Bogolyubov variational theorem

Consider $\underset{\substack{\uparrow \\ \text{Hamiltonian}}}{H} = H_0 + H_1$ ← 'easy'

Define $H(\lambda) = H_0 + \lambda H_1$

$[H(1) = H_0 + H_1]$

$$\underset{\substack{\uparrow \\ \text{free en.}}}{-\beta F(\lambda)} = \log\Big(\sum_j e^{-\beta H_j(\lambda)}\Big)$$

$$\frac{dF(\lambda)}{d\lambda} = -\beta^{-1}(-\beta)\frac{\sum_j H_1^j e^{-\beta(H_0^j + \lambda H_1^j)}}{\sum_j e^{-\beta(H_0^j + \lambda H_1^j)}} = \langle H_1 \rangle_{H(\lambda)}$$

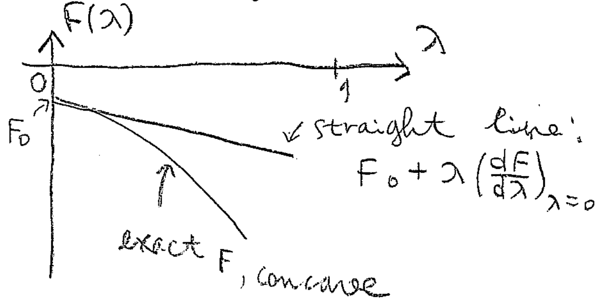
Likewise, $\dfrac{d^2F}{d\lambda^2} = -\beta\left[\langle H_1^2\rangle_{H(\lambda)} - \langle H_1\rangle^2_{H(\lambda)}\right] =$

$$= -\beta \underbrace{\langle H_1 - \langle H_1\rangle_{H(\lambda)}\rangle^2_{H(\lambda)}}_{\geq 0} \leq 0, \text{ for all } \lambda$$

So, $F(\lambda)$ is concave everywhere $\Rightarrow$

$\Rightarrow F(\lambda) \leq F(0) + \lambda\left(\dfrac{dF}{d\lambda}\right)_{\lambda=0}$ validity of expansion?

$\underline{\lambda = 1}$: $F \leq F_0 + \langle H_1\rangle_0 = F_0 + \langle H - H_0\rangle_0$



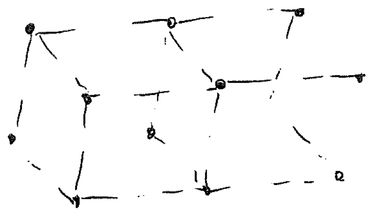
, always above exact F

Mean-field theory

So, $F \leq F_0 + \langle \mathcal{H} - \mathcal{H}_0 \rangle_0$,

$$F_{mf} = \min_{\mathcal{H}_0} \{ \underbrace{F_0 + \langle \mathcal{H} - \mathcal{H}_0 \rangle_0}_{\equiv\ \Phi} \}.$$

Consider a 3D Ising model on a sc lattice



e.g. $z = 6$ ($\#$ nnb on sc)

N sites ; $\underbrace{H=0 \text{ (no field)}}_{\text{so only the } J \text{ term in } \mathcal{H}}$

Try $\mathcal{H}_0 = -\underset{\substack{\uparrow \\ \text{mean field}}}{H_0} \sum_{i=1}^{N} \overset{\pm 1}{s_i}$ paramagnet

$$Z = \left(e^{-\beta H_0} + e^{\beta H_0}\right)^N = \left(2\cosh(\beta H_0)\right)^N$$

$$F_0 = -N k_B T \log\left(2\cosh(\beta H_0)\right)$$

$$\underset{\substack{\| \\ N\langle s\rangle_0}}{\langle M \rangle_0} = -\left(\frac{\partial F}{\partial H_0}\right)_T = (+N \cancel{k_B T}) \frac{\cancel{2}\sinh(\beta H_0)}{\cancel{2}\cosh(\beta H_0)} \cancel{\beta} = N \tanh(\beta H_0).$$

