MATH327: StatMech and Thermo

Thursday, 30 April 2026

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Something to consider

We have seen different high- vs. low-temperature behaviour
even for non-interacting spin systems

What distinguishes this
from a true *phase transition* between distinct phases?

Recap

Phase transitions motivate interacting stat. systems

Ising model on d-dim'l simple cubic lattices with PBC

$$E_i = -\sum_{(jk)} s_j s_k - H \sum_n s_n$$

Plan

High-T and low-T phases

Phase transition and order parameter

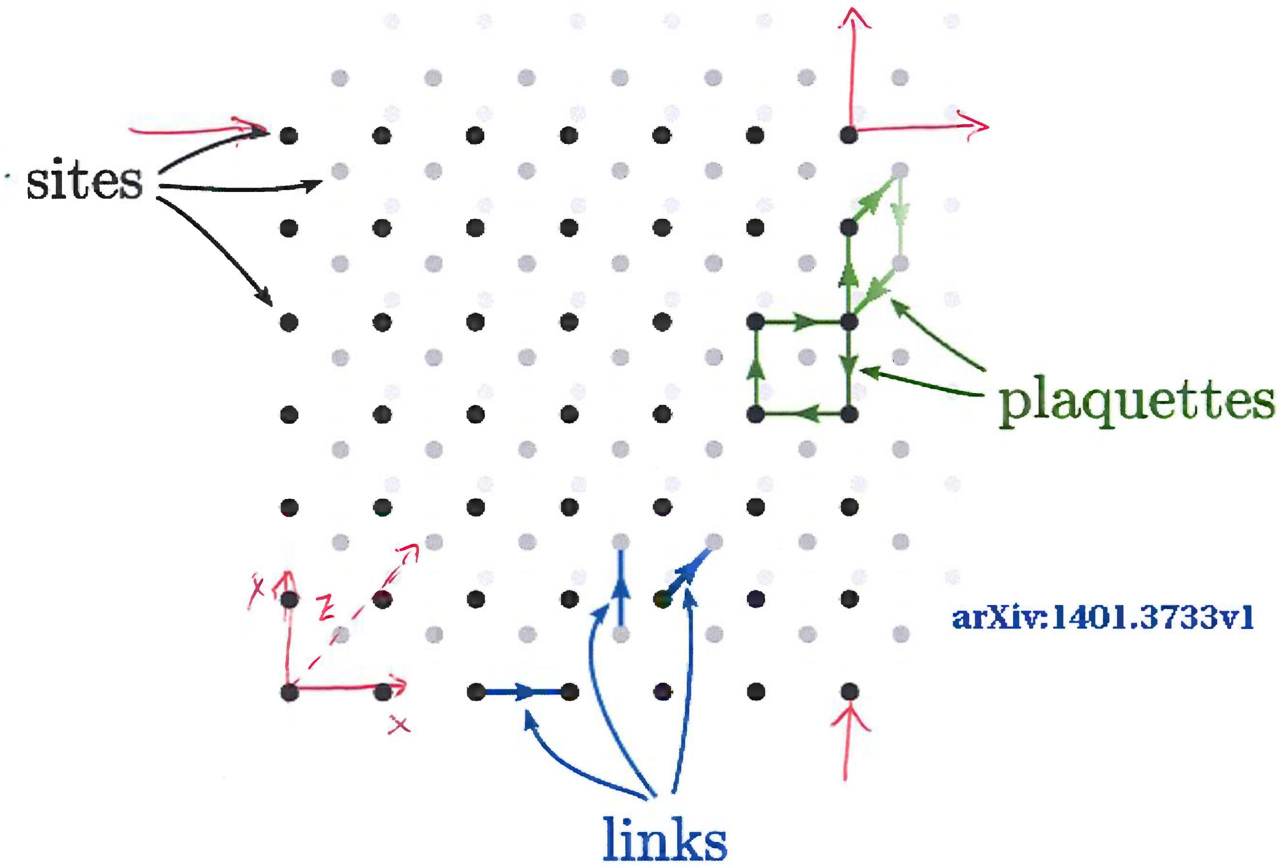
Mean-field approx.

