Handin 5 : FK7058

Author : Andreas Evensen

Date: February 22, 2024

$$\mathcal{H} = -J\sum_{\langle i,j\rangle} S_iS_j - \Delta\sum_{i=1}^{N} S_i^2 - H\sum_{i=1}^{N} S_i$$

Problem 1

Make the usual mean-field approximation to convert the term with nearest-neighbour interactions to a term over single spins and write the mean-field Hamiltonian.

Answer: We rewrite the above Hamiltonian in the following manner:

$$\begin{aligned}
\mathcal{H} &= -J\sum_{\langle i,j\rangle} S_iS_j - \Delta\sum_{i=1}^{N} S_i^2 - H\sum_{i=1}^{N} S_i \\
&= -\sum_{\langle i,j\rangle} J_{i,j}\langle S_j\rangle S_i - \Delta\sum_{i=1}^{N} S_i^2 - H\sum_{i=1}^{N} S_i \\
&= -\sum_{i}(H + \sum_{j}\langle S_j\rangle)S_i - \Delta S_i^2 \\
&= -\sum_{i} S_i(h_i + \Delta S_i),
\end{aligned}$$

where $h_i = H - J\sum_j^{2d}\langle S_j\rangle$.

Problem 2

Determine a self-consistent equation for the magnetization M.

Answer: In order to find the self-consistent equation for the magnetization, one has to find the partition function:

$$\begin{aligned}
Z &= \sum_{\{S_j\}} e^{-\beta\mathcal{H}} = \sum_{\{S_j\}} e^{\beta\sum_i S_i(h_i+\Delta S_i)} \\
&= \sum_{\{S_j\}}\prod_{i=1}^{N}\exp\left[\beta S_i(h_i+\Delta S_i)\right] = \prod_{i=1}^{N}\sum_{\{S_j\}}\exp\left[\beta S_i(h_i+\Delta S_i)\right] \\
&= \prod_{i=1}^{N}\Big(\exp\left[\beta(h_i+\Delta)\right] + \exp\left[-\beta h_i + \beta\Delta\right] + 1\Big) \\
&= \prod_{i=1}^{N} 2e^{\beta\Delta}\left(\cosh(\beta h_i) + \frac{e^{-\beta\Delta}}{2}\right) = \left[2e^{\beta\Delta}\left(\cosh(\beta(H+2dJM)) + \frac{e^{-\beta\Delta}}{2}\right)\right]^N.
\end{aligned}$$

From this, one can compute the free energy as:

$$
\begin{aligned}
\mathcal{F} &= -k_b T \ln(Z) \\
&= -k_b T N \ln\left[2e^{\beta\Delta}\left(\cosh(\beta(H+2dJM)) + \frac{e^{-\beta\Delta}}{2}\right)\right].
\end{aligned}
$$

The magnetization is thus given by:

$$
\begin{aligned}
M &= -\frac{1}{N}\frac{\partial \mathcal{F}}{\partial H} \\
&= \frac{\sinh(\beta(H+2dJM))}{\cosh(\beta(H+2dJM)) + \frac{e^{-\beta\Delta}}{2}}.
\end{aligned}
$$

Problem 3

In all that follows we put $H = 0$. From the above equation obtain an equation for the critical temperature at which the Blume-Chapel models undergoes a continuous phase transition. (Hint: Keep only the highest order term in both the numerator and denominator of the self-consistent equation! You will get a transcendental equation for the critical temperature.)

Answer: If $H = 0$, we get the following magnetization:

$$
M = \frac{\sinh(\beta 2dJM)}{\cosh(\beta 2dJM) + \frac{e^{-\beta\Delta}}{2}} = f(M, \beta)
$$

Differentiating with respect to M gives:

$$
\begin{aligned}
\frac{\partial f}{\partial M} &= \frac{\beta 2dJ \cosh(\beta 2dJM)}{\cosh(\beta 2dJM) + \frac{e^{-\beta\Delta}}{2}} - \frac{\beta 2dJ \sinh^2(\beta 2dJM)}{\left(\cosh(\beta 2dJM) + \frac{e^{-\beta\Delta}}{2}\right)^2} \\
\left.\frac{\partial f}{\partial M}\right|_{M=0} &= \frac{\beta 2dJ}{1 + \frac{e^{-\beta\Delta}}{2}} = 1. \qquad (1)
\end{aligned}
$$

Letting $\beta = \frac{1}{k_b T_c}$, by solving (1) for T_c, we get the critical temperature:

$$
k_b T_c = \frac{2dJ}{1 + \frac{e^{-\frac{\Delta}{k_b T_c}}}{2}}.
$$

Problem 4

Taylor-expand the self-consistent equation keeping terms up to M^5 and from this construct a Landau free energy.

