

(magnetic systems)
"Mean field" description of the ordering transition

Consider Ising ferromagnet as an example

$$H = -J \sum_{\langle i,j \rangle} S_i S_j - h \sum_i S_i$$

$\mu_B \cdot B$ applied external field in physical units

(qualitatively similar approach works for ~~vector~~ n-vector models as well)

Single spin in a field:

$$H_{1\text{spin}} = -h S$$

$$Z_{1\text{spin}} = e^{\beta h} + e^{-\beta h} = 2 \cosh(\beta h)$$

$$F_{1\text{spin}} = -k_B T \ln(2 \cosh(\beta h))$$

$$\boxed{m = \langle S \rangle = \frac{e^{\beta h} - e^{-\beta h}}{e^{\beta h} + e^{-\beta h}} = \tanh(\beta h)} = \frac{1}{\beta} \frac{\partial \ln Z}{\partial h} = - \frac{\partial F}{\partial h}$$

↑
"magnetization"

Collection of N noninteracting spins - multiply by N to obtain total free energy and magnetization; (properties per spin remain unchanged)

Interacting spins - try "effective medium" approximation or "mean field"

Consider a spin @ i

piece in H containing S_i :

$$- \left(J \sum_{\substack{j\text{-neighbours} \\ \text{of } i}} S_j + h \right) S_i$$

h_{eff} - effective field acting on S_i

h_{eff} depends on the configuration of spins nearby

Mean field approximation: consider "average" h_{eff} obtained by $S_i \rightarrow \langle S_i \rangle$

$$\boxed{h_{\text{eff}} = h + J \sum_{j=\text{neighbours of } i} \langle S_j \rangle = h + \underbrace{J \cdot Z \cdot m}_{\substack{\text{number} \\ \text{of neighbours}}}}$$

(remark: this is equivalent to ^{the} uniform density approximation in our treatment of interacting particles; here $J \cdot Z \sim$ integral of the attractive part of the interaction assuming uniform dens., only here interaction extends only to nearest neighbours)

But $m = \langle S_i \rangle$ is itself determined by h_{eff}
 $\Rightarrow$ self-consistent field condition

$$\boxed{m = \tanh(\beta h_{\text{eff}}) = \tanh(\beta(h + J Z m))}$$

want to solve for m as a function of h .

Example: at high temperatures and in small field
 $k_B T \gg J$ $h \ll k_B T$,
 (e.g. susceptibility is measured with $h \rightarrow 0$)
 expect also m to be small:

$$m = \tanh \beta(h + J Z m) \approx \frac{h + J Z m}{k_B T} \quad \text{Curie-Weiss}$$

$$m = \frac{h}{k_B T - J Z} \quad ; \quad \chi = \left(\frac{m}{h} \right)_{h \rightarrow 0} = \frac{1}{k_B T - J Z}$$

if J ferromagnetic $\rightarrow$ susceptibility is larger than for free spins - "spins are happy to cooperate"

(if J is antiferromagnetic, the susceptibility is smaller than free spins: spins like to be antiparallel, so aligning neighbours with the field effectively decreases the field on a given spin).

Remark: all discussions of dielectric constant or magnetic permeability constant are essentially effective "medium descriptions" in the above sense. If the "medium corrections" are small, we would stop here. Important aspect in electrostatics and magnetostatics is the long-range nature of the interactions, so one needs to work harder to calculate the average field due to the rest of the system — usually done by using e.g. Gauss' law.

