PHYSICS 210A : STATISTICAL PHYSICS
HW ASSIGNMENT #8 SOLUTIONS

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

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

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

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

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

$$\hat{H}_{\rm MF} = \tfrac{1}{2} N z J m^2 - (\mu_0 H + zJ) \sum_i \sigma_i \, .$$

(b) Using the result

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

we have

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

(c) Expanding the free energy, we obtain

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

Thus,

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

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

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

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

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

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

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 section 7.11 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

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

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

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

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

(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]

[1] This 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 $\tilde{\varrho}$, we have

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

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

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

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

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

(c) The entropy is

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

(d) The dimensionless free energy is given by

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

(e) The mean field equations are

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

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 $m \to 0$ in the first equation, we obtain $n=\theta$, hence

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

(h) The above equation may be recast as

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

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

$$\frac{\partial\delta}{\partial\theta} = \ln\bigg(\frac{2}{\theta}-2\bigg) - \frac{1}{1-\theta} \qquad \Longrightarrow \qquad \theta = \frac{\delta}{\delta+1} \ .$$

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

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

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

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

We find

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

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

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

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

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

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

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

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.