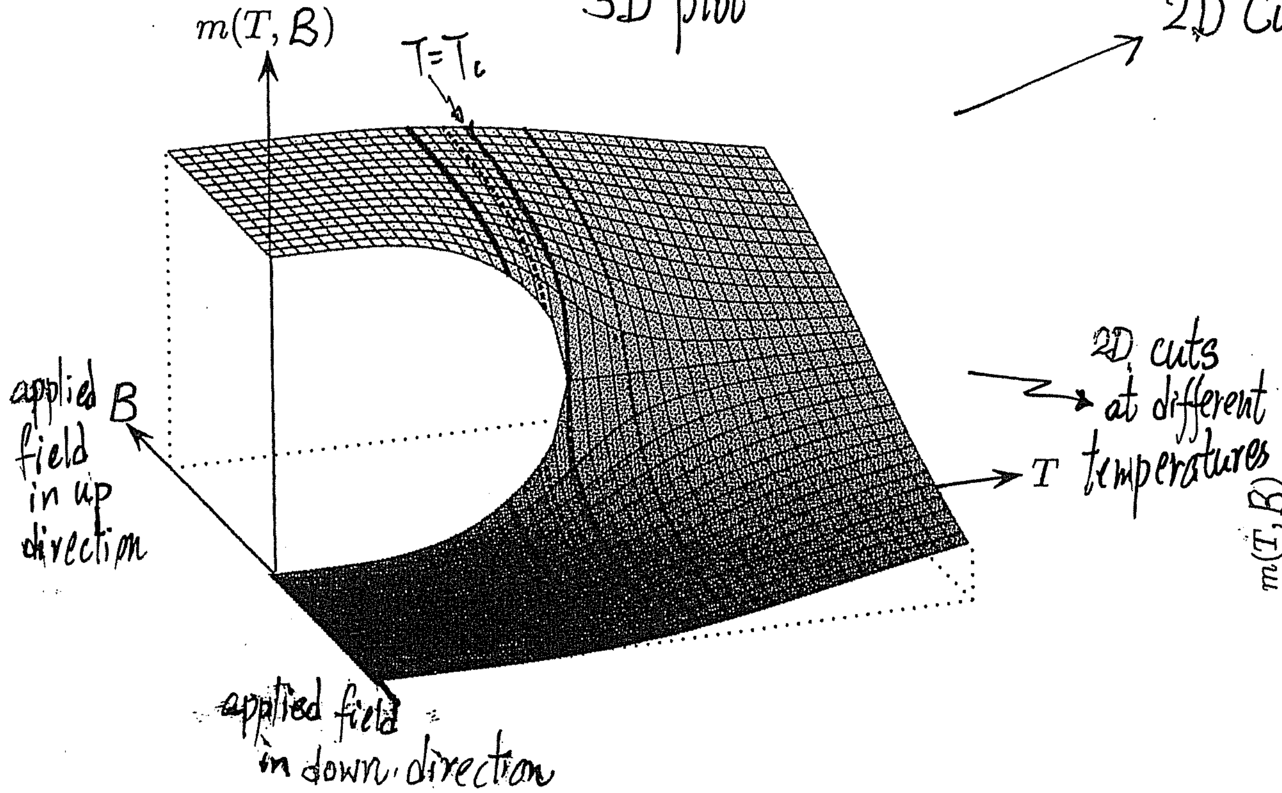
G. Critical Behavior as predicted by Mean field theory

Key equations:

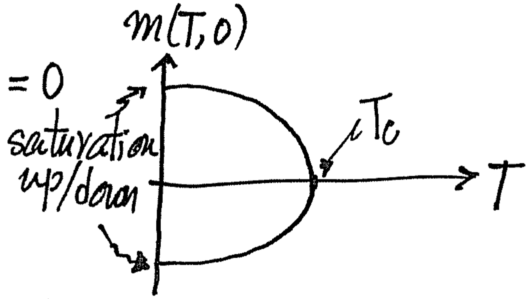
$$\boxed{\begin{aligned} m &= \tanh\left[\beta J z m + \beta B\right] \quad (4) \text{ (with applied field)} \\ m &= \tanh\left[\beta J z m\right] \quad (5)\ B_{applied} = 0 \text{ (OR } B=0) \end{aligned}}$$

