7CCMCS03 – Equilibrium Analysis of Complex Systems
Solutions 5

Question 1

We consider a system of spin-1 particles on a square lattice with periodic boundary conditions, described by the Hamiltonian

$$H(\boldsymbol{S}) = -J\sum_{(i,j)} S_i S_j - h_1 \sum_i S_1 - h_2 \sum_i S_i^2 \ , \qquad S_i \in \{0, \pm 1\} \ ,$$

and attempt to onstruct a variational mean-field theory based on the test Hamiltonian

$$H_0(\boldsymbol{S}) = -k_1 \sum_i S_1 - k_2 \sum_i S_i^2 \ ,$$

(a) The variational mean-field theory is constructed by minimizing

$$\tilde{F} = F_0 + \langle H(\boldsymbol{S}) - H_0(\boldsymbol{S})\rangle_0$$

over the coupling constants k_1 and k_2 of the test Hamiltonian H_0. Here we use $\langle \ldots \rangle_0$ to denote a Gibbs average in the test ensemble generated by H_0.

First compute the free energy F_0 of the system described by the test Hamiltonian. Get

$$Z_0 = \sum_{\boldsymbol{S}} \mathrm{e}^{-\beta H_0(\boldsymbol{S})} = \Big(\sum_{S\in\{0,\pm1\}} \mathrm{e}^{\beta k_1 S + \beta k_2 S^2} \Big)^N = (1 + 2\mathrm{e}^{\beta k_2}\cosh(\beta k_1))^N \ ,$$

where we used the fact that the test system is a collection of N independent spin-1 systems; the partition function is therefore the product of the single site partition functions. As a consequence we have

$$F_0 = -\beta^{-1} N \ln(1 + 2\mathrm{e}^{\beta k_2}\cosh(\beta k_1))$$

Next, evaluate

$$\langle S_i \rangle_0 = \frac{2\mathrm{e}^{\beta k_2}\sinh(\beta k_1)}{1 + 2\mathrm{e}^{\beta k_2}\cosh(\beta k_1)} \ ,$$

(again exploiting the independence of individual spins – you should fill in the details of this argument!) and similarly

$$\langle S_i^2 \rangle_0 = \frac{2\mathrm{e}^{\beta k_2}\cosh(\beta k_1)}{1 + 2\mathrm{e}^{\beta k_2}\cosh(\beta k_1)} \ .$$

Similarly, because of the independence of spins in the test ensemble, the expectation of products of spins factorizes,

$$\langle S_i S_j \rangle_0 = \langle S_i \rangle_0 \langle S_j \rangle_0 = \Big(\frac{2\mathrm{e}^{\beta k_2}\sinh(\beta k_1)}{1 + 2\mathrm{e}^{\beta k_2}\cosh(\beta k_1)} \Big)^2$$

Introducing the abbreviations $m = \langle S_i \rangle_0$ and $a = \langle S_i^2 \rangle_0$ for the i independent magentizations and 'activities', we can write the variational free energy $\tilde{F}$ as

$$\tilde{F} = N\Big[-\beta^{-1}\ln(1 + 2\mathrm{e}^{\beta k_2}\cosh(\beta k_1)) - 2Jm^2 - (h_1 - k_1)m - (h_2 - k_2)a \Big]$$

The variational equations of state are given by

$$\begin{aligned}
\frac{\partial \tilde{F}}{\partial k_1} &= N\Big[-m - 4Jm\frac{\partial m}{\partial k_1} - (h_1 - k_1)\frac{\partial m}{\partial k_1} - (h_2 - k_2)\frac{\partial a}{\partial k_1} + m \Big] = 0 \\
\frac{\partial \tilde{F}}{\partial k_2} &= N\Big[-a - 4Jm\frac{\partial m}{\partial k_2} - (h_1 - k_1)\frac{\partial m}{\partial k_2} - (h_2 - k_2)\frac{\partial a}{\partial k_2} + a \Big] = 0
\end{aligned}$$

which can be rewritten as

$$\begin{aligned}
\frac{\partial m}{\partial k_1}[4Jm + h_1 - k_1] + \frac{\partial a}{\partial k_1}[h_2 - k_2] \quad &= 0 \\
\frac{\partial m}{\partial k_2}[4Jm + h_1 - k_1] + \frac{\partial a}{\partial k_2}[h_2 - k_2] \quad &= 0 \ .
\end{aligned}$$

This can be seen as linear homogeneous system of equations for the variables $[4Jm+h_1 - k_1]$ and $[h_2 - k_2]$ with matrix of coefficients given by

$$A = \begin{pmatrix} \frac{\partial m}{\partial k_1} & \frac{\partial a}{\partial k_1} \\ \frac{\partial m}{\partial k_2} & \frac{\partial a}{\partial k_2} \end{pmatrix} = \beta^2 \begin{pmatrix} a - m^2 & m - m^2 \\ m - am & a - a^2 \end{pmatrix}$$

Using $m = \tan(\beta k_1)a$ one can show that $\det(A) \neq 0$, [you should convince yourself of this fact !], so the only solution is

$$k_1 = 4Jm + h_1 \ , \qquad k_2 = h_2 \ .$$

Given the definitions of m and a in terms of averages over the test ensemble, we thus have the equations of state

$$m = \frac{2\mathrm{e}^{\beta h_2}\sinh(\beta(4Jm + h_1))}{1 + 2\mathrm{e}^{\beta h_2}\cosh(\beta(4Jm + h_1))} \ , \quad \text{and} \quad a = \frac{2\mathrm{e}^{\beta h_2}\cosh(\beta(4Jm + h_1))}{1 + 2\mathrm{e}^{\beta h_2}\cosh(\beta(4Jm + h_1))} \ .$$

Question 2
Given the Hamiltonian of a Curie-Weiss RFIM

$$H(\boldsymbol{S}) = -\frac{J}{N}\sum_{(i,j)} S_i S_j - \sum_i h_i S_i$$

with the h_i denoting independent identically distributed random fields.

