Introduction to Critical phenomena

Chapter 0 - Lecture 2

Thursday 04 April

Phase transitions and Critical phenomena

Lecture 2

Plan:

Phases and Phases diagrams

Continuous VS discontinuous phase transitions

Critical phenomena

From micro to macro: example of the Ising model

Questions: Is everyone in a working group?

Campuswire?

Overlapping course or exam? Let us know **here**.

Expectations: Participate in the discussions, take notes

References: Various books from bachelor in physics in Thermodynamics...

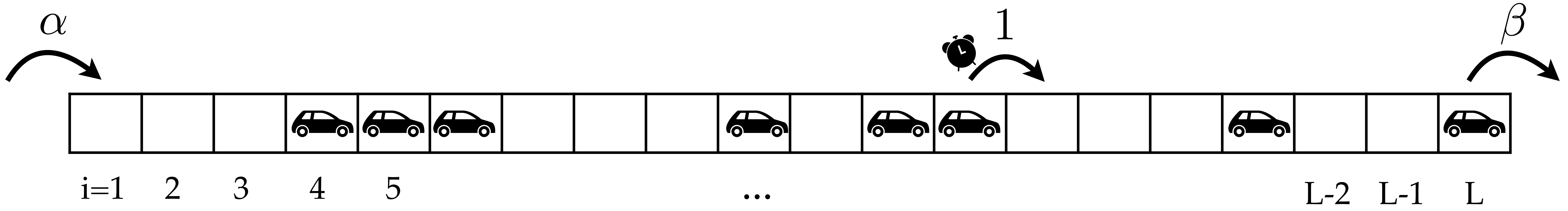
Before we begin: The word **"critical"** is used in science with different meanings.

Here we use it in the **context of critical phenomena**, in connections with phase transitions.

In this context, **"critical"** describes a **system at the border between order and disorder**.

Introduction: Ex. TASEP
Results of the numerical experiment

Cars move at random times: models the random small fluctuations in the speed of each driver



Two parameters:

α = **rate** at which cars **enter from the left** of the lattice

β = **rate** at which cars **exit from the right** of the lattice

TASEP — Numerical Experiment

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Simulation: With different choices for (α, β)

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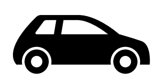
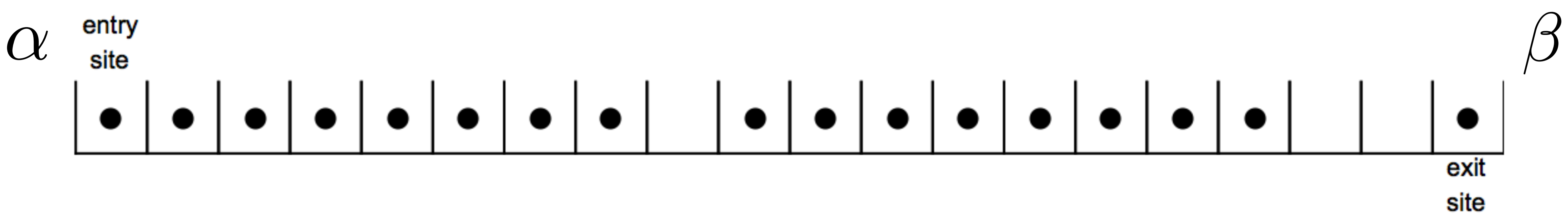
$\bullet$ = 

$(\alpha, \beta) = (1, 0.1)$



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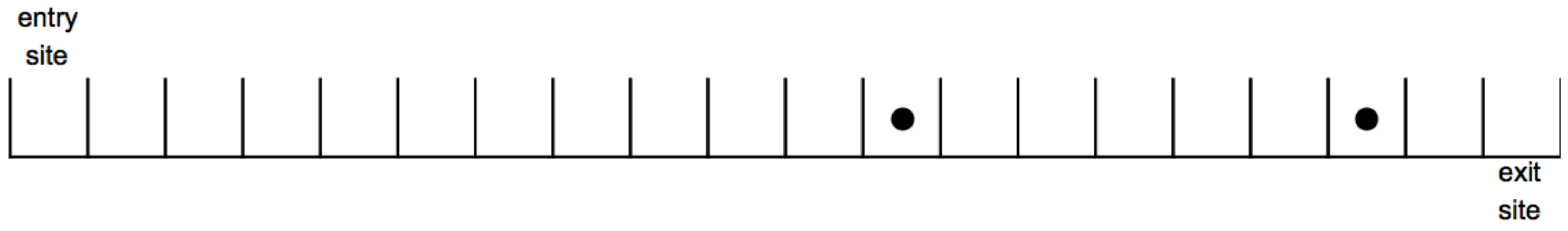

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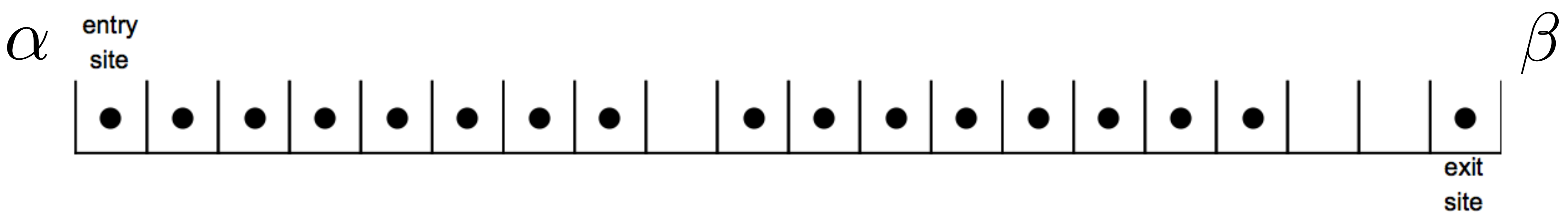
Quantities of interest at stationarity:

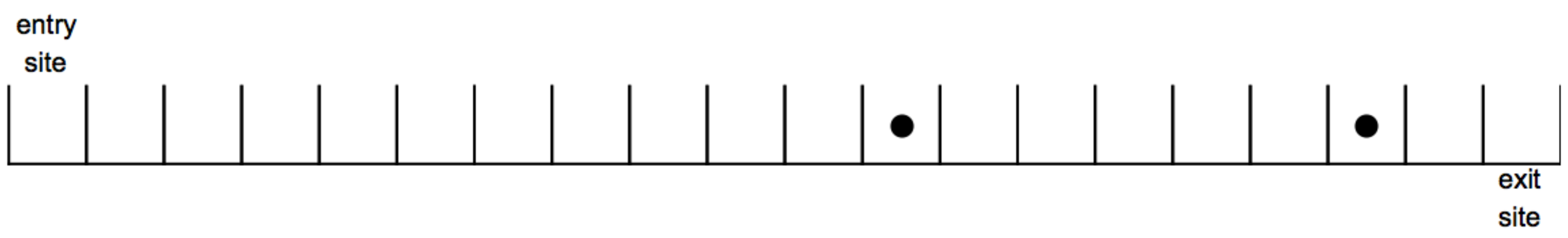
$\overline{n_i}$ = **density of cars** at site *i* = average number of cars at site *i*

$\bullet$ = 

$(\alpha,\, \beta) = (1,\, 0.1)$ Very dense



$(\alpha,\, \beta) = (0.1,\, 1)$ Much less dense!



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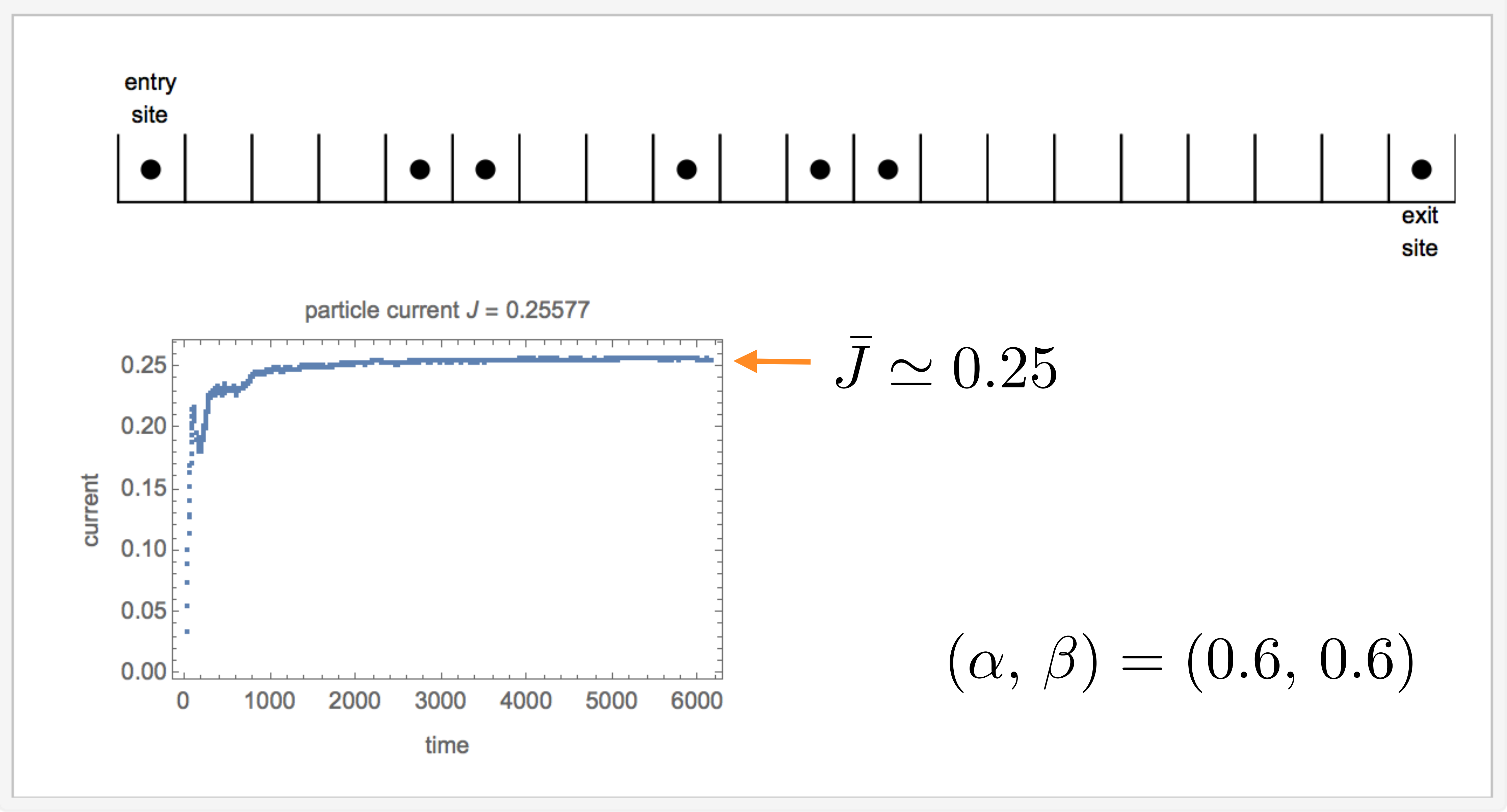
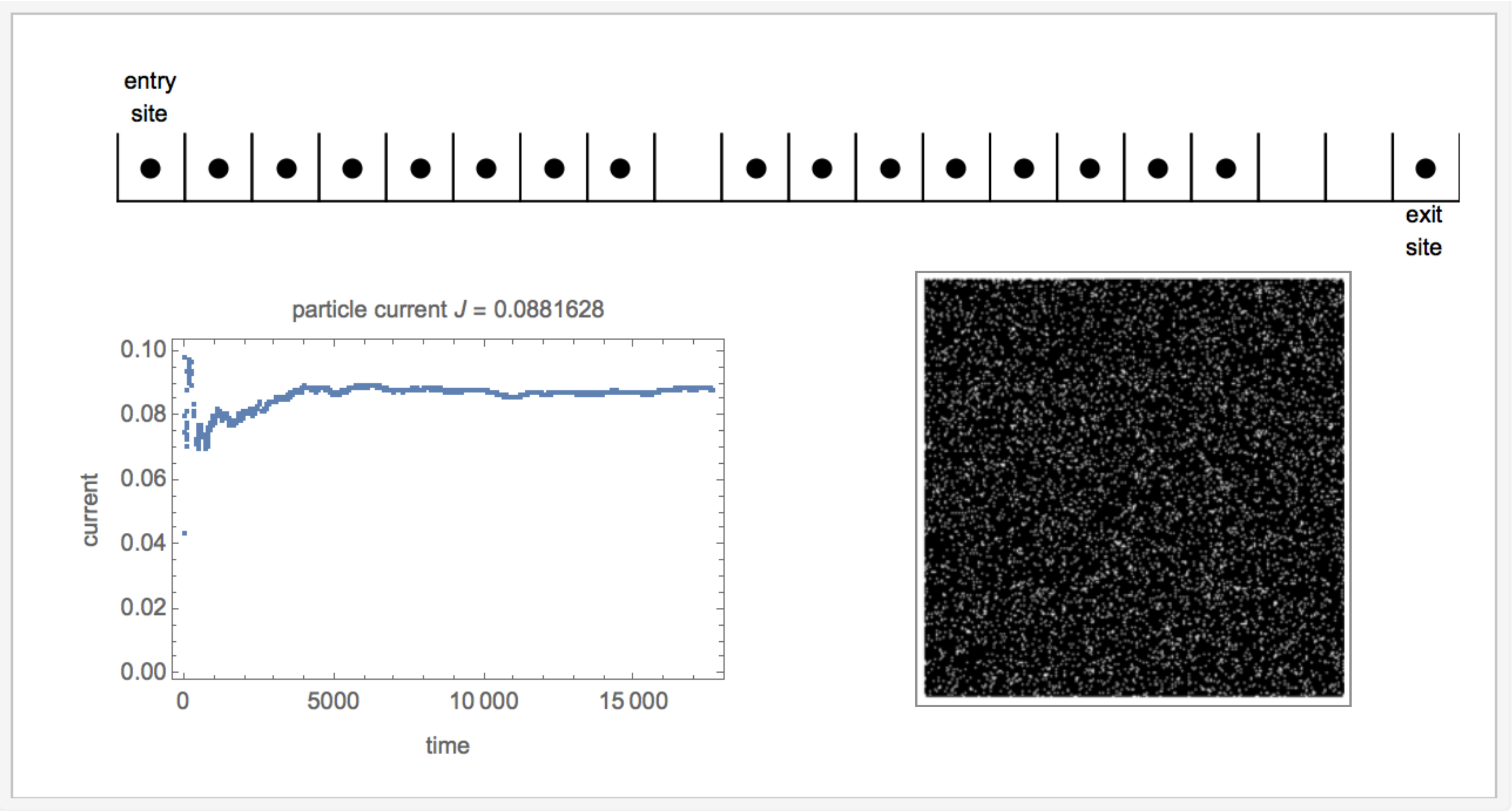
$\bar{J}$ = average **current of cars** across the system at stationarity



beta \ alpha	0,1	0,2	0,3	0,4	0,5	0,6	0,7	0,8	0,9	1,0
1,0	0,09	0	0	0	0	0	0	0	0	0
0,9	0	0	0	0	0	0	0	0	0	0
0,8	0	0	0	0	0	0	0	0	0	0
0,7	0	0	0	0	0	0	0,25	0	0	0
0,6	0	0,17	0	0	0	0,25	0	0	0	0
0,5	0	0	0	0	0,25	0	0	0	0	0
0,4	0	0	0	0	0	0	0	0	0	0
0,3	0	0	0	0	0	0	0	0	0	0
0,2	0	0,15	0	0	0	0	0	0	0	0
0,1	0	0	0	0	0	0	0	0	0	0,09

TASEP — Different macroscopic behaviours?

$(\alpha,\, \beta) = (1,\, 0.1)$ High density $\bar{J} \simeq 0.09$



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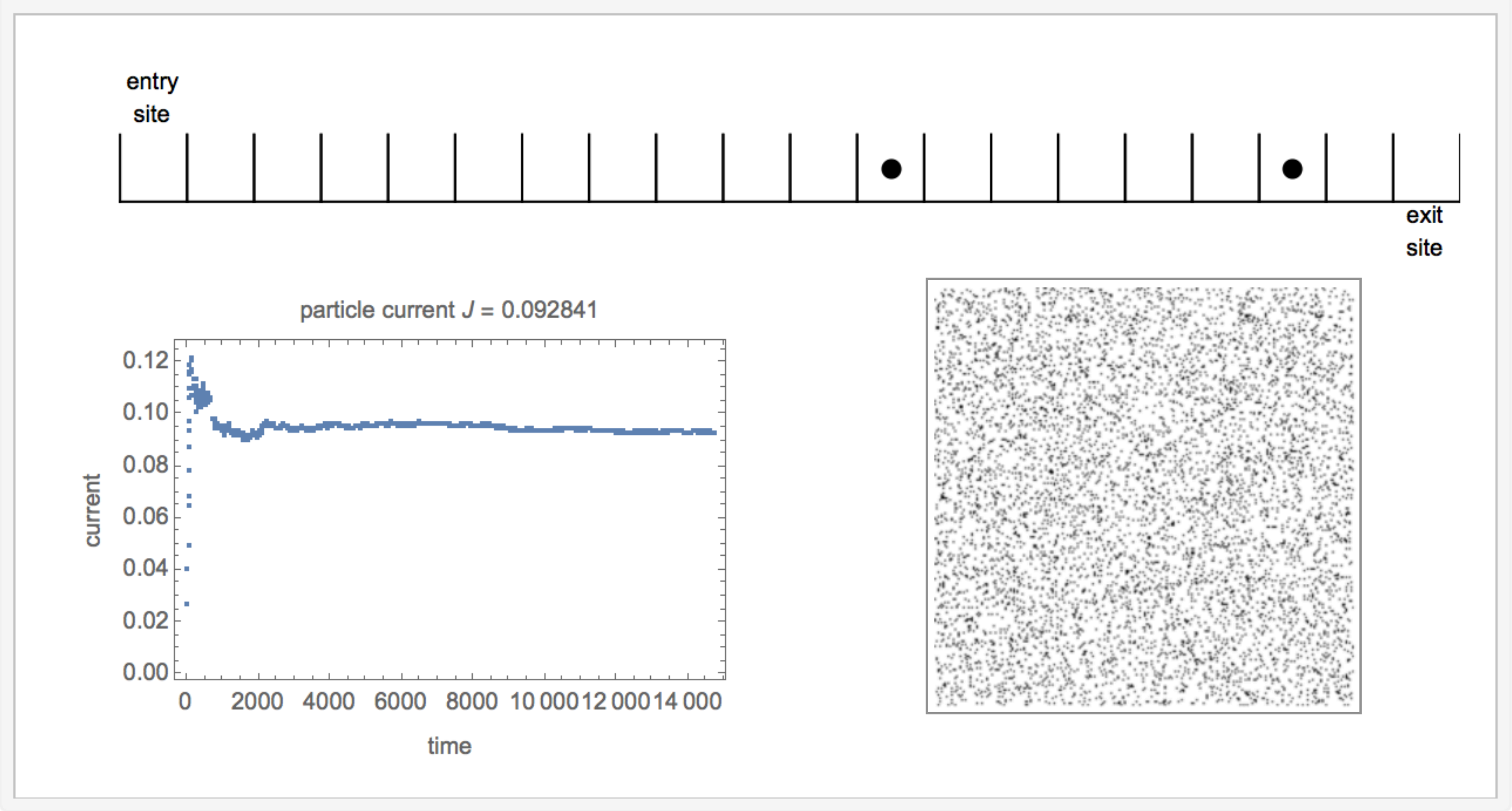

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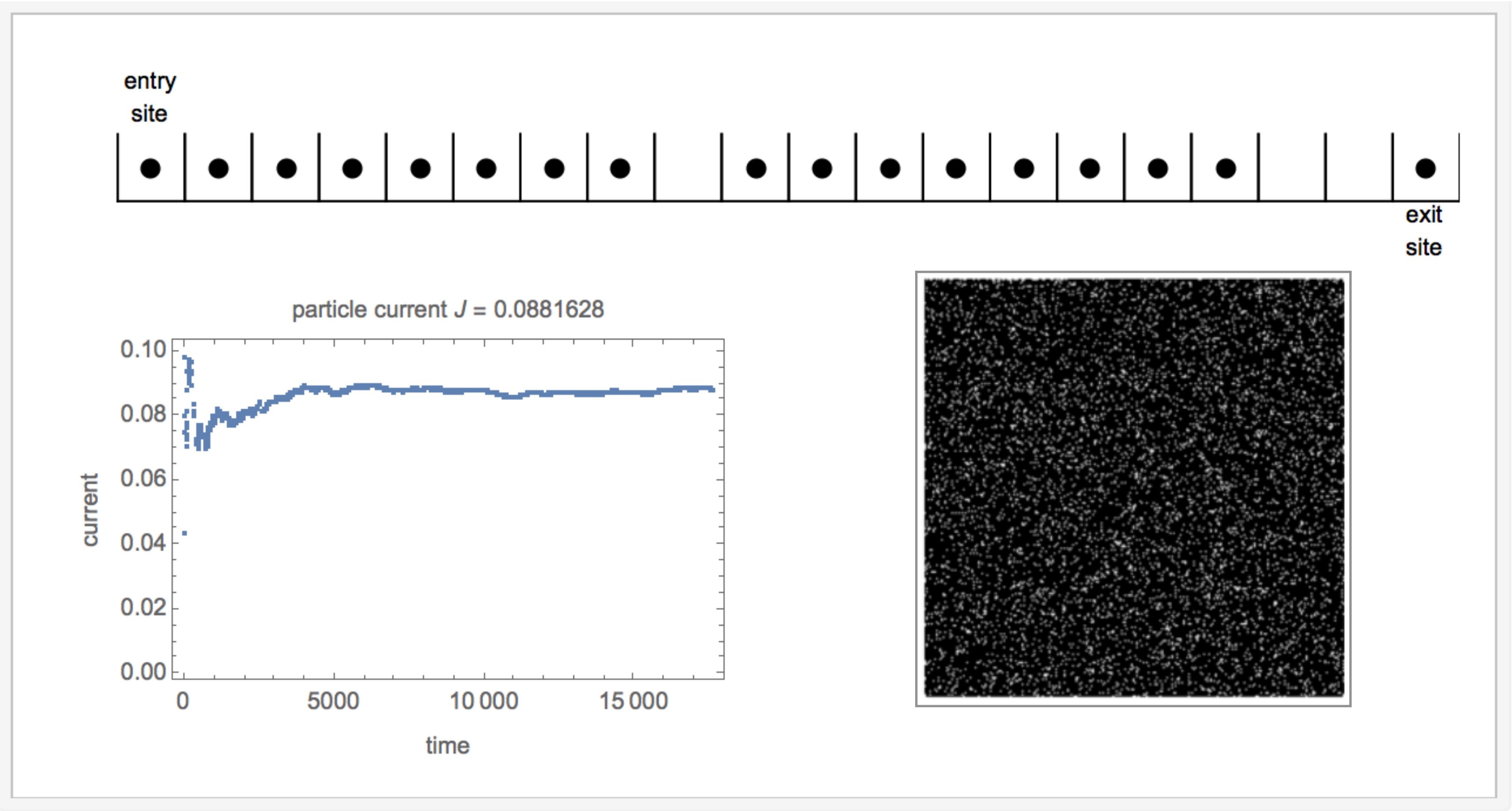

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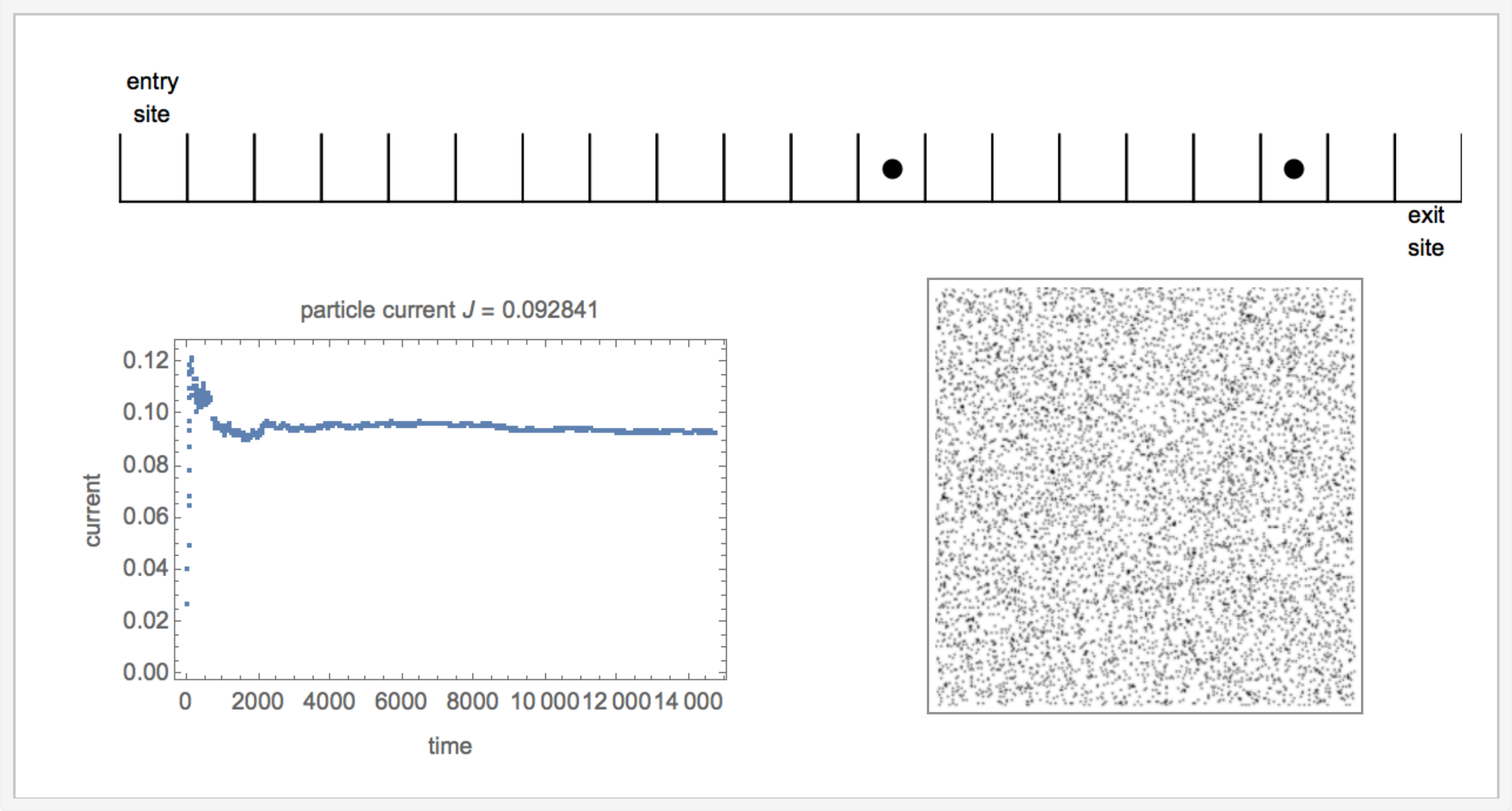
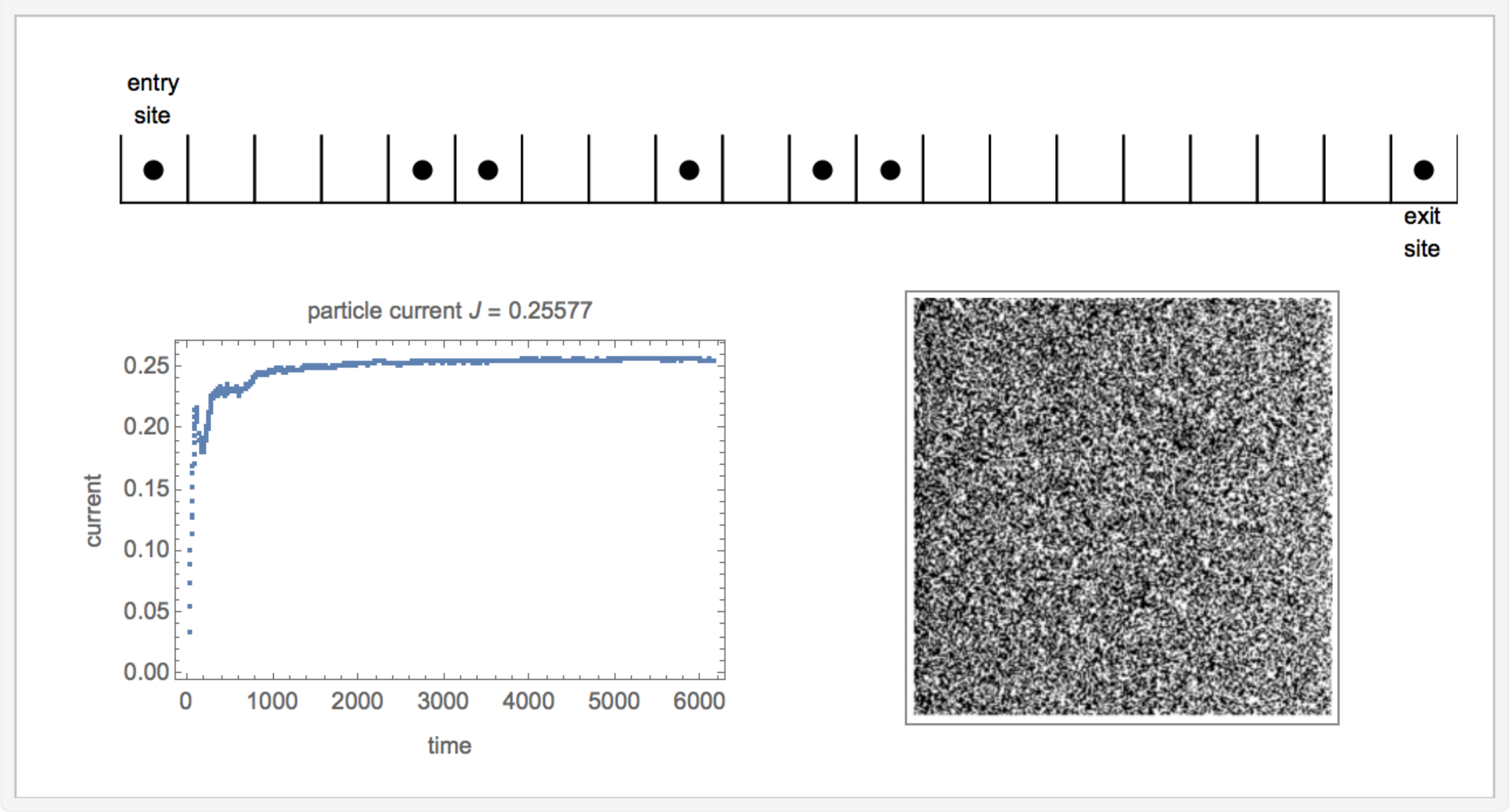


