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

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

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

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

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

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

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

structure factor

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

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

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

lattice constant.

mean-field results:

$r \gg \xi$: $\qquad \boxed{G(r) \sim \frac{1}{r^{\frac{d-1}{2}}} e^{-r/\xi}}$ ← 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: $\xi \sim |T - T_c|^{-\nu}$ $\qquad \boxed{\nu = 1/2}$ ← mean-field values

definition of the exponent η:

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

Review of inhomogeneous mean-field results:

$G(i,j) = \langle s_i s_j \rangle - \langle s_i \rangle \langle s_j \rangle$ (two-point correlation function)

$r \equiv |i-j|$ $\quad G(i,j) = G(r)$ translational invariance + isotropic structures

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

inhomogeneous mean-field (from Ising model)

$$\boxed{\tilde{G}(\bar{k}) = \frac{\text{Const.}}{k^2 + \xi^{-2}}}$$

$$\xi \sim \frac{1}{|t|^{1/2}} = |t|^{-\nu} \qquad \boxed{\nu = 1/2}$$

correlation length

$$\chi_T = \frac{1}{k_B T} \sum_{\bar{r}} G(\bar{r}) = \frac{1}{k_B T} \lim_{\bar{k}\to 0} \tilde{G}(\bar{k}) = \text{Const.}\ \xi^2 \sim |t|^{-2\nu}$$

(susceptibility sum rule)

$$\chi_T \sim |t|^{-\gamma} \quad \Rightarrow \quad \boxed{\gamma = 2\nu = 1}$$

real-space correlations:

$$G(r) = \frac{1}{N} \sum_{\bar{k}} \tilde{G}(\bar{k}) e^{i\bar{k}\cdot\bar{r}} \simeq \text{Const.} \int \frac{d^d k}{(2\pi)^d} \frac{e^{i\bar{k}\cdot\bar{r}}}{k^2 + \xi^{-2}}$$

modified Bessel function

$$= \text{const.} \frac{1}{(2\pi)^{d/2}} \frac{1}{(r\xi)^{\frac{d-2}{2}}} \cdot K_{\frac{d-2}{2}}(r/\xi)$$

asymptotic behavior of modified Bessel function:

$$\boxed{K_\nu(x) \simeq \begin{cases} \frac{\Gamma(\nu)}{2}\left(\frac{2}{x}\right)^\nu & x \ll 1 \quad (\nu \neq 0) \\ \sqrt{\frac{\pi}{2x}}\, e^{-x} & x \gg 1 \end{cases}}$$

Thus, when $T \neq T_c$, ξ = finite, and

$T \neq T_c$

$$\boxed{G(r) \simeq \text{const.}\ \frac{1}{\xi^{\frac{d-3}{2}}}\ \frac{1}{r^{\frac{d-1}{2}}}\ e^{-r/\xi}} \qquad r \gg \xi$$

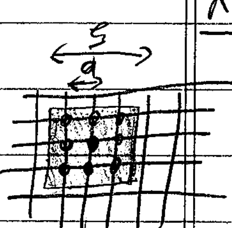
~ exponential (fast) decay
(weakly interacting subsystems)

$T \to T_c$
$(\xi \to \infty)$

$$\boxed{G(r) \simeq \text{const.}\ \frac{1}{r^{d-2}}}$$

correlations decay "much slower" (in a power law fashion) at the critical point. The system then consists of many strongly interacting components. Central-limit theorem, etc., is expected to break down

<u>Role of fluctuations: the breakdown of the mean-field approximat.</u>
(Ginzburg criterion)



correlation volume: $V_\xi = \xi^d$

$N_\xi = \left(\frac{\xi}{a}\right)^d$

$$m_\xi = \frac{1}{N_\xi} \sum_{i \in I_\xi} s_i \qquad \langle m_\xi \rangle = \langle s_i \rangle = m \quad i \in I_\xi$$

$\boxed{T \lesssim T_c}$

$$\langle (\Delta m)^2 \rangle = \frac{1}{N_\xi^2} \sum_{i,j \in I_\xi} (s_i - m)(s_j - m) = \frac{1}{N_\xi^2} \sum_{i,j \in I_\xi} G(ij) \simeq \frac{1}{N_\xi} \sum_i G(i)$$

$$\frac{\langle (\Delta m)^2 \rangle}{\langle m_\xi \rangle^2} = \frac{\frac{1}{N_\xi} \sum_i G(i)}{m^2} = \frac{\sum_i G(i)}{N_\xi m^2} \sim \frac{k_B T \chi_T}{\left(\frac{\xi}{a}\right)^d m^2} = a^d k_B T \frac{\chi_T}{\xi^d m^2}$$

$$\sim \frac{|t|^{-\gamma}}{|t|^{-\nu d} |t|^{2\beta}} = |t|^{-\gamma - 2\beta + \nu d} \xrightarrow[T \to T_c]{} \begin{cases} 0 & \nu d - \gamma - 2\beta > 0 \\ \infty & \nu d - \gamma - 2\beta < 0 \end{cases}$$

thus, <u>fluctuations are small</u> in a self-consistent fashion only if <u>$\nu d - \gamma - 2\beta > 0$</u>

$\Rightarrow \boxed{d > \frac{2\beta + \gamma}{\nu}} = d_c$ (<u>upper critical dimension</u>) | Ising: $\boxed{d_c = 4}$

Ginzburg criterion tells us that mean-field behavior (and exponents) will be asymptotically exact for $d > d_c$
for Ising model $d_c = 4$.
What about $d = 1, 2, 3$? Is there a phase transition at all ?

London - Peierls arguments

$H = 0$ $\mathcal{H} = -J \sum_{\langle ij \rangle} s_i s_j$ $J > 0$ (ferromagnet)

$d=1$ ground-state $(T=0)$ $\cdots \uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow \cdots$ $E_0 = -(N-1)J$
(or, equivalently, $\cdots \downarrow\downarrow\downarrow\downarrow\downarrow \cdots$)

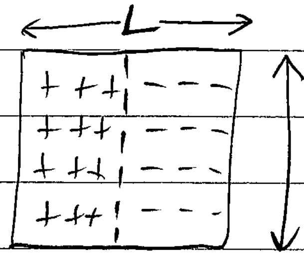
consider an open-end system:
$\boxed{T \gtrsim 0}$ lowest energy configuration: (single domain wall)
$\cdots \uparrow\uparrow\uparrow\uparrow\uparrow | \downarrow\downarrow\downarrow\downarrow\downarrow \cdots$

$N-1$ possible location of the domain wall

$F = E - TS$ $\Delta S = k_B \ln(N-1)$
$\Delta F = \Delta E - T\Delta S = 2J - T k_B \ln(N-1) < 0$ for sufficiently large N
$N \to \infty$ entropy "wins", introduction of domain wall is favorable from the viewpoint of minimizing the free energy
Thus, for $T \gtrsim 0$, fluctuation will destroy the long-range order $\boxed{T > 0 \Rightarrow m = 0}$

There can be no phase transition in the $d=1$ Ising model

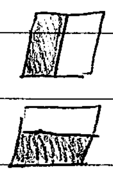
$\boxed{d = 2}$



$N = L^2$ $\quad (L = \sqrt{N})$

$T = 0$: $F_{GS} = E_{GS}$

$F_{DW} - F_{GS}$



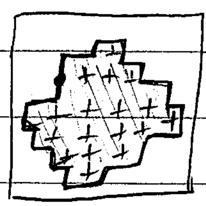
$$\Delta F = \Delta E - T\Delta S = 2JL - T k_B \ln(2L) = 2J\sqrt{N} - k_B T \ln(\sqrt{N}\cdot 2)$$

$$= 2J\sqrt{N} - k_B T \ln(2\sqrt{N}) > 0$$ for sufficiently large N (domain walls are unfavorable

But, the above expression underestimates the entropy

Let's overestimate entropy:

Consider more complex domains with length $L \sim \sqrt{N}$



$$\Delta F = 2JL - k_B T \ln \Gamma(L)$$

degeneracy of domain walls with length L

q:  (coordination number)

$$\Gamma(L) = N \cdot q \cdot \underbrace{(q-1)(q-1)\dots(q-1)}_{L-1} \simeq N(q-1)^L$$

$$\Delta F \simeq 2JL - k_B T \ln(N(q-1)^L) = 2J\sqrt{N} - k_B T L \ln(q-1) - k_B T \ln(N)$$

$$= 2J\sqrt{N} - k_B T\sqrt{N}\ln(q-1) - k_B T \ln(N) \approx 2J\sqrt{N} - k_B T \sqrt{N} \ln(q-1)$$

$\Delta F > 0$ if $(2J - k_B T \ln(q-1))\sqrt{N} > 0$ (system prefers order)

i.e., $2J - k_B T \ln(q-1) > 0$

$$\boxed{T < \frac{2J}{k_B \ln(q-1)} \equiv T_c}$$

phase transition is possible for $T > T_c$

Landau Theory

$$\tilde{f}(T,H,m) = \frac{1}{2} J q m^2 - k_B T \ln(2) - k_B T \ln\cosh[\beta(Jqm + H)]$$

$\vdots$ (see earlier notes and HW)

$$\boxed{\tilde{f}(T,H,m) \simeq a(T) + \frac{1}{2} b(T) m^2 + \frac{1}{4} c(T) m^4 - mH}$$

provided that $c(T)$ does not change sign, and $b(T) \propto b_0 (T - T_c)$, the above "free-energy" functional describes a continuous (second-order) phase transition at $T = T_c$

Note: $\tilde{f}(T,H,m)$ is not the free energy.

The free-energy would be: $f(T,H) = \min_m \{\tilde{f}(T,H,m)\}$

$$\left.\begin{array}{l} \dfrac{\partial \tilde{f}}{\partial m} = 0 \\ \dfrac{\partial^2 \tilde{f}}{\partial m^2} > 0 \end{array}\right\} \Rightarrow m(T,H) \qquad f(T,H) = \tilde{f}(T,H,m(T,H))$$

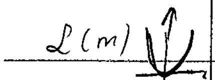
equilibrium magnetization

Landau Theory:

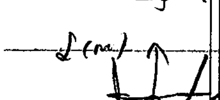
$$\boxed{\mathcal{L}(T,H,m) = a(T) + \frac{1}{2} b(T) m^2 + \frac{1}{4} c(T) m^4 - mH} \qquad L = \mathcal{L} \cdot V$$

$(H=0)$ $\quad \dfrac{\partial \mathcal{L}}{\partial m} = b(T) m + c(T) m^3 = 0 \qquad b(T) \approx b_0 (T - T_c)$

$$b_0 (T - T_c) m + C_0 m^3 = 0 \qquad c(T) \approx C_0$$



$T > T_c \qquad m = 0$



$T < T_c \qquad m = \pm\sqrt{\dfrac{b_0 (T_c - T)}{C_0}}$ (spontaneous magnetization)

$\Rightarrow \boxed{\beta = 1/2}$

inhomogeneous systems $(H \to h(\bar{r}))$

$\langle S_i \rangle = m_i \longrightarrow \varphi(\bar{r})$ (local order parameter)

Coarse-grained description

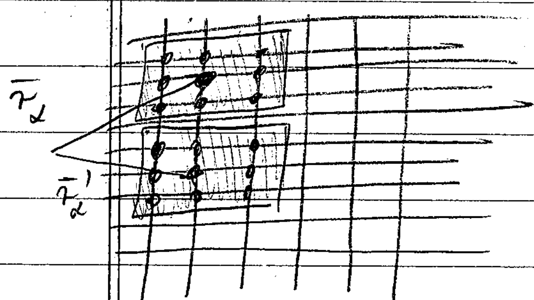
$$L = \int \mathcal{L}(T, H; \{\varphi(\bar{r})\})\, d^d r$$

$$\boxed{\mathcal{L} = \frac{\gamma}{2}(\nabla\varphi)^2 + \frac{1}{2}a \cdot t\, \varphi^2(\bar{r}) + \frac{b}{4}\varphi^4(\bar{r}) - h(\bar{r})\varphi(\bar{r})}$$

for Ising $\left(a \cdot \frac{T - T_c}{T_c} = a \cdot t\right)$

coming from domain wall energy

$$\sim [\varphi(\bar{r}) - \varphi(\bar{r} + \bar{\ell})]^2 \longrightarrow (\nabla\varphi)^2$$



$$\bar{r}_\alpha' = \bar{r}_\alpha + \bar{\ell} \qquad \ell = |\bar{\ell}|$$

$$a \ll \ell \ll \xi(T)$$

$$\varphi(\bar{r}_\alpha) = \frac{1}{N_\alpha} \sum_{i \in I_\alpha} S_i \qquad -1 \leq \varphi(\bar{r}_\alpha) \leq 1$$

$\varphi(\bar{r})$ is a slowly varying function of the lattice position $\bar{r}_\alpha$

continuum limit : $\ell =$ fixed $\quad \left.\begin{matrix} a \to 0 \\ N \to \infty \end{matrix}\right\} \; a^d N = V = \text{const}$

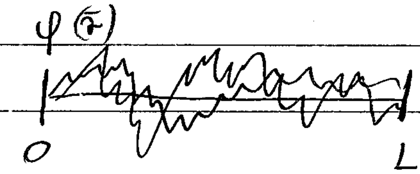
$\varphi(r_\alpha) \to \varphi(\bar{r})$ continuous, local order parameter

$$Z = \operatorname*{Tr}_{\{S_i\}} e^{-\beta \mathcal{H}[S_i]} = \sum_{\{\varphi(\bar{r})\}} \sum_{\{S_i\}} \delta\Big(\varphi(\bar{r}) - \frac{1}{N_\alpha}\sum_{i \in I_\alpha} S_i\Big)\, e^{-\beta \mathcal{H}[S_i]}$$

$$\equiv \sum_{\{\varphi(\bar{r})\}} e^{-\beta L[\{\varphi(\bar{r})\}]}$$

$$e^{-\beta L[\varphi(\vec r)]} = \sum_{\{s_i\}} \delta\left(\varphi(\vec r) - \frac{1}{N_\alpha}\sum_{i\in I_\alpha} s_i\right) e^{-\beta \mathcal{H}[\{s_i\}]}$$

L is a "constrained" free energy when the order parameter profile is constrained to $\varphi(\vec r)$



$$Z = \sum_{\{\varphi(\vec r)\}} e^{-\beta L[\{\varphi(\vec r)\}]}$$

integration over all possible order parameter profiles (functional integral)

$$\Longrightarrow \quad Z = \int \mathcal{D}\varphi(\vec r)\, e^{-\beta L[\{\varphi(\vec r)\}]}$$

$$L = \int d^d r\, \mathcal{L}(\{\varphi(\vec r)\}) \quad , \quad \mathcal{L} = \frac{\gamma}{2}(\nabla\varphi)^2 + \frac{a t}{2}\varphi^2(\vec r) + \frac{b}{4}\varphi^4(\vec r) - h(\vec r)\varphi(\vec r)$$

$a > 0$, $b > 0$, $\gamma > 0$

evaluation, e.g., by direct discretization:

$$\int \mathcal{D}\varphi = \int \prod_{i=1}^{N} d\varphi_i$$

$$\langle \varphi(\vec r)\rangle = \frac{1}{Z}\int \mathcal{D}\varphi\, \varphi(\vec r)\, e^{-\beta L} = \frac{1}{\beta}\frac{1}{Z}\frac{\delta Z}{\delta h(\vec r)}$$

$$\langle \varphi(\vec r)\varphi(\vec r\,')\rangle = \frac{1}{Z}\int \mathcal{D}\varphi\, \varphi(\vec r)\varphi(\vec r\,')\, e^{-\beta L} = \frac{1}{\beta^2}\frac{1}{Z}\frac{\delta^2 Z}{\delta h(\vec r)\delta h(\vec r\,')}$$

thermodynamic averages $\langle \dots \rangle$