V.3.3 Mean field theory of the Ising model

N spins on a d-dimensional lattice

$$H = -\varepsilon \sum_{\{i,j\}} s_i s_j - \mu B \sum_{i=1}^{N} s_i = -\frac{\varepsilon}{2} \sum_{i=1}^{N} \sum_{j \text{ neighbors of } i} s_i s_j - \mu B \sum_{i=1}^{N} s_i$$

$$= -\frac{\varepsilon}{2} \sum_{i=1}^{N} \sum_{j \text{ neighbors of } i} (s_i - \langle s_i \rangle)(s_j - \langle s_j \rangle) - \varepsilon \sum_{i=1}^{N} \sum_{j \text{ neighbors of } i} s_i \langle s_j \rangle + \frac{\varepsilon}{2} \sum_{i=1}^{N} \sum_{j \text{ neighbors of } i} \langle s_i \rangle \langle s_j \rangle - \mu B \sum_{i=1}^{N} s_i$$

$$= -\frac{\varepsilon}{2} \sum_{i=1}^{N} \sum_{j \text{ neighbors of } i} (s_i - \langle s \rangle)(s_j - \langle s \rangle) - \varepsilon \nu \langle s \rangle \sum_{i=1}^{N} s_i + \underbrace{\frac{\varepsilon N \nu}{2} \langle s \rangle^2}_{\text{constant irrelevant for physics}} - \mu B \sum_{i=1}^{N} s_i$$

ν = number of neighbors of one site
square lattice in d-dimensions : $\nu = 2d$

Mean field approximation:

neglect fluctuations

$$\rightarrow H = -(\varepsilon \nu \langle s \rangle + \mu B) \sum_{i=1}^{N} s_i$$

Problem: We do not know $\langle s \rangle$.
$\rightarrow$ self-consistent approach:

- assume we know $\langle s \rangle$
- calculate $\langle s \rangle$ as a function of $\langle s \rangle$ and the other parameters
- solve for $\langle s \rangle$

Partition function:

$$Z(T) = \sum_{s_1 = \pm 1} \cdots \sum_{s_N = \pm 1} e^{+\beta(\varepsilon \nu \langle s \rangle + \mu B) \sum_{i=1}^{N} s_i}$$

$$= \left(\sum_{s_1 = \pm 1} e^{\beta(\varepsilon \nu \langle s \rangle + \mu B) s_1} \right) \cdots \left(\sum_{s_N = \pm 1} e^{\beta(\varepsilon \nu \langle s \rangle + \mu B) s_N} \right)$$

$$= \left[e^{\beta(\varepsilon v\langle s\rangle + \mu B)} + e^{-\beta(\varepsilon v\langle s\rangle + \mu B)}\right]^N$$

$$= 2^N \cosh^N \beta(\varepsilon v\langle s\rangle + \mu B)$$

$$\langle s\rangle = \frac{1}{N}\left\langle \sum_{i=1}^{N} s_i \right\rangle = \frac{\sum_{i=1}^{N} \sum_{\{s_j\}} s_i\, e^{\beta(\varepsilon v\langle s\rangle + \mu B)\sum_{j=1}^{N} s_j}}{N\, 2^N \cosh^N \beta(\varepsilon v\langle s\rangle + \mu B)} = \frac{\sinh\left[\beta(\varepsilon v\langle s\rangle + \mu B)\right]}{\cosh\left[\beta(\varepsilon v\langle s\rangle + \mu B)\right]}$$