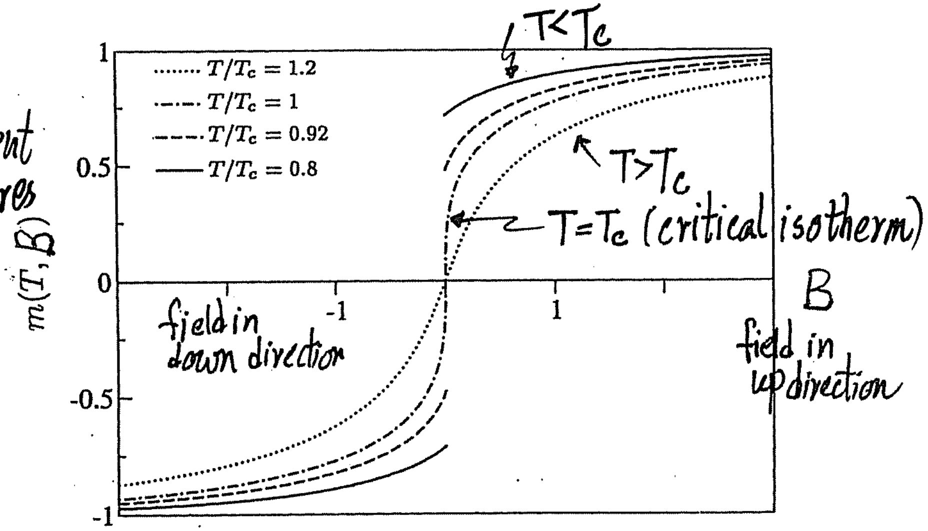
These can be solved to give m for given T and B, i.e. $m(T,B)$

3D plot

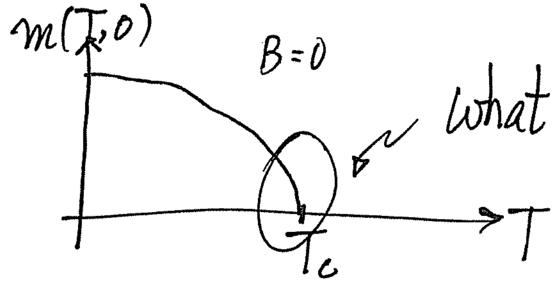


2D Cut at B = 0





Question:



what is the behavior here?

Mean field theory: $\boxed{m \sim (T_c - T)^{1/2}}$

- See how it comes out. Eq.(5) says $m = \tanh\left[\frac{T_c}{T} \cdot m\right]$

For $T \lesssim T_c$, $m \ll 1$ (m just started to grow).

$\tanh x \approx x - \frac{x^3}{3}$ for small x

$\therefore\ m \approx \frac{T_c}{T} m - \frac{1}{3}\left(\frac{T_c}{T}\right)^3 m^3 \Rightarrow 1 = \frac{T_c}{T} - \frac{1}{3}\left(\frac{T_c}{T}\right)^3 m^2$ ($m \neq 0$ solutions)

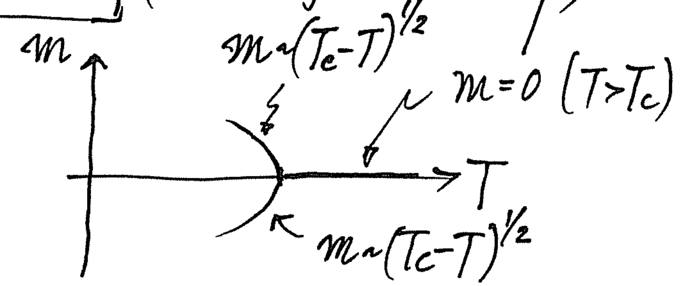
$\boxed{\begin{array}{l} m=0 \text{ is a solution} \\ \text{Valid for } T > T_c \end{array}}$

$\therefore\ m^2 = 3\left(\frac{T}{T_c}\right)^3\left[\frac{T_c}{T} - 1\right] = 3\left(\frac{T}{T_c}\right)^3\left(\frac{T_c - T}{T}\right)$

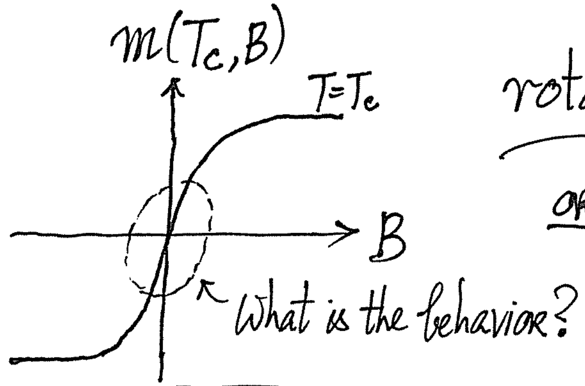
since $T \approx T_c$ ($T \lesssim T_c$), $m^2 \cong 3 \cdot \frac{1}{T_c} \cdot (T_c - T)$

$\Rightarrow \boxed{m = \pm\sqrt{\frac{3}{T_c}}\,(T_c - T)^{1/2}}$ for $T \to T_c^-$ (Mean field theory) (9)

- Comparing with $m \sim (T_c - T)^{\beta}$, $\beta_{MFT} = 1/2$

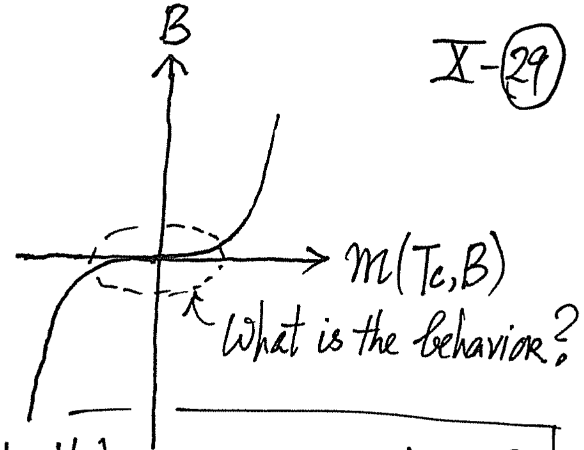


Question: Look at $T = T_c$



rotate

OR



$$m(T_c,B) \propto |B|^{1/\delta}$$

OR $\quad B \propto m^{\delta}$

What is δ_{MFT}?

$\boxed{\text{how does } m \text{ vary with } B \text{ OR (equivalently) } B \text{ vary with } m?}$

$$m = \tanh\left[\frac{zJ}{kT} m + \frac{B}{kT}\right] \quad (4)$$

Set $T = T_c$, $\frac{zJ}{kT_c} = 1$ (MFT),

$$\boxed{m = \tanh\left[m + \frac{B}{kT_c}\right]} \quad (T = T_c)$$

Look at figures, we focus on $|m| \ll 1$ (and also $\frac{B}{kT_c} \ll 1$).

$$\therefore \quad m \approx \left(m + \frac{B}{kT_c}\right) - \frac{1}{3}\left(m + \frac{B}{kT_c}\right)^3$$

$$\Rightarrow \frac{B}{kT_c} \approx \frac{1}{3}\left(m + \frac{B}{kT_c}\right)^3 \approx \underbrace{\frac{m^3}{3}}_{\text{leading term}} + \underbrace{\frac{m^2 B}{kT_c}}_{\sim m^5} + \underbrace{\cdots}_{\text{even higher}}$$

