number of sites, find $f(m,\theta)$.

(c) Is the transition second order or first order? Why?

(d) Find the equations which determine the critical temperature θ_{c}.

(e) Show that this model is equivalent to the three state Potts model. Is the $\mathbb{Z}_4$ clock model equivalent to the four state Potts model? Why or why not?

Solution :

(a) We can solve the mean field theory on a general lattice of coordination number z. The mean field Hamiltonian is

$$\hat{H}_{\text{MF}} = \tfrac{1}{2} N z J m^2 - zJm\,\hat{\mathbf{e}}_1 \cdot \sum_i \hat{\boldsymbol{n}}_i \quad .$$

(b) We have

$$\begin{aligned} f(m,\theta) &= \tfrac{1}{2}m^2 - \theta \ln \operatorname*{Tr}_{\hat{\boldsymbol{n}}} \exp\big(m\,\hat{\mathbf{e}}_1 \cdot \hat{\boldsymbol{n}}/\theta\big) \\ &= \tfrac{1}{2}m^2 - \theta \ln\Big(\tfrac{1}{3}e^{m/\theta} + \tfrac{2}{3}e^{-m/2\theta}\Big) \\ &= \frac{1}{2}\bigg(1 - \frac{1}{2\,\theta}\bigg)m^2 - \frac{m^3}{24\,\theta^2} + \frac{m^4}{64\,\theta^3} + \mathcal{O}(m^5) \quad . \end{aligned}$$

Here we have defined $\mathsf{Tr}_{\hat{\boldsymbol{n}}} = \frac{1}{3}\sum_{\hat{\boldsymbol{n}}}$ as the normalized trace. The last line is somewhat tedious to obtain, but is not necessary for this problem.

(c) Since $f(m,\theta) \neq f(-m,\theta)$, the Landau expansion of the free energy (other than constants) should include terms of all orders starting with $\mathcal{O}(m^2)$. This means that there will in general be a cubic term, hence we expect a first order transition.

(d) At the critical point, the magnetization $m = m_{\text{c}}$ is finite. We then have to solve two equations to determine m_{c} and θ_{c}. The first condition is that the free energy have degenerate minima at the transition, *i.e.* $f(m=0,\theta=\theta_{\text{c}}) = f(m=m_{\text{c}},\theta=\theta_{\text{c}})$. Thus,

$$\tfrac{1}{2}m^2 = \theta \ln\Big(\tfrac{1}{3}e^{m/\theta} + \tfrac{2}{3}e^{-m/2\theta}\Big) \quad .$$

The second is the mean field equation itself, *i.e.*

$$\frac{\partial f}{\partial m} = 0 \qquad \Rightarrow \qquad m = \frac{e^{m/\theta} - e^{-m/2\theta}}{e^{m/\theta} + 2\,e^{-m/2\theta}} \quad .$$

These equations for $(m,\theta) = (m_c, \theta_c)$ are nonlinear and hence we cannot expect to solve them analytically.

If, however, the transition were *very weakly* first order, then m_c is by assumption small, which means we should be able to get away with the fourth order Landau expansion of the free energy. For a free energy $f(m) = \frac{1}{2}am^2 - \frac{1}{3}ym^3 + \frac{1}{4}bm^4$, setting $f(m) = f'(m) = 0$ we obtain $m = 3a/y$ and $y^2 = 9ab$. For our system, $a = 1 - \frac{1}{2\theta}$, $y = \frac{1}{8\theta^2}$, and $b = \frac{1}{16\theta^3}$. We then obtain $\theta_c = \frac{5}{9}$. Note that the second order term in $f(m)$ changes sign at $\theta^* = \frac{1}{2}$, so $\theta_c > \theta^*$ is consistent with the fact that the second order transition is preempted by the first order one. Now we may ask, just how good was our assumption that the transition *is* weakly first order. To find out, we compute $m_c = 3a/y = 24\,\theta_c(\theta_c - \frac{1}{2}) = \frac{20}{27}$ which is not particularly small compared to unity. Hence the assumption that our transition is weakly first order is not justified.

(e) Let $\varepsilon(\hat{\boldsymbol{n}}, \hat{\boldsymbol{n}}') = -J\hat{\boldsymbol{n}} \cdot \hat{\boldsymbol{n}}'$ be the energy for a given link. The unit vectors $\hat{\boldsymbol{n}}$ and $\hat{\boldsymbol{n}}'$ can each point in any of three directions, which we can label as $0°$, $120°$, and $240°$. The matrix of possible bond energies is shown in Tab. 1.

$\varepsilon^{\text{clock}}_{\sigma\sigma'}$	$0°$	$120°$	$240°$
$0°$	$-J$	$\frac{1}{2}J$	$\frac{1}{2}J$
$120°$	$\frac{1}{2}J$	$-J$	$\frac{1}{2}J$
$240°$	$\frac{1}{2}J$	$\frac{1}{2}J$	$-J$

Table 1: $\mathbb{Z}_3$ clock model energy matrix.

Now consider the $q = 3$ Potts model, where the local states are labeled $|\,\mathrm{A}\,\rangle$, $|\,\mathrm{B}\,\rangle$, and $|\,\mathrm{C}\,\rangle$. The Hamiltonian is

$$\hat{H} = -\tilde{J} \sum_{\langle ij \rangle} \delta_{\sigma_i, \sigma_j} \quad .$$

The interaction energy matrix for the Potts model is given in Tab. 2.

We can in each case label the three states by a local variable $\sigma \in \{1, 2, 3\}$, corresponding, respectively, to $0°$, $120°$, and $240°$ for the clock model and to A, B, and C for the Potts model. We then observe

$$\varepsilon^{\text{clock}}_{\sigma\sigma'}(J) = \varepsilon^{\text{Potts}}_{\sigma\sigma'}(\tfrac{3}{2}J) + \tfrac{1}{2}J \quad .$$

Thus, the free energies satisfy

$$F^{\text{clock}}(J) = \tfrac{1}{4}NzJ + F^{\text{Potts}}(\tfrac{3}{2}J) \quad ,$$

and the models are equivalent. However, the $\mathbb{Z}_q$ clock model and q-state Potts model are *not* equivalent for $q > 3$. Can you see why? *Hint: construct the corresponding energy matrices for* $q = 4$.

$\varepsilon^{\text{Potts}}_{\sigma\sigma'}$	A	B	C
A	$-\tilde{J}$	0	0
B	0	$-\tilde{J}$	0
C	0	0	$-\tilde{J}$

Table 2: $q = 3$ Potts model energy matrix.

(7.9) Consider the $\mathsf{U}(1)$ Ginsburg-Landau theory with

$$F = \int\! d^d\boldsymbol{r} \left[\tfrac{1}{2} a \, |\Psi|^2 + \tfrac{1}{4} b \, |\Psi|^4 + \tfrac{1}{2} \kappa \, |\boldsymbol{\nabla} \Psi|^2 \right] \quad .$$

Here $\Psi(\boldsymbol{r})$ is a complex-valued field, and both b and κ are positive. This theory is appropriate for describing the transition to superfluidity. The order parameter is $\langle \Psi(\boldsymbol{r}) \rangle$. Note that the free energy is a functional of the two independent fields $\Psi(\boldsymbol{r})$ and $\Psi^*(\boldsymbol{r})$, where Ψ^* is the complex conjugate of Ψ. Alternatively, one can consider F a functional of the real and imaginary parts of Ψ.

(a) Show that one can rescale the field Ψ and the coordinates $\boldsymbol{r}$ so that the free energy can be written in the form

$$F = \varepsilon_0 \int\! d^d x \left[\pm \tfrac{1}{2} \, |\psi|^2 + \tfrac{1}{4} \, |\psi|^4 + \tfrac{1}{2} \, |\boldsymbol{\nabla} \psi|^2 \right] \quad ,$$

where ψ and $\boldsymbol{x}$ are dimensionless, ε_0 has dimensions of energy, and where the sign on the first term on the RHS is $\mathsf{sgn}(a)$. Find ε_0 and the relations between Ψ and ψ and between $\boldsymbol{r}$ and $\boldsymbol{x}$.

(b) By extremizing the functional $F[\psi, \psi^*]$ with respect to ψ^*, find a partial differential equation describing the behavior of the order parameter field $\psi(\boldsymbol{x})$.

(c) Consider a two-dimensional system ($d = 2$) and let $a < 0$ (*i.e.* $T < T_{\rm c}$). Consider the case where $\psi(\boldsymbol{x})$ describe a *vortex* configuration: $\psi(\boldsymbol{x}) = f(r) \, e^{i\phi}$, where (r, ϕ) are two-dimensional polar coordinates. Find the ordinary differential equation for $f(r)$ which extremizes F.

