MATH327: Statistical Physics

Friday, 3 May 2024

80 54 35

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

Done w/ quantum gases for now

Now meeting interacting systems (canonical) motivated by phase transitions

What precisely distinguish interacting or not?

Recall non-interacting spin system (fixed, dist'able)

Micro-states ω_i defined by $\{s_n\}$, $s_n = \pm 1$

have energy $E_i = -H \sum_{n=1}^{N} s_n = \sum_n \varepsilon_n$

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

all pairs of nearest-neighbour (n.n.) spins

Non-interacting → factorization → very simple

$$Z_N = Z_1^N = (2\cosh(\beta H))^N$$

Definition

Consider change ΔE_j from alteration to jth particle

Non-interacting iff. ΔE_j independent of all particles $k \neq j$

Example: Flip ~~a~~ spin $s_j \to -s_j$

$$E = -H\left(s_j + \sum_{k\neq j} s_k\right) \to -H\left(-s_j + \sum_{k\neq j} s_k\right)$$

$\Delta E_j = 2Hs_j$ independent of s_k for $k \neq j$

→ non-interacting ✓

page 132

Example: Same spin flip w/ $s_j s_k$ term

$$E = -s_j \sum_{k\in(jk)} s_k - \sum_{(mk)\not\ni j} s_m s_k - H\left(s_j + \sum_{k\neq j} s_k\right)$$

$$\to +s_j \sum_{k\in(jk)} s_k - \sum_{(mk)\not\ni j} s_m s_k - H\left(-s_j + \sum_{k\neq j} s_k\right)$$