Finally,

$$\langle \mathcal{H} - \mathcal{H}_0 \rangle_0 = \frac{\sum_{\{s\}} e^{\beta H_0 \sum_i s_i} \left[-J \sum_{\langle ij \rangle} s_i s_j + H_0 \sum_i s_i \right]}{\sum_{\{s\}} e^{+\beta H_0 \sum_i s_i}} =$$

$$= -J \sum_{\langle ij \rangle} \langle s_i \rangle_0 \langle s_j \rangle_0 + H_0 \sum_{i=1}^{N} \langle s_i \rangle_0 \ =$$

Translational inv: $\langle s_i \rangle_0 = \langle s_j \rangle_0 \equiv \langle s \rangle_0$

$$= -J\underbrace{\left(\frac{NZ}{2}\right)}_{\substack{\text{total \#}\\ \text{bonds}}}\langle S\rangle_0^2 + H_0 N\langle S\rangle_0$$

So, $$\varphi = -Nk_BT\log(2\cosh(\beta H_0)) - J\frac{NZ}{2}\tanh^2(\beta H_0) + N H_0\tanh(\beta H_0)$$

$$\frac{\partial\varphi}{\partial H_0} = 0 \quad \text{yields}$$

$$-N(k_BT)\beta\cancel{\tanh}(\beta H_0) - J\cancel{N}Z\tanh(\beta H_0)\frac{1}{\cosh^2(\beta H_0)}\beta + N\cancel{\tanh}(\beta H_0) + \cancel{N}H_0\frac{\beta}{\cosh^2(\beta H_0)} = 0,$$

$\frac{d}{dx}\tanh x = \frac{1}{\cosh^2 x}$

or

$$\underline{\underline{H_0 = JZ\underbrace{\tanh(\beta H_0)}_{\langle S\rangle_0}.}}$$

$$H_0 = JZ\langle S\rangle_0$$

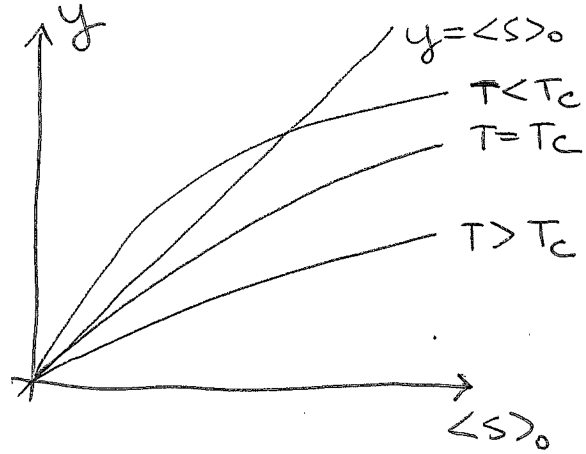
$$(*) \quad \underline{\underline{\langle S\rangle_0 = \tanh(\beta JZ\langle S\rangle_0).}}$$

self-consistent eq'n for $\langle S\rangle_0$

So, $$F_{mf} = -Nk_BT\log[2\cosh(\beta JZ\langle S\rangle_0)] - J\frac{NZ}{2}\langle S\rangle_0^2 + N(JZ\langle S\rangle_0)\langle S\rangle_0 =$$

$$= -Nk_BT\log[\ldots] + N\frac{JZ}{2}\langle S\rangle_0^2.$$

Study (*):



$y = \tanh(\beta J z \langle S\rangle_0)$

If $\langle S\rangle_0 = 0 \rightarrow H_0 = 0$

$\underbrace{\phi = -N k_B T \log(2)}_{\text{entropic term}}$

$\underline{T>T_c}$: $\langle S\rangle_0 = 0$ is the only solution (paramagnetic phase)

$\underline{T<T_c}$: 2 solutions $\Rightarrow$ $\langle S\rangle_0 = 0$ &

$\langle S\rangle_0$ finite $\leftarrow$ minimize free en.

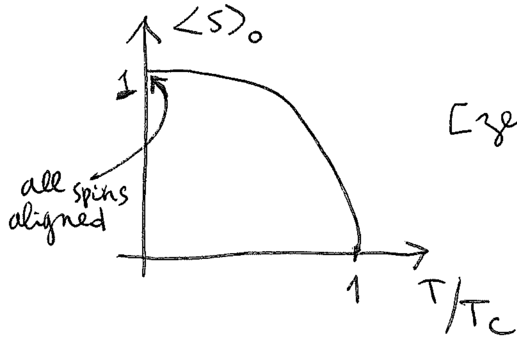
ferromagnetic stable phase

$\underline{T=T_c}$: $\langle S\rangle_0 \simeq \beta_c J z \langle S\rangle_0$ ($\langle S\rangle_0$ small)

$\downarrow$

$k_B T_c = J z$ [equate the slopes]

Note that T_c depends only on z, not on the other details of the lattice structure such as # dims $\rightarrow$ incorrectly predicts finite T_c for 1D Ising model



[zero field]

$\beta \rightarrow \infty$: $\langle S\rangle_0 \rightarrow \dfrac{e^{\beta J z \langle S\rangle_0}}{e^{\beta J z \langle S\rangle_0}} \rightarrow 1$

Calculate $\overset{\text{mean-field}}{\vee}$ critical exponents

$$t = \frac{T - T_c}{T_c} \Rightarrow T = T_c + tT_c = T_c(1+t) =$$
$$= \frac{Jz}{k_B}(1+t)$$

Hence $$\langle s\rangle_0 = \tanh\left(\frac{\cancel{Jz}}{\cancel{k_B}\left(\frac{\cancel{Jz}}{\cancel{k_B}}\right)(1+t)}\langle s\rangle_0\right) =$$

$$= \tanh\left(\frac{\langle s\rangle_0}{1+t}\right).$$

Expand in $\langle s\rangle_0$ & t:

$$\langle s\rangle_0 \simeq \frac{\langle s\rangle_0}{1+t} - \frac{\langle s\rangle_0^3}{3(1+t)^3} + \ldots \simeq$$

$$\approx \langle s\rangle_0(1-t) - \frac{\langle s\rangle_0^3}{3} \ldots$$

$\langle s_0\rangle^2 \simeq -3t$ just below T_c

So, $$-t \simeq \frac{\langle s_0\rangle^2}{3} \Rightarrow \underline{\underline{\langle s_0\rangle \sim (-t)^{1/2}}}.$$

Neglected $\underbrace{t^2,\ \langle s\rangle_0^2 t,\ \langle s\rangle_0^4}_{\text{all } \sim t^2 \text{, ok to neglect}}$.

So, $\boxed{\beta_{mf} = \frac{1}{2}}$

Can show that $\boxed{\gamma_{mf} = 1}$ (see below, pp. 8-9)

$(\chi_T \sim |t|^{-\gamma})$

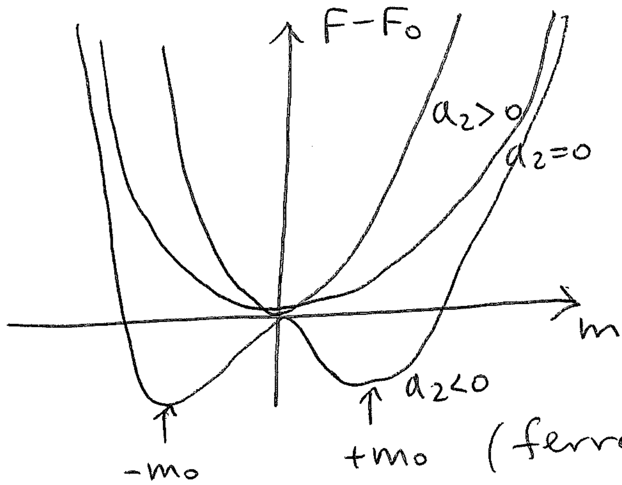
Landau theory

Assume that free energy F can be expanded:

$$F = F_0 + a_2 m^2 + a_4 m^4$$

$\uparrow$ order prm (magnetization)

F: inv under $m \to -m$, no odd powers



(ferromagnetic phase)

Note that $a_4 > 0$ in physical systems (magnet'n must be bounded)

$a_2 = 0 \Rightarrow$ critical temperature,

$$a_2 = \tilde{a}_2 t$$

Magnetization becomes non-zero continuously as a_2 changes sign $\Rightarrow$ 2nd order (cont.) phase transition