$(\alpha,\,\beta) = (0.6,\,0.6)$ $\bar{J} \simeq 0.25$ High current



$\alpha = \beta$

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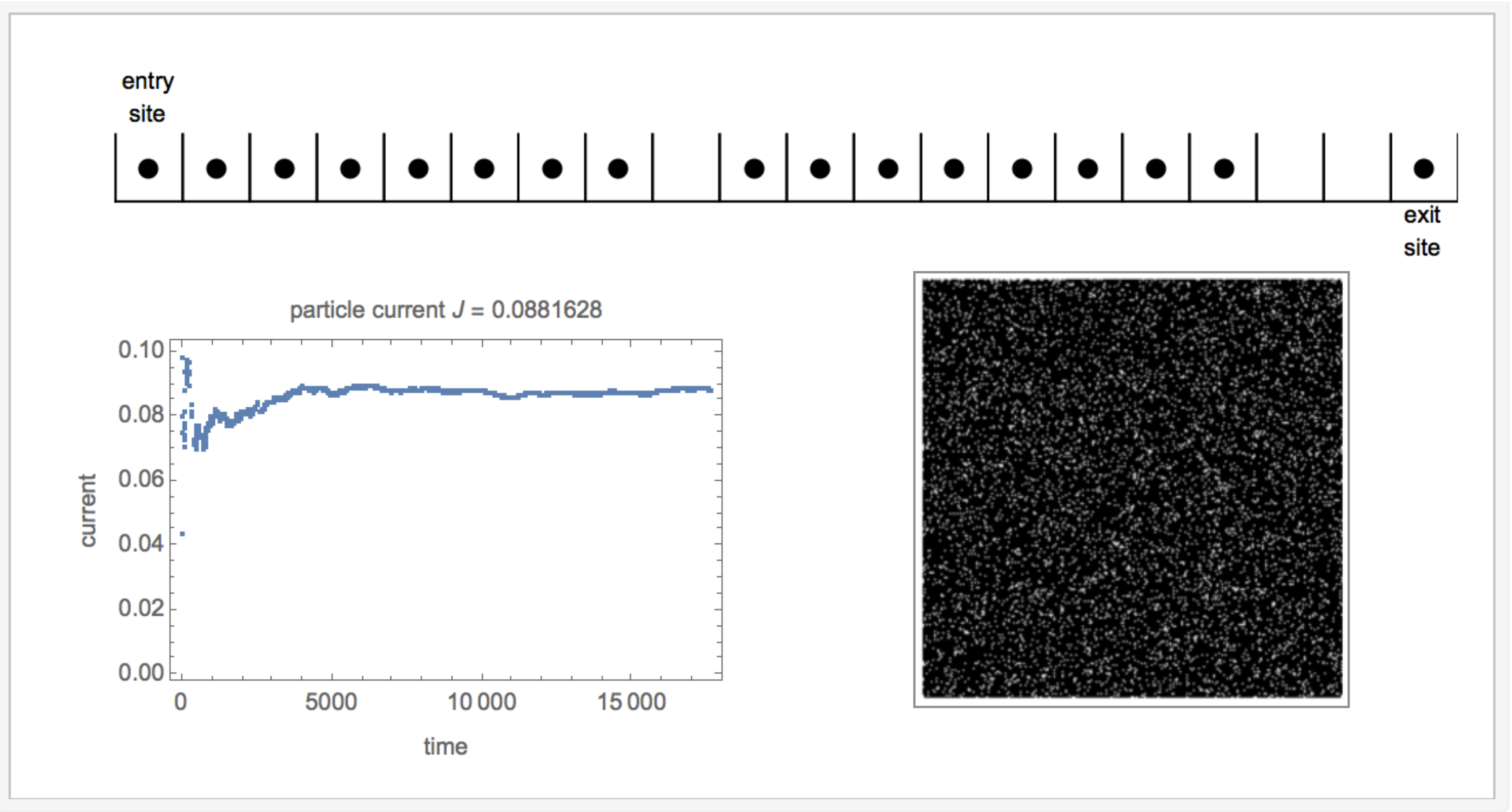

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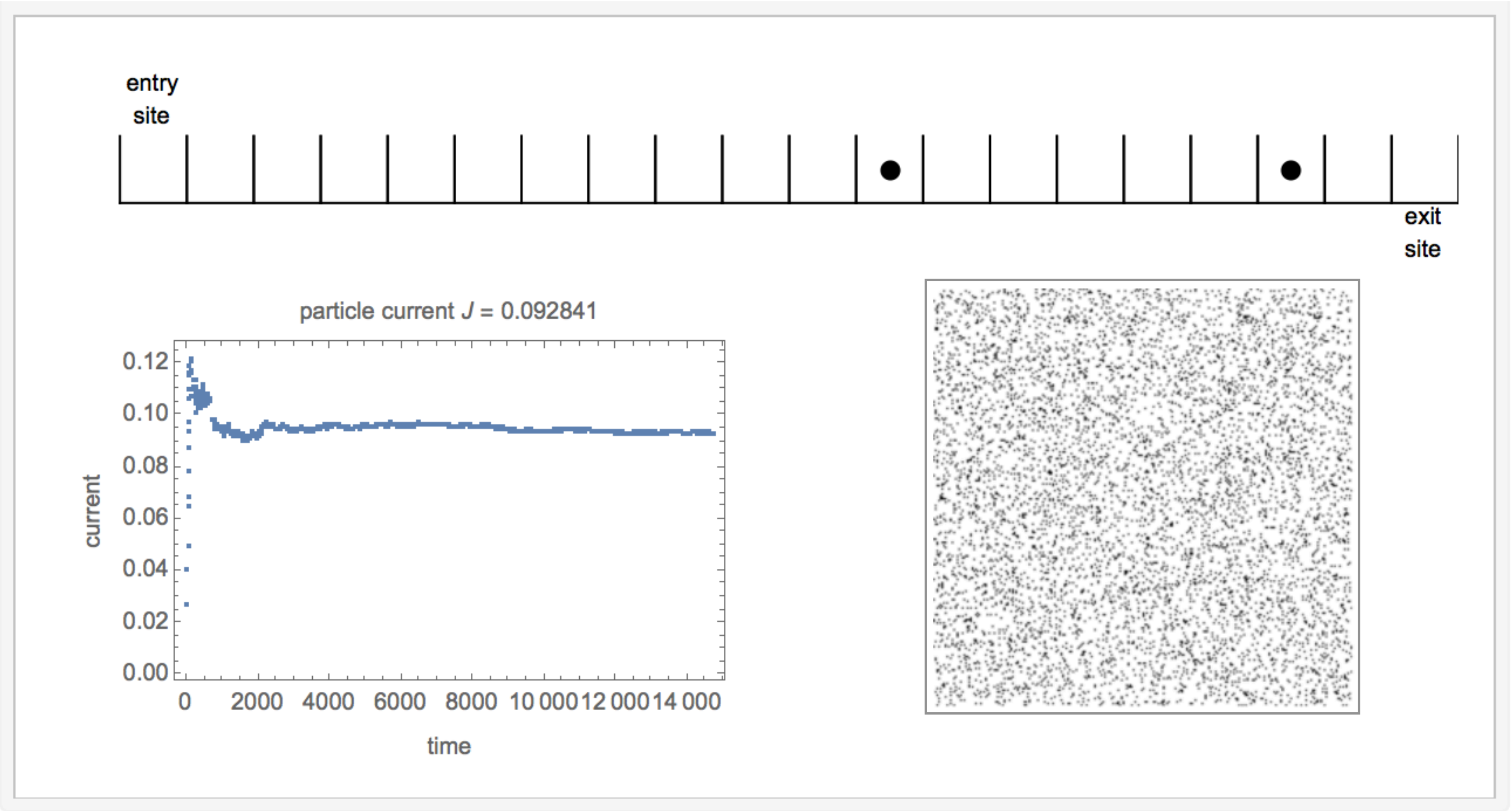

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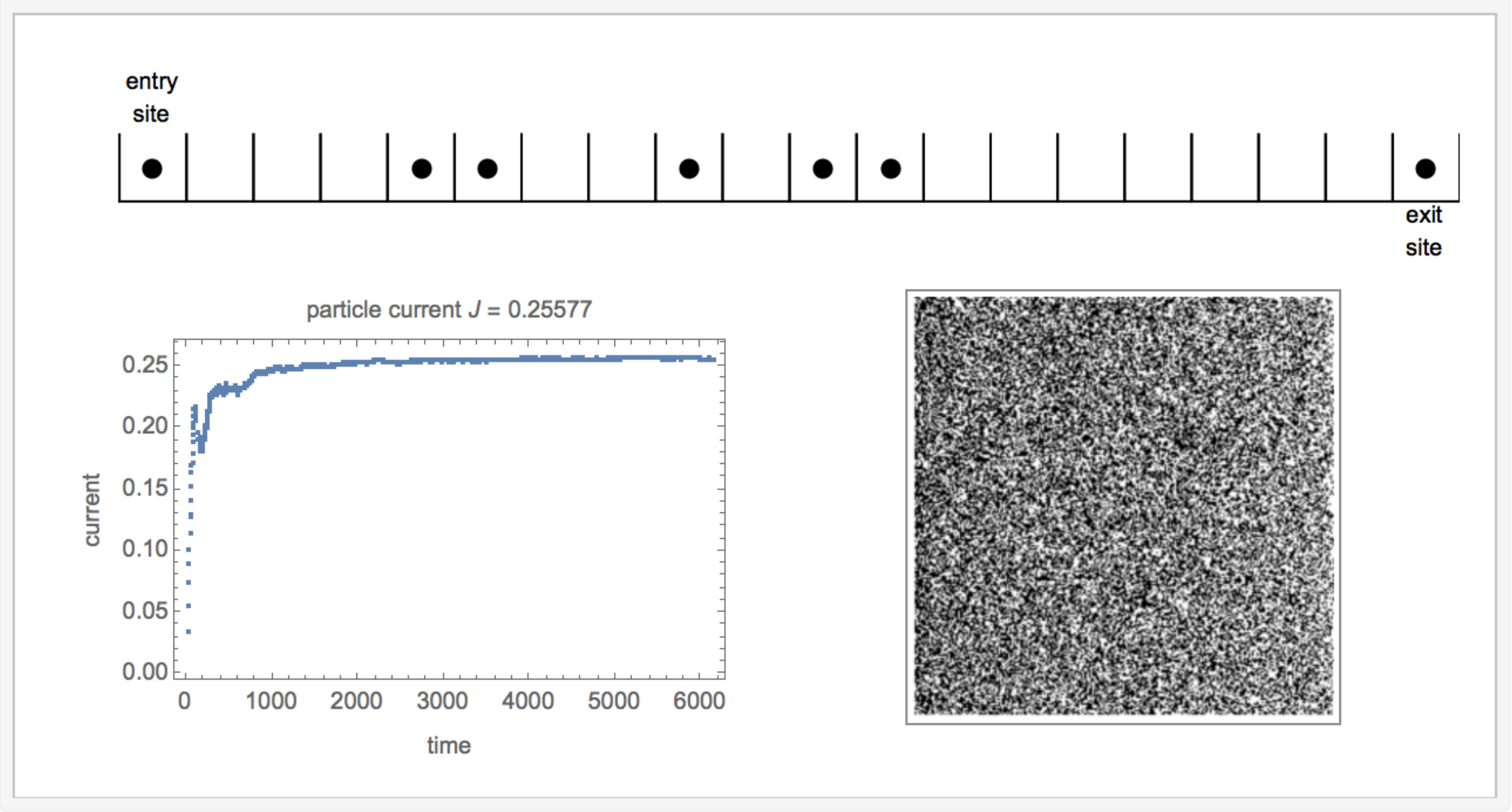
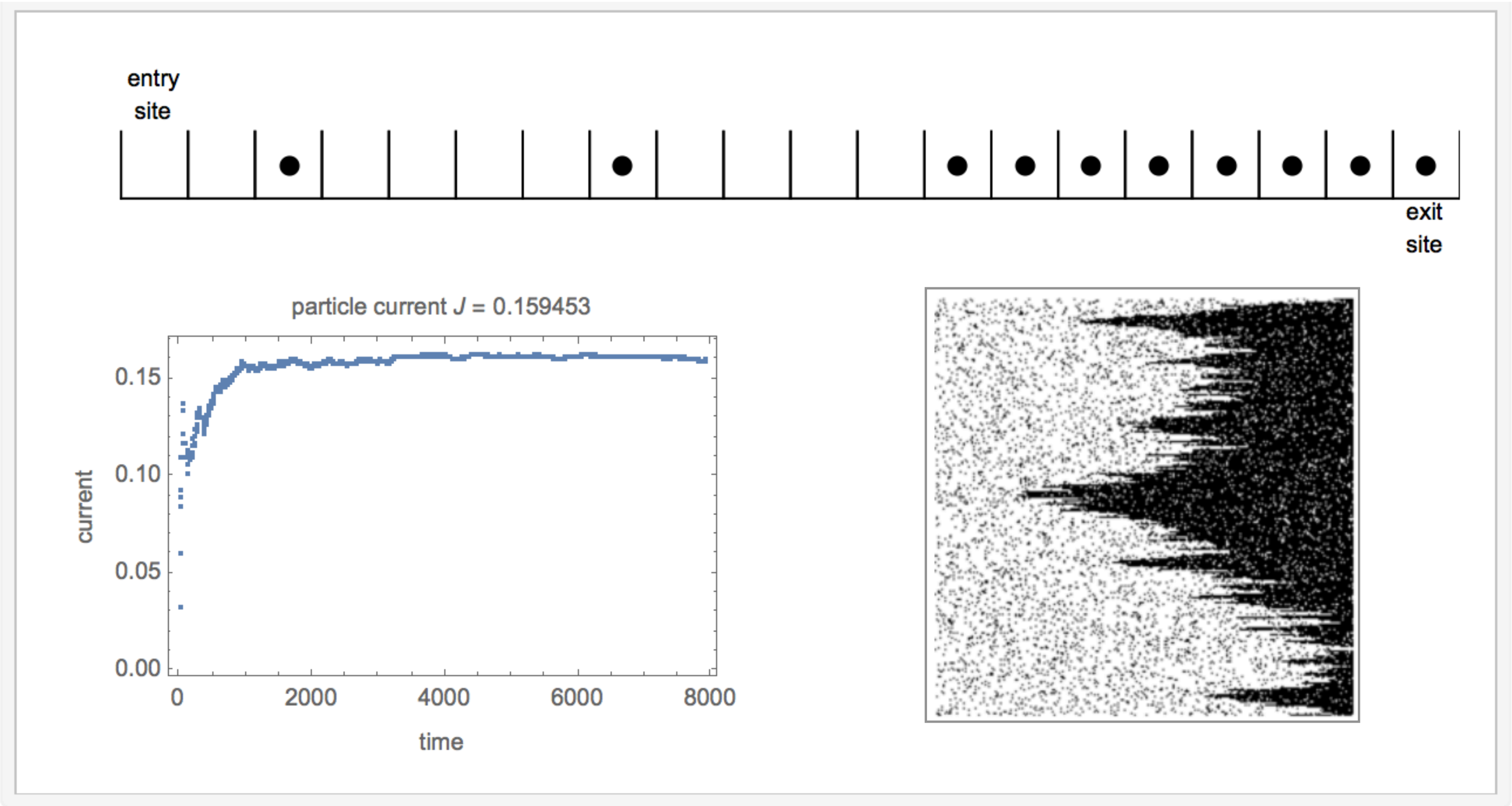


$\alpha = \beta$

$(\alpha,\, \beta) = (0.2,\, 0.2)$ $\bar{J} \simeq 0.15$ “Traffic jam”!



Boundary between two phases?

TASEP — Diagram of the Current

Two parameters:

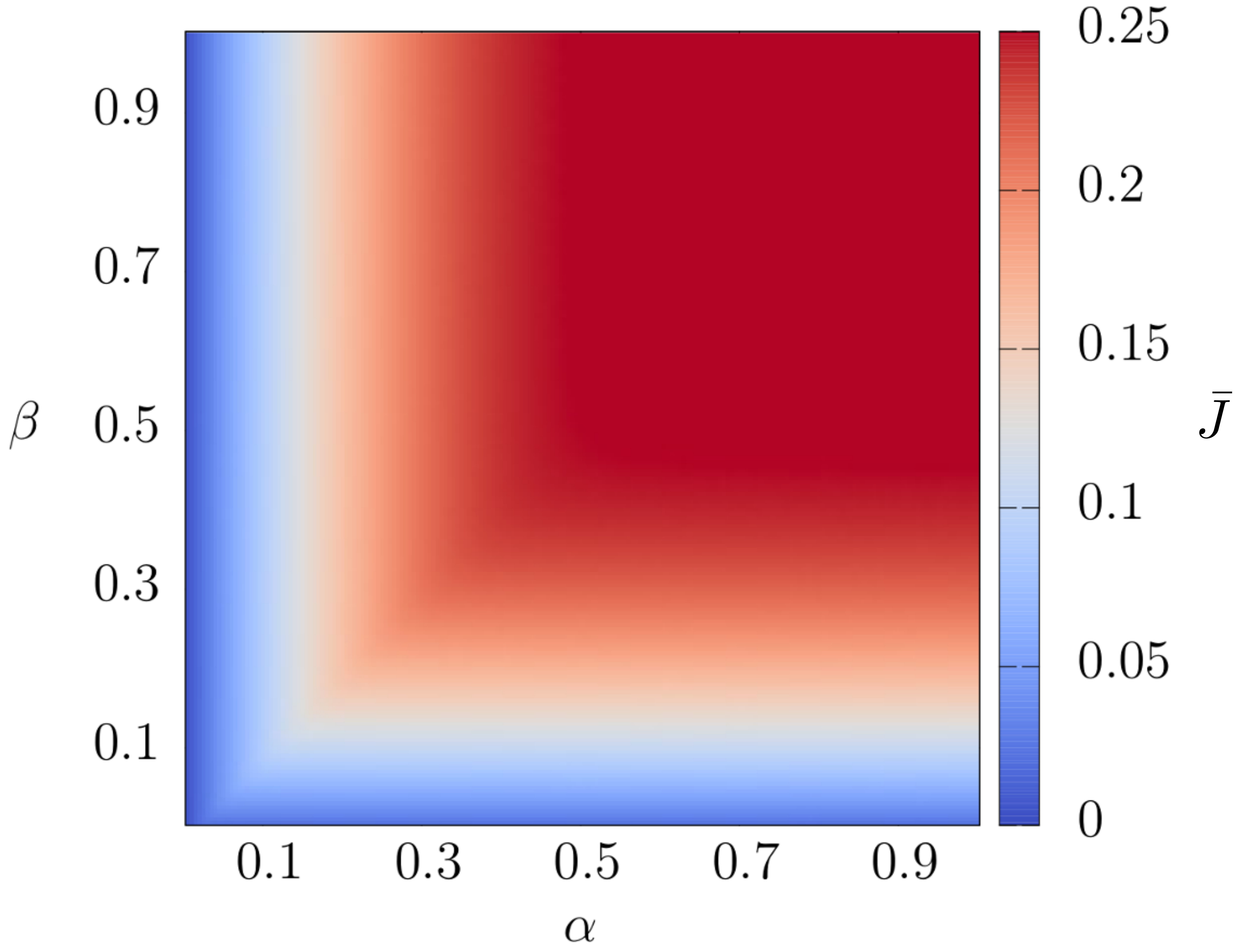
α = **rate** at which cars **enter from the left** of the lattice

β = **rate** at which cars **exit from the right** of the lattice

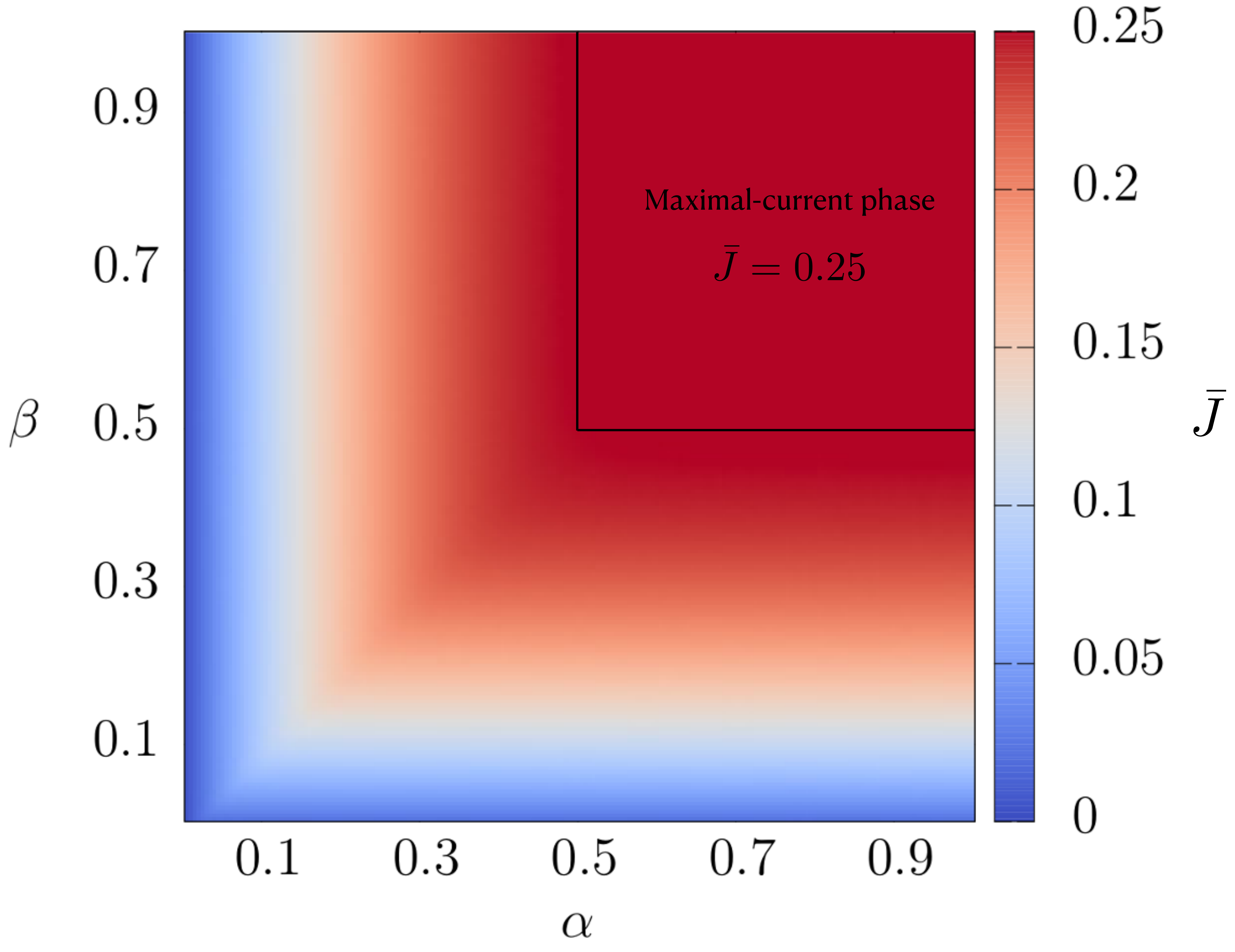
Average current across the system at stationarity: $\bar{J}$

beta \ alpha	0,1	0,2	0,3	0,4	0,5	0,6	0,7	0,8	0,9	1,0
1,0	0,09	0,158	0,21	0,23	0,25	0,256	0,27	0,27	0,27	0,26
0,9	0,09	0	0	0	0	0,255	0	0,27	0,26	0,265
0,8	0.09	0	0,21	0	0	0	0	0	0	0,27
0,7	0,09	0	0	0,24	0	0	0,25	0.23	0,25	0
0,6	0	0,17	0	0	0	0,25	0	0,22	0	0
0,5	0,09	0,16	0	0,24	0,25	0,25	0,25	0,26	0	0,25
0,4	0	0	0	0,23	0	0	0,25	0,25	0	0
0,3	0,09	0	0,19	0	0	0,21	0	0,2	0	0
0,2	0	0,15	0,16	0	0,15	0	0,17	0	0,15	0,16
0,1	0,09	0	0,09	0	0,09	0	0,09	0	0	0,09

TASEP — Current



TASEP — Phase diagram



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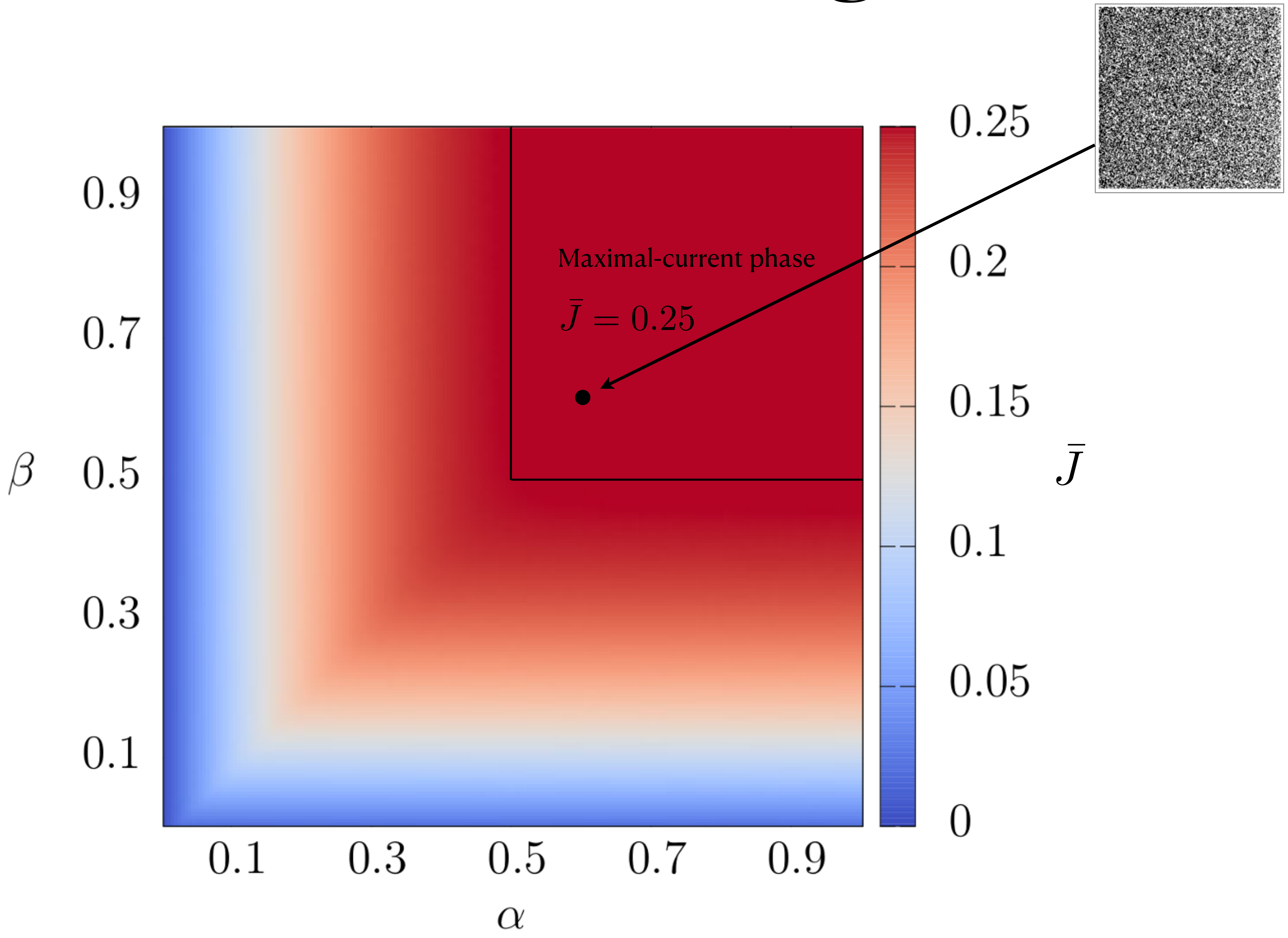

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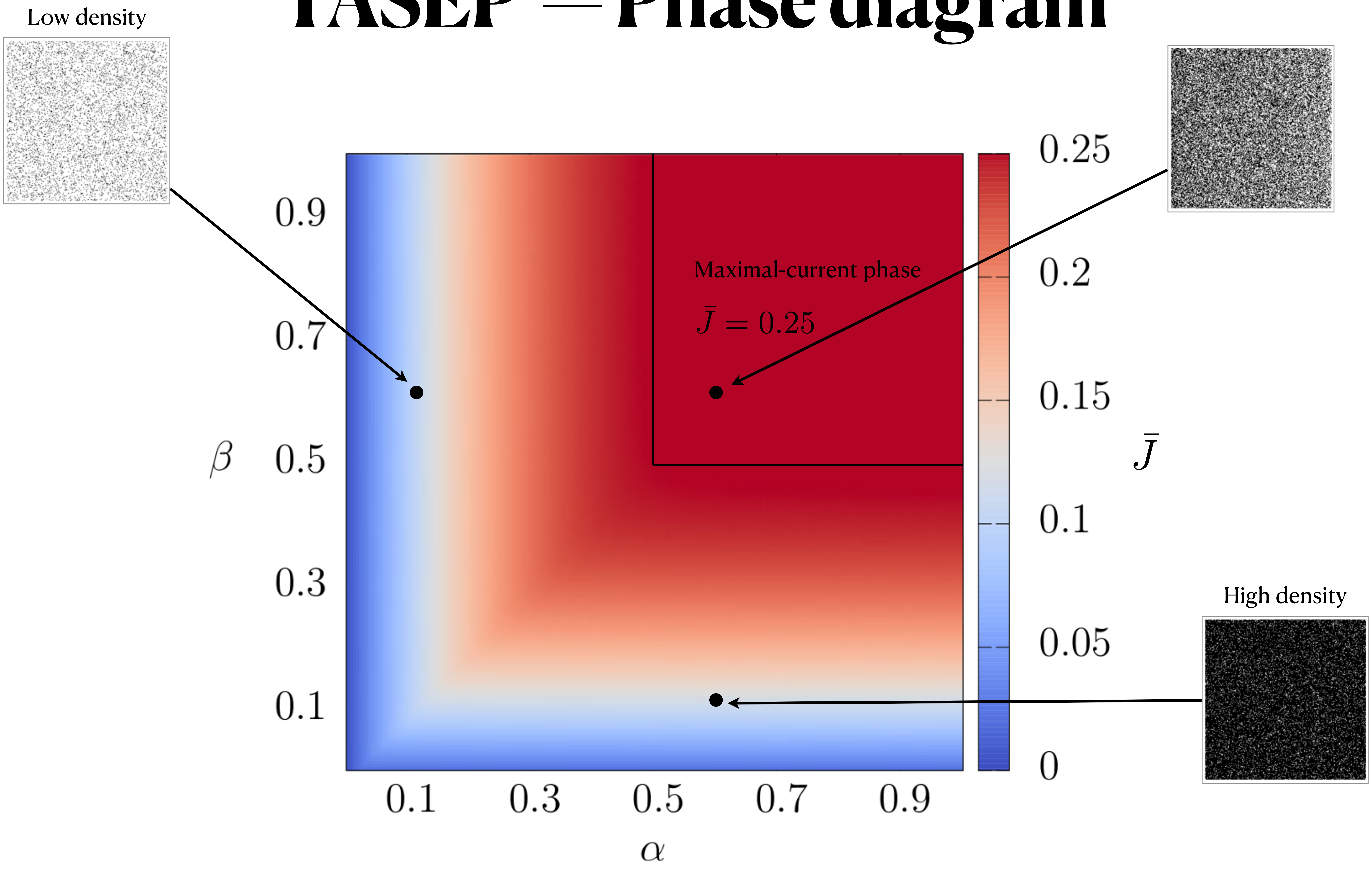

