Bogolyubov variational theorem

Consider $H = H_0 + H_1$

H ← Hamiltonian; H_0 ← 'easy'

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

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

$$-\beta F(\lambda) = \log\left(\sum_j e^{-\beta H_j(\lambda)}\right)$$

F ← free en.

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

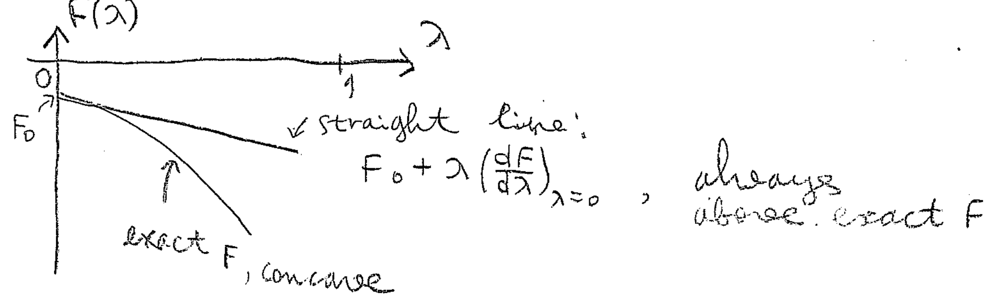
Likewise, $$\frac{d^2F}{d\lambda^2} = -\beta\left[\langle H_1^2\rangle_{H(\lambda)} - \langle H_1\rangle_{H(\lambda)}^2\right] =$$

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

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

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

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

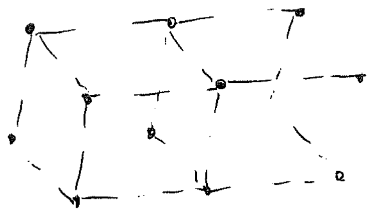


Mean-field theory

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

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

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

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

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

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

So, $\Phi = -Nk_BT\log\left(2\cosh(\beta H_0)\right) - J\frac{Nz}{2}\tanh^2(\beta H_0) + NH_0\tanh(\beta H_0)$

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

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

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

or

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

$$H_0 = Jz\langle S\rangle_0$$

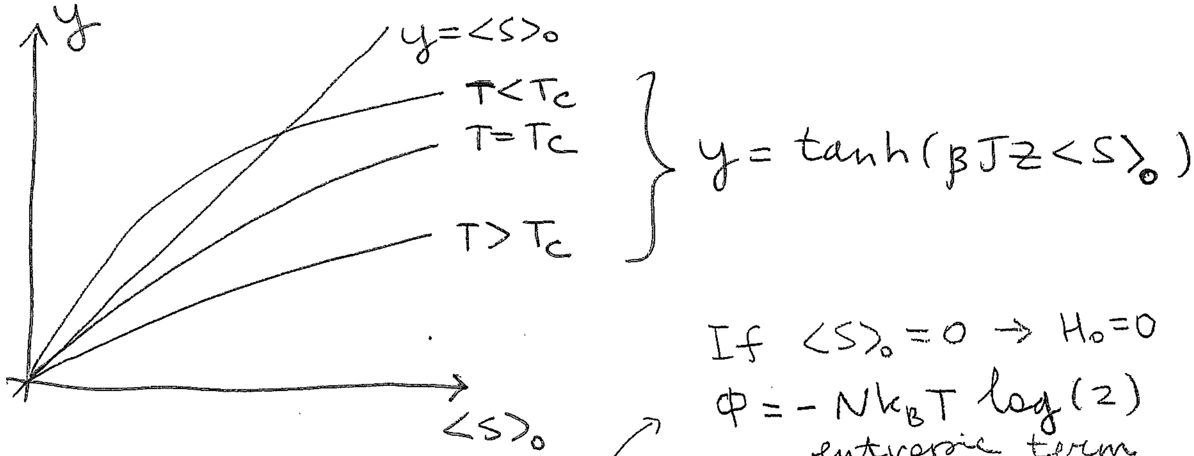
$$(*)\quad \langle S\rangle_0 = \tanh(\beta Jz\langle S\rangle_0).$$

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 (*):



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

$\Phi = -Nk_BT\log(2)$
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.

