

Handin 5 : FK7058

Author : Andreas Evensen

Date: February 22, 2024

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

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:

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

where $h_i = H - J \sum_j \langle S_j \rangle$.

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:

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

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:

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

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:

$$\begin{aligned}
\text{LHS: } f(0) + f'(0) \cdot M + \frac{f''(0)}{2}M^2 + \frac{f^{(3)}(0)}{6}M^3 + \frac{f^{(4)}(0)}{24}M^4 + \frac{f^{(5)}(0)}{120}M^5 \\
= 0 + \left(1 + \frac{1}{2}e^{-\frac{\Delta}{k_b T}}\right) \cdot M + (0) \cdot M^2 + 2 \left(\frac{Jd}{k_b T}\right)^2 \cdot M^3 + (0) \cdot M^4 + \frac{2}{3} \left(\frac{Jd}{k_b T}\right)^4 \cdot M^5 \\
\text{RHS: } Q(0) + Q'(0) \cdot M + \frac{Q''(0)}{2}M^2 + \frac{Q^{(3)}(0)}{6}M^3 + \frac{Q^{(4)}(0)}{24}M^4 + \frac{Q^{(5)}(0)}{120}M^5 \\
= 0 + 2 \left(\frac{Jd}{k_b T}\right) \cdot M + (0) \cdot M^2 + \frac{8}{6} \left(\frac{Jd}{k_b T}\right)^3 \cdot M^3 + (0) \cdot M^4 + \frac{4}{15} \left(\frac{Jd}{k_b T}\right)^5 \cdot M^5.
\end{aligned}$$

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

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

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:

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

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

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

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: