From Micro to Macro
Example of the Ising model

Chapter II. Lecture 1

Thursday 11 April

From micro to macro
Example of the Ising model

Chapter II — Lecture 1

Plan:

1) Spontaneous magnetization
   a) Model with no interactions (J=0)
   b) H=0, Spontaneous magnetization
   c) Symmetry breaking??

2) Phase transition in the Ising model
   a) Control parameter and Order parameter
   b) 1d Ising model: continuous phase transition
   c) 2d Ising model

3) Properties at the critical point: Infinite Clusters of Correlated Spins
   a) Correlation length diverging at Tc
   b) Susceptibility diverging at Tc
   c) Properties at criticality

Expectations: Participate in the discussions, take notes, try to do the analytical derivations

References: Book "Complexity and Criticality", K. Christensen, N. Moloney, Chapter 2, Ising model

Yesterday: Ising model

Microscopic description:

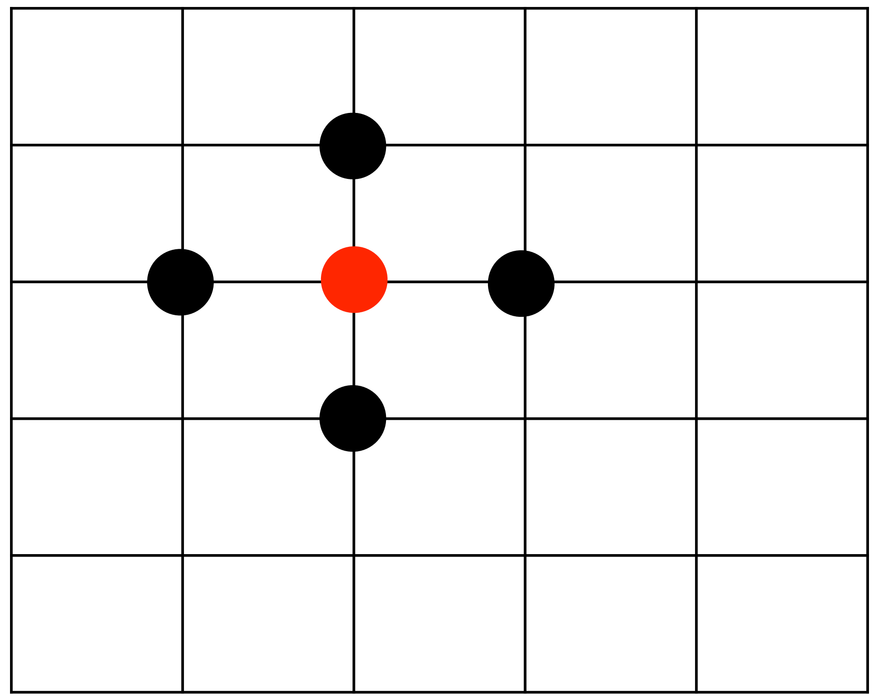
Energy of the system: $E(\vec{s}) = -J \sum_{<i,j>} s_i\, s_j$ with $J > 0$

Scalar spin $s_i = \pm 1$

Sum over closest neighbours only

Microscopic description

Ex. In 2D



From Microscopic to macroscopic description:

State probability: $P(s_1, \cdots, s_N) = \dfrac{\exp(-\beta\, E(\vec{s}))}{Z}$ where $\beta = \dfrac{1}{k_b\, T}$

Partition function: $Z = \sum_{s_1, \cdots, s_N} \exp(-\beta\, E(\vec{s}))$ Normalisation

Contains all the information about the system!

OK!

Free energy: $F = -k_b\, T\, \log(Z)$

Thermodynamic potential

Macroscopic description

Partition function

Statistical (microscopic) description

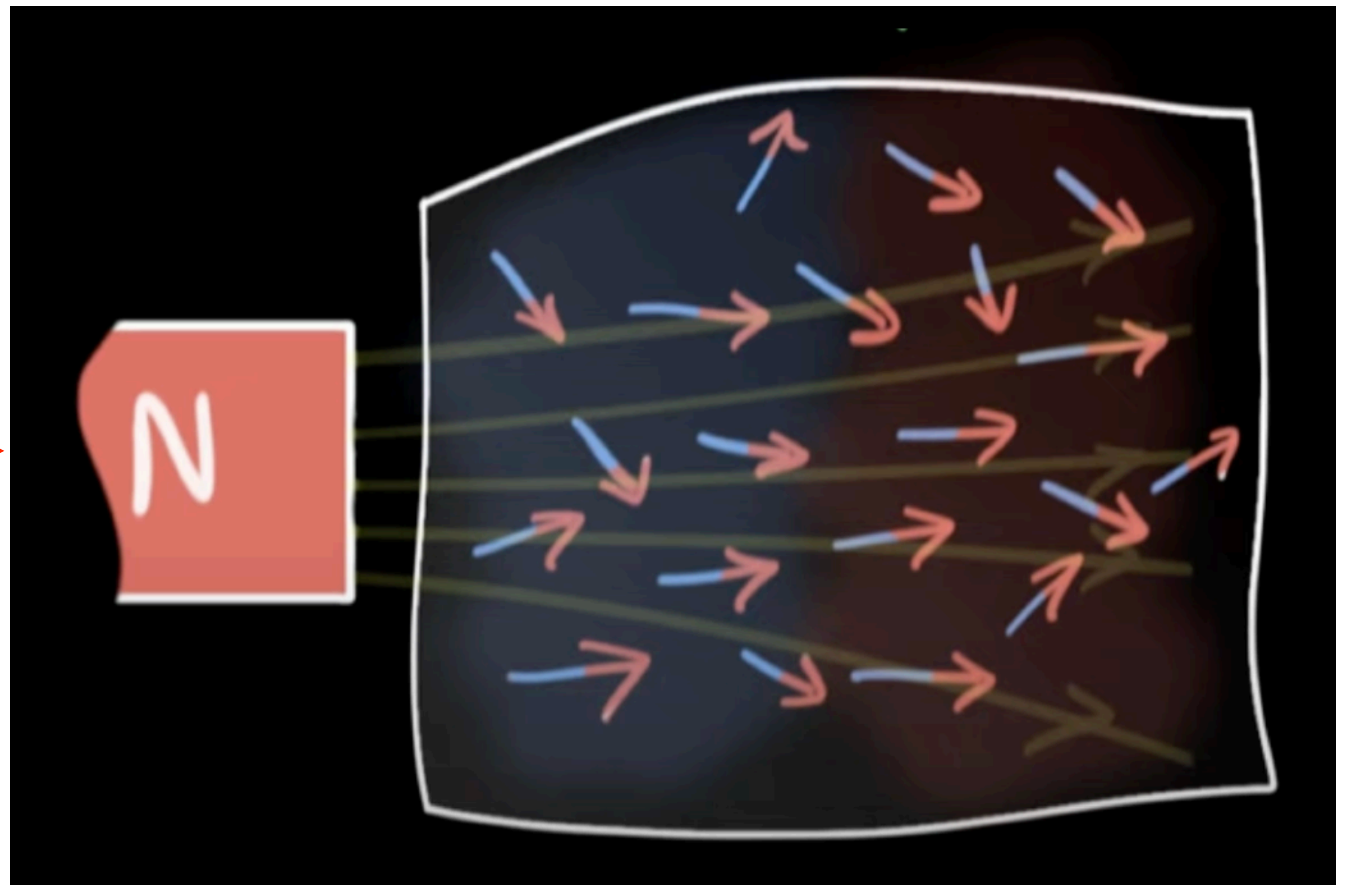
Ferromagnetic - Paramagnetic material

In the presence of an external magnetic field

Paramagnetic material:

Magnet

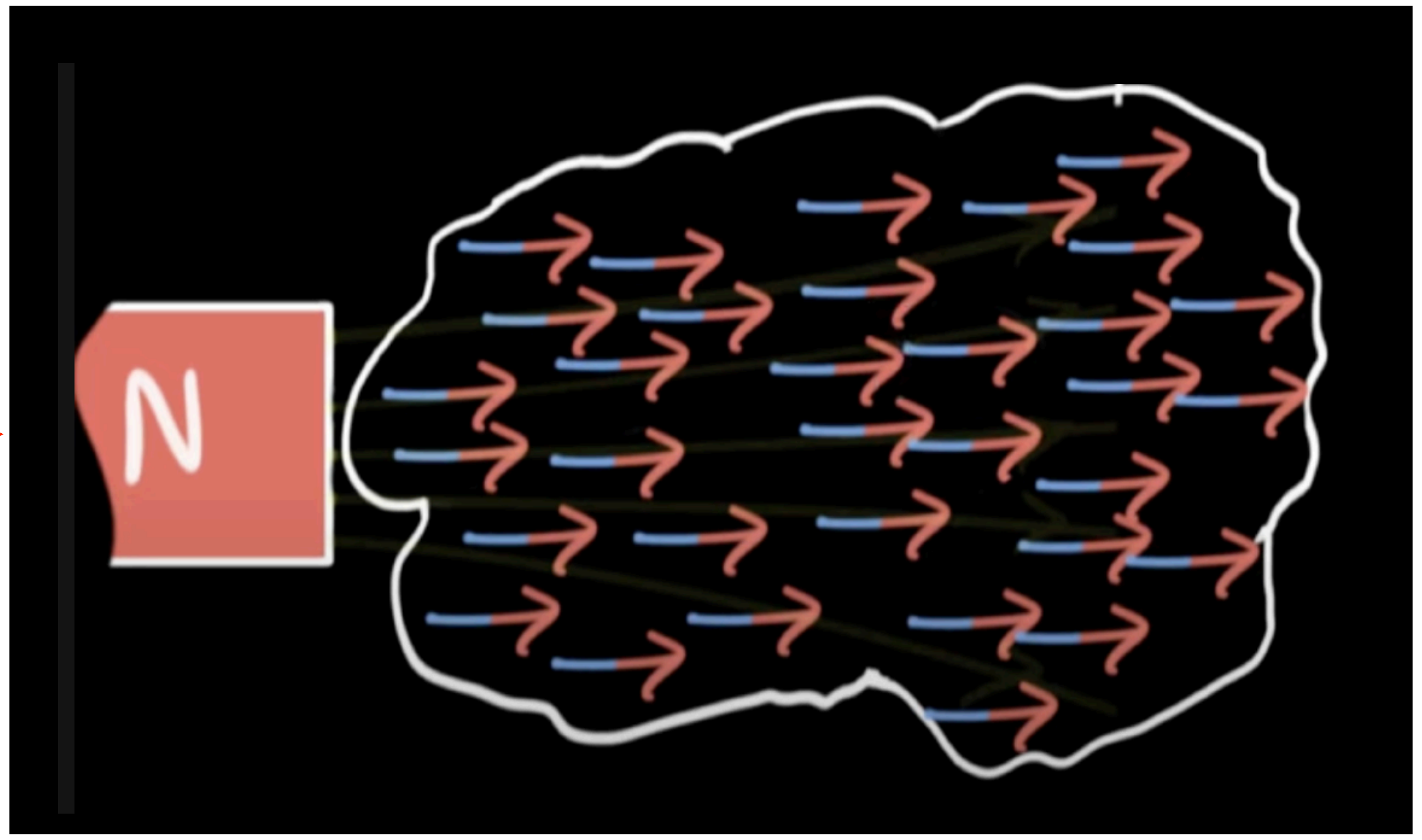
H



Weak alignment of the “tiny” magnet

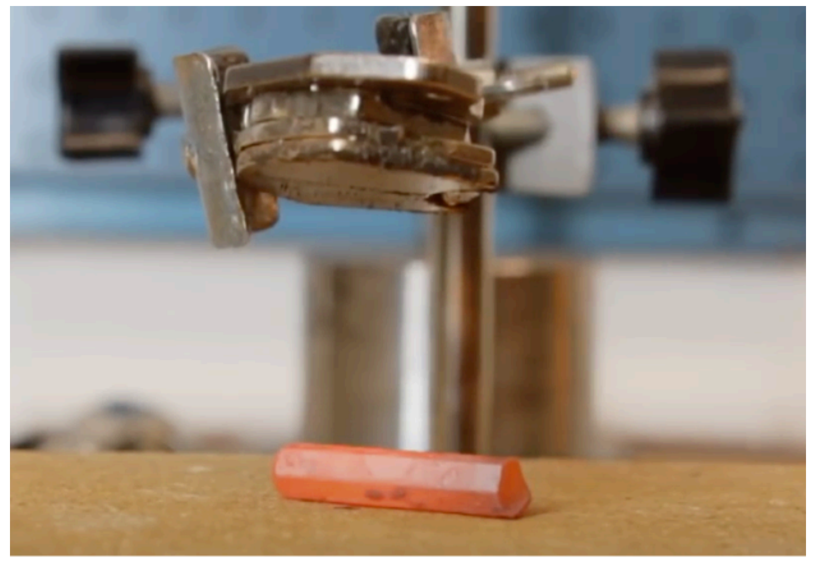
Ferromagnetic material:

Magnet

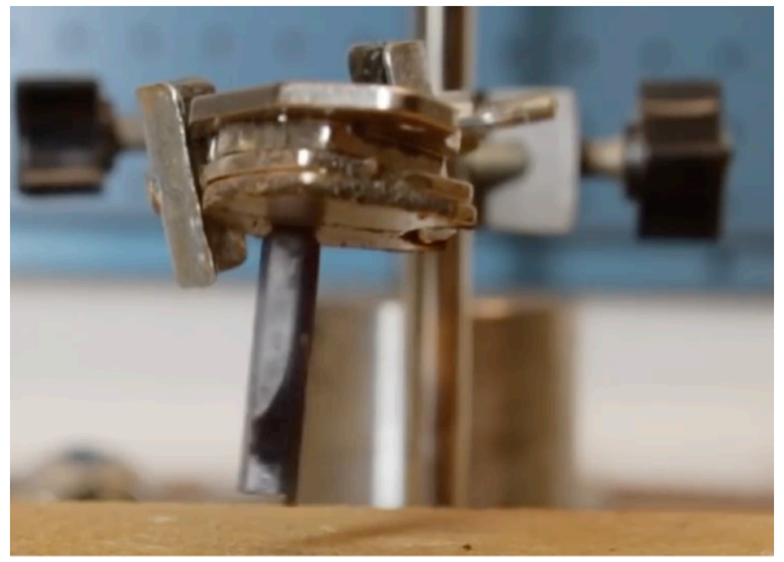


Entire domains align.

Material very slightly magnetised ==> not attracted to magnet



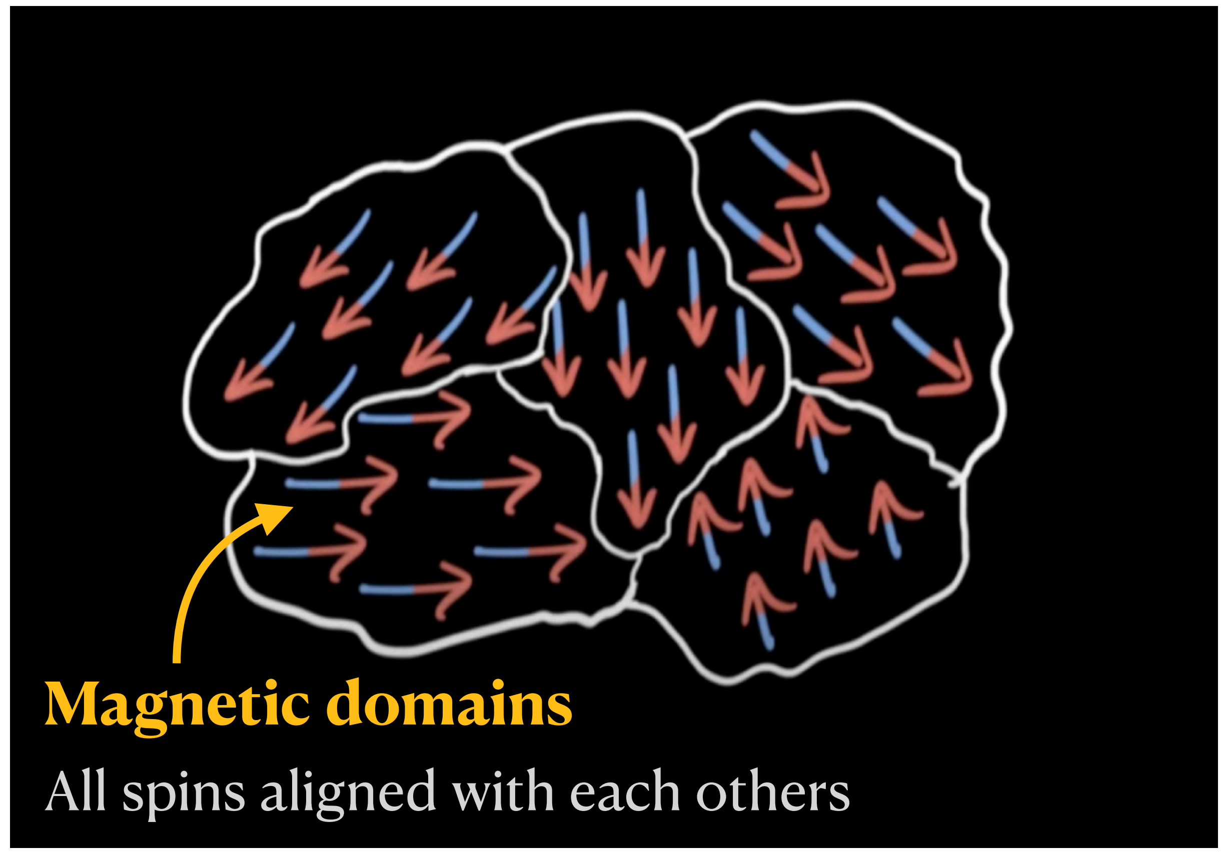
Material strong magnetisation ==> strong attraction to magnet



Ferromagnetic - Paramagnetic material

In the absence of an external magnetic field

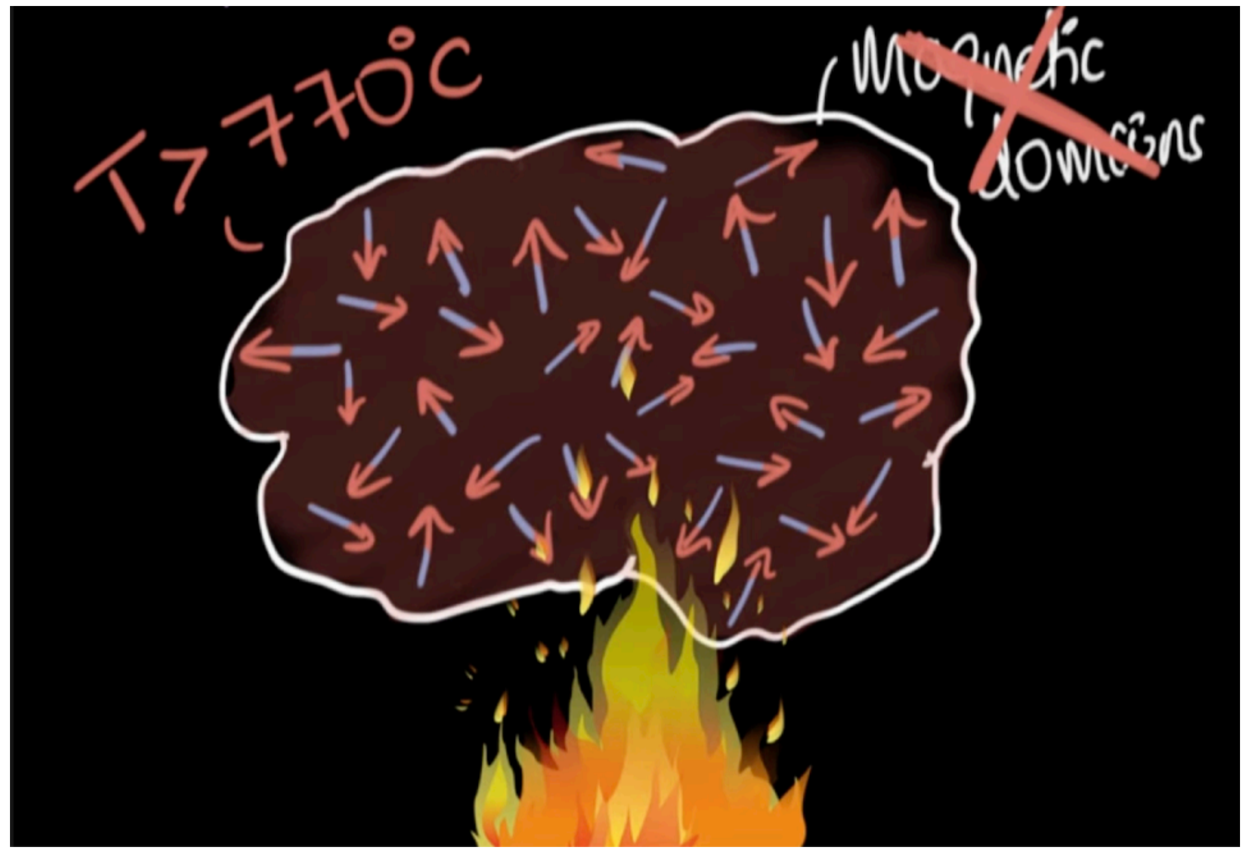
T < Tc: Ferromagnetic material



Increase T

Iron (Fe): Tc = 770 C

T > Tc: Paramagnetic material:



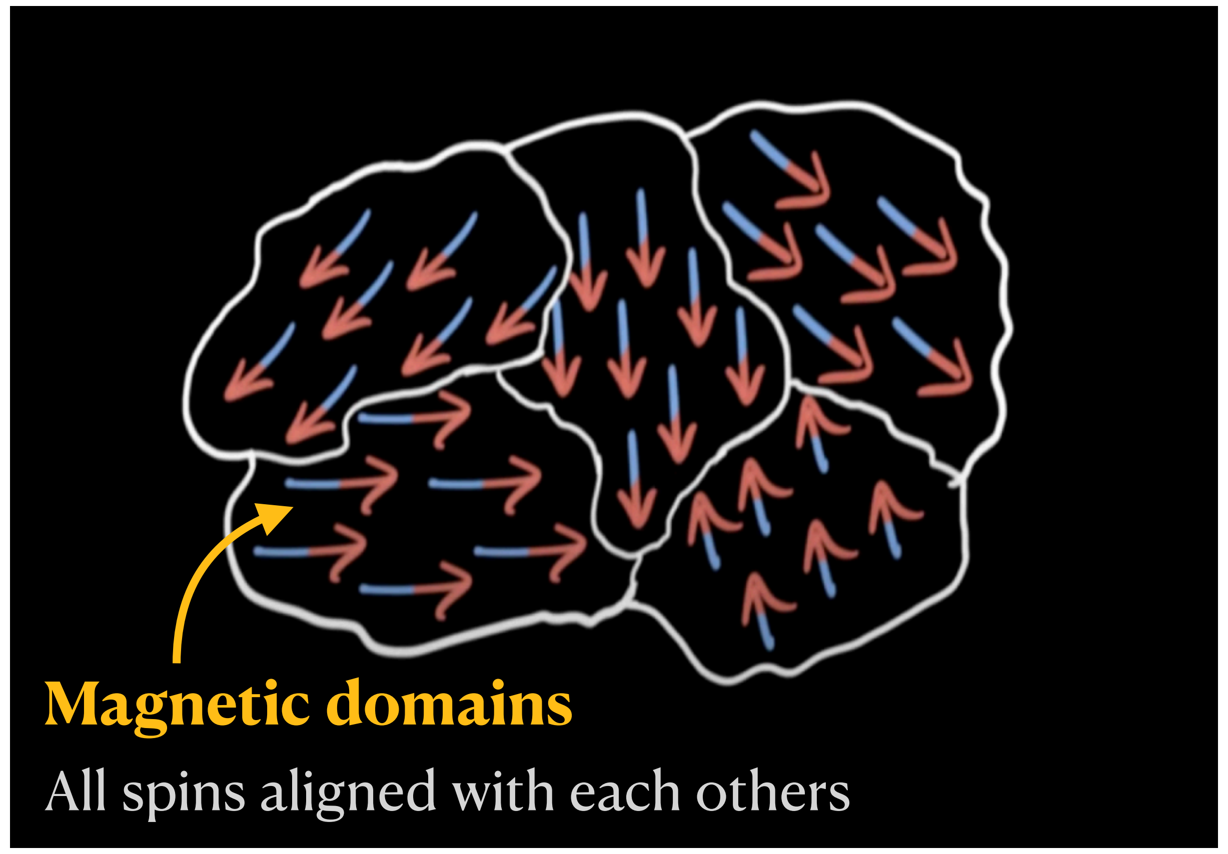
Below Tc: the domains have **non-zero magnetisation even in absence of external field**

Above Tc: the magnetisation of the domains is zero

Ferromagnetic - Paramagnetic material

In the absence of an external magnetic field

T < Tc: Ferromagnetic material



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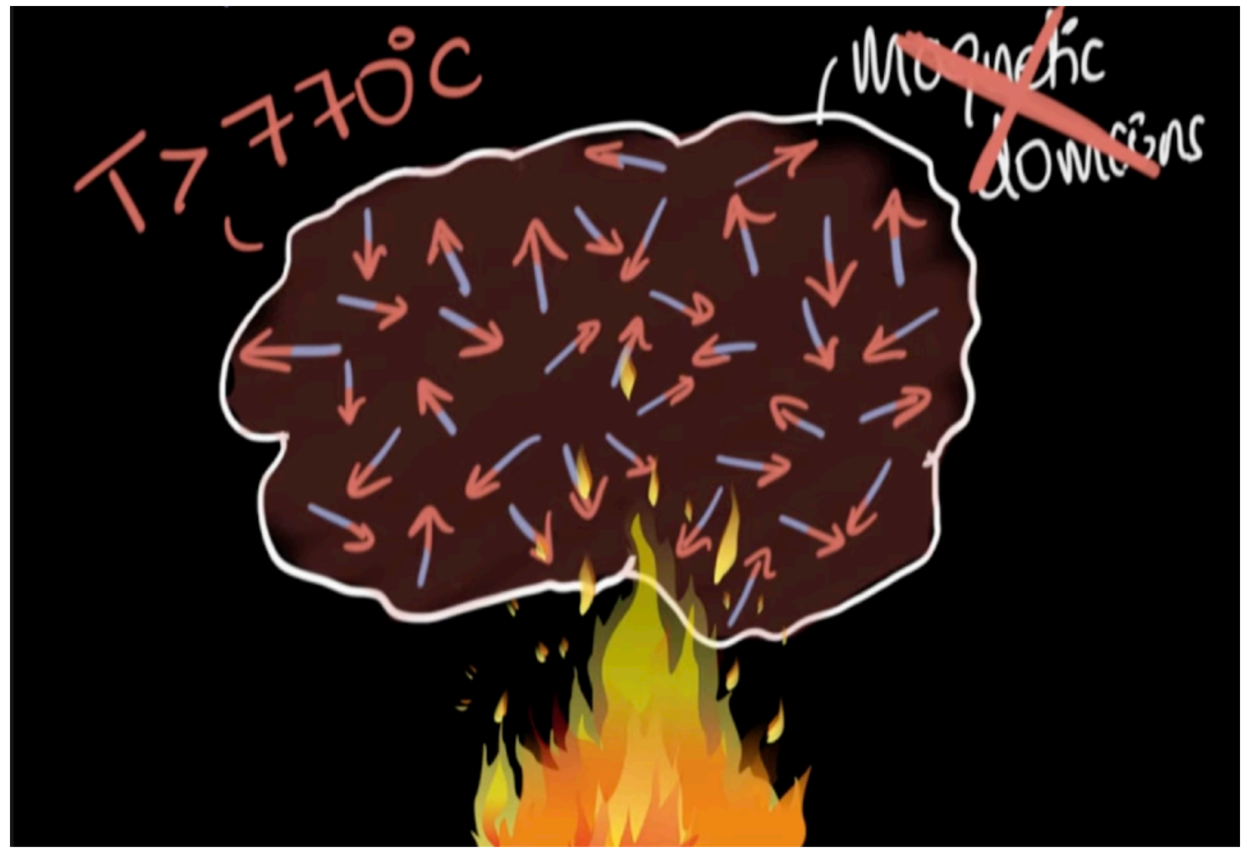

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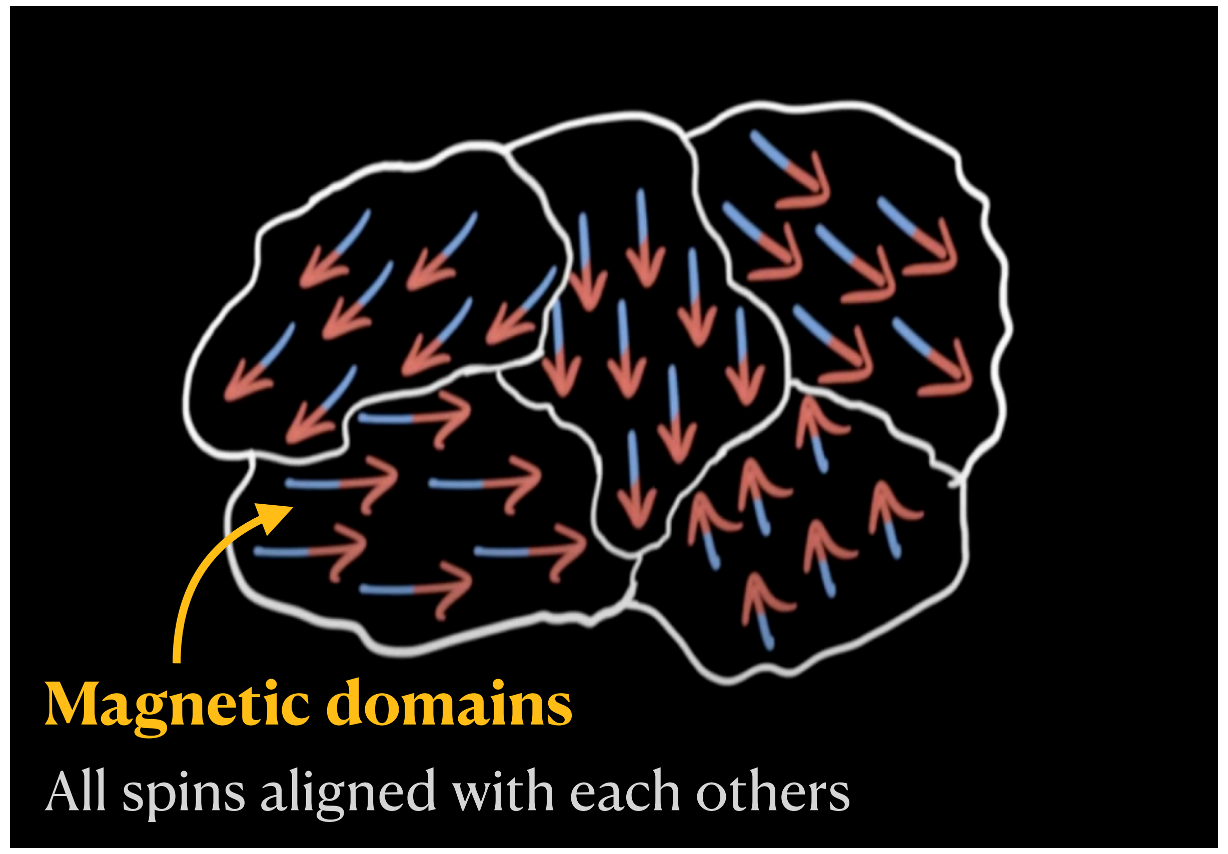
Above Tc: the magnetisation of the domains is zero

Ferromagnetism: emergence of a **"spontaneous magnetisation"** at **T<Tc**.

