The conditional (or constrained) free energy

$$F_N(T,H) = -kT \ln Z_N(T,H) \Rightarrow e^{-\frac{F_N(T,H)}{kT}} = Z_N(T,H)$$

$$f(T,H) = \frac{1}{N} F_N(T,H)$$ free-energy per spin

$$\tilde{F}_N(m,T,H) = -kT \ln Z_N(m,T,H) \Rightarrow e^{-\frac{\tilde{F}_N(m,T,H)}{kT}} = Z_N(m,T,H)$$

$$\tilde{f}(m,T,H) = \frac{1}{N} \tilde{F}_N(m,T,H)$$ variational (conditional or constrained) free-energy per spin

$$e^{-\frac{F_N(T,H)}{kT}} = Z_N(T,H) = \sum_{\{S_i\}} e^{-\frac{\mathcal{H}[\{S_i\}]}{kT}} =$$

$$= \int dm \sum_{\substack{\{S_i\} \\ \langle S_i \rangle = m}}{}' e^{-\mathcal{H}[\{S_i\}]} = \int dm\, Z_N(m,T,H) =$$

$$= \int dm\, e^{-\frac{\tilde{F}_N(m,T,H)}{kT}} = \int dm\, e^{-\frac{N\tilde{f}(m,T,H)}{kT}} \simeq$$

$$\simeq \text{const}(N)\, e^{-\frac{N\tilde{f}(m^*,T,H)}{kT}}$$

where $\tilde{f}(m^*,T,H) = \max_m \{\tilde{f}(m,T,H)\}$

i.e. $\frac{\partial \tilde{f}(m,T,H)}{\partial m} = 0$

$\Downarrow$

$m^* = m(T,H)$

$$F_N(T,H) = o\,\ln(N) + N\tilde{f}(m^*,T,H)$$

$$\boxed{f_N(T,H) = \lim_{N\to\infty} \frac{F_N(T,H)}{N} \simeq \tilde{f}(m^*,T,H)}$$

Landau Free Energy per spin

$$\tilde{f}(m,T,H) \longrightarrow \mathcal{L}(m,T,H) \simeq a(T) + \frac{b(T)}{2}m^2 + \frac{c(T)}{4}m^4 - mH$$

(in general)

$$\lim_{T\to T_c} a(T) = a(T_c) \quad \text{(non-singular)}$$

$$b(T) \simeq b_0(T-T_c) \quad \text{when} \quad \left|\frac{T-T_c}{T_c}\right| \ll 1$$

$b_0 > 0$ clearly changes sign @ T_c (in the vicinity of T_c)

$$\lim_{T\to T_c} c(T) = c(T_c) > 0$$

(i) $$\left.\frac{\partial \mathcal{L}}{\partial m}\right|_{m^*} = 0 \quad \Rightarrow \quad m = m^* = m(T,H)$$

(ii) $$f(T,H) = \mathcal{L}(m^*,T,H) = \mathcal{L}(m(T,H),T,H)$$

(*) Notes on the Free energy in magnetic system

$$dE = TdS - MdH$$

$$F = E - TS \quad \Rightarrow \quad dF = -S\,dT - M\,dH$$

$$S = -\left(\frac{\partial F}{\partial T}\right)_H \qquad M = -\left(\frac{\partial F}{\partial H}\right)_T$$

Correlation length in the "inhomogeneous" mean-field theory

$$G(i,j) = \langle S_i S_j \rangle - \langle S_i \rangle \langle S_j \rangle = \langle (S_i - \langle S_i \rangle)(S_j - \langle S_j \rangle) \rangle$$

$$Z_N(T,H) = \sum_{\{S_i\}} e^{\beta J \sum_{\langle ij \rangle} S_i S_j + \beta H \sum_i S_i}$$

$$m = \frac{1}{N} \left\langle \sum_{i=1}^{N} S_i \right\rangle = \langle S_i \rangle = \frac{1}{N} \frac{1}{\beta} \frac{\partial}{\partial H} \ln Z_N(T,H)$$

$$\chi = \frac{\partial m}{\partial H} = \frac{1}{N} \frac{1}{\beta} \frac{\partial^2}{\partial H^2} \ln Z_N = \frac{1}{N\beta} \frac{\partial}{\partial H} \left(\frac{1}{Z} \frac{\partial Z}{\partial H} \right) = \frac{1}{N\beta} \left[\frac{1}{Z} \frac{\partial^2 Z}{\partial H^2} - \left(\frac{\partial Z / \partial H}{Z} \right)^2 \right]$$