(d) Show that the free energy, up to a constant, may be written as

$$F = 2\pi\varepsilon_0 \int\limits_0^R \! dr \, r \left[\tfrac{1}{2} \big(f'\big)^2 + \frac{f^2}{2r^2} + \tfrac{1}{4} \big(1 - f^2\big)^2 \right] \quad ,$$

where R is the radius of the system, which we presume is confined to a disk. Consider a *trial solution* for $f(r)$ of the form

$$f(r) = \frac{r}{\sqrt{r^2 + a^2}} \quad ,$$

where a is the variational parameter. Compute $F(a, R)$ in the limit $R \to \infty$ and extremize with respect to a to find the optimum value of a within this variational class of functions.

Solution :

(a) Taking the ratio of the second and first terms in the free energy density, we learn that Ψ has units of $A \equiv \big(|a|/b\big)^{1/2}$. Taking the ratio of the third to the first terms yields a length scale $\xi = \big(\kappa/|a|\big)^{1/2}$. We therefore write $\Psi = A \, \psi$ and $\tilde{\boldsymbol{x}} = \xi x$ to obtain the desired form of the free energy, with

$$\varepsilon_0 = A^2 \, \xi^d \, |a| = |a|^{2 - \frac{1}{2}d} \, b^{-1} \, \kappa^{\frac{1}{2}d} \quad .$$

(b) We extremize with respect to the field ψ^*. Writing $F = \varepsilon_0 \int d^3x \, \mathcal{F}$, with $\mathcal{F} = \pm\frac{1}{2} \, |\psi|^2 + \frac{1}{4} \, |\psi|^4 + \frac{1}{2} \, |\boldsymbol{\nabla} \psi|^2$,

$$\frac{\delta(F/\varepsilon_0)}{\delta \psi^*(\boldsymbol{x})} = \frac{\partial \mathcal{F}}{\partial \psi^*} - \boldsymbol{\nabla} \cdot \frac{\partial \mathcal{F}}{\partial \, \boldsymbol{\nabla} \psi^*} = \pm \tfrac{1}{2} \, \psi + \tfrac{1}{2} \, |\psi|^2 \, \psi - \tfrac{1}{2} \, \nabla^2 \psi \quad .$$

Thus, the desired PDE is

$$-\nabla^2 \psi \pm \psi + |\psi|^2 \, \psi = 0 \quad ,$$

which is known as the time-independent nonlinear Schrödinger equation.

(c) In two dimensions,

$$\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{1}{r}\,\frac{\partial}{\partial r} + \frac{1}{r^2}\,\frac{\partial^2}{\partial \phi^2} \quad .$$

Plugging in $\psi = f(r)\, e^{i\phi}$ into $\nabla^2\psi + \psi - |\psi|^2\psi = 0$, we obtain

$$\frac{d^2 f}{dr^2} + \frac{1}{r}\,\frac{df}{dr} - \frac{f}{r^2} + f - f^3 = 0 \quad .$$

(d) Plugging $\boldsymbol{\nabla}\psi = \hat{\boldsymbol{r}}\, f'(r) + \frac{i}{r}\, f(r)\,\hat{\boldsymbol{\phi}}$ into our expression for F, we have

$$\begin{aligned} \mathcal{F} &= \tfrac{1}{2}\,|\boldsymbol{\nabla}\psi|^2 - \tfrac{1}{2}\,|\psi|^2 + \tfrac{1}{4}\,|\psi|^4 \\ &= \tfrac{1}{2}\big(f'\big)^2 + \frac{f^2}{2r^2} + \tfrac{1}{4}\,\big(1 - f^2\big)^2 - \tfrac{1}{4} \quad , \end{aligned}$$

which, up to a constant, is the desired form of the free energy. It is a good exercise to show that the Euler-Lagrange equations,

$$\frac{\partial\,(r\mathcal{F})}{\partial f} - \frac{d}{dr}\bigg(\frac{\partial\,(r\mathcal{F})}{\partial f'}\bigg) = 0$$

results in the same ODE we obtained for f in part (c). We now insert the trial form for $f(r)$ into F. The resulting integrals are elementary, and we obtain

$$F(a,R) = \tfrac{1}{4}\pi\varepsilon_0 \Bigg\{ 1 - \frac{a^4}{(R^2+a^2)^2} + 2\ln\bigg(\frac{R^2}{a^2} + 1\bigg) + \frac{R^2\,a^2}{R^2+a^2} \Bigg\} \quad .$$

Taking the limit $R \to \infty$, we have

$$F(a, R\to\infty) = 2\ln\bigg(\frac{R^2}{a^2}\bigg) + a^2 \quad .$$

We now extremize with respect to a, which yields $a = \sqrt{2}$. Note that the energy in the vortex state is logarithmically infinite. In order to have a finite total free energy (relative to the ground state), we need to introduce an *antivortex* somewhere in the system. An antivortex has a phase winding which is opposite to that of the vortex, *i.e.* $\psi = f\, e^{-i\phi}$. If the vortex and antivortex separation is r, the energy is

$$V(r) = \tfrac{1}{2}\pi\varepsilon_0 \ln\bigg(\frac{r^2}{a^2} + 1\bigg) \quad .$$

This tends to $V(r) = \pi\varepsilon_0 \ln(d/a)$ for $d \gg a$ and smoothly approaches $V(0) = 0$, since when $r = 0$ the vortex and antivortex annihilate leaving the ground state condensate. Recall that two-dimensional point charges also interact via a logarithmic potential, according to Maxwell's equations. Indeed, there is a rather extensive analogy between the physics of two-dimensional models with $\mathsf{O}(2)$ symmetry and $(2+1)$-dimensional electrodynamics.

(7.10) Consider a two-state Ising model, with an added dash of quantum flavor. You are invited to investigate the *transverse Ising model*, whose Hamiltonian is written

$$\hat{H} = -\tfrac{1}{2} \sum_{i,j} J_{ij} \sigma_i^x \sigma_j^x - H \sum_i \sigma_i^z \quad ,$$

where the σ_i^α are Pauli matrices:

$$\sigma_i^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}_i \qquad , \qquad \sigma_i^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}_i \quad .$$

(a) Using the trial density matrix,

$$\varrho_i = \tfrac{1}{2} + \tfrac{1}{2}\, m_x\, \sigma_i^x + \tfrac{1}{2}\, m_z\, \sigma_i^z$$

compute the mean field free energy $F/N\hat{J}(0) \equiv f(\theta, h, m_x, m_z)$, where $\theta = k_B T/\hat{J}(0)$, and $h = H/\hat{J}(0)$. *Hint: Work in an eigenbasis when computing* Tr $(\varrho \ln \varrho)$.

(b) Derive the mean field equations for m_x and m_z.

(c) Show that there is always a solution with $m_x = 0$, although it may not be the solution with the lowest free energy. What is $m_z(\theta, h)$ when $m_x = 0$?

(d) Show that $m_z = h$ for all solutions with $m_x \neq 0$.

(e) Show that for $\theta \leq 1$ there is a curve $h = h^*(\theta)$ below which $m_x \neq 0$, and along which m_x vanishes. That is, sketch the mean field phase diagram in the (θ, h) plane. Is the mean field transition at $h = h^*(\theta)$ first order or second order?

(f) Sketch, on the same plot, the behavior of $m_x(\theta, h)$ and $m_z(\theta, h)$ as functions of the field h for fixed θ. Do this for $\theta = 0$, $\theta = \frac{1}{2}$, and $\theta = 1$.

Solution :

(a) We have Tr $(\varrho\, \sigma^x) = m_x$ and Tr $(\varrho\, \sigma^z) = m_z$. The eigenvalues of ϱ are $\frac{1}{2}(1 \pm m)$, where $m = (m_x^2 + m_z^2)^{1/2}$. Thus,

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

(b) Differentiating with respect to m_x and m_z yields

$$\frac{\partial f}{\partial m_x} = 0 = -m_x + \frac{\theta}{2} \ln\left(\frac{1+m}{1-m}\right) \cdot \frac{m_x}{m}$$
$$\frac{\partial f}{\partial m_z} = 0 = -h + \frac{\theta}{2} \ln\left(\frac{1+m}{1-m}\right) \cdot \frac{m_z}{m} \quad .$$

Note that we have used the result

$$\frac{\partial m}{\partial m_\mu} = \frac{m_\mu}{m}$$

where m_α is any component of the vector $\boldsymbol{m}$.