(a) To compute the $\{h_i\}$-dependent free energy per spin, evaluate the partition function at given configuration of the random fields. Exploit the fact that, up to an $\mathcal{O}(1)$ contribution, the interaction term can be written as a complete square, which is then linearized using a standard identity for Gaussian integrals. This gives

$$\begin{aligned}
Z_N &= \sum_{\boldsymbol{S}} \exp\left\{\frac{\beta J}{2N}\Big(\sum_i S_i\Big)^2 - \frac{\beta J}{2} + \beta\sum_i h_i S_i\right\} \\
&\simeq \sum_{\boldsymbol{S}} \int \frac{\mathrm{d}m}{\sqrt{2\pi/(\beta J N)}} \exp\left\{-\frac{N\beta J}{2}m^2 + \beta\sum_i (Jm + h_i)S_i\right\} \\
&= \int \frac{\mathrm{d}m}{\sqrt{2\pi/(\beta J N)}} \exp\left\{N\Big[-\frac{\beta J}{2}m^2 + \frac{1}{N}\sum_i \ln[2\cosh(\beta(Jm + h_i))]\Big]\right\} \\
&= \int \frac{\mathrm{d}m}{\sqrt{2\pi/(\beta J N)}} \exp\left\{N\Big[-\frac{\beta J}{2}m^2 + \langle \ln[2\cosh(\beta(Jm + h))]\rangle_h\Big]\right\}
\end{aligned}$$

where the $\mathcal{O}(1)$ contribution in the exponent is neglected after the first line, and the LLN is invoked to obtain the last line.

Evaluating the m integral via the Laplace method requies finding the stationary point of the exponential, leading to the FPE

$$m = \langle \tanh(\beta(Jm + h))]\rangle_h$$

and the free energy in the thermodynamic limit is given by

$$-\beta f(\beta) = \lim_{N\to\infty} N^{-1} \ln Z_N = -\frac{\beta J}{2} m^2 + \langle \ln[2\cosh(\beta(Jm+h))]\rangle_h \ ,$$

with m a solution of the FPE which gives rise to the (absolute) minimum of $f(\beta)$. The solution of the FPE and the free energy per site in the thermodynamic do not depend on the specific configuration of the random fields (as a consequence of the LLN invoked above).

(b) To compute the average of the replicated partition function, we omit $\mathcal{O}(1)$ contributions from start. Begin by writing interaction terms as complete squares for each replica, which are then linearized using Gaussian integral identites as in **(a)**. Doing the sum over states before field average, one obtains

$$\begin{aligned}\langle Z_N^n\rangle_h &\simeq \left\langle \sum_{\{\boldsymbol{S}^a\}} \exp\left\{\frac{\beta J}{2N}\sum_a \Big(\sum_i S_i^a\Big)^2 + \beta \sum_{ia} h_i S_i^a\right\}\right\rangle_h \\ &= \int \prod_a \frac{\mathrm{d}m_a}{\sqrt{2\pi/(\beta J N)}} \exp\left\{-N\frac{\beta J}{2}\sum_a m_a^2\right\} \times \left\langle \prod_{ia}[2\cosh(\beta(Jm_a+h_i))]\right\rangle_h\end{aligned}$$

Using the fact that the average over the random fields factors w.r.t. i, and is i-independent, one gets

$$\begin{aligned}\langle Z_N^n\rangle_h &= \int \prod_a \frac{\mathrm{d}m_a}{\sqrt{2\pi/(\beta J N)}} \exp\left\{N\Big[-\frac{\beta J}{2}\sum_a m_a^2\right. \\ &\qquad\qquad \left. + \ln\Big\langle \prod_a [2\cosh(\beta(Jm_a+h))]\Big\rangle_h\Big]\right\}\end{aligned}$$

as claimed.

(c) Evaluating the m_a integrals via the Laplace method, we look for the stationary point of the exponent w.r.t. variations of the m_a, and get the FPEs

$$\begin{aligned} m_\alpha &= \frac{\Big\langle \sinh(\beta(Jm_\alpha+h))]\prod_{a(\neq\alpha)}[2\cosh(\beta(Jm_a+h))]\Big\rangle_h}{\Big\langle \prod_a[2\cosh(\beta(Jm_a+h))]\Big\rangle_h} \\ &= \frac{\Big\langle \tanh(\beta(Jm_\alpha+h))]\prod_{a}[2\cosh(\beta(Jm_a+h))]\Big\rangle_h}{\Big\langle \prod_a[2\cosh(\beta(Jm_a+h))]\Big\rangle_h}\ , \qquad \alpha = 1,\dots,n.\end{aligned}$$

Assuming replica symmetry $m_a = m$, we have

$$\prod_a [2\cosh(\beta(Jm_a+h))] = [2\cosh(\beta(Jm+h))]^n \to 1$$

as $n \to 0$, and we get a fixed point equation for m which is identical to that of the direct calculation.

Also, the free energy in this case is

$$-\beta f(\beta) = \lim_{N\to\infty} N^{-1} \lim_{n\to 0} \frac{1}{n} \ln\langle Z_N^n\rangle = -\frac{\beta J}{2} m^2 + \langle \ln[2\cosh(\beta(Jm+h))]\rangle_h$$