$$\Delta E_j = 2s_j\left(H + \sum_{k\in(jk)} s_k\right)$$

page 132 Depends on s_k with ~~...~~ $k \neq j$ → interacting ✓

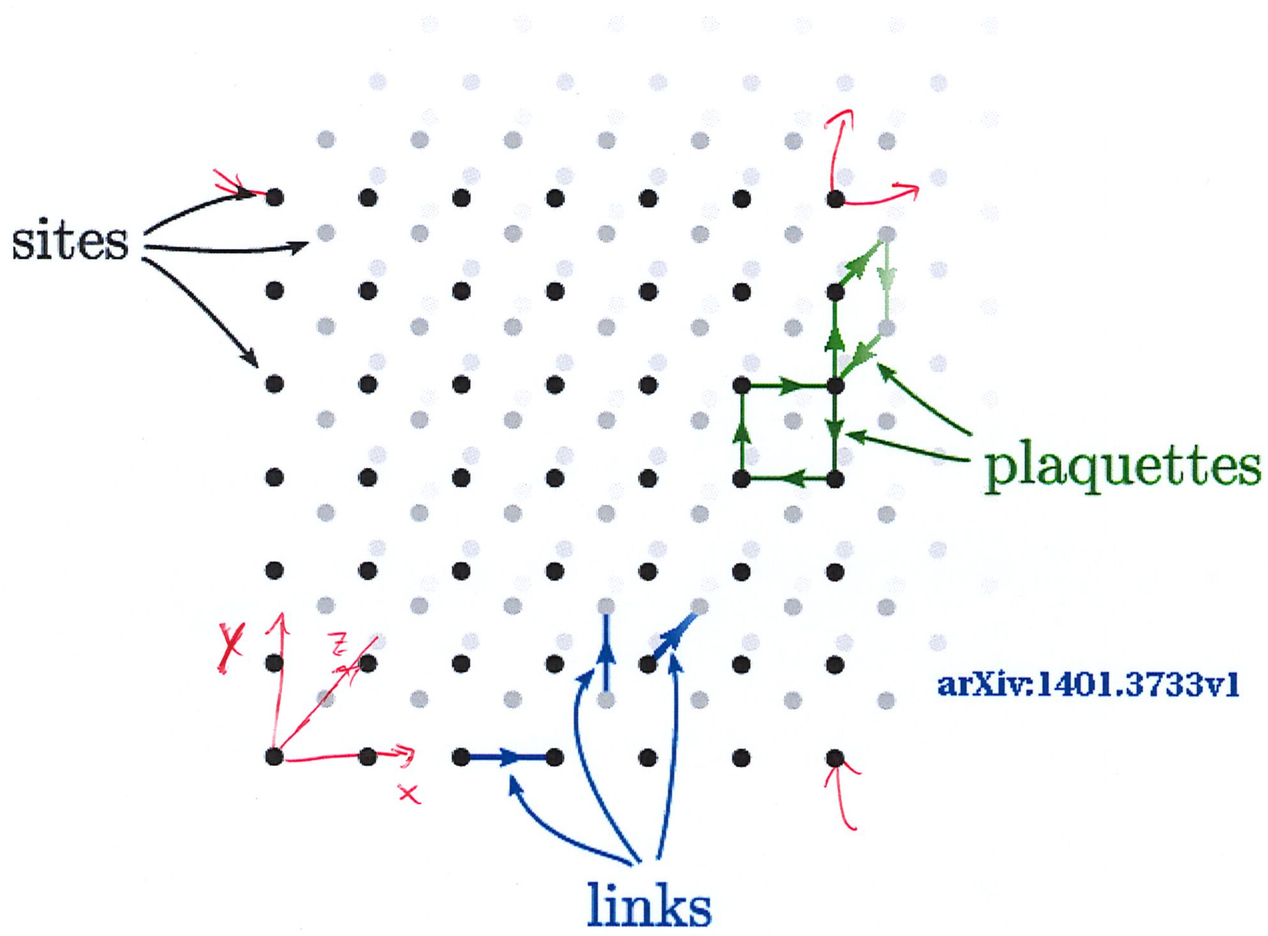
n.n. pairs depend on lattice structure

$E(s_n) \supset \sum_{(jk)} s_j s_k$ & lattice → Ising model

d-dim'l cubic lattice

"Sites" where spins are located

"Links" correspond to n.n. pairs



arXiv:1401.3733v1

Number of links per site is coordination #

$C = 2d$ for d-dim'l cubic lattice w/periodic boundary conditions

Each link shared by two sites

$\rightarrow$ total number $\#\ell = \frac{2d \cdot N}{2} = d \cdot N$ page 134

Can we solve the Ising model canonical part. func.?

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

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

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

$3 \le d < \infty$: 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

Plan for interacting systems:

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

Set $H=0$ for simplicity

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

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

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>

$$m = \frac{n_+ - n_-}{n_+ + n_-} = \frac{n_+ - n_-}{N}$$

$$-1 \leq m \leq 1$$

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

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

To find $\lim_{T\to\infty} \langle |m| \rangle = \lim_{T\to\infty} \sum_i |m|_i p_i$

just need to count equally probable 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

excited states exponentially suppressed

$p_i \sim e^{-\beta E_i}$

$H = 0 \to 2$ degenerate ground states

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

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

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

$$(n_+, n_-) = (N-1, 1) \text{ and } (1, N-1)$$
$$N + N = 2N \text{ degen. micro-states}$$

Prob. depends on $\boxed{E_1 = 2d - (d \cdot N - 2d) = -(d \cdot N - 4d)}$ page 137

Excited ~~states~~ micro-states have lower prob.

vs. higher degeneracy...

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

Ground state wins — exponentially approach $\langle |m| \rangle \to 1$

as $T \to 0$, $\beta \to \infty$

"ordered phase"

Magnetization is Ising model order parameter (OP)

Distinguish $\langle |m| \rangle \to 0$ high-T disordered phase

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

In general phases distinguished by zero vs. non-zero $N \to \infty$ order param.

