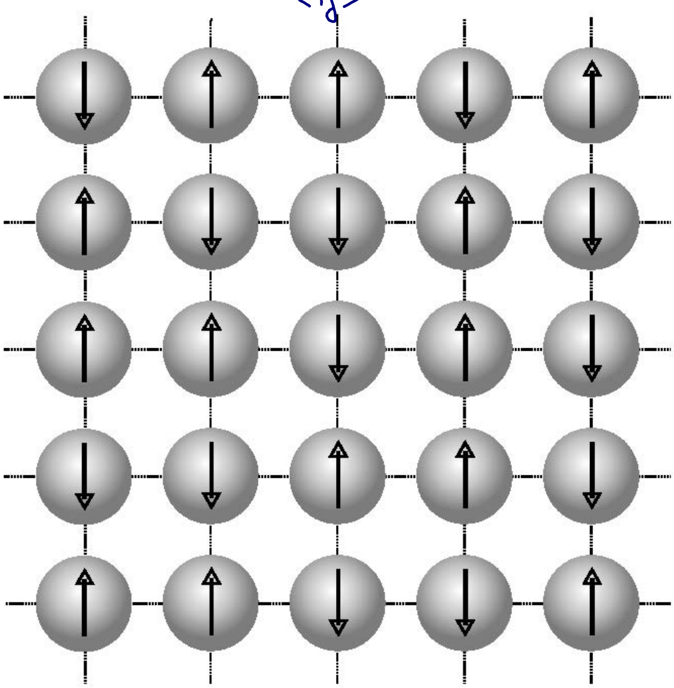
LECTURE 8: Mean-field theory of phase transitions

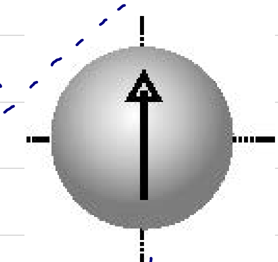
↳ a META THEORY which specifies how to construct approximative theory with a single degree of freedom by starting from original classical or quantum many-body theory

1° Mean-field theory (MFT) for the classical Ising model

$$H = -J \sum_{\langle ij \rangle} S_i \cdot S_j - h \sum_i S_i$$



MFT



single spin interacts with the effective field generated by all other spins so $\{S_i\}$ is only 2

$$Z = \sum_{\{S_i\}} e^{-\beta H}$$

no. of microstates cannot be found even numerically $\Rightarrow$ modest lattice 32×32 has $\sim 10^{300}$ $\{S_i\}$, while fastest supercomputer can generate about 10^{40} during the age of the universe

$\langle m \rangle = \langle S_i \rangle$, $\delta S_i = S_i - \langle S_i \rangle$

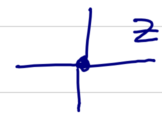
MFT $\Leftrightarrow$ assumes fluctuations are small, so $\delta S_i \cdot \delta S_j \to 0$

$$H_{MF} = -J \sum'_{\langle ij\rangle} (m+\delta s_i)(m+\delta s_j) - h\sum_i s_i$$

$$\approx -Jm^2 N_B - Jm \sum'_{\langle ij\rangle}(\delta s_i+\delta s_j) - h\sum'_i s_i$$

↳ no. of interacting pairs of spins

$$= -Jm^2 N_B - Jmz\sum'_i \delta s_i - h\sum'_i s_i$$


z=4 example

↳ no. of bonds from a single site

$$= -Jm^2 N_B - Jmz\sum'_i (s_i - m) - h\sum'_i s_i$$

$$= -Jm^2\underbrace{\frac{zN}{2}}_{N_B} + JmzN - (Jmz+h)\sum'_i s_i$$

$$= NzJm^2/2 - \underbrace{(Jmz+h)}_{h_{eff}} \sum'_i s_i$$

$$h_{eff} = \underbrace{h_{MF}}_{\text{mean-field internal}} + \overbrace{h}^{\text{external}}$$

i) fast algorithm to find H_{MF} in homeworks & exams:

$$H_{MF} = -J\sum'_{\langle ij\rangle} s_i \overbrace{\langle s_j\rangle}^{\langle m\rangle} - h\sum'_i s_i = \sum'_i H_i = -(Jmz+h)\sum_i s_i$$