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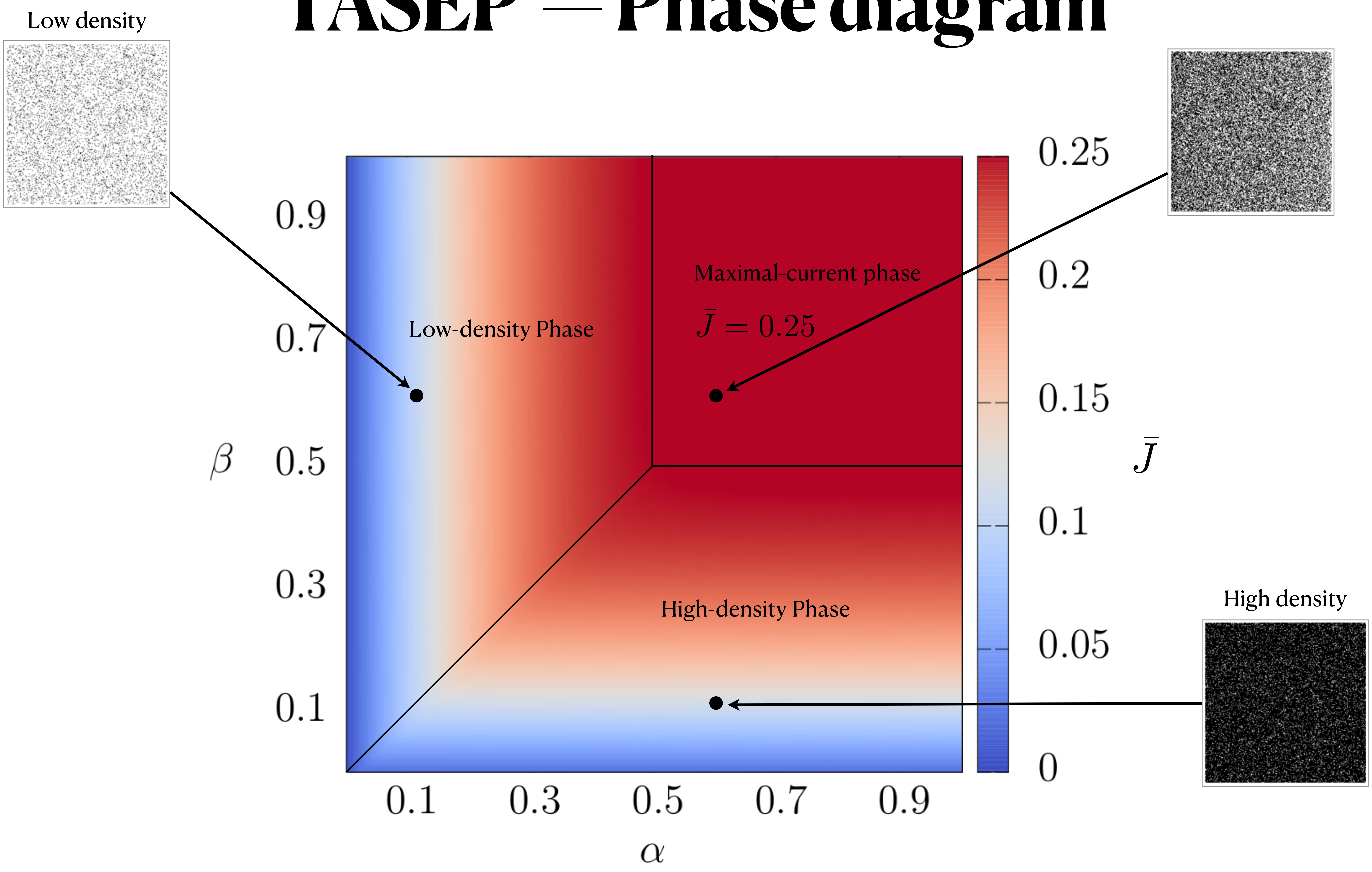

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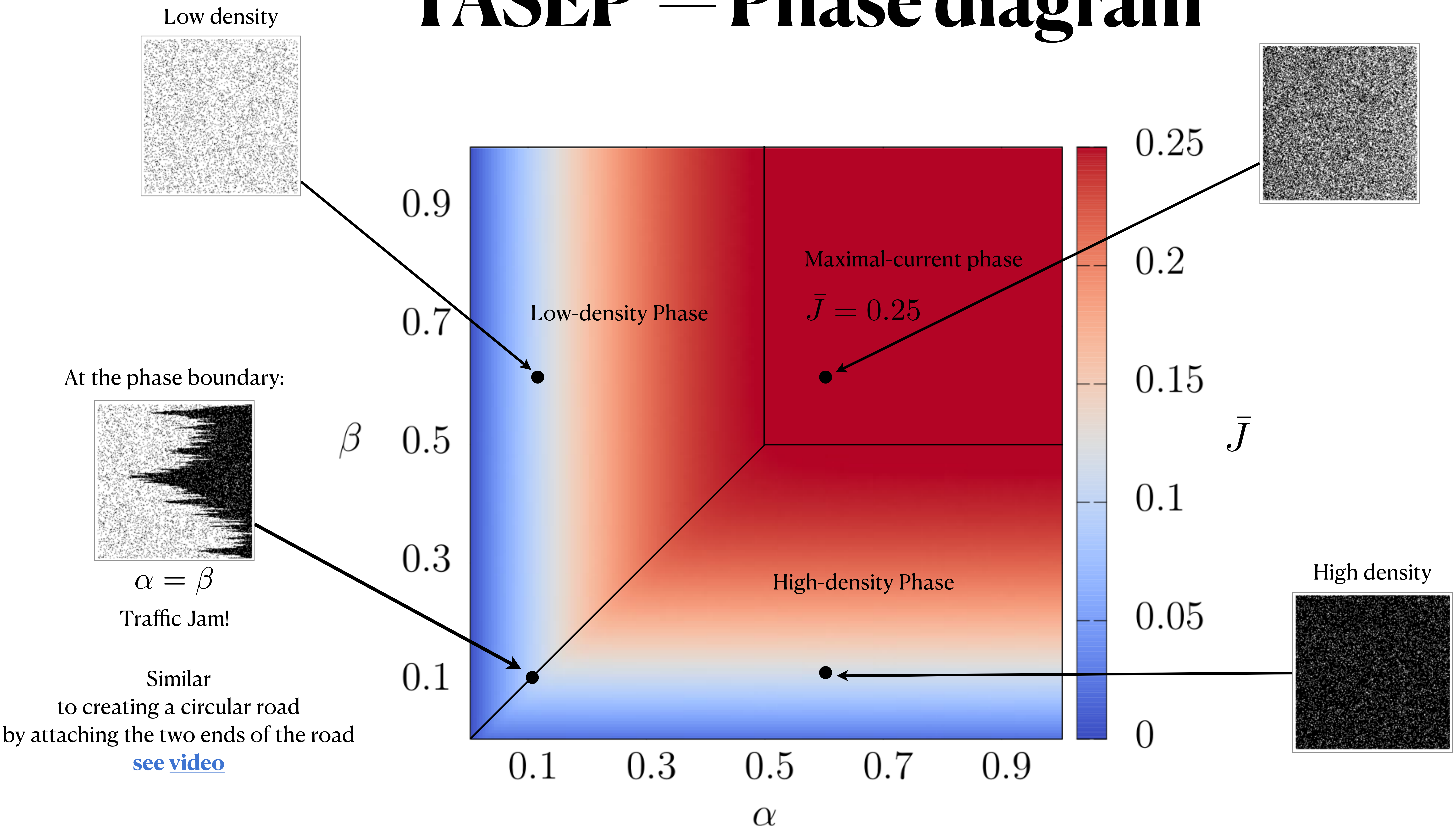
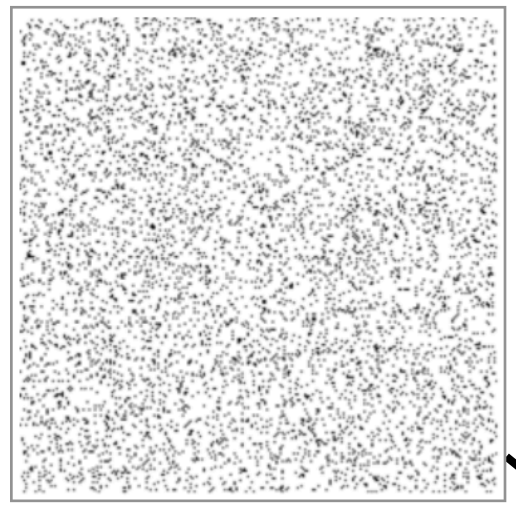
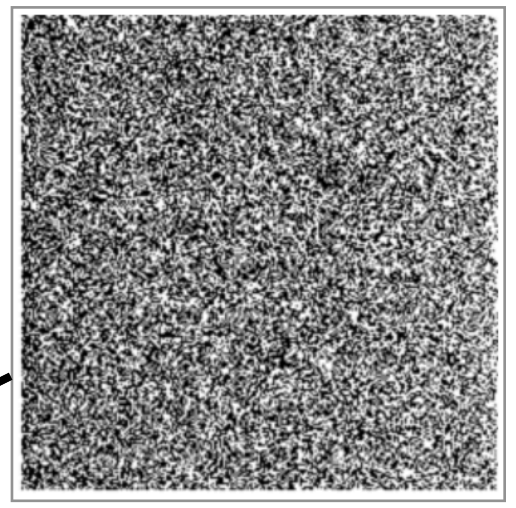


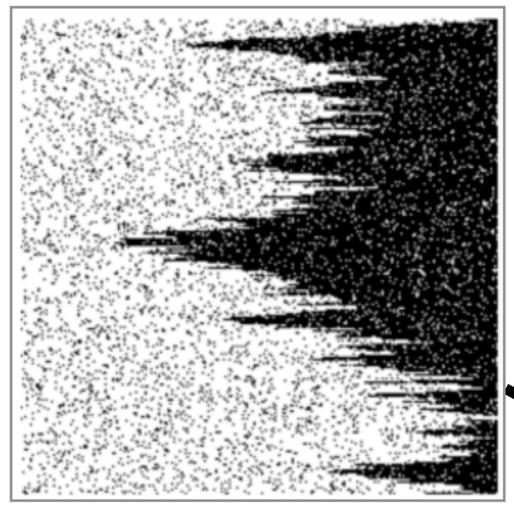
TASEP — Phase diagram

Low density





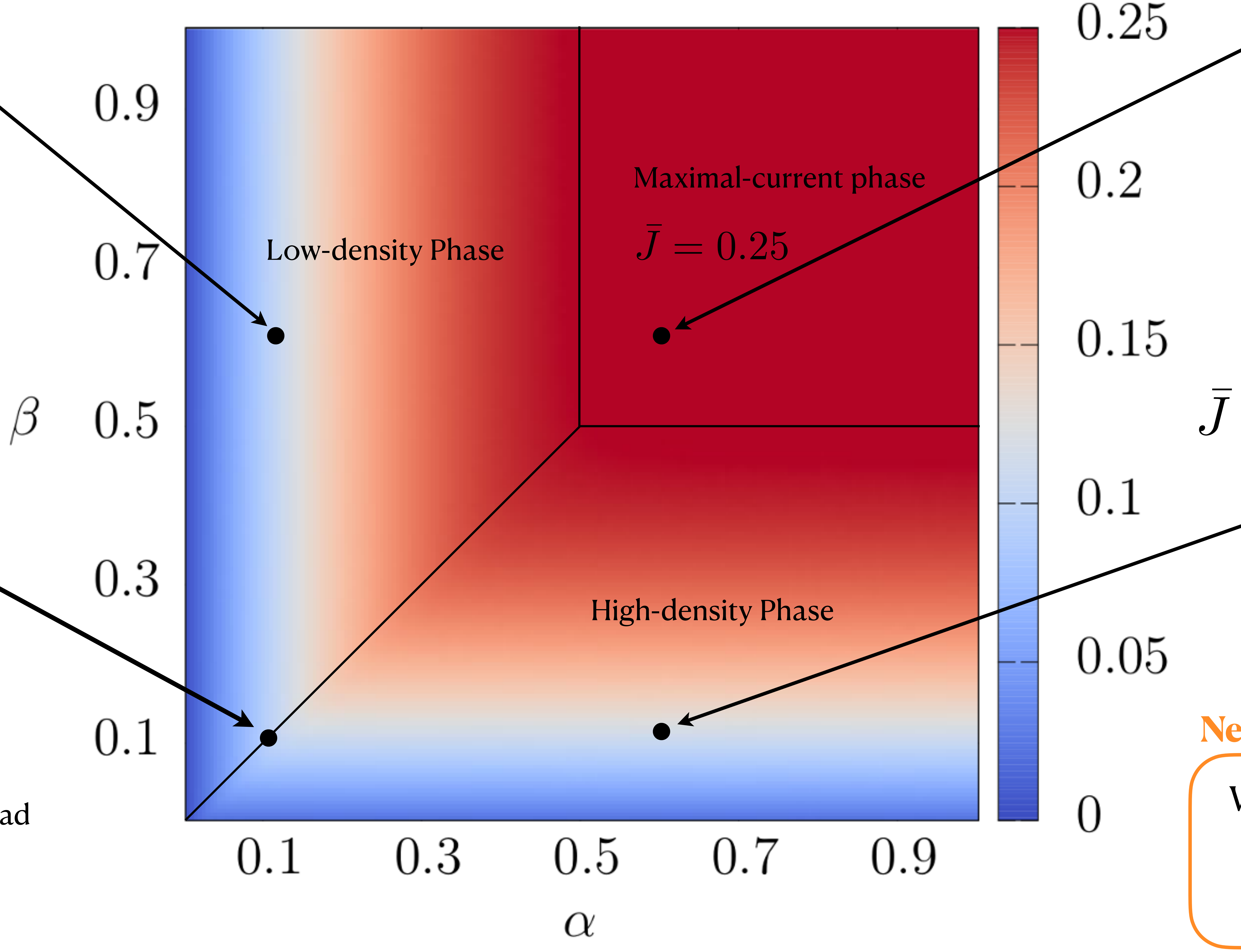
At the phase boundary:



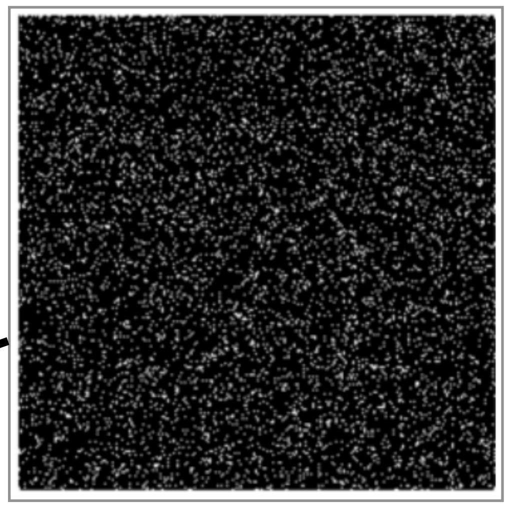
$\alpha = \beta$

Traffic Jam!

Similar
to creating a circular road
by attaching the two ends of the road
see video



High density



Next: tutorial T4

We will see later how to prove that these are the different phases of this system.

Phases and phase diagrams

Phase

Phase: a **macroscopic state** of a system that has **physical properties** that are **uniform on a macroscopic length scale**.

Ex.

Phase

Phase: a **macroscopic state** of a system that has **physical properties** that are **uniform on a macroscopic length scale**.

Ex. Different phases of water

Liquid (water)

Solid (Ice)

Gas (water vapours)

Phase

Phase: a **macroscopic state** of a system that has **physical properties** that are **uniform on a macroscopic length scale**.

Roughly speaking

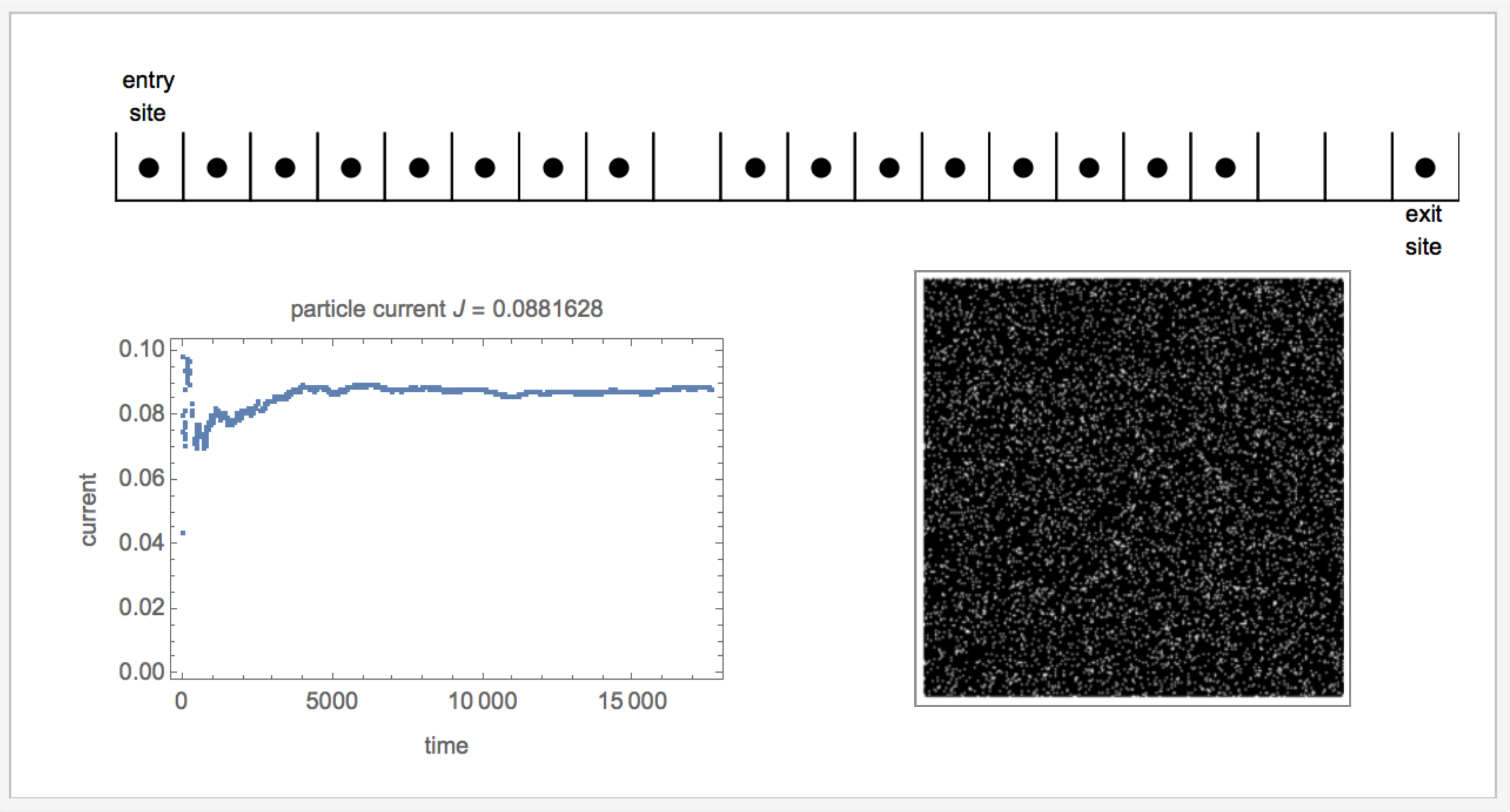
microscopic scale: In physics/chemistry: atomic scale

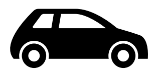
Scale of the individual component of the complex systems

macroscopic scale: Physics/chemistry: our "daily life scale"

complex systems: scale at which the system display non-trivial collective behaviour

$(\alpha, \beta) = (1, 0.1)$ High density $\bar{J} \simeq 0.09$



Microscopic states: Position of all the cars: $\bullet$ = 

$$P(s_1, \cdots, s_N)$$

Macroscopic properties:

$\overline{n_i}$ = **density of cars** at site i = average number of cars at site i

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Phase Diagram

The **phase** of system is **determined** by the values of **a few parameters**, such as the **temperature** and the **pressure**.

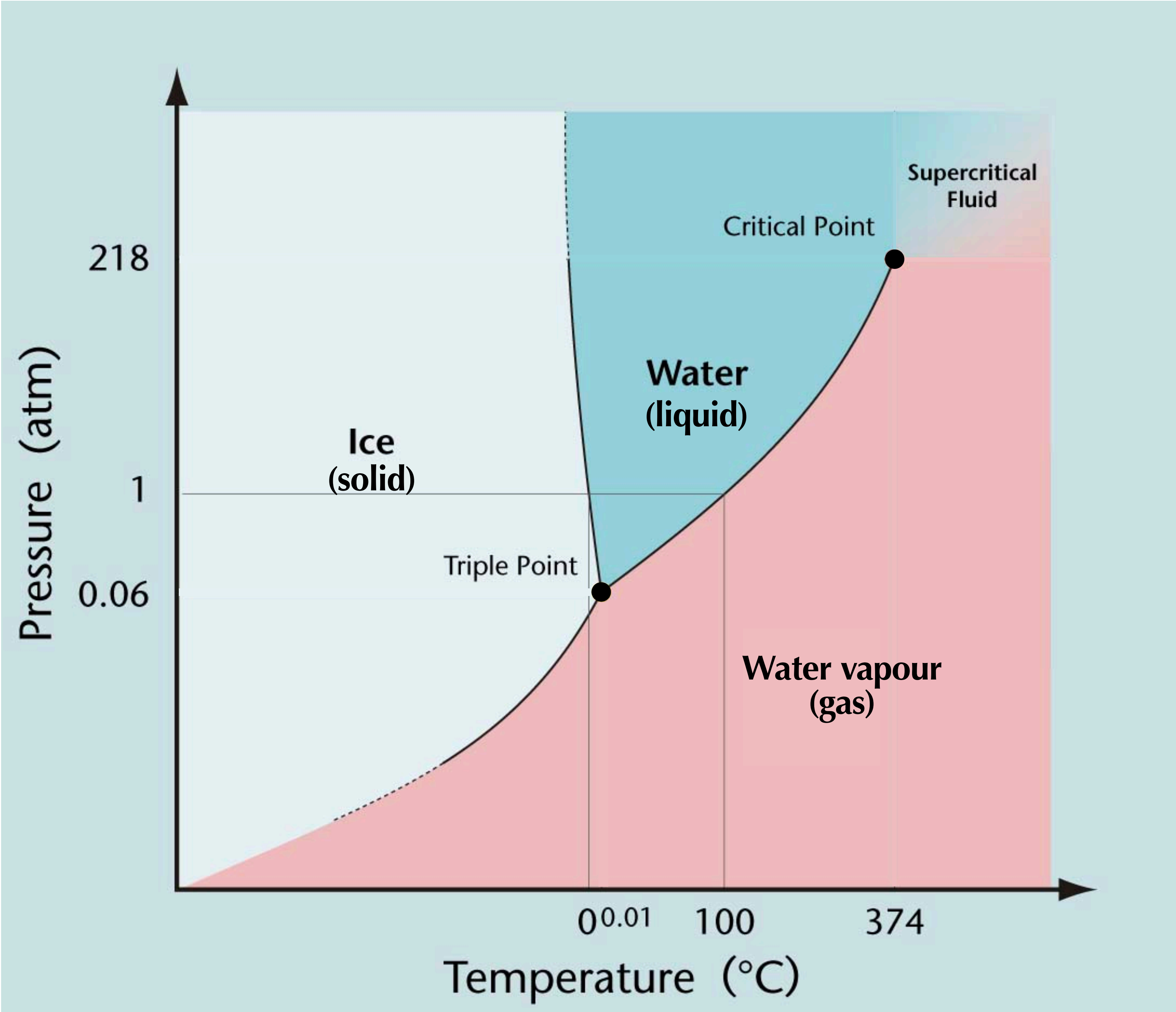
Ex. At the atmospheric pressure, at T = 25 ^oC, water exists as a ....?

at T = -4 ^oC, water exists as a ....?

at T = 105 ^oC, water exists as ....?

Phase Diagram: is a graph with those parameters as the axes, on which the phase is specified for each point.

Phase Diagram for water



Phase Diagram

The **phase** of system is **determined** by the values of **a few parameters**, such as the **temperature** and the **pressure**.

Ex. At the atmospheric pressure, at T = 25 °C, water exists as a liquid

at T = -4 °C, water exists as a solid

at T = 105 °C, water exists as a gas

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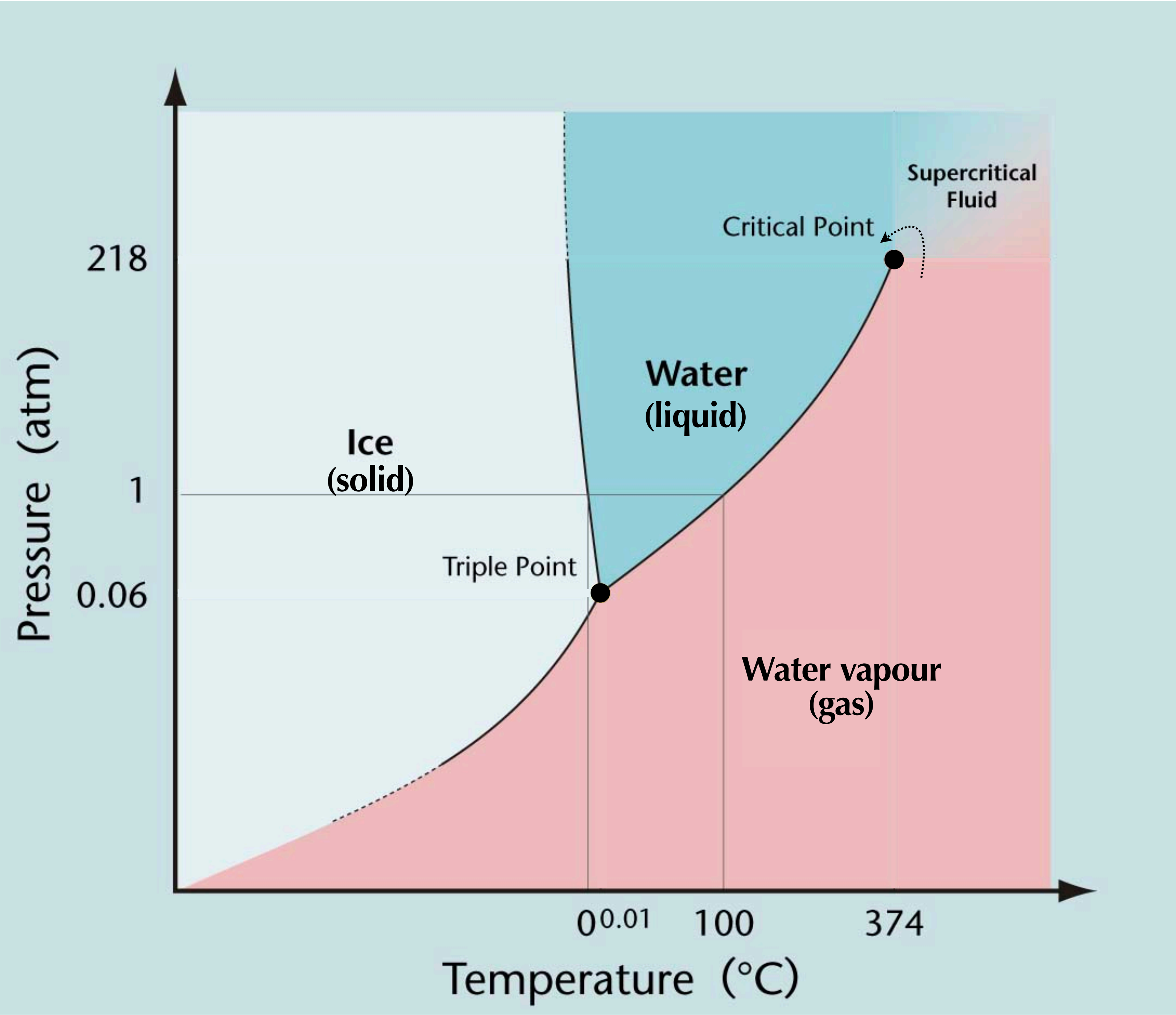
for water



Phase boundaries:

Coexistence of two phases at the boundary

Triple points:

Coexistence of the three phases at this point

Critical point:

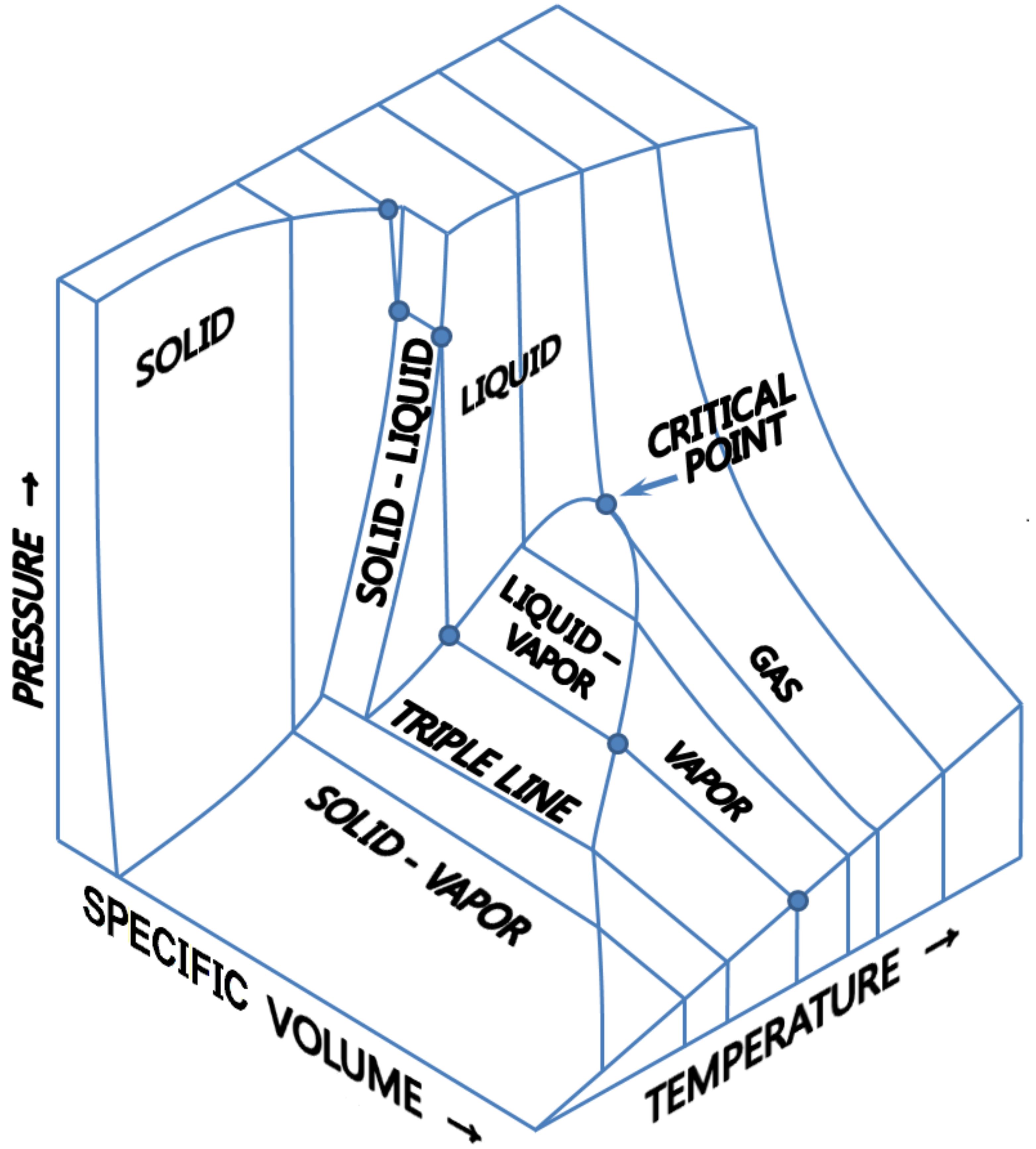
Beyond the critical point, there is no distinction between liquid and gas.

It is possible to go from liquid to gas without crossing any boundary curve

Phase Diagram

There are **not necessarily only two parameters** that define the phase of a system.

Ex. 3D Typical phase diagram for a pure substance:



Triple line

Coexistence of the three phases along this line.