(c) If we set $m_x = 0$, the first mean field equation is satisfied. We then have $m_z = m\, \mathrm{sgn}(h)$, and the second mean field equation yields $m_z = \tanh(h/\theta)$. Thus, in this phase we have

$$m_x = 0 \qquad , \qquad m_z = \tanh(h/\theta) \quad .$$

(d) When $m_x \neq 0$, we divide the first mean field equation by m_x to obtain the result

$$m = \frac{\theta}{2} \ln\left(\frac{1+m}{1-m}\right) \quad ,$$

which is equivalent to $m = \tanh(m/\theta)$. Plugging this into the second mean field equation, we find $m_z = h$. Thus, when $m_x \neq 0$,

$$m_z = h \quad , \quad m_x = \sqrt{m^2 - h^2} \quad , \quad m = \tanh(m/\theta) \quad .$$

Note that the length of the magnetization vector, m, is purely a function of the temperature θ in this phase and thus does not change as h is varied when θ is kept fixed. What does change is the canting angle of $\boldsymbol{m}$, which is $\alpha = \tan^{-1}(h/m)$ with respect to the $\hat{\boldsymbol{z}}$ axis.

(e) The two solutions coincide when $m = h$, hence

$$h = \tanh(h/\theta) \qquad \Longrightarrow \qquad \theta^*(h) = \frac{2h}{\ln\left(\frac{1+h}{1-h}\right)} \quad .$$

Inverting the above transcendental equation yields $h^*(\theta)$. The component m_x, which serves as the order parameter for this system, vanishes smoothly at $\theta = \theta_c(h)$. The transition is therefore second order.

(f) See fig. 2.

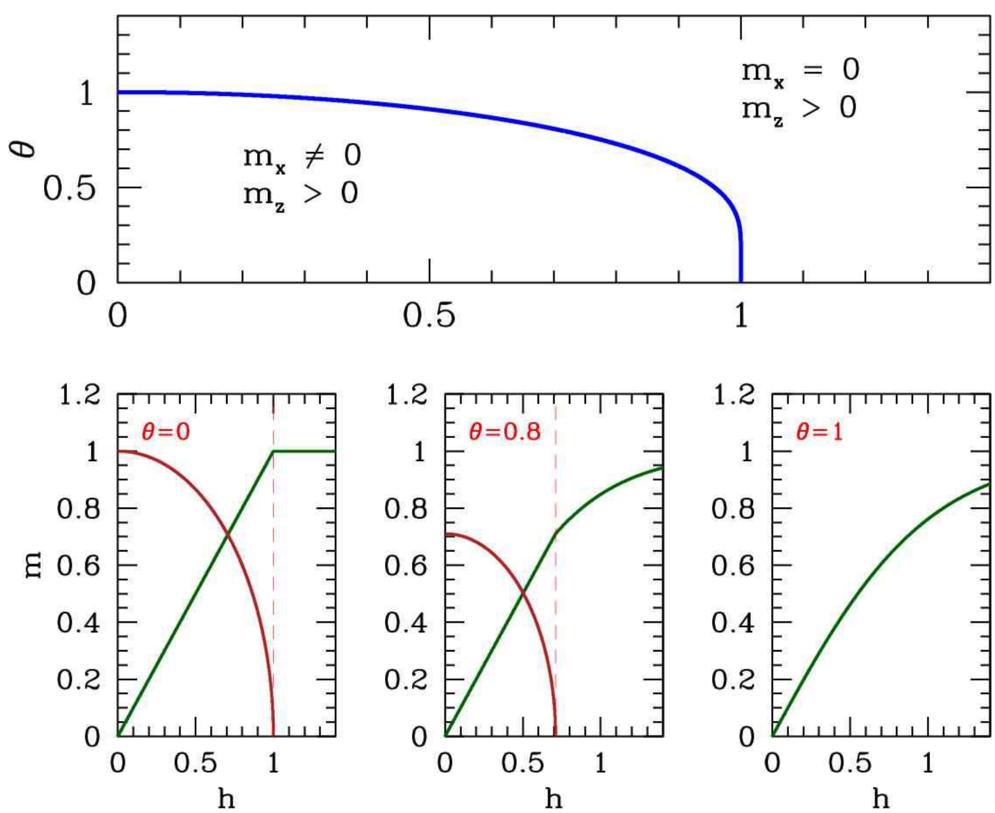

Figure 2: Solution to the mean field equations for problem 2. Top panel: phase diagram. The region within the thick blue line is a canted phase, where $m_x \neq 0$ and $m_z = h > 0$; outside this region the moment is aligned along $\hat{\boldsymbol{z}}$ and $m_x = 0$ with $m_z = \tanh(h/\theta)$.

(7.11) The Landau free energy of a crystalline magnet is given by the expression

$$f = \frac{1}{2}\alpha\, t\, (m_x^2 + m_y^2) + \frac{1}{4} b_1 (m_x^4 + m_y^4) + \frac{1}{2} b_2\, m_x^2\, m_y^2 \quad ,$$

where the constants α and b_1 are both positive, and where t is the dimensionless reduced temperature, $t = (T - T_c)/T_c$.

(a) Rescale, so that f is of the form

$$f = \varepsilon_0 \Big\{ \frac{1}{2} t\, (\phi_x^2 + \phi_y^2) + \frac{1}{4} (\phi_x^4 + \phi_y^4 + 2\lambda\, \phi_x^2\, \phi_y^2) \Big\} \quad ,$$

where $m_{x,y} = s\, \phi_{x,y}$, where s is a scale factor. Find the appropriate scale factor and find expressions for the energy scale ε_0 and the dimensionless parameter λ in terms of α, b_1, and b_2.

(b) For what values of λ is the free energy unbounded from below?

(c) Find the equations which minimize f as a function of $\phi_{x,y}$.

(d) Show that there are three distinct phases: one in which $\phi_x = \phi_y = 0$ (phase I), another in which one of $\phi_{x,y}$ vanishes but the other is finite (phase II) and one in which both of $\phi_{x,y}$ are finite (phase III). Find f in each of these phases, and be clear to identify any constraints on the parameters t and λ.

(e) Sketch the phase diagram for this theory in the (t, λ) plane, clearly identifying the unphysical region where f is unbounded, and indicating the phase boundaries for all phase transitions. Make sure to label the phase transitions according to whether they are first or second order.

Solution :

(a) It is a simple matter to find

$$m_{x,y} = \sqrt{\frac{\alpha}{b_1}}\, \phi_{x,y} \quad , \quad \varepsilon_0 = \frac{\alpha^2}{b_1} \quad , \quad \lambda = \frac{b_2}{b_1} \quad .$$

(b) Note that

$$f = \frac{1}{4}\, \varepsilon_0\, \begin{pmatrix} \phi_x^2 & \phi_y^2 \end{pmatrix} \begin{pmatrix} 1 & \lambda \\ \lambda & 1 \end{pmatrix} \begin{pmatrix} \phi_x^2 \\ \phi_y^2 \end{pmatrix} + \frac{1}{2}\, \varepsilon_0\, \begin{pmatrix} \phi_x^2 & \phi_y^2 \end{pmatrix} \begin{pmatrix} t \\ t \end{pmatrix} \tag{1}$$

We need to make sure that the quartic term goes to positive infinity when the fields $\phi_{x,y}$ tend to infinity. Else the free energy will not be bounded from below and the model is unphysical. Clearly the matrix in the first term on the RHS has eigenvalues $1 \pm \lambda$ and corresponding (unnormalized) eigenvectors $\binom{1}{\pm 1}$. Since $\phi_{x,y}^2$ cannot be negative, we only need worry about the eigenvalue $1 + \lambda$. This is negative for $\lambda < -1$. Thus, $\lambda \le -1$ is unphysical.

