# MATH327: StatMech and Thermo

Wednesday, 30 April 2025

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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

Phases → interacting stat. systems

Ising model on d-dim'l cubic lattice

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

Plan

Finish formulating Ising model

High-T & low-T phases

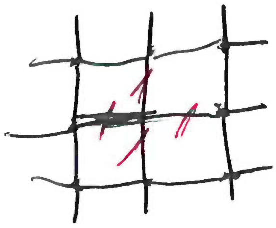
Phase transition & order param.

Mean-field approx.

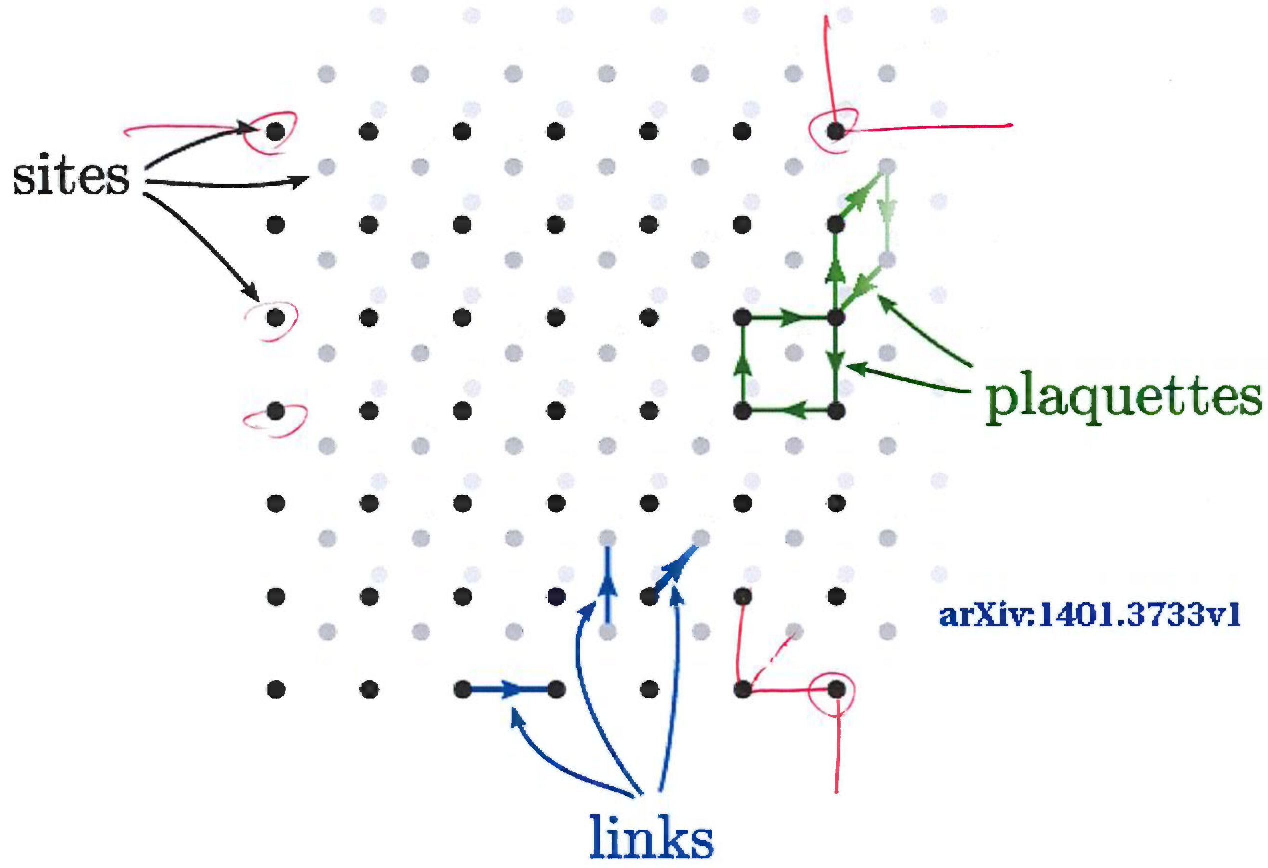
How many links given N spins?