Critical point

Phase Diagram

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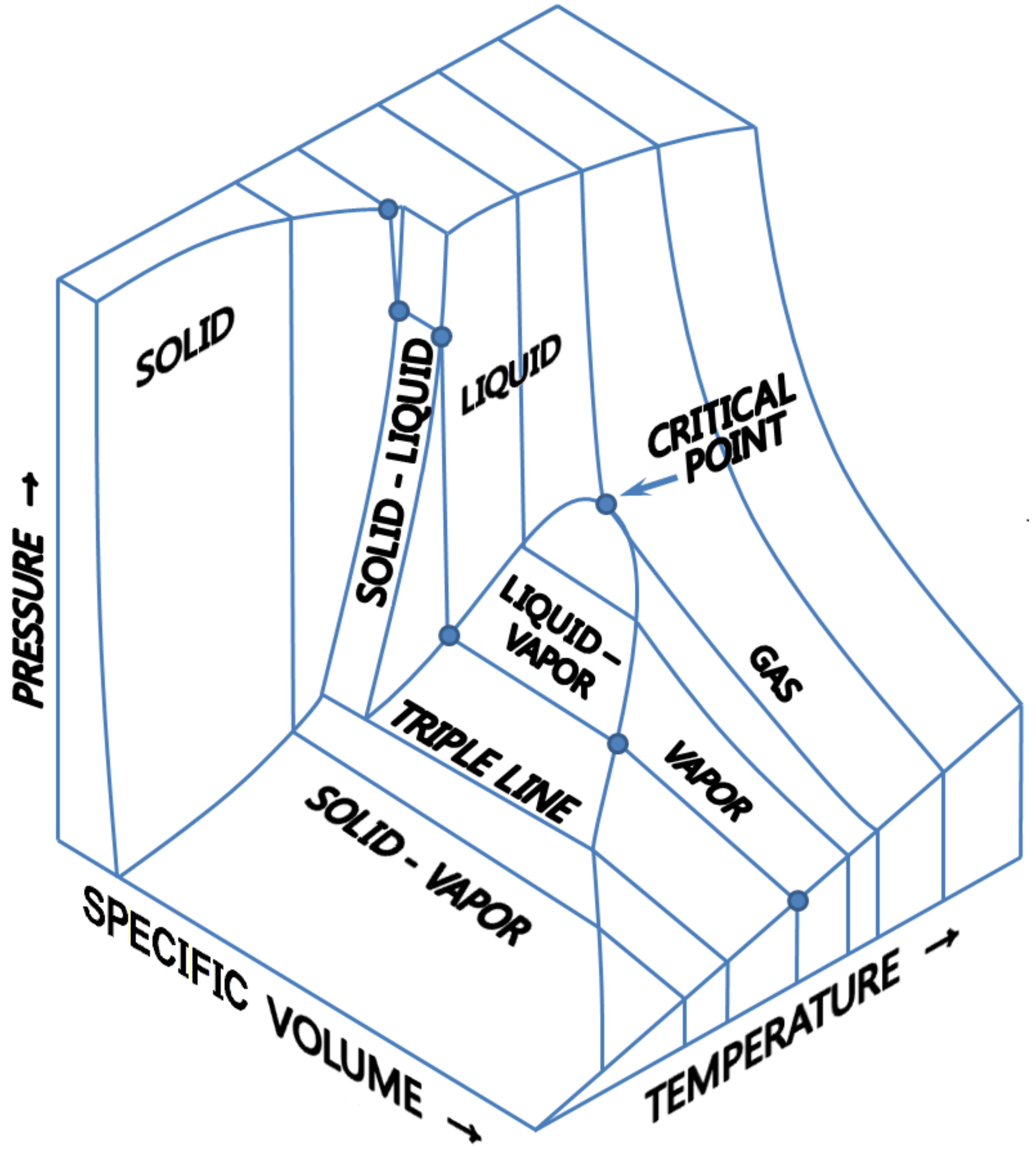

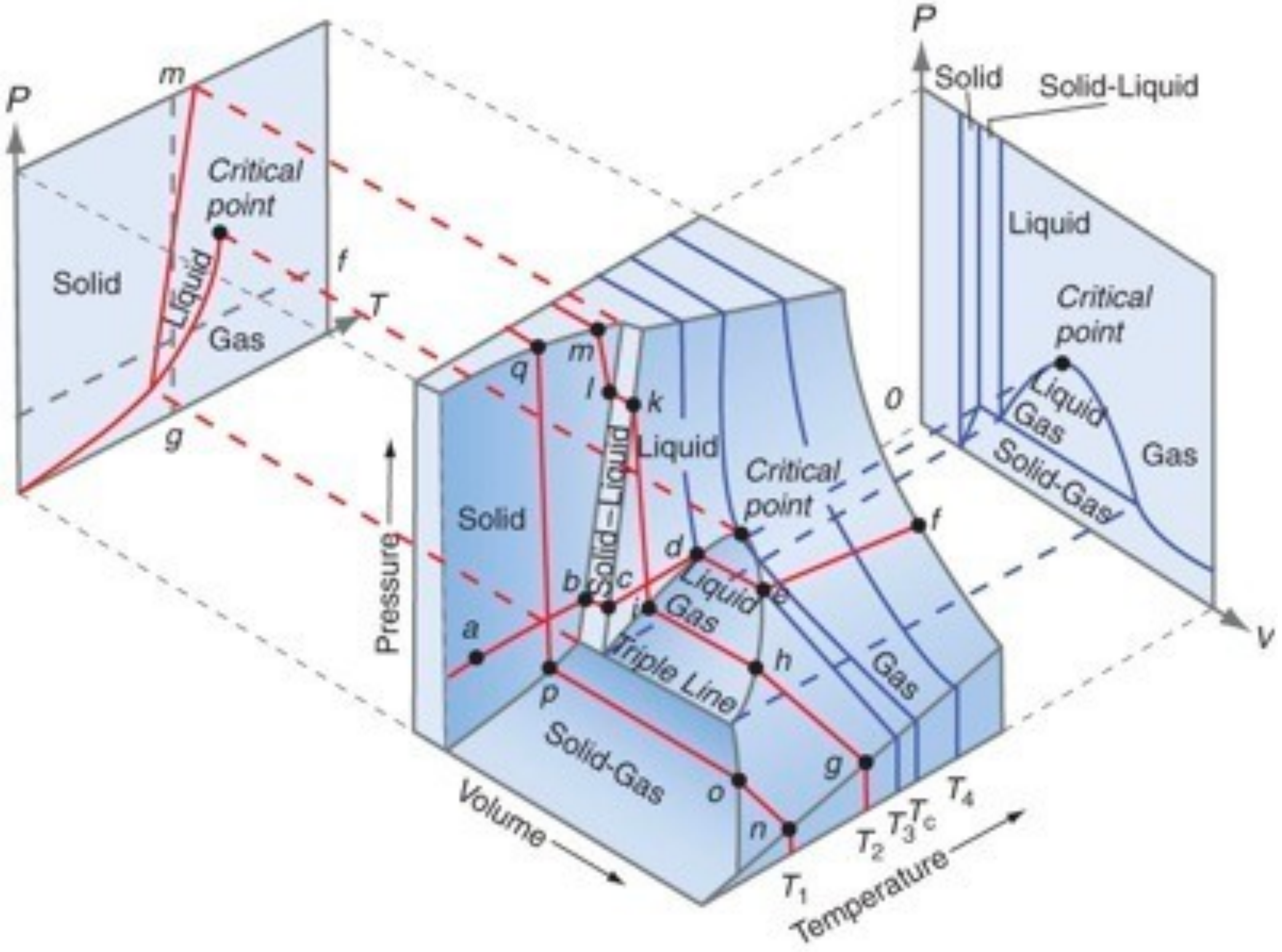

Two ways we will study the macroscopic states/properties of a system

1) **Using statistical physics approach to thermodynamics** —>> this coming lectures

2) **Compute equation of evolution for the probability distribution over the microstates** —>>> Master Equation
Solve it at stationarity

—>> later on, going there

Thermodynamic potentials

Phases of system are characterised by thermodynamic functions.

Thermodynamic potential:

is a **function of the parameters of the system** and external constraints (e.g. pressure, temperature) that **decreases during the evolution of the system** until reaching a **minimum at equilibrium**.

The variation of this function thus allow to **predict the directions of evolution of a system** and the **stability of the equilibrium**.

Common examples:

Internal energy:	**U**	T = temperature of the system
Free energy:	$\mathbf{F = U - TS}$	P = Pressure of the system
Enthalpie:	$\mathbf{H = U - PV}$	S = Entropy of the system
Gibbs free energy:	$\mathbf{G = H - TS}$	

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Common thermodynamic potential:

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Free energy:	**F = U - TS**	when **V** and **T** are **fixed**
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Proof: by combining 1rst and 2nd law of thermodynamics

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Common thermodynamic potential:

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Free energy:	$F = U - TS$	when V and T are **fixed**
Enthalpie:	$H = U + PV$	when P and S are **fixed**
Gibbs free energy:	$G = H - TS$	when P and T are **fixed**

For many simple models of complex systems:

Look at systems with
— fixed size (~ volume)
— and fixed temperature

Temperature = level of noise

Phase Transitions

Phase Transitions

Phase Transition:

When a system undergoes a **drastic change in its macroscopic properties** in response to **a small change in the environment**.

Ex. At atmospheric pressure, ice turns to liquid water at exactly 0°C

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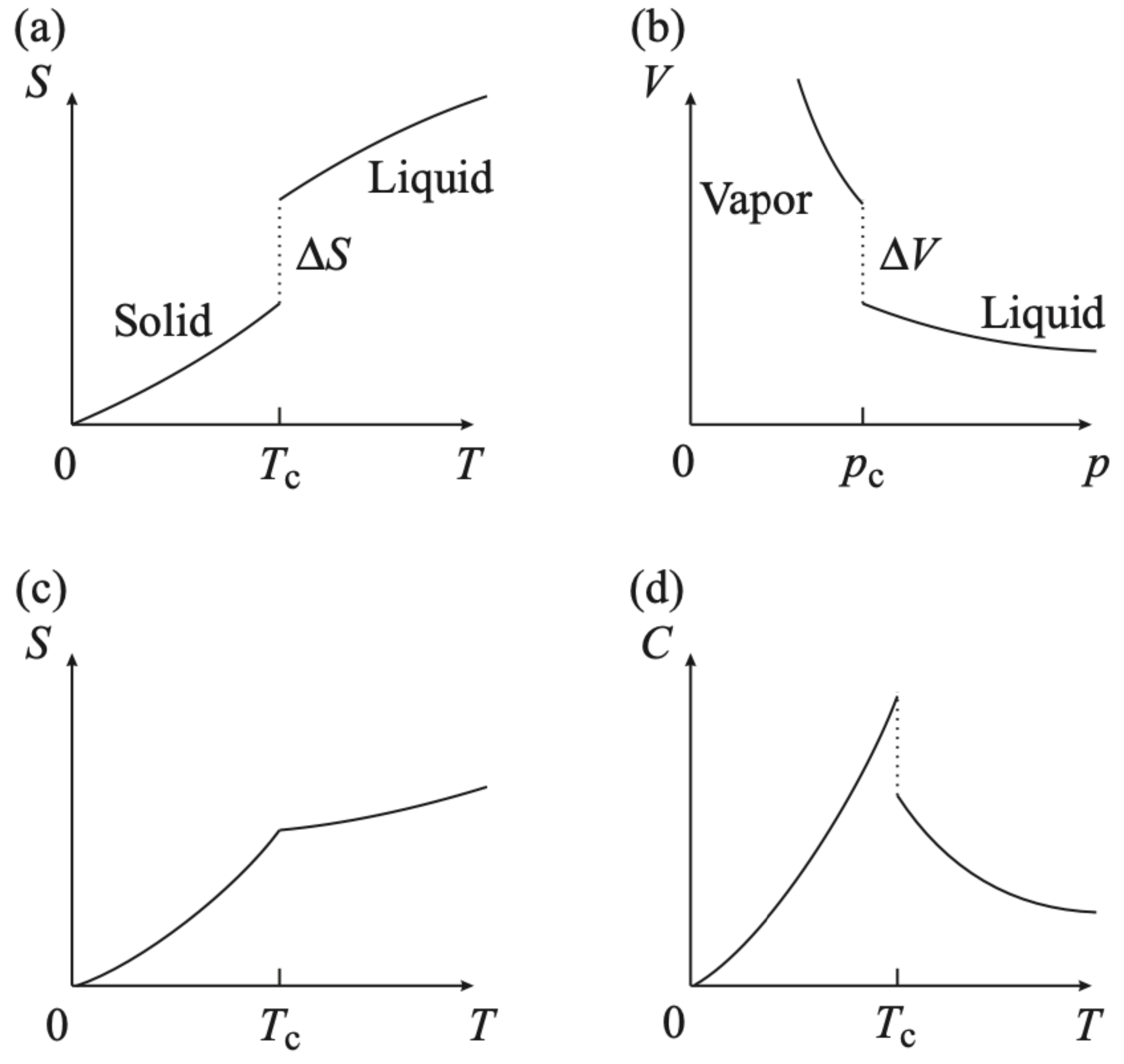
This **drastic change** is described theoretically by **singularities in the physical quantities** characterising the system.



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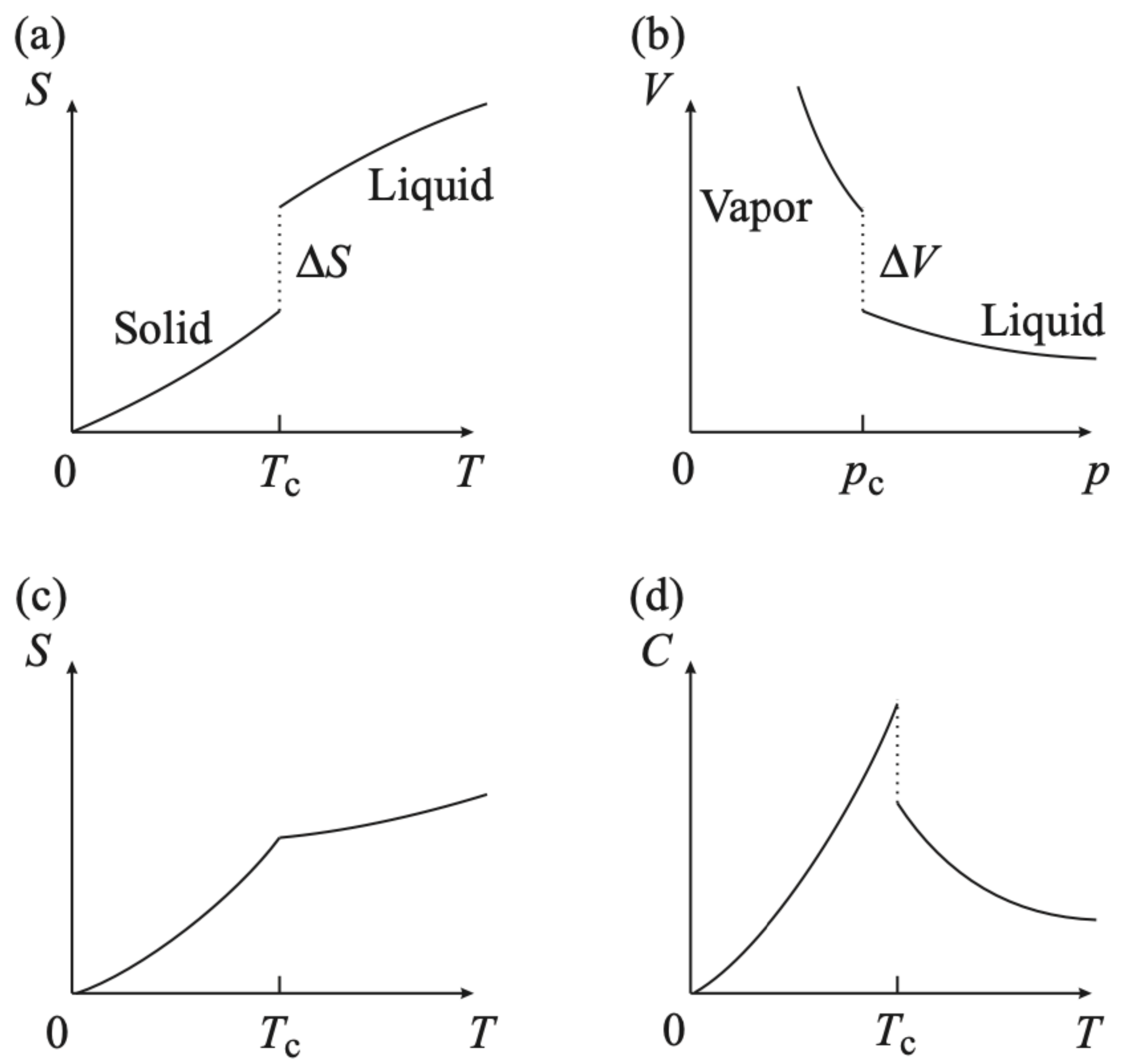


Two broad categories:

Discontinuous phase transitions (or "first order" phase transitions)

Continuous phase transitions (or "second order" phase transitions)

Discontinuous phase transitions

Most phase transitions are **not critical**, but are **abrupt**.

Discontinuous phase transitions:

At the transition, the **system has discontinuities in most physical properties**

(entropy, density, compressibility, viscosity, specific heat, thermal conductivity, .. all jump to a new value)

Ex.

When water starts boiling, it undergoes a phase transition from liquid to gas.

For each phases, the **equation of state** is a well-defined regular function.

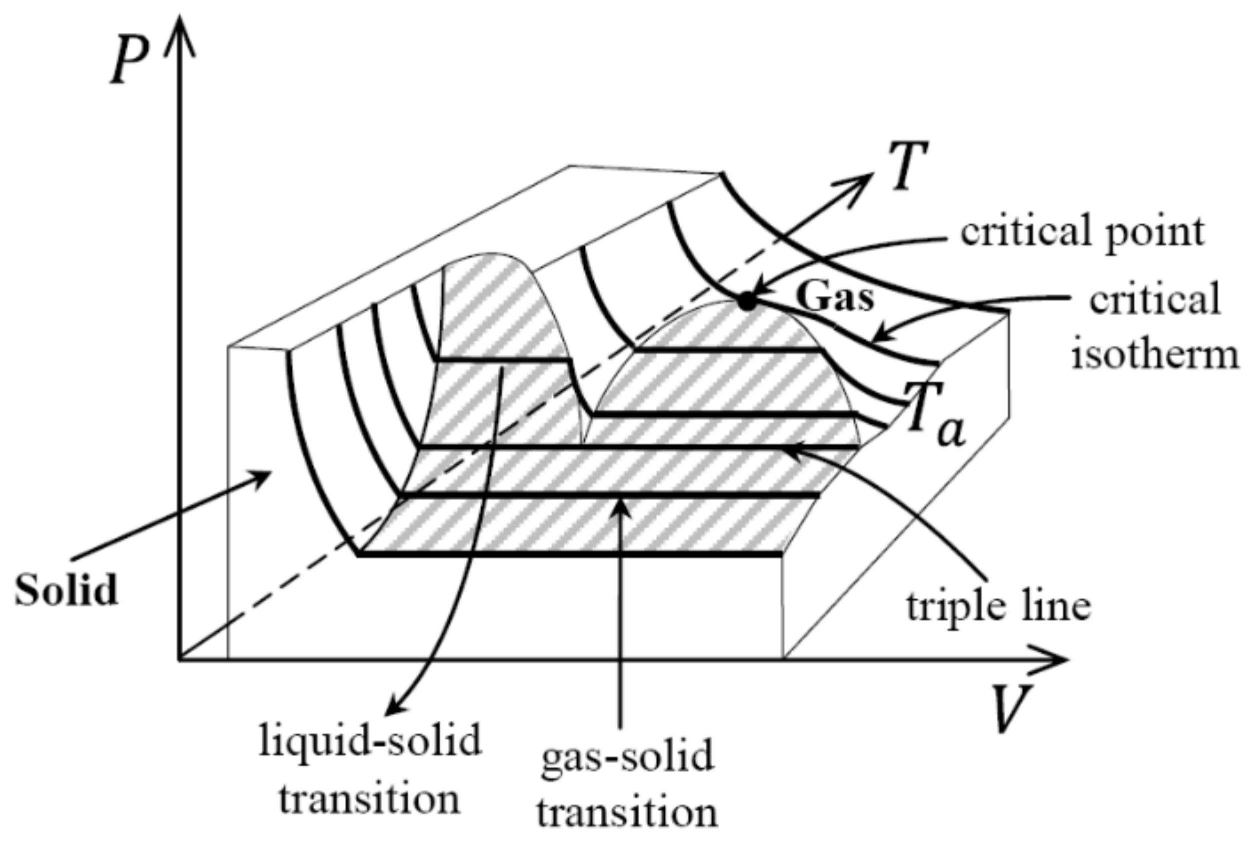
Going from liquid to gas one function "abruptly" changes to the other function.

In most cases these **transitions happen with no precursors**, **no hint** that a change is about to occur.

Ex. water vapor at 101°C has no little droplets of water inside.

Boiling water: Discontinuity of the Volume

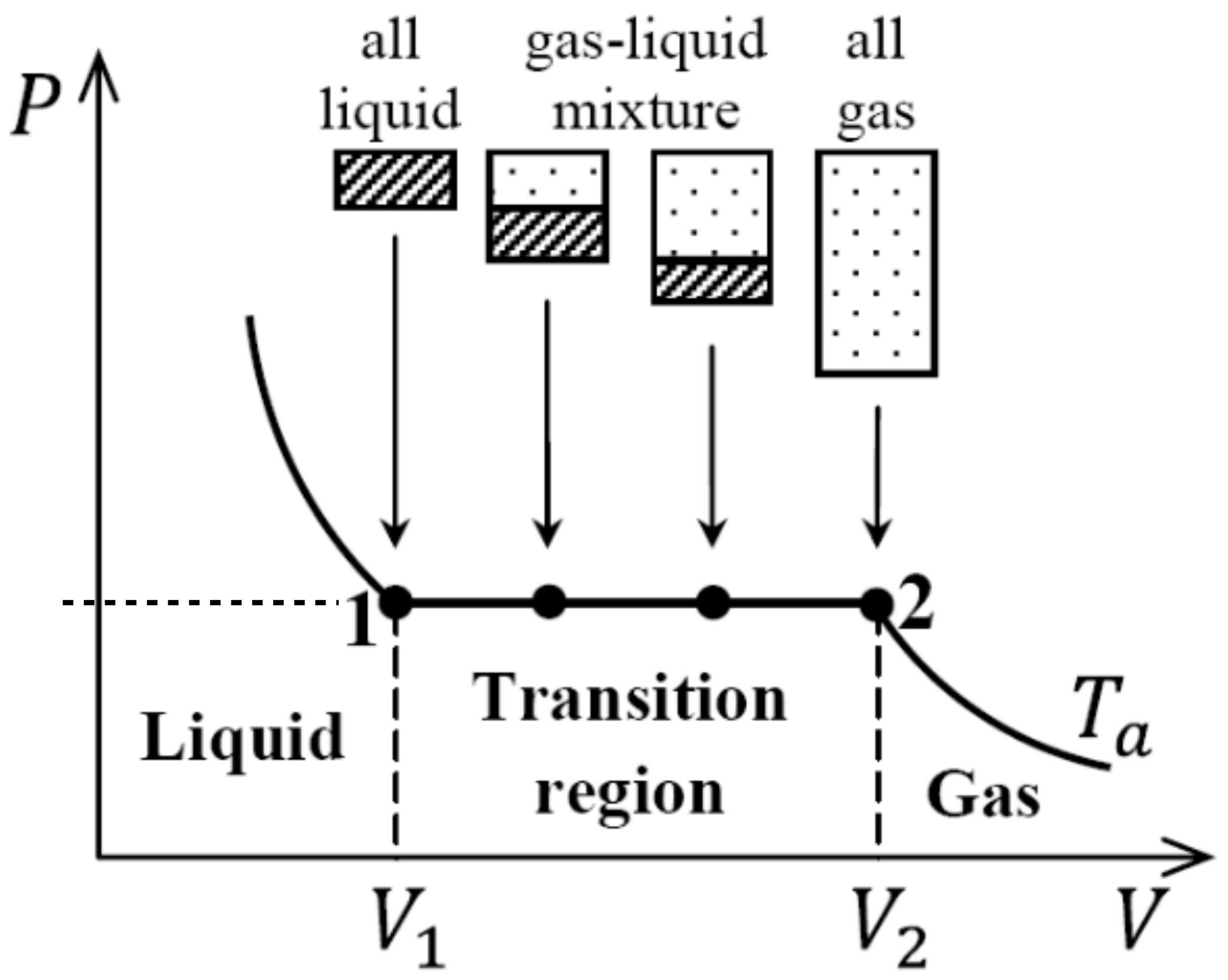
More thermodynamics: **Ex.** Boiling water $P = 1$ atm and $T = 100°C$ are **fixed**



Coexistence of two phases

$T = 100°C$

$P = 1$ atm



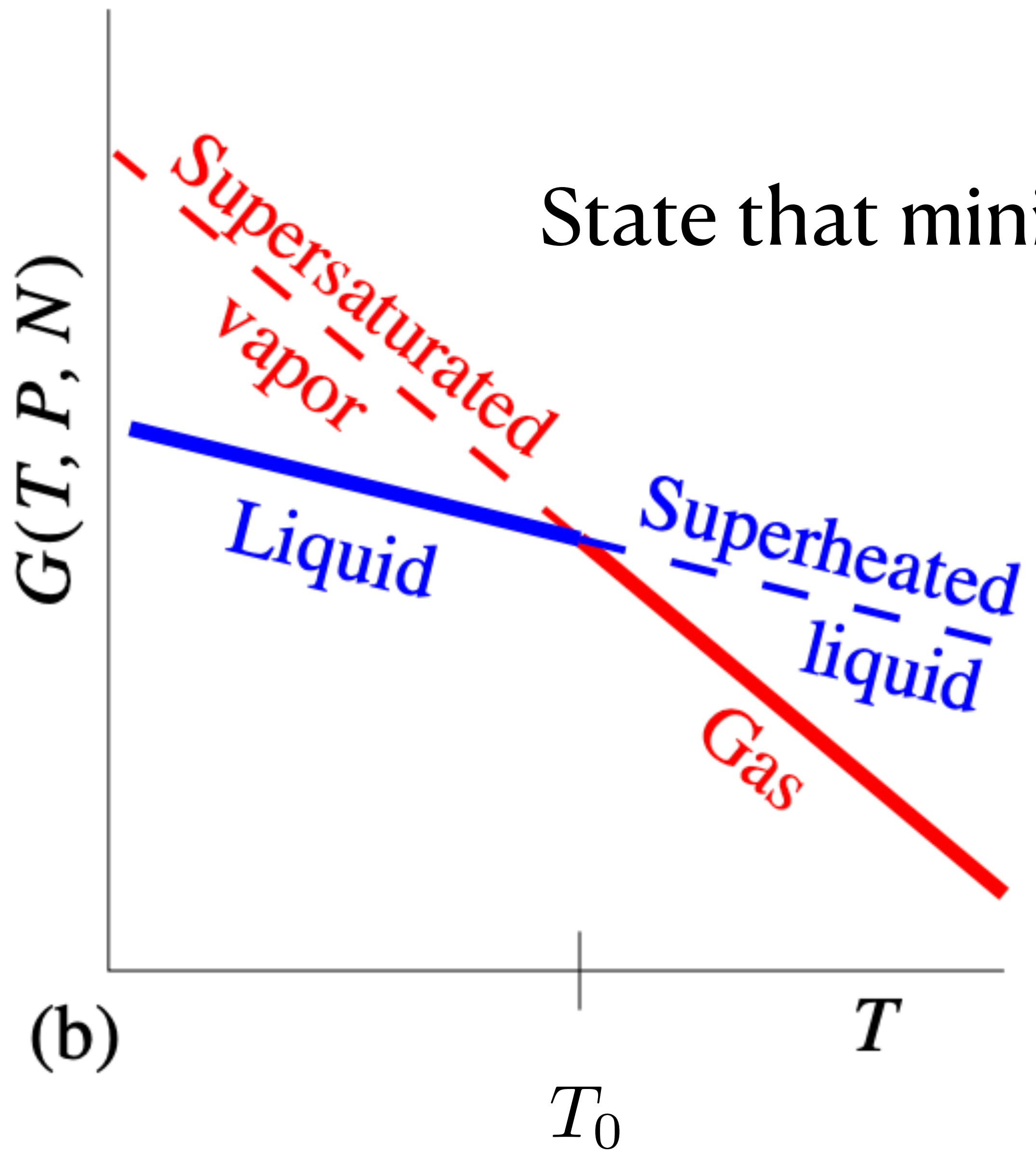
Discontinuity in V

Discontinuity of the Entropy

Ex. Boiling water $P = 1$ atm and $T = 100°C$ are **fixed**

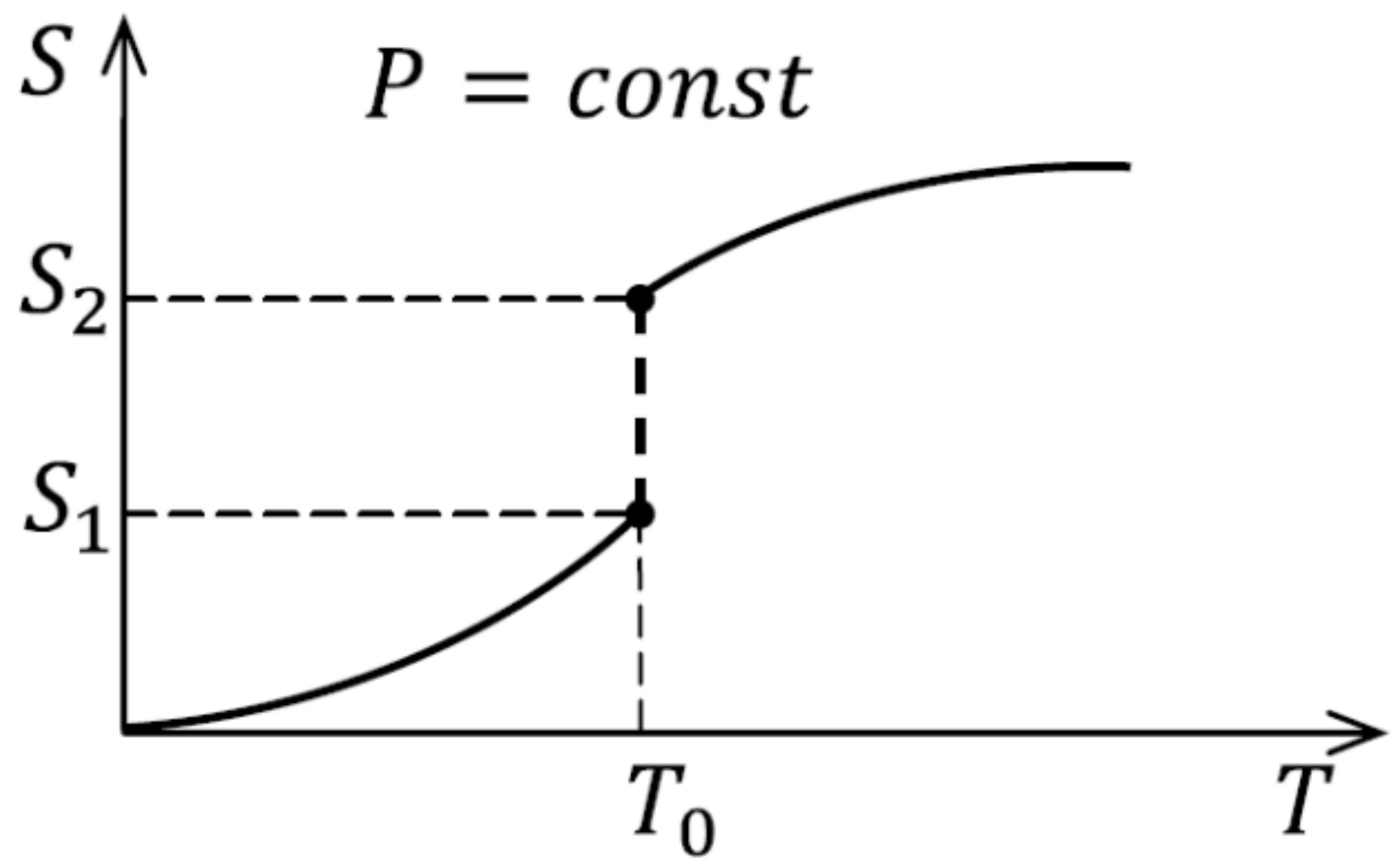
Potential thermodynamics: Gibbs free energy: **G = H - TS**

State that minimises G "wins"!



G is continuous, but with a singularity in T_0

$$\left(\frac{\partial G}{\partial T}\right)_P = -S$$



Discontinuity in S

Discontinuity in S: Two phases L-G coexisting at T_0 have different entropies S_1 and S_2.

The system must absorb or release heat during the transition, "**latent heat**": $\Delta Q = T_0\, \Delta S$

Continuous Phase Transition
and
Critical Phenomena

Continuous phase transitions and Critical phenomena

Continuous phase transitions: are synonymous with **critical phenomena**.