(c) Differentiating with respect to $\phi_{x,y}$ yields the equations

$$\frac{\partial f}{\partial \phi_x} = \big(t + \phi_x^2 + \lambda\, \phi_y^2\big)\, \phi_x = 0 \quad , \quad \frac{\partial f}{\partial \phi_y} = \big(t + \phi_y^2 + \lambda\, \phi_x^2\big)\, \phi_y = 0 \quad .$$

(d) Clearly phase I with $\phi_x = \phi_y = 0$ is a solution to these equations. In phase II, we set one of the fields to zero, $\phi_y = 0$ and solve for $\phi_x = \sqrt{-t}$, which requires $t < 0$. A corresponding solution exists if we exchange $\phi_x \leftrightarrow \phi_y$. In phase III, we solve

$$\begin{pmatrix} 1 & \lambda \\ \lambda & 1 \end{pmatrix} \begin{pmatrix} \phi_x^2 \\ \phi_y^2 \end{pmatrix} = -\begin{pmatrix} t \\ t \end{pmatrix} \qquad \Rightarrow \qquad \phi_x^2 = \phi_y^2 = -\frac{t}{1+\lambda} \quad .$$

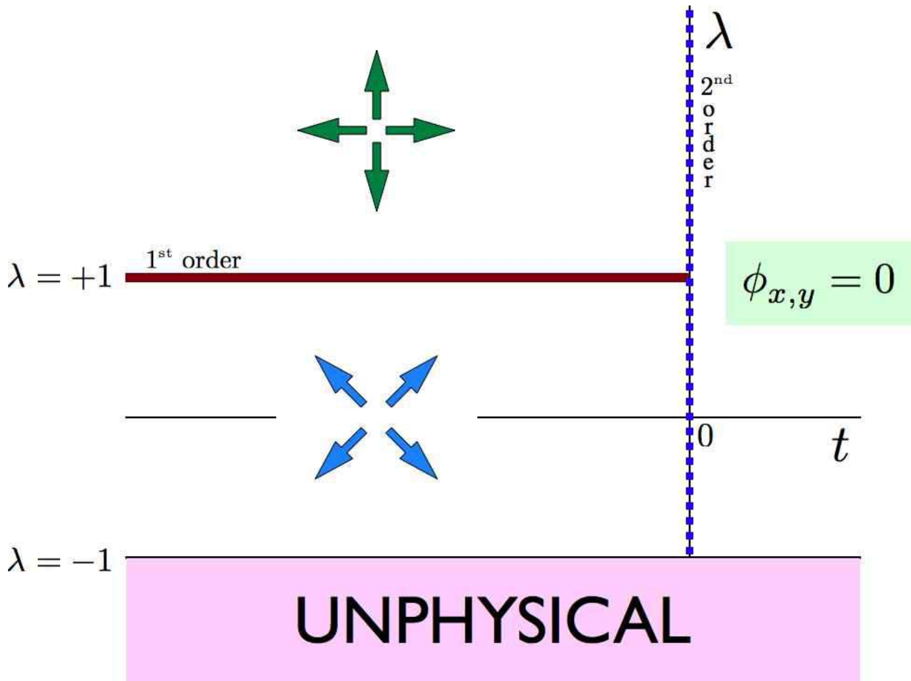

Figure 3: Phase diagram for problem (2e).

This phase also exists only for $t < 0$, and $\lambda > -1$ as well, which is required if the free energy is to be bounded from below. Thus, we find

$$(\phi_{x,\mathrm{I}}\,,\,\phi_{y,\mathrm{I}}) = (0,0) \quad , \quad f_{\mathrm{I}} = 0$$

and

$$(\phi_{x,\mathrm{II}}\,,\,\phi_{y,\mathrm{II}}) = (\pm\sqrt{-t}\,,\,0) \text{ or } (0\,,\,\pm\sqrt{-t}) \quad , \quad f_{\mathrm{II}} = -\tfrac{1}{4}\varepsilon_0\,t^2$$

and

$$(\phi_{x,\mathrm{III}}\,,\,\phi_{y,\mathrm{III}}) = \pm\sqrt{\tfrac{-t}{1+\lambda}}\,(1\,,\,1) \text{ or } \pm\sqrt{\tfrac{-t}{1+\lambda}}\,(1\,,\,-1) \quad , \quad f_{\mathrm{III}} = -\frac{\varepsilon_0\,t^2}{2\,(1+\lambda)} \quad .$$

(e) To find the phase diagram, we note that phase I has the lowest free energy for $t > 0$. For $t < 0$ we find

$$f_{\mathrm{III}} - f_{\mathrm{II}} = \tfrac{1}{4}\,\varepsilon_0\,t^2\,\frac{\lambda-1}{\lambda+1} \quad , \qquad (2)$$

which is negative for $|\lambda| < 1$. Thus, the phase diagram is as depicted in fig. 3.

(7.12) A system is described by the Hamiltonian

$$\hat{H} = -J \sum_{\langle ij \rangle} \varepsilon(\mu_i, \mu_j) - H \sum_i \delta_{\mu_i, \mathrm{A}} \quad , \tag{3}$$

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 $\varepsilon(\mu, \mu')$ is given in the following table:

ε	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

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

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, $E(x, T, H)/N$?

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

(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 $H = 0$ 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 $\mathrm{Tr}(\varrho_1) = x + 3y = 1$.

(b) We have

$$\frac{E}{N} = -\tfrac{1}{2} z J \big(x^2 - 4\,xy + 3\,y^2 - 4\,y^2\big) - Hx \quad ,$$

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

$$\frac{E}{N} = \tfrac{1}{18} z J \big(1 + 10\,x - 20\,x^2\big) - Hx$$

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

(c) The variational entropy per site is

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

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

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

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

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

(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 ch. 7 of the lecture 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 $a = a_{\rm c}^+$ to $m_0 = \frac{2}{3}\,b^{-1}y$ at $a = a_{\rm c}^-$. For our problem here, we have $a = 3\big(\theta - \frac{3}{4}\big)$, $y = 3\theta$, and $b = 7\theta$. This gives

$$
\theta_{\rm c} = \tfrac{63}{76} \approx 0.829 \qquad , \qquad \varepsilon_0 = \tfrac{2}{7} \quad .
$$

As θ decreases further below $\theta_{\rm c}$ to $\theta = 0$, ε increases to $\varepsilon(\theta = 0) = 1$. No sketch needed!

(7.13) Consider a q-state Potts model on the body-centered cubic (BCC) lattice. The Hamiltonian is given by

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

where $\sigma_i \in \{1, \ldots, q\}$ on each site.

(a) Following the mean field treatment in ch. 7 of the lecture notes, write $x = \langle \delta_{\sigma_i\,,\,1} \rangle = q^{-1} + s$, and expand the free energy in powers of s up through terms of order s^4. Neglecting all higher order terms in the free energy, find the critical temperature θ_c, where $\theta = k_B T / zJ$ as usual. Indicate whether the transition is first order or second order (this will depend on q).

(b) For second order transitions, the truncated Landau expansion is sufficient, since we care only about the sign of the quadratic term in the free energy. First order transitions involve a discontinuity in the order parameter, so any truncation of the free energy as a power series in the order parameter involves an approximation. Find a way to numerically determine $\theta_c(q)$ based on the full mean field (*i.e.* variational density matrix) free energy. Compare your results with what you found in part (a), and sketch both sets of results for several values of q.

Solution :

(a) The expansion of the free energy $f(s, \theta)$ is given in ch. 7 of the lecture notes (set $h = 0$). We have

$$f = f_0 + \tfrac{1}{2} a\, s^2 - \tfrac{1}{3} y\, s^3 + \tfrac{1}{4} b\, s^4 + \mathcal{O}(s^5) \quad ,$$

with

$$a = \frac{q(q\theta - 1)}{q - 1} \quad , \quad y = \frac{(q-2)\, q^3 \theta}{2(q-1)^2} \quad , \quad b = \tfrac{1}{3} q^3 \theta \Big[1 + (q-1)^{-3} \Big] \quad .$$

For $q = 2$ we have $y = 0$, and there is a second order phase transition when $a = 0$, *i.e.* $\theta = q^{-1}$. For $q > 2$, there is a cubic term in the Landau expansion, and this portends a first order transition. Restricting to the quartic free energy above, a first order at $a > 0$ transition preempts what would have been a second order transition at $a = 0$. The transition occurs for $y^2 = \frac{9}{2} ab$. Solving for θ, we obtain

$$\theta_c^{L} = \frac{6(q^2 - 3q + 3)}{(5q^2 - 14q + 14)\, q} \quad .$$

The value of the order parameter s just below the first order transition temperature is

$$s(\theta_c^-) = \sqrt{2a/b} \quad ,$$

where a and b are evaluated at $\theta = \theta_c$

(b) The full variational free energy, neglecting constants, is

$$f(x, \theta) = -\tfrac{1}{2} x^2 - \frac{(1-x)^2}{2(q-1)} + \theta\, x \ln x + \theta\, (1 - x) \ln\!\left(\frac{1-x}{q-1} \right) \quad .$$

Therefore

$$\frac{\partial f}{\partial x} = -x + \frac{1-x}{q-1} + \theta \ln x - \theta \ln\!\left(\frac{1-x}{q-1} \right)$$

$$\frac{\partial^2 f}{\partial x^2} = -\frac{q}{q-1} + \frac{\theta}{x(1-x)} \quad .$$

Solving for $\frac{\partial^2 f}{\partial x^2} = 0$, we obtain

$$x_\pm = \frac{1}{2} \pm \frac{1}{2} \sqrt{1 - \frac{\theta}{\theta_0}} \quad ,$$