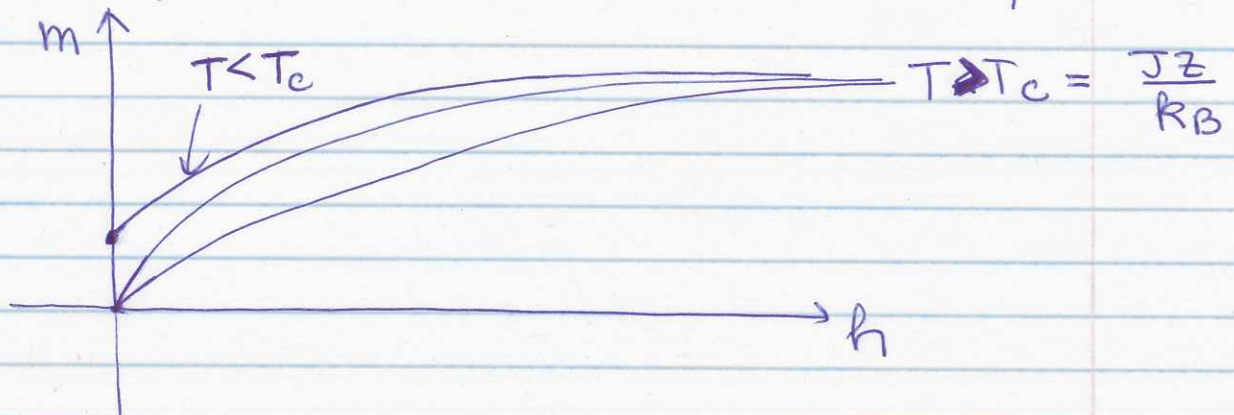
Note:

$$\chi = \frac{1}{k_B T - Jz} \rightarrow \infty \text{ for } T \rightarrow T_c = \frac{Jz}{k_B}$$

$$m = \tanh\left(\frac{h + Jzm}{k_B T}\right) \Rightarrow m(h)$$

Can

~~argue~~ argue that for $T > T_c$ this has unique solution,



while for $T < T_c$ the solution is not unique and the stable branch starts with nonzero magnetization @ $h=0$

Indeed, consider $h=0$ first:

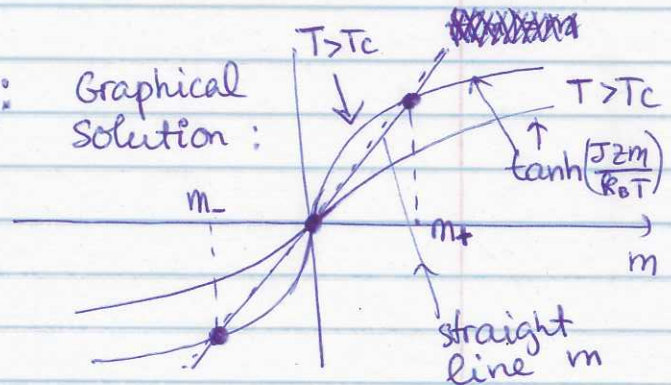
$$m = \tanh\left(\frac{Jzm}{k_B T}\right)$$



for small m ,

behaves as $\sim \frac{Jzm}{k_B T} \rightarrow \text{slope } \frac{Jz}{k_B T}$

Graphical Solution:



- For $k_B T > Jz$, the initial slope is < 1 , and there is unique solution $m=0$
- For $k_B T < Jz$, the initial slope is > 1 , and there are three solutions: $m=0, m_+, m_- = -|m_+|$