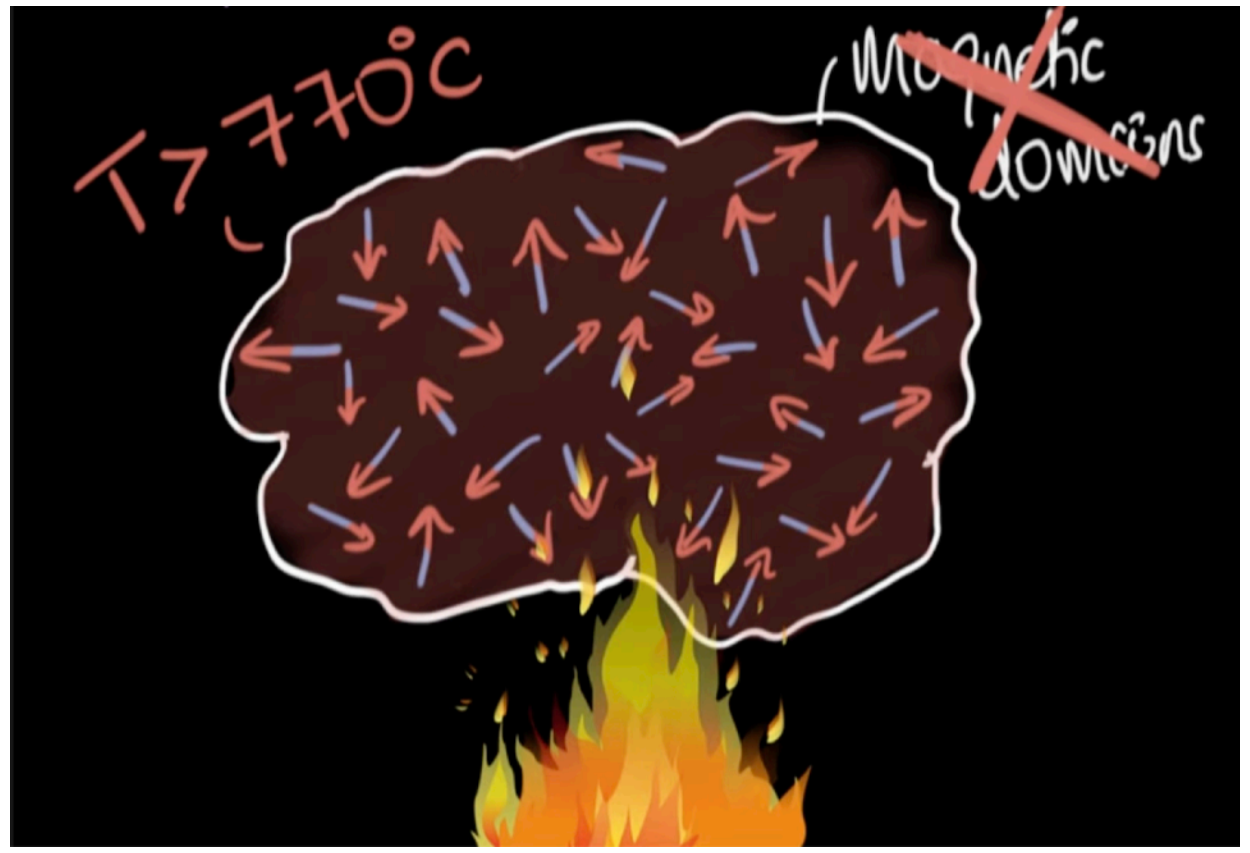
Ferromagnetic - Paramagnetic material

In the absence of an external magnetic field

T < Tc: Ferromagnetic material



T > Tc: Paramagnetic material:



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Microscopic description: model for a small domain

Energy of the system: $E(\vec{s}) = -J \sum_{<i,j>} s_i \, s_j$ with $J > 0$

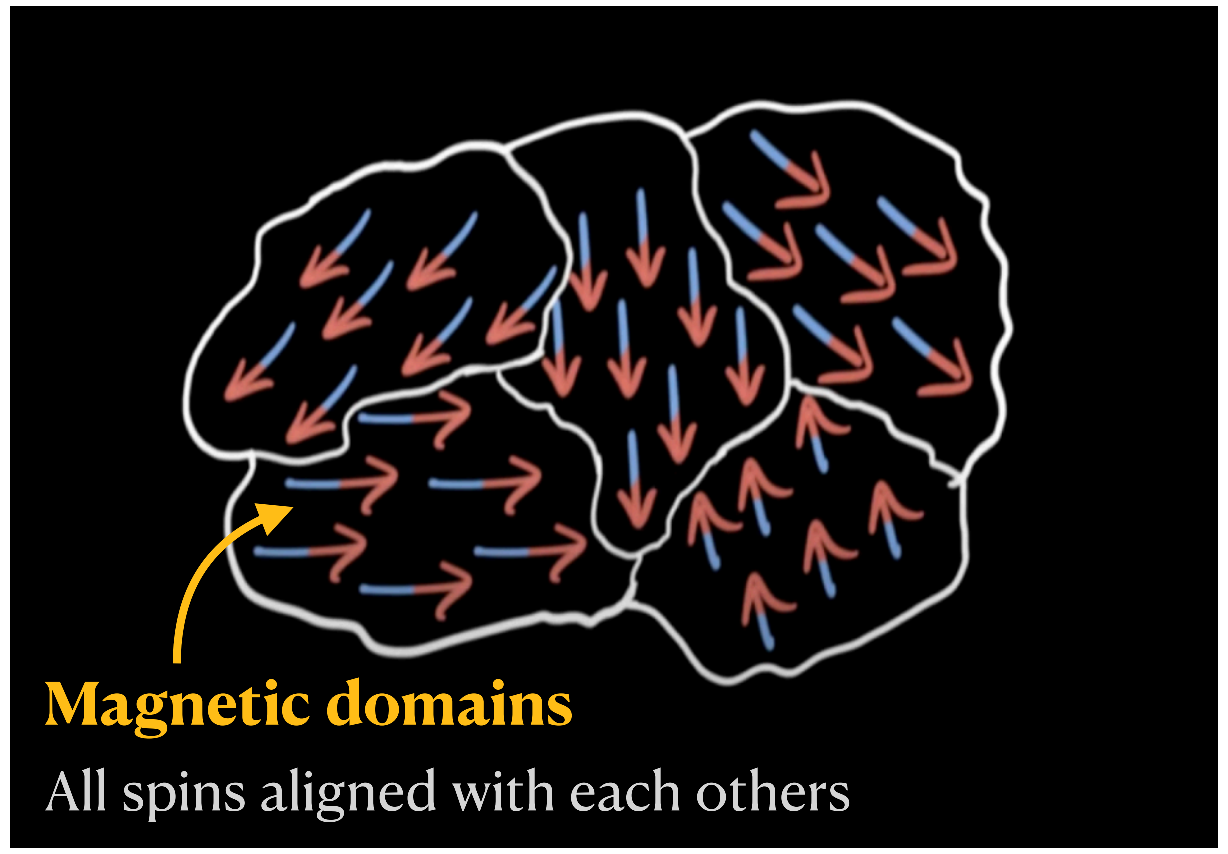
Sum over **closest neighbours** only

Scalar spin $s_i = \pm 1$

Ferromagnetic - Paramagnetic material

In the absence of an external magnetic field

T < Tc: Ferromagnetic material



Increase T

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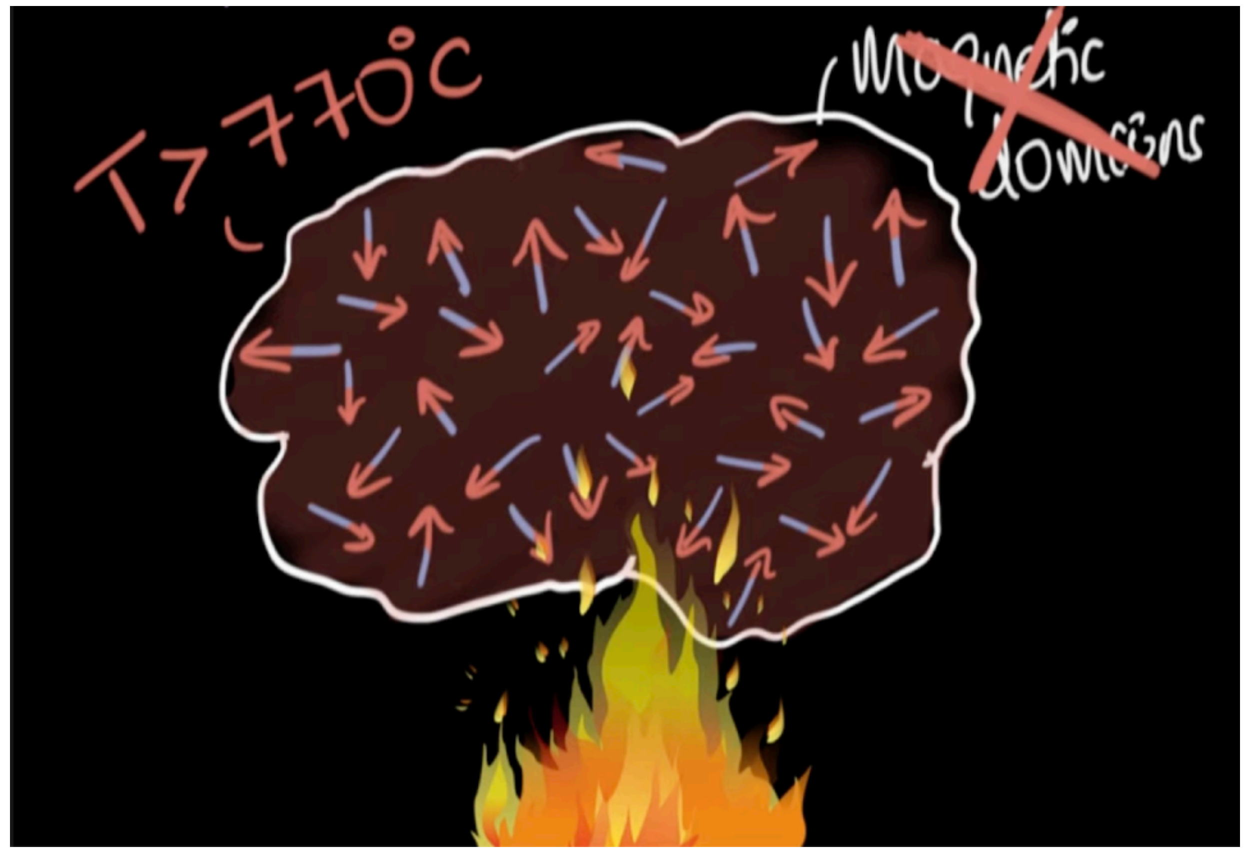

Below Tc: the domains have **non-zero magnetisation even in absence of external field**

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Ferromagnetism: emergence of a **"spontaneous magnetisation"** at **T<Tc**.

Microscopic description: model for a small domain

Energy of the system: $$E(\vec{s}) = -J \sum_{<i,j>} s_i \, s_j \qquad \text{with} \quad J > 0$$

Sum over **closest neighbours** only

Scalar spin $s_i = \pm 1$

Can **microscopic interactions** explain the emergence of a **spontaneous magnetisation**?

Plan

Chapter I — Lecture 2

Question 1

Can the **microscopic interactions between nearest neighbors** explain the emergence of a **spontaneous magnetization over a whole domain**?

Question 2

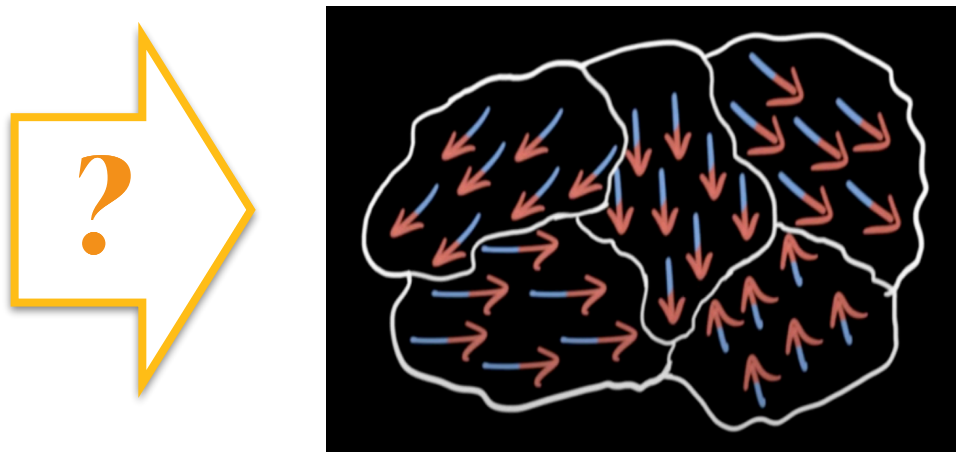
Is there a **Phase Transition?**

if so: **What type**?

Question 3

Properties of the system **at criticality?**

$$E(\vec{s}) = -J \sum_{<i,j>} s_i \, s_j$$



I - Spontaneous magnetization

1) Model with no interactions (J=0)
2) H=0, Spontaneous magnetization
3) "Symmetry breaking"??

II - Phase transition in the Ising model

a) Control parameter and Order parameter

b) 1d Ising model: continuous phase transition

c) 2d Ising model

III - Properties at the critical point: Infinite Clusters of Correlated Spins

I- Spontaneous magnetization

1) Non-interacting Spins

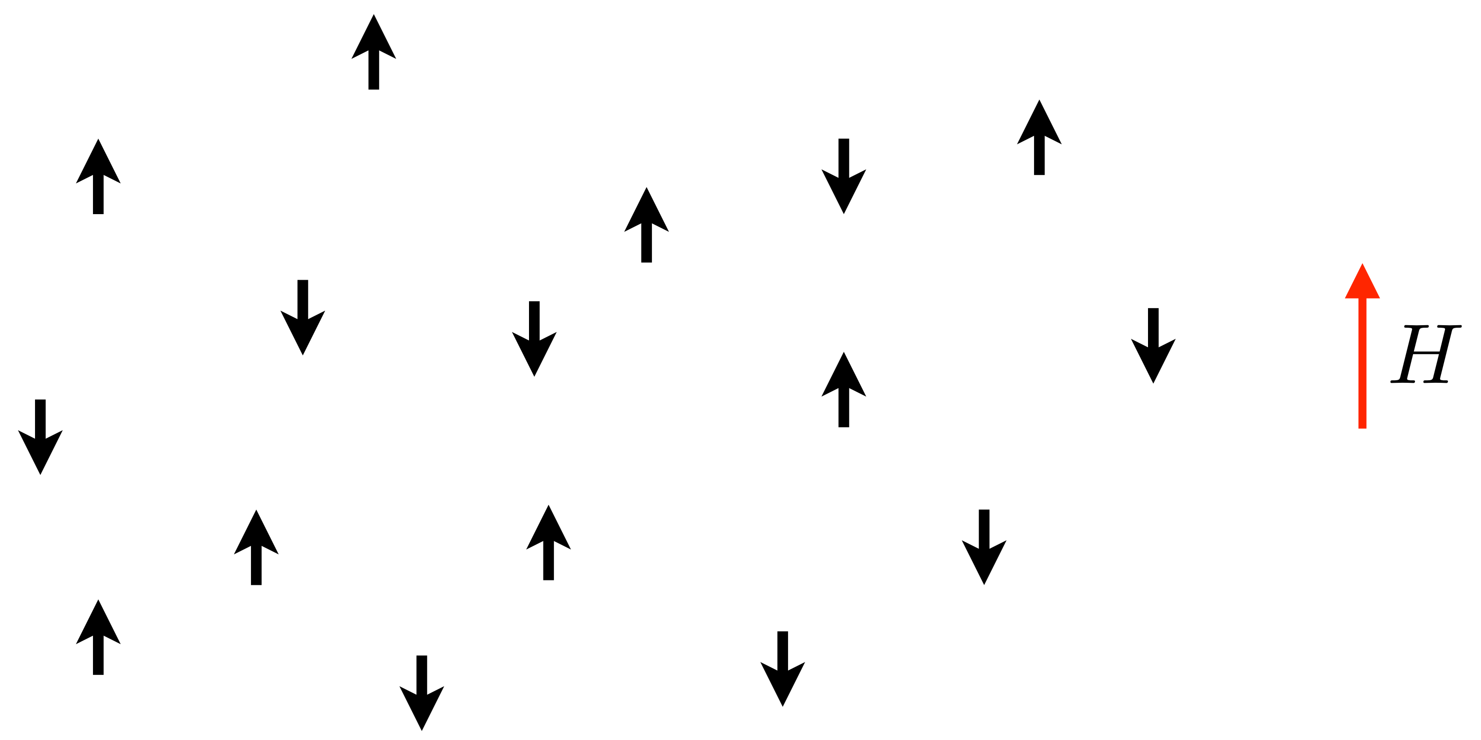
—>> Spontaneous magnetization???

No interaction!

Energy of the system: $E(\vec{s}) = -H \sum_{i=1}^{N} s_i$

External field H = constant

$s_i = \pm 1$



As the spin are non-interacting,
the problem is **independent of the underlying lattice and dimensionality**.

No interaction!

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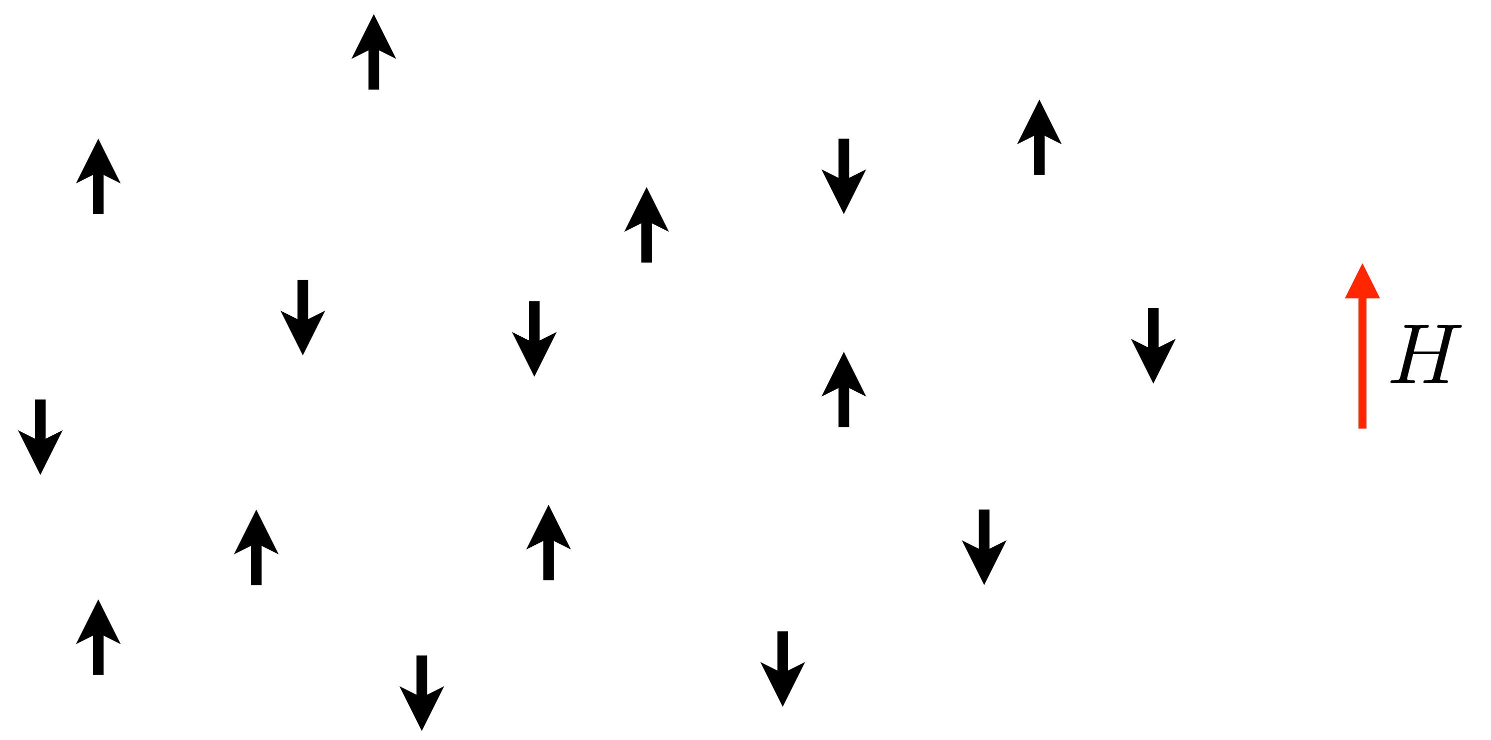
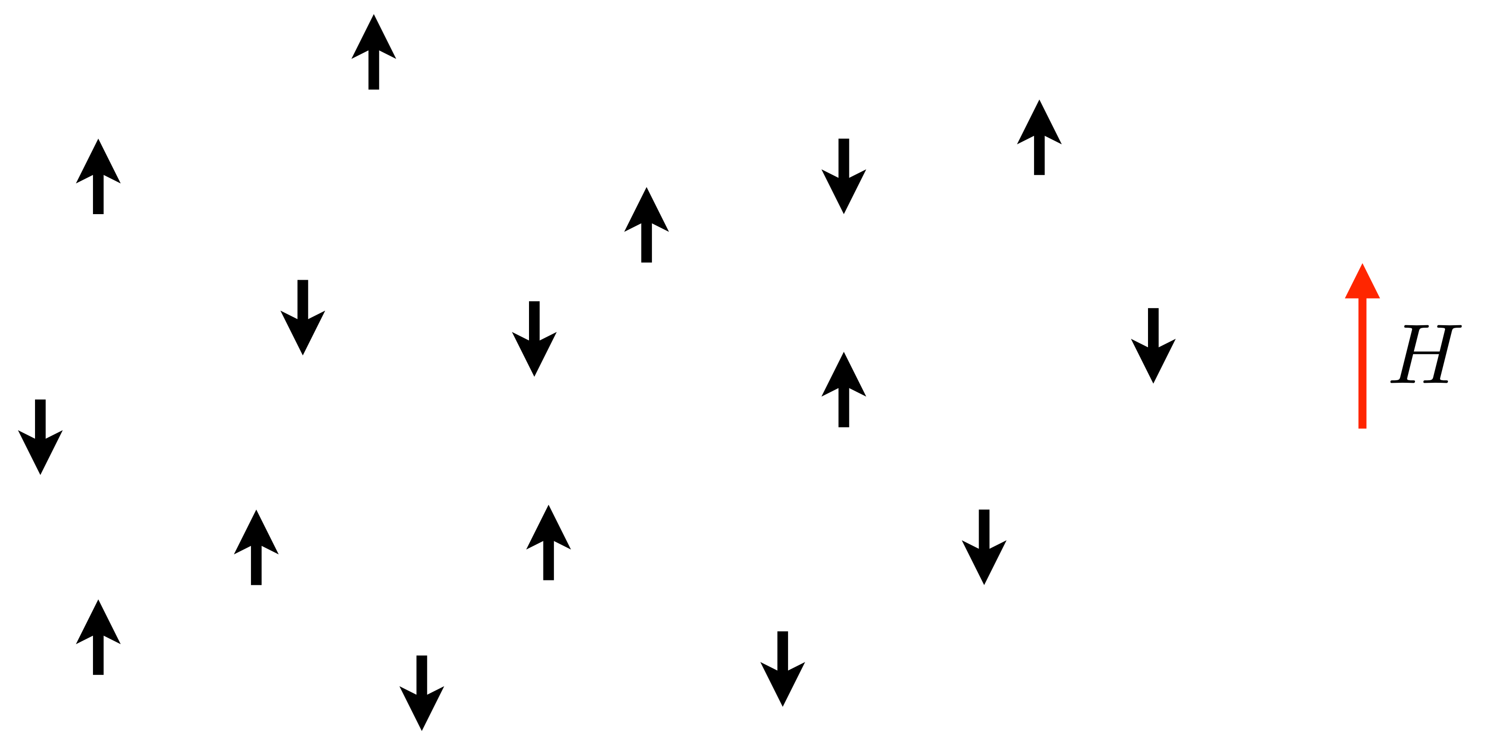


Distribution of the microstates: $$P(\vec{s}) = \frac{\exp(-\beta\, E(\vec{s}))}{Z}$$

The behaviour of the system is determined by **competition** between:

- **the external field** ——>> tends to align the spin
- **thermal energy** ——>> tends to disorganise

No interaction!



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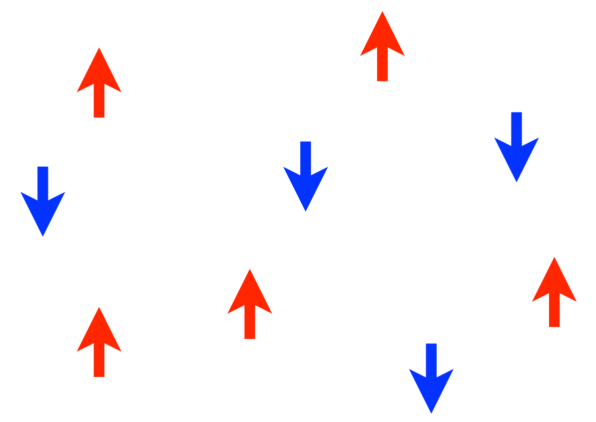
Limit $\dfrac{H}{k_B T} \to 0$ **:** the **thermal energy ``wins"** over the external field

Most probable microstates: **spins randomly pointing up and down**

$\langle M \rangle = 0 \qquad \langle E \rangle = 0$



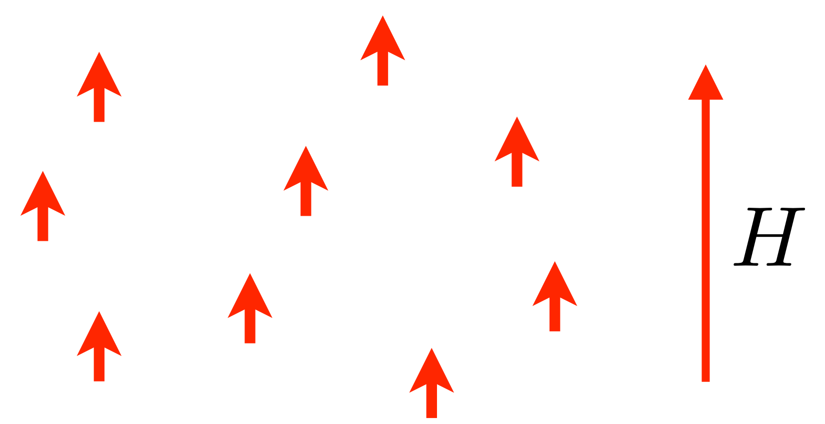
Limit $\dfrac{H}{k_B T} \to \pm\infty$ **:** the **external field ``wins"** over the thermal energy

Most probable microstates: **all spins aligned in the same direction than H**

If $H > 0$ then $\langle M \rangle = N$

If $H < 0$ then $\langle M \rangle = -N$

$\langle E \rangle = -N|H|$



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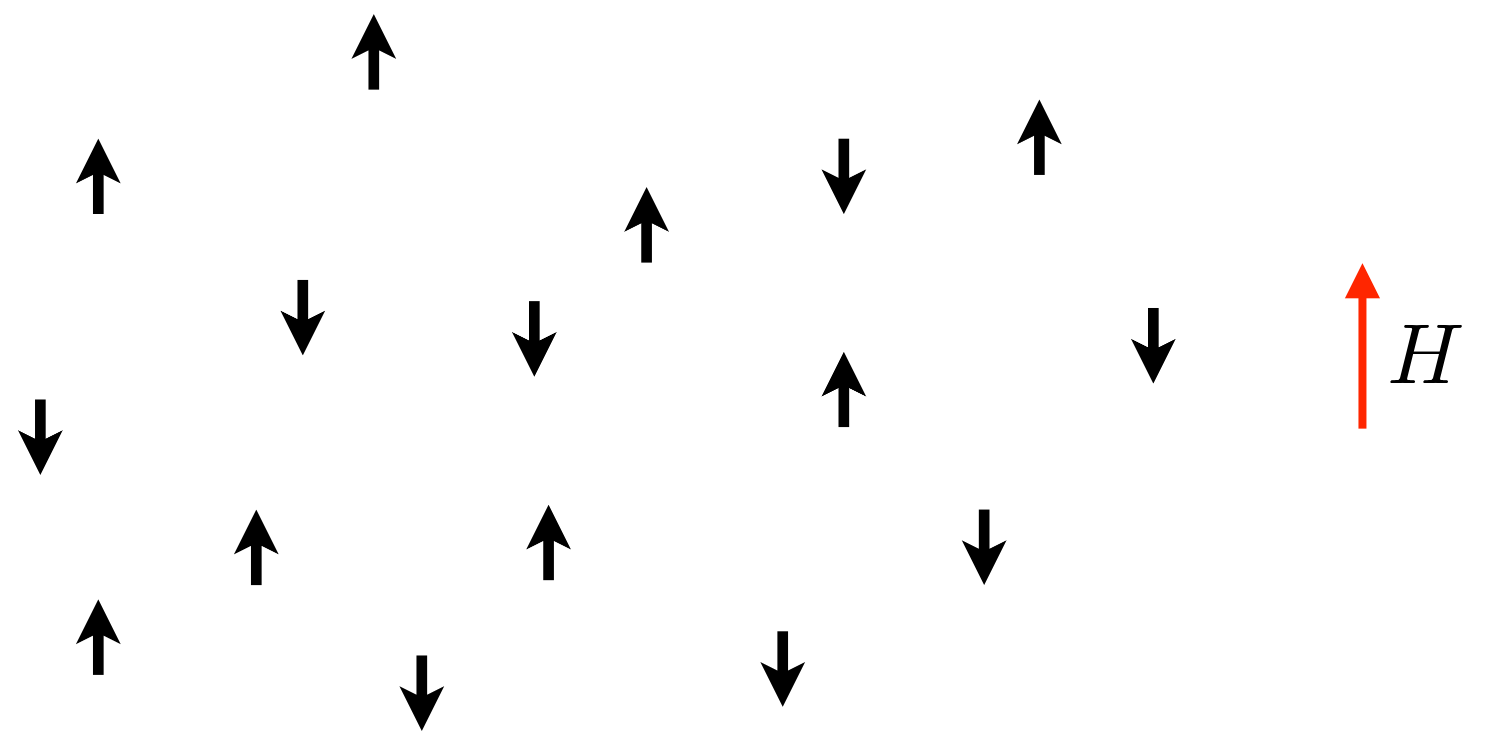

Energy of the system: $E(\vec{s}) = -H\sum_{i=1}^{N} s_i$ $\qquad s_i = \pm 1$

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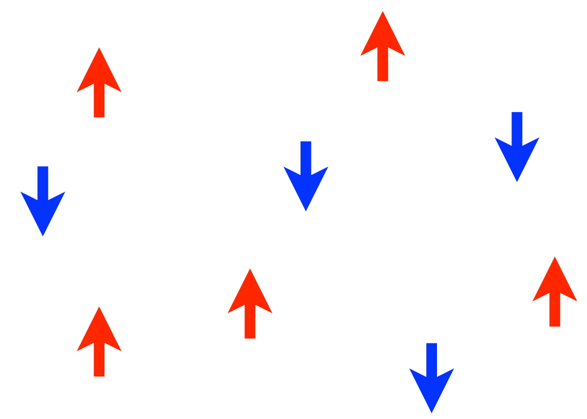

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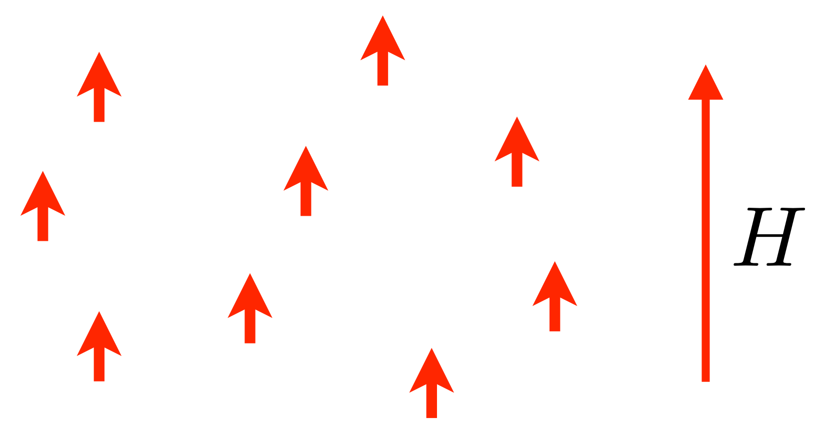
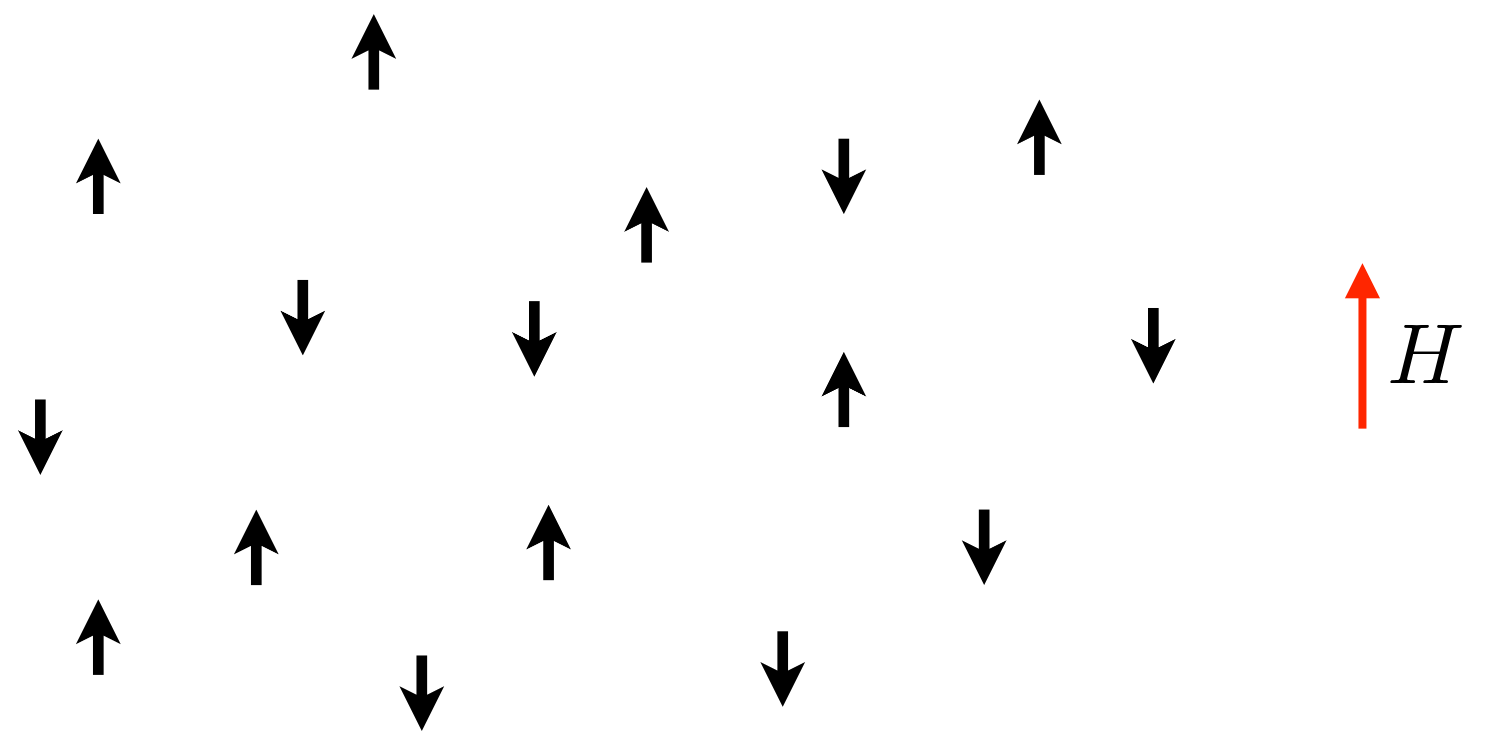


Rem: Extensive quantities —— >>>> $m = \dfrac{\langle M \rangle}{N} \qquad \epsilon = \dfrac{\langle E \rangle}{N}$ **Intensive**

No interaction!