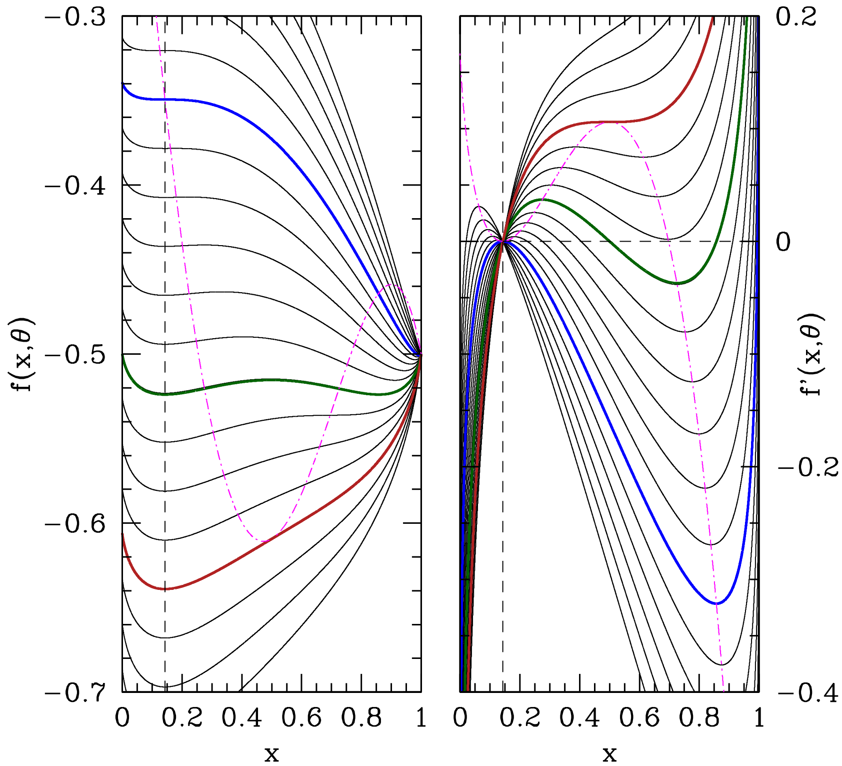

Figure 4: Variational free energy of the $q = 7$ Potts model *versus* variational parameter x. Left: free energy $f(x, \theta)$. Right: derivative $f'(x, \theta)$ with respect to the x. The dot-dash magenta curve in both cases is the locus of points for which the second derivative $f''(x, \theta)$ with respect to x vanishes. Three characteristic temperatures are marked $\theta = q^{-1}$ (blue), where the coefficient of the quadratic term in the Landau expansion changes sign; $\theta = \theta_0$ (red), where there is a saddle-node bifurcation and above which the free energy has only one minimum at $x = q^{-1}$ (symmetric phase); and $\theta = \theta_c$ (green), where the first order transition occurs.

where

$$\theta_0 = \frac{q}{4(q-1)} \quad .$$

For temperatures below θ_0, the function $f(x, \theta)$ has three extrema: two local minima and one local maximum. The points $x_\pm$ lie between either minimum and the maximum. The situation is depicted in fig. 4 for the case $q = 7$. To locate the first order transition, we must find the temperature θ_c for which the two minima are degenerate. This can be done numerically, but there is an analytic solution:

$$\theta_c^{\text{MF}} = \frac{q-2}{2(q-1)\ln(q-1)} \quad , \quad s(\theta_c^-) = \frac{q-2}{q} \quad .$$

A comparison of with results from part (a) is shown in fig. 5. Note that the truncated free energy is sufficient to obtain the mean field solution for $q = 2$. This is because the transition for $q = 2$ is continuous (*i.e.* second order), and we only need to know $f(\theta, m)$ in the vicinity of $m = 0$.

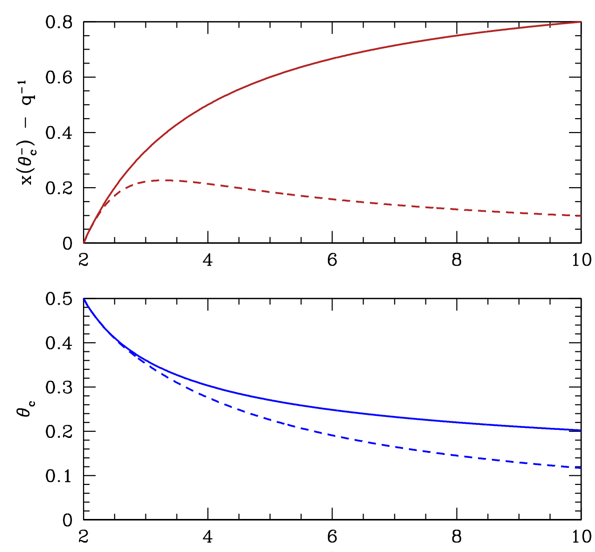

Figure 5: Comparisons of order parameter jump at θ_c (top) and critical temperature θ_c (bottom) for untruncated (solid lines) and truncated (dashed lines) expansions of the mean field free energy. Note the agreement as $q \to 2$, where the jump is small and a truncated expansion is then valid.

(7.14) The Blume-Capel model is a $S = 1$ Ising model described by the Hamiltonian

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

where $J_{ij} = J(\boldsymbol{R}_i - \boldsymbol{R}_j)$ and $S_i \in \{-1, 0, +1\}$. The mean field theory for this model is discussed in ch. 7 of the lecture notes, using the 'neglect of fluctuations' method. Consider instead a variational density matrix approach. Take $\varrho(S_1, \ldots, S_N) = \prod_i \tilde{\varrho}(S_i)$, where

$$\tilde{\varrho}(S) = \left(\frac{n+m}{2}\right)\delta_{S,+1} + (1-n)\,\delta_{S,0} + \left(\frac{n-m}{2}\right)\delta_{S,-1} \quad .$$

(a) Find $\langle 1 \rangle$, $\langle S_i \rangle$, and $\langle S_i^2 \rangle$.

(b) Find $E = \mathsf{Tr}\,(\varrho H)$.

(c) Find $S = -k_{\rm B}\,\mathsf{Tr}\,(\varrho \ln \varrho)$.

(d) Adimensionalizing by writing $\theta = k_{\rm B}T/\hat{J}(0)$, $\delta = \Delta/\hat{J}(0)$, and $f = F/N\hat{J}(0)$, find the dimensionless free energy per site $f(m, n, \theta, \delta)$.

(e) Write down the mean field equations.

(f) Show that $m = 0$ always permits a solution to the mean field equations, and find $n(\theta, \delta)$ when $m = 0$.

(g) To find $\theta_{\rm c}$, set $m = 0$ but use both mean field equations. You should recover the result in ch. 7 of the lecture notes.

(h) Show that the equation for $\theta_{\rm c}$ has two solutions for $\delta < \delta_*$ and no solutions for $\delta > \delta_*$. Find the value of δ_*.[1]

(i) Assume $m^2 \ll 1$ and solve for $n(m, \theta, \delta)$ using one of the mean field equations. Plug this into your result for part (d) and obtain an expansion of f in terms of powers of m^2 alone. Find the first order line. You may find it convenient to use `Mathematica` here.

Solution :

(a) From the given expression for $\tilde{\varrho}$, we have

$$\langle 1 \rangle = 1 \qquad , \qquad \langle S \rangle = m \qquad , \qquad \langle S^2 \rangle = n \quad ,$$

where $\langle A \rangle = \mathsf{Tr}(\tilde{\varrho}\, A)$.

(b) From the results of part (a), we have

$$\begin{aligned} E &= \mathsf{Tr}(\tilde{\varrho}\,\hat{H}) \\ &= -\tfrac{1}{2} N \hat{J}(0)\, m^2 + N\Delta\, n \quad , \end{aligned}$$

assuming $J_{ii} = 0$ for al i.

(c) The entropy is

$$\begin{aligned} S &= -k_{\rm B}\,\mathsf{Tr}\,(\varrho \ln \varrho) \\ &= -Nk_{\rm B}\left\{\left(\frac{n-m}{2}\right)\ln\!\left(\frac{n-m}{2}\right) + (1-n)\ln(1-n) + \left(\frac{n+m}{2}\right)\ln\!\left(\frac{n+m}{2}\right)\right\} \quad . \end{aligned}$$

[1] *Nota bene* : (θ_*, δ_*) is not the tricritical point.