Critical exponents:

$$\frac{dF}{dm} = 2\tilde{a}_2 t m + 4 a_4 m^3 = 0,$$

$$m \sim (-t)^{1/2} \quad \beta_{mf} \text{ as before}$$

$$m^2 = -\frac{\tilde{a}_2 t}{2 a_4}$$

$$F = F_0 - \frac{(\tilde{a}_2 t)^2}{2 a_4} + a_4 \left(\frac{\tilde{a}_2 t}{2 a_4}\right)^2 = F_0 - \frac{(\tilde{a}_2 t)^2}{4 a_4}$$

$\underline{t<0}$

$$C_H = T\left(\frac{\partial S}{\partial T}\right)_H = -T\left(\frac{\partial^2 F}{\partial T^2}\right)_H \sim |t|^{-\alpha}$$

As $t \to 0^-$, $C_H \to$ const

$t>0$: $m=0$ @ equilibrium, F is const $\Rightarrow C_H \to \emptyset$

So, $\alpha_{mf} = \emptyset$ & there is a jump discontinuity in specific heat.

$\Rightarrow$ All critical exponents match our explicit calc'n above

Indeed, from 6.4

$$F_{mf} = -N k_B T \log(2\cosh(\beta J z \langle S\rangle_0)) + \frac{NJz}{2}\langle S\rangle_0^2 \simeq$$

neglected $\mathcal{O}(\langle S\rangle_0^4)$

$$\simeq \underbrace{-N k_B T \log(2)}_{F_0} - N k_B T \frac{(\beta J z \langle S\rangle_0)^2}{2} + \frac{NJz}{2}\langle S\rangle_0^2 =$$

$$= F_0 + \frac{NJz}{2}\langle S\rangle_0^2 \left[1 - \beta J z\right]$$

same as Landau theory at small magnetization...

$$\Downarrow$$

$$a_2 = \frac{NJz}{2}\underbrace{(1-\beta J z)}_{1-\frac{T_c}{T} = \frac{T-T_c}{T} = \frac{T_c}{T}\frac{T-}{T}} \qquad \tilde{a}_2 = \frac{NJz}{2}\frac{T_c}{T} = \frac{N k_B T_c}{2T}$$

$a_2 = 0 \Rightarrow \underline{k_B T_c = Jz}$, as before

If the coeff. in front of $\langle S\rangle_0^4$ is negative, have to include $\langle S\rangle_0^6$...

$$\boxed{\mathcal{H} = -J \sum_{\langle ij \rangle} S_i S_j - H \sum_i S_i , \quad S_i = \pm 1}$$ ← add magnetic field to $\mathcal{H}$

So, $\varphi = -N k_B T \log(2\cosh(\beta H_0)) -$

$$- J\left(\frac{Nz}{2}\right)\langle S\rangle_0^2 + (H_0 - H) N \langle S \rangle_0 =$$

$$= -N k_B T \log(2\cosh(\beta H_0)) - J\frac{Nz}{2}\tanh^2(\beta H_0) + $$
$$+ N(H_0 - H)\tanh(\beta H_0)$$

$\langle S\rangle_0 = \tanh(\beta H_0)$

$$\frac{\partial \varphi}{\partial H_0} = 0 \implies \cancel{-NJz\tanh(\beta H_0)\beta\frac{1}{\cosh^2(\beta H_0)}}^{-N\cancel{\beta^{-1}}\tanh(\beta H_0)\cancel{\beta}} +$$
$$+ (H_0 - H) N \frac{1}{\cosh^2(\beta H_0)}\beta + \frac{N\tanh(\beta H_0)}{} = 0$$, or

$$H_0 = H + Jz \underbrace{\tanh(\beta H_0)}_{\langle S\rangle_0}$$

If $J=0$, $H_0 = H$ & $\varphi = -N k_B T \log(2\cosh(\beta H))$, as expected

Then $\langle S\rangle_0 = \dfrac{H_0 - H}{Jz}$, $\implies H_0 = H + Jz\langle S\rangle_0$

$$\langle S\rangle_0 = \tanh(\beta H_0) = \tanh(\beta H + \beta J z \langle S\rangle_0).$$