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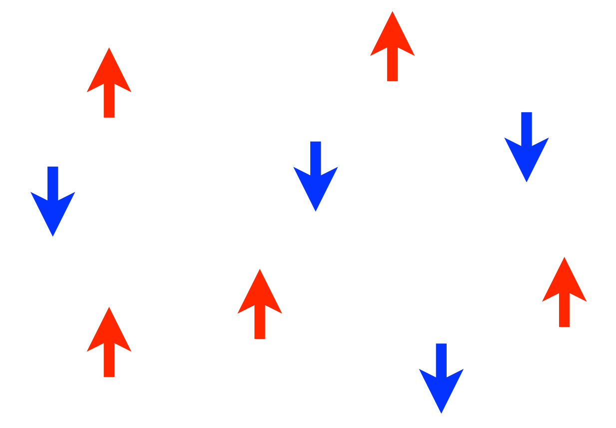

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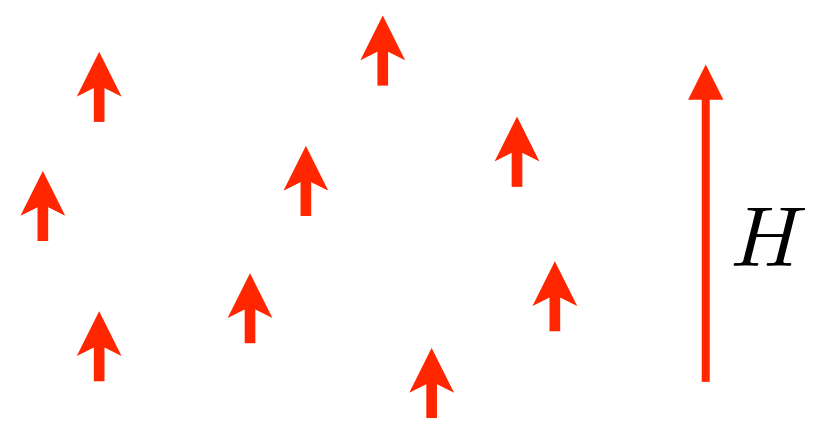
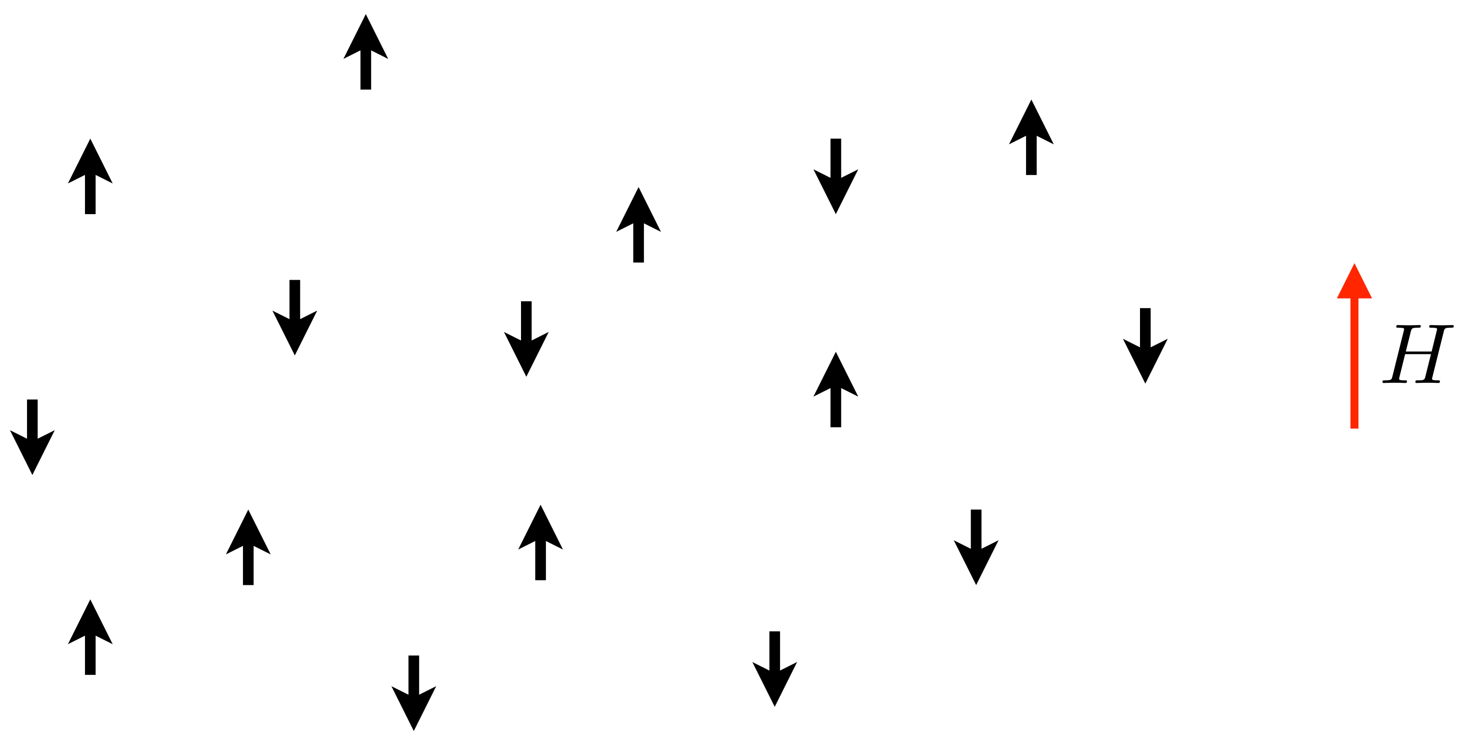


Is there a phase transition???

At H=0: spontaneous magnetization?

No interaction!



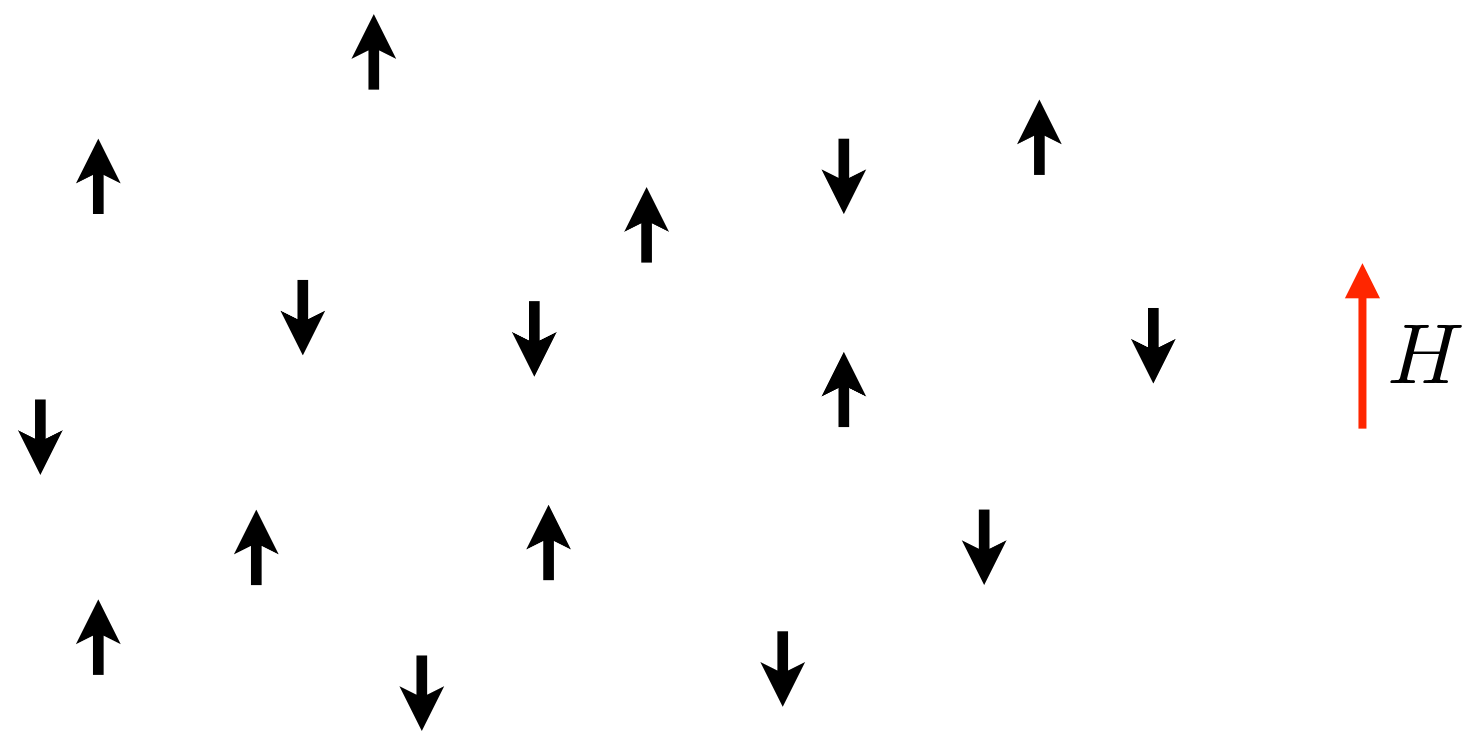
Energy of the system: $$E(\vec{s}) = -H\sum_{i=1}^{N} s_i \qquad s_i = \pm 1$$

External field H = constant

Partition function: $$Z(T,H) = \sum_{\vec{s}} \exp(-\beta E(\vec{s})) \quad \text{where} \quad \beta = \frac{1}{k_b\, T}$$

Free energy: $$F = -k_b\, T\, \log(Z)$$

No interaction!



Energy of the system: $$E(\vec{s}) = -H \sum_{i=1}^{N} s_i$$ $s_i = \pm 1$

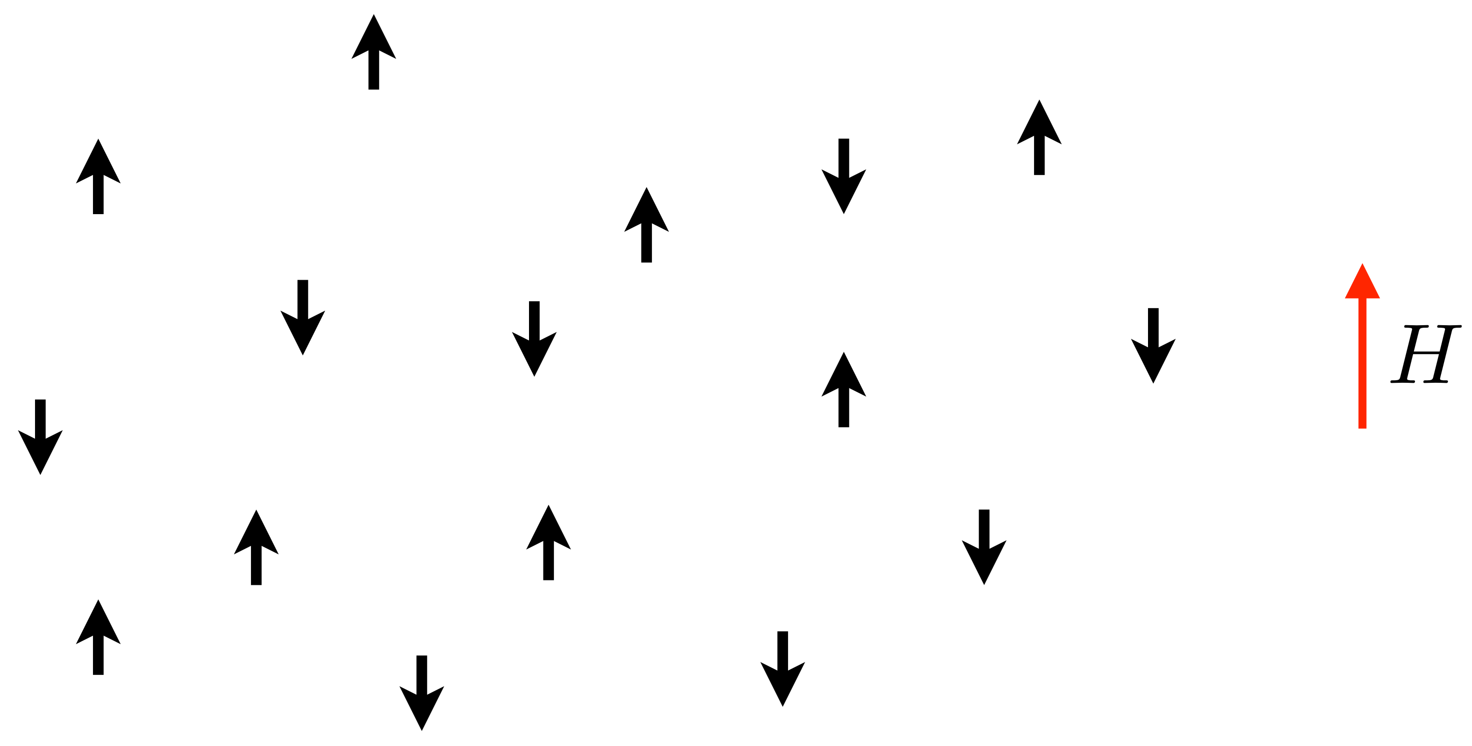
External field H = constant

Partition function:

$$\begin{aligned} Z(T,H) &= \sum_{\vec{s}} \exp(-\beta E(\vec{s})) \\ &= \sum_{s_1=-1}^{+1} \exp(\beta H s_1) \sum_{s_2=-1}^{+1} \exp(\beta H s_2) \cdots \sum_{s_N=-1}^{+1} \exp(\beta H s_N) \\ &= (2\,\cosh(\beta H))^N \end{aligned}$$

Free energy: $$F = -k_b T \log(Z)$$

No interaction!



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External field H = constant

Partition function:

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$$= \sum_{s_1=-1}^{+1} \exp(\beta H s_1) \sum_{s_2=-1}^{+1} \exp(\beta H s_2) \cdots \sum_{s_N=-1}^{+1} \exp(\beta H s_N)$$
$$= (2\, \cosh(\beta H))^N$$

Free energy: $F = -k_b\, T\, \log(Z)$

Free energy: $$F(T,H) = -N\, k_B T \log(2 \cosh(\beta H))$$

Rem: F is extensive

No interaction!

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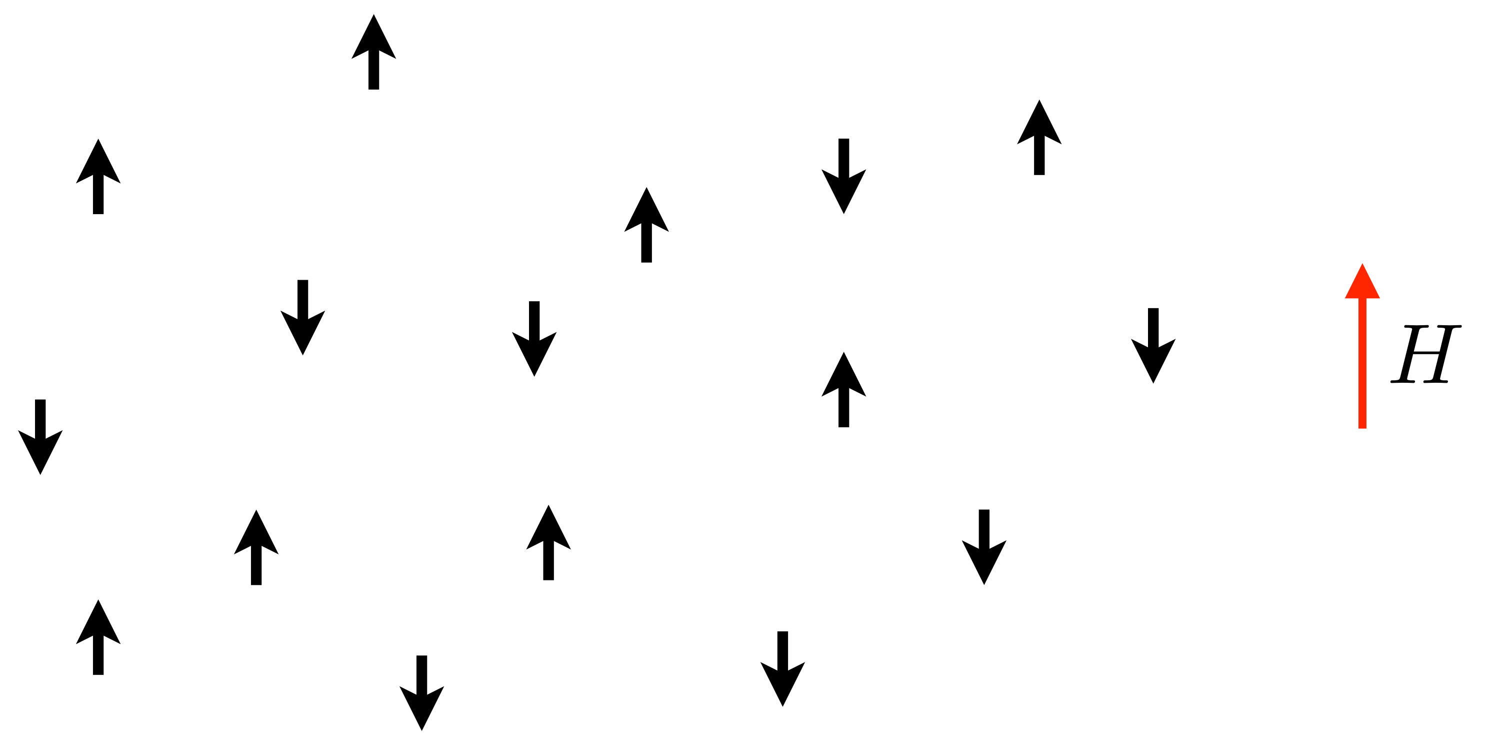
External field H = constant



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Free energy: $$F = -k_b T \log(Z)$$

Free energy: $$F(T,H) = -N\, k_B T \log(2\cosh(\beta H))$$

Rem: F is extensive

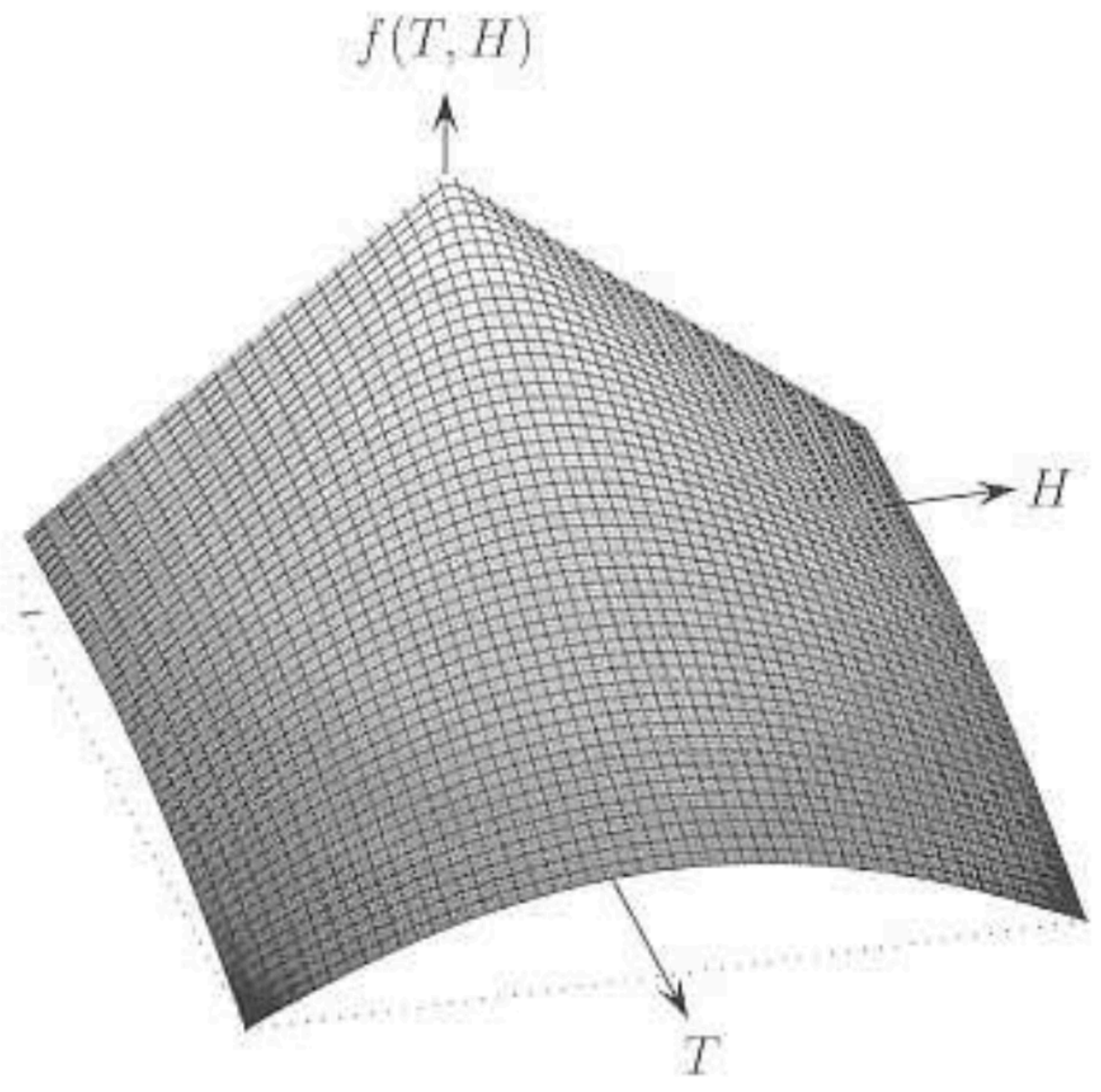
Free energy per spin: $$f(T,H) = -k_B T \log(2\cosh(\beta H))$$

$$f(T,H) = F(T,H)/N$$ **is intensive**

No interactions

No interaction, no spontaneous magnetization!

Free energy per spin: $f(T,H) = -k_B T \log(2\cosh(\beta H))$



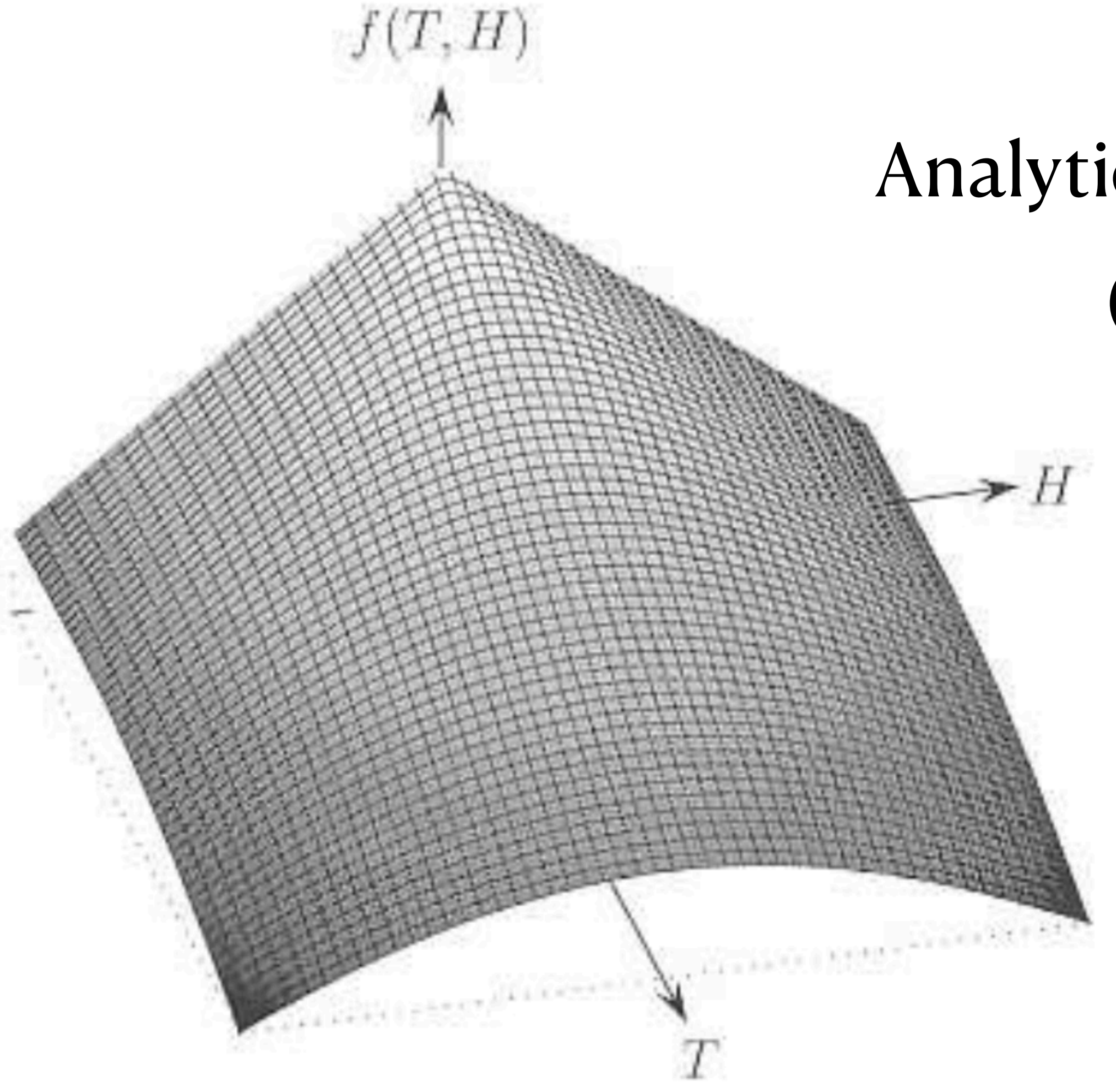
Analytic everywhere: no phase transition

(but in T=0, H=0)

No interaction, no spontaneous magnetization!

Free energy per spin: $f(T,H) = -k_B T \log(2\cosh(\beta H))$

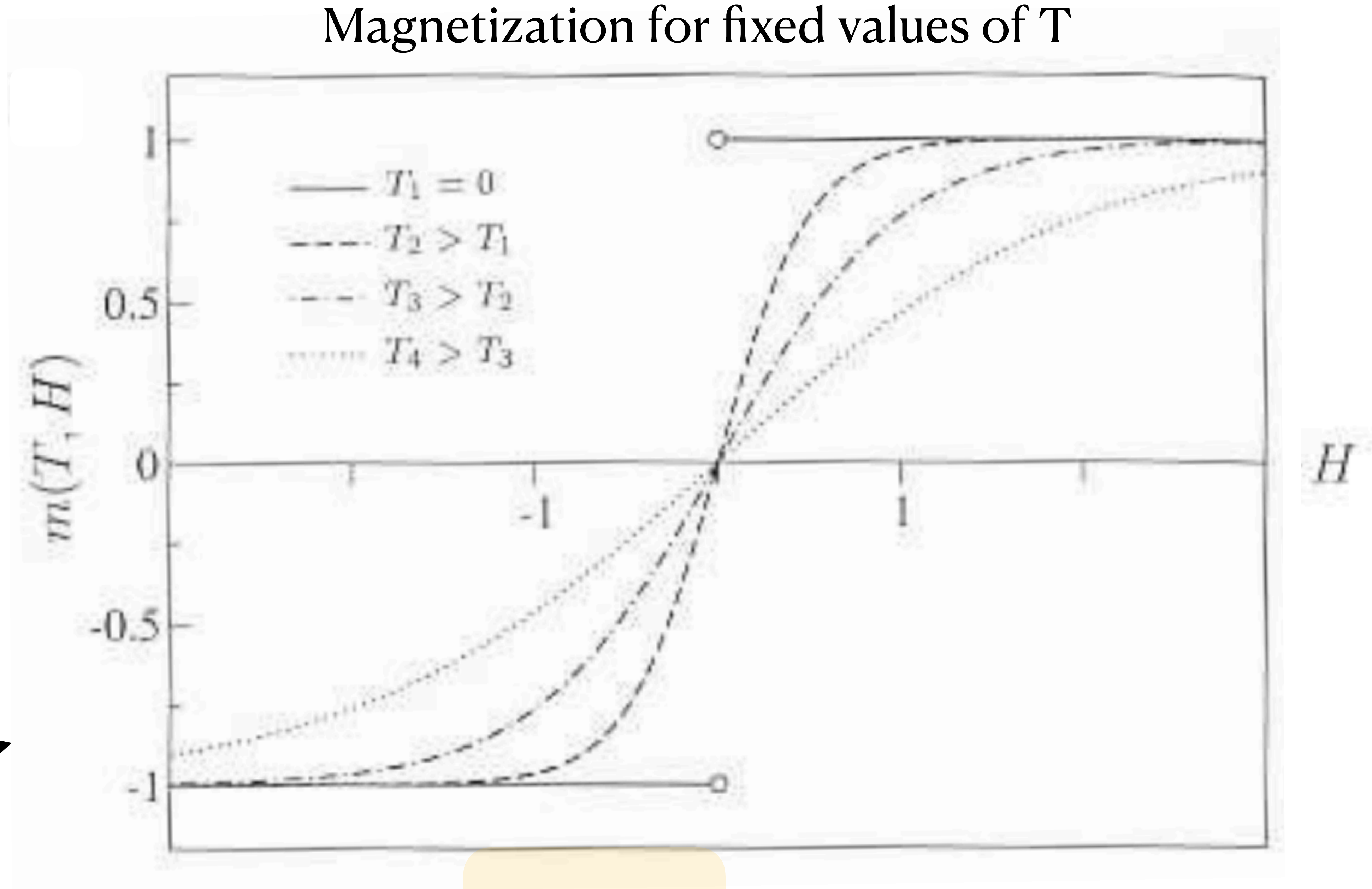
$$m(T,H) = -\left(\frac{\partial f}{\partial H}\right)_T = \tanh(\beta H)$$



Analytic everywhere: no phase transition

(but in T=0, H=0)

Magnetization for fixed values of T



$H \neq 0$

$H = 0$

High T: a strong H must be applied to align the spins

Smaller T: spins align more easily

T = 0: all the spins are aligned with H

Any T >= 0: $m(T,0) = 0$

$m(T,H)$ becomes steeper as T approaches zero

At T—> 0: Step function $\lim_{H\to 0^\pm} m(T,H) = \pm 1$

No spontaneous magnetization for any temperature in a **system with non-interacting spins**

1) Non-interacting Spins

===>> NO spontaneous magnetization

2) Interacting Spins

—>> spontaneous magnetization

No external field

$$E(\vec{s}) = -J \sum_{<i,j>} s_i s_j$$

Spontaneous magnetization: Can the short range nearest-neighbor interactions give rise to a spontaneous magnetization in absence of an external field?

Spontaneous magnetization

No external field

$$E(\vec{s}) = -J \sum_{<i,j>} s_i s_j$$

Spontaneous magnetization: Can the short range nearest-neighbor interactions give rise to a spontaneous magnetization in absence of an external field?

- **Large temperatures** $\frac{J}{k_B T} \ll 1$ **:**

No external field

$$E(\vec{s}) = -J \sum_{<i,j>} s_i s_j$$

Spontaneous magnetization: Can the short range nearest-neighbor interactions give rise to a spontaneous magnetization in absence of an external field?

- **Large temperatures** $\frac{J}{k_B T} \ll 1$ **:** **Thermal energy dominates:** spins are randomly up or down $m(T) = 0$

No external field

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Spontaneous magnetization: Can the short range nearest-neighbor interactions give rise to a spontaneous magnetization in absence of an external field?

- **Large temperatures** $\frac{J}{k_B T} \ll 1$ **:** **Thermal energy dominates:** spins are randomly up or down $m(T) = 0$
- **Low temperatures** $\frac{J}{k_B T} \gg 1$ **:**

No external field

$$E(\vec{s}) = -J \sum_{<i,j>} s_i s_j$$

Spontaneous magnetization: Can the short range nearest-neighbor interactions give rise to a spontaneous magnetization in absence of an external field?

- **Large temperatures** $\frac{J}{k_B T} \ll 1$ **:** **Thermal energy dominates:** spins are randomly up or down $m(T) = 0$
- **Low temperatures** $\frac{J}{k_B T} \gg 1$ **:** **Interaction term dominates:** spin tends to align to minimize the total energy

T=0: Configuration with minimal energy all the spin are aligned: $E_{\text{min}} = -J\, N_{\text{pairs}}$

either **all spins up:** $m(T) = +1$

or **all spins down:** $m(T) = -1$

—> **Spontaneous magnetization**

"symmetry breaking"

No external field

$$E(\vec{s}) = -J \sum_{<i,j>} s_i s_j$$

Spontaneous magnetization: Can the short range nearest-neighbor interactions give rise to a spontaneous magnetization in absence of an external field?