↑
unstable solution

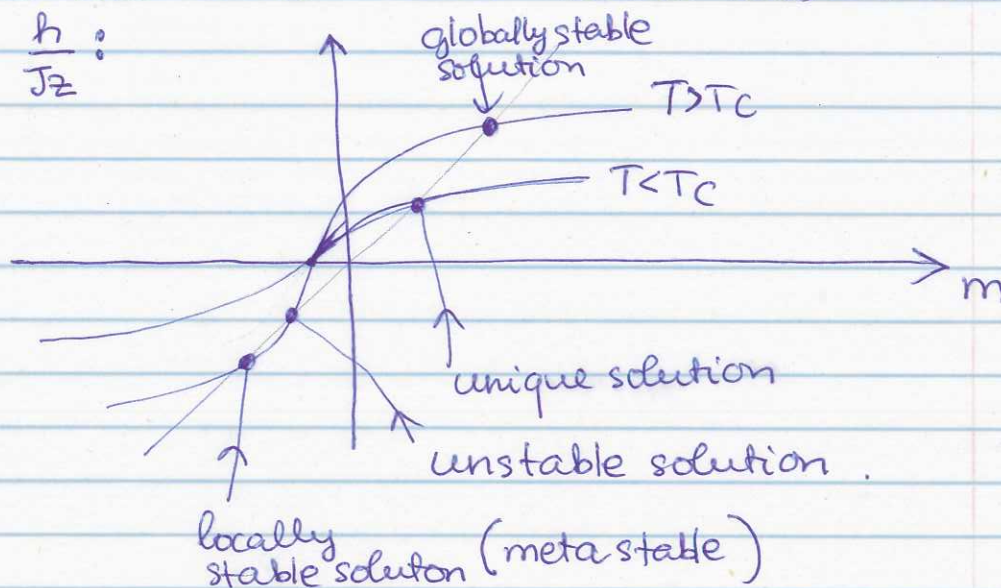
↖ ↗
stable solutions

↖ in the sense to be made clear below.

- $k_B T_c = Jz$ - critical point

For $h \neq 0$, $\tanh\left(\frac{Jz m + h}{k_B T}\right) = \tanh\left(\frac{Jz(m + \frac{h}{Jz})}{k_B T}\right) -$

- gives the same "tanh" curve shifted to the left by $\frac{h}{Jz}$:



"Variational" perspective on this mean field (so-called Bragg-Williams theory)

Consider trial density matrix where spins are independent — for example, can define the trial density matrix by hess

$$H_0 = -\text{hess} \sum_i S_i$$

or equivalently

$$p_+ = \frac{e^{\beta \text{hess}}}{\mathcal{Z}_{1\text{spin}}} \quad p_+ + p_- = 1$$

$$p_- = \frac{e^{-\beta \text{hess}}}{\mathcal{Z}_{1\text{spin}}} \quad p_+ - p_- = m = \tanh(\beta \text{hess})$$

(can parametrize the trial state by either hess or m)

$$F_{\text{trial}} = \langle H \rangle_{\rho_{\text{trial}}} + k_B T \cdot \text{Tr}(\rho_{\text{trial}} \ln \rho_{\text{trial}})$$

$$\begin{aligned}
 \langle H \rangle_{\text{trial}} &= -J \sum_{\langle ij \rangle} \underbrace{\langle S_i \rangle}_m \underbrace{\langle S_j \rangle}_m - h \sum_i \underbrace{\langle S_i \rangle}_m = \\
 &= N \cdot \left(-Jm^2 \cdot \underbrace{\frac{Z}{2}}_{\substack{\text{each bond} \\ \text{is shared between 2}}} - hm \right);
 \end{aligned}$$

$$\begin{aligned}
 \text{Tr } \rho_{\text{trial}} \ln \rho_{\text{trial}} &= N \cdot (p_+ \ln p_+ + p_- \ln p_-) = \\
 &= N \left(\frac{1+m}{2} \ln \frac{1+m}{2} + \frac{1-m}{2} \ln \frac{1-m}{2} \right)
 \end{aligned}$$

$$\Rightarrow \boxed{\frac{F_{\text{trial}}}{N} = -Jm^2 \frac{Z}{2} - hm + k_B T \times \left\{ \frac{1+m}{2} \ln \frac{1+m}{2} + \frac{1-m}{2} \ln \frac{1-m}{2} \right\}}$$