$$Z_{MF} = e^{-\beta NzJm^2/2}\sum_{\{s_i\}} e^{\beta(Jmz+h)\sum'_i s_i}$$

$$= e^{-\beta NzJm^2/2}\prod_i \left[e^{\beta(h+zJm)} + e^{-\beta(h+zJm)}\right]$$

$$= e^{-\beta NzJm^2/2}\left\{2\cosh\left[\beta(Jzm+h)\right]\right\}^N$$

$$f_{MF} = F_{MF}/N = -\frac{1}{N} k_B T \ln Z_{MF}$$

$$= \frac{zJm^2}{2} - k_B T \ln\left\{2\cosh\left[\beta(zJm+h)\right]\right\}$$

$$\partial f_{MF}/\partial m\Big|_{m_0} = 0 \Rightarrow m_0 = \tanh\left[\beta(zJm_0+h)\right] \leftarrow \text{self-consistency condition}$$

ii) fast algorithm for homeworks & exams:

$$m = \langle S_i \rangle \Rightarrow m = \sum_{S_i=\pm1} S_i e^{\beta(Jmz+h)S_i} \Big/ \sum_{S_i=\pm1} e^{\beta(Jmz+h)S_i}$$

$$= \tanh \beta(Jmz+h)$$

- solve graphically or by Taylor expansion

→ for $h \neq 0$ f_{MF} has minimum at $m_0 \neq 0$

→ for $h = 0$ existence of nontrivial solution $m_0 \neq 0$ depends on temperature:

$T < zJ/k_B \Rightarrow$ two solutions $m_0 \neq 0$

$T > zJ/k_B \Rightarrow m_0 \equiv 0$

iii) fast algorithm to get T_c for homeworks & exams

$$T_c: \quad \partial m/\partial m\Big|_{m=0} = 1 = \frac{\partial}{\partial m} \tanh \beta J m z\Big|_{m=0} = \frac{1}{k_B T_c} Jz \cdot (1 - \tanh^2 \beta J m z)$$

$$T_c = \frac{Jz}{k_B} = \frac{2dJ}{k_B} \quad \text{on cubic lattice in } d \text{ dimensions}$$

1D: exact solution in 1D is $T_c \equiv 0$, not $T_c = 2J/k_B$

→ Peierls argument show importance of fluctuations in 1D

$T = 0 \Rightarrow E = -(N-1)J$, $S = 0$

$T > 0 \Rightarrow \uparrow\uparrow\uparrow\downarrow\downarrow\downarrow\downarrow$ domain wall $\Delta E = 2J$ cost

$\Delta F = 2J - T\Delta S < 0$ for $N \gg 1$, $\Delta S = ?$

↳ so, proliferation of domain walls lowers F until $m = 0$

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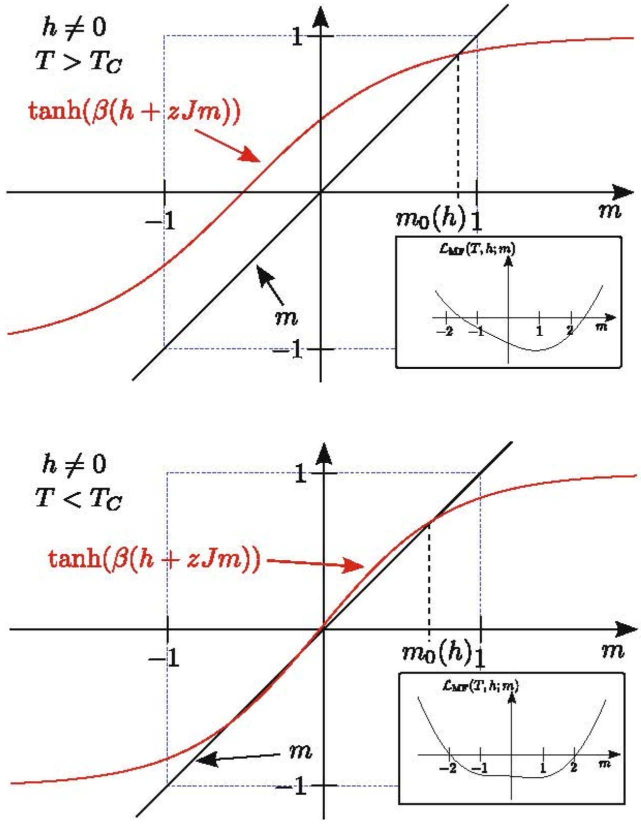