If OP or its derivative(s) discontinuous or divergence

Then phase transition at critical point of control params

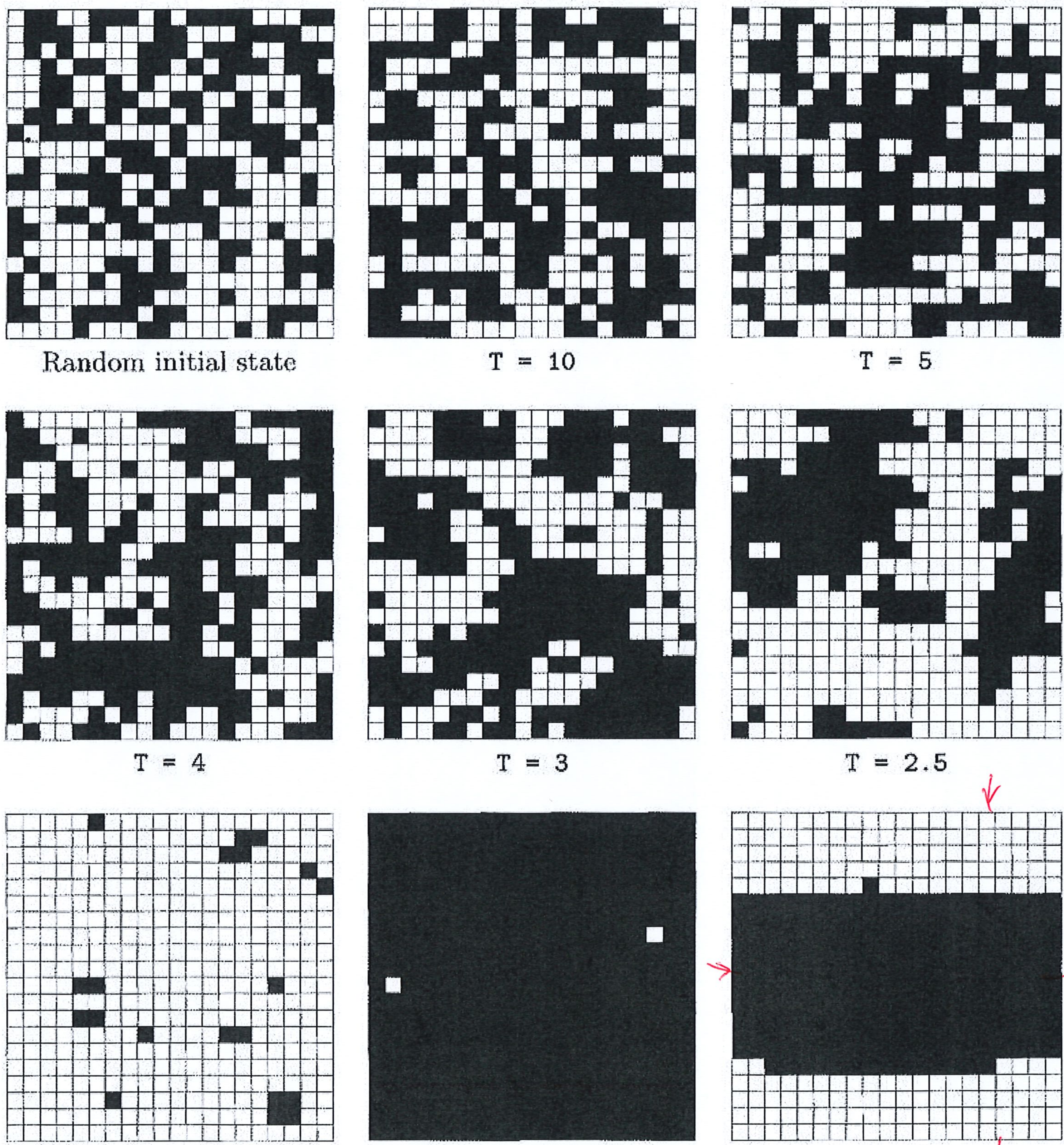
Otherwise crossover instead of true transition