- **Large temperatures** $\frac{J}{k_B T} \ll 1$ **:** **Thermal energy dominates:** spins are randomly up or down $m(T) = 0$
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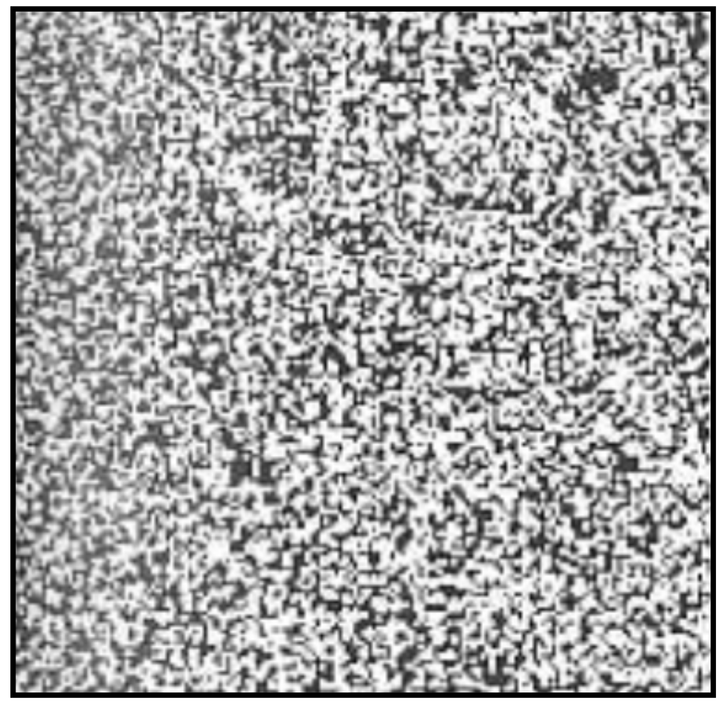
—> Spontaneous magnetization

$L = 150$

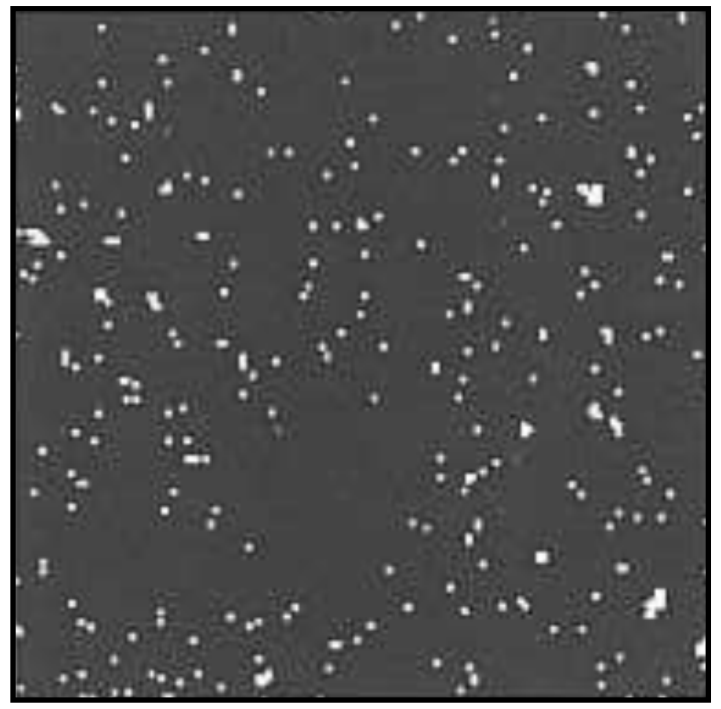
T "very large"



$T/T_c = 4$

Reduce T

T "very small"



$T/T_c = 0.75$

For T sufficiently small

—> Spontaneous magnetization

"symmetry breaking"

No external field

$$E(\vec{s}) = -J \sum_{<i,j>} s_i s_j$$

Spontaneous magnetization: Can the short range nearest-neighbor interactions give rise to a spontaneous magnetization in absence of an external field?

- **Large temperatures** $\frac{J}{k_B T} \ll 1$ **:** **Thermal energy dominates:** spins are randomly up or down $m(T) = 0$
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T=0: Configuration with minimal energy all the spin are aligned: $E_{\text{min}} = -J\, N_{\text{pairs}}$

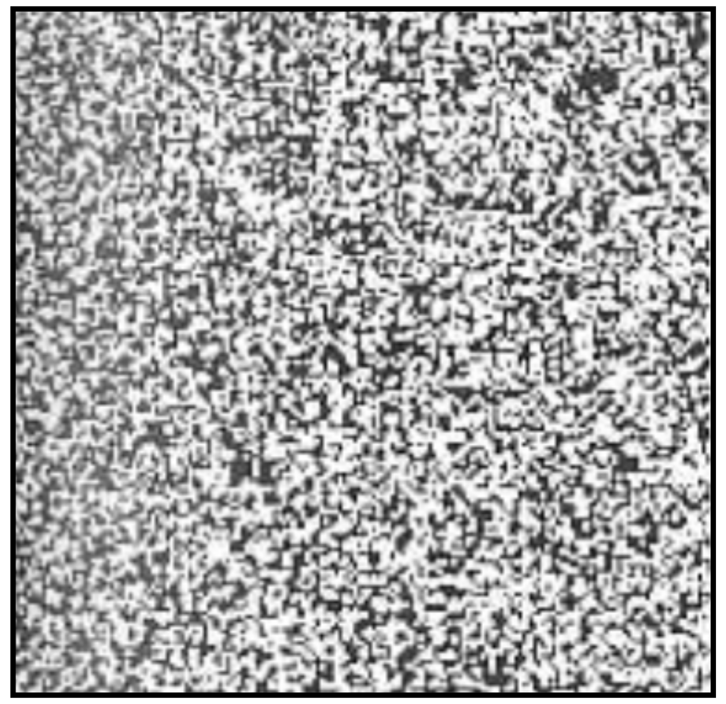
either **all spins up:** $m(T) = +1$

or **all spins down:** $m(T) = -1$

—> Spontaneous magnetization

$L = 150$

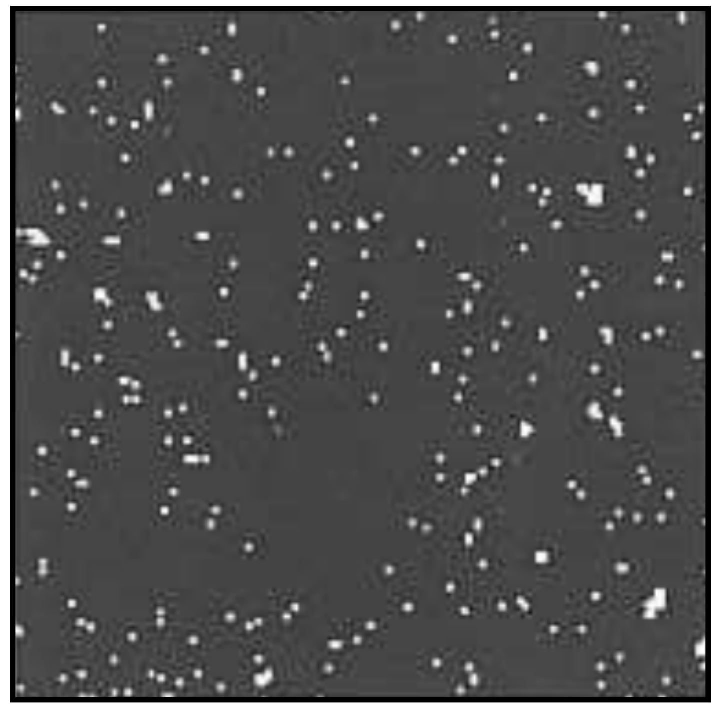
T "very large"



$T/T_c = 4$

Reduce T

T "very small"



$T/T_c = 0.75$

For T sufficiently small

—> Spontaneous magnetization

"symmetry breaking"

Possible phase transition when the thermal energy $k_B T$ and the interaction energy J are comparable.

Spontaneous magnetization

No external field

$$E(\vec{s}) = -J \sum_{<i,j>} s_i s_j$$

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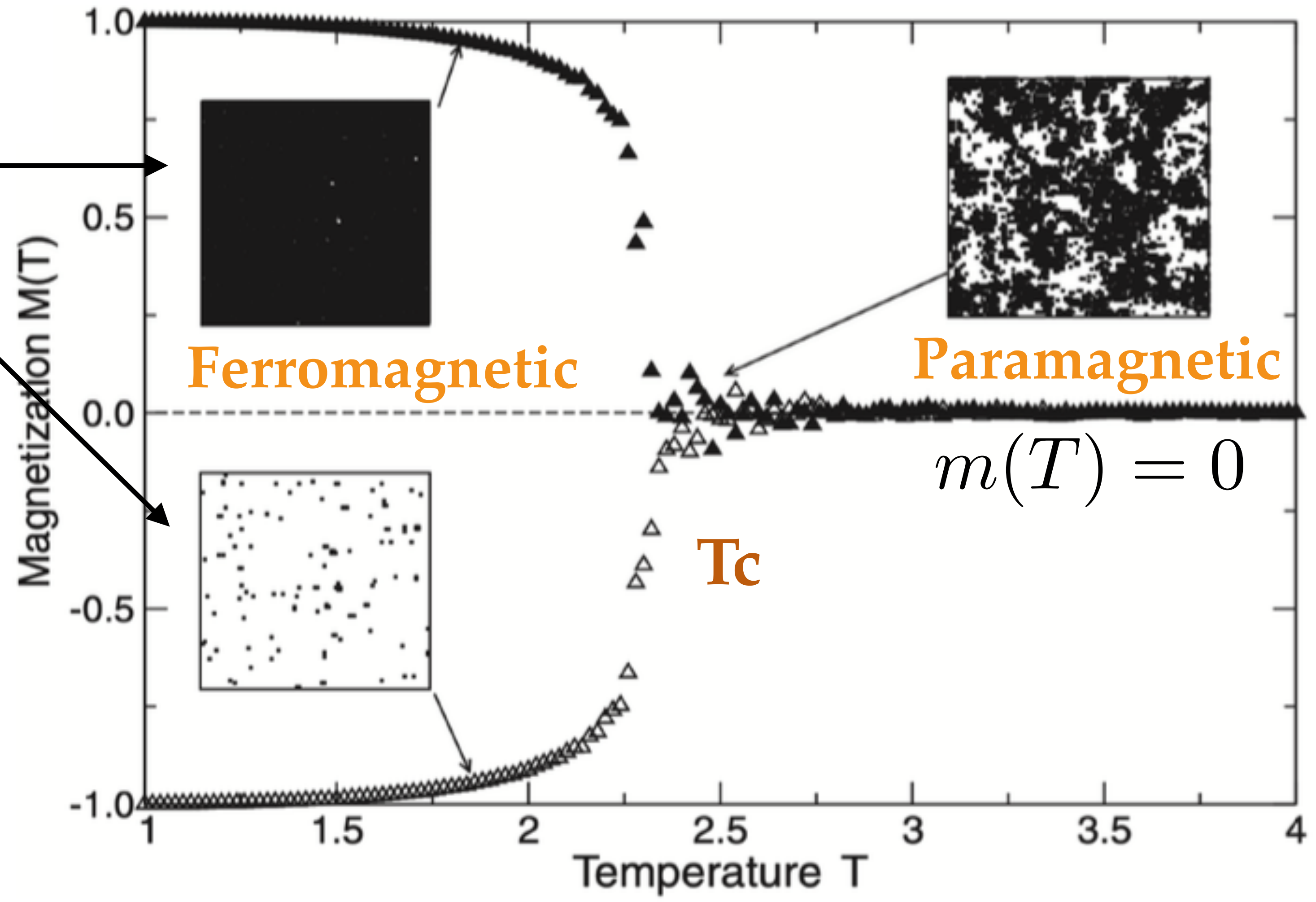
—> **Spontaneous magnetization**

$m(T) \neq 0$

Symmetry breaking

a symmetric state spontaneously ends up in an asymmetric state



$m(T) = 0$

Phase transition at Tc

Spontaneous magnetization

2) Interacting Spins

===>> Spontaneous magnetization

3) Symmetry breaking??

Symmetry breaking??

System with no field: $H = 0$ $$E(\vec{s}) = -J \sum_{<i,j>} s_i s_j$$ $$P(\vec{s}) = \frac{\mathrm{e}^{-\beta E(\vec{s})}}{Z}$$

Symmetry breaking??

System with no field: $H = 0$ $\qquad E(\vec{s}) = -J \sum_{<i,j>} s_i s_j \qquad P(\vec{s}) = \frac{e^{-\beta E(\vec{s})}}{Z}$

Take the microstates $\vec{s}$ and $-\vec{s}$: (all spin flipped)

They have — **same energy:** $E(\vec{s}) = E(-\vec{s}) \longrightarrow P(\vec{s}) = P(-\vec{s})$

— **opposite magnetization:** $M(\vec{s}) = -M(-\vec{s})$

Symmetry breaking??

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Average total magnetization: $\langle M \rangle = \sum_{\vec{s}} M(\vec{s})\, P(\vec{s})$

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Average total magnetization: $\langle M \rangle = \sum_{\vec{s}} M(\vec{s})\, P(\vec{s}) = 0$

as, for each state, there's a symmetric state with same probability but opposite magnetization

Symmetry breaking??

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Average total magnetization: $\langle M \rangle = \sum_{\vec{s}} M(\vec{s})\, P(\vec{s}) = 0$ at any T for $H = 0$

What's going on? Where is the phase transition???

Symmetry breaking??

System with very small field: $H \neq 0$
(we will take H —> 0 later)

$$E(\vec{s}) = -J \sum_{<i,j>} s_i s_j - H \sum_{i=1}^{N} s_i$$

$$P(\vec{s}) = \frac{\mathrm{e}^{-\beta E(\vec{s})}}{Z}$$

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Take the microstates $\vec{s}$ **and** $-\vec{s}$ **:**

Energy difference: $E(\vec{s}) - E(-\vec{s}) = -2H\, M(\vec{s})$ $\longrightarrow$ $\dfrac{P(\vec{s})}{P(-\vec{s})} = \exp(2\beta H M(\vec{s}))$

We recall that **M is an extensive quantity:** $\alpha(\vec{s}) = M(\vec{s})/N$ intensive $\longrightarrow$ $\dfrac{P(\vec{s})}{P(-\vec{s})} = \exp(2\beta H N \alpha(\vec{s}))$

- **Limit** $H \to 0$**:** we recover the previous result

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Thermodynamic limit $N \to \infty$**:**

Take a state $\vec{s}$ for which $M(\vec{s}) > 0$: Taking the **thermodynamic limit before taking H to 0**, we get:

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$$\lim_{H \to 0^{\pm}} \lim_{N \to \infty} \frac{P(\vec{s})}{P(-\vec{s})} = \begin{cases} \infty, & \text{for } H \to 0^{+} \\ 0, & \text{for } H \to 0^{-} \end{cases}$$

for $H \to 0^{+}$ $\xrightarrow{\text{i.e.}}$ configurations with $M(\vec{s}) > 0$ have probability 1

for $H \to 0^{-}$ $\longrightarrow$ configurations with $M(\vec{s}) < 0$ have probability 1

Symmetry breaking??

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(we will take H —> 0 later)

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A tiny H breaks the symmetry among the spin configurations!

Symmetry breaking??

Thermodynamic limit $N \to \infty$ **and limit** $H \to 0^{\pm}$ **are not interchangeable:**

$$\lim_{N\to\infty} \lim_{H\to 0^{\pm}} \langle M \rangle = 0$$

$$\lim_{H\to 0^{\pm}} \lim_{N\to\infty} \langle M \rangle \neq 0$$

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$$\lim_{H\to 0^{\pm}} \lim_{N\to\infty} \langle M \rangle = N m_0 \neq 0 \longrightarrow \textbf{Spontaneous magnetization}$$

definition of m_0

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Below Tc:

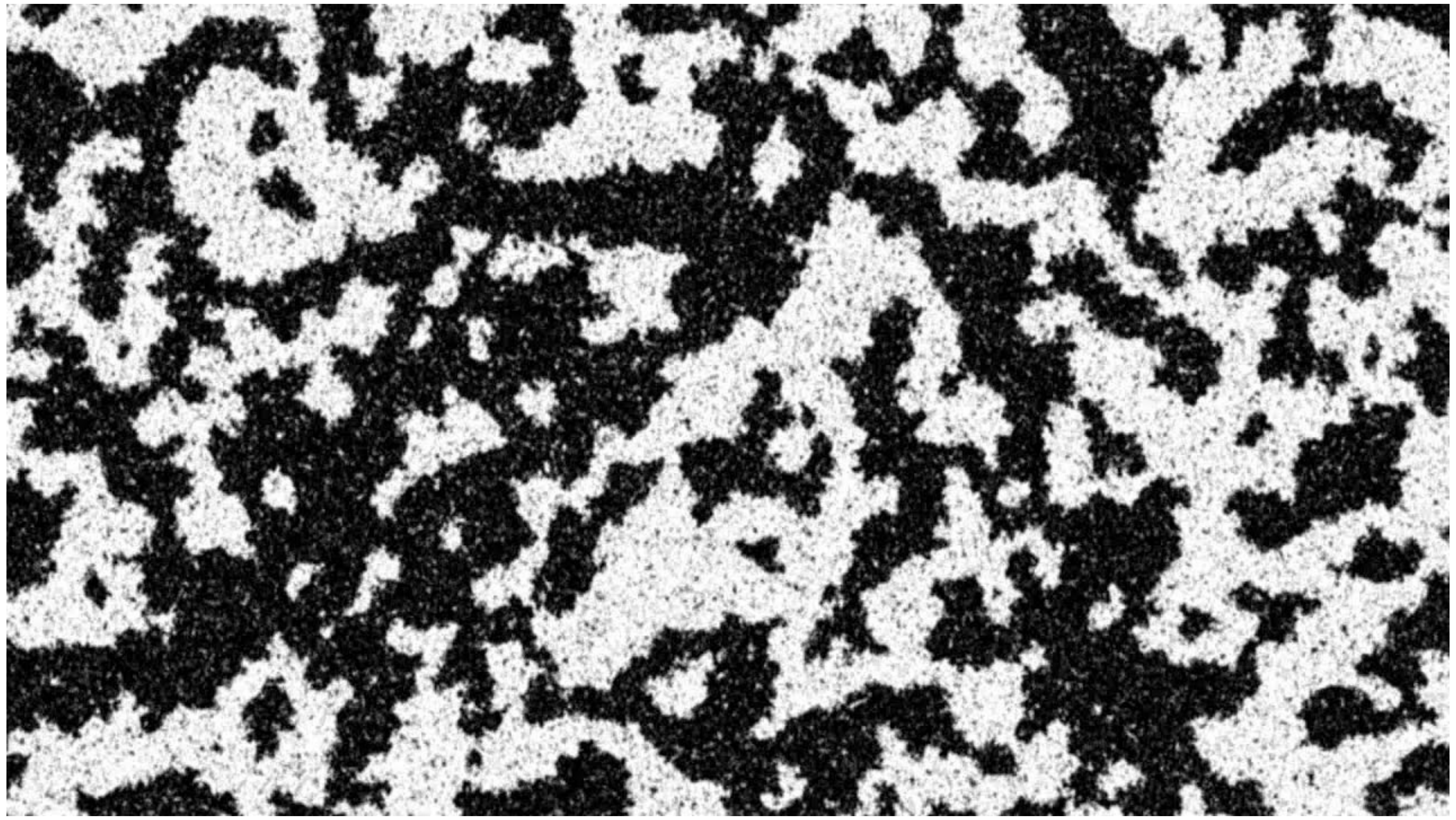
Finite size system: Temporal average of the magnetization over a sufficiently long time will give 0

as the system spend equal time in ***m*** and ***-m***

Infinite size system: spontaneous symmetry breaking

System will spend all its time in only one phase determined by the initial conditions.

II - Phase transition in the Ising model



1) Control parameter, Order parameter

Continuous phase transition?

$$E(\vec{s}) = -J \sum_{<i,j>} s_i s_j$$

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either **all spins up:** $m(T) = +1$

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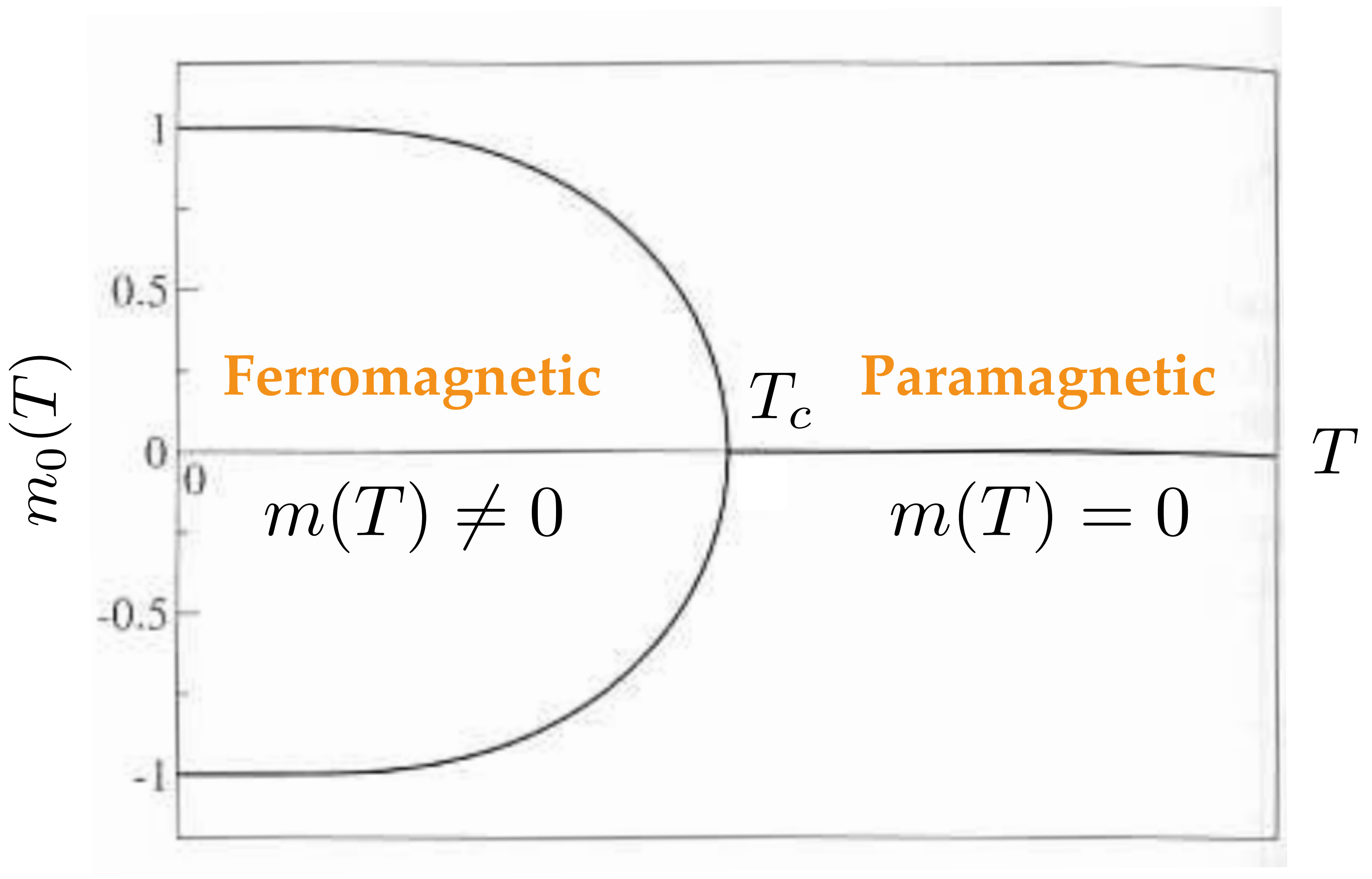
——>>> **There may be a phase transition when the thermal energy** $k_B T$ **and the interaction energy** J **are comparable.**



Control parameter: T

By changing T we expect to have a phase transition when kT ~ J

Order parameter: $m(T) = \dfrac{\langle M(T) \rangle}{N}$

For T > Tc, disorder **:** $m(T) = 0$

For T < Tc, order **:** $m(T) \neq 0$

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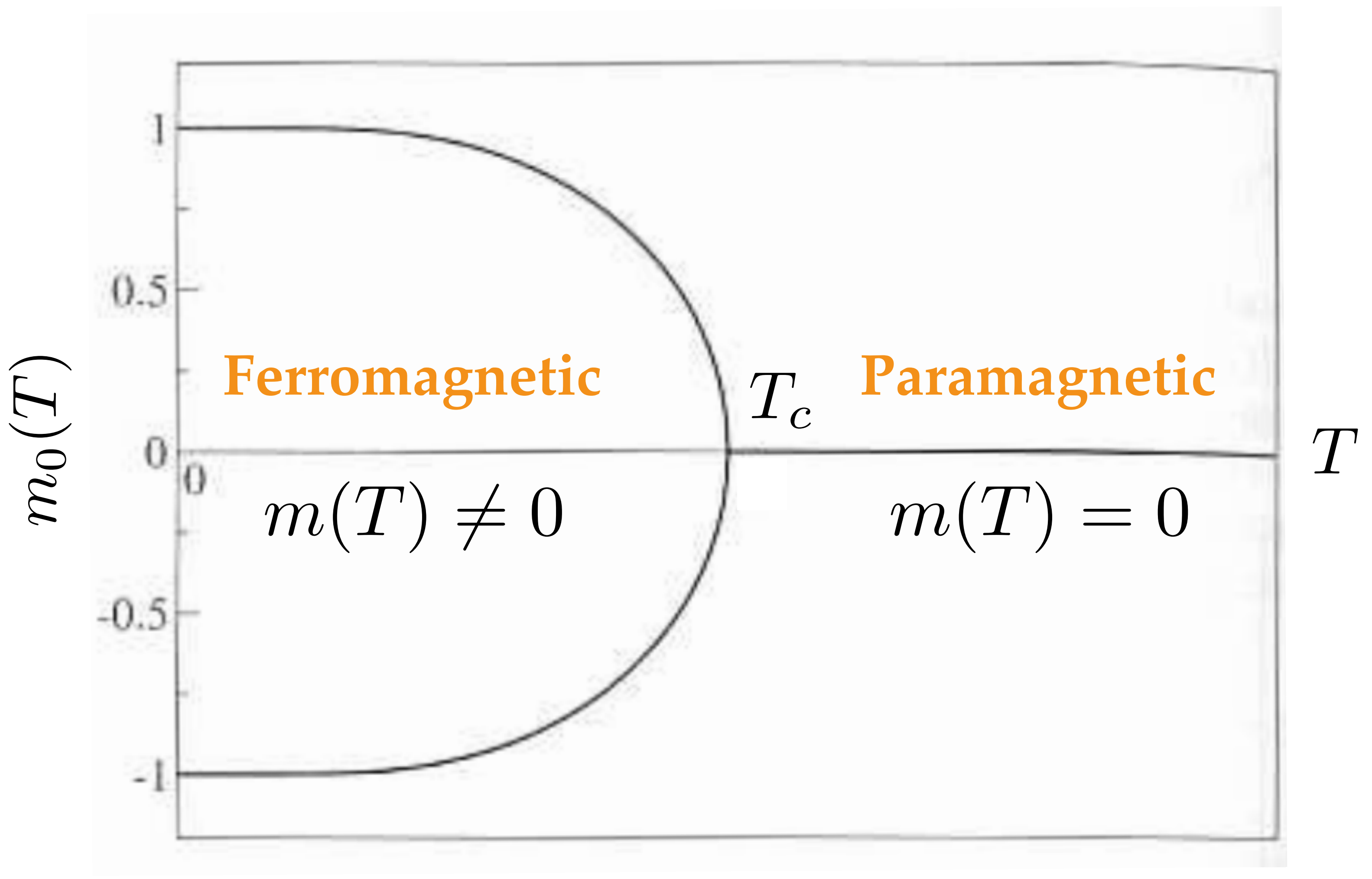

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a continuous but sudden pick-up of a magnetization at the critical temperature

(cf. curve for the difference in density in the fluid to liquid-solid phase transition)

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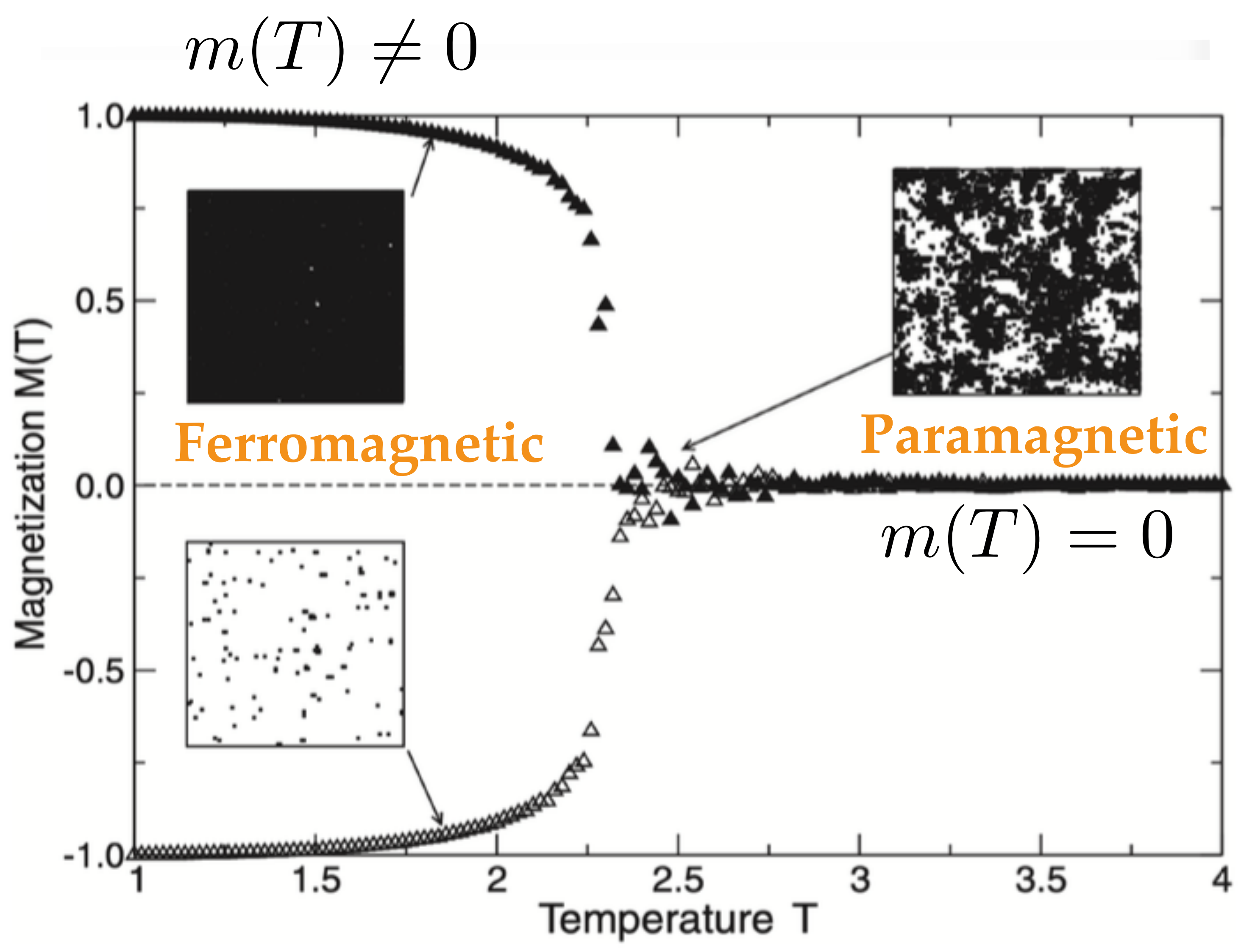

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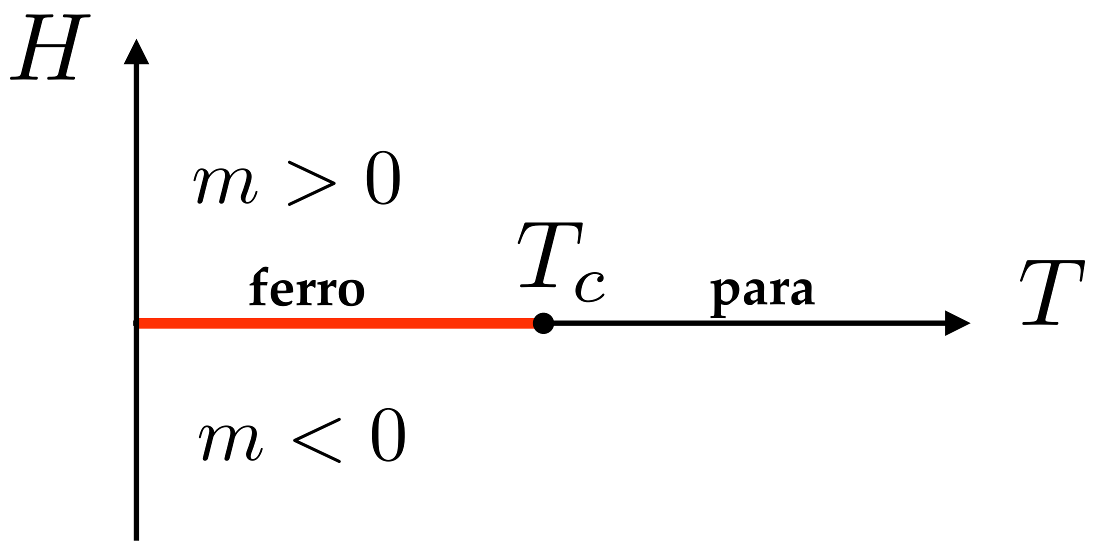
Analogy: ferromagnetic materials and fluids