$$= \frac{1}{N\beta} \Big[\underbrace{\beta^2 \Big\langle \Big(\sum_i S_i \Big)^2 \Big\rangle}_{\langle M^2 \rangle} - \underbrace{\beta^2 \Big\langle \sum_i S_i \Big\rangle^2}_{\langle M \rangle^2} \Big] = \frac{1}{NkT} \Big[\sum_{i,j} \langle S_i S_j \rangle - \sum_{i,j} \langle S_i \rangle \langle S_j \rangle \Big]$$

$$= \frac{1}{Nk_BT} \sum_{i,j} \underbrace{\left(\langle S_i S_j \rangle - \langle S_i \rangle \langle S_j \rangle \right)}_{G(i,j)} = \frac{1}{Nk_BT} \sum_{i,j} G(i,j) = \frac{1}{k_BTN} \langle (\Delta M)^2 \rangle$$

<u>a technical tool: inhomogeneous "field"</u> $H \to \{H_i\}$ $\quad H_i$ at site i

$$Z_N(T,\{H_i\}) = \sum_{\{S_i\}} e^{\beta J \sum_{\langle ij \rangle} S_i S_j + \beta \sum_i H_i S_i}$$

$$m_i = \langle S_i \rangle = \frac{1}{\beta} \frac{\partial}{\partial H_i} \ln Z_N(T,\{H_i\}) =$$

$$\chi_{ij} = \frac{\partial m_i}{\partial H_j} = \frac{1}{\beta} \frac{\partial^2}{\partial H_j \partial H_i} \ln Z_N = \frac{1}{\beta} \frac{\partial}{\partial H_j} \left(\frac{\partial Z / \partial H_i}{Z} \right) = \frac{1}{\beta} \left[\frac{1}{Z} \frac{\partial^2 Z}{\partial H_j \partial H_i} - \left(\frac{\frac{\partial Z}{\partial H_i}}{Z} \right) \left(\frac{\frac{\partial Z}{\partial H_j}}{Z} \right) \right]$$

($H_i \equiv H$ at the end)

$$= \frac{1}{\beta} \left[\beta^2 \langle S_i S_j \rangle - \beta^2 \langle S_i \rangle \langle S_j \rangle \right] = \frac{1}{kT} G(i,j)$$

$$\boxed{\chi_T = \frac{1}{Nk_BT} \sum_{ij} G(i,j) \qquad \chi_{ij} = \frac{1}{k_BT} G(i,j)}$$

general linear response theory

H_j is small:

$$m_i(\{H_j\}) \cong m_i(0) + \sum_j \frac{\partial m_i}{\partial H_j}\Big|_{\{H_j = 0\}} H_j$$

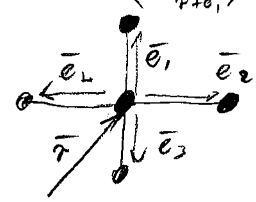
$$= m_i(0) + \sum \chi_{ij} H_j$$

the divergence of χ suggest the divergence of $\sum_{\bar r} G(\bar r)$

$$\chi_T = \frac{1}{NkT} \sum_{R,\bar r} G(R, R+\bar r) = \frac{1}{kT} \sum_{\bar r} G(\bar r) \quad \leftarrow \underline{\text{susceptibility "sum" rule}}$$

Inhomogeneous "mean-field"

$\langle s_{\bar r+\bar e_1} \rangle = m_{\bar r+\bar e_1}$



$$m = \tanh\left[\beta(Jqm + H)\right] \Rightarrow$$

$$\boxed{m_{\bar r} = \tanh\left[\beta\left(J\sum_{\bar e} m_{\bar r+\bar e} + H_{\bar r}\right)\right]}$$

at the end ; $H_i \to H$

$T \to T_c + 0$ focusing on behavior near T_c ; $T > T_c$ nearest neighbors $= \bar r + \bar e$

$|\bar e| = a$ lattice constant

$\bar r$: on discrete lattice

$$m_{\bar r} = \tanh\left[\beta\left(J\sum_{\bar e} m_{\bar r+\bar e} + H_{\bar r}\right)\right]$$

$$\approx \beta J \sum_{\bar e} m_{\bar r+\bar e} + \beta H_{\bar r}$$

$$\underbrace{N_x \cdot N_y \cdot N_z \cdots}_{d} = N$$

$$\frac{\partial m_{\bar r}}{\partial H_{\bar r'}} = \beta J \sum_{\bar e} \frac{\partial m_{\bar r+\bar e}}{\partial H_{\bar r'}} + \beta\, \delta_{\bar r,\bar r'}$$

$$k_x = \frac{2\pi}{N_x a} n_x$$

$$n_x = -\frac{N_x}{2}, \dots, \frac{N_x}{2}$$

$$\chi_{\bar r,\bar r'} = \beta J \sum_{\bar e} \chi_{\bar r+\bar e,\bar r'} + \beta\, \delta_{\bar r,\bar r'}$$