Minimize w.r.t. m :

$$\begin{aligned}
 0 \stackrel{!}{=} \frac{\partial F}{\partial m}: 0 \stackrel{!}{=} -JmZ - h + k_B T \left\{ \frac{1}{2} \ln \frac{1+m}{2} + \frac{1+m}{2} \cdot \frac{2}{1+m} \cdot \frac{1}{2} + \right. \\
 \left. + \frac{-1}{2} \ln \frac{1-m}{2} + \frac{1-m}{2} \cdot \frac{2}{1-m} \cdot \frac{-1}{2} \right\} = -JmZ - h + \frac{k_B T}{2} \ln \frac{1+m}{1-m}
 \end{aligned}$$

$$\underbrace{\frac{1}{2} \ln \frac{1+m}{1-m}}_{\text{atanh}(m)} = \frac{h + JmZ}{k_B T}$$

$$\triangleright \tanh(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}} = \frac{e^{2x} - 1}{e^{2x} + 1} = \frac{\frac{1+m}{1-m} - 1}{\frac{1+m}{1-m} + 1} = m \quad \checkmark \quad \triangle$$

$\uparrow$
 $x = \frac{1}{2} \ln \frac{1+m}{1-m}$

$$\Rightarrow \boxed{m = \tanh \frac{h + JmZ}{k_B T}} \quad - \text{precisely the self-consistency condition!}$$

This is not magic but ^{is} dictated by the structure of the variational meanfield:

general site-dep.:

$$H_0 = - \sum_i h_i^z S_i^z$$

$$F_{\text{trial}} = - \sum_{\langle ij \rangle} J_{ij} m(h_i) m(h_j) + \sum_i \underbrace{\left(F_{\text{spin}}(h_i) + h_i m(h_i) \right)}_{F_0 - \langle H_0 \rangle_0}$$

Minimize wrt h_i :

$$\frac{\delta F_{\text{trial}}}{\delta h_i} = - \sum_{j \in \text{neighbours of } i} J_{ij} m(h_j) \frac{\delta m(h_i)}{\delta h_i} + \left(\frac{\partial F_{\text{spin}}}{\partial h_i} + m(h_i) + h_i \frac{\delta m(h_i)}{\delta h_i} \right) =$$

||
0!

$$= \left(h_i - \sum_{j \in i} J_{ij} m(h_j) \right) \frac{\delta m}{\delta h_i} = \text{require equal to } 0.$$

$$\Rightarrow \boxed{h_i = \sum_{j \in i} J_{ij} m(h_j)} \text{ — self-consistent field equation}$$

Analysis of the solutions of the self-consistency conditions is the same as before, but now for each solution we can calculate $F_{\text{trial}}(m)$, and check which one is global minimum (if there are several).

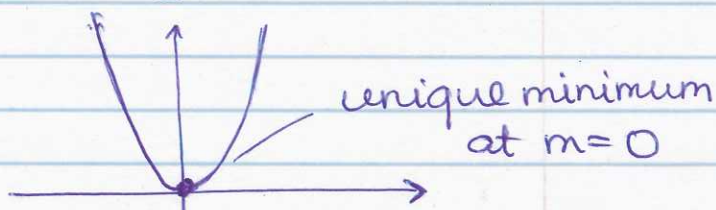
Analysis of F_{trial} for small m :

$$\begin{aligned} \frac{F_{\text{trial}}}{N} &\approx \underset{\substack{\uparrow \\ \text{expand to } O(m^4)}}{-Jm^2 \cdot \frac{Z}{2} - hm + k_B T \times \left\{ \frac{1+m}{2} \cdot (-\ln 2 + \right.} \\ &\quad \left. + m - \frac{m^2}{2} + \frac{m^3}{3} - \frac{m^4}{4} \right\} + \frac{1-m}{2} \left(-\ln 2 - m - \frac{m^2}{2} - \frac{m^3}{3} - \frac{m^4}{4} \right) \Big\} \\ &= -Jm^2 \cdot \frac{Z}{2} - hm + k_B T \times \left\{ 1 \cdot \left(-\ln 2 - \frac{m^2}{2} - \frac{m^4}{4} \right) + \right. \\ &\quad \left. + m \cdot \left(m + \frac{m^3}{3} \right) \right\} = \cancel{-T \cdot k_B \ln 2} + \frac{(k_B T - JZ)m^2}{2} \\ &\quad + \frac{k_B T}{12} \cdot m^4 - hm \end{aligned}$$