(d) The dimensionless free energy is given by

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

(e) The mean field equations are

$$\begin{aligned}0 &= \frac{\partial f}{\partial m} = -m + \tfrac{1}{2}\theta\,\ln\!\left(\frac{n-m}{n+m}\right)\\ 0 &= \frac{\partial f}{\partial n} = \delta + \tfrac{1}{2}\theta\,\ln\!\left(\frac{n^2-m^2}{4\,(1-n)^2}\right) \quad .\end{aligned}$$

These can be rewritten as

$$\begin{aligned}m &= n\tanh(m/\theta)\\ n^2 &= m^2 + 4\,(1-n)^2\,e^{-2\delta/\theta} \quad .\end{aligned}$$

(f) Setting $m=0$ solves the first mean field equation always. Plugging this into the second equation, we find

$$n = \frac{2}{2+\exp(\delta/\theta)} \quad .$$

(g) If we set $m \to 0$ in the first equation, we obtain $n = \theta$, hence

$$\theta_{\rm c} = \frac{2}{2+\exp(\delta/\theta_{\rm c})} \quad .$$

(h) The above equation may be recast as

$$\delta = \theta\ln\!\left(\frac{2}{\theta} - 2\right)$$

with $\theta = \theta_{\rm c}$. Differentiating, we obtain

$$\frac{\partial\delta}{\partial\theta} = \ln\!\left(\frac{2}{\theta}-2\right) - \frac{1}{1-\theta} \qquad \Longrightarrow \qquad \theta = \frac{\delta}{\delta+1} \quad .$$

Plugging this into the result for part (g), we obtain the relation $\delta\, e^{\delta+1} = 2$, and numerical solution yields the maximum of $\delta(\theta)$ as

$$\theta_* = 0.3164989\ldots \qquad , \qquad \delta = 0.46305551\ldots \quad .$$

This is *not* the tricritical point.

(i) Plugging in $n = m/\tanh(m/\theta)$ into $f(n,m,\theta,\delta)$, we obtain an expression for $f(m,\theta,\delta)$, which we then expand in powers of m, obtaining

$$f(m,\theta,\delta) = f_0 + \tfrac{1}{2}am^2 + \tfrac{1}{4}bm^4 + \tfrac{1}{6}cm^6 + \mathcal{O}(m^8) \quad .$$

We find

$$a = \frac{2}{3\theta}\left\{\delta - \theta\ln\!\left(\frac{2(1-\theta)}{\theta}\right)\right\}$$

$$b = \frac{1}{45\,\theta^3}\left\{4(1-\theta)\,\theta\ln\!\left(\frac{2(1-\theta)}{\theta}\right) + 15\theta^2 - 5\theta + 4\delta(\theta-1)\right\}$$

$$c = \frac{1}{1890\,\theta^5(1-\theta)^2}\left\{24\,(1-\theta)^2\,\theta\ln\!\left(\frac{2(1-\theta)}{\theta}\right) + 24\delta(1-\theta)^2 + \theta\left(35 - 154\,\theta + 189\,\theta^2\right)\right\} \quad .$$

The tricritical point occurs for $a = b = 0$, which yields

$$\theta_{\rm t} = \tfrac{1}{3} \qquad , \qquad \delta_{\rm t} = \tfrac{2}{3}\ln 2 \quad .$$

If, following Landau, we consider terms only up through order m^6, we predict a first order line given by the solution to the equation

$$b = -\tfrac{4}{\sqrt{3}}\sqrt{ac} \quad .$$

The actual first order line is obtained by solving for the locus of points (θ, δ) such that $f(m, \theta, \delta)$ has a degenerate minimum, with one of the minima at $m = 0$ and the other at $m = \pm m_0$. The results from Landau theory will coincide with the exact mean field solution at the tricritical point, where the $m_0 = 0$, but in general the first order lines obtained by the exact mean field theory solution and by a truncated sixth order Landau expansion of the free energy will differ.

(7.15) Consider the following model Hamiltonian,

$$\hat{H} = \sum_{\langle ij \rangle} E(\sigma_i, \sigma_j) \quad ,$$

where each σ_i may take on one of three possible values, and

$$E(\sigma, \sigma') = \begin{pmatrix} -J & +J & 0 \\ +J & -J & 0 \\ 0 & 0 & +K \end{pmatrix} \quad ,$$

with $J > 0$ and $K > 0$. Consider a variational density matrix $\varrho_{\rm v}(\sigma_1, \ldots, \sigma_N) = \prod_i \tilde{\varrho}(\sigma_i)$, where the normalized single site density matrix has diagonal elements

$$\tilde{\varrho}(\sigma) = \left(\frac{n+m}{2}\right)\delta_{\sigma,1} + \left(\frac{n-m}{2}\right)\delta_{\sigma,2} + (1-n)\,\delta_{\sigma,3} \quad .$$

(a) What is the global symmetry group for this Hamiltonian?

(b) Evaluate $E = \mathsf{Tr}\,(\varrho_{\rm v}\,\hat{H})$.

(c) Evaluate $S = -k_{\rm B}\,\mathsf{Tr}\,(\varrho_{\rm v} \ln \varrho_{\rm v})$.

(d) Adimensionalize by writing $\theta = k_{\rm B}T/zJ$ and $c = K/J$, where z is the lattice coordination number. Find $f(n, m, \theta, c) = F/NzJ$.

(e) Find all the mean field equations.

(f) Find an equation for the critical temperature $\theta_{\rm c}$, and show graphically that it has a unique solution.

Solution :

(a) The global symmetry group is $\mathbb{Z}_2$. If we label the spin values as $\sigma \in \{1, 2, 3\}$, then the group elements can be written as permutations, $1 = \binom{123}{123}$ and $\mathcal{J} = \binom{123}{213}$, with $\mathcal{J}^2 = 1$.

(b) For each nearest neighbor pair (ij), the distribution of $\{\sigma_, \sigma_j\}$ is according to the product $\tilde{\varrho}(\sigma_i)\,\tilde{\varrho}(\sigma_j)$. Thus, we have

$$\begin{aligned} E &= \tfrac{1}{2} NzJ \sum_{\sigma,\sigma'} \tilde{\varrho}(\sigma)\,\tilde{\varrho}(\sigma')\,\varepsilon(\sigma,\sigma') \\ &= \tfrac{1}{2} NzJ \cdot \Bigg\{ \overbrace{\left(\frac{n+m}{2}\right)^2}^{\tilde{\varrho}^2(1)} (-J) + \overbrace{\left(\frac{n-m}{2}\right)^2}^{\tilde{\varrho}^2(2)} (-J) + \overbrace{2\left(\frac{n+m}{2}\right)\left(\frac{n-m}{2}\right)}^{2\,\tilde{\varrho}(1)\,\tilde{\varrho}(2)} (+J) + \overbrace{(1-n)^2}^{\tilde{\varrho}^2(3)} (+K) \Bigg\} \\ &= -\tfrac{1}{2} Nz \Big[Jm^2 - K(1-n)^2 \Big] \quad . \end{aligned}$$

(c) The entropy is

$$\begin{aligned} S &= -Nk_{\rm B}\,\mathsf{Tr}\,(\tilde{\varrho} \ln \tilde{\varrho}) \\ &= -Nk_{\rm B} \left\{ \left(\frac{n+m}{2}\right) \ln\left(\frac{n+m}{2}\right) + \left(\frac{n-m}{2}\right) \ln\left(\frac{n-m}{2}\right) + (1-n)\ln(1-n) \right\} \quad . \end{aligned}$$

(d) This can be solved by inspection from the results of parts (b) and (c):

$$f = -\tfrac{1}{2}m^2 + \tfrac{1}{2}c\,(1-n)^2 + \theta\left[\left(\frac{n+m}{2}\right)\ln\left(\frac{n+m}{2}\right) + \left(\frac{n-m}{2}\right)\ln\left(\frac{n-m}{2}\right) + (1-n)\ln(1-n)\right] \quad .$$

(e) There are two mean field equations, obtained by extremizing with respect to n and to m, respectively:

$$\begin{aligned}\frac{\partial f}{\partial n} &= 0 = c\,(n-1) + \tfrac{1}{2}\theta\,\ln\left(\frac{n^2-m^2}{4\,(1-n)^2}\right)\\ \frac{\partial f}{\partial m} &= 0 = -m + \tfrac{1}{2}\theta\,\ln\left(\frac{n-m}{n+m}\right) \quad .\end{aligned}$$

These may be recast as

$$\begin{aligned}n^2 &= m^2 + 4\,(1-n)^2\,e^{-2c(n-1)/\theta}\\ m &= n\tanh(m/\theta) \quad .\end{aligned}$$

(f) To find θ_c, we take the limit $m \to 0$. The second mean field equation then gives $n = \theta$. Substituting this into the first mean field equation yields

$$\theta = 2\,(1-\theta)\,e^{-2c(\theta-1)/\theta} \quad .$$

If we define $u \equiv \theta^{-1} - 1$, this equation becomes

$$2u = e^{-cu} \quad .$$

It is clear that for $c > 0$ this equation has a unique solution, since the LHS is monotonically increasing and the RHS is monotonically decreasing, and the difference changes sign for some $u > 0$. The low temperature phase is the ordered phase, which spontaneously breaks the aforementioned $\mathbb{Z}_2$ symmetry. In the high temperature phase, the $\mathbb{Z}_2$ symmetry is unbroken.