$$\boxed{H_{\bar r} \to H = 0} \Rightarrow \chi_{\bar r,\bar r'} = \chi(\bar r - \bar r')$$

tr. invariance

$$\tilde\chi(k) = \sum_{\bar r} \chi(\bar r)\, e^{-i k \bar r}$$

$\bar r - \bar r' \to \bar r$

$$\chi(\bar r) = \beta J \sum_{\bar e} \chi(\bar r+\bar e) + \beta\, \delta_{\bar r,0} \quad \Big/ \; e^{-ik\bar r} \text{ and } \sum_{\bar r}$$

$$\chi(\bar r) = \frac{1}{N} \sum_{k} \tilde\chi(k)\, e^{ik\bar r}$$

$$\delta_{\bar r,0} = \frac{1}{N} \sum_{k} e^{ik\bar r}$$

$$\tilde\chi(k) = \beta J\, \tilde\chi(k) \sum_{\bar e} e^{ik\bar e} + \beta$$

$$\tilde\chi(k)\left[1 - \beta J \sum_{\bar e} e^{ik\cdot\bar e}\right] = \beta$$

$$\tilde\chi(\bar k) = \frac{\beta}{1 - \beta J \sum_{\bar e} e^{ik\bar e}}$$

hypercubic lattice: $|\bar{e}| = a$

$$\sum_{\bar{e}} e^{i\bar{k}\bar{e}} = \sum_{j=1}^{d} \left(e^{ik_j a} + e^{-ik_j a}\right) = 2\sum_{j=1}^{d} \cos(k_j a)$$

$$\simeq 2\sum_{j=1}^{d}\left(1 - \frac{k_j^2 a^2}{2}\right) = \underbrace{2d}_{q} - a^2 k^2 \qquad k^2 = \sum_{j=1}^{d} k_j^2$$

$$\tilde{\chi}(\bar{k}) = \frac{\beta}{1-\beta J(q - a^2k^2)} = \frac{\beta}{1-\beta Jq + \beta J a^2 k^2}$$

$T > T_c$ $\qquad 1-\beta J q = 1 - \frac{Jq}{kT} > 0 \qquad T_c = \frac{Jq}{k}$

$$\tilde{\chi}(\bar{k}) = \frac{1}{k(T-T_c) + Ja^2k^2} = \frac{1}{Ja^2}\,\frac{1}{\frac{k(T-T_c)}{Ja^2} + k^2}$$

$$S(\bar{k}) = \tilde{G}(\bar{k}) = \sum_{\bar{r}} G(\bar{r})\, e^{-i\bar{k}\bar{r}} \qquad \text{structure factor}$$

structure factor

$$\tilde{G}(\bar{k}) = k_B T\,\tilde{\chi}(\bar{k}) = \frac{k_B T}{Ja^2}\,\frac{1}{k^2 + \xi^{-2}} \qquad \xi = \sqrt{\frac{Ja^2}{k(T-T_c)}}$$

$$G(\bar{r}) = \frac{1}{N}\sum_{\bar{k}} \tilde{G}(\bar{k})\, e^{i\bar{k}\bar{r}} = \frac{1}{N}\,\frac{Na^d}{(2\pi)^d}\int e^{i\bar{k}\bar{r}}\,\tilde{G}(\bar{k})\, d^d k$$

$$= a^d \left(\frac{kT}{Ja^2}\right)\frac{1}{(2\pi)^d}\underbrace{\int d^d k\, e^{i\bar{k}\bar{r}}\,\frac{1}{k^2+\xi^{-2}}}$$

lattice constant.

$$\frac{1}{(2\pi)^{d/2}}\,\frac{1}{(r\xi)^{\frac{d-2}{2}}}\, K_{\frac{d-2}{2}}(r/\xi)$$

mean-field results:

$r \gg \xi$: $\boxed{G(r) \sim \frac{1}{r^{\frac{d-1}{2}}}\, e^{-r/\xi}}$ $\leftarrow$ correlation length

exponential decay

$T \to T_c + 0 \qquad \tilde{G}(\bar{k}) \sim \frac{1}{k^2} \qquad G(r) \sim \frac{1}{r^{d-2}}$ power law

critical exponents: $\xi \sim |T - T_c|^{-\nu}$ $\qquad \boxed{\nu = 1/2}$ $\leftarrow$ mean-field values

definition of the exponent η:

$\tilde{G}(\bar{k}) \sim \frac{1}{k^{2-\eta}}$ and $G(\bar{r}) \sim \frac{1}{r^{d-2+\eta}}$ $\qquad \boxed{\eta = 0}$