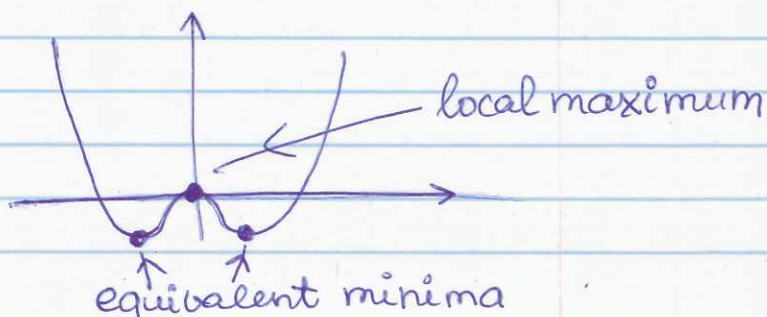
$h=0$

$$\frac{k_B T - JZ}{2} \cdot m^2 + \frac{k_B T}{12} m^4$$

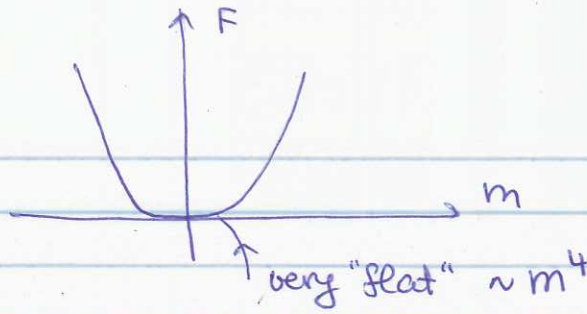
$$T > T_c = \frac{JZ}{k_B}$$



$$T < T_c$$

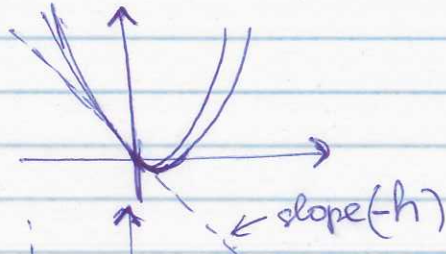


$$T = T_c$$

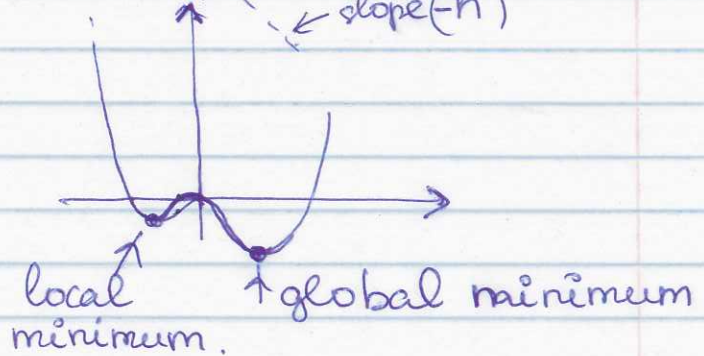


add $(-hm)$ to
 $h \neq 0$ - ~~shift~~ the above curves

$$T > T_c$$



$$T < T_c$$



Analysis near the critical point

* Self-consistency condition to $O(m^3)$:

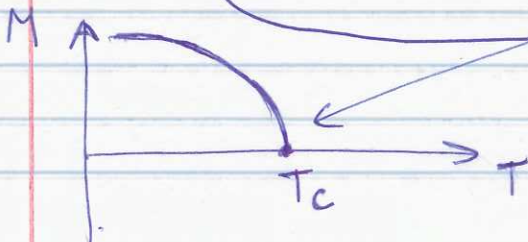
$$\boxed{(k_B T - Jz)m + \frac{k_B T}{3} m^3 - h = 0} \quad \Leftrightarrow \quad h + Jz m = \frac{1}{\beta} \tanh(\beta h) \approx \frac{1}{\beta} (m + \frac{m^3}{3})$$