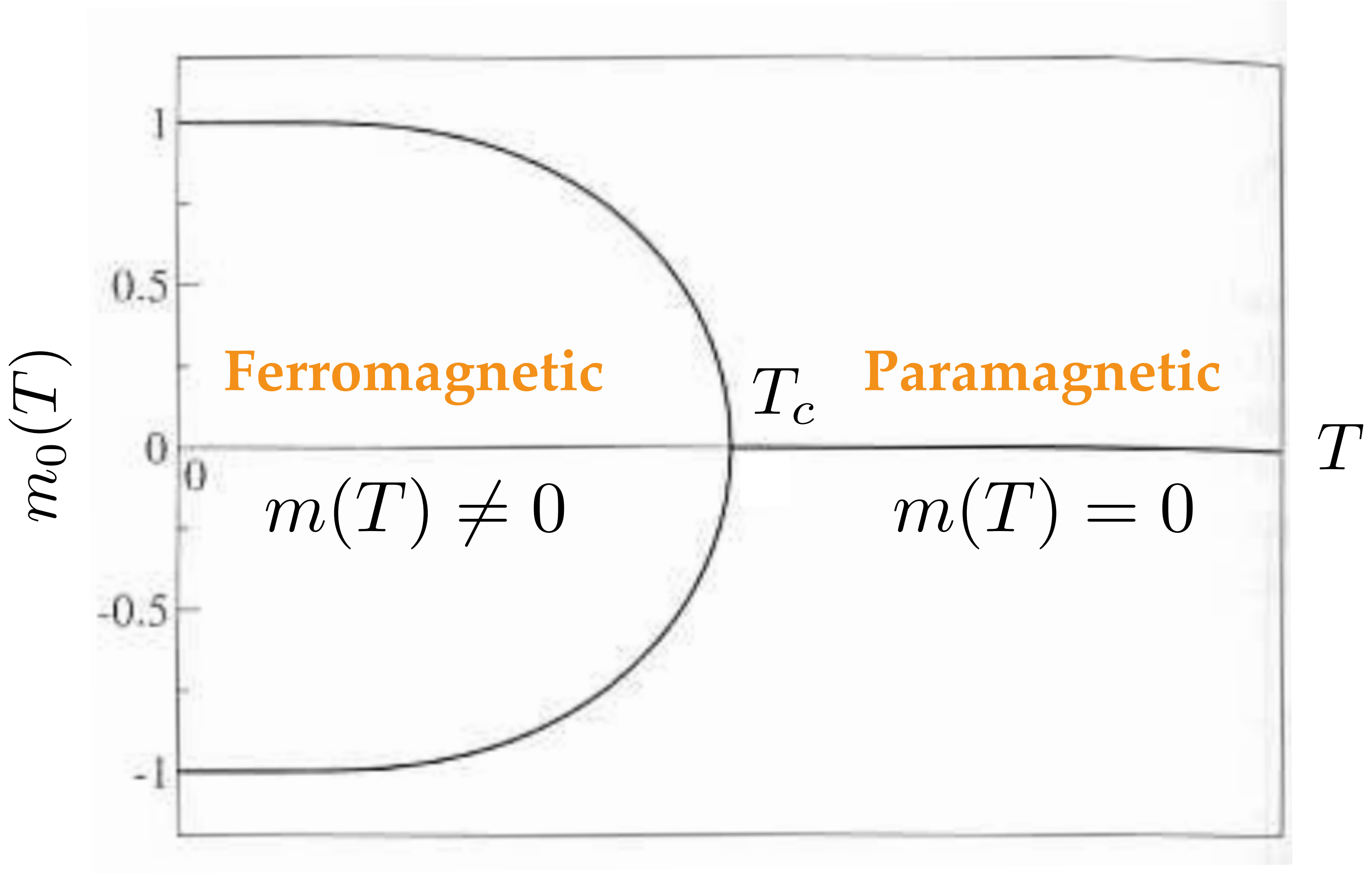
Ferromagnetic materials

Coontrol parameters: T, H

Phase diagram:



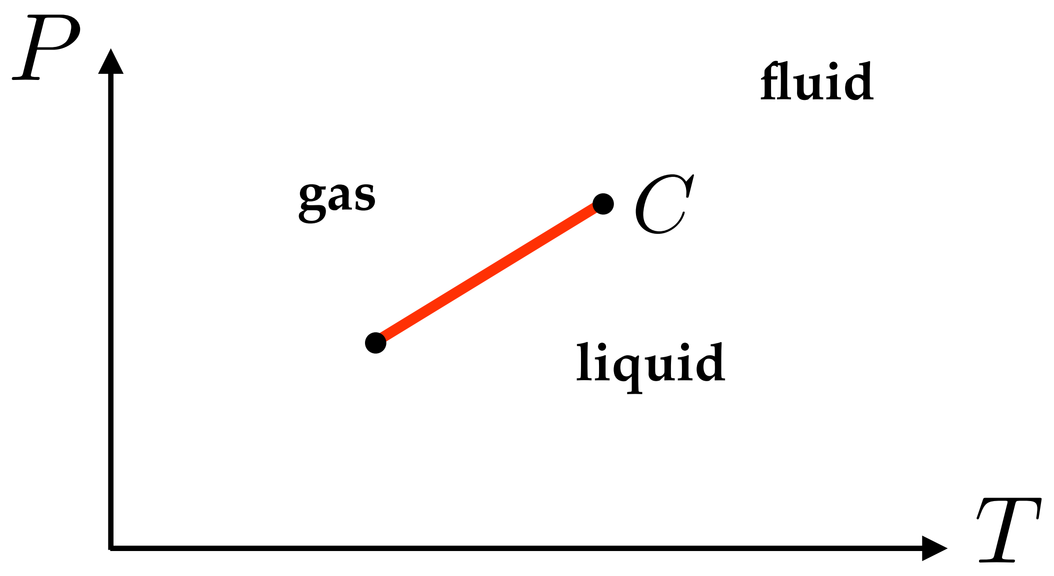
Order parameter: m



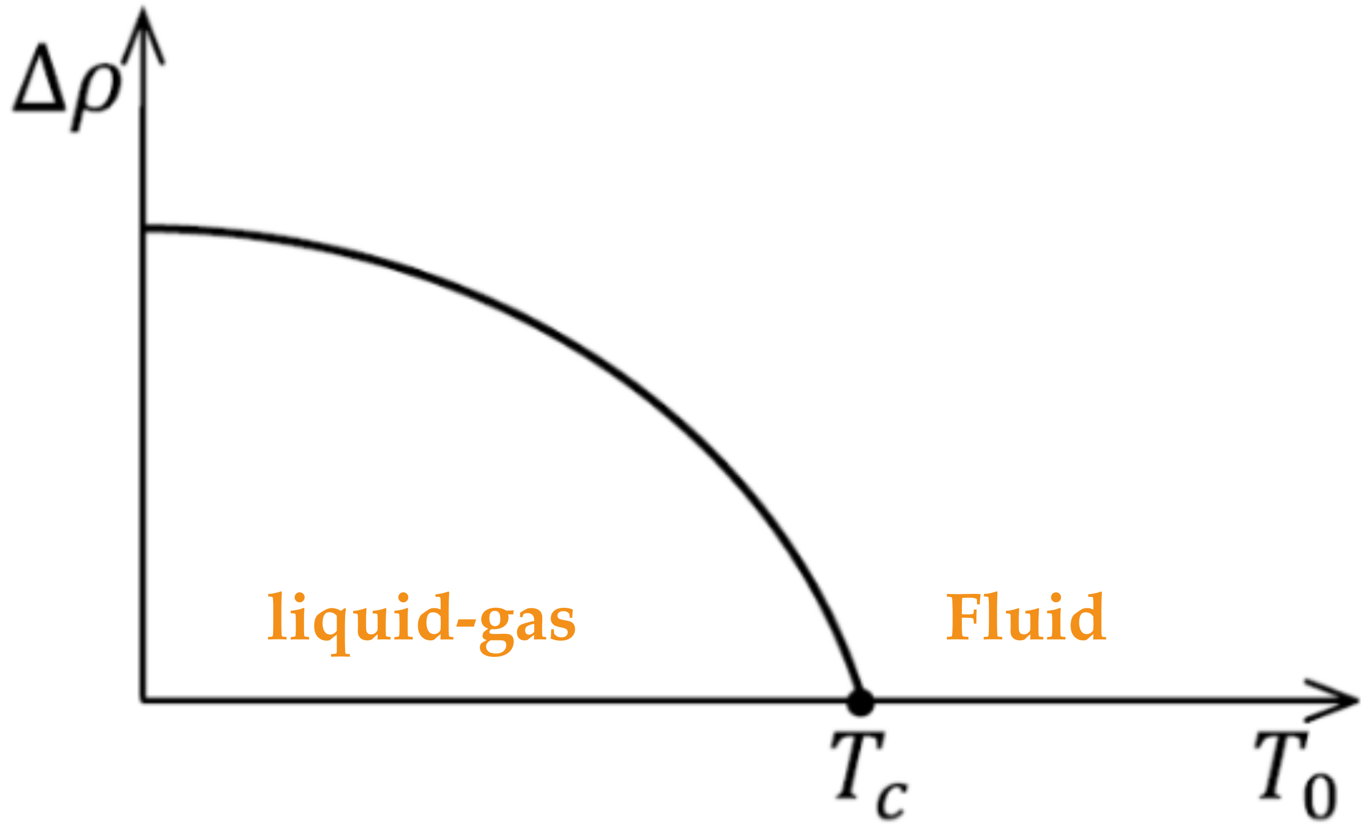
Fluids

Control parameters: T, P

Phase diagram:



Order parameter: $\Delta\rho = \rho_{liq} - \rho_{vap}$



2) 1-dimensional Ising model

1d Ising model

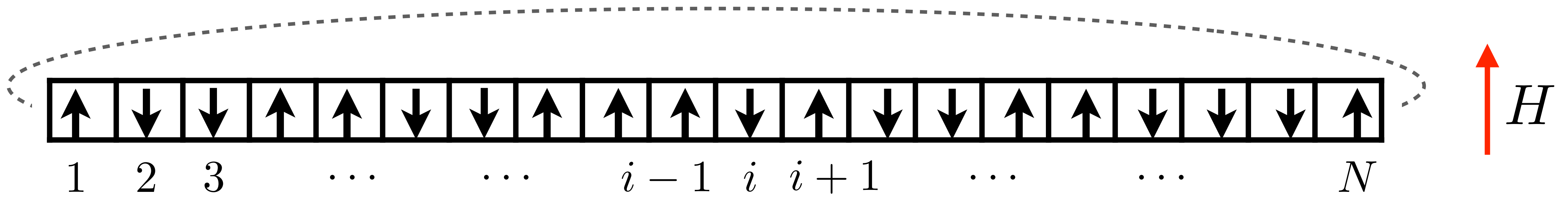
System with small field: $H \neq 0$

$$E(\vec{s}) = -J\sum_{i=1}^{N} s_i s_{i+1} - H\sum_{i=1}^{N} s_i \qquad \text{with} \qquad s_{N+1} = s_1$$

$s_i = \pm 1$

with periodic boundary conditions:

In the thermodynamic limit (N large) the boundary condition will not matter



1d Ising model

System with small field: $H \neq 0$ $\quad E(\vec{s}) = -J \sum_{i=1}^{N} s_i s_{i+1} - H \sum_{i=1}^{N} s_i$ with $s_{N+1} = s_1$

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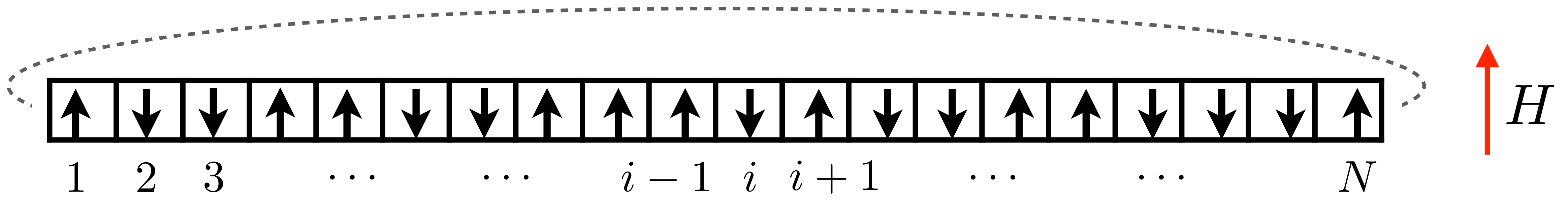

Partition function:

$$Z = \sum_{\vec{s}} \exp(-\beta E(\vec{s}))$$

$$= \sum_{\vec{s}} \exp\left(\beta J \sum_{i=1}^{N} s_i s_{i+1} + \beta H \sum_{i=1}^{N} s_i\right)$$

using the transfer matrix method (Ising 1925)

1d Ising model

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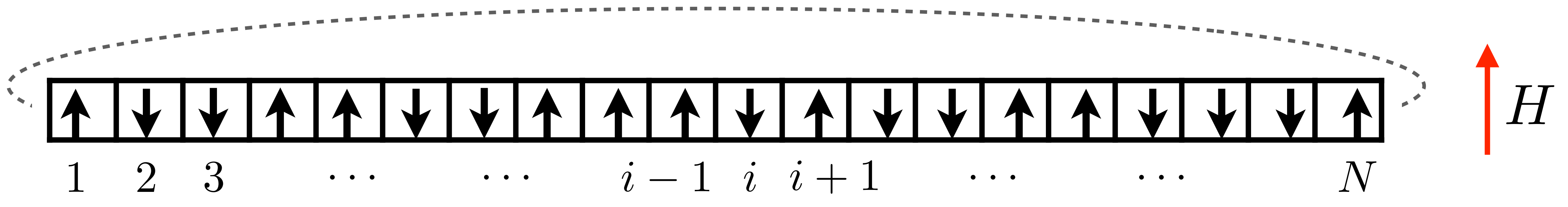

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$$= \sum_{\vec{s}} \exp\left(\beta J \sum_{i=1}^{N} s_i s_{i+1} + \beta H \sum_{i=1}^{N} s_i\right)$$

$$= \sum_{\vec{s}} \exp\left(\beta J \sum_{i=1}^{N} s_i s_{i+1} + \beta \frac{H}{2} \sum_{i=1}^{N} (s_i + s_{i+1})\right)$$

symmetric in i, i+1

$$= \sum_{\vec{s}} \exp\left(\beta J s_1 s_2 + \beta \frac{H}{2}(s_1 + s_2)\right) \cdots \exp\left(\beta J s_N s_1 + \beta \frac{H}{2}(s_N + s_1)\right)$$

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Transfer matrix: 2x2 matrix with coefficients $t_{s_i s_{i+1}} = \exp\left(\beta J s_i s_{i+1} + \beta \frac{H}{2}(s_i + s_{i+1})\right)$

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$$\boldsymbol{T} = \begin{pmatrix} t_{1,1} & t_{1,-1} \\ t_{-1,1} & t_{-1,-1} \end{pmatrix}$$

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Partition function: $Z = \sum_{\vec{s}} \prod_{i=1}^{N} t_{s_i s_{i+1}}$

$$= \sum_{s_1 = \pm 1} \cdots \sum_{s_N = \pm 1} t_{s_1 s_2} \cdots t_{s_{N-1} s_N} t_{s_N s_1}$$

Partition Function

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$$= \sum_{s_1 = \pm 1} \cdots \sum_{s_N = \pm 1} \left(\sum_{s_2 = \pm 1} t_{s_1 s_2} t_{s_2 s_3} \right) \cdots t_{s_{N-1} s_N} \, t_{s_N s_1}$$

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$$Z = \sum_{\vec{s}} \exp\left(\beta J s_1 s_2 + \beta \frac{H}{2}(s_1 + s_2)\right) \cdots \exp\left(\beta J s_N s_1 + \beta \frac{H}{2}(s_N + s_1)\right)$$

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Partition function:

$$Z = \sum_{\vec{s}} \prod_{i=1}^{N} t_{s_i s_{i+1}}$$

$$= \sum_{s_1=\pm 1} \cdots \sum_{s_N=\pm 1} t_{s_1 s_2} \cdots t_{s_{N-1} s_N} \, t_{s_N s_1}$$

$$= \sum_{s_1=\pm 1} \cdots \sum_{s_N=\pm 1} \left(\sum_{s_2=\pm 1} t_{s_1 s_2} t_{s_2 s_3} \right) \cdots t_{s_{N-1} s_N} \, t_{s_N s_1}$$

matrix multiplication:

$$(AB)_{ij} = \sum_{k=1}^{n} A_{ik} B_{kj}$$

Partition Function

$$Z = \sum_{\vec{s}} \exp\left(\beta J s_1 s_2 + \beta \frac{H}{2}(s_1 + s_2)\right) \cdots \exp\left(\beta J s_N s_1 + \beta \frac{H}{2}(s_N + s_1)\right)$$

Transfer matrix: 2x2 matrix with coefficients $t_{s_i s_{i+1}} = \exp\left(\beta J s_i s_{i+1} + \beta \frac{H}{2}(s_i + s_{i+1})\right)$

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matrix multiplication:

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matrix multiplication:

$$(AB)_{ij} = \sum_{k=1}^{n} A_{ik} B_{kj}$$

$$= \sum_{s_1=\pm 1} \sum_{s_N=\pm 1} (\boldsymbol{T}^{N-1})_{s_1 s_N} t_{s_N s_1} = \sum_{s_1=\pm 1} (\boldsymbol{T}^N)_{s_1 s_1}$$

1D Ising model

Partition Function

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$$\begin{aligned} Z &= \sum_{\vec{s}} \prod_{i=1}^{N} t_{s_i s_{i+1}} \\ &= \sum_{s_1=\pm 1} \cdots \sum_{s_N=\pm 1} t_{s_1 s_2} \cdots t_{s_{N-1} s_N} t_{s_N s_1} \\ &= \sum_{s_1=\pm 1} \cdots \sum_{s_N=\pm 1} \left(\sum_{s_2=\pm 1} t_{s_1 s_2} t_{s_2 s_3}\right) \cdots t_{s_{N-1} s_N} t_{s_N s_1} \\ &= \sum_{s_1=\pm 1} \sum_{s_N=\pm 1} (\boldsymbol{T}^{N-1})_{s_1 s_N} t_{s_N s_1} = \sum_{s_1=\pm 1} (\boldsymbol{T}^N)_{s_1 s_1} \end{aligned}$$

matrix multiplication:

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$$Z = \mathrm{Tr}(\boldsymbol{T}^N)$$

Partition Function: finally!

Partition function: $Z = \mathrm{Tr}(\boldsymbol{T}^N)$ where $\boldsymbol{T} = \begin{pmatrix} t_{1,1} & t_{1,-1} \\ t_{-1,1} & t_{-1,-1} \end{pmatrix} = \begin{pmatrix} e^{(\beta J+\beta H)} & e^{-\beta J} \\ e^{-\beta J} & e^{(\beta J-\beta H)} \end{pmatrix}$

$Z = \lambda_+^N + \lambda_-^N$ where $\lambda_\pm$ eigenvalues of $\boldsymbol{T}$

$$\lambda_\pm = \exp(\beta J)\left(\cosh\beta H \pm \sqrt{\sinh^2\beta H + \exp(-4\beta J)}\right)$$ solutions of $\det(\boldsymbol{T} - \lambda \boldsymbol{I}) = 0$

Special cases:

J=0: $\lambda_+ = 2\cosh\beta H$ and $\lambda_- = 0$ We recover $Z = (2\cosh\beta H)^N$ **OK!**

H=0: $\lambda_+ = 2\cosh\beta J$ and $\lambda_- = 2\sinh\beta J$

Thermodynamic limit: $Z(T,0) \to (2\cosh\beta J)^N$ when $N \to +\infty$ (using that $\lambda_-/\lambda_+ = \tanh\beta J < 1$)

Thermodynamic limit: $Z(T,H) \underset{N\to+\infty}{\sim} \lambda_+^N$ as $\lambda_-/\lambda_+ < 1$

Free Energy

Free energy: $F(T, H) = -k_B T \log Z$

Free Energy

Free energy:

$$
\begin{aligned}
F(T,H) &= -k_B T \log Z \\
&= -k_B T \log \lambda_+^N \qquad \text{for } N \to +\infty \\
&= -N k_B T \left[\beta J + \log \left(\cosh \beta H + \sqrt{\sinh^2 \beta H + \exp(-4\beta J)} \right) \right]
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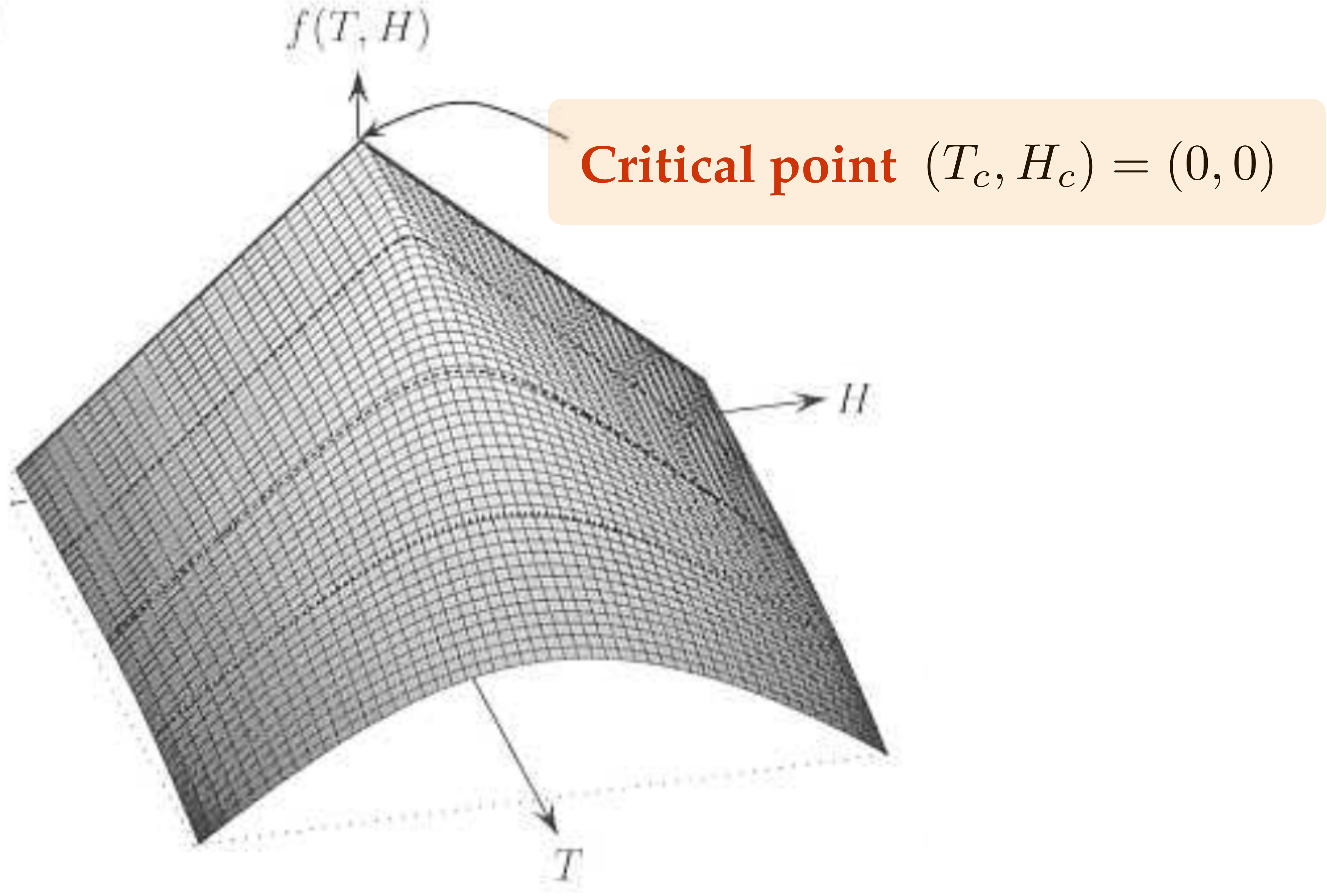


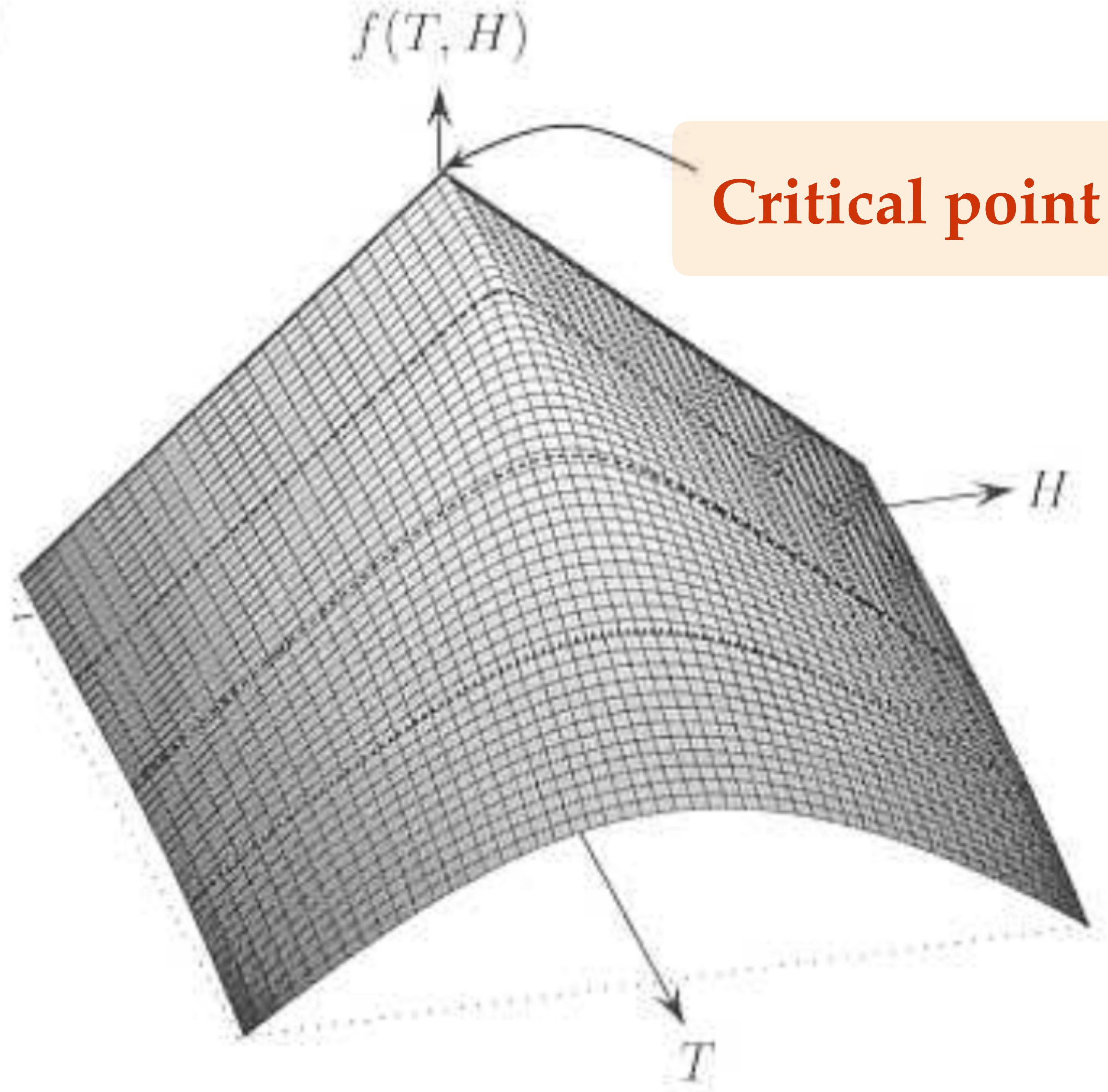
Analytic everywhere, except at $(0,0)$

1D Ising model

Free Energy

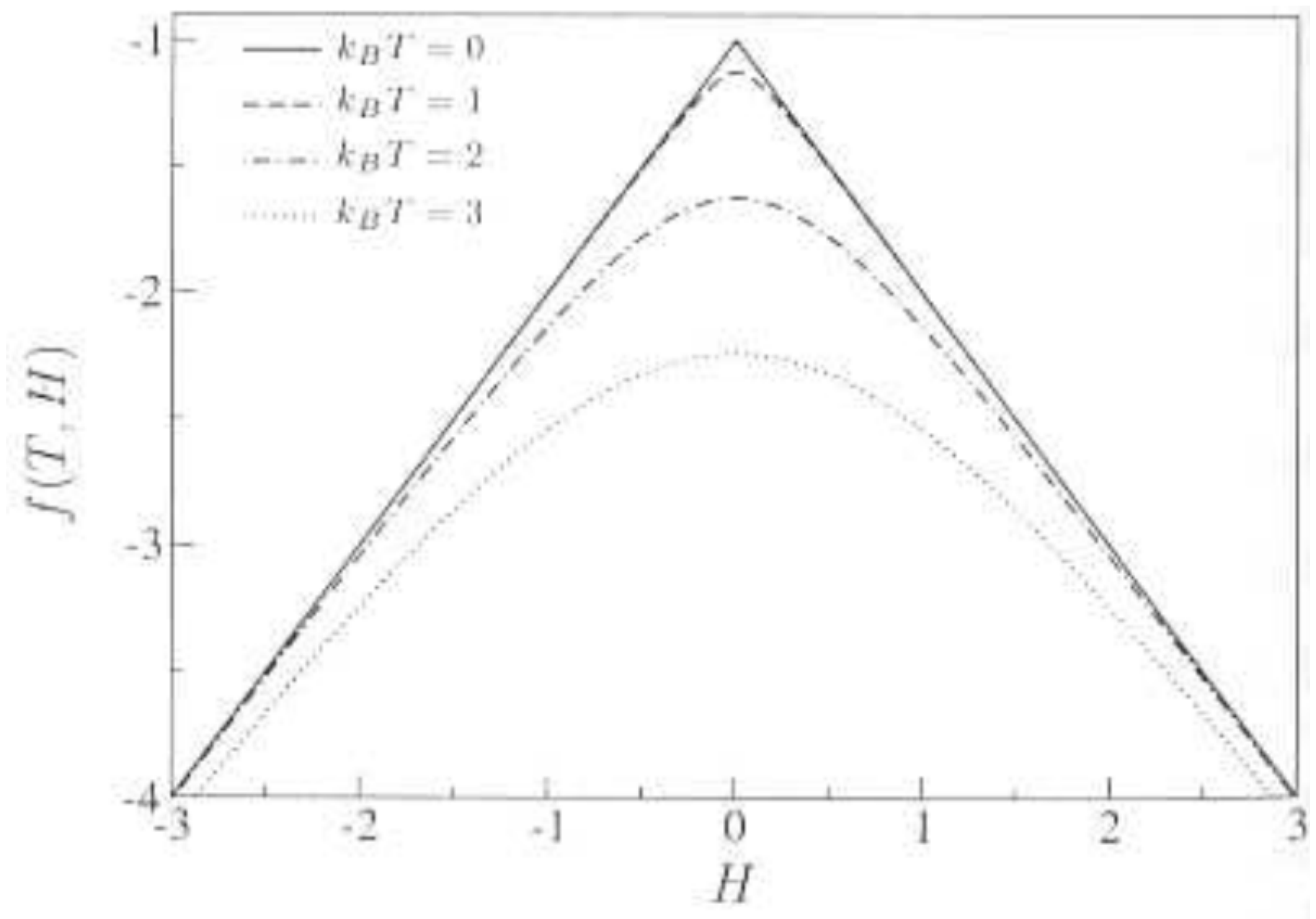
Free energy:

$$\begin{aligned} F(T,H) &= -k_B T \log Z \\ &= -k_B T \log \lambda_+^N \qquad \text{for } N \to +\infty \\ &= -N k_B T \left[\beta J + \log \left(\cosh \beta H + \sqrt{\sinh^2 \beta H + \exp(-4\beta J)} \right) \right] \end{aligned}$$