Links per site is "coordination number"

1d:  $c = 2$

2d square  $c = 4$

→ $c = 2d$ in $d$ dimensions




arXiv:1401.3733v1

Avoid edges w/ periodic boundary conditions (PBC)

$\rightarrow$ d-dim'l torus

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

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Can we solve the Ising model?

$d=1$: Exact solution by 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 impractical

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

Billion terms per second $\rightarrow 10^{23}$ seconds $\sim 10^{15}$ years

$10^9$ $\sim 500{,}000 \times$ age of universe X

Strategy for interacting systems

1) High-T and low-T limits
2) Simple approximation
3) Smarter computing

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Set $H=0$ for simplicity

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

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

$E_i$ irrelevant compared to T

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

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

$-1 \leq m \leq 1$

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

$0 \leq |m| \leq 1$

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

Just need to count micro-states

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

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

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

"disordered phase"

Low-T $\beta \to \infty$ limit dominated by ground state(s)

Excited states suppressed $\sim e^{-\beta E_j}$

$H=0 \to 2$ degenerate ground states

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

$$\boxed{E_0 = -\sum_{(jk)} s_j s_k = -\sum_{(jk)} (\pm 1)^2 = -d \cdot N}$$ page 133

Assume $d > 1$, first excited energy level flips single spin

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

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

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

Excited $w_i$ have lower $p_i = \frac{1}{Z} e^{-\beta E_i}$ vs. higher degeneracy

$$\frac{P(E_0)}{P(E_1)} = \frac{\cancel{Z}}{\cancel{Z}} \frac{2 \exp(\beta \cancel{d \cdot N})}{2N \exp(\beta(\cancel{d \cdot N} - 4d))} = \frac{\exp(4\beta d)}{N}$$

Ground states win 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 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

$H=0$ Ising model $\to$ critical temperature $T_c$

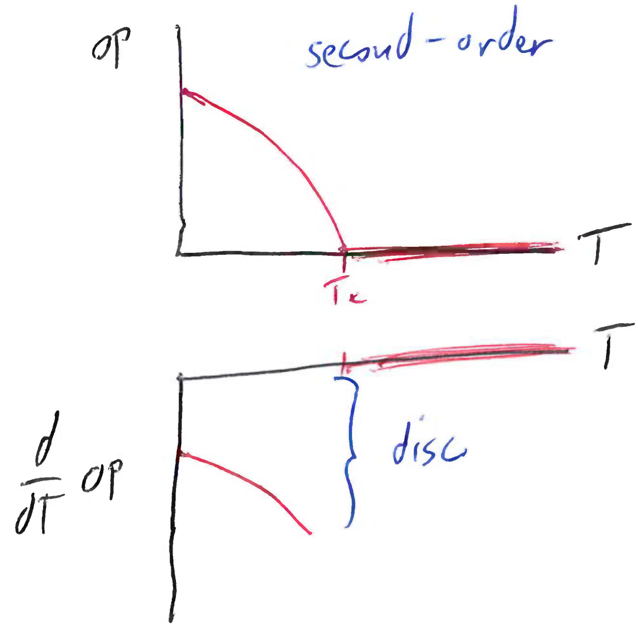
2d: $T_c = \dfrac{2}{\log(1+\sqrt{2})} \simeq 2.27$

Formally OP must be related to derivative of free energy

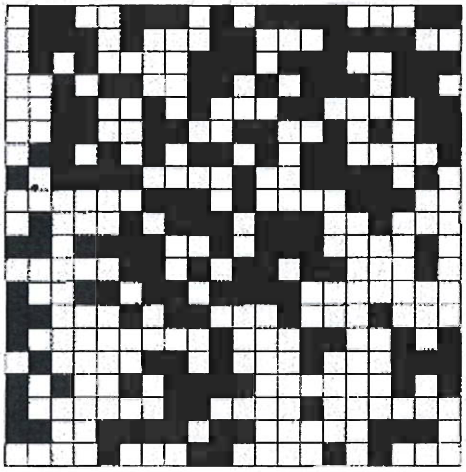
$N \to \infty$ discontinuity in OP $\to$ "~~free~~ first-order" transition

continuous OP w/ discontinuity in derivative(s)

$\to$ "second ~~...~~ order trans."