Fig. 2.1 Graphical solution of the mean-field self-consistency equation (2.11) for $h > 0$. The inset shows the behavior of the corresponding Landau function $\mathcal{L}_{\mathrm{MF}}(T, h; m)$ defined in Eq. (2.9). For $T > T_c$ or h sufficiently large the Landau function exhibits only one minimum at finite $m_0 > 0$. For $T < T_c$ and h sufficiently small, however, there is another local minimum at negative m, but the global minimum of $\mathcal{L}_{\mathrm{MF}}(T, h; m)$ is still at $m_0 > 0$

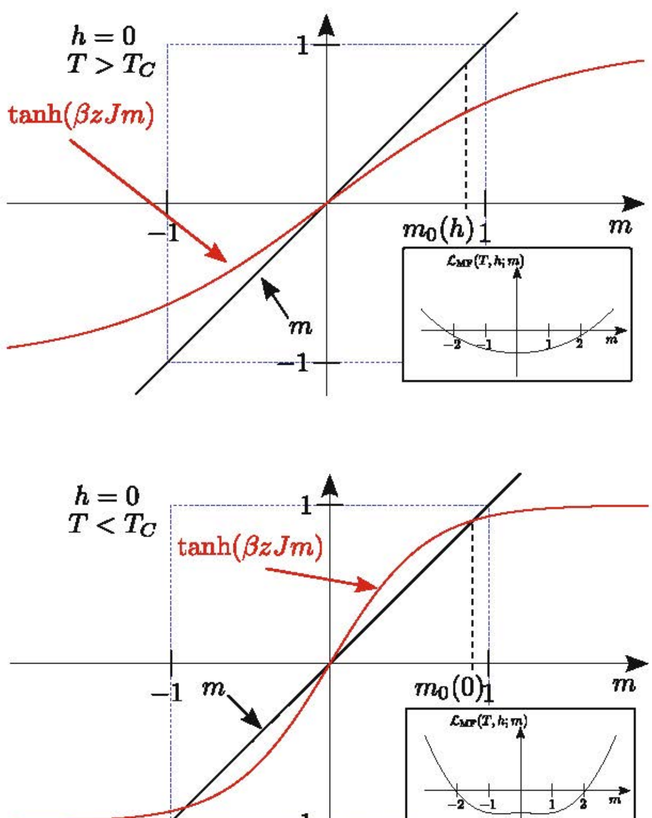


Fig. 2.2 Graphical solution of the mean-field self-consistency equation (2.11) for $h = 0$. The upper figure shows the typical behavior in the disordered phase $T > T_c$, while the lower figure represents the ordered phase $T < T_c$. The behavior of the Landau function is shown in the insets: while for $T > T_c$ it has a global minimum at $m_0 = 0$, it develops for $T < T_c$ two degenerate minima at $\pm|m_0| \neq 0$

2° Exact partition function for 1D Ising model via transfer matrix method

$$H = -J\sum_{i=1}^{N} S_i S_{i+1} - h\sum_{i=1}^{N} S_i \quad , \quad S_{N+1} = S_1$$ for periodic boundary conditions

$$Z = \sum_{S_1=\pm1}' \cdots \sum_{S_N=\pm1}' e^{\beta\left[J\sum_i' S_i S_{i+1} - \frac{1}{2}h\sum_i' (S_i + S_{i+1})\right]}$$

$$\left.\begin{aligned}
\langle S|T|S'\rangle &= e^{\beta[JSS' + h(S+S')/2]} \\
\langle 1|T|1\rangle &= e^{\beta(J+h)} \\
\langle -1|T|-1\rangle &= e^{\beta(J-h)} \\
\langle 1|T|-1\rangle &= \langle -1|H|1\rangle = e^{-\beta J}
\end{aligned}\right\}$$ defines $T \equiv$ transfer matrix