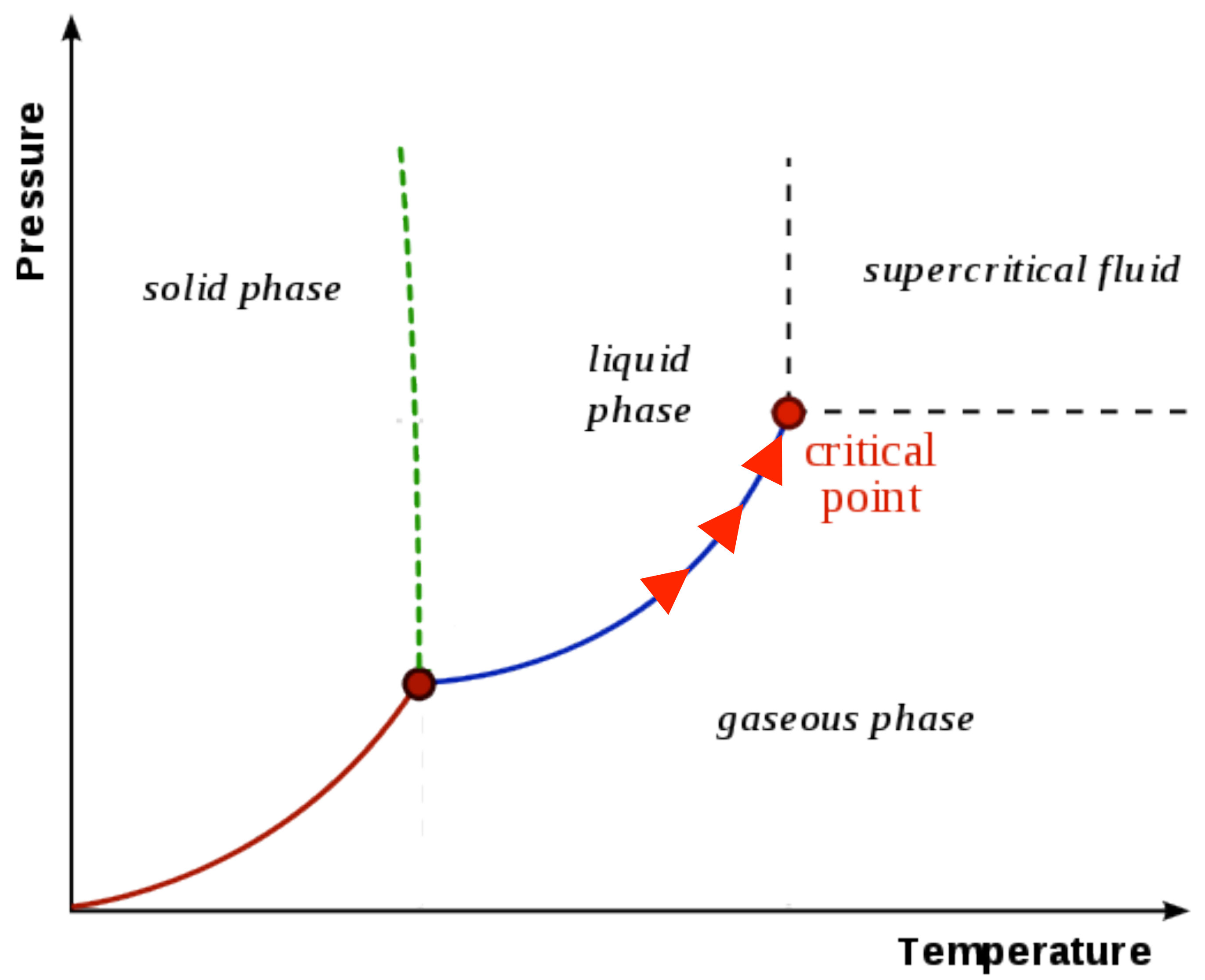
often describe a system at the **border between order and disorder**

At the critical point: **continuous** change in **entropy** (no latent heat).

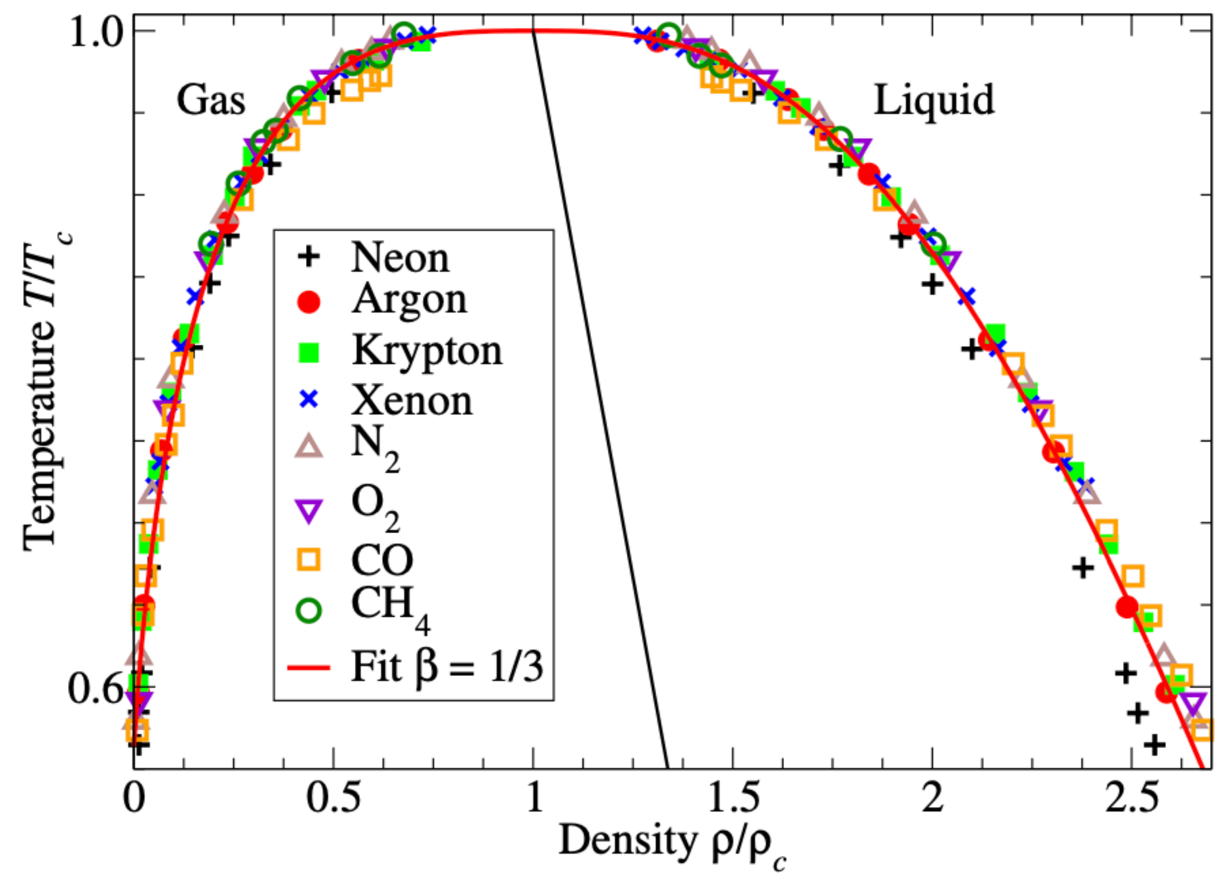
extremely large susceptibility to external factors. (divergence of the susceptibility)

strong correlation between distant parts of the system. (infinite correlation length, power law distribution of correlations)

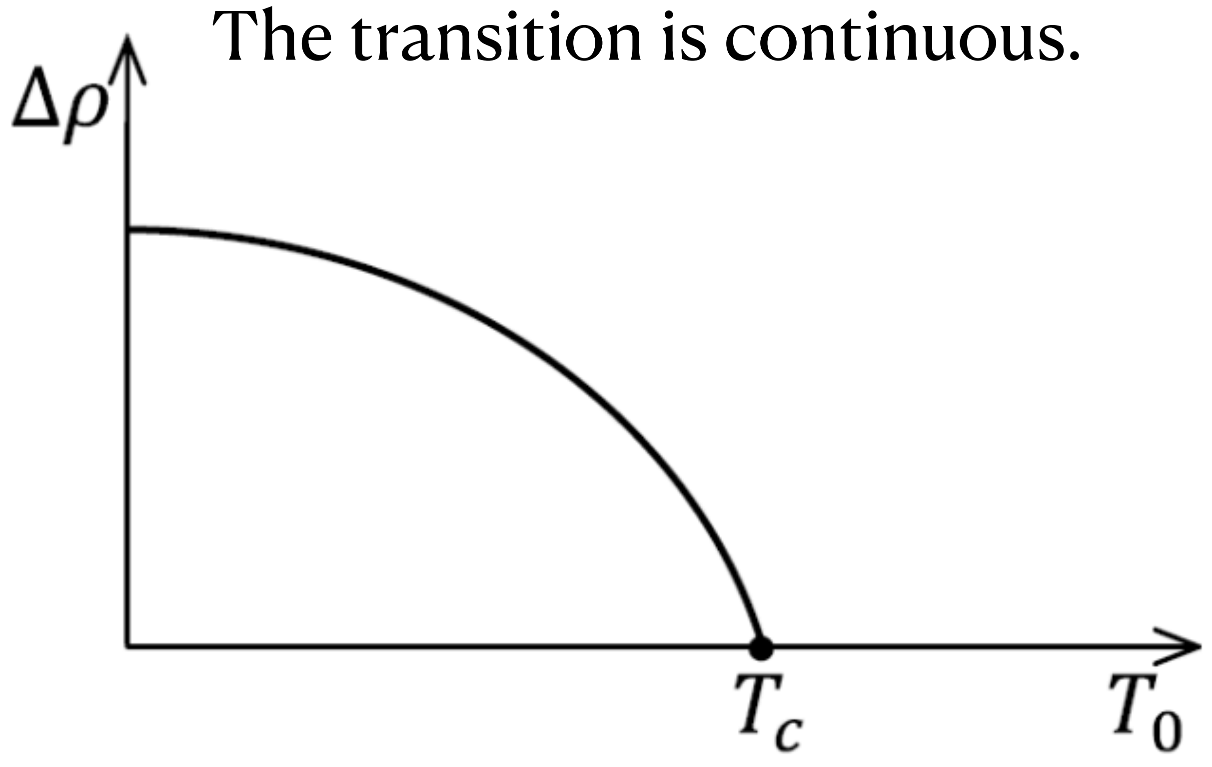
Ex. The first-order phase boundary between gas and liquid becomes second order right at the critical point **C**.



The density jump decreases along the liquid-gas line as T increases, and vanishes at Tc.

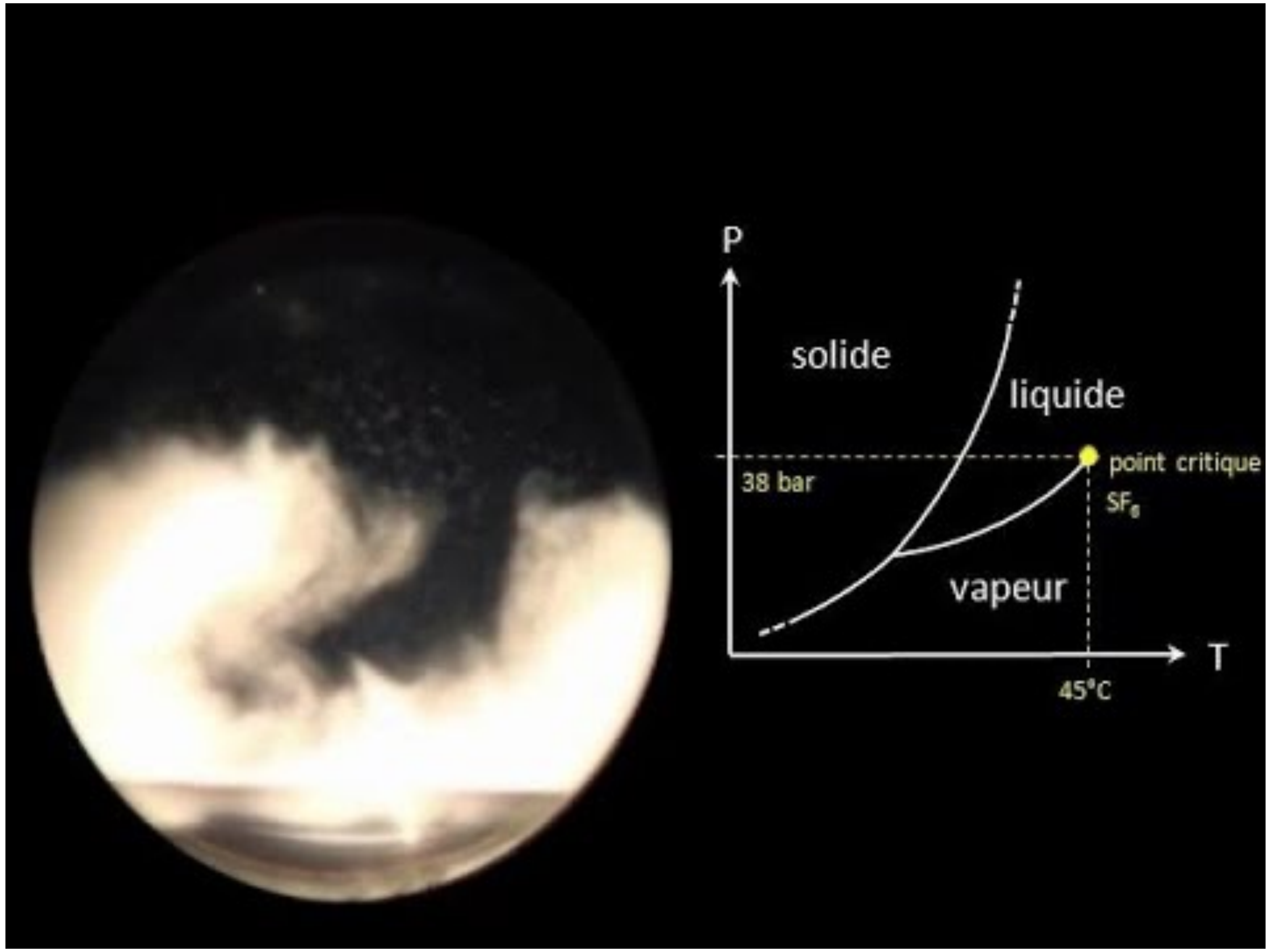


The transition is continuous.



At **C**, the **two phases** have equal densities and entropy per particle, they **become indistinguishable**.

Very large Correlation length
Critical Opalescence



Critical Opalescence:

Very large fluctuations of the density of the liquid.

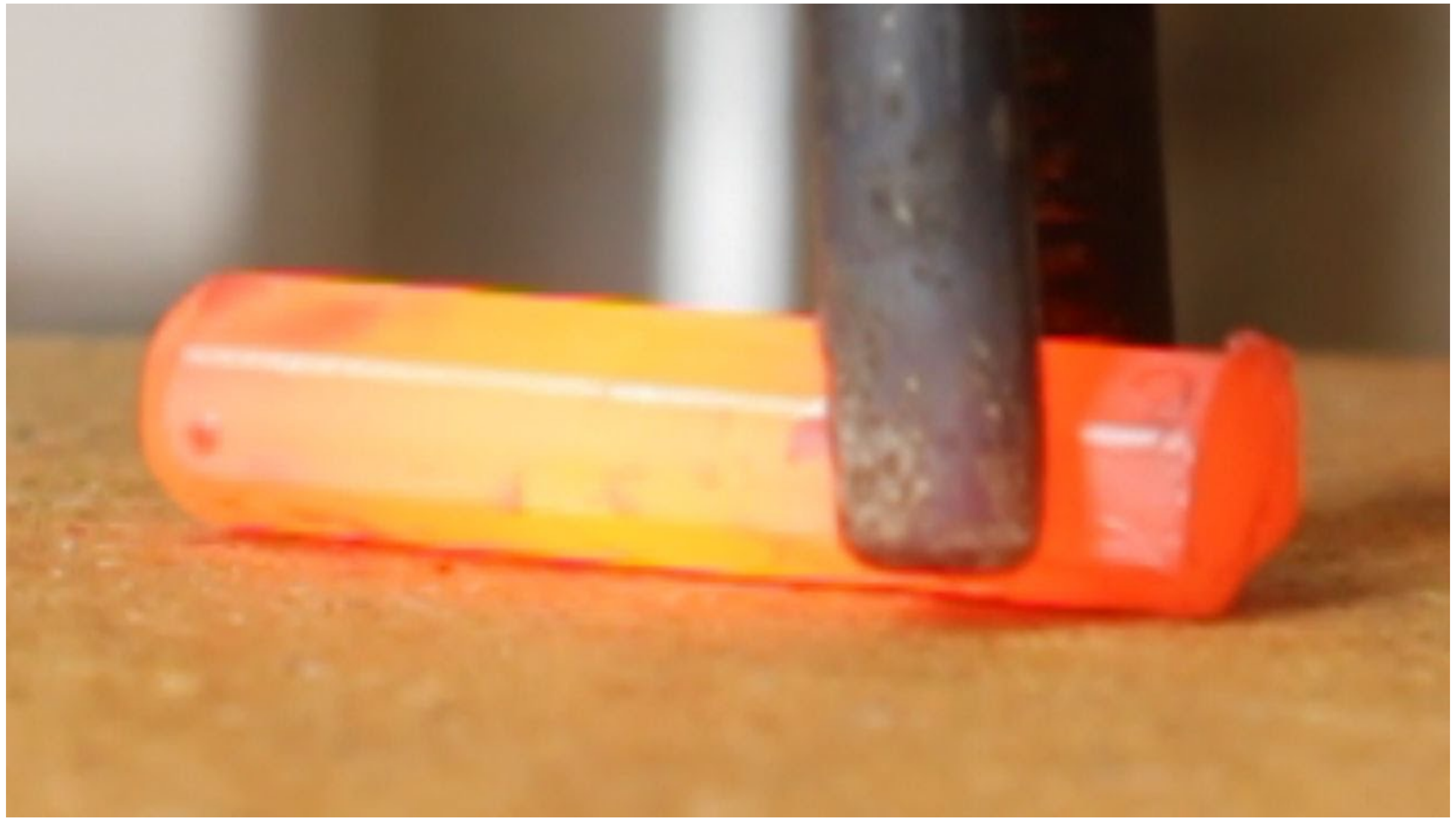
When the fluctuations become of a size comparable to the wavelength of light, the light is scattered.

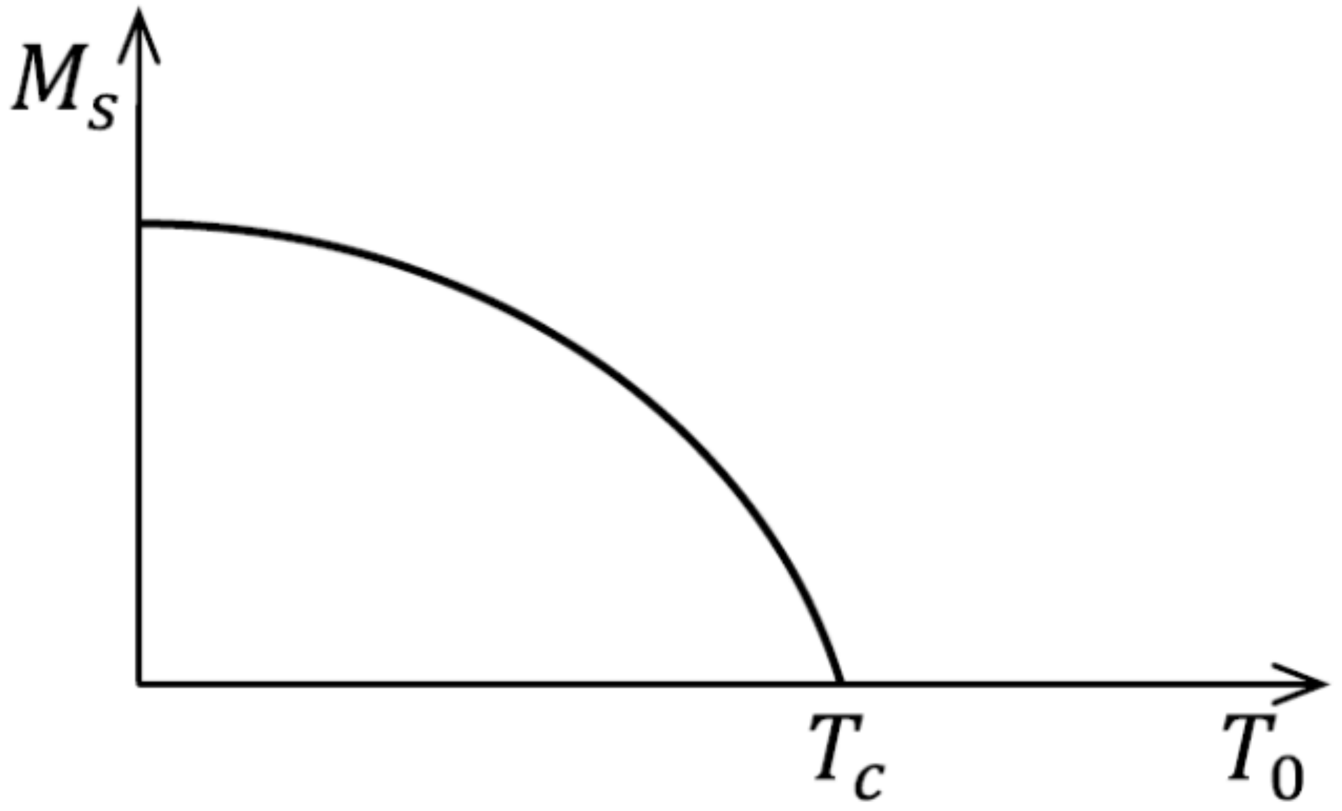
The liquid takes a milky appearance.

"Warnings"

Large fluctuations already before arriving to the critical point. They are warning that unusual behaviour is about to occur.

Ex. Ferromagnetic-paramagnetic transition

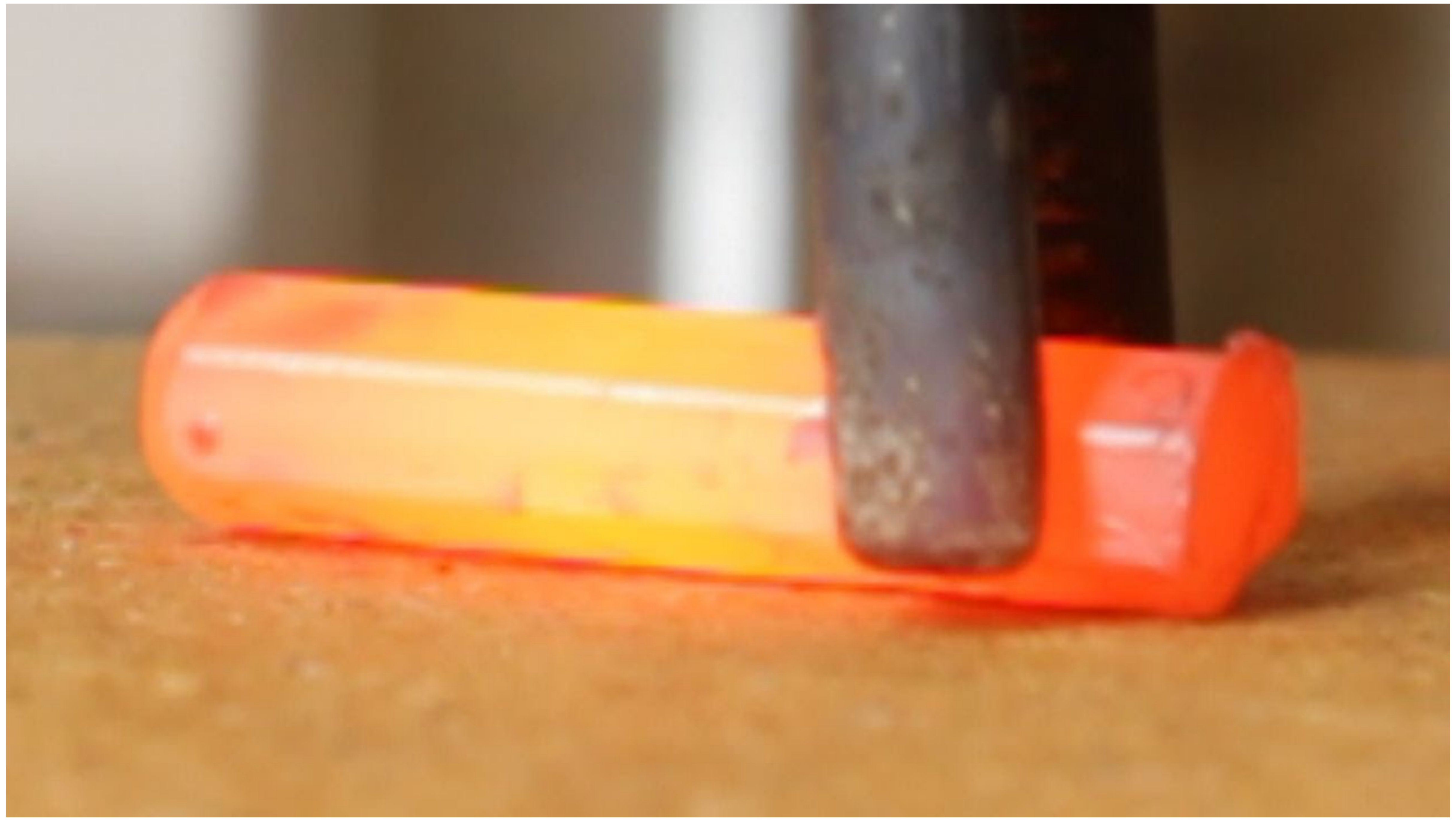




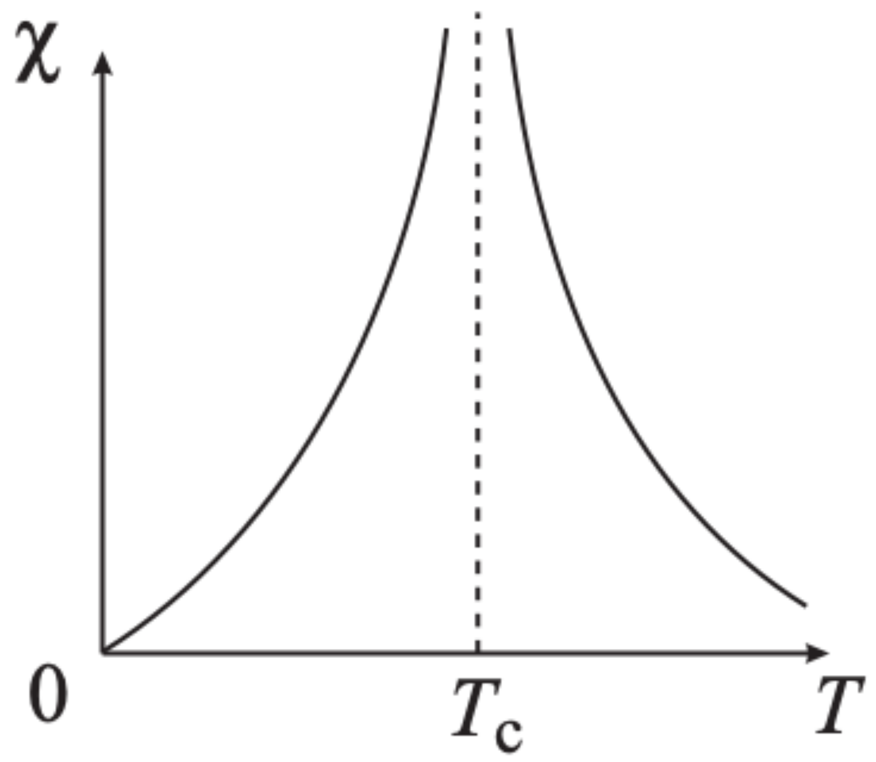
As we **raise the temperature** of a magnet, its **magnetisation** will **vanish continuously at** a critical temperature **Tc** (Curie temperature).

As the temperature of the material decreases, its spontaneous magnetisation reappears at Tc.

Ex. Ferromagnetic-paramagnetic transition



The magnetic susceptibility χ of a magnetic system diverges:



Ehrenfest classification

Ehrenfest classification of phase transitions:

The order of the lowest derivative of the thermodynamic potential showing a discontinuity.

