Exercise Sheet 3 Stat Phy — Arya Poretya, Fabio Steyer

Problem 6

We consider the Ising model:

$$H = -J \sum_{\langle ij \rangle} S_i S_j - h \sum S_i$$

By mean-field approx. we have, $S_i = m + \delta S_i$,

$$H = -J \sum_{\langle ij \rangle} (m+\delta S_i)(m+\delta S_j) - h \sum S_i$$

$$\approx -J m^2 N_B - Jm \sum_{\langle ij \rangle} (\delta S_i + \delta S_j) - h \sum_i S_i$$ ← quadratic terms removed.

$$= -J m^2 N_B - Jmz \sum_i \delta S_i - h \sum_i S_i$$ ← Introduce coordination number.

We now reintroduce the fluctuation term,

$$H \approx -J m^2 N_B - Jmz \sum_i (S_i - m) - h \sum_i S_i$$

$$= N_B J m^2 - (Jmz + h) \sum_i S_i.$$

Now we have Hamiltonian, approximated upto an additive constant

$$H \approx \sum H_i = -(Jmz + h) \sum_i S_i$$

The partial partition sum of S_i, is then

$$Z_i = \sum_{H_i} e^{-\beta H_i} = \sum_{S_i=-S}^{S} e^{\beta (Jmz+h) S_i}$$

$$Z_i - Z_i \cdot e^{\beta(Jmz+h)} = e^{-\beta(Jmz+h)S} - e^{\beta(Jmz+h)(S+1)}$$

$$\Rightarrow \quad Z_i = \frac{e^{-\beta q S} - e^{\beta q (S+1)}}{1 - e^{\beta q}} = \frac{e^{q/2}\left(e^{-q(S+\frac{1}{2})} - e^{q(S+\frac{1}{2})}\right)}{e^{q/2}\left(e^{-q/2} - e^{q/2}\right)}$$

$q = \beta(Jmz + h)$

$$= \frac{e^{q(S+\frac{1}{2})} - e^{-q(S+\frac{1}{2})}}{e^{q/2} - e^{-q/2}} = \frac{\sinh\left(q(S+\frac{1}{2})\right)}{\sinh\left(q\frac{1}{2}\right)}$$

☒ (i).

$$m = \frac{\sum_{s_i} s_i e^{q s_i}}{\sum_{s_i} e^{q s_i}} = \frac{\partial}{\partial q} \ln Z_i$$

$$= \frac{\partial}{\partial q} \ln \frac{\sinh(q(S+\frac{1}{2}))}{\sinh(q\frac{1}{2})}$$

expanding around the origin, we have

$$= \frac{\partial}{\partial q} \ln \left[\left(q(S+\tfrac{1}{2}) + \frac{q^3(S+\frac{1}{2})^3}{3!} + O(q^5) \right) \left(\frac{2}{q} - \frac{q}{2}\frac{1}{3!} + \frac{7q^3}{360} + O(q^5) \right) \right]$$

$$= \frac{\partial}{\partial q} \ln \left[1 + 2S - \frac{q^2(S+\frac{1}{2})}{12} + \frac{7q^4(S+\frac{1}{2})}{360} + q^2\frac{(S+\frac{1}{2})^3}{3} + O(q^4) \right]$$

$$= \frac{\partial}{\partial q} \ln \left\{ 1+2S + q^2 \left[\frac{(S+\frac{1}{2})^3}{3} - \frac{(S+\frac{1}{2})}{12} \right] + O(q^4) \right\}$$

$$= \frac{\partial}{\partial q} \left[\ln(1+2S) + \frac{q^2}{1+2S} \left(\frac{4(S+\frac{1}{2})^3 - (S+\frac{1}{2})}{12} \right) + O(q^4) \right]$$

$$= \frac{q}{12} \left[4(S+\tfrac{1}{2})^2 - 1 \right] + O(q^3)$$

Therefore, around the origin, and assuming $h = 0$.

