Ex 5956: Mean field approximation classical spin vector 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 for $h \to 0^+$.

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

(d) Identify exponents γ, β as $T \to T_c$ for the susceptibility $\chi \sim (T - T_c)^{-\gamma}$ above T_c and for $M \sim (T_c - T)^{\beta}$ below T_c.

(e) Show that there is a jump in C_V at T_c.

The solution:

(a) we make a roughly Mean field approximation and got the Hamiltonian for the singel spin at site i:

$$\mathcal{H}^i = -\epsilon c \langle \vec{\mathbf{s}} \rangle \vec{\mathbf{s}}_i - h \cdot \vec{\mathbf{s}}_i \tag{1}$$

lets define $\langle \vec{\mathbf{s}} \rangle = \frac{M}{N} = \vec{m}$ and $\vec{\mathbf{s}}_i = \cos\theta_i$

$$\mathcal{H}^i = -(\epsilon c m + h)\cos\theta_i \qquad so \ \ that \ \ \rightarrow \quad \mathbf{h}_{eff} = \epsilon c m + h \qquad \mathcal{H}^i = (-\mathbf{h}_{eff}\cos\theta_i)$$

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

$$Z_1 = \frac{1}{4\pi}\int_{-1}^{1} e^{\beta \mathbf{h_1}} d(\cos\theta_i) \int_0^{2\pi} d\varphi = \frac{1}{4\pi}\int_{-1}^{1} e^{\beta \mathbf{h}_{eff}\cos\theta} d(\cos\theta) \int_0^{2\pi} d\varphi = \frac{\sinh(\beta \mathbf{h}_{eff})}{\beta \mathbf{h}_{eff}} \tag{2}$$

$$Z_N = (Z_1)^N = \left(\frac{\sinh(\beta \mathbf{h}_{eff})}{\beta \mathbf{h}_{eff}}\right)^N \tag{3}$$

(b) we define $m(T) = \langle \cos\theta_i \rangle$

$$m \equiv \langle \cos(\theta_i) \rangle = \frac{1}{Z} \sum cos(\theta) e^{\beta \mathbf{h}_{eff} \cos\theta} = \frac{1}{Z} \frac{1}{\mathbf{h}_{eff}} \frac{\partial}{\partial \beta} Z \tag{4}$$

For singel spin:

$$m = \frac{1}{\mathbf{h}_{eff}} \frac{\partial}{\partial \beta} \ln Z = \frac{1}{\mathbf{h}_{eff}} \frac{\partial}{\partial \beta} \left[\ln\left(\sinh(\beta \mathbf{h}_{eff})\right) - \ln\left(\beta \mathbf{h}_{eff}\right)\right] \tag{5}$$

$$m = \coth(\beta \mathbf{h}_{eff}) - \frac{1}{\beta \mathbf{h}_{eff}} \cong \{h \to 0, \;\; T \approx T_c \Rightarrow m \to 0\} \tag{6}$$

Second approach:

$$F = -K_B T \ln Z_N = -\frac{N}{\beta}\left[-\beta \frac{1}{2} \epsilon c m^2 + \ln\left[sinh(\beta \epsilon c m) - \ln(\beta \epsilon c m)\right]\right] \tag{7}$$

$*$ we want to choose M from extremum condition.Where $\frac{M}{N} = m$

$$\frac{\partial F}{\partial M} = \frac{1}{N} \frac{\partial F}{\partial m} = \epsilon c m - \frac{1}{\beta} \frac{\cosh(\beta \epsilon c m)}{\sinh(\beta \epsilon c m)} \beta \epsilon c + \frac{1}{m\beta} = \epsilon c m - \epsilon c \coth(\beta \epsilon c m) + \frac{1}{\beta m} \;\; \Rightarrow \; 0 \tag{8}$$

$$m = \left[\coth(\beta \epsilon c m) - \frac{1}{\beta \epsilon c m}\right] \tag{9}$$

$$\coth x \cong \frac{1}{x} + \frac{x}{3} - \frac{x^3}{45} \qquad \tanh x \cong x + -\frac{x^3}{3} \quad \to \quad \coth x - \frac{1}{x} \approx \tanh x$$
$$m \approx \tanh \beta \mathbf{h}^0_{eff} \;\; \Rightarrow \;\; \tanh^{-1}(m) = \beta(\epsilon c m + h) \tag{10}$$

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

$$m = \beta \epsilon c m \qquad \to \epsilon c = K_B T_c \tag{11}$$

(c) In the mean field approximation the spins are independent of each other, and therefore $\langle \mathbf{s}_i \mathbf{s}_j \rangle = \langle \mathbf{s}_i \rangle \langle \mathbf{s}_j \rangle$. It follow that the energy is:

$$E = \langle \mathcal{H} \rangle = \left\langle -\epsilon \sum_{\langle i, \epsilon \rangle} \tilde{\mathbf{s}}_i \cdot \tilde{\mathbf{s}}_j - \mathbf{h} \cdot \sum_i \vec{\mathbf{s}}_i \right\rangle \tag{12}$$

$$E = -\frac{1}{2} \epsilon c m^2 N - \epsilon c m N h \tag{13}$$

For $h \to 0$ we get the known result for the energy $E = -\frac{1}{2} \epsilon c m^2 N$