Answer: Using the self-consistent equation, with $H = 0$, we rewrite the equation as follows:

$$
f(M) = M \cdot \left(\cosh\left(\frac{2dJM}{k_b T}\right) + \frac{e^{-\frac{\Delta}{k_b T}}}{2}\right) = \sinh\left(\frac{2dJM}{k_b T}\right) = Q(m).
$$

From this, we Taylor-expand each side of the equation: with five terms:

$$\begin{aligned}
\text{LHS:}\quad & f(0) + f'(0)\cdot M + \frac{f''(0)}{2}M^2 + \frac{f^{(3)}(0)}{6}M^3 + \frac{f^{(4)}(0)}{24}M^4 + \frac{f^{(5)}(0)}{120}M^5 \\
&= 0 + \left(1 + \frac{1}{2}e^{-\frac{\Delta}{k_bT}}\right)\cdot M + (0)\cdot M^2 + 2\left(\frac{Jd}{k_bT}\right)^2 \cdot M^3 + (0)\cdot M^4 + \frac{2}{3}\left(\frac{Jd}{k_bT}\right)^4 \cdot M^5 \\
\text{RHS:}\quad & Q(0) + Q'(0)\cdot M + \frac{Q''(0)}{2}M^2 + \frac{Q^{(3)}(0)}{6}M^3 + \frac{Q^{(4)}(0)}{24}M^4 + \frac{Q^{(5)}(0)}{120}M^5 \\
&= 0 + 2\left(\frac{Jd}{k_bT}\right)\cdot M + (0)\cdot M^2 + \frac{8}{6}\left(\frac{Jd}{k_bT}\right)^3 \cdot M^3 + (0)\cdot M^4 + \frac{4}{15}\left(\frac{Jd}{k_bT}\right)^5 \cdot M^5.
\end{aligned}$$

Moving the RHS to the LHS, and then doing the following:

$$\begin{aligned}
0 = &-\left(2\frac{Jd}{k_bT} - 1 - \frac{1}{2}e^{-\frac{\Delta}{k_bT}}\right)\cdot M - \left(\frac{8}{6}\left(\frac{Jd}{k_bT}\right)^3 - 2\left(\frac{Jd}{k_bT}\right)^2\right)\cdot M^3 \\
&- \left(\frac{4}{15}\left(\frac{Jd}{k_bT}\right)^5 - \frac{2}{3}\left(\frac{Jd}{k_bT}\right)^4\right)\cdot M^5
\end{aligned}$$

Matching the terms with a_i we get the following:

$$\begin{aligned}
\frac{\partial \mathcal{L}}{\partial M} &= a_1 M + a_3 M^3 + a_5 M^5, \\
\implies \mathcal{L} &= \frac{a_1}{2}M^2 + \frac{a_3}{4}M^4 + \frac{a_5}{6}M^6.
\end{aligned}$$

Problem 5

At the critical temperature you found in a previous step, show that the coefficient of the quadratic term goes to zero, signalling a continuous phase transition.

Answer: The quadratic term:

$$\begin{aligned}
&\left(1 + \frac{1}{2}e^{-\frac{\Delta}{k_bT}} - 2\frac{Jd}{k_bT}\right), \\
\implies &\left(1 + \frac{1}{2}e^{-\frac{\Delta}{k_bT}}\right) = 2\frac{Jd}{k_bT}
\end{aligned}$$

goes towards zero when entering a phase-transition when the temperature is at the critical temperature.

$$\begin{aligned}
\left(1 + \frac{1}{2}e^{-\frac{\Delta}{k_bT_c}}\right) &= 2\frac{Jd}{k_bT_c} \\
\left(1 + \frac{1}{2}e^{-\frac{\Delta}{k_bT_c}}\right) &= 2Jd \cdot \left(\frac{1 + \frac{e^{-\frac{\Delta}{k_bT}}}{2}}{2dJ}\right) \\
\left(1 + \frac{1}{2}e^{-\frac{\Delta}{k_bT_c}}\right) &= \left(1 + \frac{e^{-\frac{\Delta}{k_bT}}}{2}\right).
\end{aligned}$$

They are equivalent, and thus the coefficient of the quadratic term goes to zero at the critical temperature.

Problem 6

Show that there is also another temperature and a value of Δ, here the coefficients of both the quadratic and quartic terms go to zero. Hence, having another parameter in the Hamiltonian (in this case Δ) can lead to a situation where we need to the sixth-order term in the Landau free energy. We will see the implication of this in the next handin!

Answer: We begin by looking at a_3, which is the quartic term. If a_3 is zero, then we have the following:

$$\begin{aligned}\frac{8}{6}\left(\frac{Jd}{k_bT}\right)^3 &= 2\left(\frac{Jd}{k_bT}\right)^2\\ \frac{4}{6}\frac{Jd}{k_bT} &= 1\\ \frac{2}{3}\frac{Jd}{k_bT} &= 1\\ \frac{1}{3}\frac{Jz}{k_bT} &= 1.\end{aligned}$$

We use this result in the quadratic term:

$$\begin{aligned}\left(1+\frac{1}{2}e^{-\frac{\Delta}{k_bT}}\right) &= 2\frac{Jd}{k_bT}\\ \left(1+\frac{1}{2}e^{-\frac{\Delta}{k_bT}}\right) &= \frac{Jz}{k_bT}\\ \left(1+\frac{1}{2}e^{-\frac{\Delta}{k_bT}}\right) &= 3\\ \implies \frac{1}{2}e^{-\frac{\Delta}{k_bT}} &= 2\\ e^{-\frac{\Delta}{k_bT}} &= 4\\ -\frac{\Delta}{k_bT} &= \ln(4)\\ \Delta &= -k_bT\ln(4) = -\frac{Jz}{3}\ln(4)\end{aligned}$$