

Statistical Mechanics - Class Exercise 8

June 7, 2022

Exercise 5713 - Mean field approximation for a classical Heisenberg model

Apply the mean field approximation to the classical spin vector model

$$\mathcal{H} = -\epsilon \sum_{\langle i,j \rangle} \mathbf{s}_i \cdot \mathbf{s}_j - \mathbf{h} \cdot \sum_i \mathbf{s}_i$$

where \mathbf{s}_i is a unit vector and $\langle i, j \rangle$ are neighboring sites on a lattice with coordination number c . The lattice has N sites and each site has c neighbors.

1. Assume that $\mathbf{h} = (0, 0, h)$, define a mean field \mathbf{h}_{eff} , and evaluate the partition function Z in terms of \mathbf{h}_{eff} .
2. Define θ_i as the inclination angle of \mathbf{s}_i with respect to \mathbf{h} . Assume that at equilibrium $\mathbf{s}_i = (0, 0, M)$, where $M = \langle \cos \theta \rangle$. Find the equation for M , and find the transition temperature T_c .
3. Write an expression for the mean field energy of the system assuming that $M(T)$ is known.
4. Identify exponents γ and β that describe the susceptibility $\chi \sim (T - T_c)^{-\gamma}$ above T_c , and the magnetization $M \sim (T_c - T)^\beta$ below T_c .
5. Find the jump in the heat capacity C_V at T_c .

Answer

1. In the mean field approximation

$$\mathcal{H} = -\epsilon \sum_{\langle i,j \rangle} \mathbf{s}_i \cdot \langle \mathbf{s}_j \rangle - \mathbf{h} \cdot \sum_i \mathbf{s}_i = -(\epsilon c \langle \mathbf{s} \rangle + \mathbf{h}) \cdot \sum_i \mathbf{s}_i = -\mathbf{h}_{eff} \cdot \sum_i \mathbf{s}_i$$

so

$$\mathbf{h}_{eff} = (\epsilon c \langle \mathbf{s} \rangle + \mathbf{h})$$

Because $\mathbf{h} = (0, 0, h)$ we can assume $\langle \mathbf{s} \rangle = s \hat{z}$, so $\mathbf{h}_{eff} = h_{eff} \hat{z}$ and $\mathbf{h}_{eff} \cdot \mathbf{s}_i = h_{eff} \cos \theta_i$, and because the mean field approximation the problem became a sum over single spins, so the partition function

$$Z_1 = \frac{1}{4\pi} \int_0^{2\pi} d\varphi \int_{-1}^1 d(\cos \theta) e^{\beta h_{eff} \cos \theta} = \frac{1}{2\beta h_{eff}} (e^{\beta h_{eff}} - e^{-\beta h_{eff}}) = \frac{\sinh(\beta h_{eff})}{\beta h_{eff}}$$

$$Z_N = Z_1^N = \left(\frac{\sinh(\beta h_{eff})}{\beta h_{eff}} \right)^N$$

2. For $M = \langle \cos \theta \rangle$

$$\begin{aligned} M = \langle \cos \theta \rangle &= \frac{1}{Z_1} \frac{1}{4\pi} \int_0^{2\pi} d\varphi \int_{-1}^1 d(\cos \theta) \cos \theta e^{\beta h_{eff} \cos \theta} = \frac{1}{\beta} \frac{1}{Z_1} \frac{\partial Z_1}{\partial h_{eff}} = \frac{1}{\beta} \frac{\partial \ln Z_1}{\partial h_{eff}} \\ &= \frac{1}{\beta} \frac{\partial}{\partial h_{eff}} (\ln (\sinh (\beta h_{eff})) - \ln (\beta h_{eff})) = \left(\coth (\beta h_{eff}) - \frac{1}{\beta h_{eff}} \right) \\ M &= \left(\coth (\beta (\epsilon c M + h)) - \frac{1}{\beta (\epsilon c M + h)} \right) \end{aligned}$$

For $h \rightarrow 0, M \rightarrow 0$, and with $\coth (x) \approx \frac{1}{x} + \frac{x}{3} - \frac{x^3}{15}$

$$\begin{aligned} M &\approx \left(\frac{1}{\beta \epsilon c M} + \frac{\beta \epsilon c M}{3} - \frac{1}{\beta \epsilon c M} \right) = \frac{\beta \epsilon c M}{3} \\ T_c &= \frac{\epsilon c}{3} \end{aligned}$$

3. For the mean field approximation in $h \rightarrow 0$

$$E = \langle \mathcal{H} \rangle = \left\langle -\epsilon \sum_{\langle i, j \rangle} \mathbf{s}_i \cdot \langle \mathbf{s}_j \rangle \right\rangle = -\epsilon \sum_{\langle i, j \rangle} \langle \mathbf{s}_i \rangle \langle \mathbf{s}_j \rangle = -\frac{1}{2} \epsilon c N M^2$$

4. We see

$$\begin{aligned} M &= \left(\coth (\beta (\epsilon c M + h)) - \frac{1}{\beta (\epsilon c M + h)} \right) \\ &\approx \left(\frac{1}{\beta (\epsilon c M + h)} + \frac{\beta (\epsilon c M + h)}{3} - \frac{(\beta (\epsilon c M + h))^3}{15} - \frac{1}{\beta (\epsilon c M + h)} \right) = \left(\frac{(T_c M + \frac{h}{3})}{T} - \frac{9(T_c M + \frac{h}{3})^3}{5T^3} \right) \end{aligned}$$