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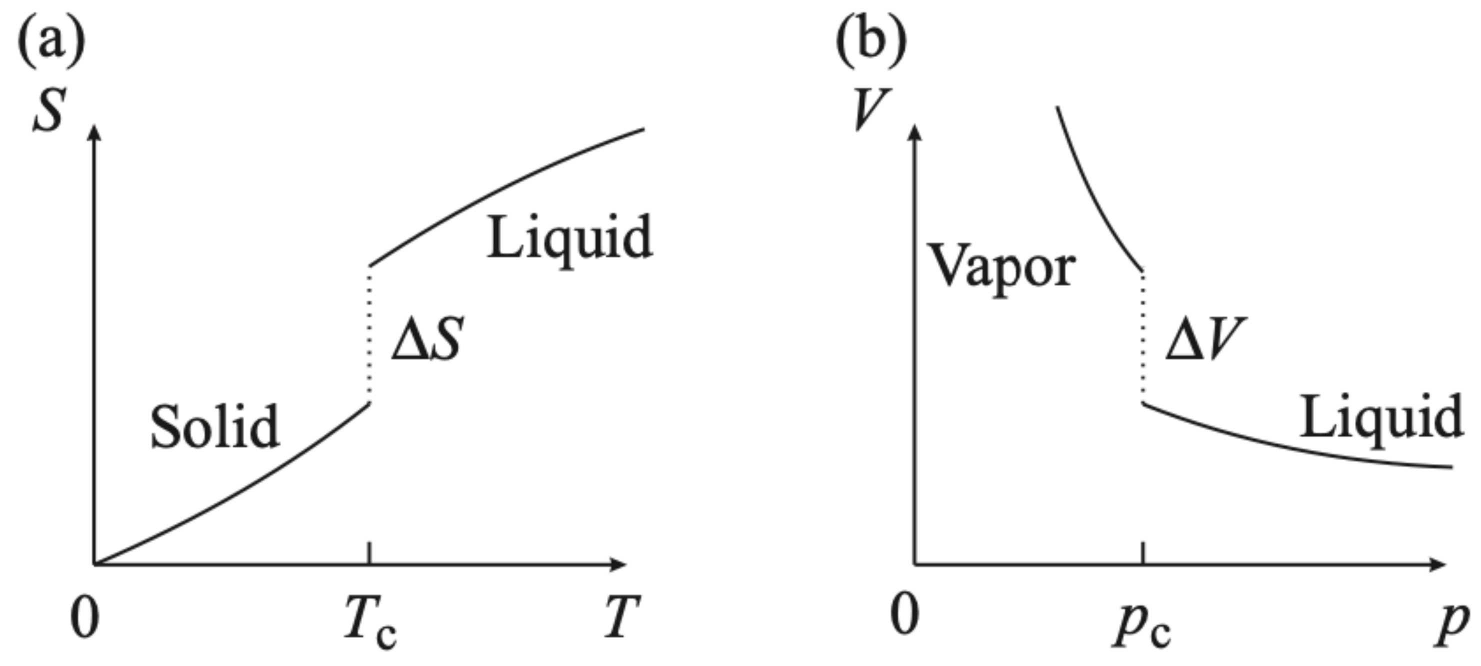
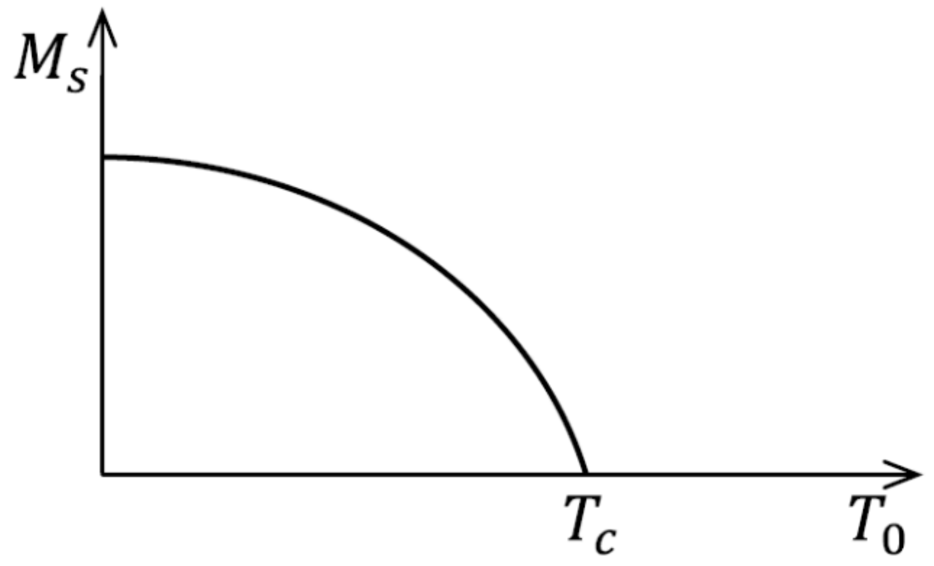
Discontinuous phase transitions

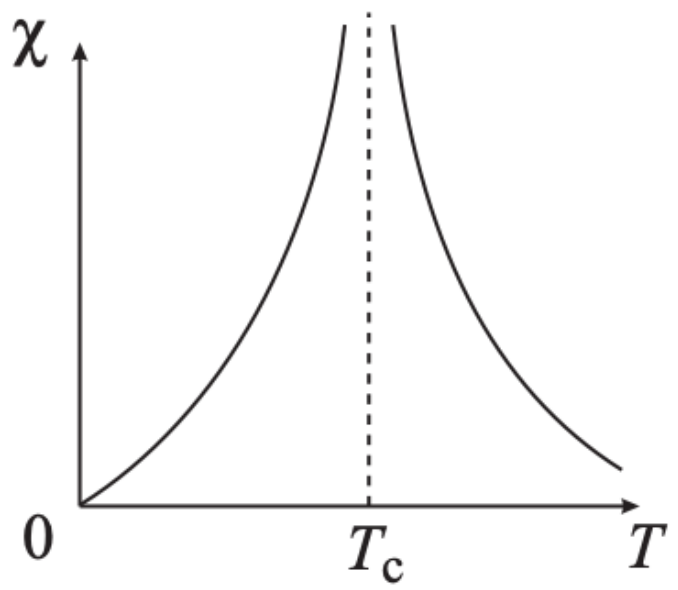


- G is continuous
- But $V = \left(\frac{\partial G}{\partial P}\right)_T$ and $S = -\left(\frac{\partial G}{\partial T}\right)_P$ are discontinuous

First order phase transition

Continuous phase transitions





- G is continuous
- $M = -\left(\frac{\partial G}{\partial H}\right)_T$ and $S = -\left(\frac{\partial G}{\partial T}\right)_H$ are continuous
- $\chi(T) = -\left(\frac{\partial^2 G}{\partial H^2}\right)_T$ is discontinuous

Second order phase transitions

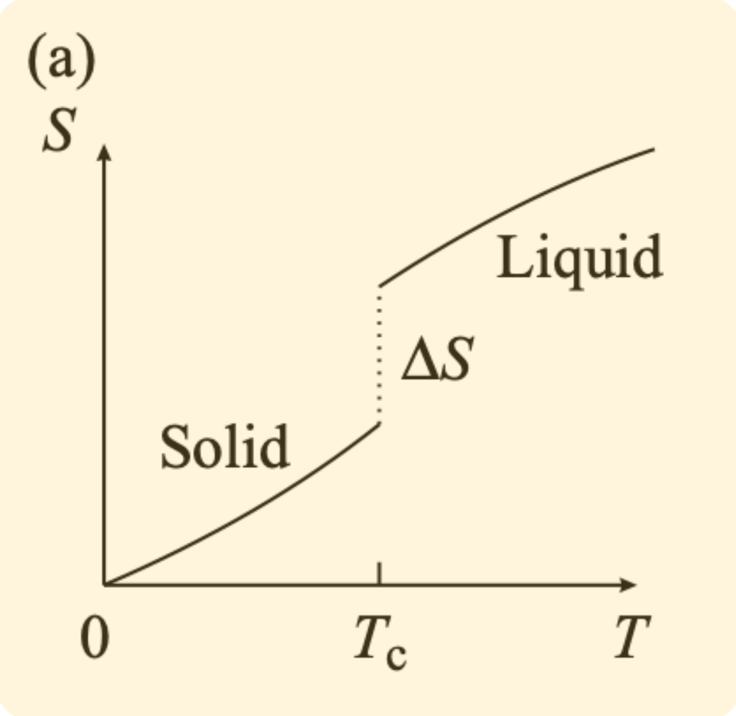
Not used anymore: As there are mainly only these two cases!

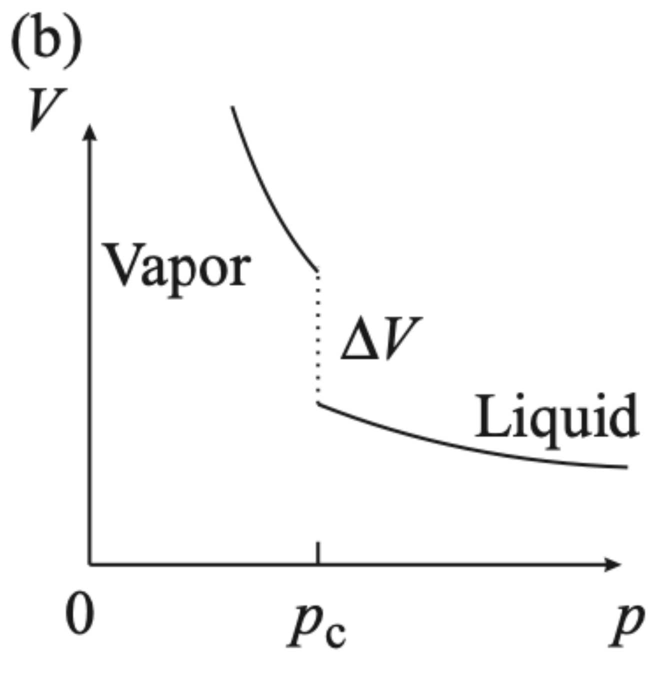
Ehrenfest classification

Ehrenfest classification of phase transitions:

The order of the lowest derivative of the thermodynamic potential showing a discontinuity.

Discontinuous phase transitions





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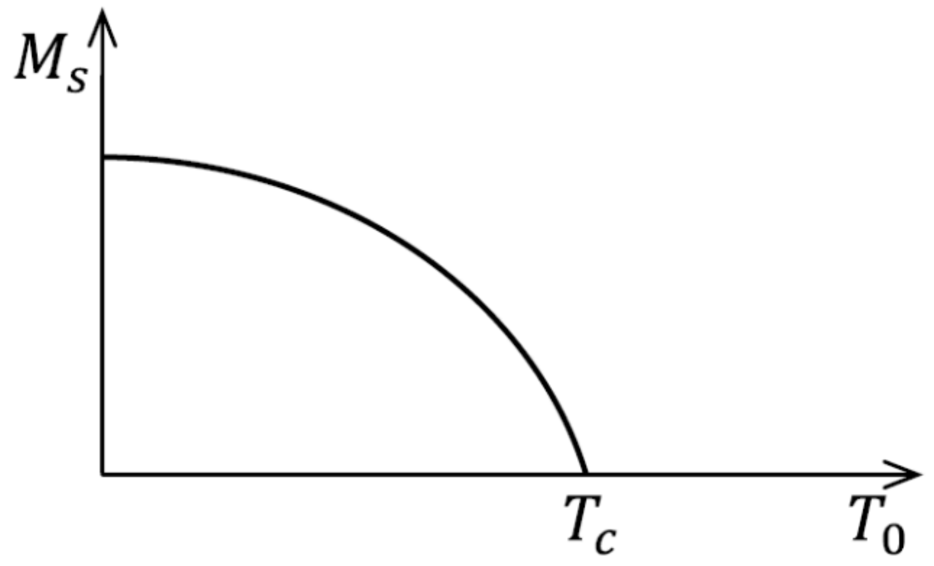

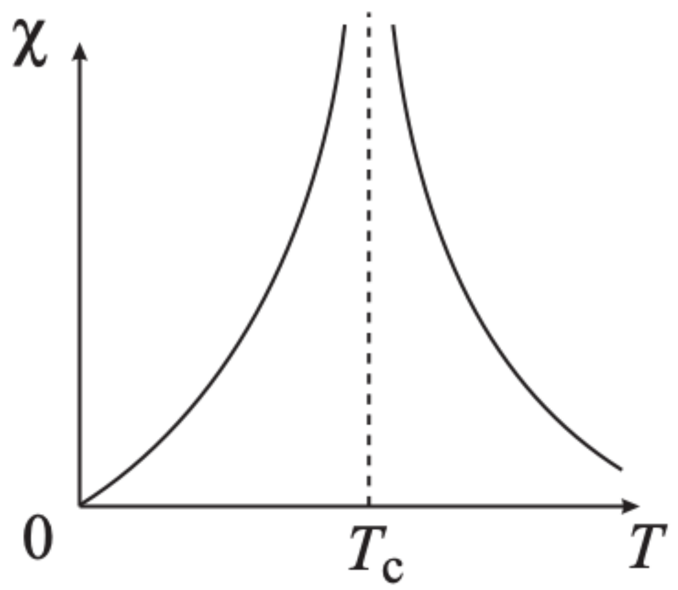

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Second order phase transitions

Instead: Use for the continuity/discontinuity of the entropy

From microscopic to macroscopic description
Example of the Ising model

Ferromagnetic - Paramagnetic material

Material: Material composed of atoms that have a magnetic moment (like a tiny magnet — due to unpaired electrons)

Paramagnetic material: Most such material barely behave like magnets. They show a very small attraction to magnets.

Ferromagnetic material: A few elements show a very strong attraction to magnets (ex. Iron, Cobalt, Nickel)

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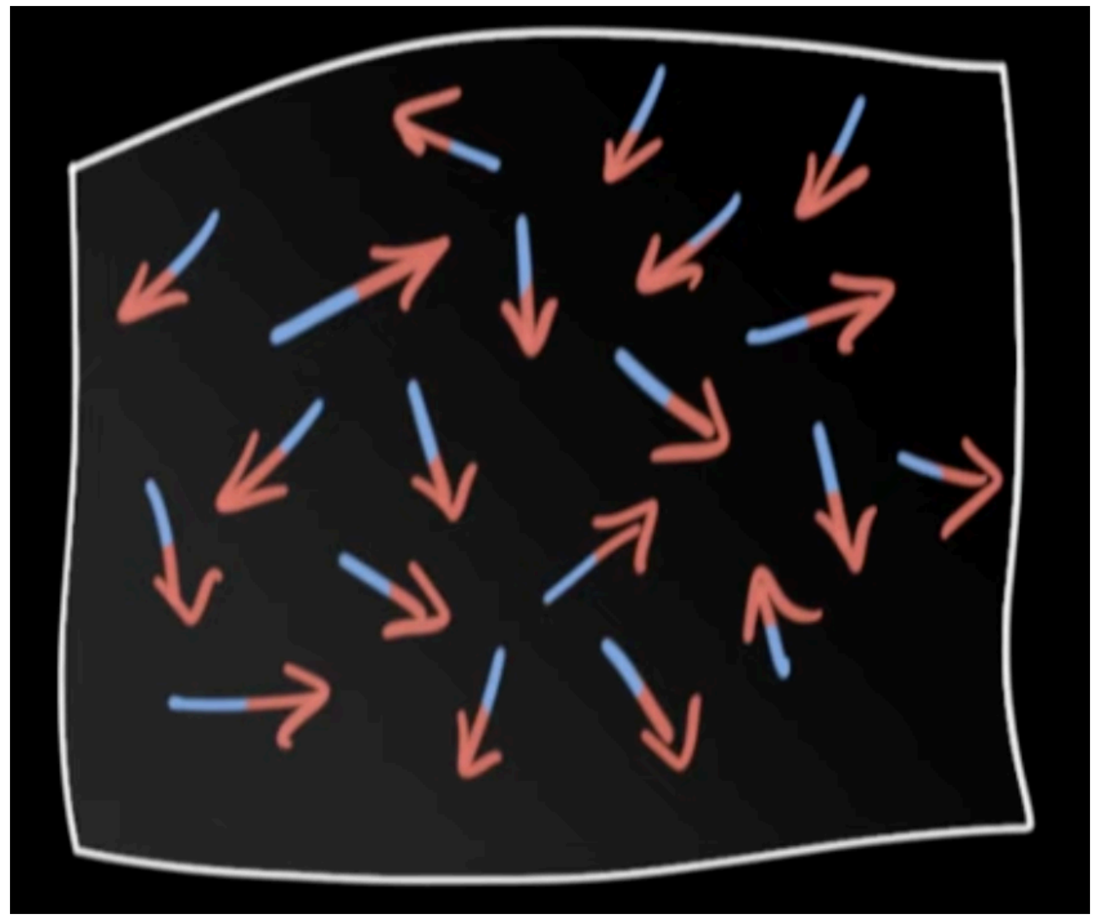

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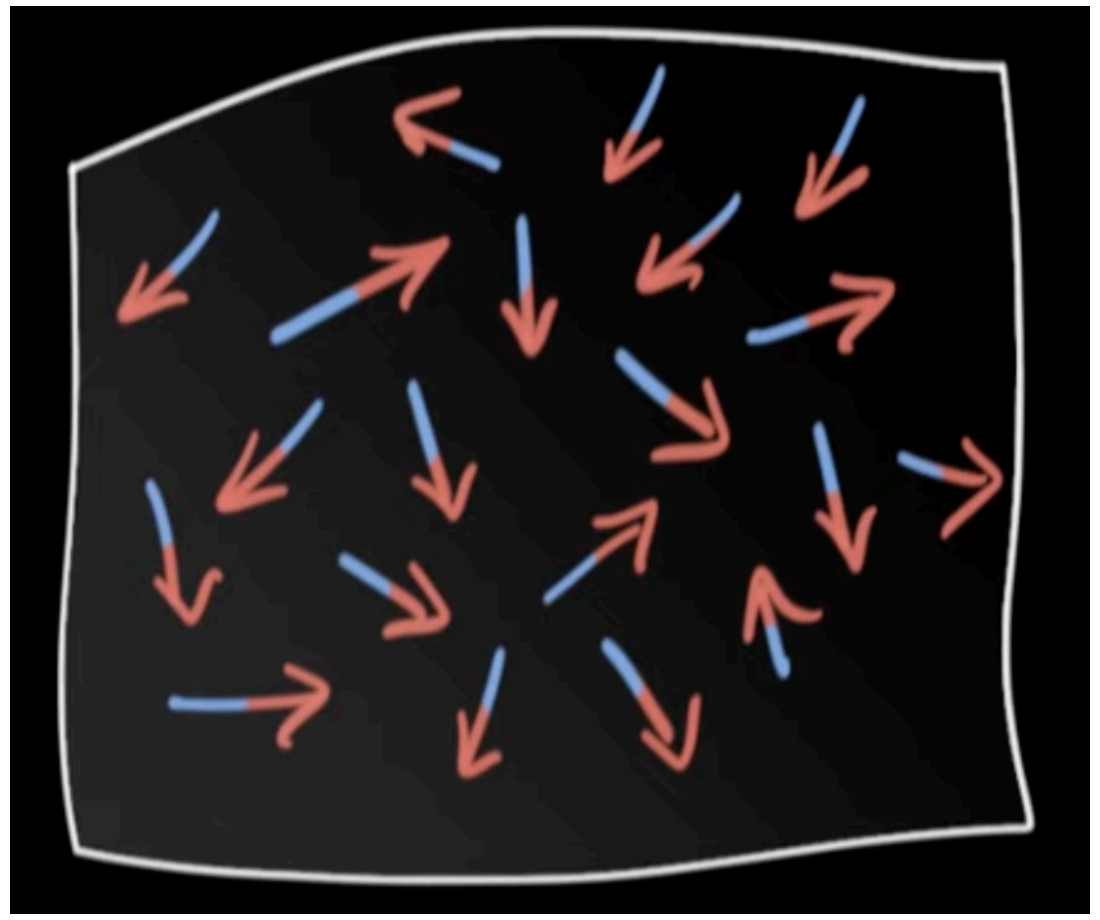

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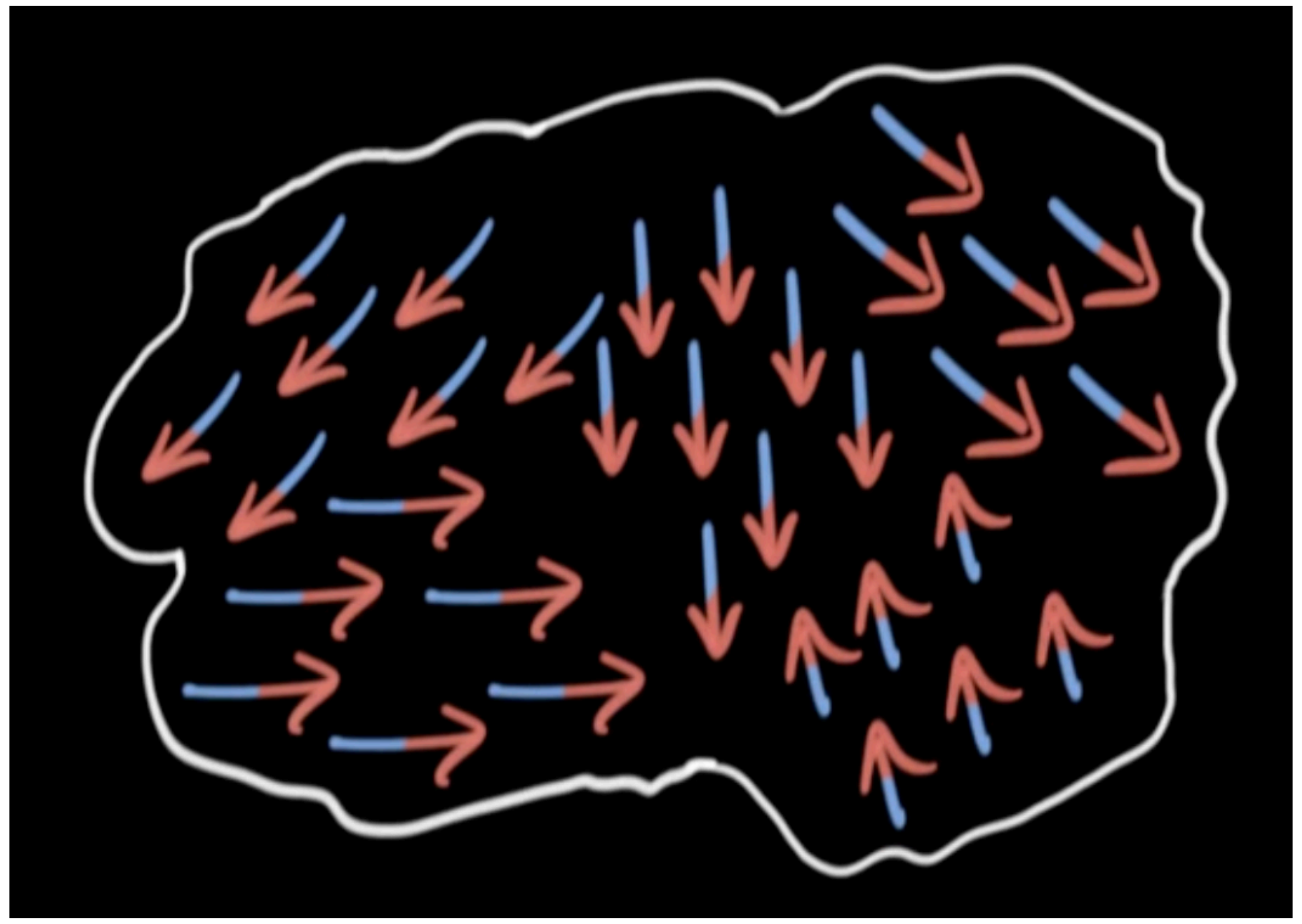

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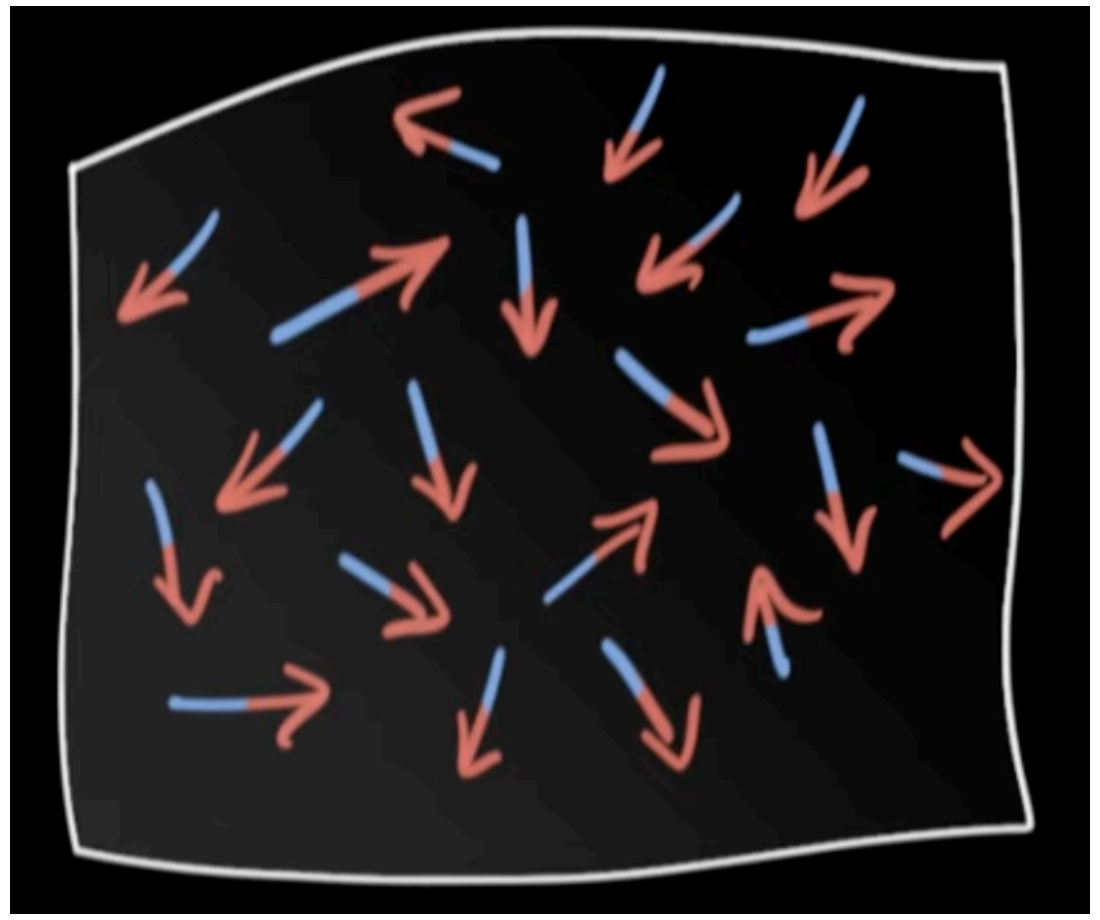

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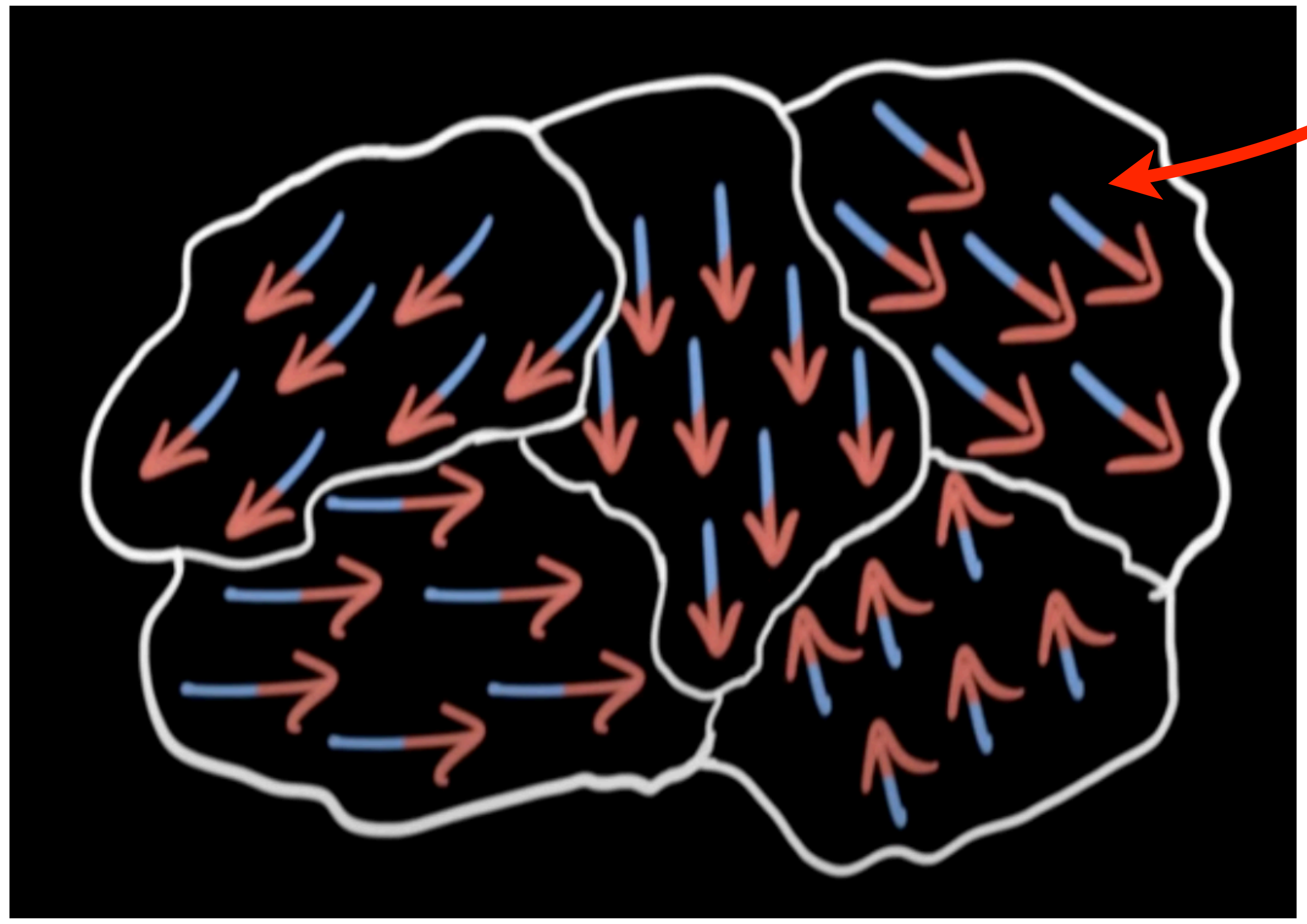
Ferromagnetic material:

Magnetic domains



Groups of "Tiny magnets" all aligned with each others

A priori, similar at the microscopic scale, but behave differently macroscopically.

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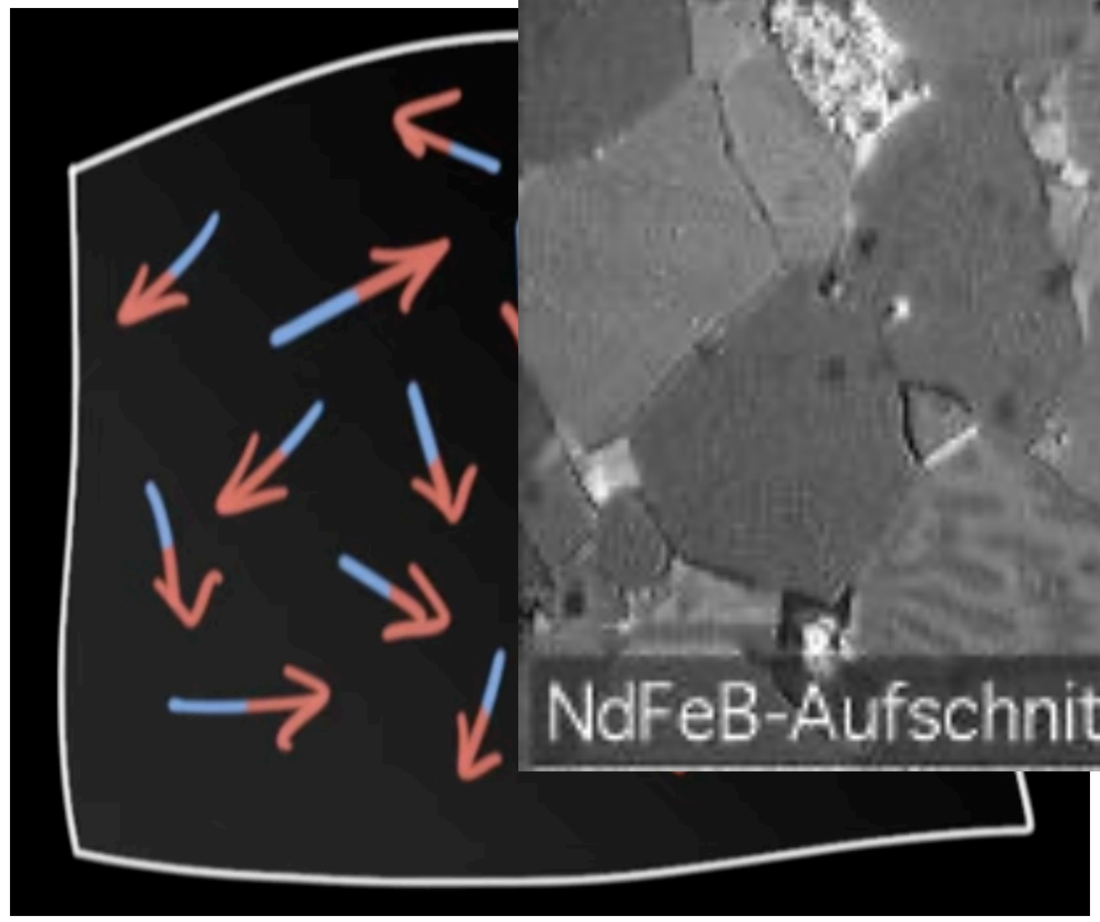