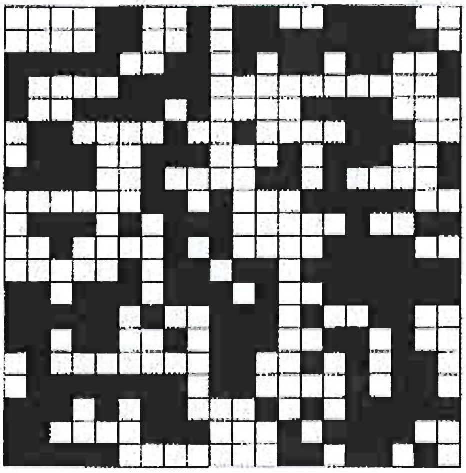



$20 \times 20 \qquad 2^{400} \sim 10^{120}$

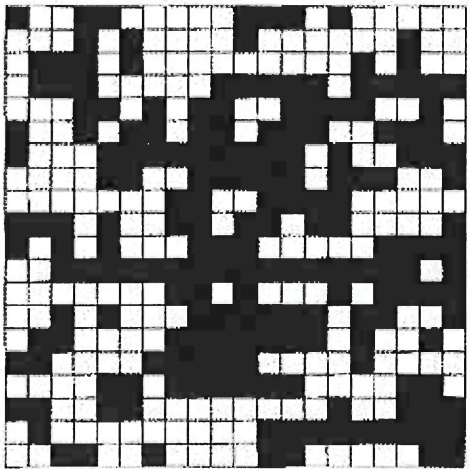


Random initial state

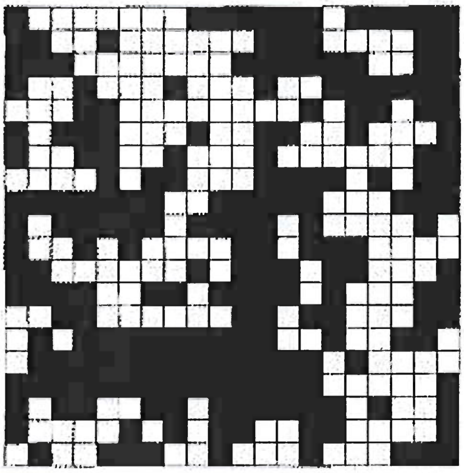
$m \approx 0$



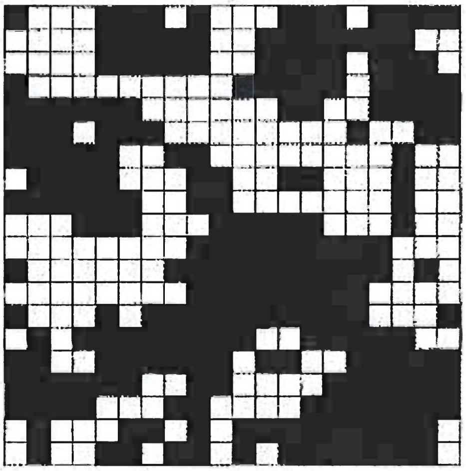
T = 10



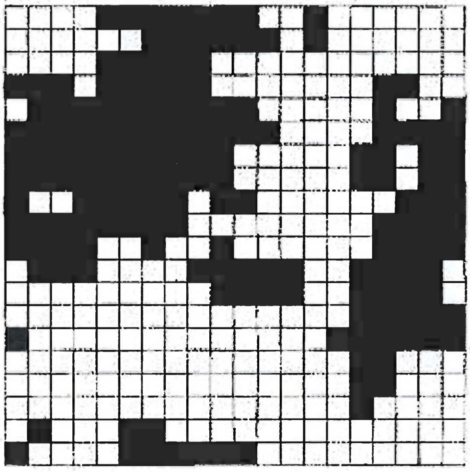
T = 5



T = 4

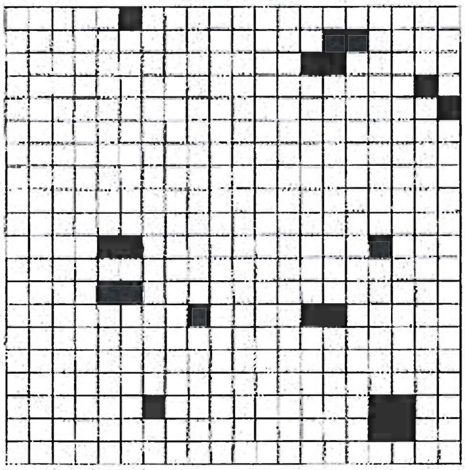


T = 3



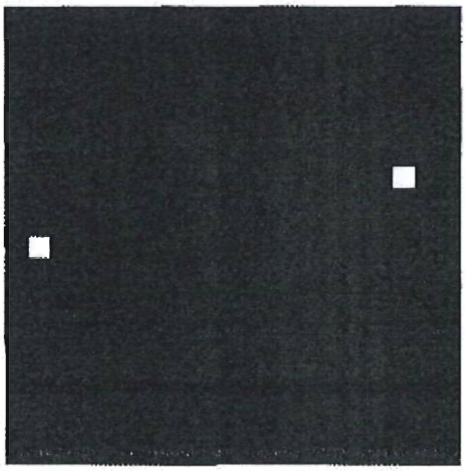
T = 2.5

$m \approx 1$

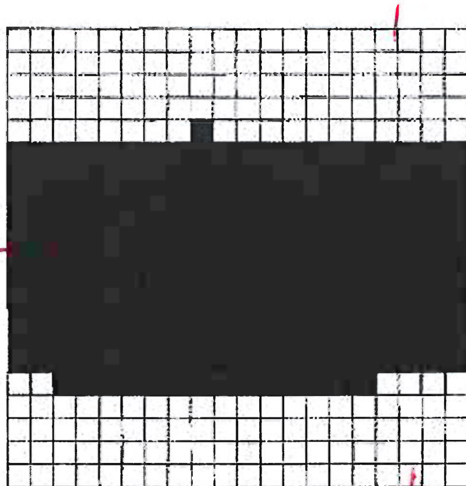


T = 2

$m \approx -1$

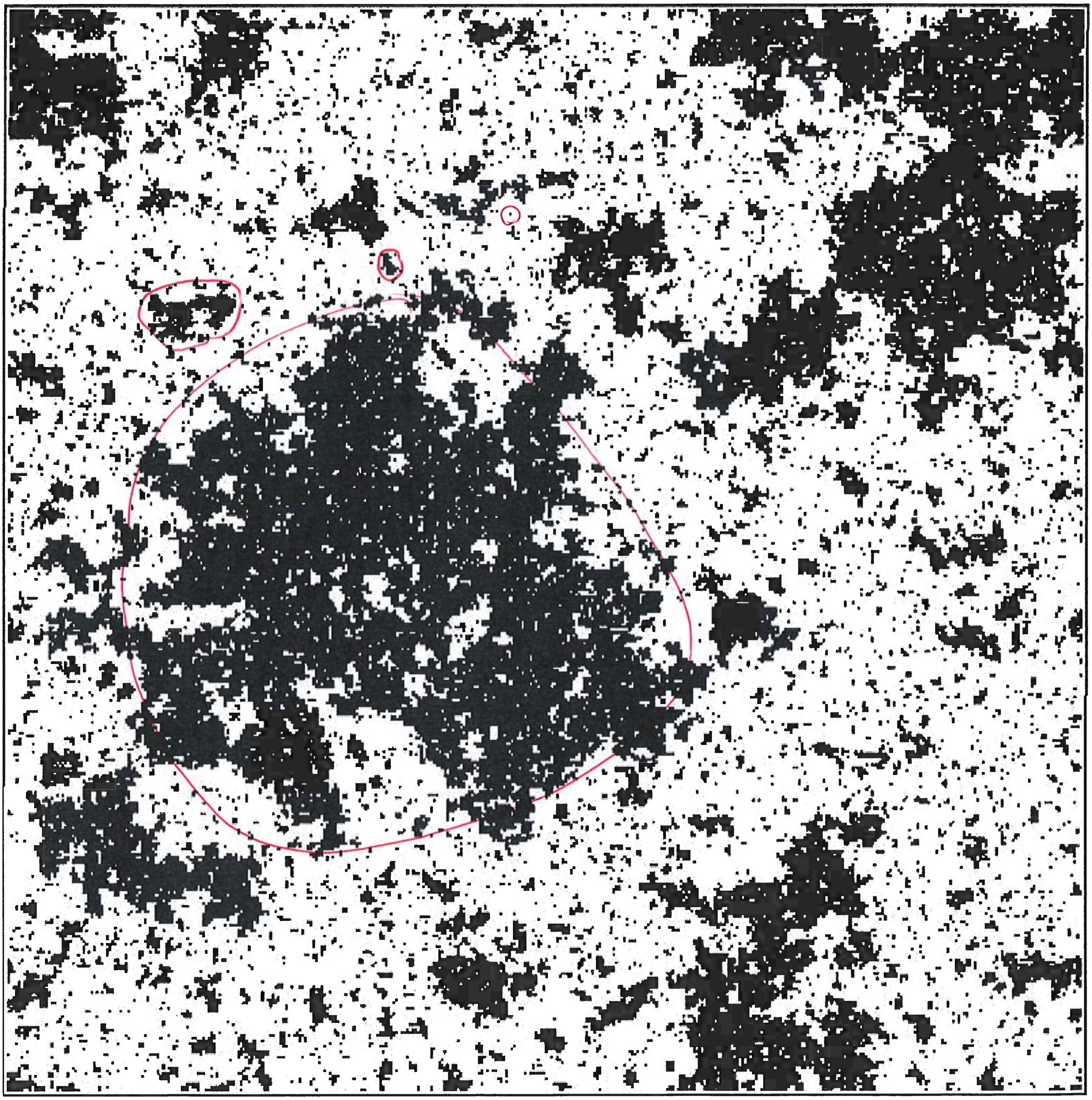


T = 1.5



T = 1

400×400 $\quad 2^{160,000} \sim 10^{48,164}$



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

Restore magnetic field

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

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

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

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

$$\boxed{\text{So } \langle m \rangle = \frac{-1}{N} \frac{\partial F}{\partial H} = \frac{1}{N\beta} \frac{\partial}{\partial H} \log Z \quad \text{is good op} \checkmark}$$

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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 all $N$ spins & $\{s_n\}$

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

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

Suppose on average only small fluctuations around mean spin

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

each spin appears $2d$ times

$$= d \cdot N \langle m \rangle^2 - \underbrace{(2d\langle m \rangle + H)}_{H_{eff}} \sum_n s_n \quad \text{is } \underline{\text{mean-field approx.}}$$

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

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

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

$$\Delta E_{MF,j} = 2 H_{eff} s_j$$

$\to$ non-interacting!

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Remnant of interaction in $H_{eff}$

Canonical part. func.

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

$$= \exp\left(-\beta d \cdot N\langle m\rangle^2\right)\left(\sum_{S_1=\pm 1} e^{\beta H_{eff} S_1}\right) \cdots \left(\sum_{S_N=\pm 1} e^{\beta H_{eff} S_N}\right)$$

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

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

$\langle m\rangle \propto \frac{\partial}{\partial H} \log Z$

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

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

<u>self-consistency condition</u> for mean-field approx.

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

Find intersection(s)