Critical point $(T_c, H_c) = (0, 0)$

Analytic everywhere, except at $(0, 0)$



For T > 0: F is analytic everywhere

For T = 0: **singular point at H=0**

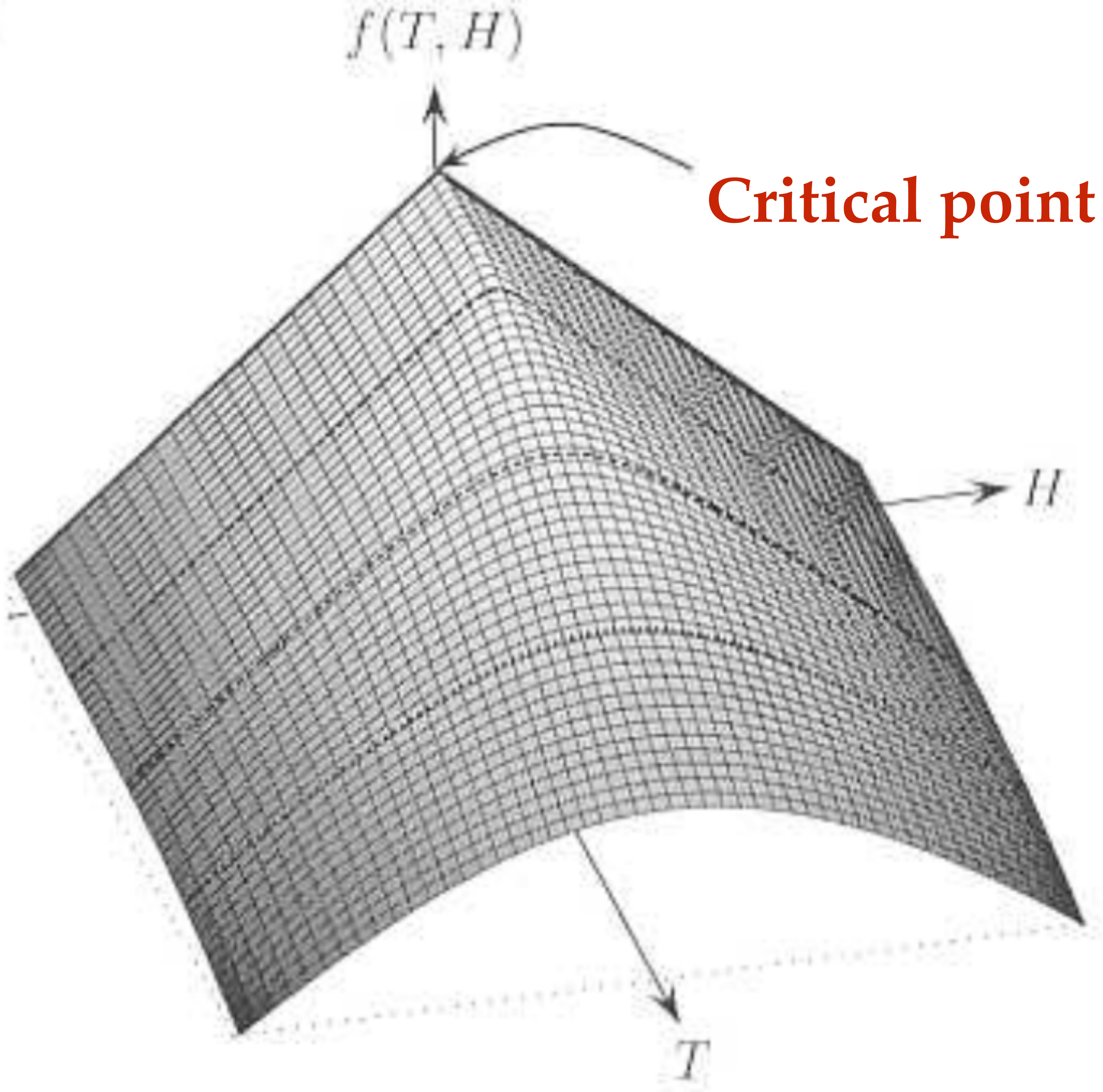
Free Energy

Free energy:

$$F(T,H) = -k_B T \log Z$$
$$= -k_B T \log \lambda_+^N \qquad \text{for } N \to +\infty$$
$$= -N k_B T \left[\beta J + \log \left(\cosh \beta H + \sqrt{\sinh^2 \beta H + \exp(-4\beta J)} \right) \right]$$

Limit H—> 0:

$$f(T,0) = -k_B T \log(2 \cosh \beta J)$$
$$\xrightarrow[N\to\infty]{} \begin{cases} -k_B T \log 2 & \text{for } T \to +\infty \\ -J & \text{for } T \to 0 \end{cases}$$



Rem: $N\,f = \langle E \rangle - TS$

for $T \to +\infty$: E=0 and f is determined by the maximization of S: $S = N k_B \log(2)$

for $T \to 0$: S=0 and f is determined by the minimization of <E>: $\langle E \rangle = -NJ$

Average Magnetization

Free energy:

$$f(T,H) = -k_B T \left[\beta J + \log\left(\cosh\beta H + \sqrt{\sinh^2\beta H + \exp(-4\beta J)} \right) \right]$$

Average magnetization per spin:

$$m(T,H) = -\left(\frac{\partial f}{\partial H}\right)_T = \frac{\sinh\beta H}{\sinh^2\beta H + \exp(-4\beta J)}$$

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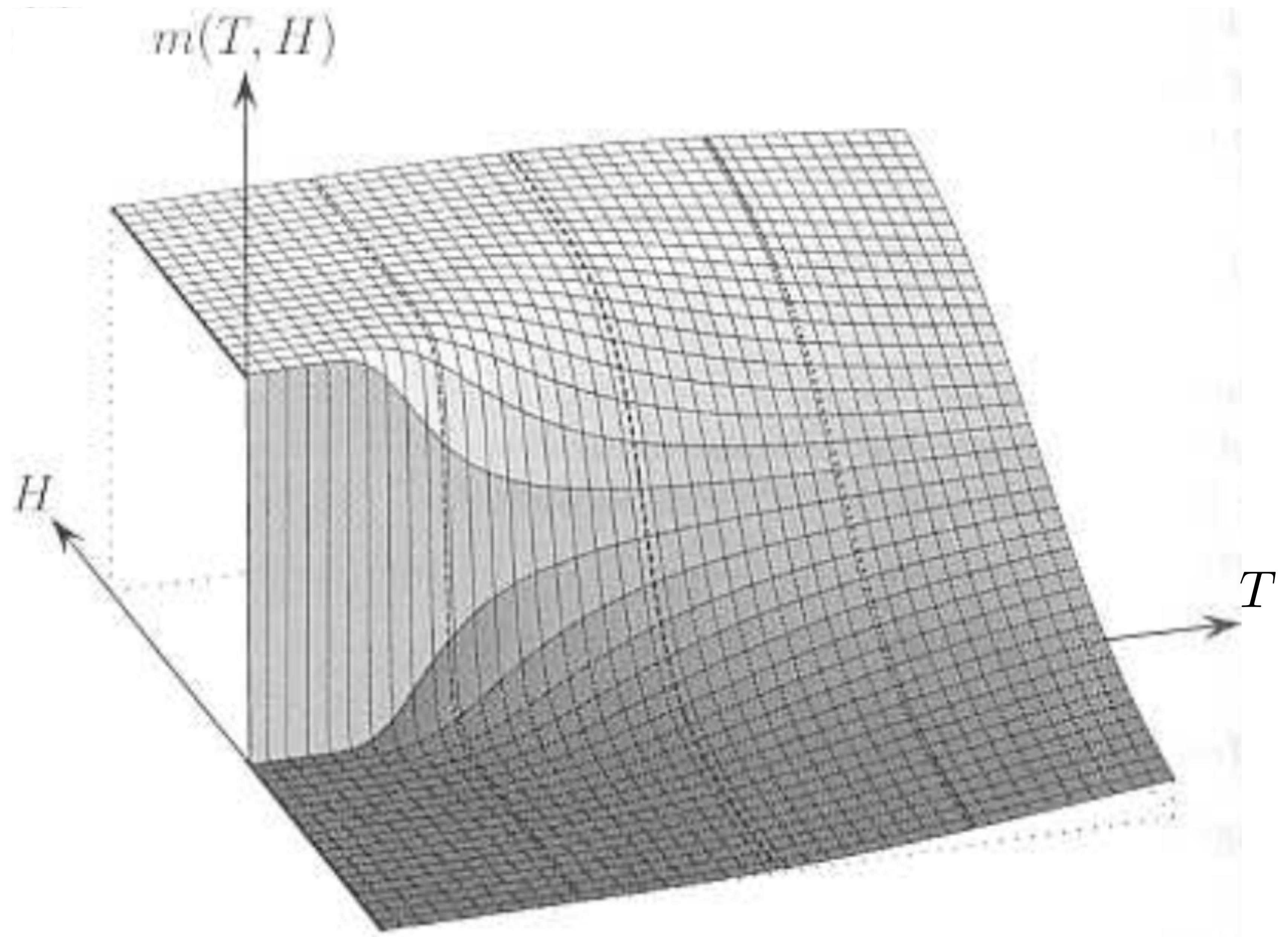
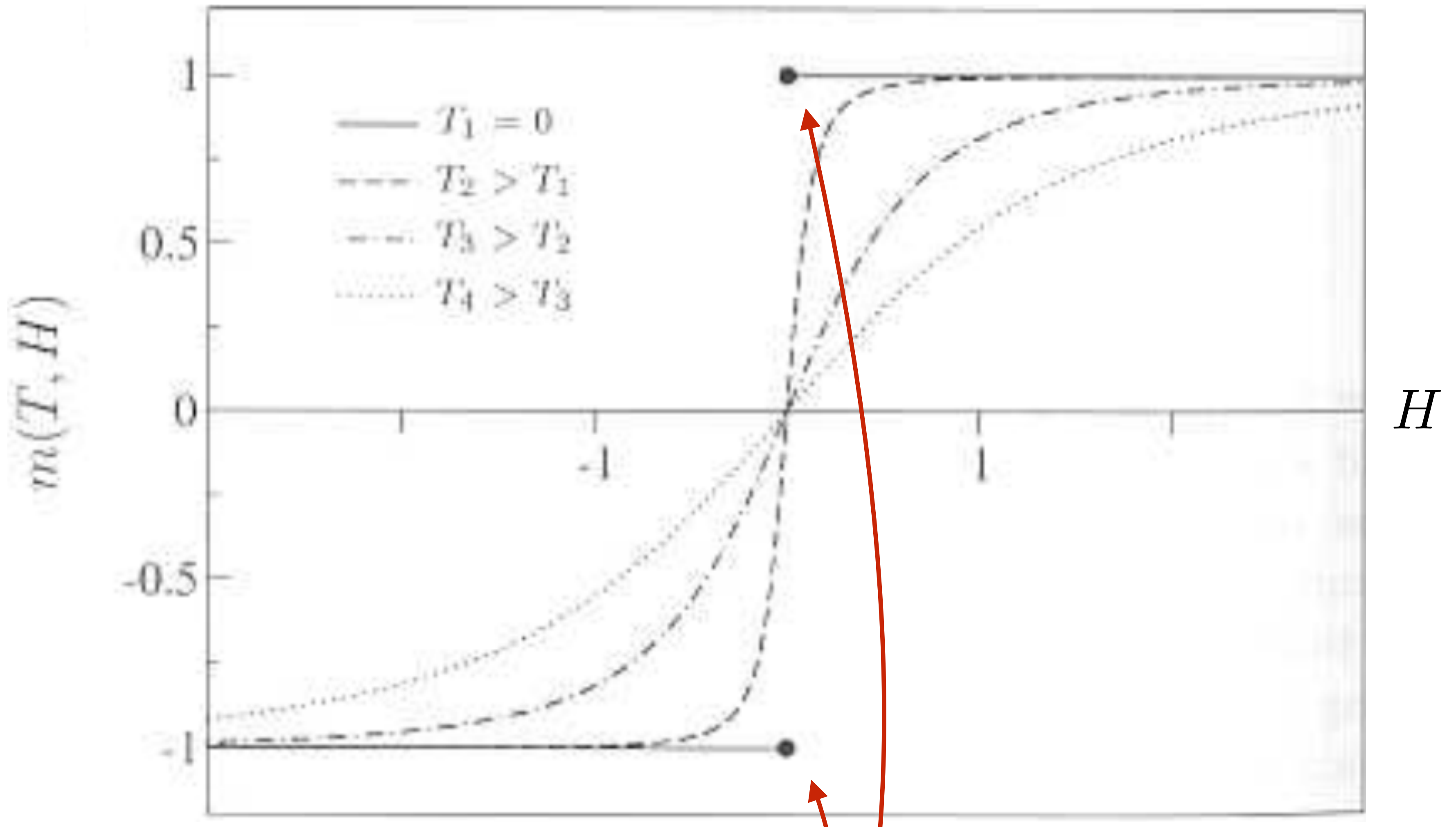


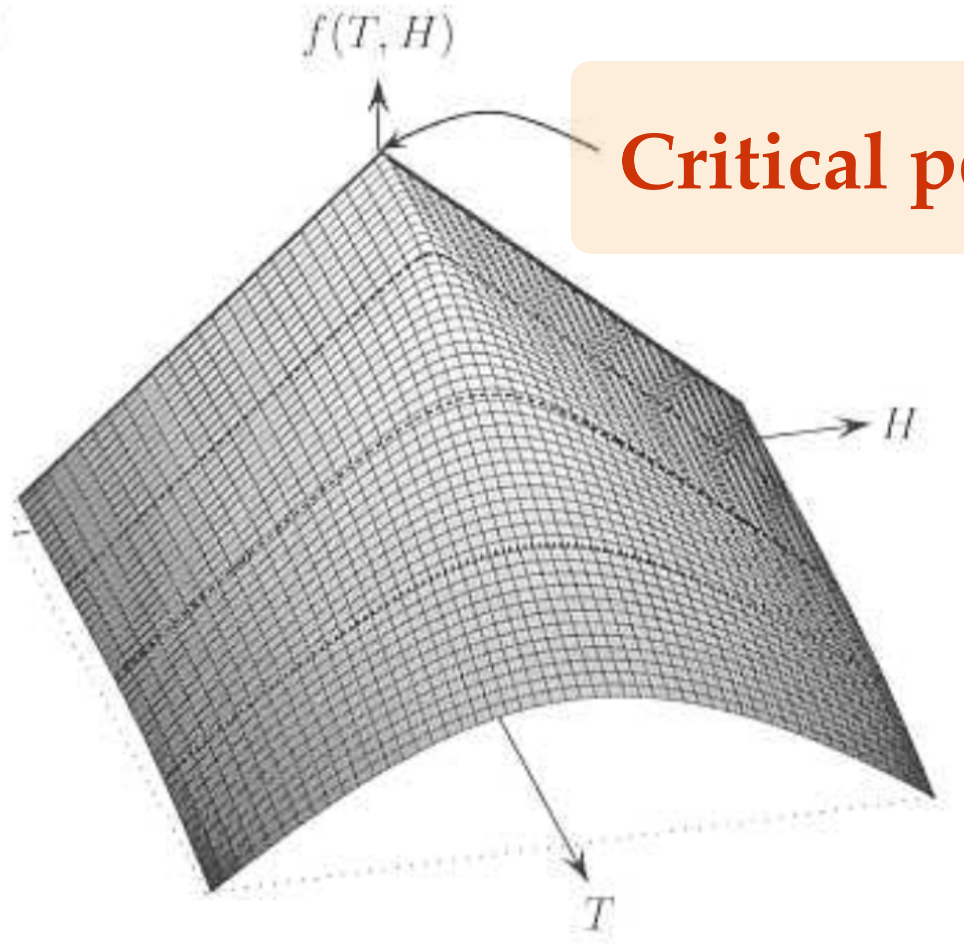


$$m_0(T) = \lim_{H\to 0^\pm} m(T,H) = \begin{cases} 0 & \text{for } T > 0 \\ \pm 1 & \text{for } T = 0 \end{cases}$$

Spontaneous magnetization at (Tc, Hc) = (0, 0) !!!!

1d Ising Summary

System with small field: $H \neq 0$ $\qquad E(\vec{s}) = -J\sum_{i=1}^{N} s_i s_{i+1} - H\sum_{i=1}^{N} s_i$ with $s_{N+1} = s_1$



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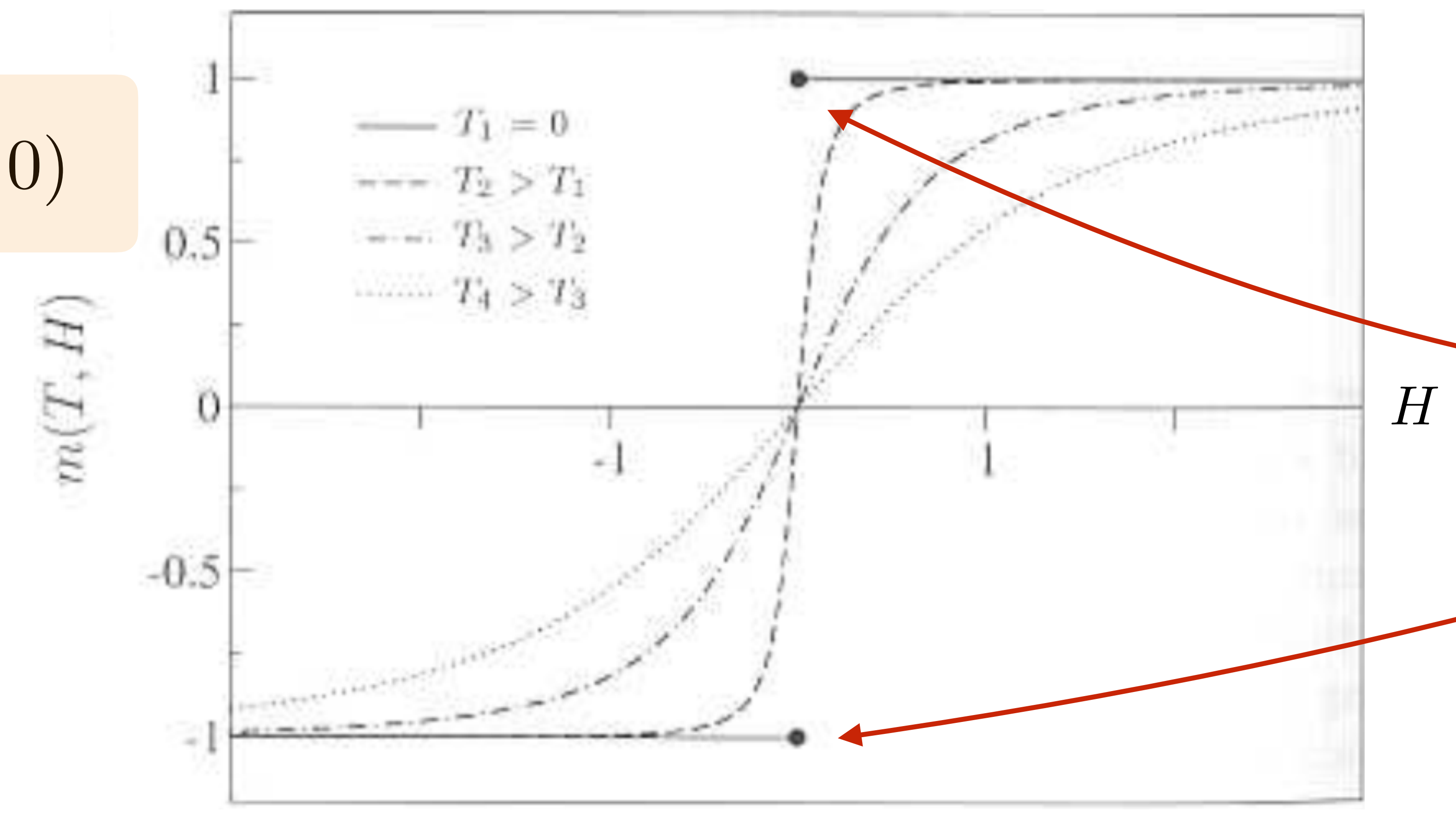

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Spontaneous magnetization !!!!

2) 2-dimensional Ising model

2D Ising model

Exact solution for H=0 by Onsager (1944):

proves the existence of a critical phase transition at $$k_B T_c = \frac{2J}{\log(1+\sqrt{2})} \simeq 2.269\,J$$

with a magnetization: $$m(T) = \lim_{H\to 0^+} \lim_{N\to +\infty} \frac{1}{N} \left\langle \sum_{i=1}^{N} s_i \right\rangle$$

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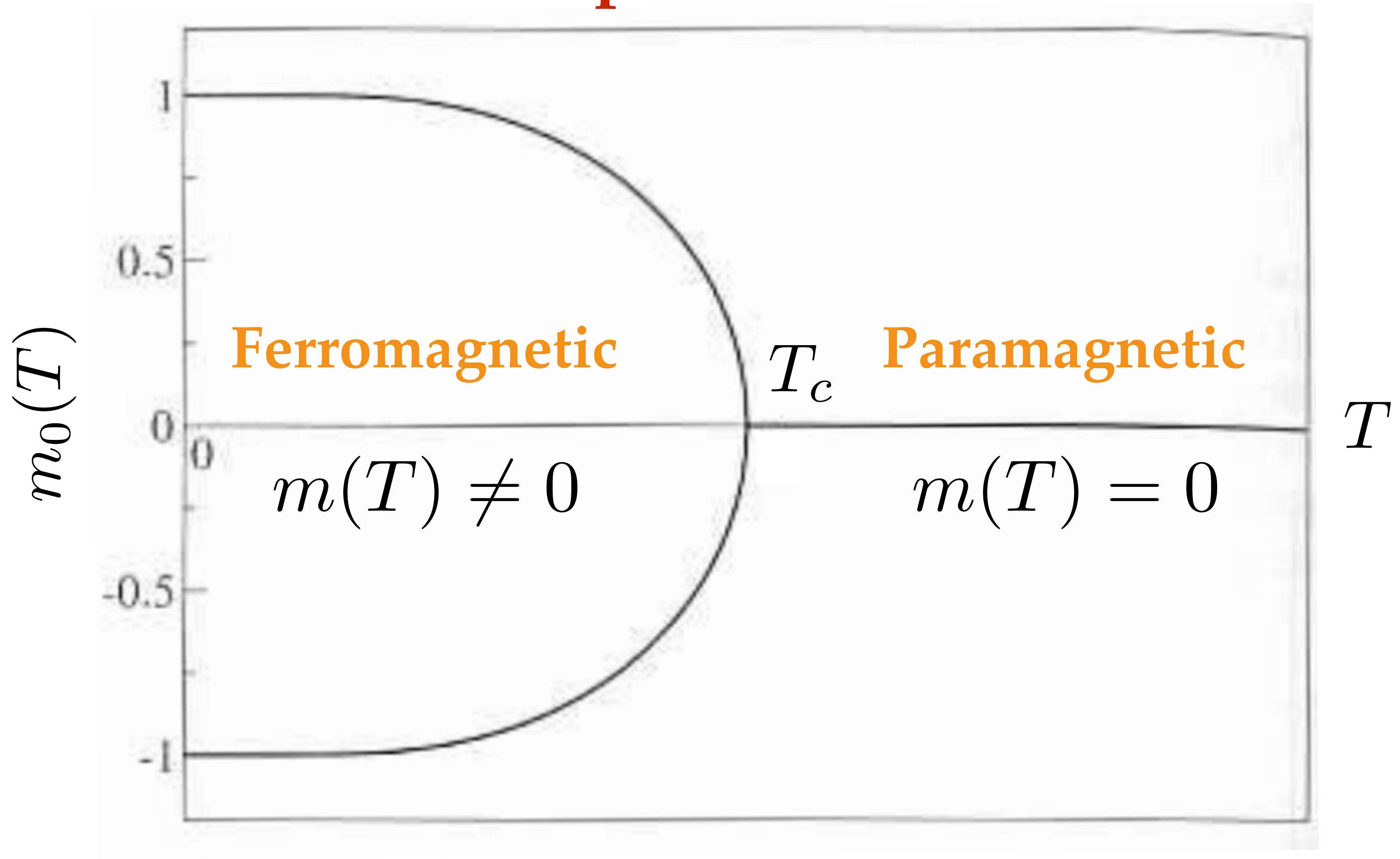
Continuous phase transition



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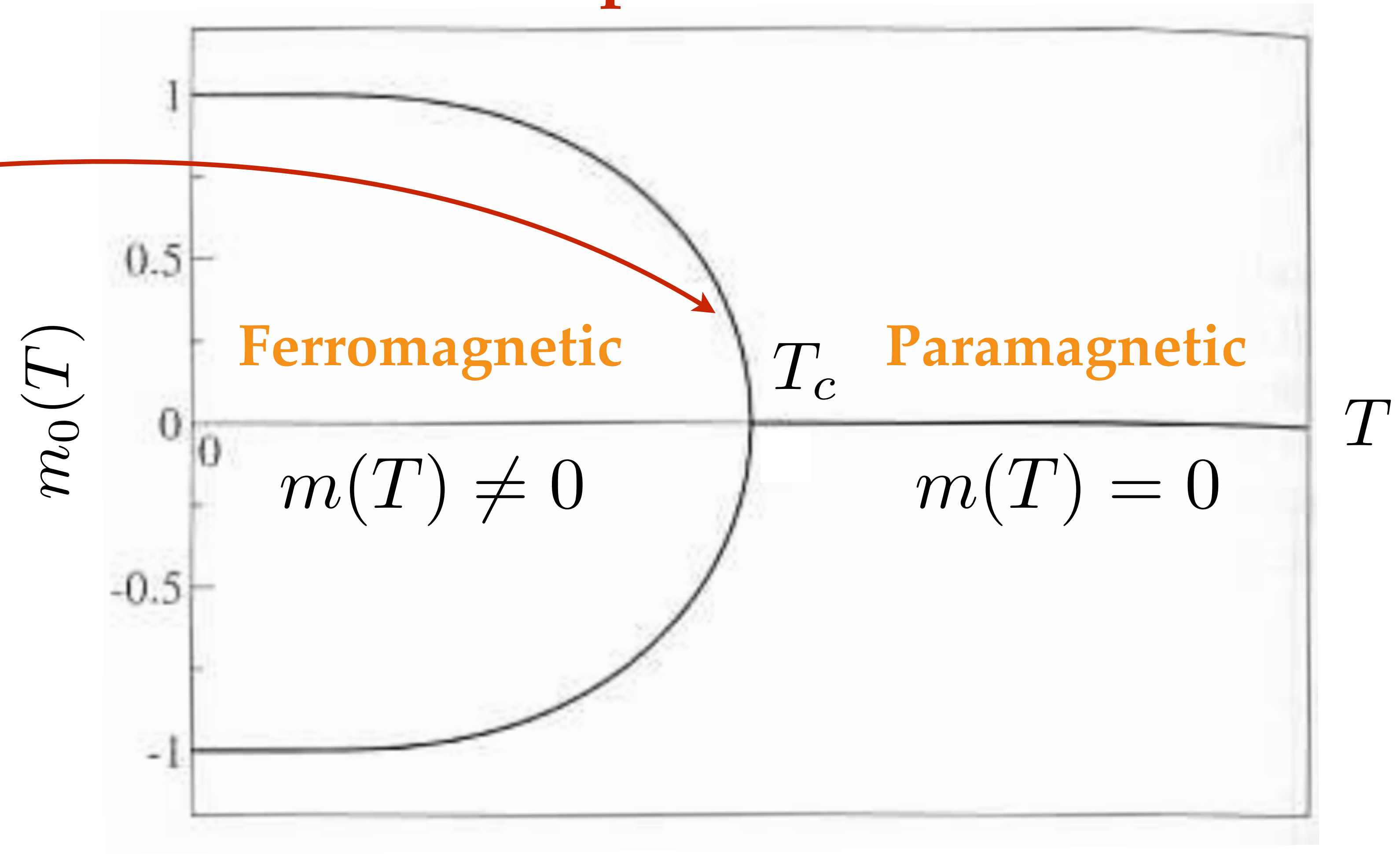
$$m(T) \underset{T_c}{\sim} (T - T_c)^{1/8}$$



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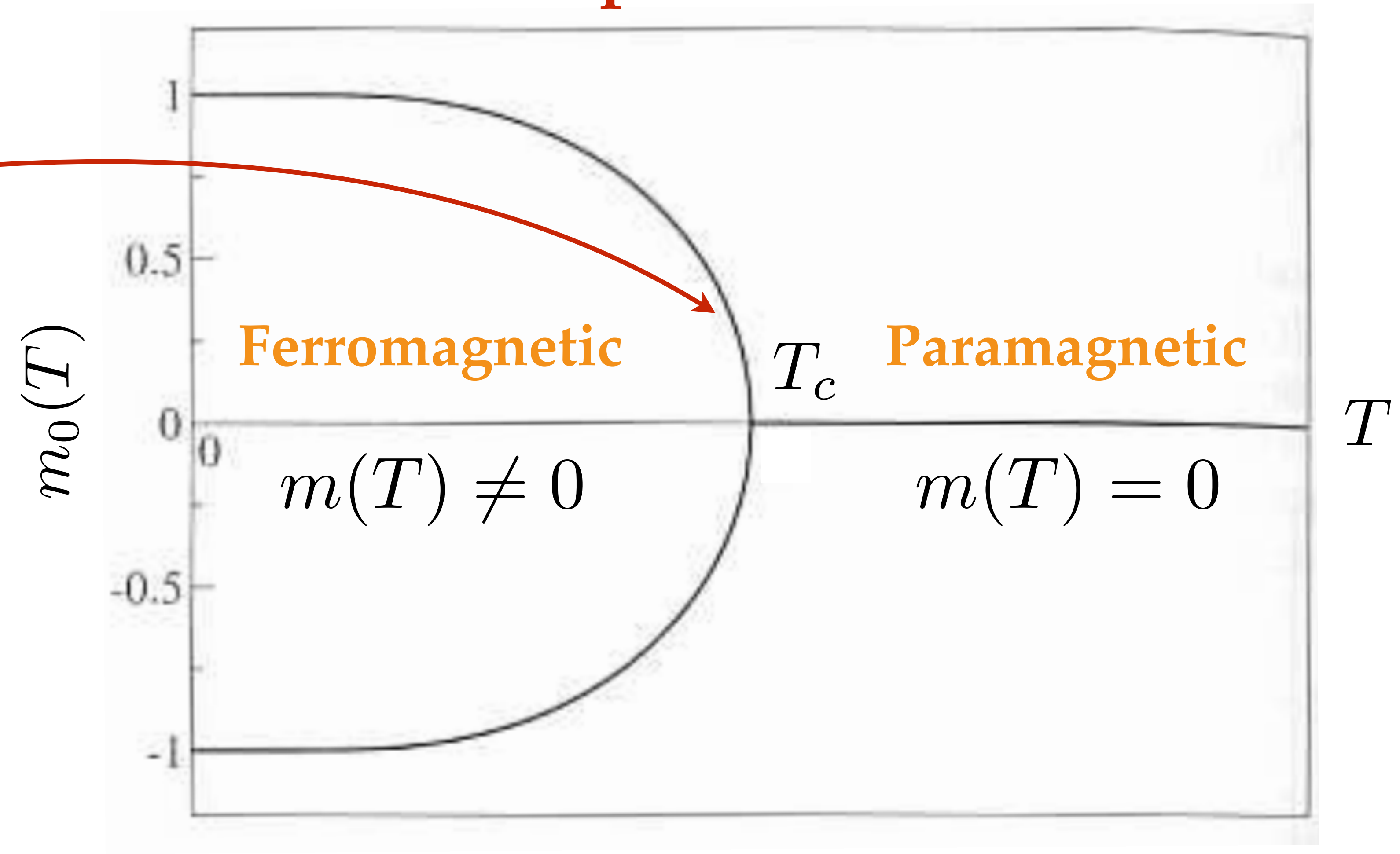

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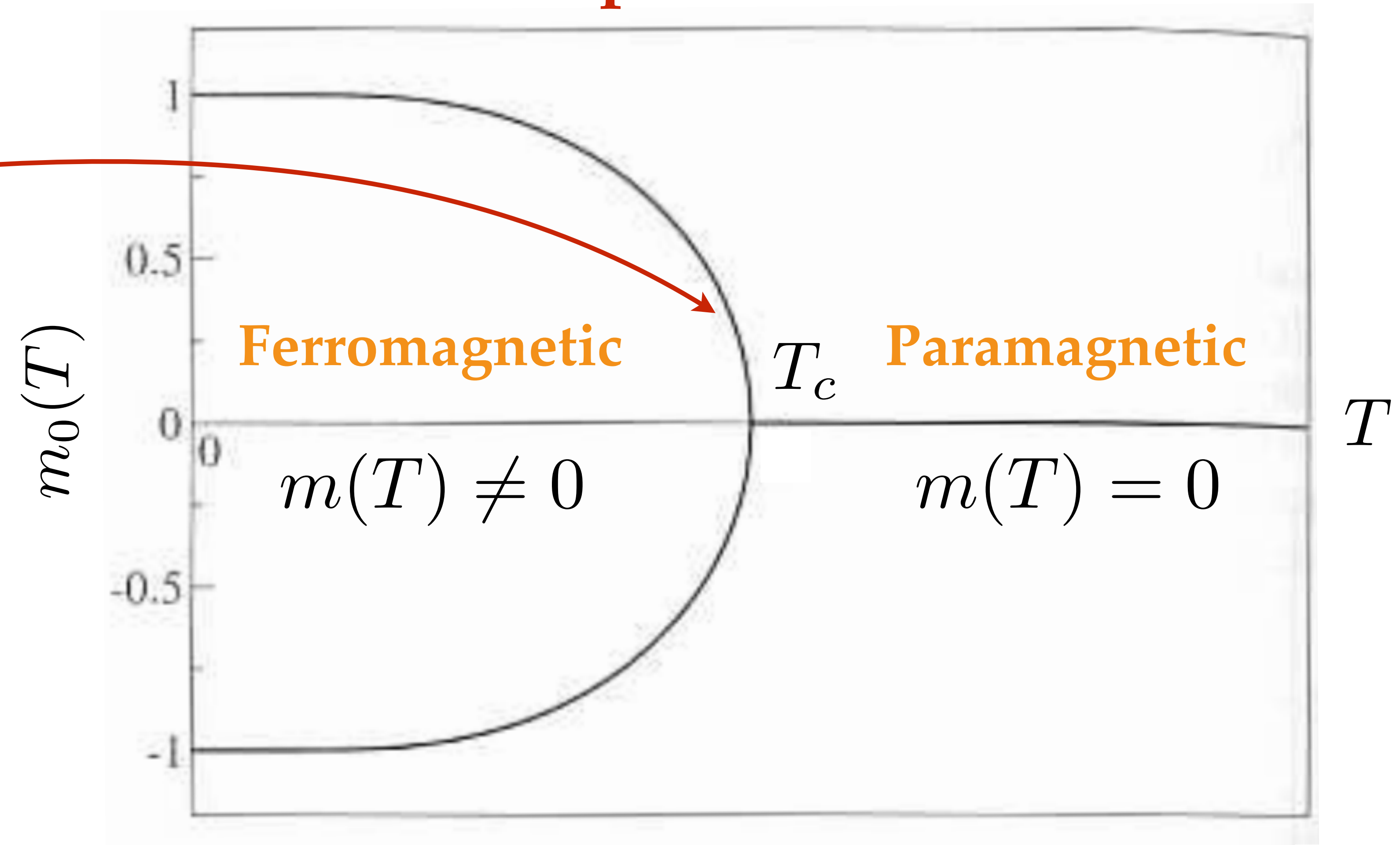