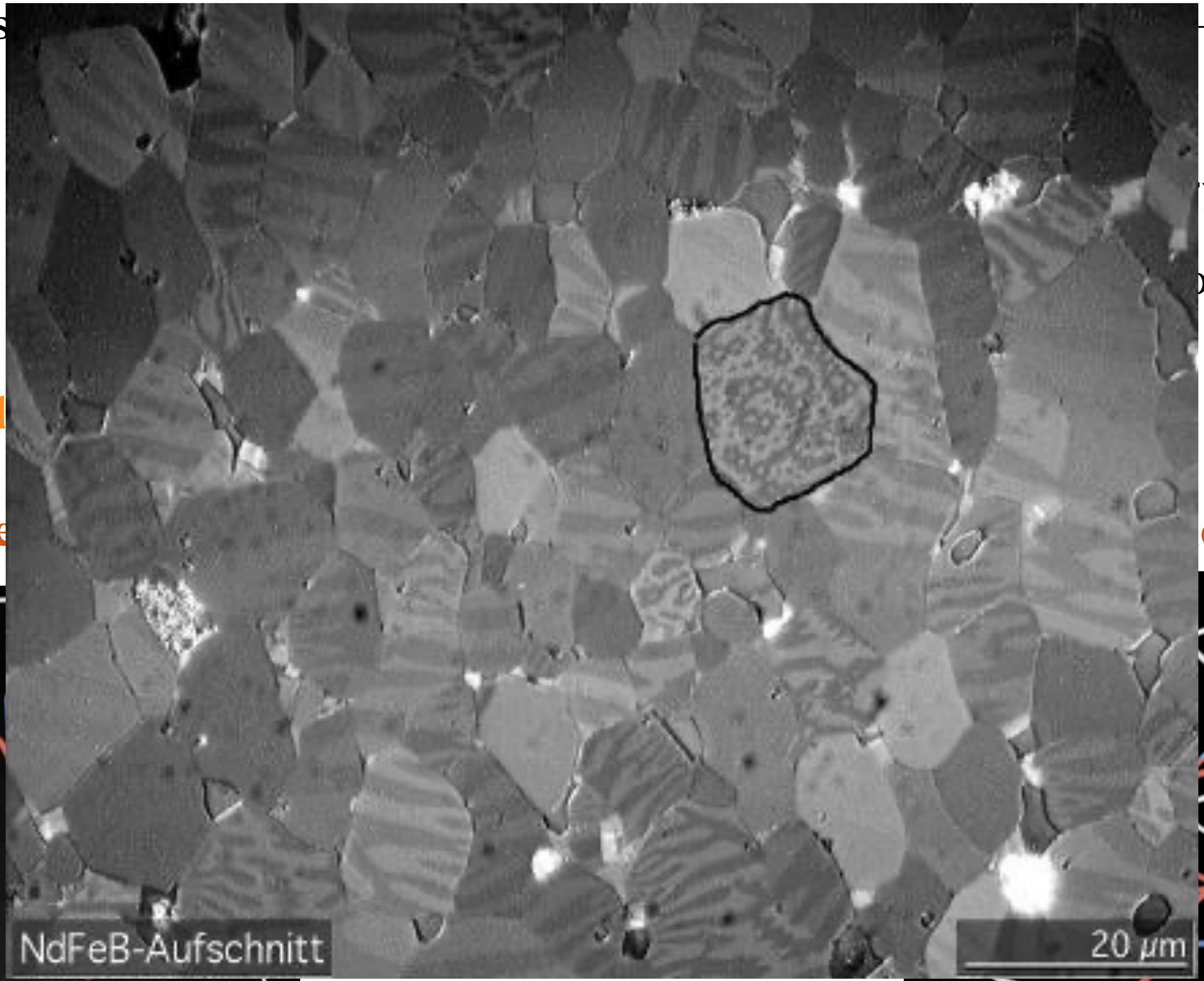

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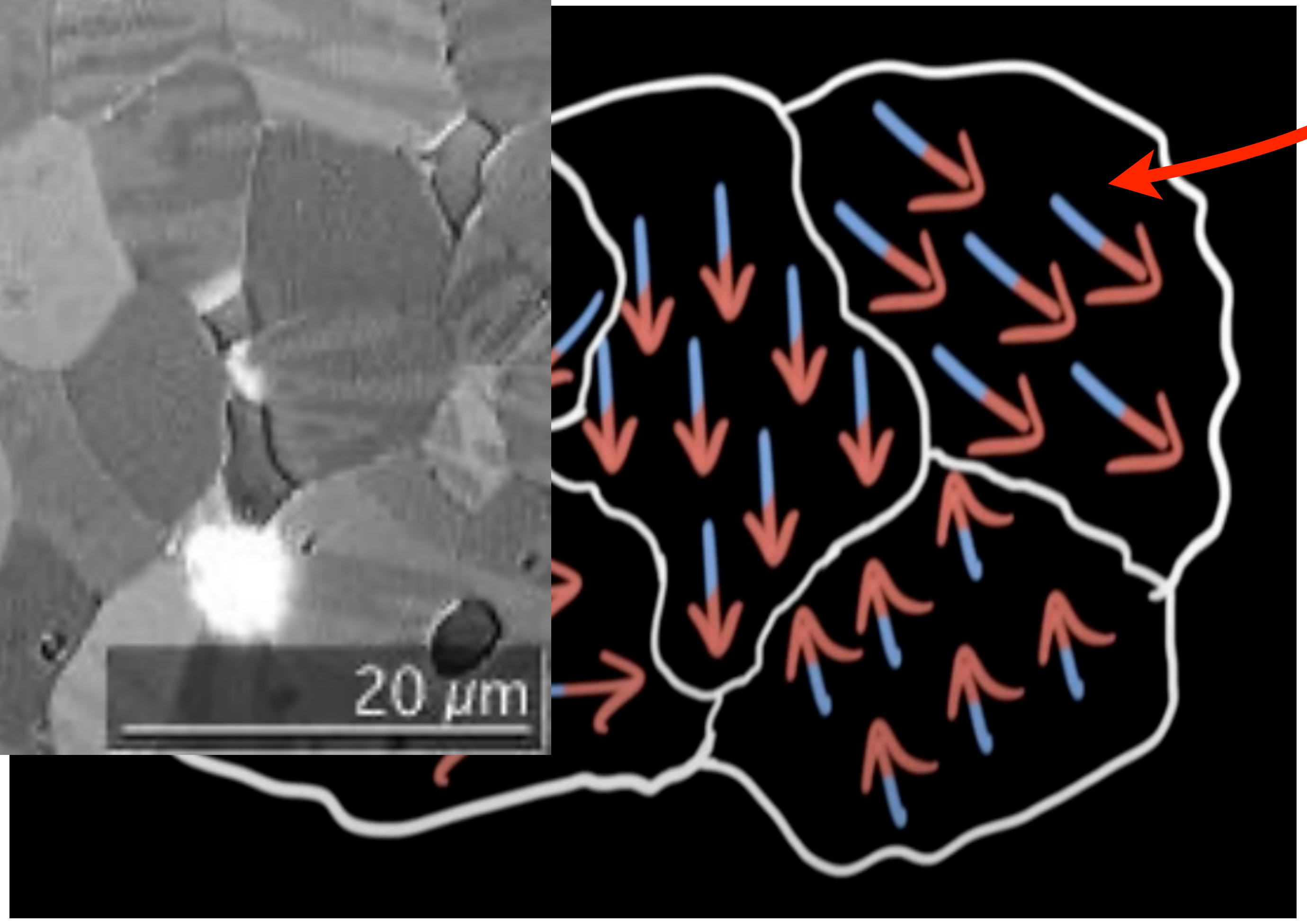

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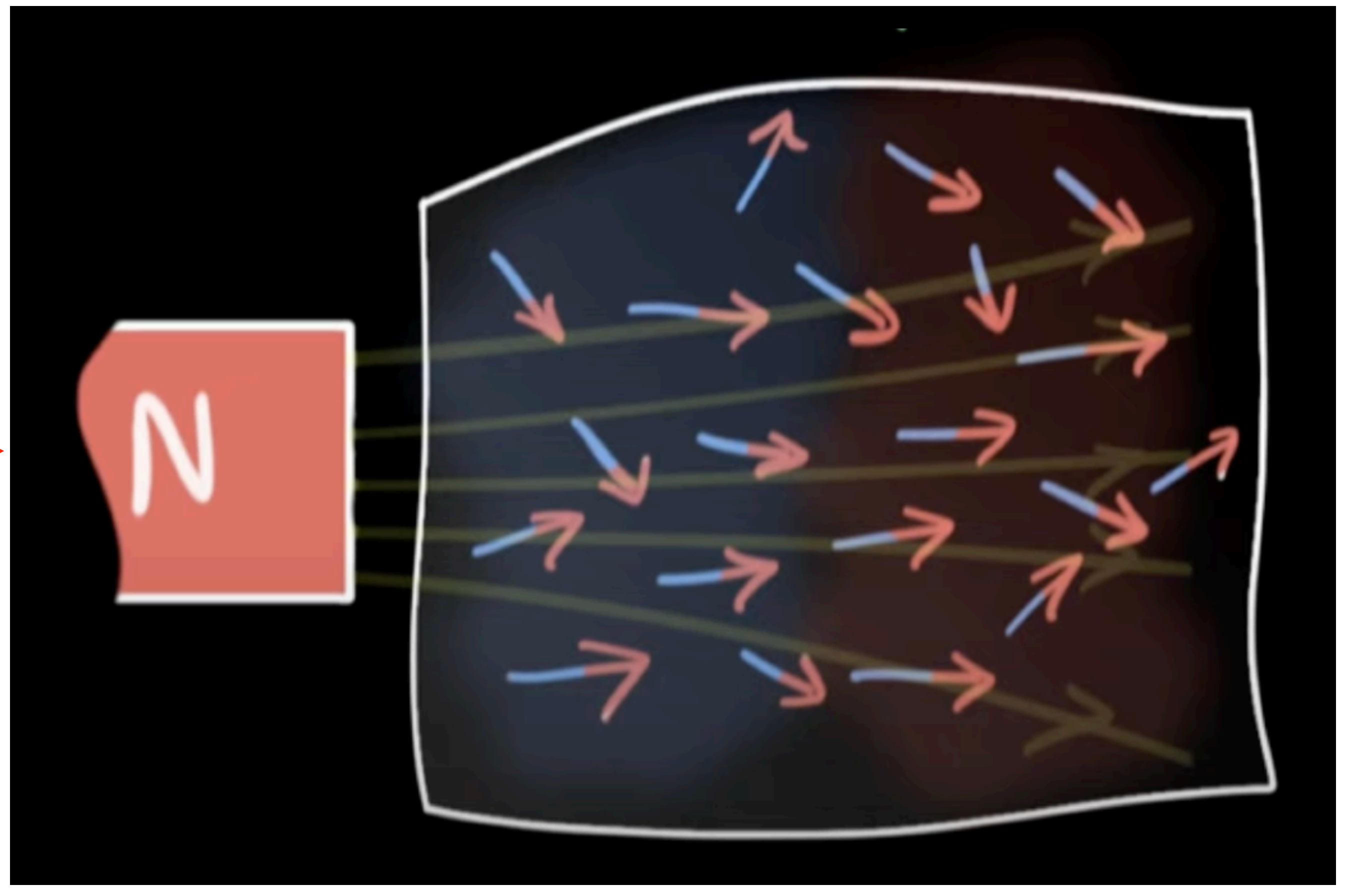

Weak alignment of the "tiny" magnet (alignment depends on temperature)

Material very slightly magnetised ==> not attracted to magnet

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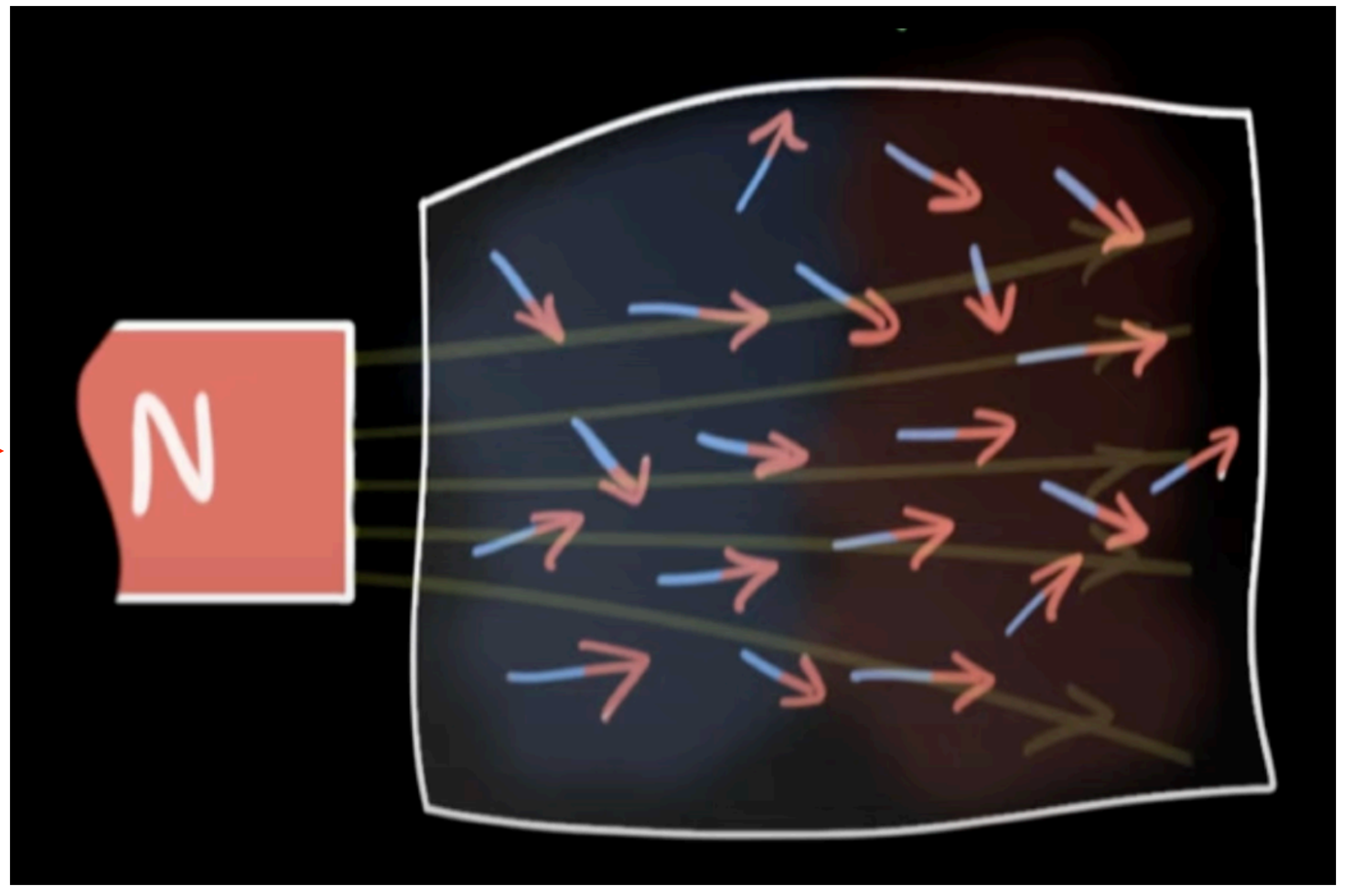

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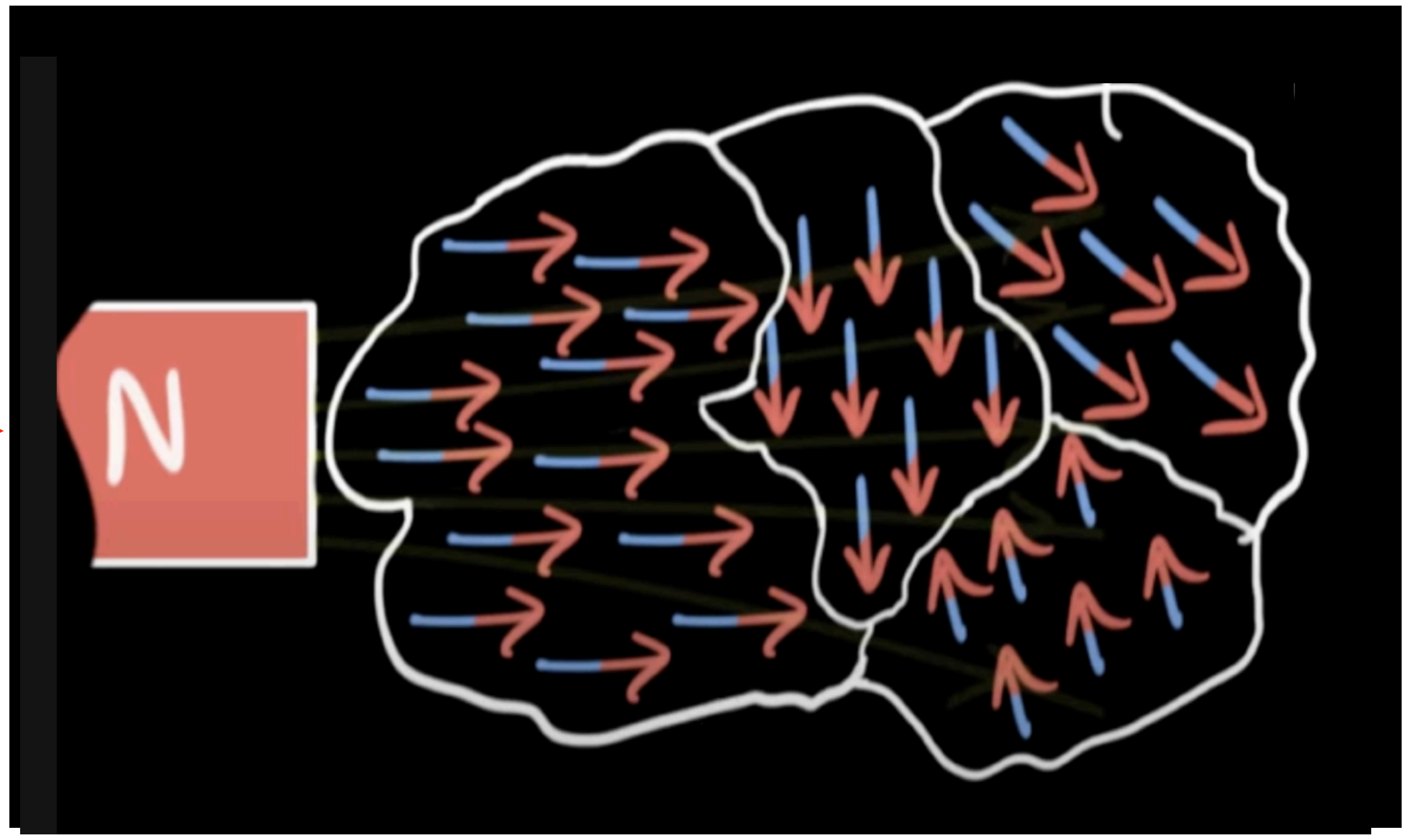

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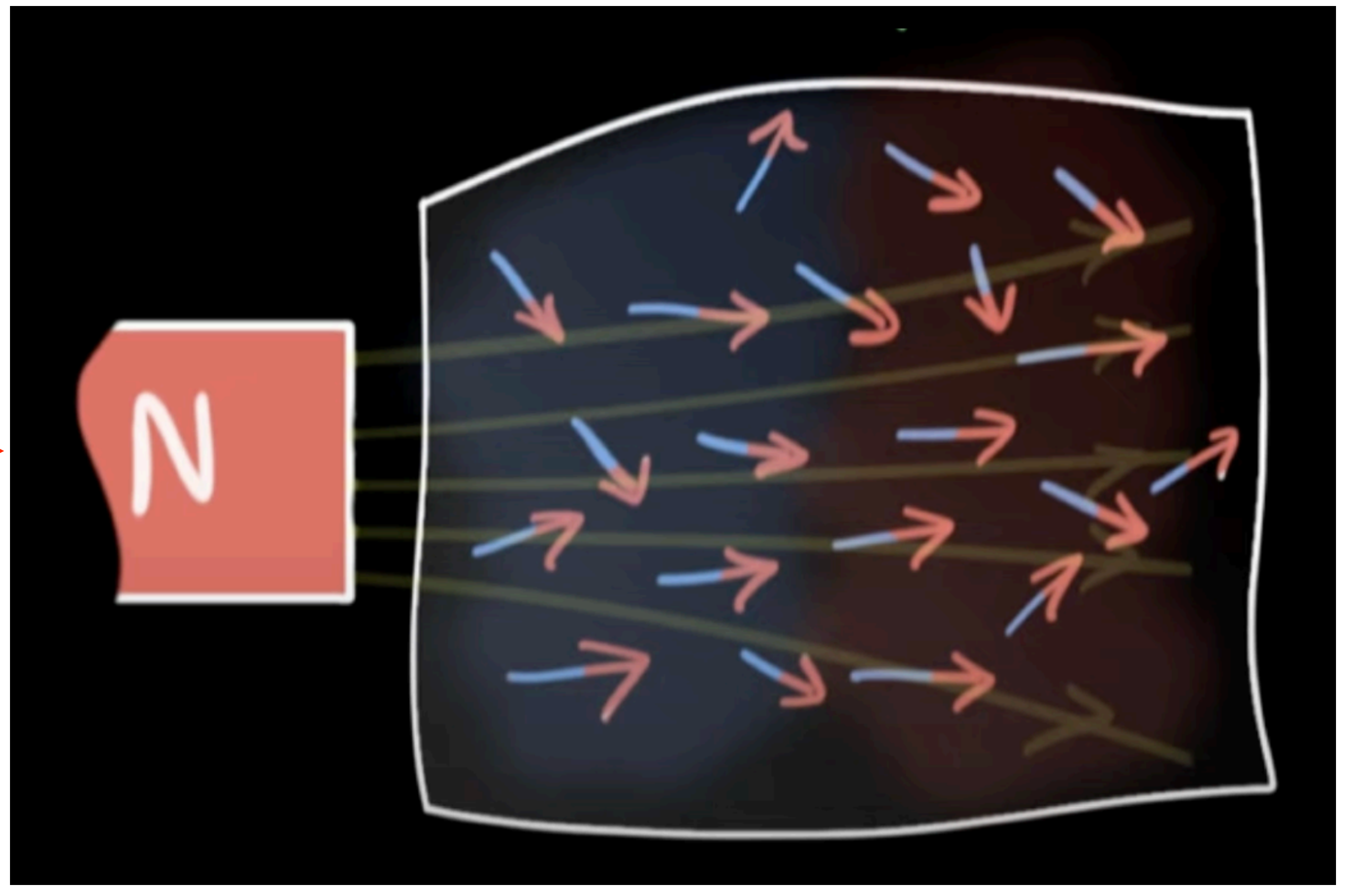

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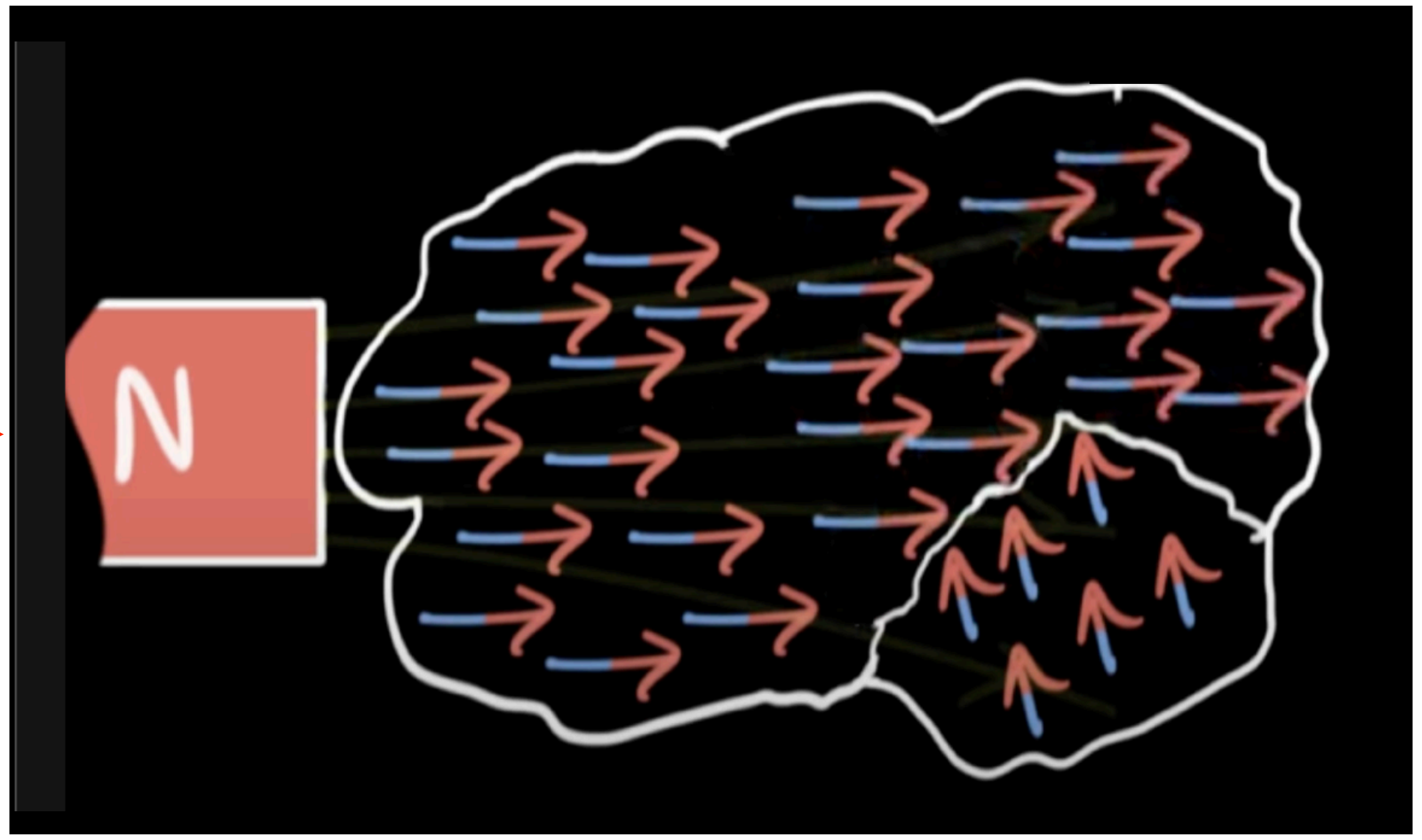

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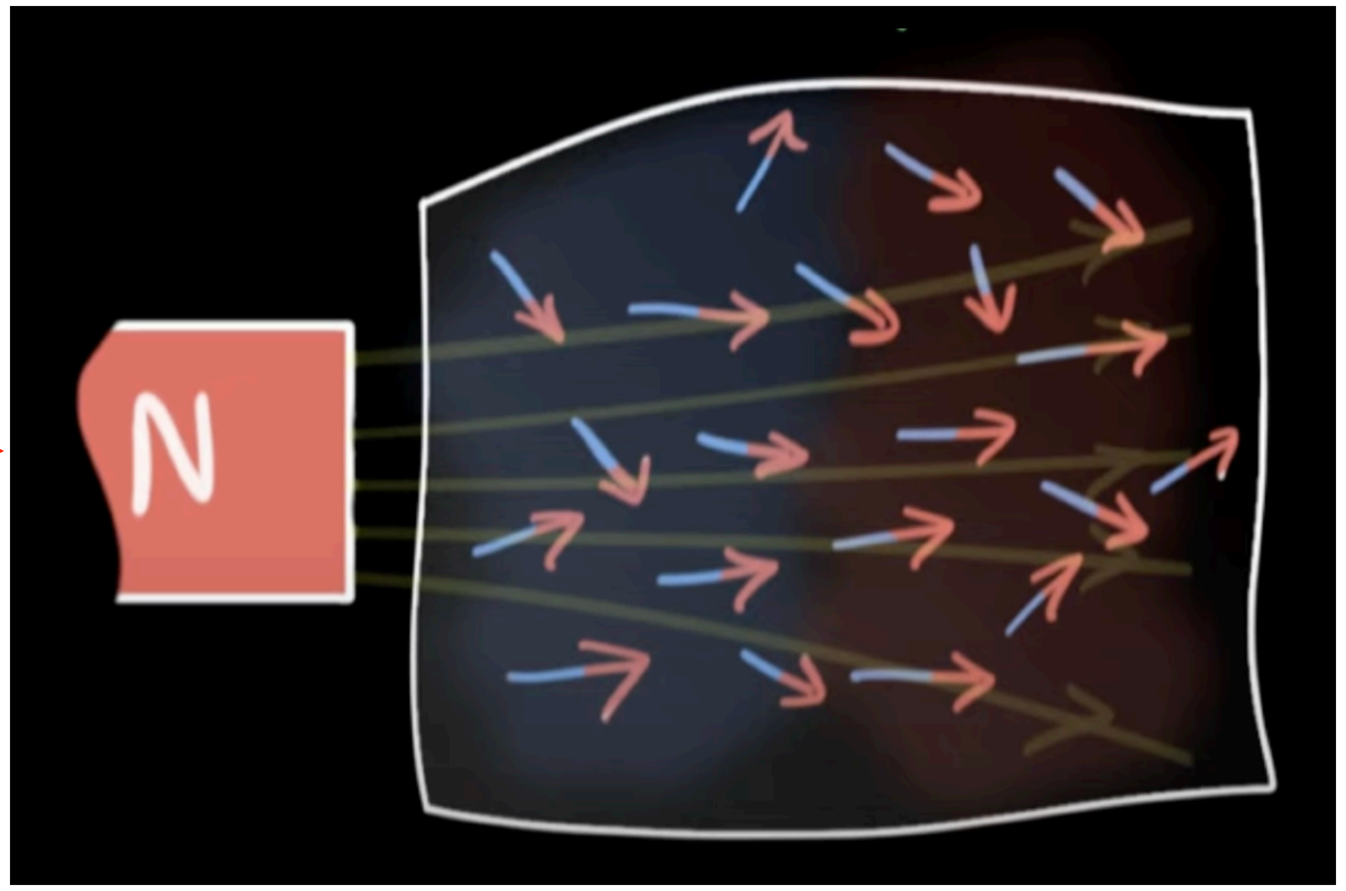

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Ferromagnetic material:

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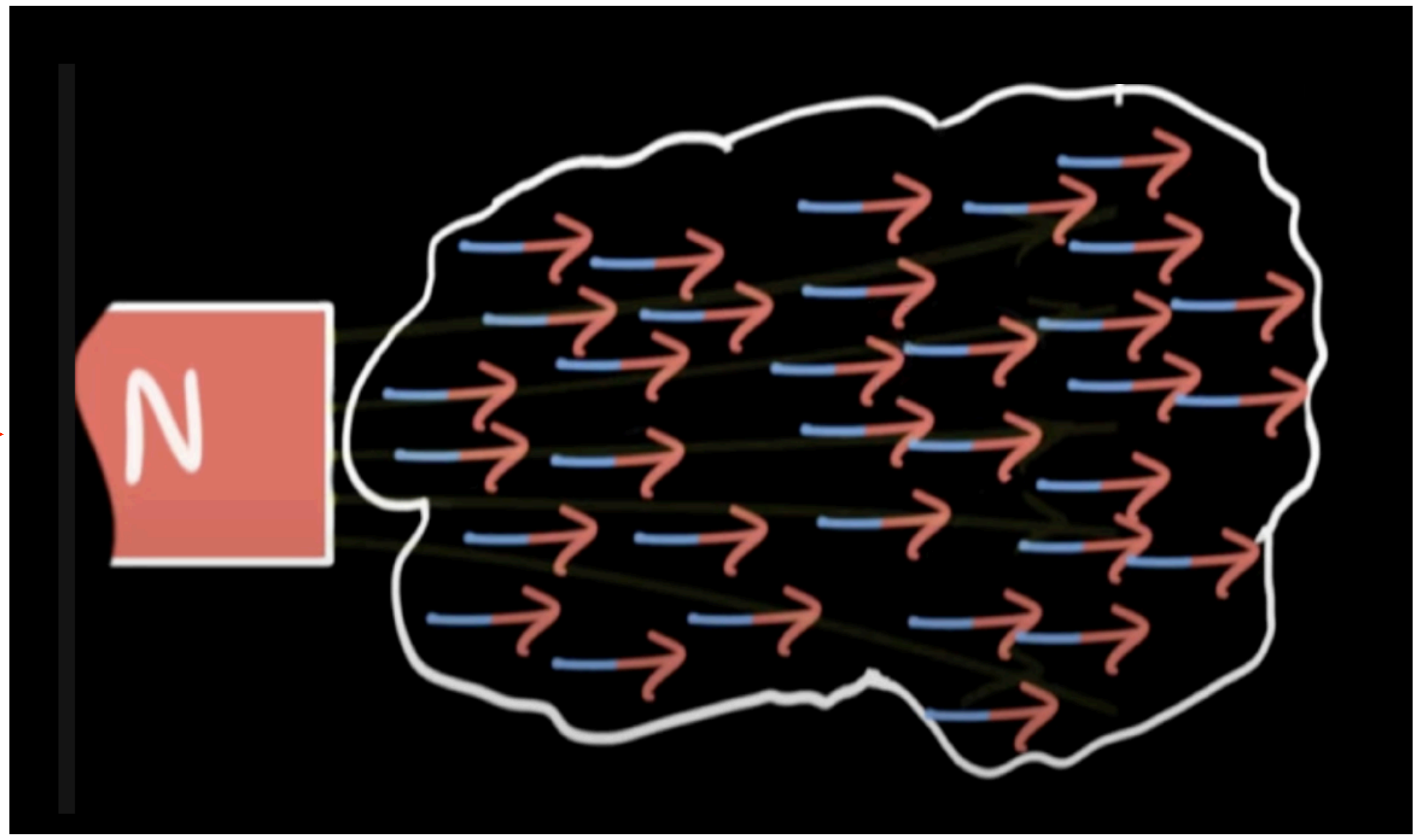


Entire domains align.