Lattice terminology:

"Sites" where spins are located

"Links" correspond to n.n. pair

$\therefore$ coordination number $c = 2d$ is links per site


sites
plaquettes
links
arXiv:1401.3733v1

With PBC $\boxed{\begin{array}{l}\text{all sites have } c = 2d \text{ links} \\ \text{all links shared by two sites} \\ \rightarrow \text{total number } \ell = \frac{2d}{2} N = d \cdot N\end{array}}$

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Can we solve the Ising model?

$$Z(\beta, N, H) = \underbrace{\sum_{\{s_n\}}}_{2^N \text{ terms}} \exp\Big[\beta \underbrace{\sum_{(jk)} s_j s_k}_{d \cdot N \text{ terms}} + \beta H \underbrace{\sum_n s_n}_{N \text{ terms}}\Big]$$

$d=1$: Exact solution by Ernst Ising (1924 PhD)

$d=2$: $H=0$ exact solution by Lars Onsager (1944)

$3 \leq d < \infty$: No known exact solution

"Brute-force" numerical evaluation

Tiny $10 \times 10 \rightarrow N = 100 \rightarrow 2^{100} \times 300 \sim 10^{32}$ terms

Billion terms per second $\rightarrow 10^{27}$ seconds $\sim 10^{15}$ years
10^9

$\sim 500{,}000 \times$ age of universe ✗

Strategy for interacting systems:
1) High-T and low-T limit
2) Simple approximation
3) Smarter computing

Set $H=0$ for simplicity

$$E_i = -\sum_{(jk)} s_j s_k \qquad Z(\beta, N) = \sum_{\{s_n\}} \exp\Big[\beta \sum_{(jk)} s_j s_k\Big]$$

High-T $\beta \to 0$ limit: $\boxed{Z \to \sum_{\{s_n\}} \exp(0) = 2^N}$ page 132

E_i irrelevant compared to T

Equal $p_i = \frac{1}{2^N}$ for all $w_i = \{s_n\}$

Characterize system by <u>magnetization</u> $m = \dfrac{n_+ - n_-}{n_+ + n_-}$

$-1 \leq m \leq 1$

$H=0$ symmetry under flipping all spins $\pm 1 \to \mp 1$

$\to$ consider $0 \leq |m| \leq 1$

$$\lim_{T\to\infty} \langle |m| \rangle = \lim_{T\to\infty} \sum_i |m|_i \, p_i = \frac{1}{2^N} \sum_i |m|_i$$

Just need to count micro-states

$$\binom{N}{n_+} = \binom{N}{n_-} = \frac{N!}{n_+! \, n_-!} = \frac{(n_+ + n_-)!}{n_+! \, n_-!}$$

$N \gg 1 \to$ sharp peak at $n_+ = n_- = \frac{1}{2}N \to |m| \doteq 0$

In thermodynamic limit $N \to \infty$, $\langle |m| \rangle = 0$

"disordered phase"

In low-T $\beta \to \infty$ limit higher-energy w_i suppressed $\sim e^{-\beta E_i}$

but larger degeneracy — what wins?