$\langle S|T|S'\rangle = T_{SS'} \rightarrow$ usage of Dirac notation purely for convenience and nothing to do with QM

$$\hat{T} = \begin{pmatrix} e^{\beta(J+h)} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-h)} \end{pmatrix}$$

$$Z = \sum_{S_1} \cdots \sum_{S_N} \langle S_1|\hat{T}|S_2\rangle\langle S_2|\hat{T}|S_3\rangle \cdots \langle S_N|\hat{T}|S_1\rangle$$

$$Z = \sum_{S_1} \langle S_1|\hat{T}^N|S_1\rangle = \mathrm{Tr}\left(\hat{T}^N\right) = \lambda_+^N + \lambda_-^N$$

$$\det\left(\hat{T} - \lambda \hat{I}_{2\times2}\right) = 0 \Rightarrow \lambda_\pm = e^{\beta J}\left[\cosh(\beta h) \pm \sqrt{\sinh^2(\beta h) + e^{-4\beta J}}\right]$$

$f = F/N \approx -k_B T \ln \lambda_+$ because $\lambda_+ > \lambda_-$ and in TD limit $\lambda_+^N \gg \lambda_-^N$

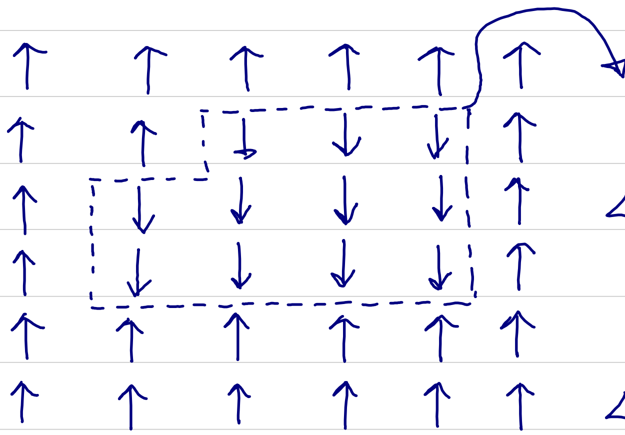
$$= -J - k_B T \ln\left[\cosh(\beta h) + \sqrt{\sinh^2(\beta h) + e^{-4\beta J}}\right]$$

$$m = M/N = -\left(\partial f/\partial h\right) = \frac{\partial}{\partial(\beta h)} \ln \lambda_+ = \frac{\sinh(\beta h) + \frac{\sinh(\beta h)\cosh(\beta h)}{\sqrt{\sinh^2(\beta h) + e^{-4\beta J}}}}{\cosh(\beta h) + \sqrt{\sinh^2(\beta h) + e^{-4\beta J}}}$$

$$h \to 0 \Rightarrow \left\{\begin{aligned} \cosh(\beta h) &\to 1 \\ \sinh(\beta h) &\to 0 \end{aligned}\right\} \Rightarrow m = 0 \text{ at any } T > T_c \text{, so } T_c \equiv 0$$

2D: exact solution by Onsager in 2D is $T_c = 2.269 \frac{J}{k_B}$

→ Peierls estimate of T_c in 2D Ising model:



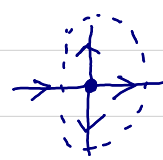
domain wall of perimeter Γ

$\Delta E = 2J\Gamma$ is energy cost to generate such domain wall

$\Delta S = k_B \ln 3^{\Gamma} \cdot N$

no. of paths to return to original position after Γ steps while passing through each bond only once

no. of sites to start from



3 choices to avoid going back to in bond

$$\Delta F = 2J\Gamma - k_B T \Gamma \ln 3 \qquad , \qquad 3^{\Gamma} \gg N \text{ as } N \to \infty$$
$$= \Gamma (2J - k_B T \ln 3)$$

$T < T_c = \frac{2J}{k_B \ln 3} = 1.8\, J/k_B \Rightarrow \Delta F > 0$ so, ferromagnetic long-range order remains stable

$T > T_c \Rightarrow$ many islands form to make $\Delta F < 0$

→ note that for long-range interactions, such as $J = J / |i-j|^n$, even 1D Ising model can have $T_c \neq 0$

→ exact partition function for 2D Ising model via transfer matrix method (Onsager 1944.)

$$H = -J\sum_{i,j}\left(S_{i,j}S_{i+1,j} + S_{i,j+1}S_{i,j}\right) - h\sum_{i,j}S_{i,j}$$

$$= \sum_{j=1}^{N}\left[\underbrace{E(\mu_j,\mu_{j+1})}_{} + \underbrace{E(\mu_j)}_{}\right]$$

$$\hookrightarrow -\sum_{i=1}^{N} S_{i,j}S_{i,k} \qquad \hookrightarrow -J\sum_{i=1}^{N}S_{i,j}S_{i+1,j} - h\sum_{i,j}S_{i,j}$$