[(here, think iteratively!) $\frac{B}{kT_c} \sim m^3 \Rightarrow \frac{m^2 B}{kT_c} \sim m^5$]

$$\Rightarrow \boxed{B = \frac{kT_c}{3} m^3 \sim m^3}$$

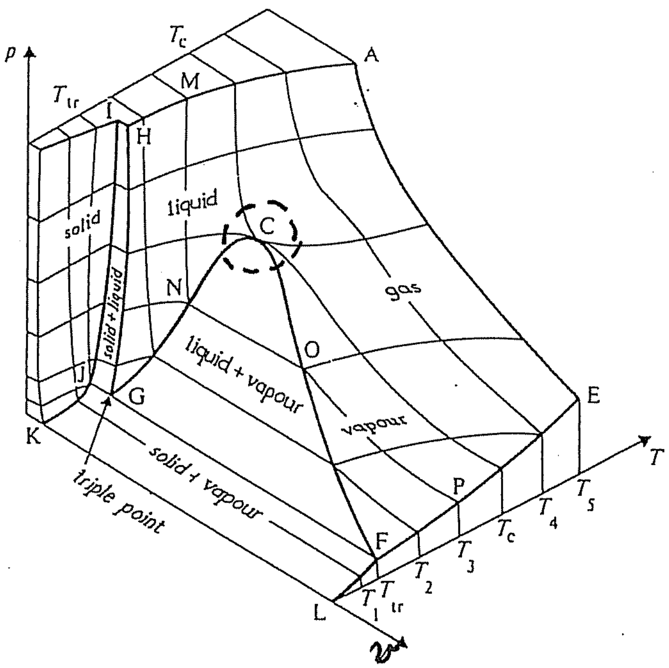
OR

$$\boxed{m = \left(\frac{3}{kT_c}\right)^{1/3} B^{1/3} \Rightarrow m \sim \operatorname{sign}(B)|B|^{1/3}} \quad (10) \quad \therefore \delta_{MFT} = 3$$

Van der Waals Equation of state

$\Delta v \sim (T_c - T)^{1/2}$; $\Delta p \sim -(\Delta v)^3$ for $T = T_c$

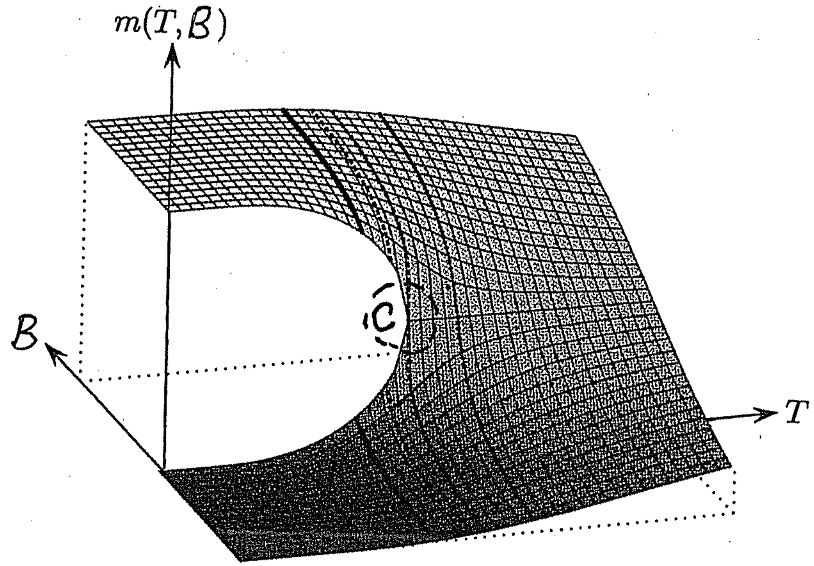
The p–V–T relation of a pure substance.



Mean Field Theory of Ferromagnetism

$m \sim (T_c - T)^{1/2}$; $B \sim m^3$ for $T = T_c$

Ising Model



- Two seemingly different physical systems behave the same way near the critical point!
- Two seemingly different theories give same behavior near critical point!

How about $T > T_c$ paramagnetic behavior?