$$m \approx \frac{\beta J m z}{12} \left[4(S+\tfrac{1}{2})^2 - 1 \right]$$

Trivial solution $m = 0$, spontaneous magnetization if non trivial solution exist, i.e $m \neq 0$. This occurs at β_c. ($k_B = 1$)

$$1 = \beta_c \frac{J z \left[4(S+\frac{1}{2})^2 - 1 \right]}{12}$$

$$\Rightarrow \boxed{T_c = \frac{J z \left[4(S+\frac{1}{2})^2 - 1 \right]}{12}}$$

Problem 5

We know that,

$$C_H = C_M + \frac{T}{N}\left(\frac{\partial M}{\partial T}\Big|_H\right)^2 \Big/ \frac{\partial M}{\partial H} \propto \chi_T.$$

Furthermore,

$$C_M, C_H \propto \tau^{-\alpha}$$

$$M \propto \tau^{\beta}$$

$$\chi_T \propto \tau^{-\gamma}$$

$$\Rightarrow C_H = a\tau^{-\alpha} + b\tau^{-\alpha+1} \cdots$$

$$C_M = c\tau^{-\alpha} + d\tau^{-\alpha+1} \cdots$$

$$M = e\tau^{\beta} + \cdots$$

$$\chi_T = f\tau^{-\gamma} + \cdots$$

$$\Rightarrow a\tau^{-\alpha} + \cdots = c\tau^{-\alpha} + \cdots + \frac{T}{N}\left(\frac{\partial \tau}{\partial T}\frac{\partial M}{\partial \tau}\Big|_H\right)^2 \Big/ \left(f\tau^{-\gamma} + \cdots\right).$$

$$= c\tau^{-\alpha} + \cdots + \frac{T}{NT_c^2}\left[\beta e \tau^{\beta-1} \cdots\right]^2 \Big/ \left(f\tau^{-\gamma} + \cdots\right)$$

$$\approx c\tau^{-\alpha} + \frac{T\beta e}{NT_c^2 f} \cdot \frac{\tau^{2\beta-2}}{\tau^{-\gamma}}$$

$$\Rightarrow a\tau^{-\alpha} \approx c\tau^{-\alpha} + \frac{T\beta e}{NT_c^2 f}\tau^{2\beta-2+\gamma}$$

$$\Rightarrow a \approx c + \frac{T\beta e}{NT_c^2 f}\tau^{\alpha+2\beta+\gamma-2}$$

i.e.

$$\frac{C_H}{\tau^{-\alpha}} = \text{const.} \iff \alpha + 2\beta + \gamma - 2 = 0 \quad \blacksquare$$

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Sheet 3

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Problem 7: Mean-field approximation for the Heisenberg model *(4 Points)*

Now we consider the Heisenberg model, where spins can freely reorient in 3 dimensions:

$$H = -J\sum_{\langle ij\rangle} \mathbf{S}_i \cdot \mathbf{S}_j - h\sum_i S_i^z,$$

with unit vectors $\mathbf{S}_i$. The direction of the magnetic field is chosen as the z-direction without loss of generality. Therefore, we can assume that $\langle \mathbf{S}_i \rangle = \mathbf{m} = m\mathbf{e}_z$.

(a) Derive the mean-field Hamiltonian of the Heisenberg model and calculate the partition sum. *Hint: Since the spins are now continuous, you need to evaluate an integral.*

$$H = -\sum_{\langle i,j\rangle} J_{ij}\,\underline{S}_i \cdot \underline{S}_j - h\sum_i S_i^z$$

Idea:
- interaction of two neighboring spins $\underline{S}_i \cdot \underline{S}_j$ can be replaced by interaction of a single spin of site i with the mean spin value of it's surrounding:

$$\underline{S}_i \cdot \underline{S}_j \longrightarrow \underline{S}_i \langle \underline{S} \rangle \quad ; \langle \underline{S} \rangle = \langle m_z e_z \rangle$$

