

PHYSICS 140B : STATISTICAL PHYSICS
HW ASSIGNMENT #5 SOLUTIONS

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

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

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

(a) Following the mean field treatment in §7.6.3 of the notes, write $x = \langle \delta_{\sigma_i, 1} \rangle = q^{-1} + s$, and expand the free energy in powers of s 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 eqn. 7.129 of the notes (set $h = 0$). We have

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

with

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

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

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

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

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

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

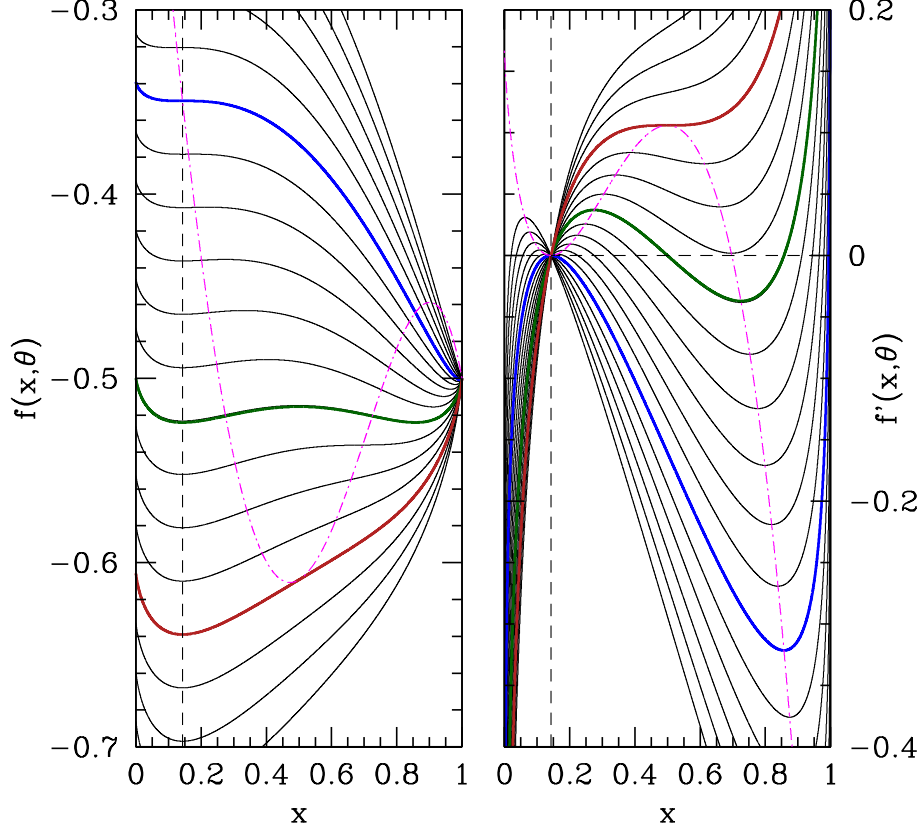


Figure 1: Variational free energy of the $q = 7$ Potts model *versus* variational parameter x . Left: free energy $f(x, \theta)$. Right: derivative $f'(x, \theta)$ with respect to the x . The dot-dash magenta curve in both cases is the locus of points for which the second derivative $f''(x, \theta)$ 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.

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

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

Therefore

$$\begin{aligned} \frac{\partial f}{\partial x} &= -x + \frac{1-x}{q-1} + \theta \ln x - \theta \ln\left(\frac{1-x}{q-1}\right) \\ \frac{\partial^2 f}{\partial x^2} &= -\frac{q}{q-1} + \frac{\theta}{x(1-x)}. \end{aligned}$$