- $T > T_c$, no spontaneous magnetization
- With applied $B \neq 0$, there is $m \neq 0$
- Again start with $m = \tanh\left[\frac{T_c}{T} \cdot m + \frac{B}{kT}\right]$

Look for how m varies with B.

$$m \approx m \frac{T_c}{T} + \frac{B}{kT}$$ (consider $\frac{B}{kT} \ll 1$ (weak field) and see how m responds)

$$\Rightarrow m\left(1 - \frac{T_c}{T}\right) = \frac{B}{kT} \Rightarrow m\left(\frac{T-T_c}{T}\right) = \frac{B}{kT} \Rightarrow \underbrace{m = \frac{B}{k}\left(\frac{1}{T-T_c}\right)}_{\text{paramagnetic behavior}}$$

Recall: $\underset{\propto m}{\vec{M}} = \chi \underset{\propto B}{\vec{H}}$

$$\therefore \chi \sim \underset{\text{agree with exp'tal observation}}{\frac{1}{T-T_c}} \sim (T-T_c)^{-1} \quad \text{for } T \to T_c^+$$

$$\sim (T-T_c)^{-\gamma} \qquad (11)$$

$$\therefore \gamma_{MFT} = +1$$

- MFT gives results the capture the key features.
- This has the merit of being simple, and yet captures the essential features.

Summary: Steps in setting up mean-field theory X-26

- Decoupling the coupling term $S_i S_j \approx S_i \langle S_j \rangle$
  [Interacting system $\approx$ effective non-interacting system]
- Evaluating $\langle S \rangle$ using the approximated $E_{MF}(\{S_i\})$ to set up self-consistent equation(s)
- Same idea can be applied to many other problems

Remarks

- included interaction in an averaged way, just sufficient to show critical phenomena
- self-consistency often enhances a theory's "accuracy"
- other spin models, many-body problems, random resistor network, etc.

We wrote down Eqs. (4), (5) [MF equations] by physical reasoning.

Q: Can we set up Eqs. (4), (5) in a more systematic way? Any insight from a more systematic approach?

H. Mean Field Theory: A More Systematic Approach

- In Stat. Mech., we often want to follow the standard path of...

  evaluate Z (despite approximately) $\rightarrow F \rightarrow$ other quantities

- Starting with the Hamiltonian of Ising Model

$$E(\{S_i\}) = \underbrace{-J\sum_{\langle ij\rangle} S_i S_j}_{\substack{\text{interaction} \\ \text{couples neighboring spins (term that causes trouble)}}} \underbrace{- B\sum_i S_i}_{\text{just paramagnetic (easy to handle)}} \qquad \text{(Ising Model)}$$

- Apply mean field approximation to 1st term
  - Idea: S_i fluctuates slightly from $\langle S_i\rangle$, so $(S_i - \langle S_i\rangle)$ is assumed to be small

1st term $\rightsquigarrow$ $$E_{interaction}(\{S_i\}) = -J\sum_{\langle ij\rangle} S_i S_j = -J\sum_{\langle ij\rangle}\left(S_i - \langle S_i\rangle + \langle S_i\rangle\right)\left(S_j - \langle S_j\rangle + \langle S_j\rangle\right) \quad \text{(still exact)}$$

$$= -J\sum_{\langle ij\rangle}\left[(S_i - \langle S_i\rangle)\langle S_j\rangle + (S_j - \langle S_j\rangle)\langle S_i\rangle + \langle S_i\rangle\langle S_j\rangle + \underbrace{\underbrace{(S_i - \langle S_i\rangle)}\underbrace{(S_j - \langle S_j\rangle)}}_{\text{small} \times \text{small}}\right] \quad \text{(still exact)}$$

$$\Rightarrow E_{int}(\{S_i\}) \approx -J\sum_{\langle ij\rangle}\left[(S_i - \langle S_i\rangle)\langle S_j\rangle + (S_j - \langle S_j\rangle)\langle S_i\rangle + \langle S_i\rangle\langle S_j\rangle\right]$$

numbers to be determined self-consistently

(approximate)

ignore! (then $S_i S_j$ interaction term is avoided)