* Order
 param;
 Magnetization

For $h=0$ and $T < T_c$

$$m \approx \sqrt{\frac{3(Jz - k_B T)}{k_B T}} =$$

$$= \left(\frac{3(T_c - T)}{T} \right)^{1/2} \sim (T_c - T)^{\beta}$$



order parameter
 exponent;

$$\boxed{\beta = \frac{1}{2} \text{ in mean field}}$$

⊗ Singularity in the susceptibility

$$T > T_c : \quad m(h) \approx \frac{h}{k_B T - Jz}$$

$$\chi(T > T_c) \approx \frac{1}{k_B T - Jz} = \frac{1}{k_B (T - T_c)} = \frac{A_+}{(T - T_c)^{\gamma_+}}$$

$$\gamma_+ = 1 \text{ in mean field}$$

$$T < T_c : \quad \bar{m} = \sqrt{\frac{3(Jz - k_B T)}{k_B T}} \quad \text{solves} \quad (k_B T - Jz)\bar{m} + \frac{k_B T - 3}{3}\bar{m}^3 = 0$$

$$\text{Write } m = \bar{m} + \delta m$$

$$(k_B T - Jz)(\bar{m} + \delta m) + \frac{k_B T}{3}(\bar{m}^3 + 3\bar{m}^2 \delta m + O(\delta m^2)) - h = 0$$

$$\Rightarrow \delta m \left(\underbrace{k_B T \cdot \bar{m}^2}_{3(Jz - k_B T)} + k_B T - Jz \right) = h$$

$$\delta m = \frac{h}{2(Jz - k_B T)}$$

$$\Rightarrow \chi(T < T_c) = \frac{1}{2k_B(T_c - T)} = \frac{A_-}{(T_c - T)^{\gamma_-}}$$

$$\begin{aligned} \gamma_+ &= \gamma_- = 1 \\ \frac{A_+}{A_-} &= 2 \end{aligned}$$

in mean field

("critical isotherm")

⊗ Behaviour at the critical temperature :

$$T = T_c$$

$$m(h) = \left(\frac{3}{k_B T} \right)^{1/3} h^{1/3} \sim h^{1/3}$$

$$\delta = 3 \text{ in mean field}$$

⊗ ~~Singularity~~ Singularity in the specific heat

- $F_{\text{trial}}(T > T_c) = -k_B T \ln 2$

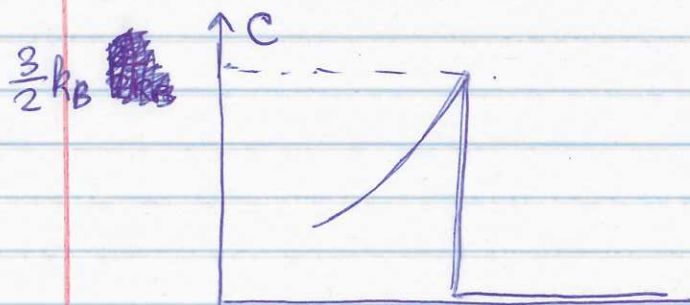
$$C = \frac{\partial u}{\partial T} = \frac{\partial}{\partial T} (F + TS) = \frac{\partial}{\partial T} (F - T \frac{\partial F}{\partial T}) = -T \frac{\partial^2 F}{\partial T^2} = 0$$

- $F_{\text{trial}}(T < T_c) = -k_B T \ln 2 + \frac{k_B(T - T_c)}{2} m(T)^2 + \frac{k_B T}{12} m(T)^4$