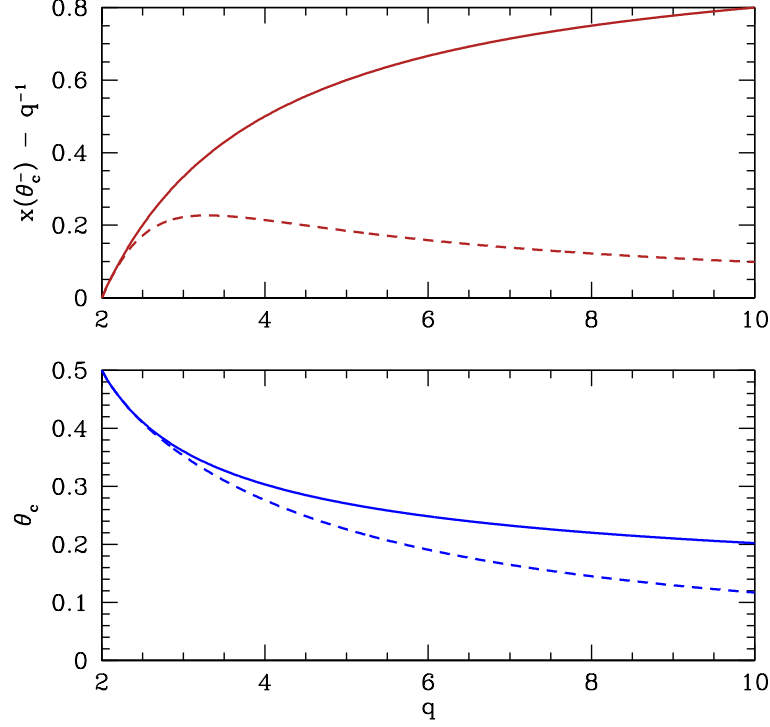


Figure 2: Comparisons of order parameter jump at θ_c (top) and critical temperature θ_c (bottom) for untruncated (solid lines) and truncated (dashed lines) expansions of the mean field free energy. Note the agreement as $q \rightarrow 2$, where the jump is small and a truncated expansion is then valid.

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

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

where $\theta_0 = q/4(q-1)$. 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. 1 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:

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

A comparison of these results with those from part (a) is shown in fig. 2.

(2) Consider the U(1) Ginsburg-Landau theory with

$$F = \int d^d \mathbf{r} \left[\frac{1}{2} a |\Psi|^2 + \frac{1}{4} b |\Psi|^4 + \frac{1}{2} \kappa |\nabla \Psi|^2 \right].$$

Here $\Psi(\mathbf{r})$ 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 $\langle \Psi(\mathbf{r}) \rangle$. Note that the free energy is a functional of the two independent fields $\Psi(\mathbf{r})$ and $\Psi^*(\mathbf{r})$, 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 \mathbf{r} so that the free energy can be written in the form

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

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

(c) Consider a two-dimensional system ($d = 2$) and let $a < 0$ (i.e. $T < T_c$). Consider the case where $\psi(\mathbf{x})$ describe a *vortex* configuration: $\psi(\mathbf{x}) = f(r) e^{i\phi}$, 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

$$F = 2\pi\varepsilon_0 \int_0^R dr r \left[\frac{1}{2} (f')^2 + \frac{f^2}{2r^2} + \frac{1}{4} (1 - f^2)^2 \right],$$

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

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

where a is the variational parameter. Compute $F(a, R)$ in the limit $R \rightarrow \infty$ 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 $A \equiv (|a|/b)^{1/2}$. Taking the ratio of the third to the first terms yields a length scale $\xi = (\kappa/|a|)^{1/2}$. We therefore write $\Psi = A\psi$ and $\tilde{\mathbf{x}} = \xi\mathbf{x}$ to obtain the desired form of the free energy, with

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

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

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

Thus, the desired PDE is

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

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

(c) In two dimensions,

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

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

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

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

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

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,

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

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

$$F(a, R) = \frac{1}{4} \pi \varepsilon_0 \left\{ 1 - \frac{a^4}{(R^2 + a^2)^2} + 2 \ln \left(\frac{R^2}{a^2} + 1 \right) + \frac{R^2 a^2}{R^2 + a^2} \right\}.$$

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

$$F(a, R \rightarrow \infty) = 2 \ln \left(\frac{R^2}{a^2} \right) + a^2.$$

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

$$V(r) = \frac{1}{2}\pi\varepsilon_0 \ln\left(\frac{r^2}{a^2} + 1\right).$$

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 $O(2)$ symmetry and $(2 + 1)$ -dimensional electrodynamics.