(7.16) Consider a set of magnetic moments on a cubic lattice ($z = 6$). Due to the cubic anisotropy, the system is modeled by the Hamiltonian

$$\hat{H} = -J \sum_{\langle ij \rangle} \hat{\boldsymbol{n}}_i \cdot \hat{\boldsymbol{n}}_j - \boldsymbol{H} \cdot \sum_i \hat{\boldsymbol{n}}_i \quad ,$$

where at each site $\hat{\boldsymbol{n}}_i$ can take one of six possible values: $\hat{\boldsymbol{n}}_i \in \{\pm\hat{\boldsymbol{x}}\,,\,\pm\hat{\boldsymbol{y}}\,,\,\pm\hat{\boldsymbol{z}}\}$.

(a) Find the mean field free energy $f(\theta, \boldsymbol{m}, \boldsymbol{h})$, where $\theta = k_{\rm B}T/6J$ and $\boldsymbol{h} = \boldsymbol{H}/6J$.

(b) Find the self-consistent mean field equation for $\boldsymbol{m}$, and determine the critical temperature $\theta_{\rm c}(\boldsymbol{h} = 0)$. How does $\boldsymbol{m}$ behave just below $\theta_{\rm c}$? *Hint: you will have to go beyond $\mathcal{O}(\boldsymbol{m}^2)$ to answer this.*

(c) Find the phase diagram as a function of θ and h when $\boldsymbol{h} = h\,\hat{\boldsymbol{x}}$.

Solution :

(a) The effective mean field is $\boldsymbol{H}_{\rm eff} = zJ\boldsymbol{m} + \boldsymbol{H}$, where $\boldsymbol{m} = \langle \hat{\boldsymbol{n}}_i \rangle$. The mean field Hamiltonian is

$$\hat{H}_{\rm MF} = \tfrac{1}{2} NzJ\boldsymbol{m}^2 - \boldsymbol{H}_{\rm eff} \cdot \sum_i \hat{\boldsymbol{n}}_i \quad .$$

With $\boldsymbol{h} = \boldsymbol{H}/zJ$ and $\theta = k_{\rm B}T/zJ$, we then have

$$\begin{aligned} f(\theta\,,\boldsymbol{h}\,,\boldsymbol{m}) &= -\frac{k_{\rm B}T}{NzJ} \ln \text{Tr}\, e^{-\hat{H}_{\rm eff}/k_{\rm B}T} \\ &= \tfrac{1}{2}\big(m_x^2 + m_y^2 + m_z^2\big) - \theta\, \ln\!\left[2\cosh\!\left(\frac{m_x + h_x}{\theta}\right) + 2\cosh\!\left(\frac{m_y + h_y}{\theta}\right) + 2\cosh\!\left(\frac{m_z + h_z}{\theta}\right)\right] \quad . \end{aligned}$$

(b) The mean field equation is obtained by setting $\frac{\partial f}{\partial m_\alpha} = 0$ for each Cartesian component $\alpha \in \{x, y, z\}$ of the order parameter $\boldsymbol{m}$. Thus,

$$m_x = \frac{\sinh\!\left(\frac{m_x + h_x}{\theta}\right)}{\cosh\!\left(\frac{m_x + h_x}{\theta}\right) + \cosh\!\left(\frac{m_y + h_y}{\theta}\right) + \cosh\!\left(\frac{m_z + h_z}{\theta}\right)} \quad ,$$

with corresponding equations for m_y and m_z. We now set $\boldsymbol{h} = 0$ and expand in powers of $\boldsymbol{m}$, using $\cosh u = 1 + \frac{1}{2}u^2 + \frac{1}{24}u^4 + \mathcal{O}(u^6)$ and $\ln(1+u) = u - \frac{1}{2}u^2 + \mathcal{O}(u^3)$. We have

$$\begin{aligned} f(\theta\,,\boldsymbol{h}=0\,,\boldsymbol{m}) &= \tfrac{1}{2}\big(m_x^2 + m_y^2 + m_z^2\big) - \theta\, \ln\!\left(6 + \frac{m_x^2 + m_y^2 + m_z^2}{\theta^2} + \frac{m_x^4 + m_y^4 + m_z^4}{12\,\theta^4} + \mathcal{O}(\boldsymbol{m}^6)\right) \\ &= -\theta \ln 6 + \tfrac{1}{2}\Big(1 - \tfrac{1}{3\theta}\Big)\big(m_x^2 + m_y^2 + m_z^2\big) + \frac{m_x^2\, m_y^2 + m_y^2\, m_z^2 + m_z^2\, m_x^2}{36\,\theta^3} + \mathcal{O}(\boldsymbol{m}^6) \quad . \end{aligned}$$

We see that the quadratic term is negative for $\theta < \theta_{\rm c} = \frac{1}{3}$. Furthermore, the quadratic term depends only on the magnitude of $\boldsymbol{m}$ and not its direction. How do we decide upon the direction, then? We must turn to the quartic term. Note that the quartic term is minimized when $\boldsymbol{m}$ lies along one of the three cubic axes, in which case the term vanishes. So we know that in the ordered phase $\boldsymbol{m}$ prefers to lie along $\pm\hat{\boldsymbol{x}}$, $\pm\hat{\boldsymbol{y}}$, or $\pm\hat{\boldsymbol{z}}$. How can we determine its magnitude? We must turn to the *sextic* term in the expansion:

$$f(\theta\,,h=0\,,m) = -\theta \ln 6 + \tfrac{1}{2}\Big(1 - \tfrac{1}{3\theta}\Big)m^2 + \frac{m^6}{3240\,\theta^5} + \mathcal{O}(m^8) \quad ,$$

which is valid provided $\boldsymbol{m} = m\hat{\boldsymbol{n}}$ lies along a cubic axis. Extremizing, we obtain

$$m(\theta) = \pm\Big[540\,\theta^4\,(\theta_{\rm c} - \theta)\Big]^{1/4} \simeq \big(\tfrac{20}{3}\big)^{1/4}(\theta_{\rm c} - \theta)^{1/4} \quad ,$$

where $\theta_c = \frac{1}{3}$. So due to an accidental cancellation of the quartic term, we obtain a nonstandard mean field order parameter exponent of $\beta = \frac{1}{4}$.

(c) When $\boldsymbol{h} = h\,\hat{\boldsymbol{x}}$, the magnetization will choose to lie along the $\hat{\boldsymbol{x}}$ axis in order to minimize the free energy. One then has

$$
\begin{aligned}
f(\theta,h,m) &= -\theta\ln 6 + \tfrac{1}{2}m^2 - \theta\ln\bigg[\tfrac{2}{3} + \tfrac{1}{3}\cosh\bigg(\frac{m+h}{\theta}\bigg)\bigg] \\
&= -\theta\ln 6 + \tfrac{3}{2}(\theta-\theta_c)\,m^2 + \tfrac{3}{40}\,m^6 - hm + \ldots \quad ,
\end{aligned}
$$

where in the second line we have assumed $\theta \approx \theta_c$, and we have expanded for small m and h. The phase diagram resembles that of other Ising systems. The h field breaks the $m \to -m$ symmetry, and there is a first order line extending along the θ axis (*i.e.* for $h=0$) from $\theta = 0$ and terminating in a critical point at $\theta = \theta_c$. As we have seen, the order parameter exponent is nonstandard, with $\beta = \frac{1}{4}$. What of the other critical exponents? Minimizing f with respect to m, we have

$$
3(\theta-\theta_c)\,m + \tfrac{9}{20}\,m^5 - h = 0 \quad .
$$

For $\theta > \theta_c$ and m small, we can neglect the $\mathcal{O}(m^5)$ term and we find $m(\theta,h) = \frac{h}{3(\theta-\theta_c)}$, corresponding to the familiar susceptibility exponent $\gamma = 1$.