Difficult to derive exact results
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Different approaches: **Mean-field theory** **Landau theory** **Renormalisation group**

Properties at the critical point:

Infinite Clusters of Correlated Spins

1) 1D Ising: Susceptibility per spin

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Susceptibility: sensitivity of the magnetization to changes in the external field at fixed temperature.

$$\chi(T, H) = \left(\frac{\partial m}{\partial H}\right)_T = \beta \, \frac{\cosh \beta H \exp(-4\beta J)}{[\sinh^2 \beta H + \exp(-4\beta J)]^{3/2}}$$

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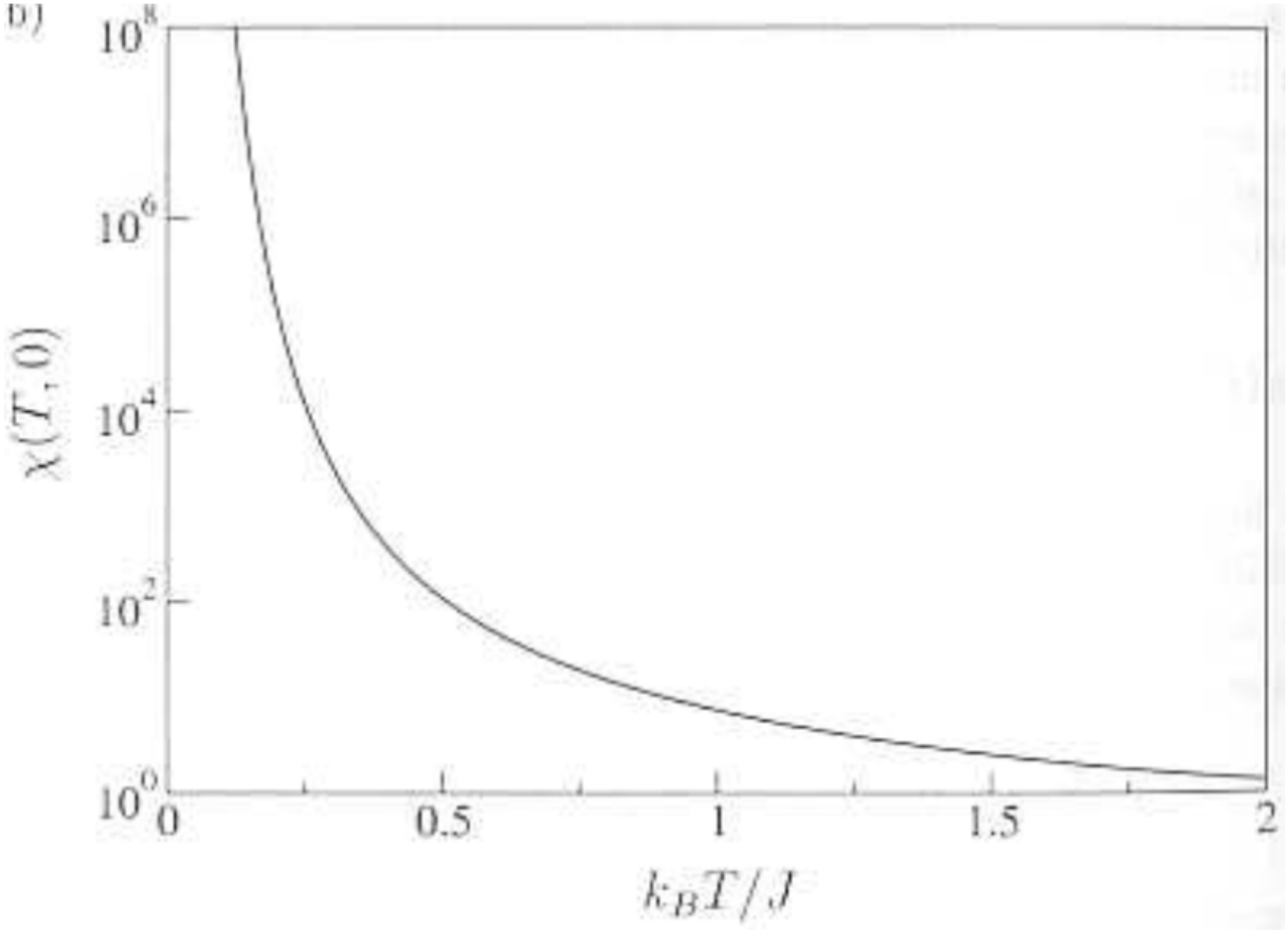

H=0:

$$\chi(T,0) = \beta \exp(2\beta J) \to \begin{cases} \beta & \text{for } T \to \infty \\ \beta \exp(2\beta J) & \text{for } T \to 0 \end{cases}$$

For T—> 0, the susceptibility diverge exponentially!

Fluctuation-dissipation theorem:

$$\frac{\langle M^2 \rangle - \langle M \rangle^2}{N} = k_B T\, \chi = \exp(2\beta J)$$

Variance of the magnetization diverges for T—> 0 !

2) 1D Ising model: Correlation function

Correlation function

Correlation function: $g(s_i, s_j) = \langle s_i s_j \rangle - \langle s_i \rangle \langle s_j \rangle$

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average magnetization is the same everywhere

g only depends on the distance between the spins

Correlation function

Correlation function: $g(s_i, s_j) = \langle s_i s_j \rangle - \langle s_i \rangle \langle s_j \rangle$

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average magnetization is the same everywhere

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Case 1d Ising model, for **H = 0:** for $T > 0$, $m_0 = 0$

$g(r) = \langle s_i s_{i+r} \rangle$ $g(r) = \tanh^r \beta J$

Correlation function

Correlation function: $g(s_i, s_j) = \langle s_i s_j \rangle - \langle s_i \rangle \langle s_j \rangle$

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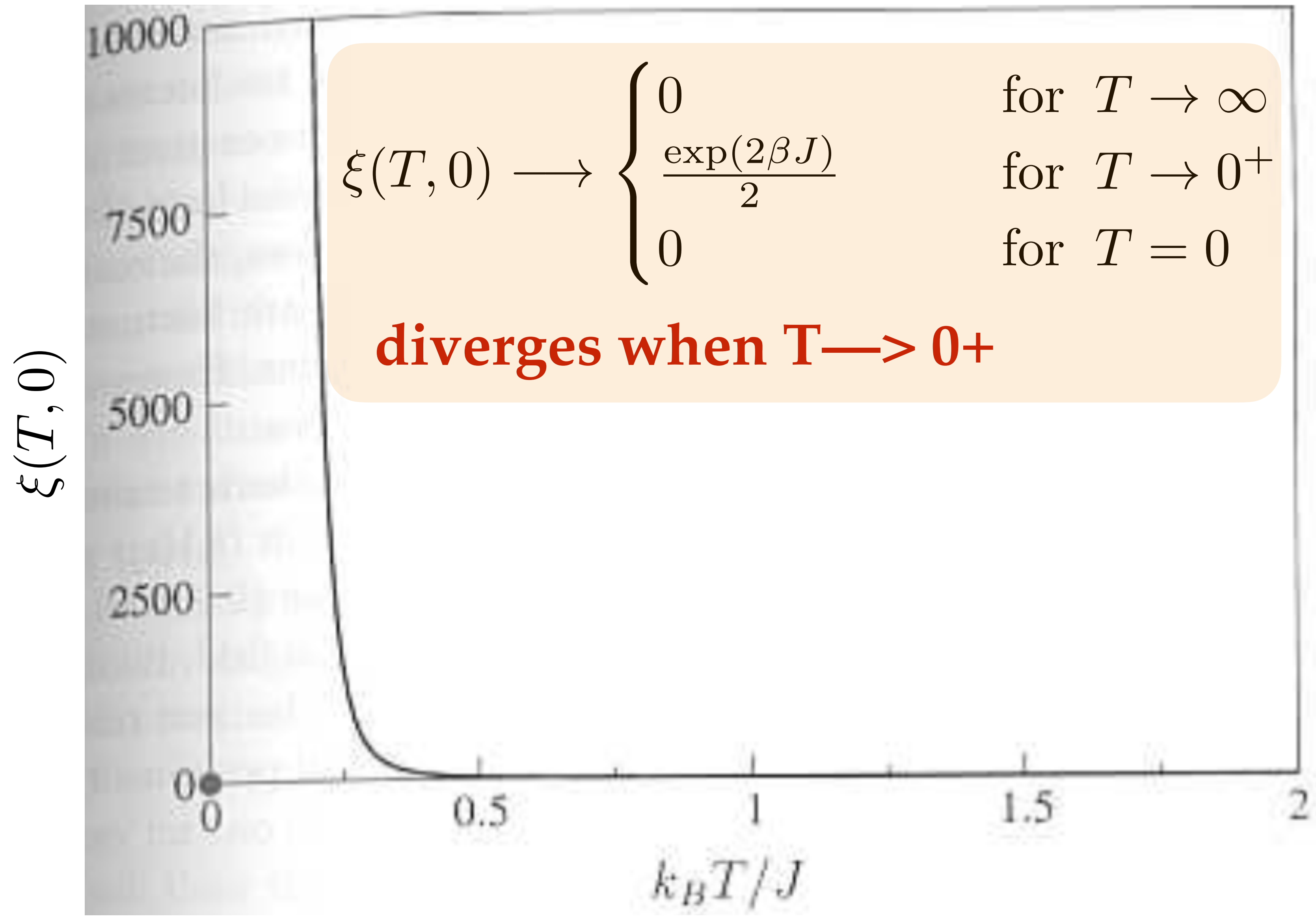
Case 1d Ising model, for **H = 0:** for $T > 0$, $m_0 = 0$

$$g(r) = \langle s_i s_{i+r} \rangle \qquad g(r) = \tanh^r \beta J \qquad = \exp(r \log(\tanh \beta J))$$

Correlation function: $g(r) = \exp(-r/\xi)$

Correlation length: $\xi(T,0) = -\dfrac{1}{\log(\tanh \beta J)}$



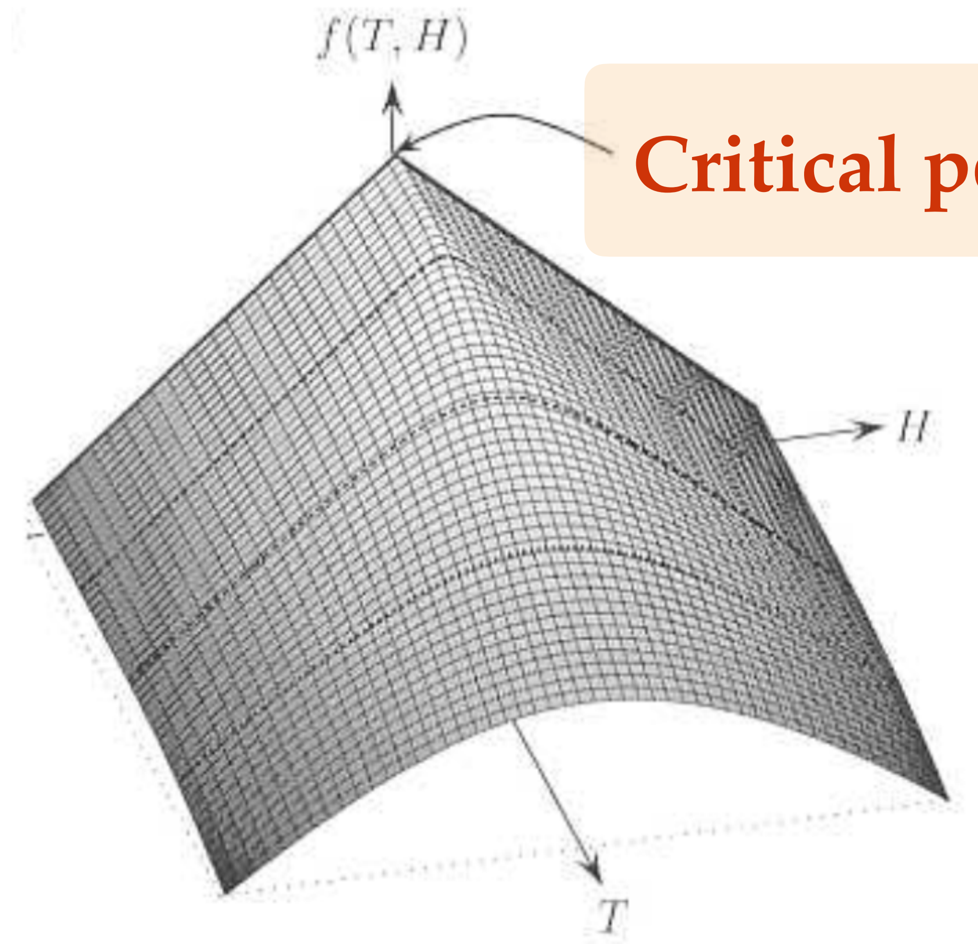
$$\xi(T,0) \longrightarrow \begin{cases} 0 & \text{for } T \to \infty \\ \frac{\exp(2\beta J)}{2} & \text{for } T \to 0^+ \\ 0 & \text{for } T = 0 \end{cases}$$

diverges when T—> 0+

1d Ising Summary

System with small field: $H \neq 0$

$$E(\vec{s}) = -J\sum_{i=1}^{N} s_i s_{i+1} - H\sum_{i=1}^{N} s_i \qquad \text{with} \qquad s_{N+1} = s_1$$



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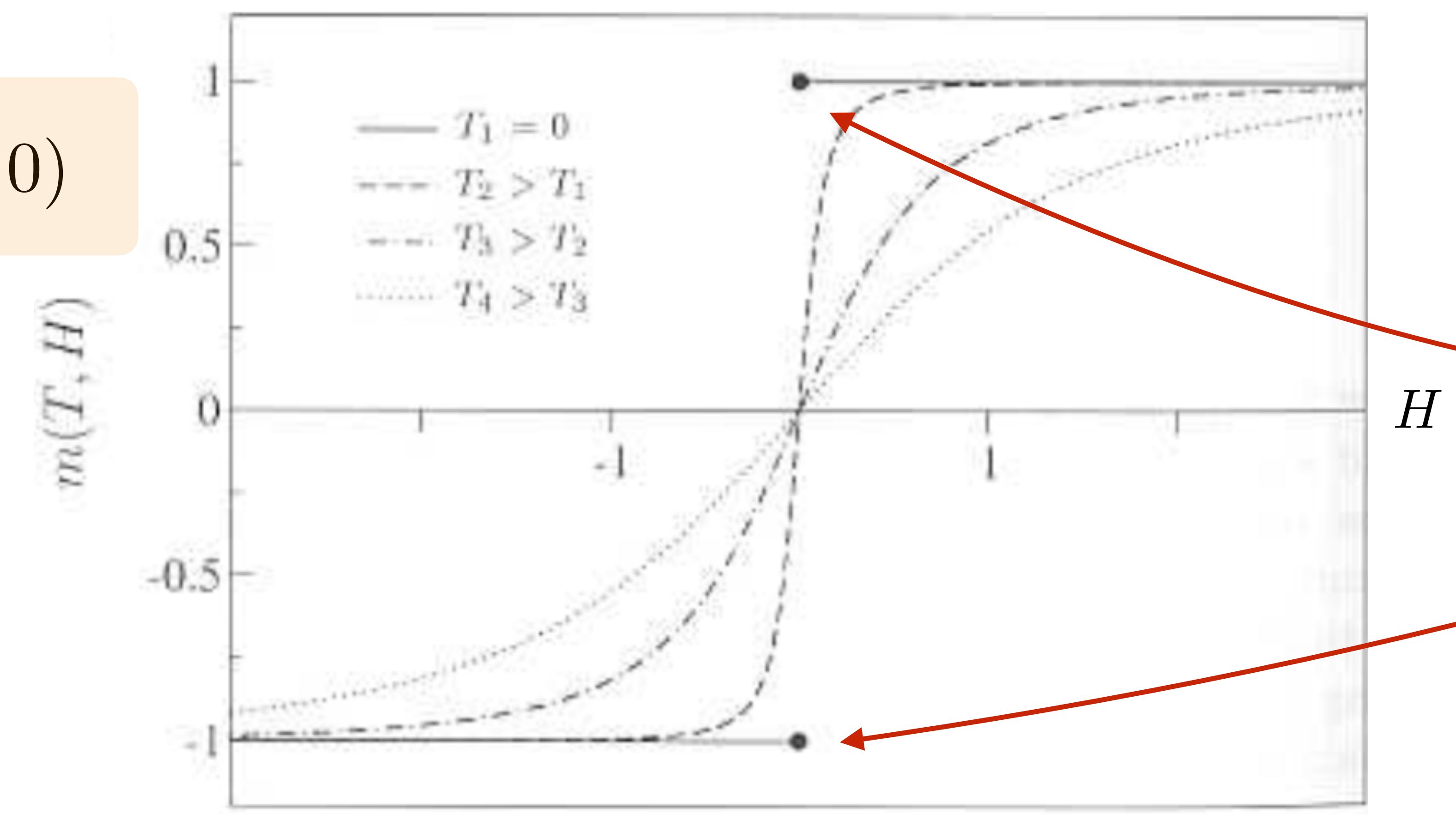

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Spontaneous magnetization !!!!

Correlation function: $g(r) = \exp(-r/\xi)$

Variance of the magnetization:

$$\frac{\langle M^2\rangle - \langle M\rangle^2}{N} = k_B T\,\chi = \exp(2\beta J)$$

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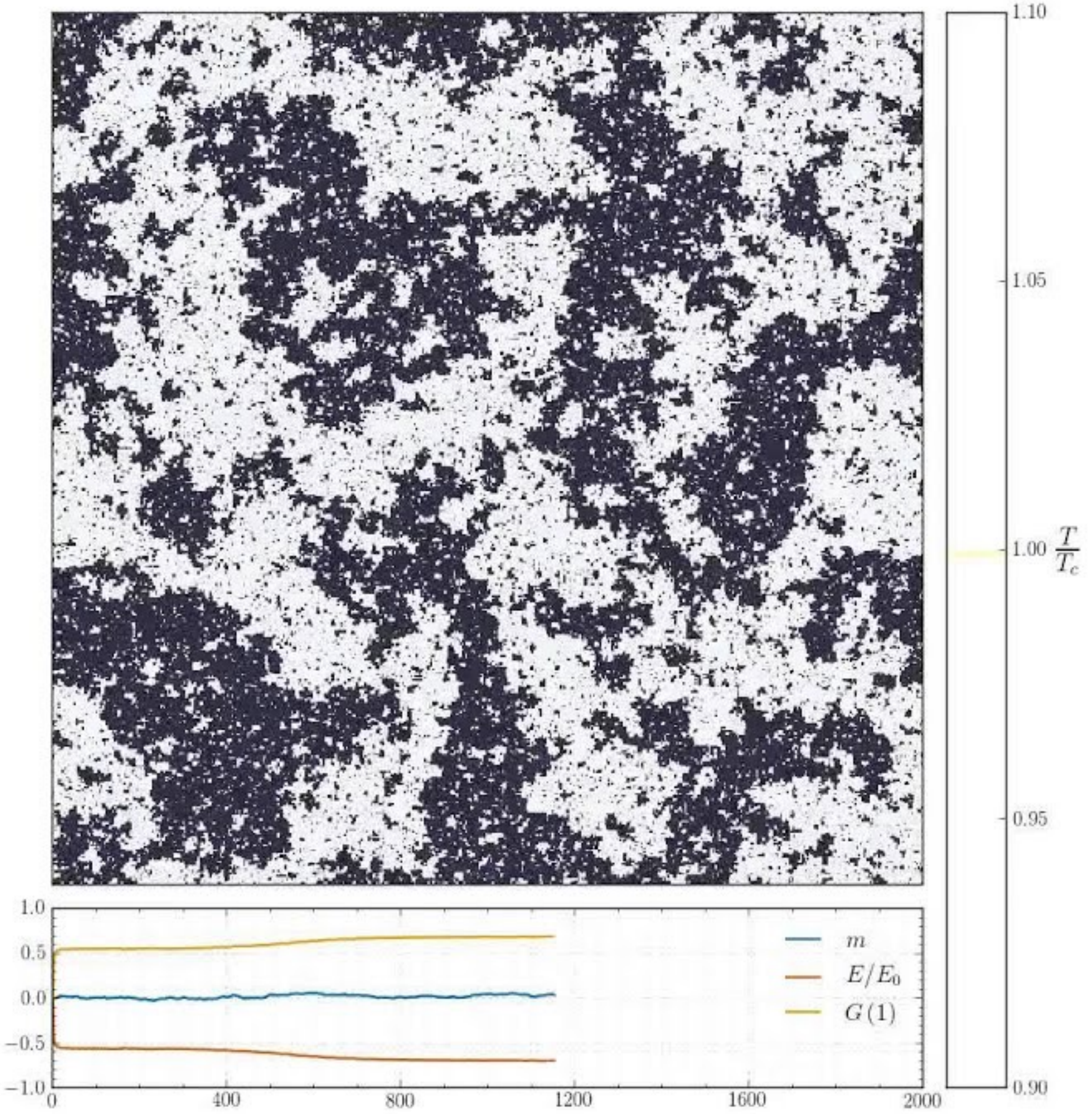
3) Critical point

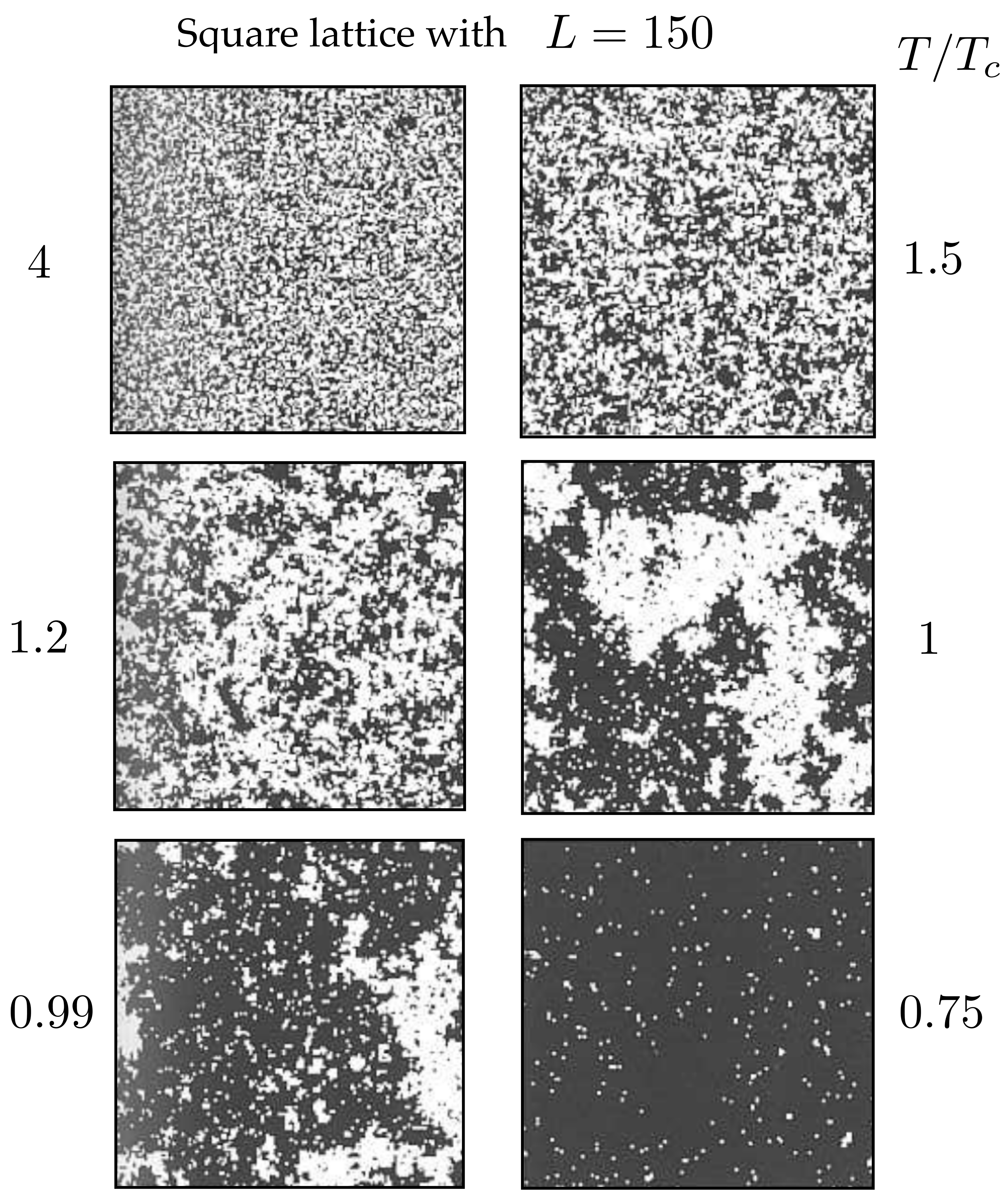


Explaining the phase transition at the microscopic scale clusters of correlated spins

Critical phase transition at: $(T, H) = (T_c, 0)$

Clusters of correlated spins: chain of spin with the same orientation

Ingredients:	**“wins”**	**Correlation length**	**Order/Disorder**
T >> Tc			
T << Tc			
T = Tc			



Link: Numerical simulation through phase transition

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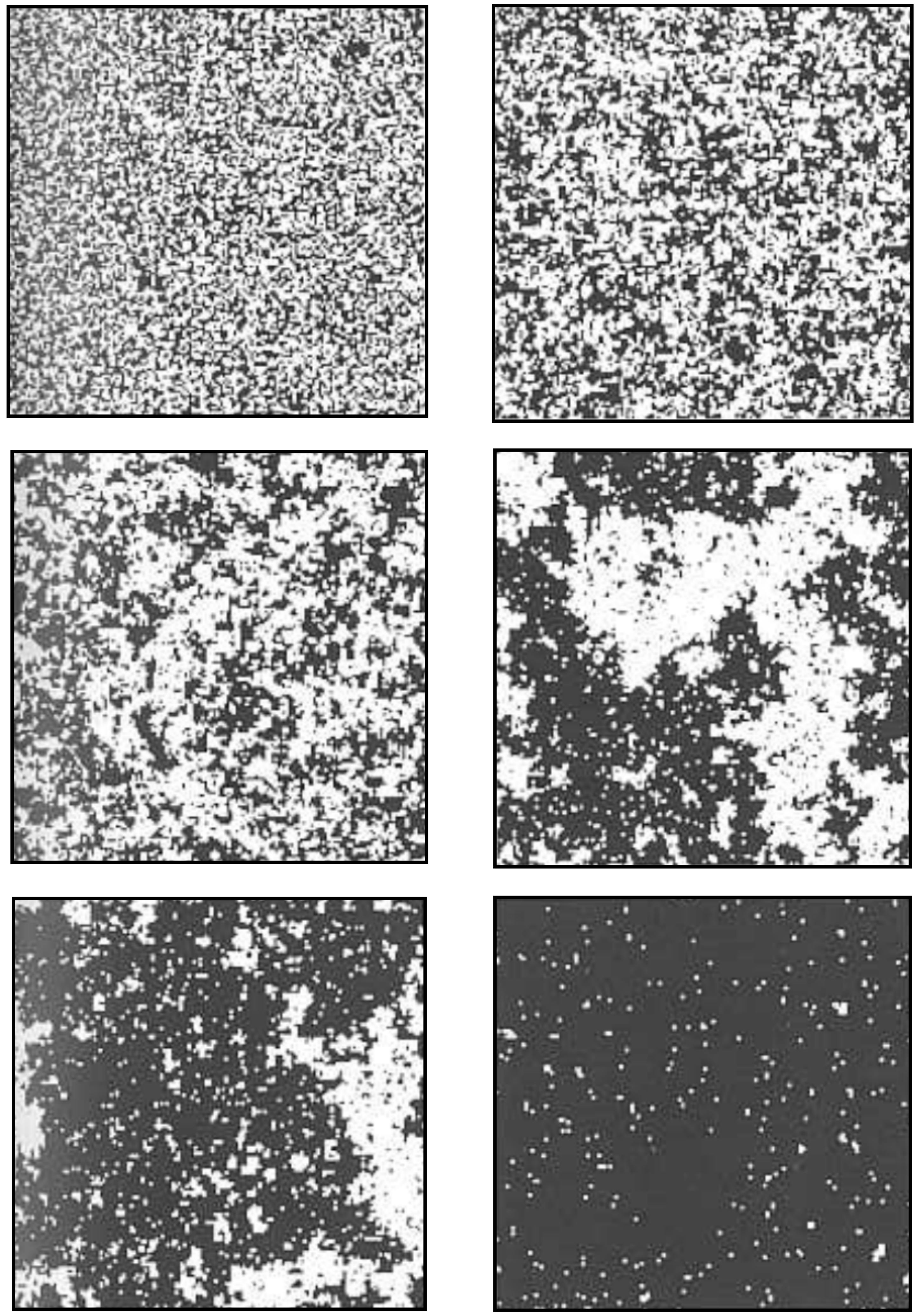
T >> Tc	thermal energy		spins are disordered
T << Tc	local spin-spin interactions		spins are aligned
T = Tc			

Square lattice with $L = 150$

T/T_c



4 1.5

1.2 1

0.99 0.75

Explaining the phase transition at the microscopic scale clusters of correlated spins

Critical phase transition at: $(T, H) = (T_c, 0)$

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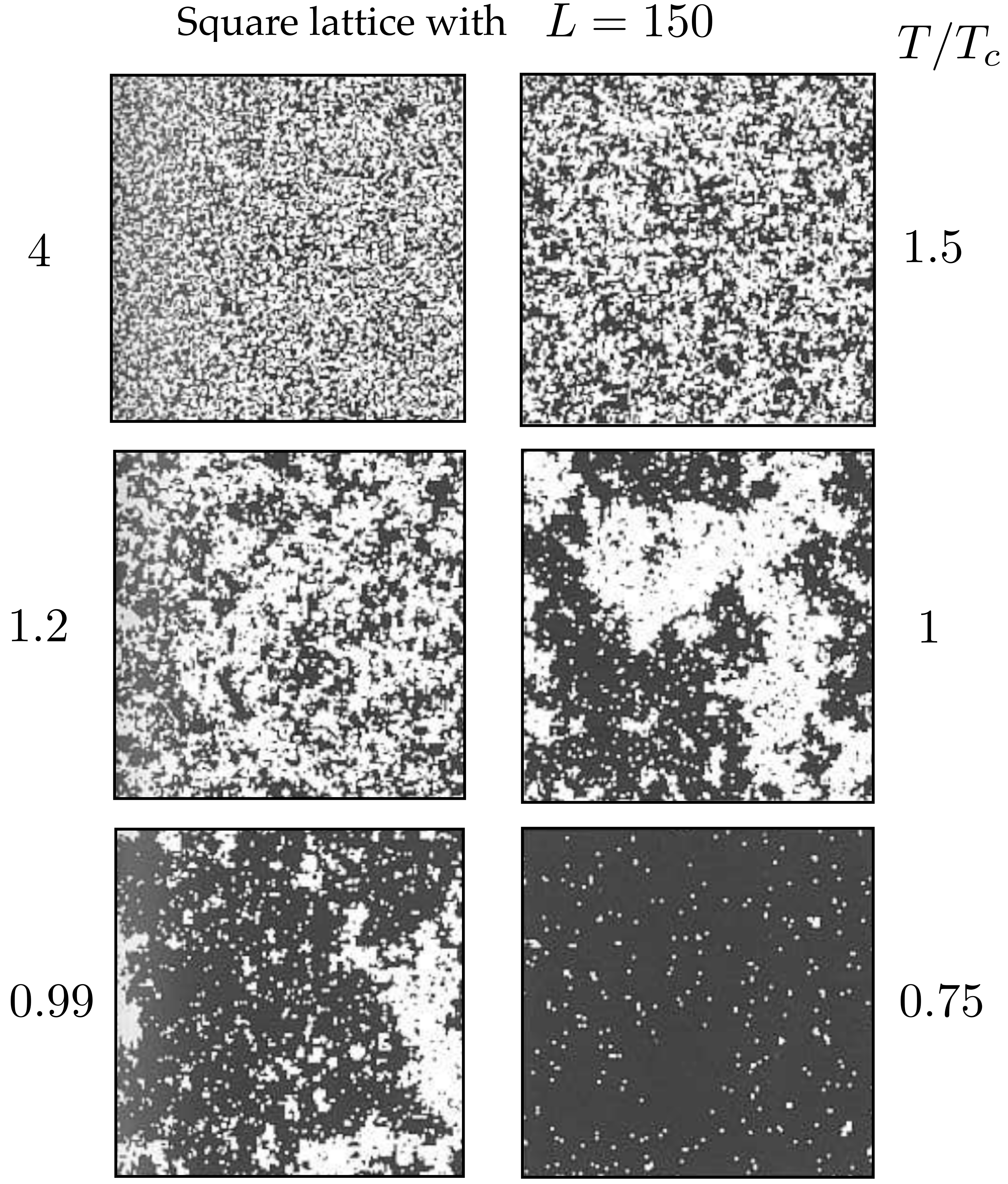