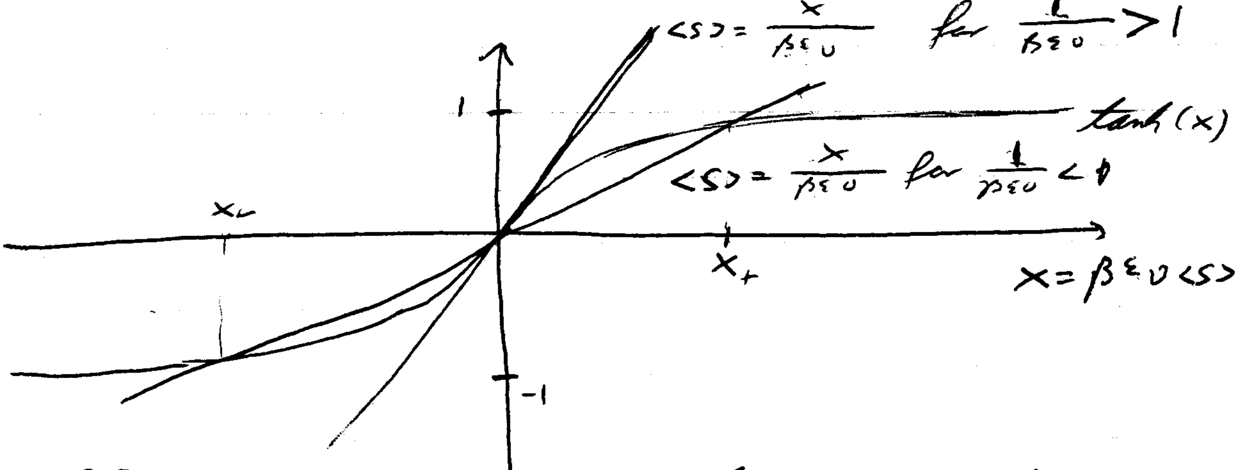
$$= \tanh\left[\beta(\varepsilon v\langle s\rangle + \mu B)\right]$$

$$\Rightarrow \boxed{\langle s\rangle = \tanh\left[\beta(\varepsilon v\langle s\rangle + \mu B)\right]}$$

self-consistent equation for $\langle s\rangle$ as a function of T and B (and the "material parameters" ε, v, and μ)

Is there a magnetization for $B \to 0$?

solve $\langle s\rangle = \tanh\left[\beta\varepsilon v\langle s\rangle\right]$



$\frac{2k_BT}{\varepsilon v} > 1 \Rightarrow$ only solution $x = 0 \Rightarrow \langle s\rangle = 0$ paramagnet

$\frac{2k_BT}{\varepsilon v} < 1 \Rightarrow$ three solutions $x = 0$, $x = x_+$, $x = x_-$ [illegible] which is the right solution?

look at free energy

$x=0$: $G=-k_BTN\ln[2\cosh(0)]=-k_BTN\ln(2)$

$x=x_\pm$ $G=-k_BTN\ln[2\cosh(x_\pm)]<-k_BTN\ln(2)$

$\Rightarrow x=x_\pm$ is the stable solution $\Rightarrow \langle s\rangle \neq 0$

$\Rightarrow$ ferromagnet

$\Rightarrow$ phase transition at T_c given by $\frac{k_BT_c}{\varepsilon\upsilon}=1$

$$\Rightarrow \boxed{T_c=\frac{\varepsilon\upsilon}{k_B}}$$

Contradiction to result in $d=1$

$\rightarrow$ mean field approximation not good in $d=1$

in fact: mean field approximation good for $d\geq 4$

How does magnetization behave?