Then $\chi_T = \left(\dfrac{\partial\langle S\rangle_0}{\partial H}\right)_T = \dfrac{\beta + \beta J z\left(\dfrac{\partial\langle S\rangle_0}{\partial H}\right)_T}{\cosh^2(\beta H + \beta J z\langle S\rangle_0)}$, or

susceptibility per spin

$$\chi_T \cosh^2(\dots) = \beta + \beta J z \chi_T ,$$

$$\chi_T = \frac{\beta}{[\underbrace{\cosh^2(\dots)}_{\frac{1}{1-\tanh^2(\dots)} = \frac{1}{1-\langle S\rangle_0^2}} - \beta J z]}$$

So, $\chi_T = \dfrac{1}{\dfrac{1}{1-\langle S\rangle_0^2}(k_B T) - Jz} =$

$$= \frac{1-\langle S\rangle_0^2}{k_B \underbrace{T_c(t+1)}_{T} - Jz(1-\langle S\rangle_0^2)} =$$

$t = \dfrac{T-T_c}{T_c} \Rightarrow T = T_c(t+1)$

$k_B T_c = Jz$ [matching slopes still OK since $H\to 0$, $\langle S_0\rangle \to 0$ still yields this expression]

$$= \frac{1-\langle S\rangle_0^2}{Jz(t+\langle S\rangle_0^2)}$$

$\underline{t>0}$: $\langle S\rangle_0 = 0$, $\chi_T = \dfrac{1}{Jzt} \sim t^{-1}$

$\underline{t<0}$: Recall that $\langle S\rangle_0^2 \simeq -3t$ just below T_c, so that

$$\chi_T \simeq \frac{1+3t}{-2(Jzt)} \simeq -\frac{1}{2Jzt}, \text{ as } t\to 0^-$$

So $\chi_T \sim |t|^{-1} \Rightarrow \gamma_{mf} = 1$

Limits of MFT applicability

MFT ignores fluct's

Typical fluct'n: $\sim k_B T$

size: $\sim \xi^d$ ← corr'n length

So, $F_{fluc} \sim \frac{k_B T}{\xi^d} \sim |t|^{\nu d}$, since $\xi \sim |t|^{-\nu}$

free en → F; F_{fluc} ← per unit volume

Specific heat: $C_H \sim |t|^{-\alpha}$

$\Downarrow$

$F \sim |t|^{2-\alpha}$ ← total free en.

Must have $F > F_{fluc}$:

$t \to 0 \Rightarrow |t|^{2-\alpha} > |t|^{\nu d}$,

$(2-\alpha) \underbrace{\log|t|} > \nu d \underbrace{\log|t|}_{<0}$

$\Downarrow$

$2-\alpha_{MF} < d\nu_{MF}$.

Since [if] $\alpha_{MF}=0$, $\underbrace{\nu_{MF} = \frac{1}{2}}_{\text{can show...}}$,

we get: $d > \underline{\underline{4}}$ ← MFT valid

$d=4$ ← upper critical dim'n

"MFT improves w/ nnb"

Critical isotherm $(t=0)$: { Extra notes

$$H \sim |M|^{\delta}\, \mathrm{sgn}(M)$$

Landau theory:

$$F = F_0 - hm + \tilde{a}_2 t\, m^2 + a_4 m^4,$$

$$\frac{dF}{dm} = -h + 2\tilde{a}_2 t\, m + 4a_4 m^3 = 0 \quad \text{@ equil.}$$

Critical isotherm: $(t=0)$

$$h \sim m^3 \Rightarrow \delta_{mf} = \underline{\underline{3}}.$$

Explicit theory:

Recall that

$$\langle S\rangle_0 = \tanh(\beta(H + Jz\langle S\rangle_0))$$

at $T=T_c \Rightarrow \beta_c Jz = 1$

$$\langle S\rangle_0 = \tanh\left(\langle S\rangle_0 + \frac{H}{Jz}\right).$$

Expand: $\langle S\rangle_0 \simeq \langle S\rangle_0 + \frac{H}{Jz} - \frac{\langle S\rangle_0^3}{3}$, or

$$H \sim \langle S_0\rangle^3 \Rightarrow \langle S\rangle_0 \sim H^{1/3}.$$

$\Uparrow$

$\delta_{mf} = 3$

Omitted terms: $\langle S\rangle_0^2 H$,

$\langle S\rangle_0 H^2$,

all higher-order H^3,

$\langle S\rangle_0^5$, ...