Consider next the heat capacity. For $\theta > \theta_c$ the free energy is $f = -\theta\ln 6$, arising from the entropy term alone, whereas for $\theta < \theta_c$ we have $m^2 = \sqrt{\frac{20}{3}}\,(\theta_c-\theta)^{1/2}$, which yields

$$
f(\theta<\theta_c\,,h=0) = -\theta\ln 6 - \sqrt{\tfrac{20}{3}}\,(\theta_c-\theta)^{3/2} \quad .
$$

Thus, the heat capacity, which is $c = -\theta\,\frac{\partial^2 f}{\partial\theta^2}$, behaves as $c(\theta) \propto (\theta_c-\theta)^{-1/2}$, corresponding to $\alpha = \frac{1}{2}$, rather than the familiar $\alpha = 0$.

Finally, we examine the behavior of $m(\theta_c\,,h)$. Setting $\theta = \theta_c$, we have

$$
f(\theta_c\,,h\,,m) = -hm + \tfrac{9}{40}\,m^6 + \mathcal{O}(m^8) \quad .
$$

Setting $\frac{\partial f}{\partial m} = 0$, we find $m \propto h^{1/\delta}$ with $\delta = 5$, which is also nonstandard.

(7.17) A magnet consists of a collection of local moments which can each take the values $S_i = -1$ or $S_i = +3$. The Hamiltonian is

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

(a) Define $m = \langle S_i \rangle$, $h = H/\hat{J}(0)$, $\theta = k_{\rm B}T/\hat{J}(0)$. Find the dimensionless mean field free energy per site, $f = F/N\hat{J}(0)$ as a function of θ, h, and m.

(b) Write down the self-consistent mean field equation for m.

(c) At $\theta = 0$, there is a first order transition as a function of field between the $m = +3$ state and the $m = -1$ state. Find the critical field $h_{\rm c}(\theta = 0)$.

(d) Find the critical point $(\theta_{\rm c}\,,\, h_{\rm c})$ and plot the phase diagram for this system.

(e) Solve the problem using the variational density matrix approach.

Solution :

(a) We invoke the usual mean field treatment of dropping terms quadratic in fluctuations, resulting in an effective field $H_{\rm eff} = \hat{J}(0)\, m + H$ and a mean field Hamiltonian

$$\hat{H}_{\rm MF} = \tfrac{1}{2} N \hat{J}(0)\, m^2 - H_{\rm eff} \sum_{i=1}^{N} S_i \quad .$$

The free energy is then found to be

$$\begin{aligned} f(\theta, h, m) &= \tfrac{1}{2}m^2 - \theta \,\ln\!\Big(e^{3(m+h)/\theta} + e^{-(m+h)/\theta}\Big) \\ &= \tfrac{1}{2}m^2 - m - h - \theta \ln\cosh\!\bigg(\frac{2(m+h)}{\theta}\bigg) - \theta \ln 2 \quad . \end{aligned}$$

(b) We extremize f with respect to the order parameter m and obtain

$$m = 1 + 2\tanh\!\bigg(\frac{2(m+h)}{\theta}\bigg) \quad .$$

(c) When $T = 0$ there are no fluctuations, and since the interactions are ferromagnetic we may examine the two uniform states. In the state where $S_i = +3$ for each i, the energy is $E_1 = \frac{9}{2}N\hat{J}(0) - 3NH$. In the state where $S_i = -1 \;\forall\, i$, the energy is $E_2 = \frac{1}{2}N\hat{J}(0) + NH$. Equating these energies gives $H = -\hat{J}(0)$, *i.e.* $h = -1$.

(d) The first order transition at $h = -1$ and $\theta = 0$ continues in a curve emanating from this point into the finite θ region of the phase diagram. This phase boundary is determined by the requirement that $f(\theta, h, m)$ have a degenerate double minimum as a function of m for fixed θ and h. This provides us with two conditions on the three quantities (θ, h, m), which in principle allows the determination of the curve $h = h_{\rm c}(\theta)$. The first order line terminates in a critical point where these two local minima annihilate with a local maximum, which requires that $\frac{\partial f}{\partial m} = \frac{\partial^2 f}{\partial m^2} = \frac{\partial^3 f}{\partial m^3} = 0$, which provides the three conditions necessary to determine $(\theta_{\rm c}\,,\, h_{\rm c}\,,\, m_{\rm c})$. Now from our

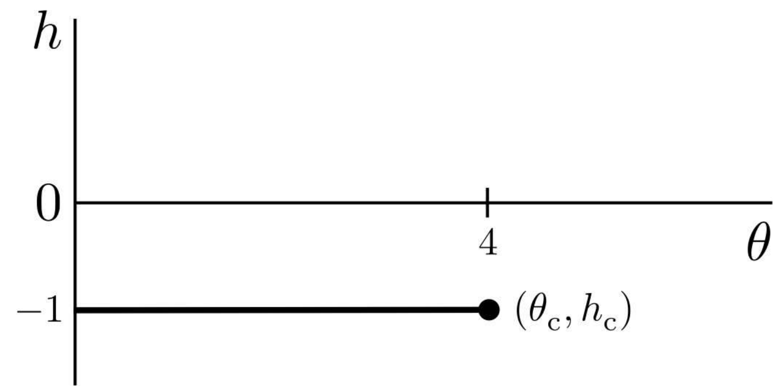

Figure 6: Phase diagram for problem 17.

expression for $f(\theta,h,m)$, we have

$$\begin{aligned}\frac{\partial f}{\partial m} &= m - 1 - 2\tanh\!\left(\frac{2(m+h)}{\theta}\right)\\ \frac{\partial^2 f}{\partial m^2} &= 1 - \frac{4}{\theta}\,\mathrm{sech}^2\!\left(\frac{2(m+h)}{\theta}\right)\\ \frac{\partial^3 f}{\partial m^3} &= \frac{16}{\theta^2}\,\tanh\!\left(\frac{2(m+h)}{\theta}\right)\mathrm{sech}^2\!\left(\frac{2(m+h)}{\theta}\right) \quad .\end{aligned}$$

Now set all three of these quantities to zero. From the third of these, we get $m+h=0$, which upon insertion into the second gives $\theta=4$. From the first we then get $m=1$, hence $h=-1$.

For a slicker derivation, note that the free energy may be written

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

Thus, when $h=-1$, we have that f is an even function of $m-1$. Expanding then in powers of $m+h$, we have

$$f(\theta,h=-1,m) = f_0 + \tfrac{1}{2}\big(1-\tfrac{4}{\theta}\big)(m-1)^2 + \tfrac{4}{3\theta^3}(m-1)^4 + \ldots \quad ,$$

whence we conclude $\theta_c = 4$ and $h_c=-1$.

(e) The most general single site variational density matrix is

$$\varrho(S) = x\,\delta_{S,-1} + (1-x)\,\delta_{S,+3} \quad .$$

This is normalized by construction. The average magnetization is

$$m = \mathrm{Tr}\,(S\varrho) = (-1)\cdot x + (+3)\cdot(1-x) = 3-4x \quad\Rightarrow\quad x = \frac{3-m}{4} \quad .$$

Thus we have

$$\varrho(S) = \frac{3-m}{4}\,\delta_{S,-1} + \frac{1+m}{4}\,\delta_{S,+3} \quad .$$

The variational free energy is then

$$\begin{aligned}F &= \mathrm{Tr}\,(\hat{H}\hat{\varrho}) + k_B T\,\mathrm{Tr}\,(\hat{\varrho}\ln\hat{\varrho})\\ &= -\tfrac{1}{2}N\hat{J}(0)\,m^2 - NHm + k_B T\left[\left(\frac{3-m}{4}\right)\ln\!\left(\frac{3-m}{4}\right) + \left(\frac{1+m}{4}\right)\ln\!\left(\frac{1+m}{4}\right)\right] \quad ,\end{aligned}$$

where we assume all the diagonal elements vanish, *i.e.* $J_{ii}=0$ for all i. Dividing by $N\hat{J}(0)$, we have

$$f(\theta,h,m) = -\tfrac{1}{2}m^2 - hm - \theta\left[\left(\frac{3-m}{4}\right)\ln\!\left(\frac{3-m}{4}\right) + \left(\frac{1+m}{4}\right)\ln\!\left(\frac{1+m}{4}\right)\right] \quad .$$

Minimizing with respect to the variational parameter m yields

$$\frac{\partial f}{\partial m} = -m - h + \tfrac{1}{4}\theta\,\ln\!\left(\frac{1+m}{3-m}\right) \quad ,$$

which is equivalent to our earlier result $m = 1 + 2\tanh\big[2(m+h)/\theta\big]$.

If we once again expand in powers of $(m-1)$, we have

$$f(\theta,h,m) = -\big(\tfrac{1}{2} + h + \theta\ln 2\big) - (h+1)(m-1) + \tfrac{1}{8}(\theta-4)(m-1)^2 + \tfrac{1}{48}(m-1)^4 + \ldots \quad .$$

Again, we see $(\theta_c, h_c) = (4,-1)$.