$\mu_j = \{S_{1j},\ldots,S_{Nj}\}$ → spins in column j of square lattice

$$\langle\mu_j|\hat{T}|\mu_k\rangle = e^{-\beta[E(\mu_j,\mu_k)+E(\mu_j)]}$$

$\hat{T}$ is $2^N \times 2^N$ matrix ; $Z = \mathrm{Tr}(\hat{T}^N)$

$$Z = \lambda_+^N \Rightarrow f \overset{h\to 0}{=} -k_BT\ln[2\cosh(2\beta J)] - \frac{k_BT}{2\pi}\int_0^{\pi} d\phi \times \ln\frac{1}{2}\left(1+\sqrt{1-K^2\sin^2\phi}\right)$$

↳ largest eigenvalue

$$K = \frac{2}{\cosh(2\beta J)\coth(2\beta J)}$$

in $h=0$ cannot use $m = -\left(\frac{\partial f}{\partial h}\right)_{h\to 0} \Rightarrow m = \lim_{j\to\infty}\langle S_{1,1}S_{1,1+j}\rangle = \left\{1-\sinh(2\beta J)^{-4}\right\}^{1/8}$

$$2\tanh^2(\beta J) = 1 \Rightarrow k_BT_c = 2.269185\,J$$

$$C = -T\left(\frac{\partial^2 f}{\partial T^2}\right)\Bigg|_{T\to T_c} = k_B\frac{2}{\pi}\left(\frac{2J}{k_BT_c}\right)^2\left[-\ln\left(1-\frac{T}{T_c}\right) + \ln\left(\frac{k_BT_c}{2J}\right) - \left(1+\pi/4\right)\right]$$

→ C diverges logarithmically as $T\to T_c$ so $\alpha = 0$

3° Landau MFT

→ for T close to T_c and small $\beta|h|$ the value of m_0 at the minimum of f_{MF} is small so we can expand it to fourth order in m and linear in $h \neq 0$:

$$f_{MF} = \frac{zJm^2}{2} - T \ln\left\{2\cosh\left[\beta(zJm + h)\right]\right\}$$

$$\ln[2\cosh x] = \ln 2 + \frac{x^2}{2} - \frac{x^4}{12} + \mathcal{O}(x^6)$$

$$f_{MF} = \underbrace{f + \frac{r}{2}m^2 + \frac{u}{4!}m^4}_{\to f_{MF}(m) = f_{MF}(-m)} - hm + \dots$$

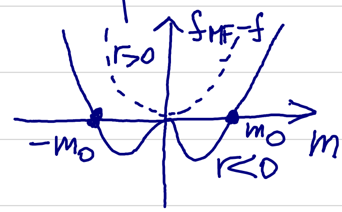
because in $h=0$: $H(S_i) = H(-S_i)$

$f = -k_BT \ln 2$, $\quad r = \frac{zJ}{2}(k_BT - zJ) \approx (T - T_c)\,k_B$

$u = 2k_BT(zJ/k_BT) \approx 2k_BT_c$

→ r changes sign at $T = T_c$, so that for $h=0$ global minimum of f_{MF} for $T > T_c$ evolves into a local minimum for $T < T_c$, and two new minima emerge at finite values of m

$$\partial f_{MF}/\partial m\Big|_{m_0} = r m_0 + \frac{u}{6}m_0^3 - h = 0$$



a) $h=0$: $\quad m_0 = \sqrt{\frac{-6r}{u}} \propto (-t)^{1/2} \Rightarrow \beta = 1/2$

b) $h \to 0$: neglect m_0^3 so that $m_0(h) \propto h/r$

$$\left.\begin{aligned} &\chi = \partial m_0(h)/\partial h \propto 1/r \propto (T - T_c)^{-1} \end{aligned}\right\} T \geq T_c$$