- Spin-i (or Spin-j) is nothing special [or no local region in a lattice is special†]

Write $\langle S_i\rangle = \langle S_j\rangle = \langle S\rangle = m$ ← to be determined self-consistently

($\langle S\rangle$: any location)

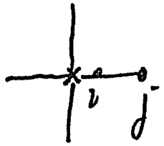
$$\therefore E_{int}(\{S_i\}) \approx -J\sum_{\langle ij\rangle}\left[(S_i - m)m + (S_j - m)m + m^2\right]$$

$$= -Jm\sum_{\langle ij\rangle} S_i - Jm\sum_{\langle ij\rangle} S_j + J\sum_{\langle ij\rangle} m^2$$

$$= -2Jm\sum_{\langle ij\rangle} S_i + J\sum_{\langle ij\rangle} m^2$$

† Technically, it is about translation invariant of the model.

$$\sum_{\langle ij \rangle} S_i = \frac{z}{2} S_i$$



z neighbors

$\Rightarrow z$ pairs involving i

$$\sum_{\langle ij \rangle} S_i \stackrel{?}{=} z \sum_{i=1}^{N} S_i$$

No! RHS will double count a pair (ij) and (ji)

$$\therefore \sum_{\langle ij \rangle} S_i = \frac{z}{2} \sum_{i=1}^{N} S_i$$

$$\therefore E_{int}(\{S_i\}) \cong -zJm \sum_{i=1}^{N} S_i + \frac{Jz}{2} \sum_{i=1}^{N} m^2 = -zJm \sum_{i=1}^{N} S_i + \frac{NJz}{2} m^2$$

to be determined (just a number)

e.g. 1D chain

×	×	×	×	×
1	2	$\boxed{3}$	4	

$(z=2)$

$-J \sum_{\langle ij \rangle} (S_i + S_j) m$ has the terms $-J(S_2+S_3)m - J(S_3+S_4)m$

$\Rightarrow -2JmS_3$ for site $i=3$

$\Rightarrow -zJmS_i$ for site i

- Adding back the term for the external applied field

$$E_{MFT}(\{S_i\}) \approx \underbrace{-zJm}_{\text{mean field acting on } S_i} \sum_{i=1}^{N} S_i + \frac{NJz}{2} m^2 - B \sum_{i=1}^{N} S_i$$

$\boxed{\text{this is the mean-field Hamiltonian}}$

$$= \underbrace{-(Jzm + B) \sum_{i=1}^{N} S_i}_{\text{like an independent spin problem}} + \underbrace{\frac{NJz}{2} m^2}_{\text{just a constant}} \qquad (12)$$

contains the unknown m

- <u>Partition Function</u>

$$Z_{MF} = e^{-\frac{\beta N J z m^2}{2}} \sum_{\text{all strings } \{S_i\}} e^{\beta (Jzm+B)\left(\sum_{i=1}^{N} S_i\right)} \quad \text{(formally)}$$

$$= e^{-\beta N \frac{Jzm^2}{2}} \left[\sum_{S_i=+1,-1} e^{\beta (Jzm+B) S_i} \right]^N \quad (\text{just like } Z = z^N \text{ for independent spins in paramagnetism})$$

$$= e^{-\beta N \frac{Jzm^2}{2}} \left[2 \cosh(\beta J z m + \beta B) \right]^N \quad \text{(copying paramagnetic result)}$$

$$= \left[2\, e^{-\beta \frac{Jzm^2}{2}} \cdot \cosh(\beta J z m + \beta B) \right]^N = z^N \qquad (13) \quad \text{(exact within mean field theory)}$$