know: $\langle s\rangle=0$ for $T>T_c$

$$\langle s\rangle=\tanh\left[\frac{T_c}{T}\langle s\rangle\right]$$

$T\to 0$ $\Rightarrow$ $\langle s\rangle \Rightarrow \tanh(\pm\infty)=\pm 1$

$T\approx T_c$: $\frac{T}{T_c}=1+\delta$ $0<\delta\ll 1$

$\delta=\frac{T_c-T}{T_c}$

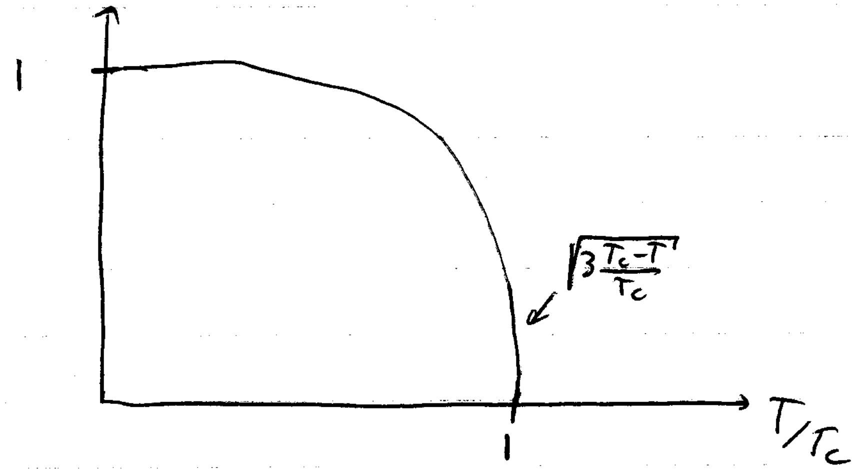
assume $\langle s\rangle$ small

$$\langle s\rangle=\tanh\left[\frac{\langle s\rangle}{1-\delta}\right]\approx\frac{\langle s\rangle}{1-\delta}-\frac{1}{3}\frac{\langle s\rangle^3}{(1-\delta)^3}+O(\langle s\rangle^5)$$

$$\langle s\rangle\left(1-\frac{1}{1-\delta}\right)\approx -\frac{1}{3}\ \frac{\langle s\rangle^3}{(1-\delta)^3}$$

$$\langle s\rangle^2 \approx 3\ \frac{\delta}{1-\delta}(1-\delta)^3 = 3\delta + O(\delta^2)$$

$$\Rightarrow \langle s\rangle \approx \pm\sqrt{3\delta}$$



→ continuous phase transition

Is it second order? → calculate heat capacity

$$U = \langle H\rangle = -\varepsilon \sum_{\{i,j\}} \langle s_i s_j\rangle = -N\frac{\varepsilon}{2}\nu\langle s\rangle^2 = -\frac{N}{2}k_B T_c\langle s\rangle^2$$

$$C_N = \left(\frac{\partial U}{\partial T}\right)_N = -N k_B T_c \langle s\rangle \left(\frac{\partial \langle s\rangle}{\partial T}\right)_N$$

$$\left(\frac{\partial\langle s\rangle}{\partial T}\right)_N = \frac{\partial}{\partial T}\tanh\left(\frac{T_c}{T}\langle s\rangle\right) = \frac{-\frac{T_c}{T^2}\langle s\rangle + \frac{T_c}{T}\left(\frac{\partial\langle s\rangle}{\partial T}\right)_N}{\cosh^2\left(\frac{T_c}{T}\langle s\rangle\right)}$$

$$\Rightarrow \frac{T_c}{T^2}\langle s\rangle = \left[\frac{T_c}{T} - \cosh^2\left(\frac{T_c}{T}\langle s\rangle\right)\right]\left(\frac{\partial\langle s\rangle}{\partial T}\right)_N$$

$$\Rightarrow \left(\frac{\partial\langle s\rangle}{\partial T}\right)_N = \frac{\langle s\rangle}{T - \frac{T^2}{T_c}\cosh^2\left(\frac{T_c}{T}\langle s\rangle\right)}$$

$$C_N = \frac{N k_B \langle s\rangle^2}{\left(\frac{T}{T_c}\right)^2 \cosh^2\left(\frac{T_c}{T}\langle s\rangle\right) - \frac{T}{T_c}}$$

$T > T_c$: $\quad \langle s\rangle = 0 \quad \Rightarrow C_N = 0$

$T \ll T_c$: $\quad \langle s\rangle = \pm 1 \quad \Rightarrow C_N = \dfrac{N k_B}{\underbrace{\left(\frac{T}{T_c}\right)^2 \cosh^2\left(\frac{T_c}{T}\right)}_{\approx \left(\frac{e^{\frac{T_c}{T}}}{2}\right)^2} - \frac{T}{T_c}} \sim 4 N k_B \left(\frac{T_c}{T}\right)^2 e^{-2\frac{T_c}{T}}$