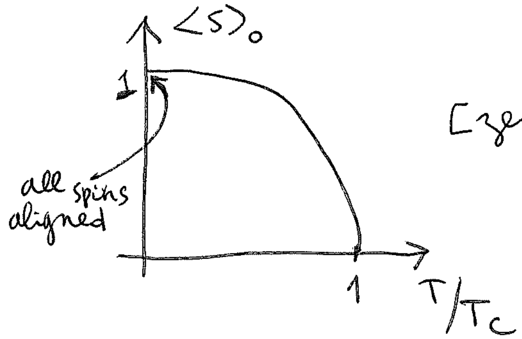
ferromagnetic stable phase

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

$\downarrow$

$k_BT_c = Jz$ [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]

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

Calculate mean-field 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 $$\langle s \rangle_0 = \tanh\left(\frac{Jz}{k_B\left(\frac{Jz}{k_B}\right)(1+t)}\langle s \rangle_0\right) =$$

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

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

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

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

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

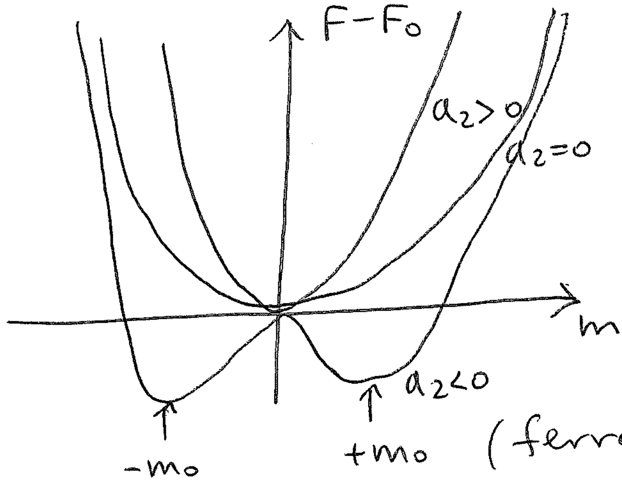
Landau theory

Assume that free energy F can be expanded:

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

m ↑ 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:

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

$m \sim (-t)^{1/2}$ ← β_{mf} as before

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

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

$\underline{t<0}$

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

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 64

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

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...

$$1 - \frac{T_c}{T} = \frac{T-T_c}{T} = \frac{T_c}{T}\,\frac{T-}{T}$$

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

$a_2 = 0 \Rightarrow \underline{k_B T_c = Jz}$, 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, $\varphi = -Nk_BT\log(2\cosh(\beta H_0)) - J\left(\frac{Nz}{2}\right)\langle S\rangle_0^2 + (H_0-H)N\langle S\rangle_0 =$

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

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

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

, or

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

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

Then $\langle S\rangle_0 = \frac{H_0-H}{Jz}$, $\Rightarrow H_0 = H + Jz\langle S\rangle_0$

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

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

↑ susceptibility per spin

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

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

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

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

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

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

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

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

$\underline{t<0}$: 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, $\underset{\substack{\uparrow \\ \text{per unit volume}}}{F_{fluc}}^{\swarrow \text{free en}} \sim \frac{k_B T}{\xi^d} \sim |t|^{\nu d}$, since $\xi \sim |t|^{-\nu}$

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] $\alpha_{MF} = 0$, $\underbrace{\nu_{MF} = \frac{1}{2}}$, can show...

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

$d = 4$ ← upper critical dim'n

"MFT improves w/ nnb"

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

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

<u>Landau theory:</u>

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

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

Critical isotherm: ($t=0$)

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

<u>Explicit theory:</u>

Recall that

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

at $T = T_c \Rightarrow \beta_c J z = 1$

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

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

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

$$\Uparrow$$

$$\delta_{mf} = 3$$

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

$\langle S \rangle_0 H^2$,

H^3,

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

all higher-order