- we assume that all angular momenta point in the direction of the external magnetic field:

$$\underline{S}_i \longrightarrow S_i^z$$

$$\Rightarrow H_{MF} = -J\sum_{\langle ij\rangle} \underbrace{\underline{S}_i}_{S_i^z} \cdot z\langle \underline{S}\rangle - \underbrace{h}_{\mu B^z}\sum_i S_i^z + \sum_{\langle ij\rangle} J\langle \underline{S}\rangle^2 \; ; \; z := \text{number of nearest partners}$$

$$= -\left[\mu B^z + \underbrace{zJ\langle \underline{S}\rangle}_{B^z_{MF}}\right]\sum_i S_i^z + \sum_{\langle ij\rangle} J\langle \underline{S}\rangle^2$$

$$= -\mu B^z_{total}\sum_i S_i^z + \frac{JzN}{2}\langle \underline{S}\rangle^2 \;/\!/$$

$$Z = \sum_{\{S_i\}} \exp(-\beta H_{MF}) = \exp\left(-\frac{\beta JzN}{2}\langle \underline{S}\rangle^2\right) 2^N \cosh^N(\beta\mu B^z + zJ\langle \underline{S}\rangle)$$

b) with free enthalpie follows:

$$G(T,B) = -\left(\frac{1}{\beta}\right)\ln(Z) = \frac{zJN}{2}\langle \underline{S}\rangle^2 - \left(\frac{N}{\beta}\right)\ln\left[2\cosh(\beta_g \beta + zJ\beta\langle \underline{S}\rangle)\right]$$

=> for magnetisation we obtain:

$$M = -\left(\frac{\partial G}{\partial B_{total}}\right)_T = N\mu \tanh(\mu\beta B_{total})$$

$$M = N\mu\langle \underline{S}\rangle$$

$$\Rightarrow \langle \underline{S}\rangle = \tanh\left[\mu\beta B^z + \beta z J\langle \underline{S}\rangle\right] \; ; \; \langle \underline{S}\rangle = m$$

with $\langle \underline{S}\rangle = m$ and free enthalpie $G(T,B)$ follows:

$$\cosh(\beta\mu B + \beta J z m) = \frac{1}{\sqrt{1-\tanh^2(\beta\mu B + \beta J z m)}} = \frac{1}{\sqrt{1-m^2}}$$

$$\overset{(B=H)}{\Rightarrow} G(T,H) = Nk_BT\left[-\ln(2) + \frac{1}{2}\ln(1-m^2)\right] + \frac{N}{2}Jzm^2$$

$$\Rightarrow m = \tanh(\beta\mu H + \beta J z m)$$

with free energie $F(T,M) = G(T,H) + MH$ and $M = N\mu\langle S\rangle = N\mu m$ follows:

$$\beta\mu H = \operatorname{arctanh}(m) - \beta J z m = \frac{1}{2}\ln\left(\frac{1+m}{1-m}\right) - \beta J z m$$

$$\Leftrightarrow \beta(\mu H + J z m) = \frac{1}{2}\ln\left(\frac{1+m}{1-m}\right)$$

$$\Leftrightarrow \beta = \frac{\ln\left(\frac{1+m}{1-m}\right)}{2(\mu H + J z m)} \;/\!/$$

c)
- $h \to 0$ ($\hookrightarrow \mu B \to 0$), in the limits of small m:

$$\left[\beta = \frac{1}{k_B T} \; ; \; T_c = \frac{Jz}{k_B}\right]$$

$$m = \beta J z m - \frac{1}{3}(\beta J z m)^3 + \dots$$

$$= \frac{Jzm}{k_BT} - \frac{1}{3}\left(\frac{Jzm}{k_BT}\right)^3 + \dots$$

$$\simeq \frac{T_c \cdot m}{T} - \frac{1}{3}\left(\frac{T_c \cdot m}{T}\right)^3 + \dots$$

[NR:

$$m = \frac{T_c \cdot m}{T} - \frac{1}{3}\left(\frac{T_c \cdot m}{T}\right)^3 \quad | \cdot m$$

$$\Rightarrow 1 = \frac{T_c}{T} - \frac{1}{3}\left(\frac{T_c}{T}\right)^3 m^2$$

$$\Leftrightarrow m^2 = \frac{3\left(1-\frac{T_c}{T}\right)}{\left(\frac{T_c}{T}\right)^3} = \frac{3(T_c - T)}{T_c}$$