$H=0 \to 2$ degenerate ground states

$(n_+, n_-) = (N, 0)$ and $(0, N) \to |m| = 1$

$$\boxed{E_0 = -J \cdot N = -\sum_{(jk)} (\pm 1)^2}$$

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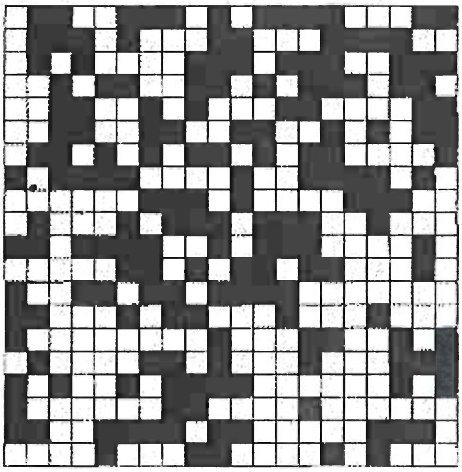
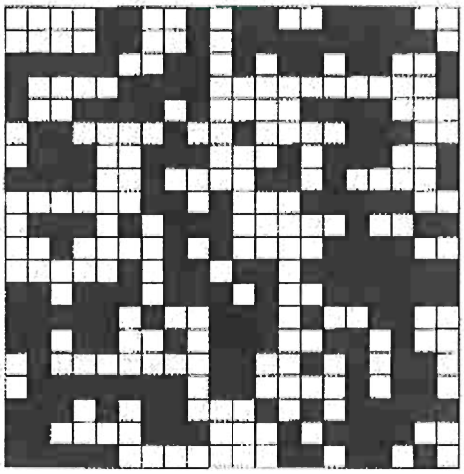
$20 \times 20 \rightarrow 2^{400} \sim 10^{120}$