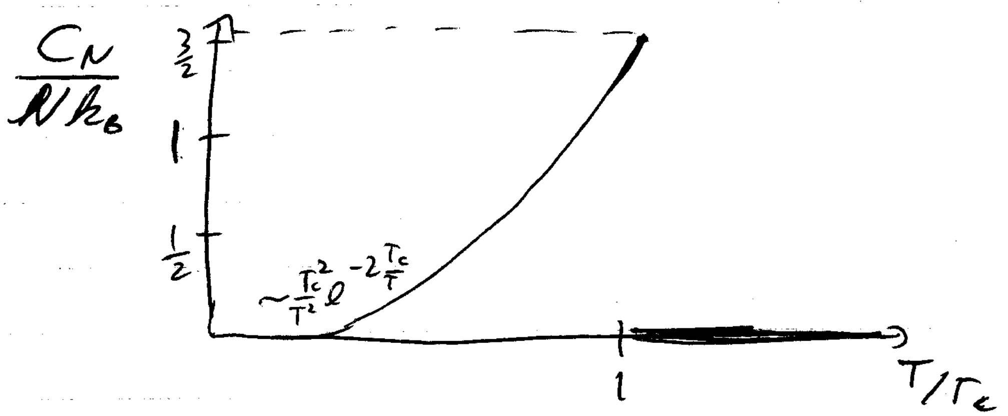
small compared to

$T < T_c$ but close to T_c, $\quad \frac{T}{T_c} = 1 - \delta$, $\quad \langle s\rangle \approx \sqrt{3\delta}$

$$C_N \approx \frac{N k_B 3\delta}{(1-\delta)^2 \cosh^2\left(\frac{\sqrt{3\delta}}{1-\delta}\right) - (1-\delta)} \approx \frac{3 N k_B \delta}{(1-\delta)^2\left(1 + \frac{1}{2}\frac{3\delta}{(1-\delta)^2}\right)^2 - 1 + \delta}$$

$$\approx \frac{3 N k_B \delta}{-2\delta + 2\frac{3}{2}\delta + \delta} = \frac{3N}{2} k_B$$

$\rightarrow$ jump in C_N $\rightarrow$ second order transition



Magnetic susceptibility:

$$\chi_{T,N}(B) = \left(\frac{\partial \langle M\rangle}{\partial B}\right)_{T,N} = N\mu \left(\frac{\partial \langle s\rangle}{\partial B}\right)_{T,N}$$

$$\langle s\rangle = \tanh\left[\frac{T_c}{T}\langle s\rangle + \beta\mu B\right]$$

$$\left(\frac{\partial \langle s \rangle}{\partial B}\right)_{T,N} = \frac{\frac{T_c}{T}\left(\frac{\partial \langle s \rangle}{\partial B}\right)_{T,N} + \beta\mu}{\cosh^2\left[\frac{T_c}{T}\langle s \rangle + \beta\mu B\right]}$$

$$\Rightarrow \left(\frac{\partial \langle s \rangle}{\partial B}\right)_{T,N} = \frac{\beta\mu}{\cosh^2\left[\frac{T_c}{T}\langle s \rangle + \beta\mu B\right] - \frac{T_c}{T}}$$

at $B=0$:

$$\chi_{T,N}(B) = N\mu \frac{\beta\mu}{\cosh^2\left[\frac{T_c}{T}\langle s \rangle\right] - \frac{T_c}{T}}$$

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$T \gg T_c$: $\langle s \rangle = 0$ $\qquad \chi_{T,N}(B) = \dfrac{N\mu^2\beta}{1 - \frac{T_c}{T}} = \dfrac{N\mu^2}{k_B}\dfrac{1}{T-T_c}$

$T \ll T_c$: $\qquad \chi_{T,N}(B) = \dfrac{N\mu^2}{k_B}\dfrac{1}{T\underbrace{\cosh^2\left(\frac{T_c}{T}\right)}_{\approx\left(2e^{T_c/T}\right)^2} - T_c} \approx \dfrac{4N\mu^2}{k_B T} e^{-2\frac{T_c}{T}}$

$T < T_c$ but $T \approx T_c$ $\qquad \dfrac{T}{T_c} = 1-\delta \qquad 0 < \delta \ll 1$

$\langle s \rangle \approx \sqrt{3\delta}$

$$\chi_{T,N}(B) \approx \frac{N\mu^2}{k_B T_c}\frac{1}{1-\delta}\frac{1}{\cosh^2\left(\frac{\sqrt{3\delta}}{1-\delta}\right) - \frac{1}{1-\delta}}$$

$$\approx \frac{N\mu^2}{k_B T_c}\frac{1}{1-\delta}\frac{1}{\left[1+\frac{1}{2}\frac{3\delta}{(1-\delta)^2}\right]^2 - 1 - \delta} \approx \frac{N\mu^2}{k_B T_c}\frac{1}{2\delta} = \frac{N\mu^2}{2k_B}\frac{1}{T-T_c}$$

$\chi_{T,N}(B)$ diverges like $\dfrac{1}{T-T_c}$ close to T_c