$$\chi \propto |T - T_c|^{-1} \text{ for } T < T_c$$

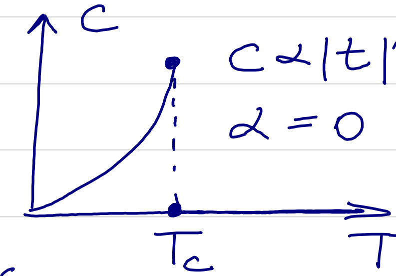
$$\Downarrow\ \gamma = 1$$

c) at the critical point setting $r=0$ leads to

$m_0(h) \propto (h/u)^{1/3}$ so $\delta = 3$

d) $C = -T\, \partial^2 f_{MF} / \partial T^2$
↳ per spin

$h=0$: $T > T_c \Rightarrow f_{MF} = f$ because $m_0 = 0$
$C \equiv 0$



$C \propto |t|^0$
$\alpha = 0$

$T < T_c \Rightarrow f_{MF} = f - \frac{3}{2}\frac{r^2}{u}$

$C \approx -T_c\, \partial^2 f / \partial T^2 + \underbrace{3T_c/u}_{3/2 \text{ because } u \approx 2T_c}$

$2 - \alpha = 2\beta + \gamma = \beta(\delta + 1)$
↳ MF exponents satisfy scaling relations

Table 1.1 Critical exponents of the Ising, XY, and Heisenberg universality classes. The corresponding symmetry groups of the order parameter are Z_2 for the Ising universality class, $O(2)$ for the XY universality class, and $O(3)$ for the Heisenberg universality class. The small subscripts in the first line denote the dimensionality. While the exponents of the two-dimensional Ising universality class are exact, the exponents in three dimensions are only known approximately. The numbers for Ising$_3$ and the error estimates are from the review by Pelissetto and Vicari (2002). For XY$_3$ we give rounded values for α, γ, ν, and η up to two significant figures, as compiled in Pelissetto and Vicari (2002, Table 19). The values for β and δ are obtained using the scaling relations (1.33b) and (1.33d). For Heisenberg$_3$ we quote the results by Holm and Janke (1993)

Exponent	Ising$_2$	Ising$_3$	XY$_3$	Heisenberg$_3$	Ising$_{MF}$
α	0 (log)	0.110(1)	–0.015	–0.10	0
β	1/8	0.3265(3)	0.35	0.36	1/2
γ	7/4	1.2372(5)	1.32	1.39	1
δ	15	4.789(2)	4.78	5.11	3
ν	1	0.6301(4)	0.67	0.70	1/2
η	1/4	0.0364(5)	0.038	0.027	0

4° Ginzburg criterion for validity of MFT.

→ accumulated fluctuations up to ξ length

$$\sigma_m^2 = \int_0^\xi \langle (S_r - \langle S_r\rangle)(S_0 - \langle S_0\rangle) \, d^3r$$

$$= \int_0^\xi \left(\langle S_r S_0\rangle - \langle S_r\rangle\langle S_0\rangle\right) d^3r = k_B T \chi$$

χ requires $\int_0^\infty$ but integration outside of $\int_0^\xi$ gives very small contribution

fluctuations were assumed small when deriving MFT

$$\int_0^\xi \langle S_r\rangle\langle S_0\rangle \, d^3r \propto m^2 \xi \Rightarrow \underbrace{k_B T \chi \ll m^2 \xi^d}$$

close to T_c

$$k_B T \, (T_c - T)^{-\gamma} \ll (T_c - T)^{2\beta} (T_c - T)^{-\nu d}$$

$$\underset{=1}{\gamma} < \underset{=1/2}{\nu} d - 2\underset{=1/2}{\beta} \Rightarrow d > 4 \text{ MFT is valid}$$

→ alternative is to find the size of temperature interval where fluctuations dominate and MFT is invalid

$$\frac{\sigma_m^2 \propto \chi \propto |t|^{-1}}{\underbrace{\int_0^\xi \langle S_r\rangle\langle S_0\rangle d^3r}_{R^d |t|^{1-d/2}}} \ll 1 \Leftrightarrow \varepsilon R^{-d} \ll |t|^{(4-d)/2}$$

↳ of order 1

because $m^2 \propto |t|$ and $\xi \propto R|t|^{-1/2}$

↳ range of interactions like exchange

i) for liquid ^4He or antiferromagnets $R \sim 1$ nm and $|t|$ has to be large, so MFT valid only away from T_c

ii) for low temperature superconductors $R \sim 100$ nm and critical region is too small to be accessible to experiment