Link: Numerical simulation through phase transition

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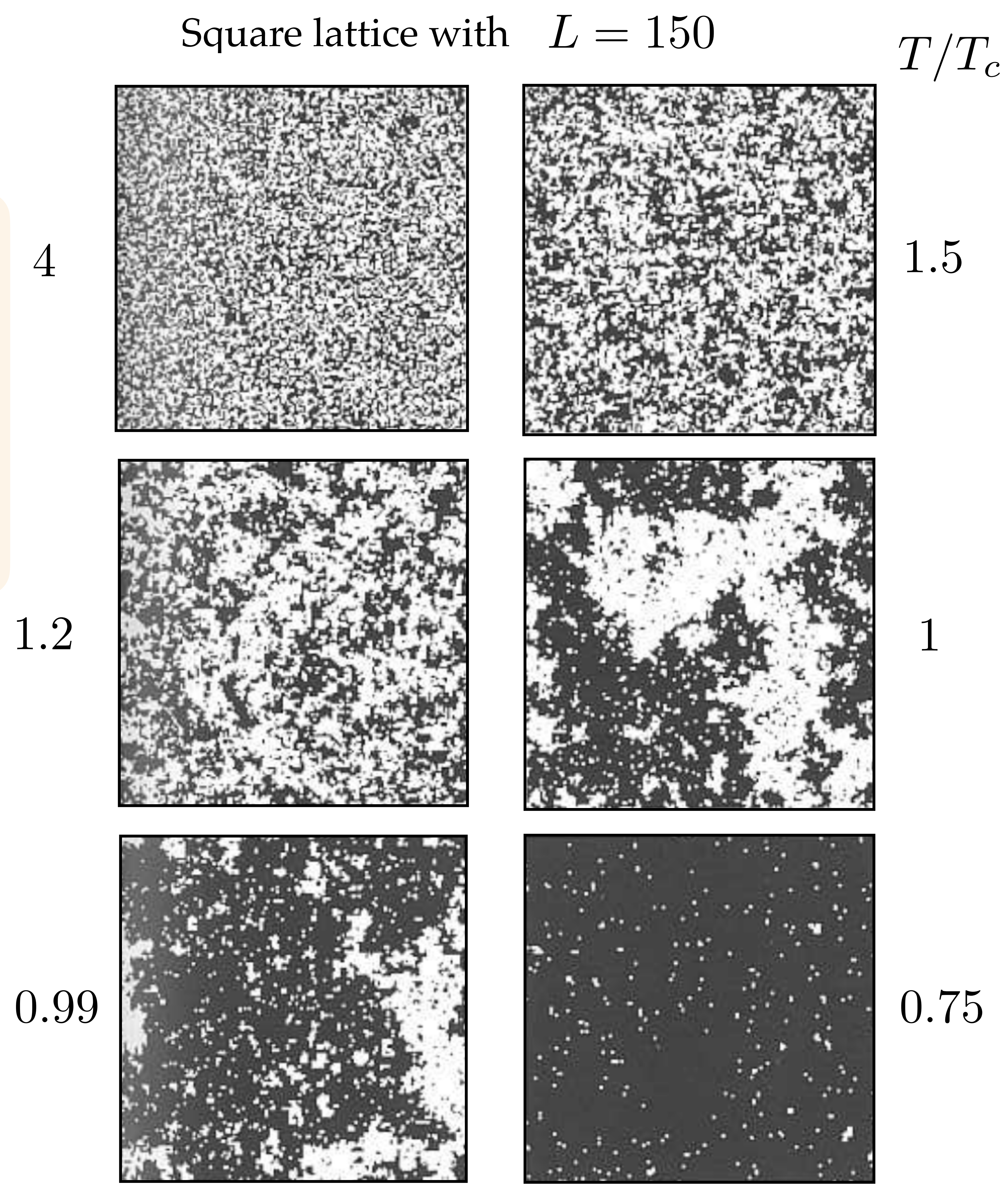

Explaining the phase transition at the microscopic scale
clusters of correlated spins

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Starting from T >> Tc: Spin randomly up/down. No correlation.

Lower T: spin interaction are less suppressed

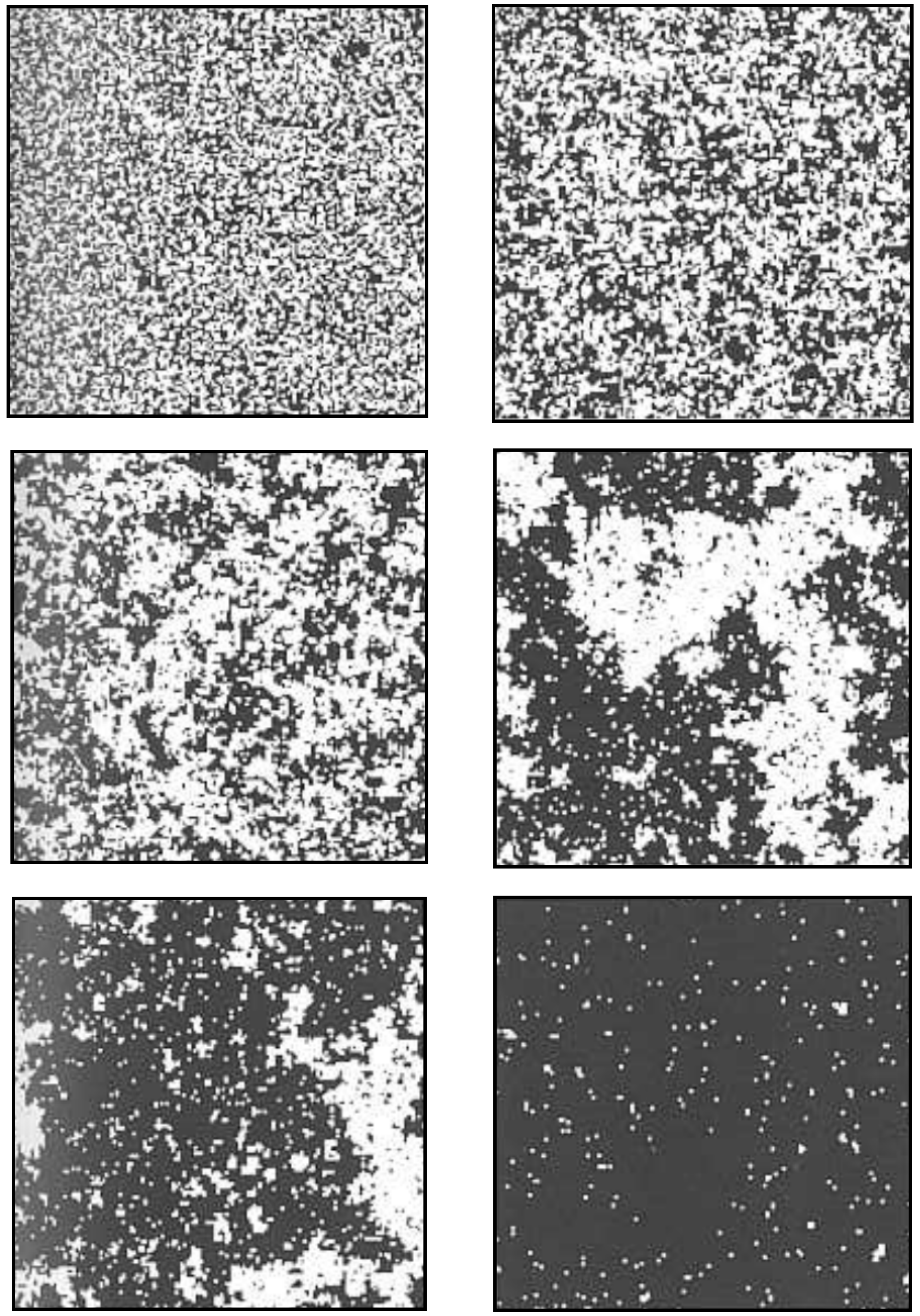
larger and larger clusters of correlated spins

clusters are finite in size and equally likely to be up or down ==> m=0

Local effects can't give rise to a **spontaneous magnetization…**

Square lattice with $L = 150$

T/T_c



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larger and larger clusters of correlated spins

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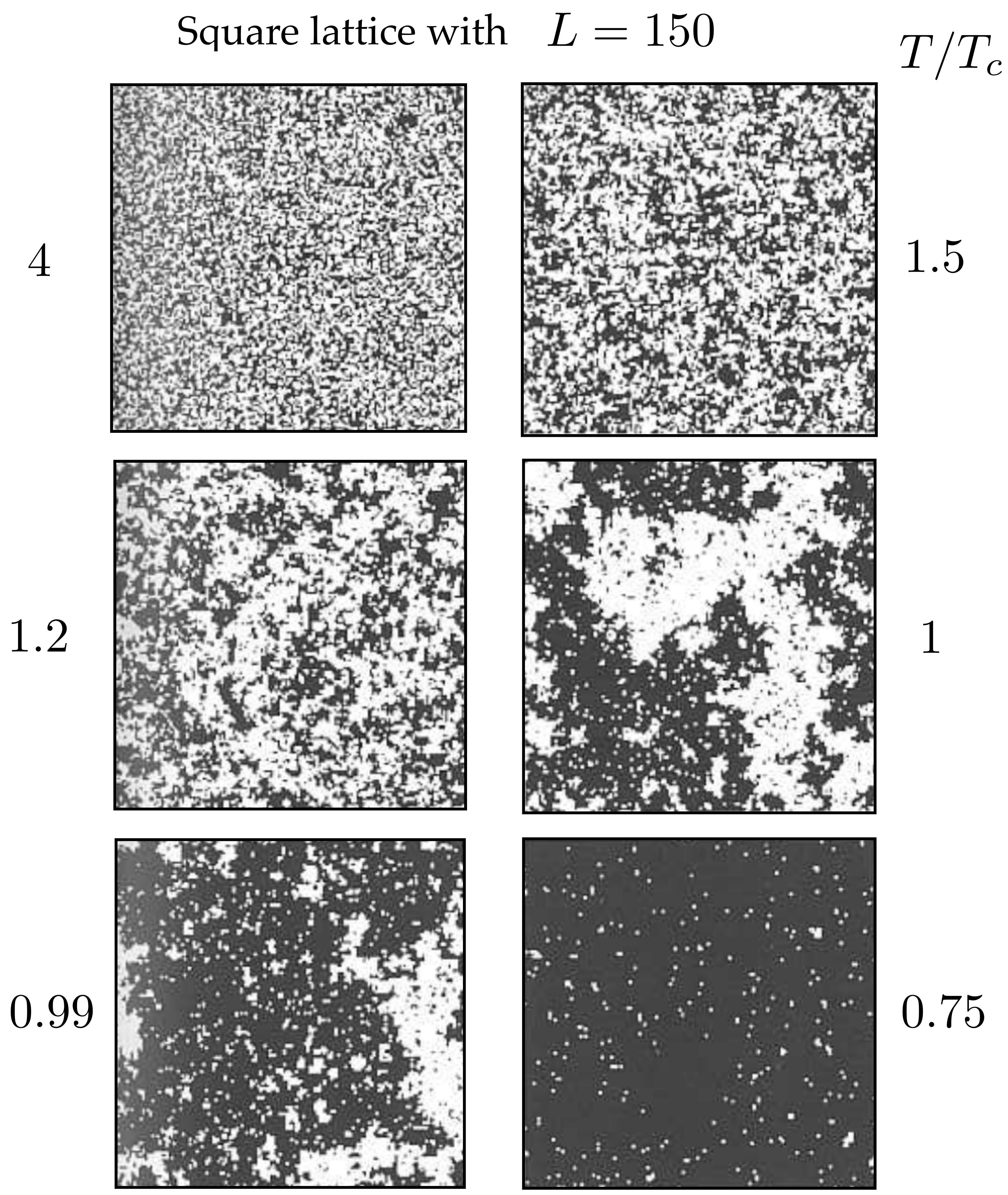
At Tc: Emergence of a **"macro-cluster" of correlated spins** associated with the divergence of the correlation length as T approach Tc from above

These **non-local effect** can give rise to a **spontaneous magnetization** as T passes Tc.



Explaining the phase transition at the microscopic scale clusters of correlated spins

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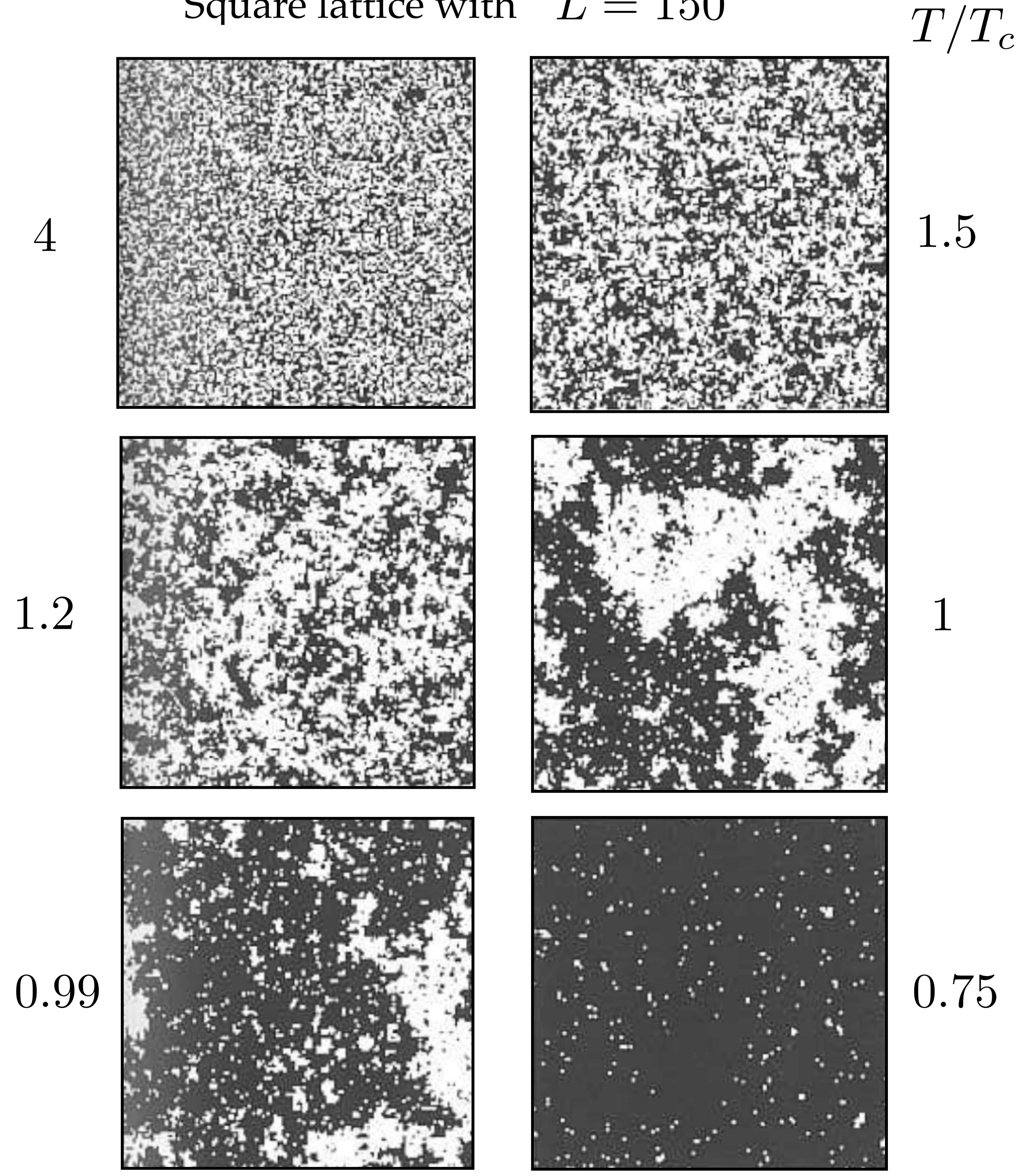
Starting from T << Tc: Spin almost all aligned. Correlation spin-to-spin.

Increase T: thermal noise increases ==> increase the correlation length

magnetization persists as long as the correlation length remains finite

Square lattice with $L = 150$



Explaining the phase transition at the microscopic scale clusters of correlated spins

Critical phase transition at: $(T, H) = (T_c, 0)$

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Starting from T << Tc: Spin almost all aligned. Correlation spin-to-spin.

Increase T: thermal noise increases ==> increase the correlation length

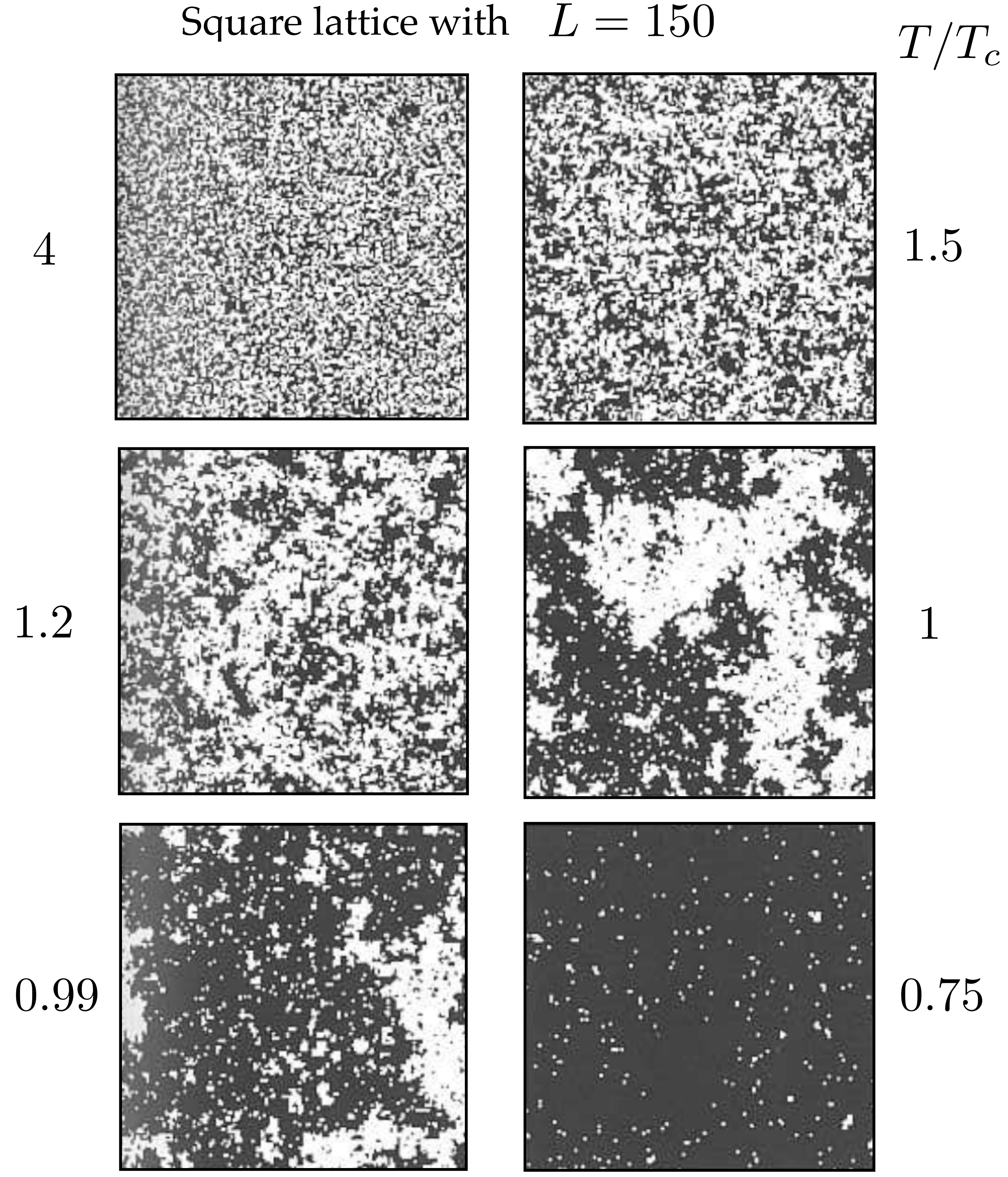
magnetization persists as long as the correlation length remains finite

At Tc: the divergence of the correlation length as T approach Tc from below

Increasing correlation length due to thermal noise: magnetization vanishes

These non-local effect destroys the magnetization as T passes Tc.

Square lattice with $L = 150$



Explaining the phase transition at the microscopic scale clusters of correlated spins

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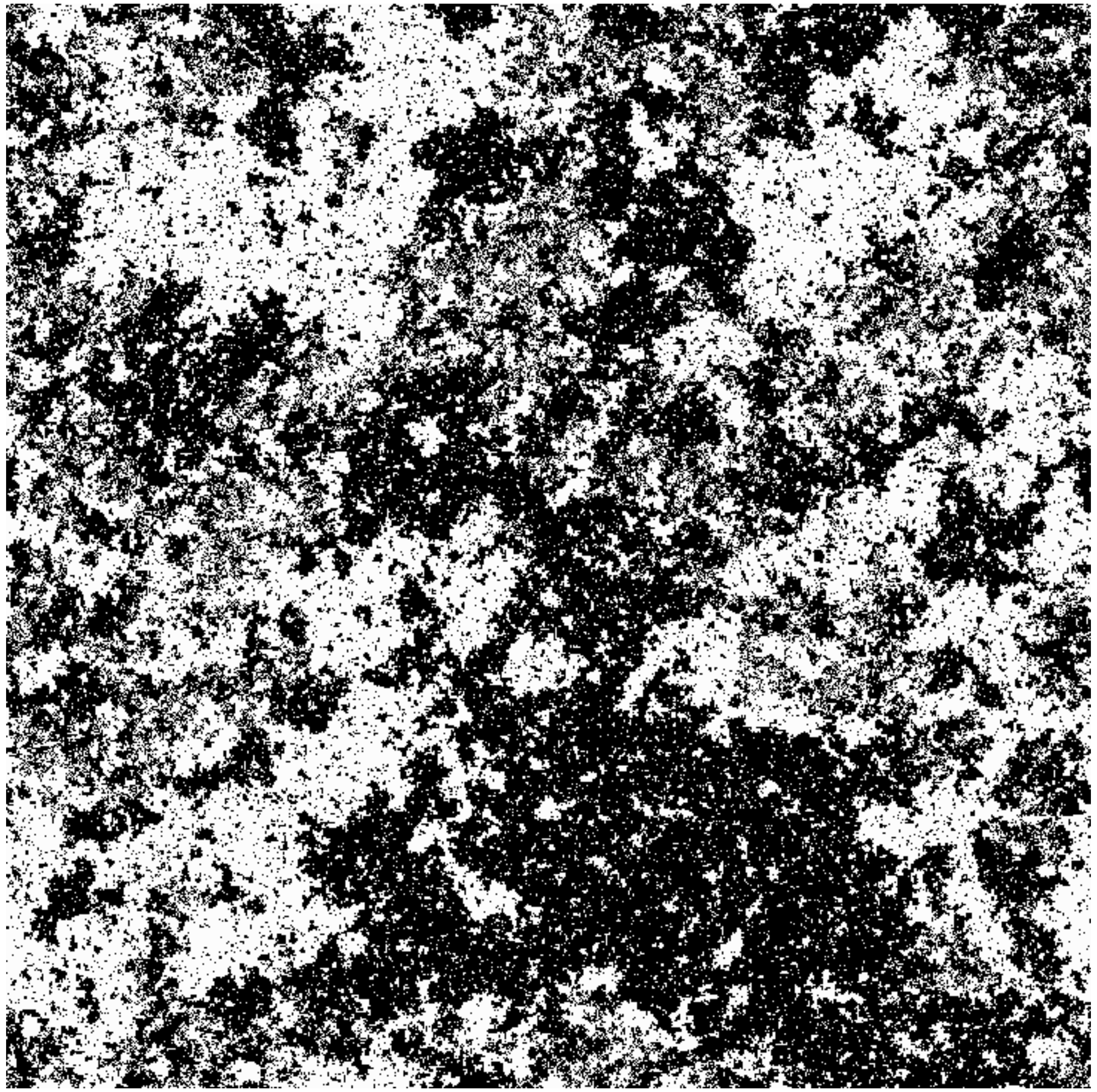


Ising model close to Tc

At T = Tc: **Macroscopic cluster** of correlated spins

This macro-cluster:

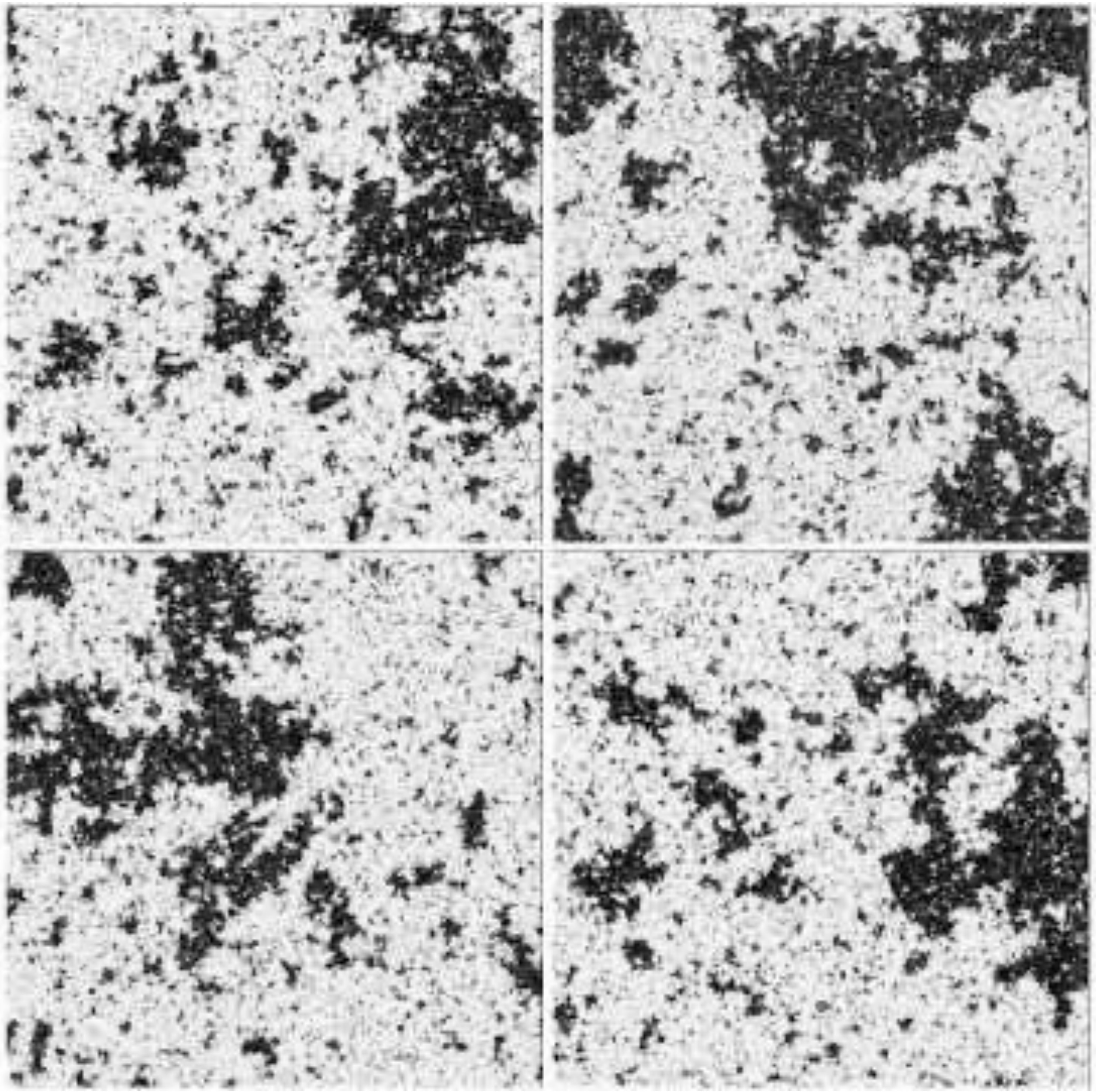
has an **infinite size** (spans the entire system)

is **fractal**: i.e. it **contains clusters of all sizes** of opposite spins, which themselves contain clusters of all sizes of opposite spins, and so on…

Signatures of **Fluctuations at all scales…**

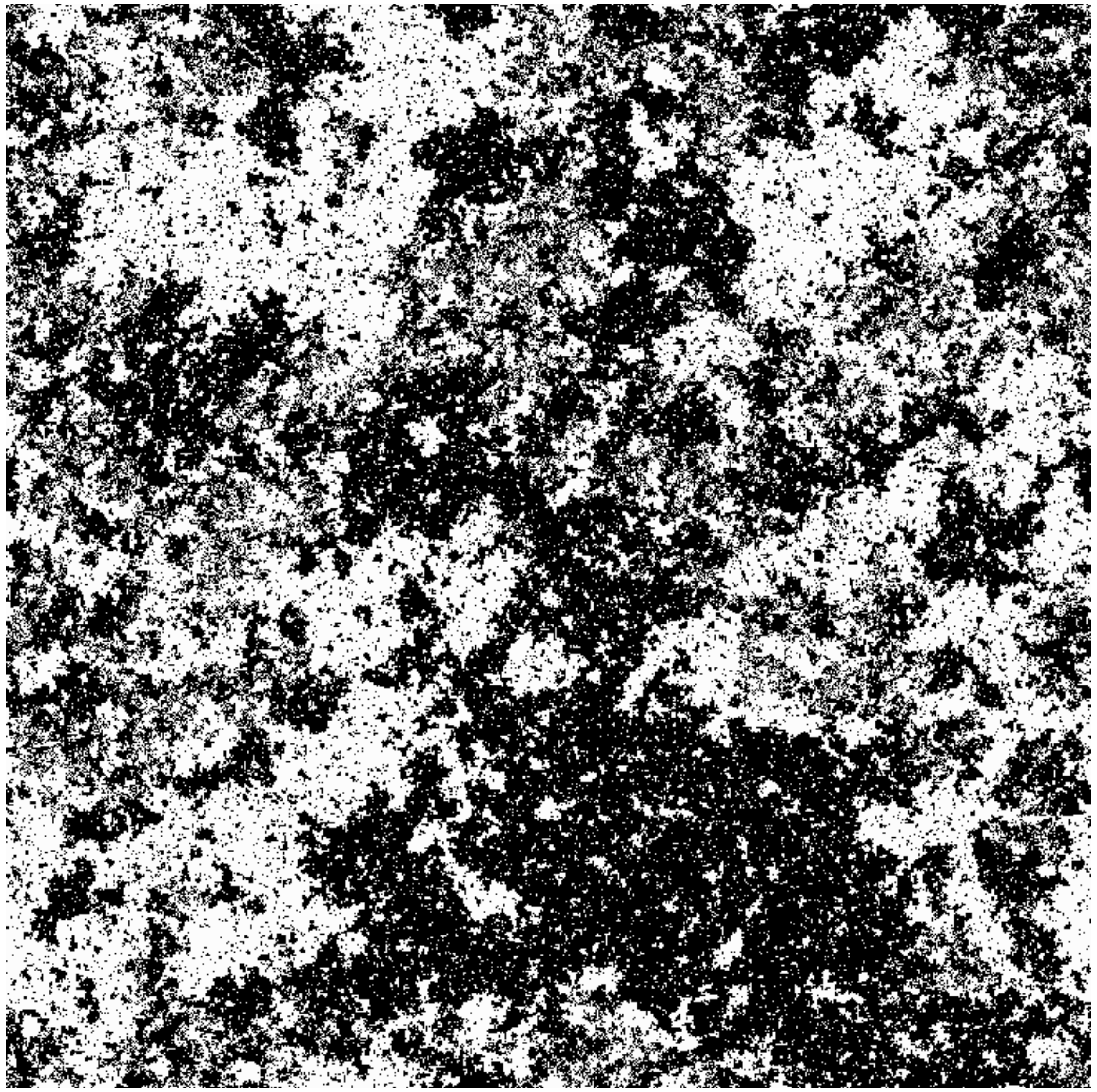
Clusters at all scales

At T = Tc:



Coming up

Coming tutorial: Help!!! Review of calculations on Ising model.
(and more…)



Homework:

Using Ising model for modeling US Supreme Court
(and more…)

Coming lecture:

Mean-field approach on the 2D Ising.
Discussing more properties of critical phenomena.

Questions?