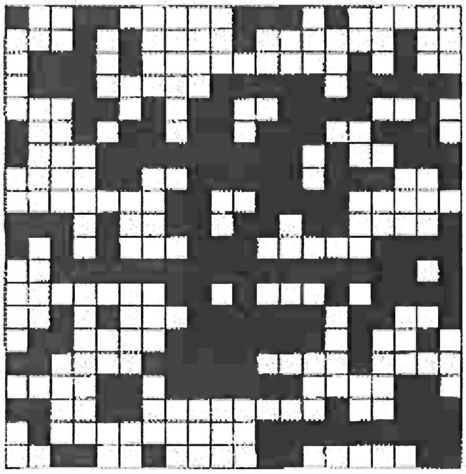
$m \approx 0$



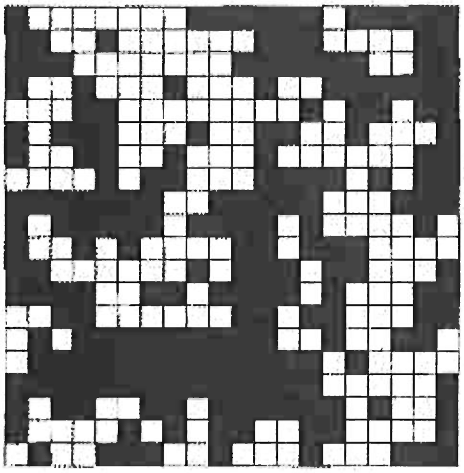
Random initial state



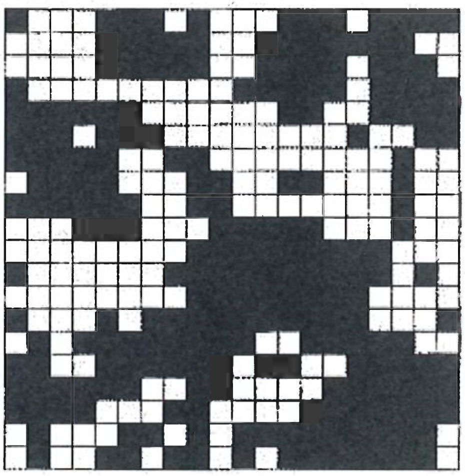
T = 10



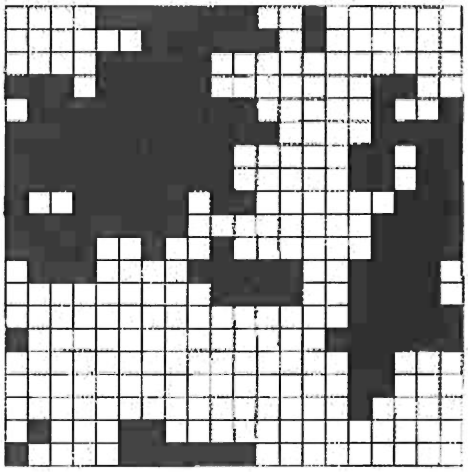
T = 5



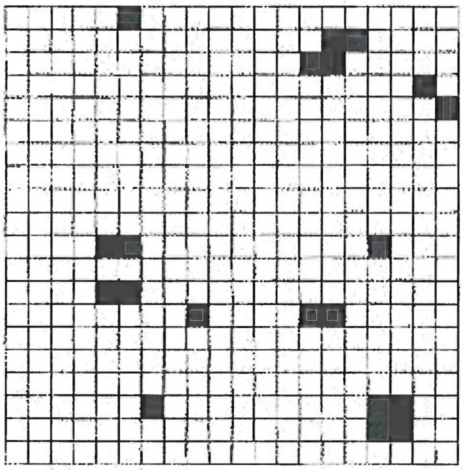
T = 4



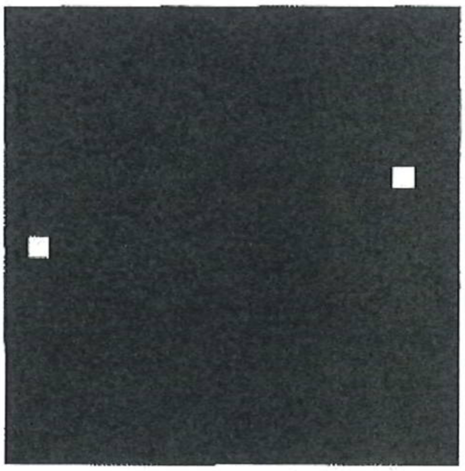
T = 3



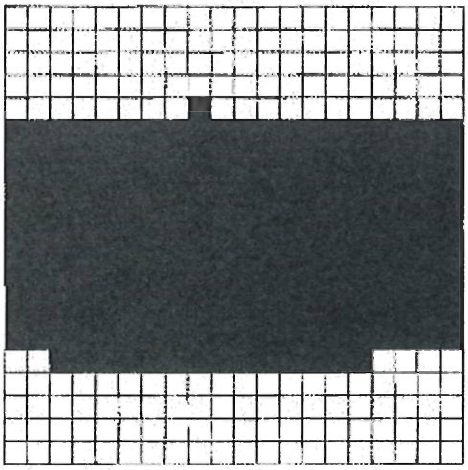
T = 2.5



T = 2 $m \approx 1$



T = 1.5 $m \approx -1$



T = 1

For $d>1$ next-lowest energy from flipping single spin

$(n_+, n_-) = (N-1, 1)$ and $(1, N-1)$ $\rightarrow$ $2N$ degeneracy

$$|m| = \frac{N-2}{N} = 1 - \frac{2}{N}$$

$$\boxed{E_1 = 2d - (d \cdot N - 2d) = -(d \cdot N - 4d)}$$ page 133

So $$\frac{P(E_0)}{P(E_1)} = \frac{\cancel{Z}}{\cancel{Z}} \, \frac{2\exp(\beta d \cdot N)}{2N \exp\left(\beta(d \cdot N - 4d)\right)} = \frac{e^{4\beta d}}{N}$$

$\therefore$ ground state(s) dominate as $T \to 0$ $\beta \to \infty$

Exponentially approach $\langle |m| \rangle \to 1$ "ordered phase"

Magnetization is Ising model <u>order parameter</u> (OP)

Distinguish $\langle |m| \rangle \to 0$ $(N \to \infty)$ high-T disordered phase

$\langle |m| \rangle \to 1$ low-T ordered phase

In general phases distinguished by OP being zero vs. non-zero in $N \to \infty$ limit

<u>Phase transition</u> means $N \to \infty$ discontinuity in OP or derivative(s)

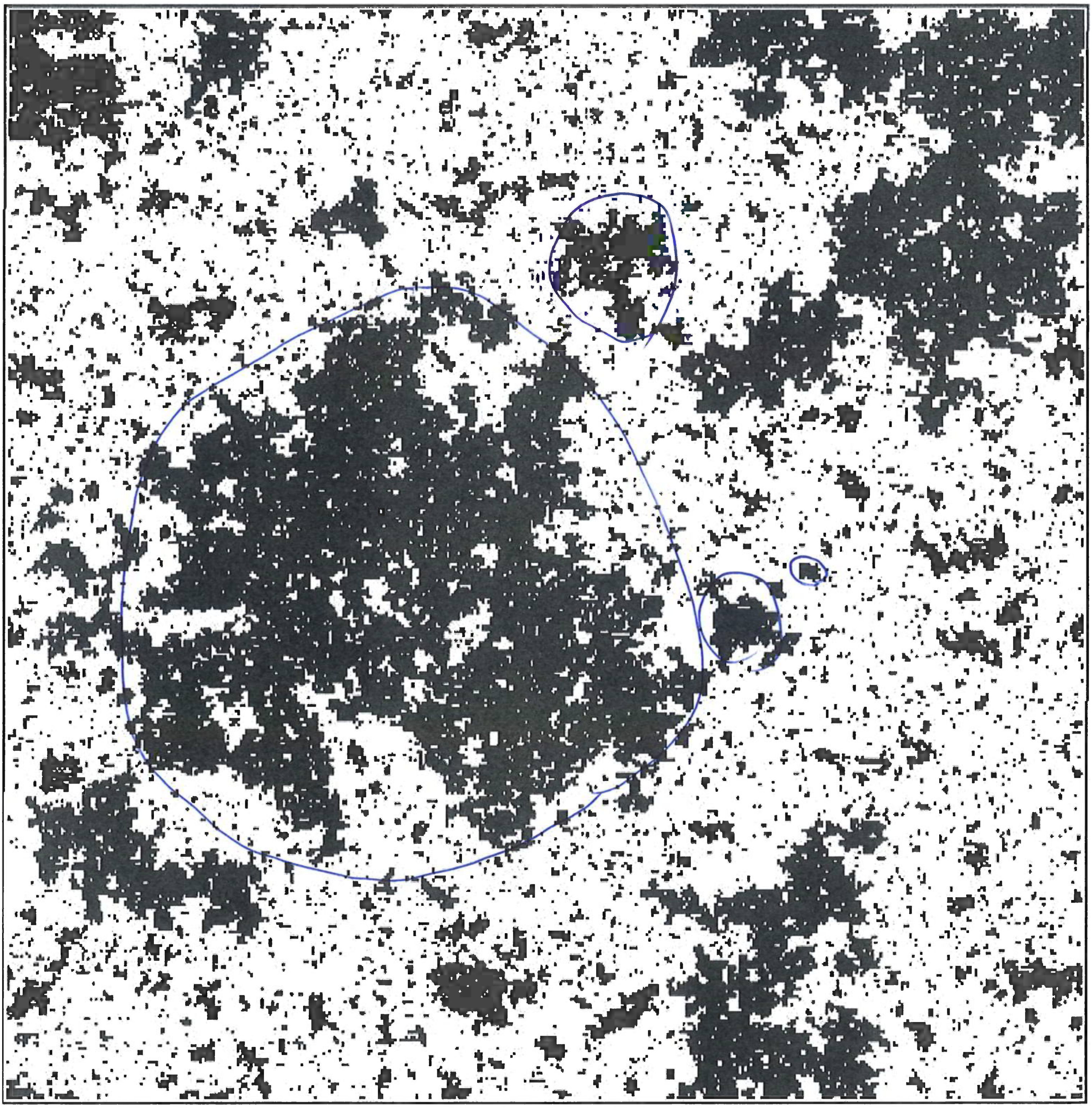
Otherwise <u>crossover</u> instead of true transition

Transition occurs at "critical point" of control params.

Critical temperature T_c for $H=0$ Ising model

$2d$ $$T_c = \frac{2}{\log(1+\sqrt{2})} \approx 2.27$$

$T=2.27$ 400×400 $2^{160,000} \sim 10^{48,164}$

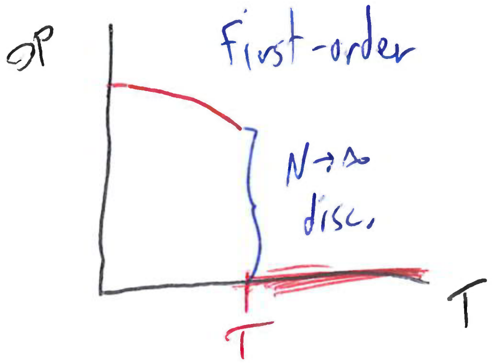


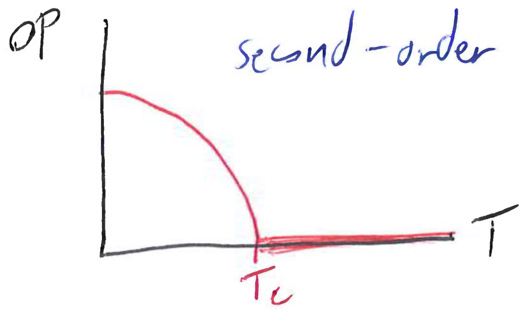
Formally OP must be related to derivative of free energy

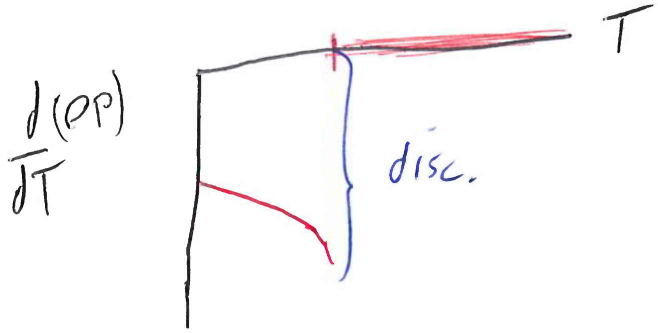
$N\to\infty$ discontinuity in OP → "first-order" transition

continuous OP with discontinuity in derivative(s)

→ "second-order" transition







Need to relate $\langle m\rangle$ to a derivative of $F=-T\log Z$

Restore magnetic field

$$E_i = -\sum_{(jk)} s_j s_k - H\sum_n s_n = -\sum_{(jk)} s_j s_k - HNm$$

$$m = \frac{n_+-n_-}{N} = \frac{1}{N}\sum_n s_n$$

$$Z = \sum_{\{s_n\}} \exp\left[\beta\sum_{(jk)} s_j s_k + \beta HNm\right]$$

$$\boxed{\frac{\partial F}{\partial H} = -T\frac{1}{Z}\frac{\partial Z}{\partial H} = -\cancel{T}\frac{1}{Z}\sum_{\{s_n\}} \cancel{\beta} N m e^{-\beta E} = -N\langle m\rangle}$$

So $\langle m\rangle = -\frac{1}{N}\frac{\partial F}{\partial H} = \frac{1}{N\beta}\frac{\partial}{\partial H}\log Z$ is good OP ✓

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Next step is simple approximation based on

$$\langle m \rangle = \frac{1}{N} \sum_n \langle s_n \rangle$$

mean value of spin averaged over both N and 2^N $w_i = \{s_n\}$

Expand $s_j s_k = \left[(s_j - \langle m \rangle) + \langle m \rangle \right] \times \left[(s_k - \langle m \rangle) + \langle m \rangle \right]$

$$= \underbrace{(s_j - \langle m \rangle)(s_k - \langle m \rangle)}_{\text{negligible}} + (s_j + s_k)\langle m \rangle - \langle m \rangle^2$$

Suppose on average only small fluctuations around mean spin

$$\to E_{MF} = -\sum_{\langle jk \rangle} \left[(s_j + s_k)\langle m \rangle - \langle m \rangle^2 \right] - H \sum_n s_n$$

each spin appears $2d$ times

$$= d \cdot N \langle m \rangle^2 - \underbrace{(2d \langle m \rangle + H)}_{H_{eff}} \sum_n s_n$$

mean-field approx.

Effective magnetic field averaging over $2d$ n.n. of s_n

Upon flipping $s_j \to -s_j$ $\quad E_{MF} = d \cdot \cancel{N} \langle m \rangle^2 - H_{eff}\left(s_j + \cancel{\sum_{k \neq j}} s_k\right)$

$$\to d \cdot \cancel{N} \langle m \rangle^2 - H_{eff}\left(-s_j + \cancel{\sum_{k \neq j}} s_k\right)$$

page 137 $\Delta E_j = 2 H_{eff} s_j$ $\therefore$ non-interacting!

Remnant of interactions in H_{eff}

Canonical part. func.

$$Z_{MF} = \sum_{\{s_n\}} \exp\left[-\beta d \cdot N \langle m\rangle^2 + \beta H_{eff} \sum_n s_n\right]$$

$$= \exp(-\beta d \cdot N\langle m\rangle^2) \left(\sum_{s_1=\pm 1} e^{\beta H_{eff} s_1}\right) \cdots \left(\sum_{s_N=\pm 1} e^{\beta H_{eff} s_N}\right)$$

$$= C\left(2\cosh(\beta H_{eff})\right)^N$$

$$= C\left(2\cosh\left[\beta\left(2d\langle m\rangle + H\right)\right]\right)^N$$

$\propto \frac{\partial}{\partial H} \log Z$

Demand $\langle m\rangle = \frac{1}{N\beta} \frac{\partial}{\partial H} \log Z_{MF}$

$$= \frac{\cancel{N\beta}}{\cancel{N\beta}} \frac{\sinh(\beta(2d\langle m\rangle + H))}{\cosh(\beta(2d\langle m\rangle + H))} = \tanh(\beta(2d\langle m\rangle + H))$$

Self-consistency consistent for mean-field approx.

Plot $\langle m\rangle$ and $\tanh(\beta(2d\langle m\rangle + H))$ vs. $\langle m\rangle$ find intersections

$T=4 \quad d=2 \quad H=0 \rightarrow \langle m\rangle = 0 \rightarrow$ disordered phase

Turn on $H \neq 0 \rightarrow$ shifts tanh

$\langle m\rangle = \pm m_0 \neq 0 \rightarrow$ ordered phase, aligned with mag. field