$\langle m\rangle = 0 \to$ disordered phase

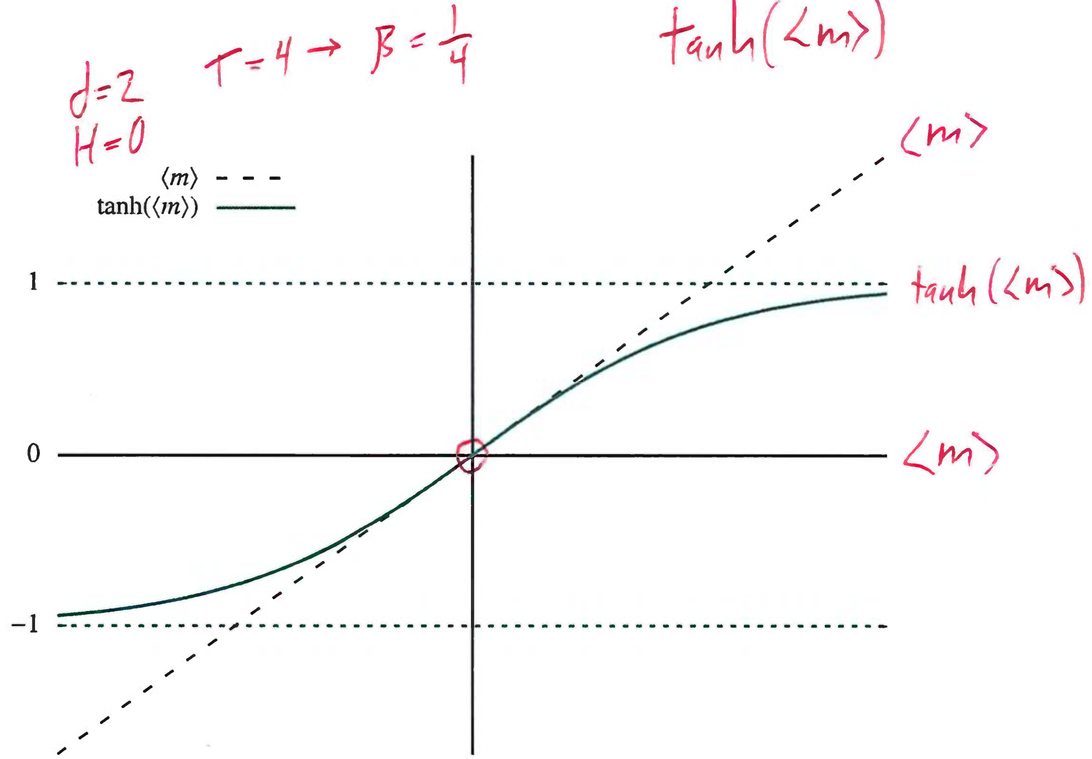
Turn on $H \neq 0 \to$ shifts tanh

Intersections at $\langle m\rangle = \pm m_0 \neq 0 \to$ ordered phase aligned w/ mag. field

$m_0 \approx 0{,}88$ for $H = \pm 2$

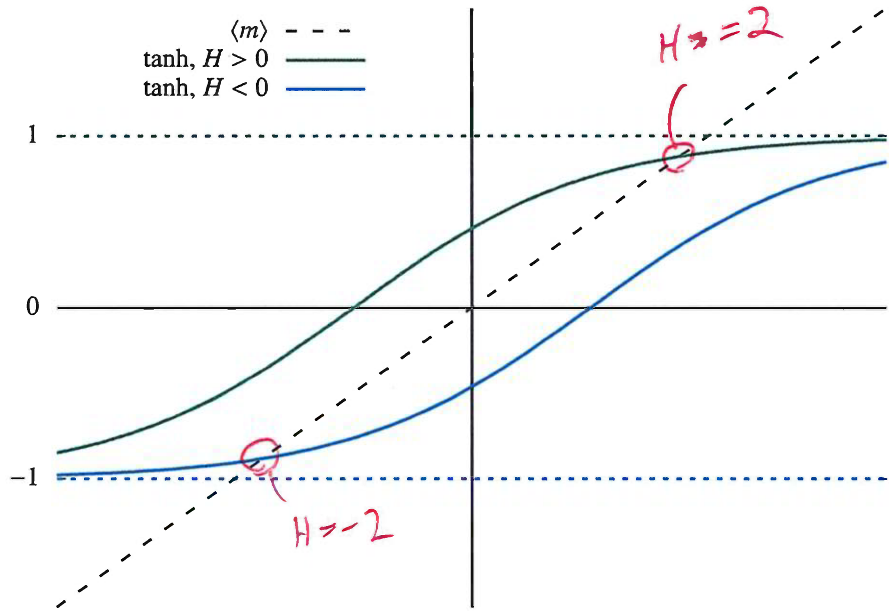
Reduce temperature $\to$ faster change vs. $\langle m\rangle$

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



$d=2$
$H=0$
$T=4 \to \beta=\frac{1}{4}$
$\tanh(\langle m\rangle)$
$\langle m\rangle$
$\tanh(\langle m\rangle)$
1
0
−1
$\langle m\rangle$

$J=2 \quad T=4$



$d=2 \quad T=2$