- <u>Helmholtz Free Energy F</u>

$$F = -kT\ln Z = N\cdot(-kT\ln z) \equiv N\cdot f$$

Helmholtz free energy per spin (per magnetic moment)

$$\boxed{f = -kT\ln\left[2\cosh(\beta Jzm+\beta B)\right] + \frac{Jzm^2}{2}} \quad (14) \qquad \beta \equiv \frac{1}{kT}$$

(exact within MFT)

Key result!

m is the mean $\langle S\rangle$ to be determined

- From here, there are several ways to get at $m = \tanh(\beta Jzm + \beta B)$ [MF equation]
- <u>Formal Viewpoint</u>

$f(T,B)$ and $m = -\left(\frac{\partial f}{\partial B}\right)_T$ [recall paramagnetic case]

gives $m(T,B)$ and everything follows!

- <u>A wonderful twist</u>

Eq.(14) hints at viewing f as a function of m and T.

This view is the beginning of <u>Landau Theory of Continuous Phase Transitions</u>

Formal Viewpoint

$$m = -\left(\frac{\partial f}{\partial B}\right)_T \qquad \text{[See Eq. (14) for } f\text{, we expect } m \text{ to depend on } B]$$

$$= -Jzm\left(\frac{\partial m}{\partial B}\right)_T + kT\,\frac{2\sinh(\beta Jzm+\beta B)}{2\cosh(\beta Jzm+\beta B)}\cdot\left(\beta Jz\left(\frac{\partial m}{\partial B}\right)_T+\beta\right)$$

$$= Jz\left(\frac{\partial m}{\partial B}\right)_T\left[\tanh(\beta Jzm+\beta B)-m\right] + \tanh(\beta Jzm+\beta B)$$

$$\Rightarrow \underbrace{\Big[1+Jz\underbrace{\left(\frac{\partial m}{\partial B}\right)_T}_{\text{positive (proportional to }\chi)}\Big]}_{\text{can't be zero}}\underbrace{\left[\tanh(\beta Jzm+\beta B)-m\right]}_{=0} = 0$$

$$\Rightarrow \boxed{m = \tanh(\beta Jzm+\beta B)}$$

Mean-field equation

everything discussed in Sec. G follows!

<u>Gained Something</u>: Recall (see p. X-23) there could be 3 roots for m at $T < T_c$.

Which solution(s) is (are) physical?

Plug m into f (Eq. (14)), <u>physical one(s) would minimize f</u> [equilibrium condition]

Formal Viewpoint: Emphasizing self-consistency

single-spin partition function $\mathcal{Z} = e^{-\beta J z m^2/2}\left(\underbrace{e^{\beta(Jzm+B)}}_{S=+1} + \underbrace{e^{-\beta(Jzm+B)}}_{S=-1}\right)$

Applying physical meaning of the terms in $\mathcal{Z}$:

$$\underbrace{m}_{\text{quantity wanted to get}} = \underbrace{\langle S\rangle}_{\substack{\text{mean value of } S \\ \text{(same for all spins } i)}} = \left[\underbrace{\frac{e^{-\beta J z m^2/2}\, e^{\beta(Jzm+B)}}{\mathcal{Z}}}_{\text{prob. of having } S=+1} - \underbrace{\frac{e^{-\beta J z m^2/2}\, e^{-\beta(Jzm+B)}}{\mathcal{Z}}}_{\text{prob. of having } S=-1}\right]$$

RHS also depends on quantity wanted to get

$$\Rightarrow \boxed{m \underset{\text{self-consistency}}{=} \tanh(\beta J z m + \beta B)}$$

Mean field equation again!