(d) From section b we get:

$$m = \coth(\beta \mathbf{h}_{eff}) - \frac{1}{\beta \mathbf{h}_{eff}} \qquad \coth x - \frac{1}{x} \approx \tanh x \tag{14}$$

so we get the known result for m:

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

we take $h \to 0$

$$\epsilon c m = k_B T m + k_B T \frac{m^3}{3} \qquad \frac{3(T_c - T)}{T} m = m^3$$

$$m = \sqrt{3(\frac{T_c}{T} - 1)} \Rightarrow \qquad \beta = \frac{1}{2} \tag{15}$$

$$h = T tanh^{-1}(m) - \epsilon c m \Rightarrow (For \ \ T > T_c \quad m \to 0) \ \ h \cong T(m + \frac{m^3}{3}) - T_c m$$

$$\chi = \frac{\partial m}{\partial h}|_{h \to 0} = \frac{1}{\frac{\partial h}{\partial m}} = \frac{1}{(T - T_c) + m^2} \cong (T - T_c)^{-1} \quad \Rightarrow \quad \gamma = 1 \tag{16}$$

(e)

$$U = -\frac{\partial \ln Z}{\partial \beta} = -\frac{\partial T}{\partial \beta} \frac{\partial \ln Z}{\partial T} = K_B T^2 \frac{\partial \ln Z}{\partial T} \tag{17}$$

$$C_v = \frac{\partial U}{\partial T} = 2 K_B T \frac{\partial \ln Z}{\partial T} + K_B T^2 \frac{\partial^2 \ln Z}{\partial T^2} \tag{18}$$

$$-\frac{\partial^2 F}{\partial T^2} = \frac{\partial}{\partial T^2}(KT \ln Z) = \frac{\partial}{\partial T}(K \ln Z + KT \frac{\partial \ln Z}{\partial T}) = 2K \frac{\ln Z}{\partial T} + KT \frac{\partial^2 \ln Z}{\partial T^2} \tag{19}$$

$$\Rightarrow \ \ C_v = -T \frac{\partial^2 F}{\partial T^2} = -T \frac{\partial}{\partial T}(\frac{\partial F}{\partial m} \cdot \frac{\partial m}{\partial T}) \tag{20}$$

From section b we got: $m \approx \sqrt{\frac{T_c}{T} - 1}$ to get: $\frac{\partial m}{\partial T} \approx \frac{-T_c/T^2}{2\sqrt{\frac{T_c}{T} - 1}}$

$$F = -K_B T \ln Z_N = -\frac{N}{\beta} \left[-\beta \frac{1}{2} \epsilon c m^2 + \ln \left[sinh(\beta \epsilon c m) - \ln(\beta \epsilon c m) \right] \right] \tag{21}$$

$$\frac{\partial F}{\partial m} = \frac{N}{\beta}(\beta \epsilon c m - \coth(\beta \epsilon c m) \beta \epsilon c + \frac{1}{m}) \qquad [\epsilon c \approx T_c]$$

$$\cong N(\epsilon c m - \epsilon c(\frac{1}{\beta \epsilon c m} - \frac{\beta \epsilon c m}{3} \ \ ) + \frac{1}{\beta m}) \cong N \epsilon c m (1 - \frac{T_c}{T}) \tag{22}$$

$$C_v = -T\frac{\partial}{\partial T}(\frac{\partial F}{\partial M}\cdot\frac{\partial M}{\partial T}) = -T\frac{\partial}{\partial T}\left(NT_c m(1-\frac{T_c}{T})\right)\left(\frac{-T_c/T^2}{2\sqrt{\frac{T_c}{T}-1}}\right) \tag{23}$$

$$C_v \cong T\frac{\partial}{\partial T}\left(N\frac{T_c^2}{T^2}(1-\frac{T_c}{T})\right) \tag{24}$$

We search C_v close to T_c so $(T-T_c) << 1$ and $\frac{T_c^2}{T^2} \cong 1$

$$C_v \cong T_c N\frac{\partial}{\partial T}\left(\frac{T-T_c}{T_c}\right) = NT_c \tag{25}$$

We can see the jump in C_v for $T > T_c$ $(m = 0)$ and as a result $C_v = 0$,for $T < T_c$
$C_v = const$
Additional approach: we consider the mean field energy $E = -\frac{1}{2}\epsilon c m^2 N$:

$$C_v = \frac{\partial U}{\partial T} = \frac{\partial}{\partial T}(-\frac{1}{2}\epsilon c m^2 N) \tag{26}$$

$$C_v = -\frac{1}{2}NT_c\frac{\partial m^2}{\partial T} = -\frac{1}{2}NT_c\frac{\partial}{\partial T}\left(\frac{T_c}{T}-1\right) \cong -\frac{1}{2}NT_c\frac{\partial}{\partial T}(T_c - T) \cong NT_c \tag{27}$$