With $H=0$, just critical temperature T_c for Ising model

$d=1$: crossover

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

$m \approx 0$



Random initial state

T = 10

T = 5

T = 4

T = 3

T = 2.5

T = 2

T = 1.5

T = 1

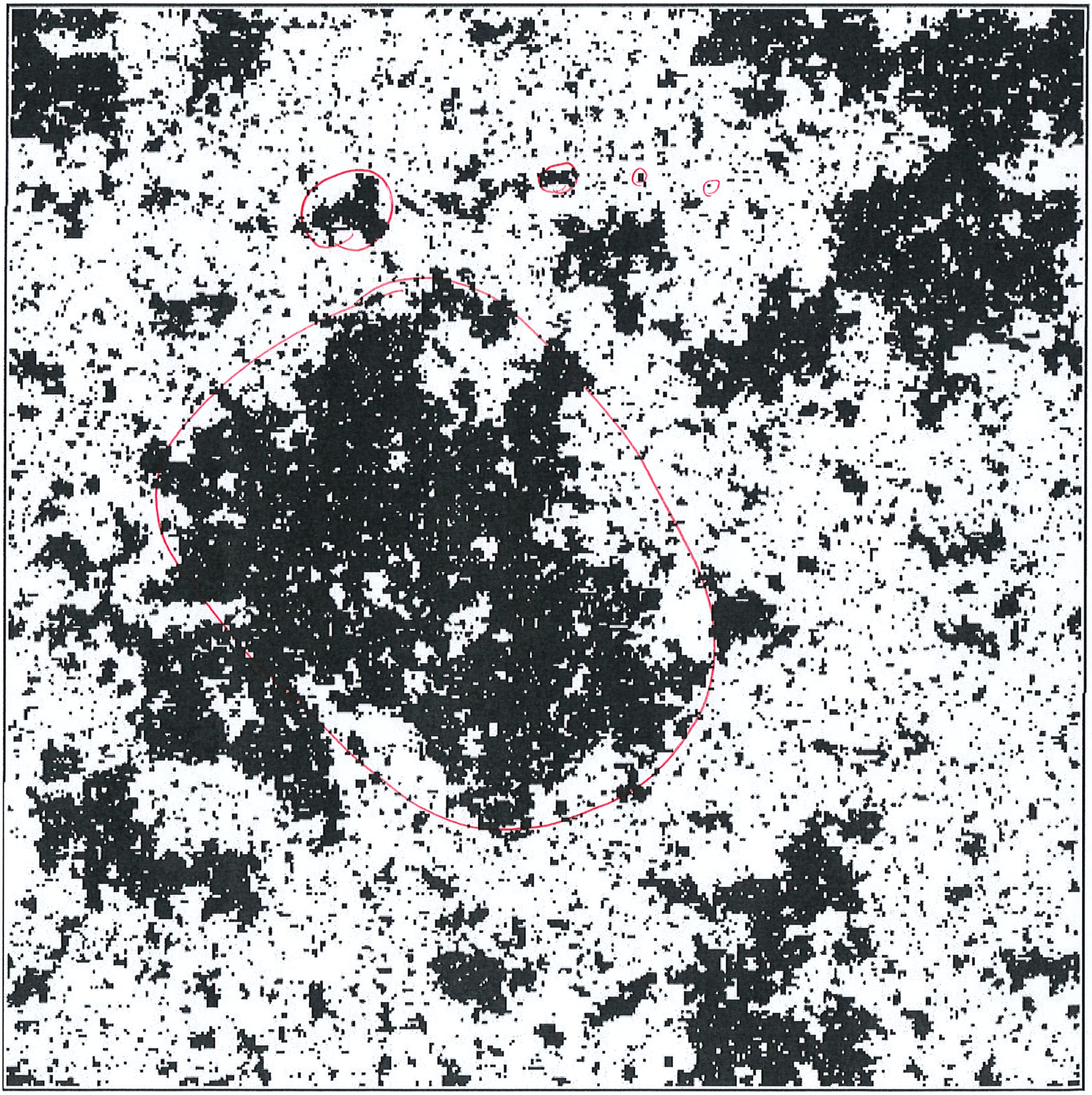
$m \approx 1$

$m \approx -1$

20×20

$2^{400} \sim 10^{120}$

T=2.27



400 × 400

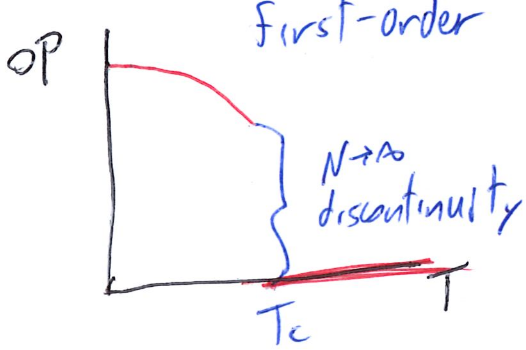
$2^{160,000} \sim 10^{48,164}$

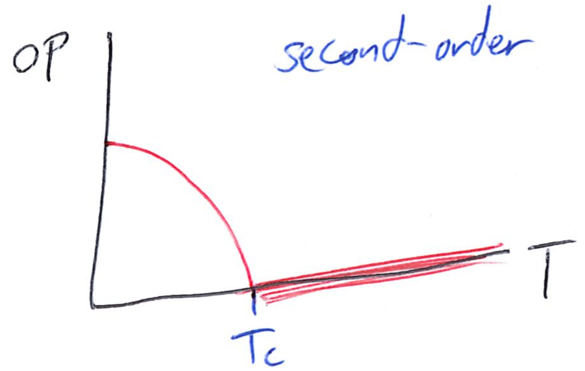
Formally OP must be related to derivative of free energy

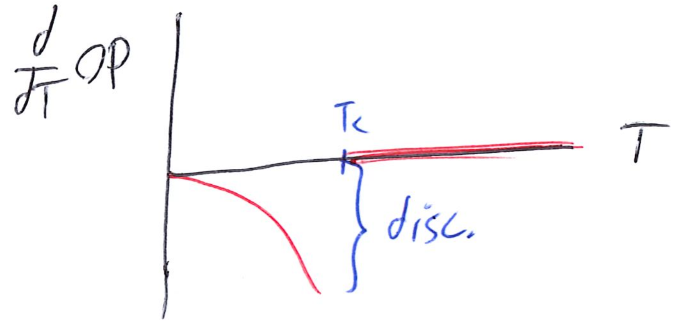
$N \to \infty$ discontinuous OP → "first-order" transition

continuous OP w/ discontinuous or divergent derivative(s)

→ "second-order" transition







Relate $\langle m \rangle$ and a derivative of $F = -T \log Z$

Restore magnetic field

$$E_i = -\sum_{\langle jk \rangle} s_j s_k - H \sum_n s_n = -\sum_{\langle jk \rangle} s_j s_k - HNm$$

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

So $$Z = \sum_{\{s_n\}} \exp\left(\beta \sum_{\langle jk \rangle} s_j s_k + \beta H N m\right)$$

$$\frac{dF}{dH} = -T \frac{1}{Z} \frac{\partial Z}{\partial H} = -\cancel{T} \frac{1}{Z} \sum_{\{s_n\}} \cancel{\beta} N m \exp\left(\beta \sum_{\langle jk \rangle} s_j s_k + \beta H N m\right)$$

$$= -N \langle m \rangle$$

$\therefore$ $\langle m \rangle = \dfrac{-1}{N} \dfrac{\partial F}{\partial H} = \dfrac{1}{N\beta} \dfrac{\partial}{\partial H} \log Z$ as promised for order param

page 139