Ex 5713: Mean field approximation for a classical Heisenberg model

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The problem:

Apply the mean field approximation to the classical spin vector model

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

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

(a) Assume that $\vec{h} = (0, 0, h)$, define a mean field $\mathbf{h}_{eff}$,and evaluate the partition function Z in terms of $\mathbf{h}_{eff}$.

(b) Define θ_i as the inclination angle of $\mathbf{s_i}$ with respect to $\vec{h}$. Assume that at equilibrium $< \mathbf{s_i} >= (0, 0, M)$ where $M =< \cos\theta >$. Find the equation for M and find the transition temperature T_c .

(c) Write an expression for the mean field energy of the system assuming that $M(T)$ is known.

(d) 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.

(e) Find the jump in the heat capacity C_V at T_c.

The solution:

(a) We make a rough Mean field approximation and get the Hamiltonian:

$$\mathcal{H} = -\epsilon c \langle \vec{\mathbf{s}} \rangle \sum_i \vec{\mathbf{s}}_i - \vec{h} \cdot \sum_i \vec{\mathbf{s}}_i = -(\epsilon c \langle \vec{\mathbf{s}} \rangle + \vec{h}) \cdot \sum_i \vec{\mathbf{s}}_i = -\vec{h}_{eff} \cdot \sum_i \vec{\mathbf{s}}_i \tag{1}$$

we define $\vec{h}_{eff} = \epsilon c M + \vec{h}$ where $M = \langle \vec{\mathbf{s}} \rangle$.

we can see this is in fact a sum of single spin hamiltonians, each of the form:

$$\mathcal{H}^{(i)} = -\vec{h}_{eff} \cdot \vec{\mathbf{s}}_i = -\vec{h}_{eff} \cdot cos\theta_i \tag{2}$$

Notice that the Mean field approximation transforms the problem from multi particle problem to a single particle problem (without a direct interaction) and the spins are pinned to their positions so that $Z_N = {Z_1}^N$.

$$Z_1 = \frac{1}{4\pi} \int_{-1}^{1} e^{\beta \mathcal{H}^{(i)}} d(\cos\theta_i) \int_0^{2\pi} d\varphi = \frac{1}{4\pi} \int_{-1}^{1} e^{\beta \mathbf{h}_{eff} \cos\theta} d(\cos\theta) \int_0^{2\pi} d\varphi = \frac{\sinh(\beta \mathbf{h}_{eff})}{\beta \mathbf{h}_{eff}} \tag{3}$$

$$Z_N = (Z_1)^N = \left(\frac{\sinh(\beta \mathbf{h}_{eff})}{\beta \mathbf{h}_{eff}} \right)^N \tag{4}$$

(b) we define $M(T) = \langle \cos\theta_i \rangle$ For a single spin:

$$M \equiv \langle \cos(\theta_i) \rangle = \frac{1}{Z}\int_{-1}^{1} cos(\theta) e^{\beta \mathbf{h}_{eff}\cos\theta} d(\cos\theta) \int_0^{2\pi} d\varphi = \frac{1}{Z}\frac{1}{\mathbf{h}_{eff}}\frac{\partial}{\partial\beta}Z \tag{5}$$

$$M = \frac{1}{\mathbf{h}_{eff}}\frac{\partial}{\partial\beta}\ln Z = \frac{1}{\mathbf{h}_{eff}}\frac{\partial}{\partial\beta}\left[\ln\left(\sinh(\beta\mathbf{h}_{eff})\right) - \ln\left(\beta\mathbf{h}_{eff}\right)\right] \tag{6}$$

$$M = \coth(\beta\mathbf{h}_{eff}) - \frac{1}{\beta\mathbf{h}_{eff}} \tag{7}$$

$$\coth x \approx \frac{1}{x} + \frac{x}{3} - \frac{x^3}{45} \qquad \tanh x \approx x - \frac{x^3}{3} \quad \rightarrow \quad \coth x - \frac{1}{x} \approx \tanh x \tag{8}$$

$$M \approx \tanh\left(\beta\mathbf{h}_{eff}\right) \;\Rightarrow\; \tanh^{-1}(M) = \beta(\epsilon c M + h) \tag{9}$$

To first order $\tanh^{-1}(M) \cong M$ and to find T_c we take $h \to 0$.

$$M = \frac{\epsilon c M}{T_c} \qquad \rightarrow T_c = \epsilon c \tag{10}$$

(c) In the mean field approximation the spins are independent of each other, and therefore $\langle \mathbf{s}_i \mathbf{s}_j \rangle = \langle \mathbf{s}_i \rangle \langle \mathbf{s}_j \rangle$. When calculating the energy we take $h \to 0$.

It follow that the energy is:

$$E = \langle \mathcal{H} \rangle = -\epsilon \sum_{\langle i,j \rangle} \langle \tilde{\mathbf{s}}_i \rangle \cdot \langle \tilde{\mathbf{s}}_j \rangle \tag{11}$$

$$E = -\frac{1}{2} N \epsilon c M^2 \tag{12}$$

(d) From section b we get:

$$M = \coth(\beta\mathbf{h}_{eff}) - \frac{1}{\beta\mathbf{h}_{eff}} \approx \tanh\beta\mathbf{h}_{eff} \tag{13}$$

so we get the known result for M:

$$M = \tanh(\beta\mathbf{h}_{eff}) \Rightarrow \tanh^{-1}(M) = \beta\mathbf{h}_{eff} \qquad \tanh^{-1}(M) \approx M + \frac{M^3}{3}$$

$$\frac{1}{T}(\epsilon c M + h) = M + \frac{M^3}{3} \quad \Rightarrow \quad h = (T - T_c)M + T_c\frac{M^3}{3} \tag{14}$$

For the last term in the final expression we replaced T with T_c, since we are looking only at temperatures close to T_c.

First we look at $T > T_c$: there is only the trivial solution $m \to 0$

$$h = (T - T_c)M \tag{15}$$

$$M = (T - T_c)^{-1}h = \chi h \quad \Rightarrow \quad \gamma = 1 \tag{16}$$

Now for $T < T_c$ we take $\quad h \to 0^+$

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

$$M = \sqrt{3\left(\frac{T_c - T}{T_c}\right)} \quad \Rightarrow \quad \beta = \frac{1}{2} \tag{17}$$

(e) We consider the mean field energy $E = -\frac{1}{2}N\epsilon c M^2$:

$$C_v = \frac{\partial E}{\partial T} = \frac{\partial}{\partial T}(-\frac{1}{2}N\epsilon c M^2) \tag{18}$$

The only dependence of T in the energy is $M(T)$. The dependence is different below T_c and above it.

for $T > T_c$:

$$M = (T - T_c)^{-1}h \ , \quad h \to 0 \quad \Rightarrow \quad M(T) = 0 \quad \Rightarrow \quad C_v(T) = 0 \tag{19}$$

and for $T < T_c$:

$$C_v = -\frac{1}{2}NT_c \frac{\partial M^2}{\partial T} = -\frac{1}{2}NT_c \cdot \frac{\partial}{\partial T}\left[3\left(\frac{T_c - T}{T_c}\right)\right] \cong \frac{3}{2}NT_c \cdot \frac{1}{T_c} = \frac{3}{2}N \tag{20}$$

Since we are used $T \approx T_c$, we got a constant. So the jump in C_v is:

$$C_v(T_c^+) - C_v(T_c^-) = 0 - \frac{3}{2}N = -\frac{3}{2}N. \tag{21}$$