Statistical Mechanics - Class Exercise 8

December 25, 2022

Exercise 5713 - Mean field approximation for a classical Heisenberg model

Apply the mean field approximation to the classical spin vector model

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

where $\boldsymbol{s}_i$ 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 $\boldsymbol{h} = (0, 0, h)$, define a mean field $\boldsymbol{h}_{eff}$, and evaluate the partition function Z in terms of $\boldsymbol{h}_{eff}$.
2. Define θ_i as the inclination angle of $\boldsymbol{s}_i$ with respect to $\boldsymbol{h}$. Assume that at equilibrium $\boldsymbol{s}_i = (0, 0, M)$, 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

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

so

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

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

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

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

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

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

$$M = \left(\coth\left(\beta\left(\epsilon c M + h\right)\right) - \frac{1}{\beta\left(\epsilon c M + h\right)}\right)$$

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

$$M \approx \left(\frac{1}{\beta\epsilon c M} + \frac{\beta\epsilon c M}{3} - \frac{1}{\beta\epsilon c M}\right) = \frac{\beta\epsilon c M}{3}$$

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

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

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

4. We see

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

Above T_c

$$M \approx \frac{\left(T_c M + \frac{h}{3}\right)}{T}$$

$$M = \frac{1}{3\left(T - T_c\right)}h = \chi h$$

So $\gamma = 1$
below T_c for $h \to 0$ and $T \approx T_c$

$$M = \frac{T_c M}{T} - \frac{9T_c^3 M^3}{5T^3}$$

$$\left(T - T_c\right)M = -\frac{9T_c M^3}{5}$$

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

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

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

$$E=-\frac{1}{2}\epsilon cNM^2$$

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

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

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

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 $\sigma(n)=\pm1$ 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

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

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 Nspins)

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

For $N\gg1$ we can go to the continuum limit, define $x=n,y=n',dx=dy=1$

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

For $\gamma>2$

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

For $N \to \infty$

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

This is finite value so

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

is negative for any finite temperature.
But for $\gamma = 2$

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

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

So

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

so for $T = 2b$ the energy cost is large of the entropy gain.
For $1 < \gamma < 2$

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

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

So we never get domain wall