Above T_c

$$\begin{aligned} M &\approx \frac{(T_c M + \frac{h}{3})}{T} \\ M &= \frac{1}{3(T - T_c)} h = \chi h \end{aligned}$$

So $\gamma = 1$

below T_c for $h \rightarrow 0$ and $T \approx T_c$

$$\begin{aligned} M &= \frac{T_c M}{T} - \frac{9T_c^3 M^3}{5T^3} \\ (T - T_c) M &= -\frac{9T_c M^3}{5} \\ M &= \frac{\sqrt{5}}{3} \left(\frac{T_c - T}{T_c} \right)^{\frac{1}{2}} \end{aligned}$$

So $\beta = \frac{1}{2}$

5. We calculate the mean field energy in $h = 0$

$$E = -\frac{1}{2}\epsilon c N M^2$$

$$C_V = \frac{\partial E}{\partial T} = -\epsilon c N \frac{\partial M}{\partial T}$$

Above T_c

$$M = \chi h = 0$$

$$\rightarrow C_V = 0$$

below T_c

$$M = \frac{\sqrt{5}}{3} \left(\frac{T_c - T}{T_c} \right)^{\frac{1}{2}}$$

using that $T_c = \frac{\epsilon c}{3}$

$$\rightarrow C_V = -\frac{3}{2} N T_c \frac{\partial M^2}{\partial T} = \frac{5}{6} N$$

Exercise 5825 - Ising model 1D, domain walls

Consider the one dimensional Ising model with the Hamiltonian $\mathcal{H} = -\sum_{n,n'} J(n-n')\sigma(n)\sigma(n')$ with $\sigma(n) = \pm 1$ at each site n , and long range interaction $J(n) = b/n^\gamma$ with $b > 0$. Find the energy of a domain wall at $n = 0$, i.e. all the $n < 0$ spins are “down” and the others are “up”. Show that the standard argument for the absence of spontaneous magnetization at finite temperatures fails if $\gamma < 2$.

Answer

In the case of short range interaction (nearest neighbors) the energy gain a domain wall is $2J$, and the domain wall can be in N different site, so the change in the free energy is

$$\Delta F = 2J - T \ln(N)$$

so for huge N this is negative for any finite temperature, making this transition favorable.

In our case all the spins are interact with each other, so the the energy gain is (for N spins)

$$\Delta E = 2 \sum_{n=0}^{\frac{N}{2}} \sum_{n'=-1}^{-\frac{N}{2}} \frac{b}{(n-n')^\gamma} = 2 \sum_{n=0}^{\frac{N}{2}} \sum_{n'=1}^{\frac{N}{2}} \frac{b}{(n+n')^\gamma}$$

For $N \gg 1$ we can go to the continuum limit, define $x = n, y = n', dx = dy = 1$

$$\Delta E = 2b \int_0^{\frac{N}{2}} dx \int_1^{\frac{N}{2}} dy \frac{1}{(x+y)^\gamma}$$

For $\gamma > 2$

$$\begin{aligned} \Delta E &= 2b \int_0^{\frac{N}{2}} dx \frac{1}{(\gamma-1)} \left((x+1)^{-\gamma+1} - \left(x + \frac{N}{2}\right)^{-\gamma+1} \right) \\ &= 2b \frac{1}{(\gamma-1)(\gamma-2)} \left[1 - \left(\frac{N}{2} + 1\right)^{-\gamma+2} - \left(\frac{N}{2}\right)^{-\gamma+2} + N^{-\gamma+2} \right] \end{aligned}$$

For $N \rightarrow \infty$

$$\Delta E = \frac{2b}{(\gamma - 1)(\gamma - 2)}$$

This is finite value so

$$\Delta F = \frac{2b}{(\gamma - 1)(\gamma - 2)} - T \ln(N)$$

is negative for any finite temperature.

But for $\gamma = 2$

$$\begin{aligned} \Delta E &= 2b \int_0^{\frac{N}{2}} dx \int_1^{\frac{N}{2}} dy \frac{1}{(x+y)^2} = 2b \int_0^{\frac{N}{2}} dx \left[\frac{1}{(x+1)} - \frac{1}{(x+\frac{N}{2})} \right] \\ &= 2b \left[\ln\left(\frac{N}{2} + 1\right) - \ln(N) + \ln\left(\frac{N}{2}\right) \right] \end{aligned}$$

$$\Delta E = 2b \ln\left(\frac{N+2}{4}\right) \approx 2b \ln(N) - 2b \ln(4)$$

So

$$\Delta F = 2b \ln(N) - T \ln(N)$$

so for $T = 2b$ the energy cost is large of the entropy gain.

For $1 < \gamma < 2$

$$\Delta E = 2b \frac{1}{(\gamma - 1)(\gamma - 2)} \left[1 - \left(\frac{N}{2} + 1\right)^{-\gamma+2} - \left(\frac{N}{2}\right)^{-\gamma+2} + N^{-\gamma+2} \right] \approx [2 - 2^\gamma] b \frac{N^{2-\gamma}}{(\gamma - 1)(\gamma - 2)}$$

$$\Delta F = [2 - 2^\gamma] b \frac{N^{2-\gamma}}{(\gamma - 1)(\gamma - 2)} - T \ln(N)$$

So we never get domain wall