~~$$\frac{\partial F}{\partial T} = -k_B \ln 2 + \frac{k_B}{2} m(T)^2 + \frac{k_B(T - T_c)}{2} 2m(T) \frac{dm}{dT} + \frac{k_B T}{3} m(T)^3 \frac{dm}{dT} + k_B m(T)^3$$~~

$$\begin{aligned} &= -k_B T \ln 2 + k_B(T - T_c) \cdot \frac{3(T_c - T)}{k_B T} + \frac{k_B T}{12} \frac{3(T_c - T)^2}{k_B T} \\ &= -k_B T \ln 2 - \frac{3}{4} k_B \frac{(T - T_c)^2}{T} \end{aligned}$$

$C \approx$
near T_c $\frac{3}{2} k_B$



In the mean field,
C is discontinuous
across the transition

$$C \sim |t|^{-\alpha} \text{ with formal } \alpha = 0$$

⊗ One more exponent — so-called "correlation length exponent"

$\xi \sim |t|^{-\nu}$ will be discussed when we consider

Landau - Ginzburg theory with inhomogeneous order parameter,
(spatially varying)

Remarks

- * Ordering transition in the Ising ferromagnet is an example of continuous phase transition: the ordered phase grows continuously below T_c .
(^{e.g.} order parameter)

Thermodynamic potentials ($U, S, F, \dots$) are continuous at T_c , but their derivatives ("susceptibilities") are not in general

$h=0$ $m(T < T_c) \sim (T_c - T)^\beta$	$; \quad m(h, T = T_c) \sim h^{1/\delta}$
$\chi(T \gtrsim T_c) \sim \frac{A_{\chi}}{ T - T_c ^{\gamma}}$	$\left. \begin{array}{l} \leftarrow \text{diverges if } \gamma > 0 \\ \leftarrow \text{diverges if } d > 0 \end{array} \right\}$
$C(T \gtrsim T_c) \sim \frac{A_C}{ T - T_c ^d}$	