Eq. (14) with a twist

$$f = \frac{Jzm^2}{2} - kT \ln\left[2\cosh(\beta Jzm + \beta B)\right] \quad (14)$$

Think

We saw that when MF equation allows multiple roots, the order parameter m should be the one(s) that minimizes (minimize) f

How about setting $\left(\frac{\partial f}{\partial m}\right)_{T,B} = 0$? [Here, f is seen to be $f(m, T, B)$]

$$\frac{\partial f}{\partial m} = Jzm - kT\,\frac{2\sinh(\beta Jzm + \beta B)}{2\cosh(\beta Jzm + \beta B)} \cdot \frac{Jz}{kT} = Jz\left(m - \tanh(\beta Jzm + \beta B)\right)$$

$$\therefore \frac{\partial f}{\partial m} = 0 \Rightarrow \boxed{m = \tanh(\beta Jzm + \beta B)}$$ mean field equation again!

extremum of f only

[Again, at equilibrium, m should minimize f]

Hinted at: Look at the function $f(m, T)$ and inspect its minimum is meaningful!

order parameter

Remarks

- [†]Could obtain mean energy $\langle E \rangle_{\text{per spin}}$ from $-\frac{\partial \ln Z}{\partial \beta}$
- Hence, could [†]obtain heat capacity and study behavior as $T \to T_c^{\pm}$
- We studied the susceptibility[†] χ for $\underbrace{T \to T_c^{+}}_{\text{from above}}$. Could also study χ for $\underbrace{T \to T_c^{-}}_{\text{from below}}$.
- 2D Ising model can be solved exactly.
  See K. Huang, "Statistical Mechanics". (there is a chapter on Ising model)

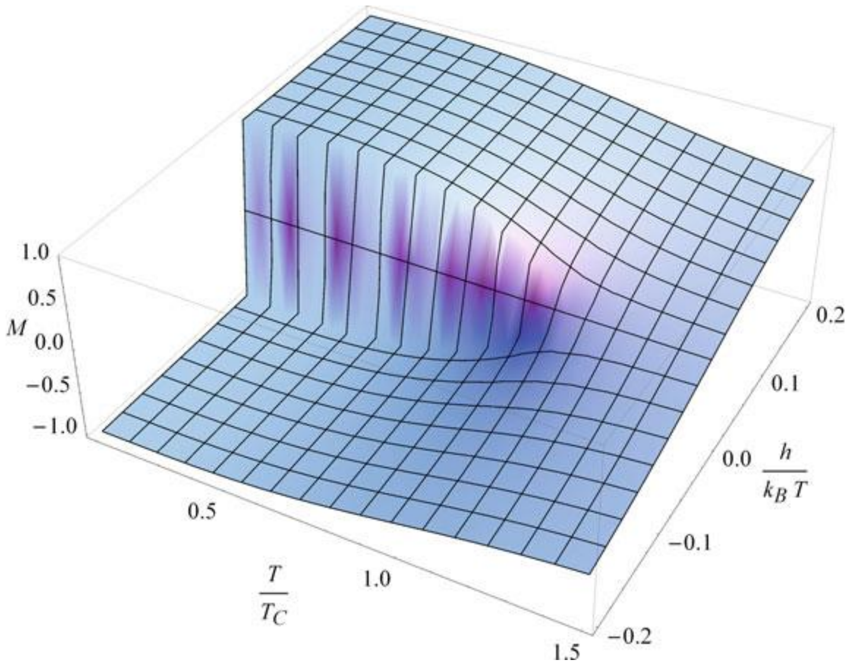
[†] We will not work them out here. Interested students could work them out starting from Z or f (Eqs. (13), (14))

Summary

- The mean field equation $m = \tanh\left(\frac{Jzm}{kT} + \frac{B}{kT}\right)$ can be obtained in many ways, e.g. physical argument and statistical mechanics formula.
- MFT gives critical phenomena
- However, critical exponents β, δ, γ predicted by MFT are often not accurate.

	2D	3D	4D	MFT
β	1/8	0.326	1/2	1/2
δ	15	4.790	3	3
γ	7/4	1.237	1	1

- MF results are off in 2D, 3D
- MF results agree with 4D results!
- Higher dimensions, what are ignored in MF turned out to be something that can be ignored!
- 4D is the "upper critical dimension" of Ising Model



A clearer T-B-M diagram of the Ising Model. The x-axis is temperature, the y-axis is the applied magnetic field, the z-axis is magnetization. This goes with the picture on the first page of Chapter 10 Part 3.