(3) A system is described by the Hamiltonian

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

where on each site i there are four possible choices for μ_i : $\mu_i \in \{A, B, C, D\}$. 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

$$\varrho(\mu_1, \dots, \mu_N) = \prod_{i=1}^N \varrho_1(\mu_i)$$

$$\varrho_1(\mu) = x \delta_{\mu, A} + y(\delta_{\mu, B} + \delta_{\mu, C} + \delta_{\mu, D}).$$

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

(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 $\text{Tr}(\varrho_1) = x + 3y = 1$.

(b) We have

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

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

$$\frac{E}{N} = \frac{1}{18}zJ(1 + 10x - 20x^2) - Hx$$

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

(c) The variational entropy per site is

$$\begin{aligned} s(x) &= -k_B \text{Tr}(\varrho_1 \ln \varrho_1) \\ &= -k_B (x \ln x + 3y \ln y) \\ &= -k_B \left[x \ln x + (1 - x) \ln \left(\frac{1 - x}{3} \right) \right]. \end{aligned}$$

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

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

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

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

(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

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

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 $a = 3(\theta - \frac{3}{4})$, $y = 3\theta$, and $b = 7\theta$. This gives

$$\theta_c = \frac{63}{76} \approx 0.829 \quad , \quad \varepsilon_0 = \frac{2}{7} .$$

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

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

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

where $J_{ij} = J(\mathbf{R}_i - \mathbf{R}_j)$ and $S_i \in \{-1, 0, +1\}$. The mean field theory for this model is discussed in section 7.11 of the Lecture Notes, using the ‘neglect of fluctuations’ method. Consider instead a variational density matrix approach. Take $\varrho(S_1, \dots, S_N) = \prod_i \tilde{\varrho}(S_i)$, where

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

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

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

(c) Find $S = -k_B \text{Tr}(\varrho \ln \varrho)$.

(d) Adimensionalizing by writing $\theta = k_B T / \hat{J}(0)$, $\delta = \Delta / \hat{J}(0)$, 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 θ_c , set $m = 0$ but use both mean field equations. You should recover eqn. 7.322 of the Lecture Notes.

(h) Show that the equation for θ_c has two solutions for $\delta < \delta_*$ and no solutions for $\delta > \delta_*$, and find the value of δ_* .¹

¹This problem has been corrected: (θ_*, δ_*) is not the tricritical point.

(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 $\tilde{\rho}$, we have

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

where $\langle A \rangle = \text{Tr}(\tilde{\rho} A)$.

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

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

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

(c) The entropy is

$$\begin{aligned} S &= -k_B \text{Tr}(\rho \ln \rho) \\ &= -N k_B \left\{ \left(\frac{n-m}{2} \right) \ln \left(\frac{n-m}{2} \right) + (1-n) \ln(1-n) + \left(\frac{n+m}{2} \right) \ln \left(\frac{n+m}{2} \right) \right\} . \end{aligned}$$

(d) The dimensionless free energy is given by

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

(e) The mean field equations are

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

These can be rewritten as

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

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

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

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

$$\theta_c = \frac{2}{2 + \exp(\delta/\theta_c)}.$$

(h) The above equation may be recast as

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

with $\theta = \theta_c$. Differentiating, we obtain

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

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

$$\theta_* = 0.3164989\dots, \quad \delta = 0.46305551\dots$$

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

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

We find

$$\begin{aligned} a &= \frac{2}{3\theta} \left\{ \delta - \theta \ln\left(\frac{2(1-\theta)}{\theta}\right) \right\} \\ b &= \frac{1}{45\theta^3} \left\{ 4(1-\theta)\theta \ln\left(\frac{2(1-\theta)}{\theta}\right) + 15\theta^2 - 5\theta + 4\delta(\theta-1) \right\} \\ c &= \frac{1}{1890\theta^5(1-\theta)^2} \left\{ 24(1-\theta)^2\theta \ln\left(\frac{2(1-\theta)}{\theta}\right) + 24\delta(1-\theta)^2 + \theta(35 - 154\theta + 189\theta^2) \right\}. \end{aligned}$$

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

$$\theta_t = \frac{1}{3}, \quad \delta_t = \frac{2}{3} \ln 2.$$

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

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

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.