$\alpha, \beta, \gamma, \delta$ - critical exponents

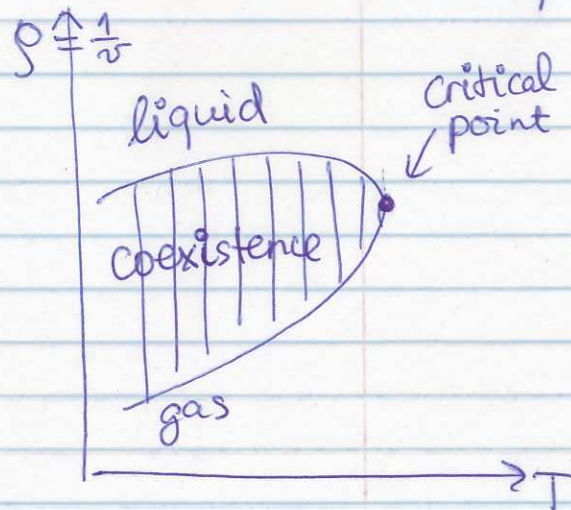
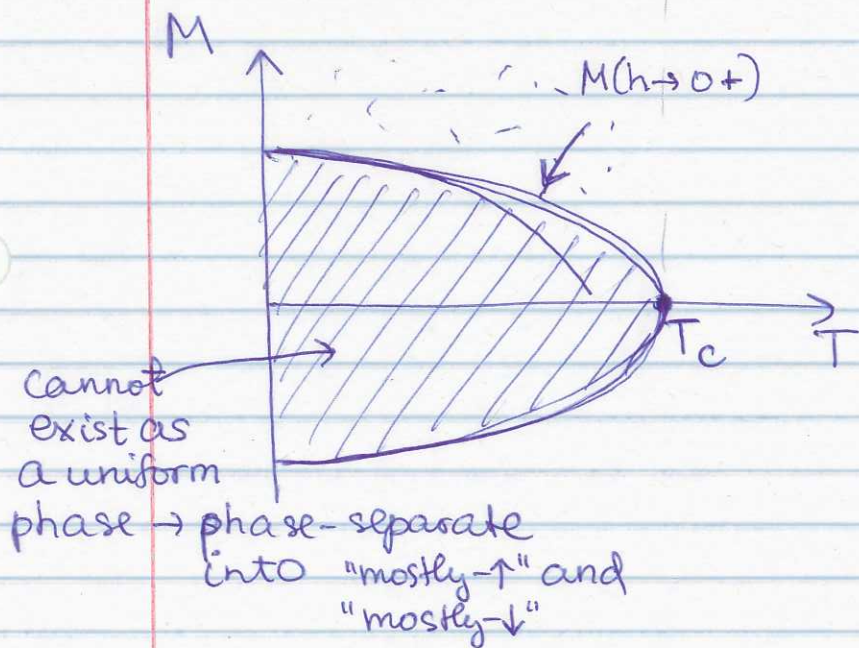
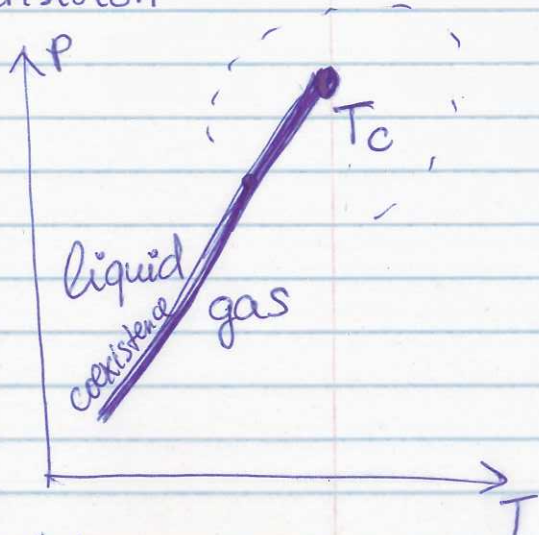
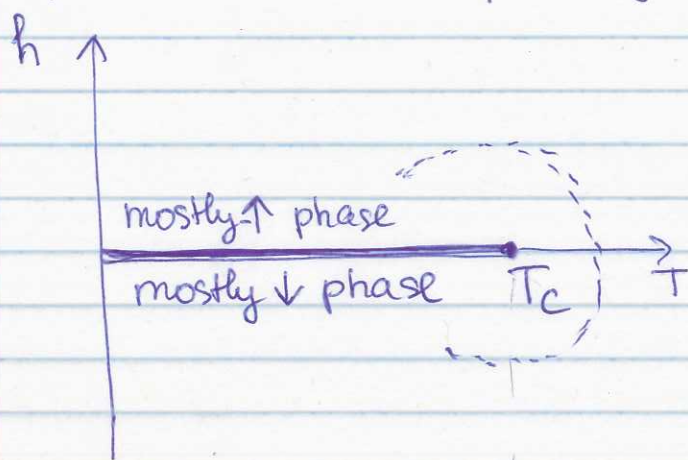
Mean field exponents: $\left\{ \beta_{mf} = \frac{1}{2}, \gamma_{mf} = 1, d_{mf} = 0, \delta_{mf} = 3 \right\}$ - "universal" in mft.

In general, $\alpha, \beta, \gamma, \delta$ are universal (system-indep) for problems within the same symmetry class (Ising; XY; Heisenberg).

For n -vector models, mean field exponents are the same, but this is not true for $d \leq 3$: different $O(n)$ models each has its own exponents.

- * Mean field exponents are accurate when $d \geq 4$, but fail for $d \leq 3$. The reason is that mft ignores fluctuations, which are important at the second-order transition since the two phases are quantitatively the same and the system easily "fluctuates"

Analogy between Ising transition and critical point in the liquid-gas transition



different h values correspond to different points in the M - T phase diagram

Critical properties of the Ising model near T_c

$\leftrightarrow$ critical properties of the liquid-gas transition near the crit. point.