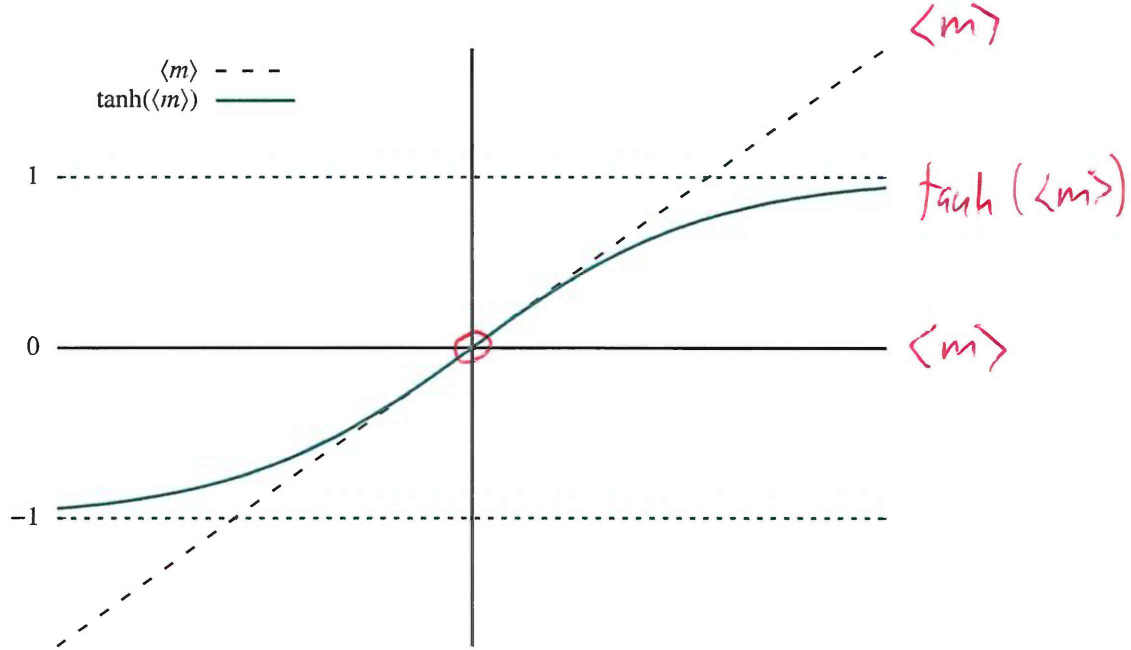
$m_0 \approx 0.88$ for $H = \pm 2$

Reduce temperature $\rightarrow$ larger β in tanh

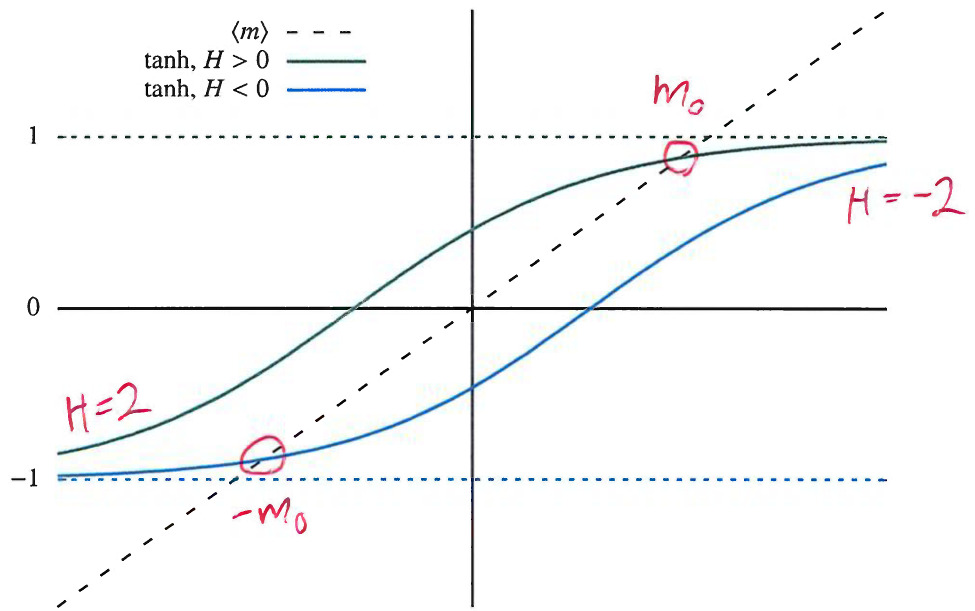
$\rightarrow$ faster change vs. $\langle m\rangle$

$\rightarrow m_0 \approx 1$ (max. magnitude)

$d=2 \quad H=0 \quad T=4 \rightarrow \beta = \frac{1}{4} \quad 2d\beta = 1$



$J=2, \quad T=4$



$d=2 \quad T=2 \quad \beta=\frac{1}{2}$