Material strong magnetisation ==> strong attraction to magnet

Ferromagnetic - Paramagnetic material

Ferromagnetic material:

Increase T

Attracted to magnet

Below Tc the domains have non-zero magnetisation

Ferromagnetic - Paramagnetic material

Ferromagnetic material:

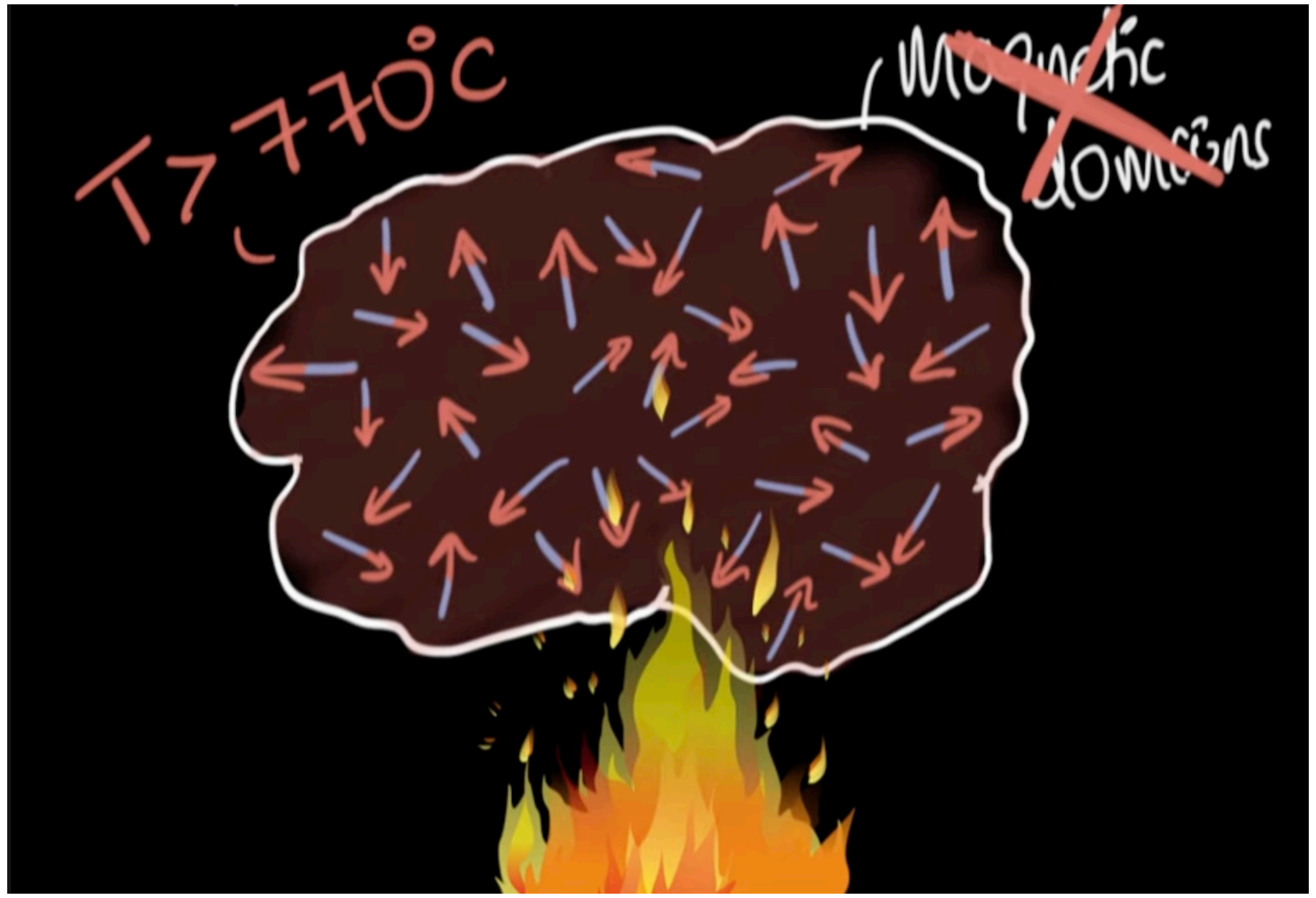
Attracted to magnet

Below Tc the domains have non-zero magnetisation

Increase T

Paramagnetic material:

Iron (Fe): Tc = 770 C



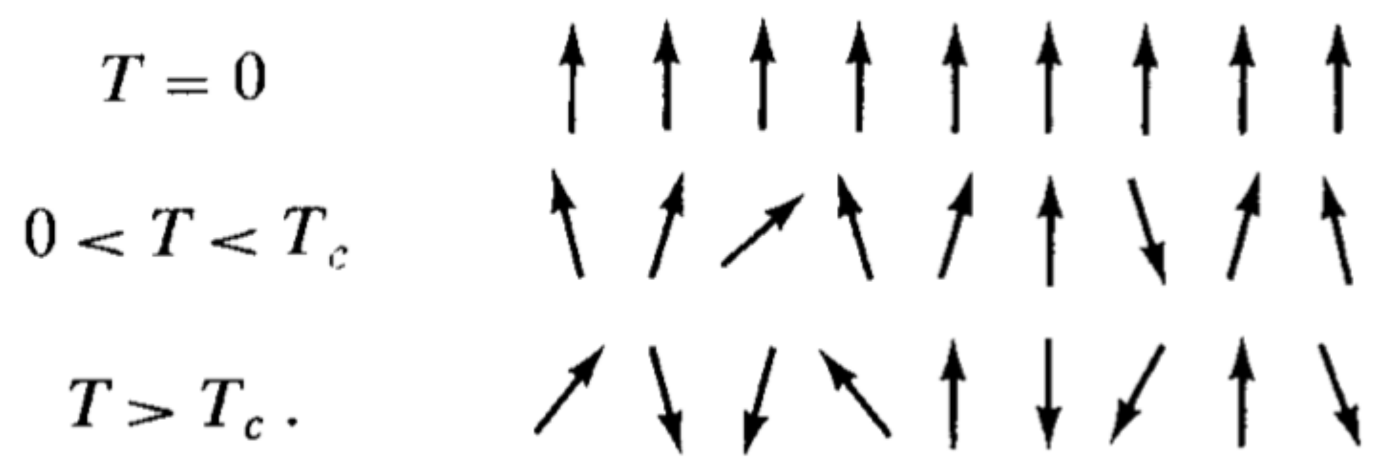
Only very weakly attracted to magnet

Above Tc the magnetisation of the domains is zero

How to model this?

How to model?

We are interested in modelling what happens inside a domain:



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$T < Tc$, as T decreases, M increases

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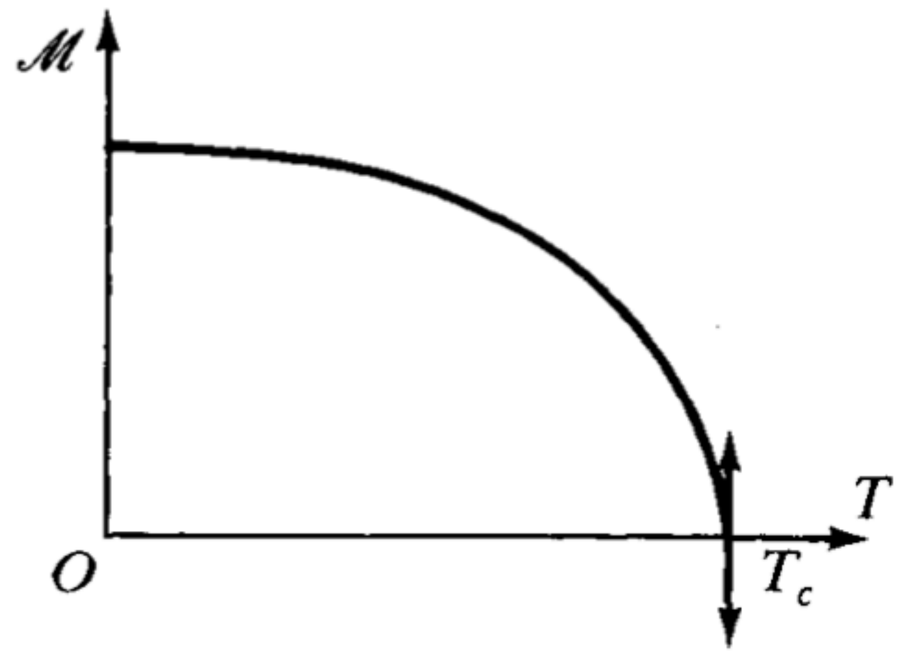


"Tiny magnet" = **spin**

For the model: What seems important in ferromagnetism is the **interaction between spin** that push them to **align with each other**.

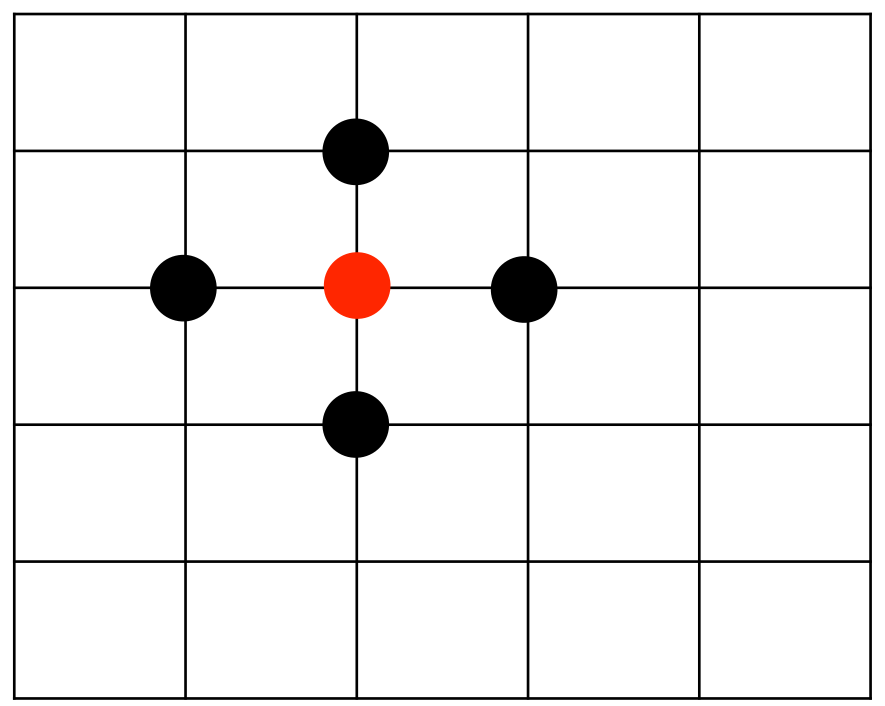
— We replace each atom of the material by just the spin.

— We place the spins on a lattice (square, cubic), similar to atoms in the material

— Interactions between spins are of small range:

we will consider that a spin ● only interact with its closest neighbours ●

Ex. In 2D



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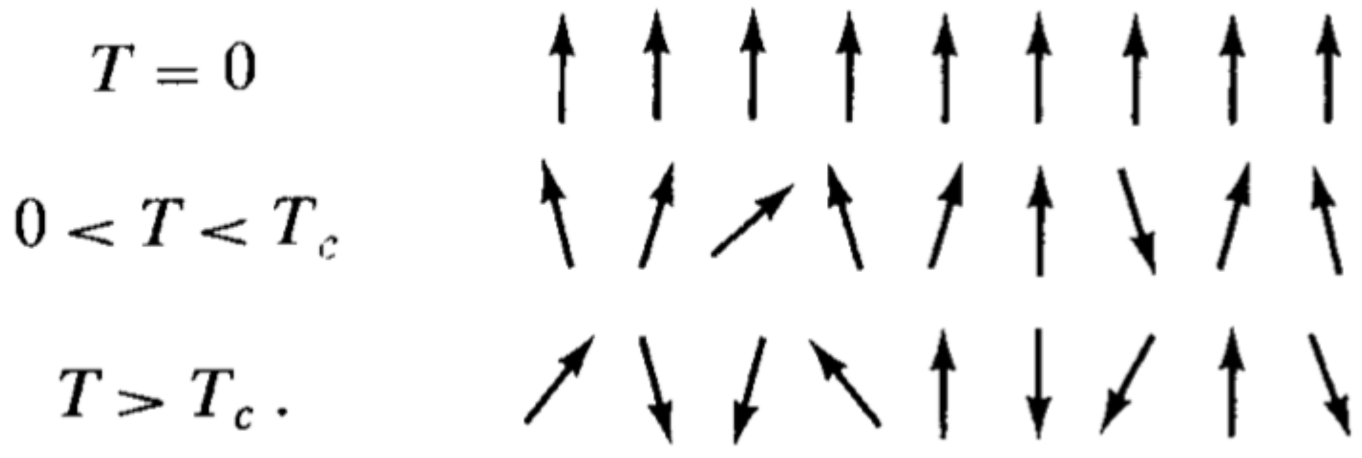

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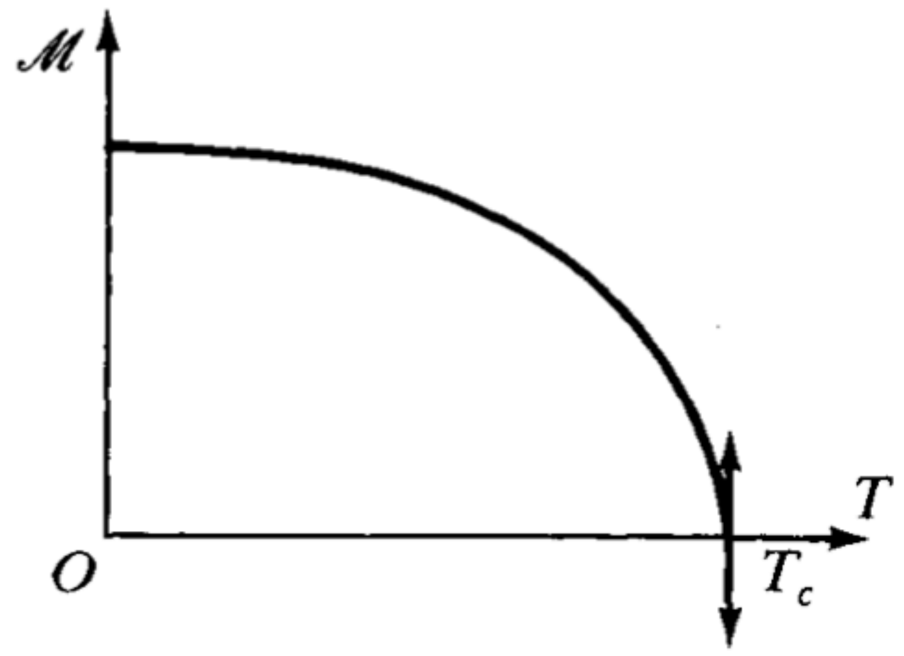

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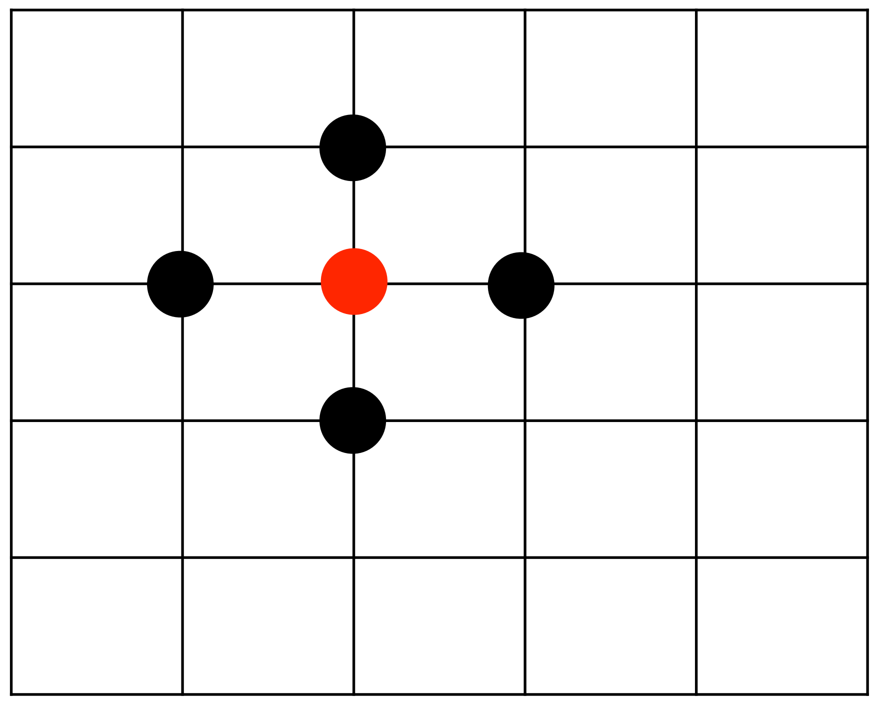

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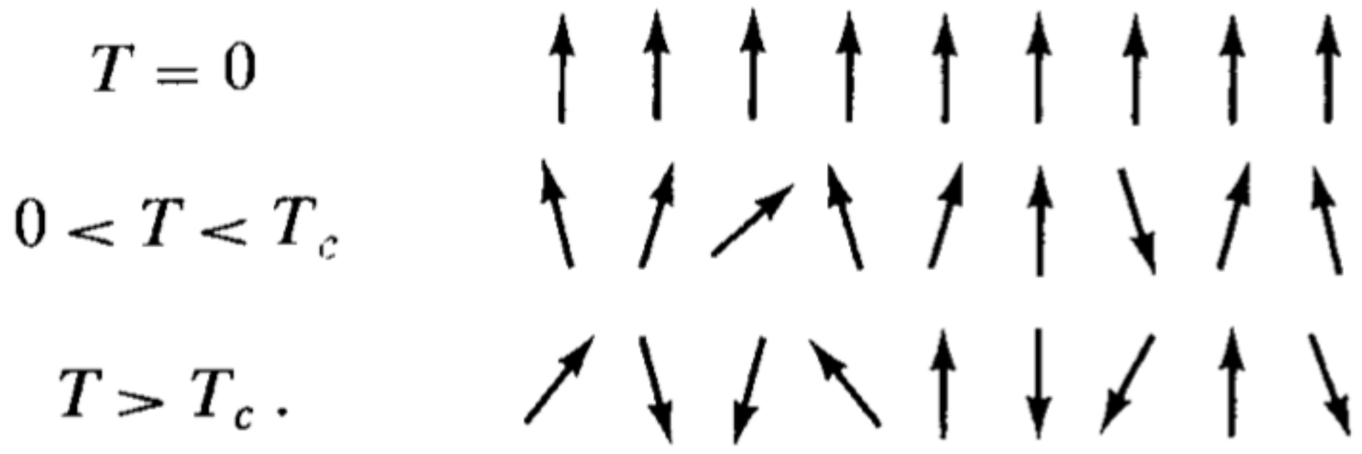

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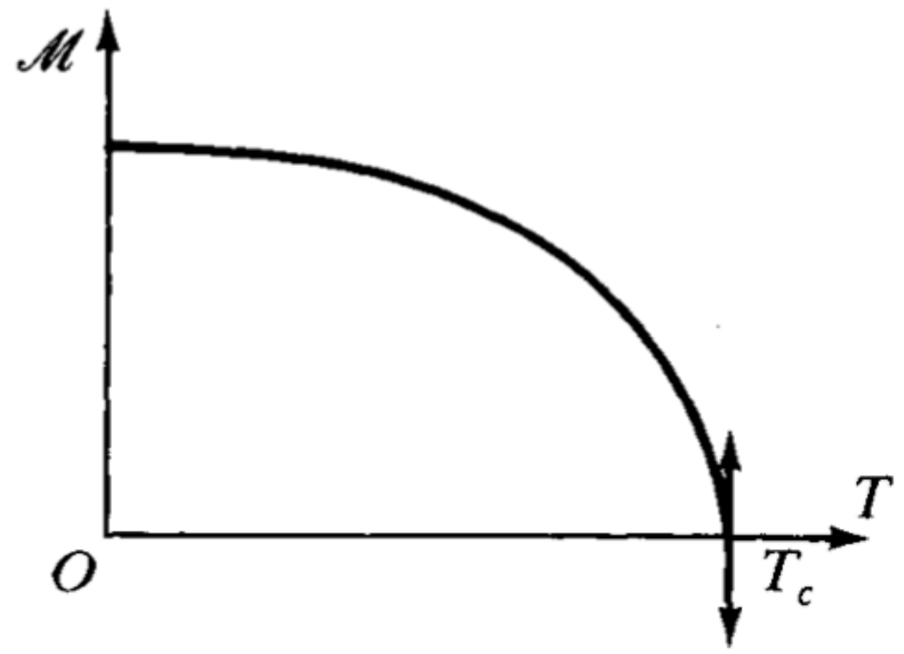

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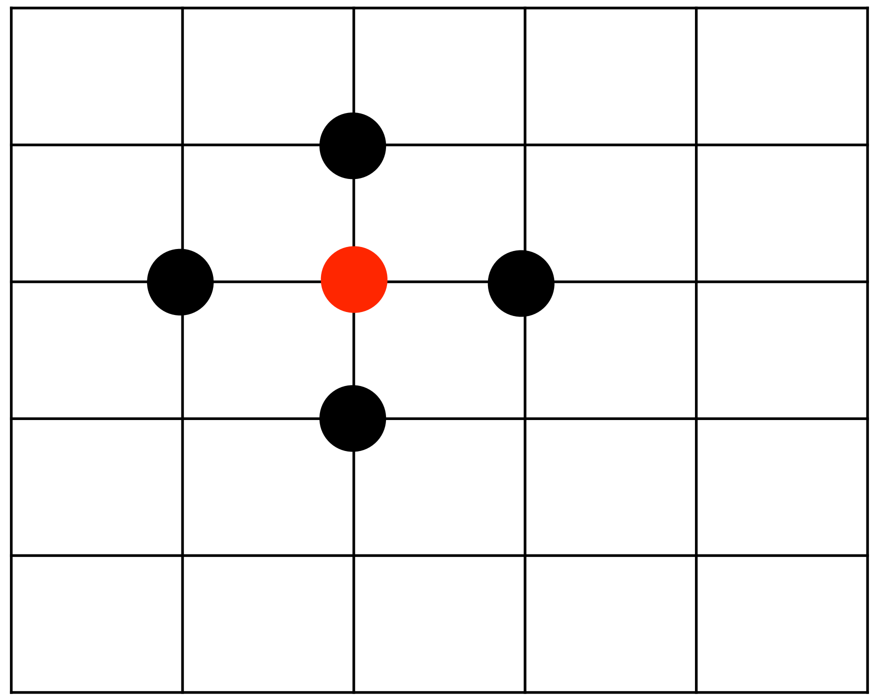
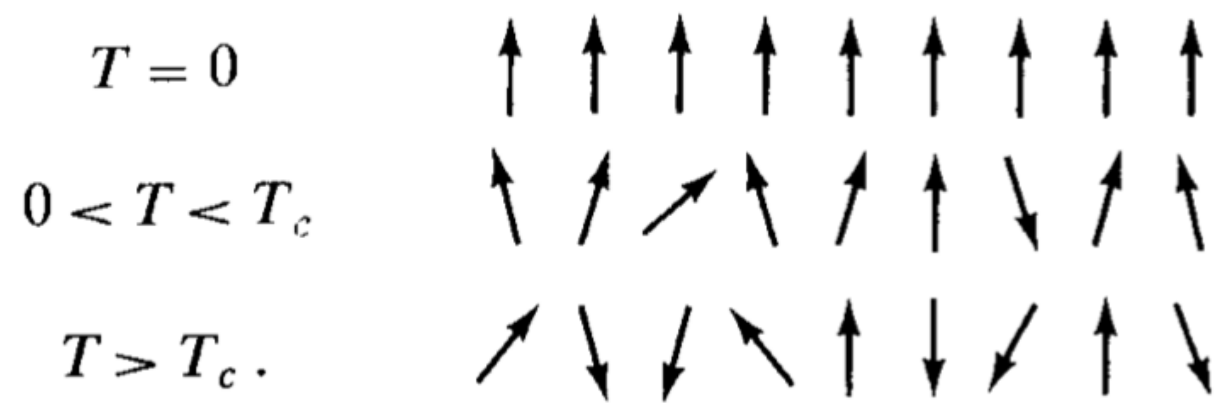
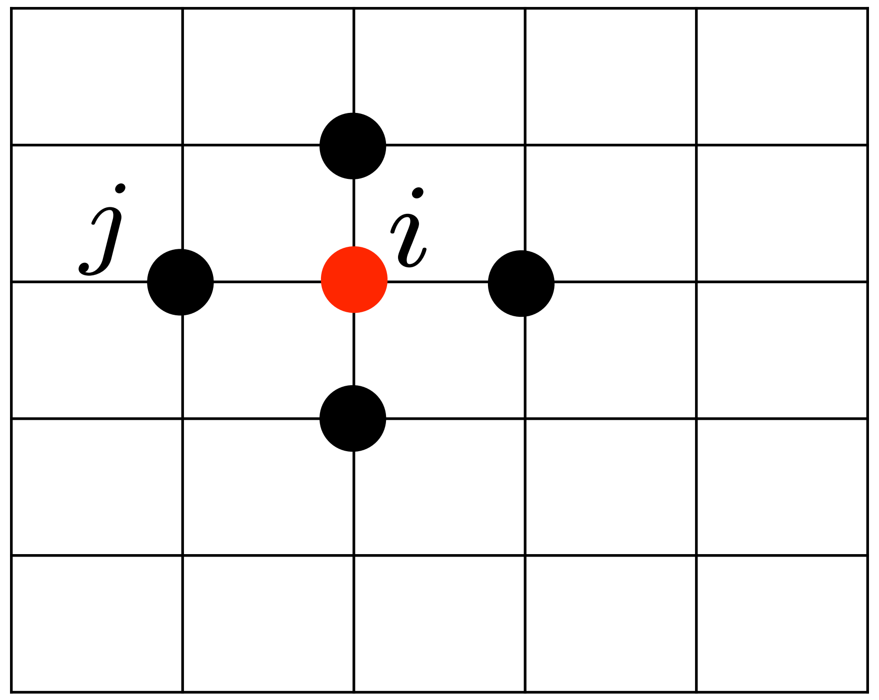




Ising model

Ex. In 2D



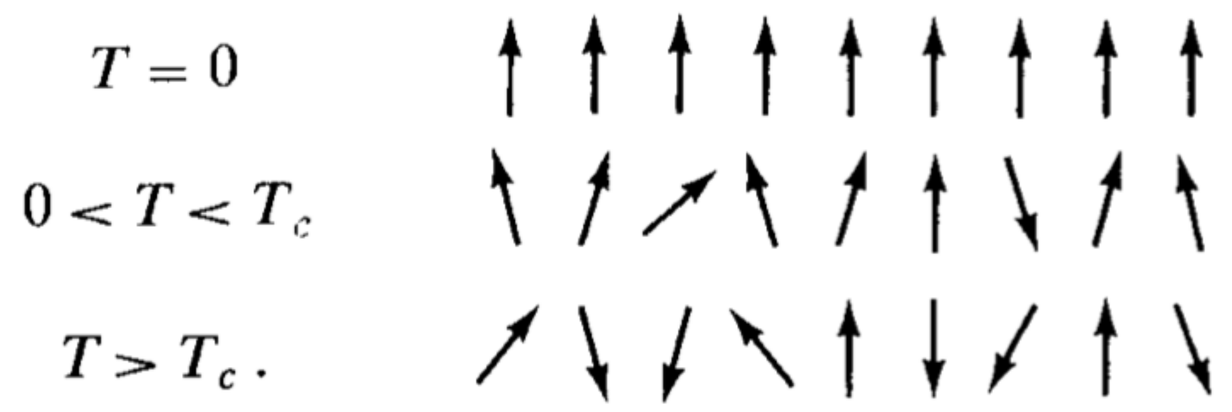
For the classical Heisenberg model: The simplest energy function that tend to align spin is:

$$H = -J \sum_{<i,j>} \vec{s}_i \cdot \vec{s}_j \qquad \text{with} \quad J > 0$$

Normalised vectors

Sum over closest neighbours only

Still too complicated....



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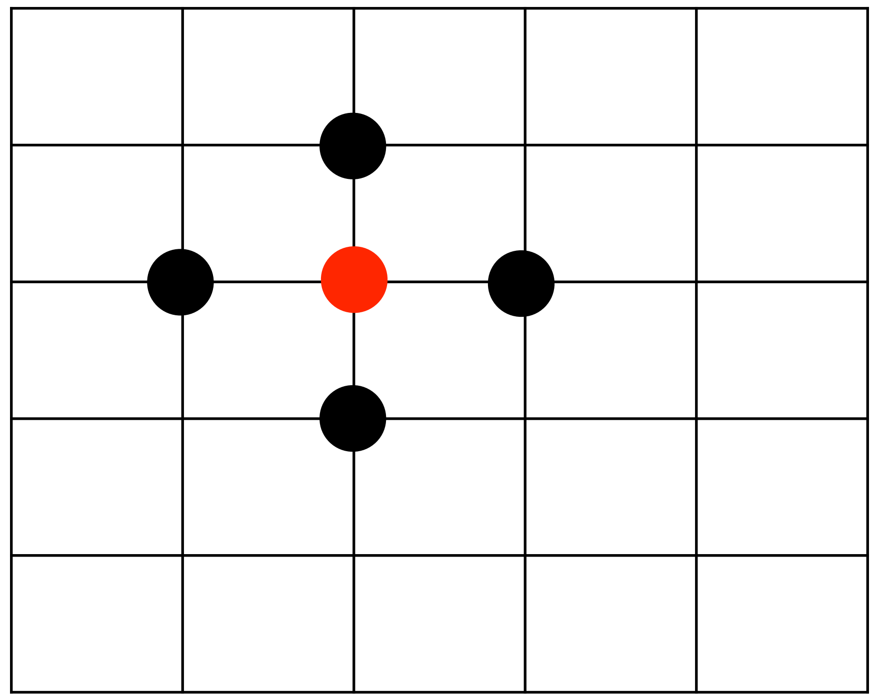

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For the Ising model: We replace the vectors by simple scalars spin, which can only take two values $s_i = +1$ and $s_i = -1$

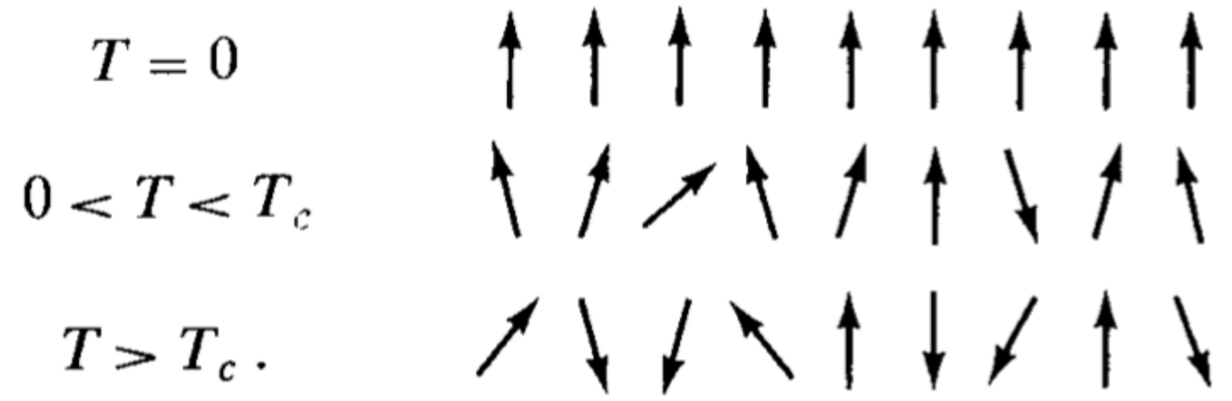
Energy of the system: $$H = -J \sum_{<i,j>} s_i \, s_j \qquad \text{with} \quad J > 0$$

Scalar spin $s_i = \pm 1$

Sum over closest neighbours only

Qualitatively a good model of ferromagnetism.

Quantitatively, some predictions are not precisely correct.



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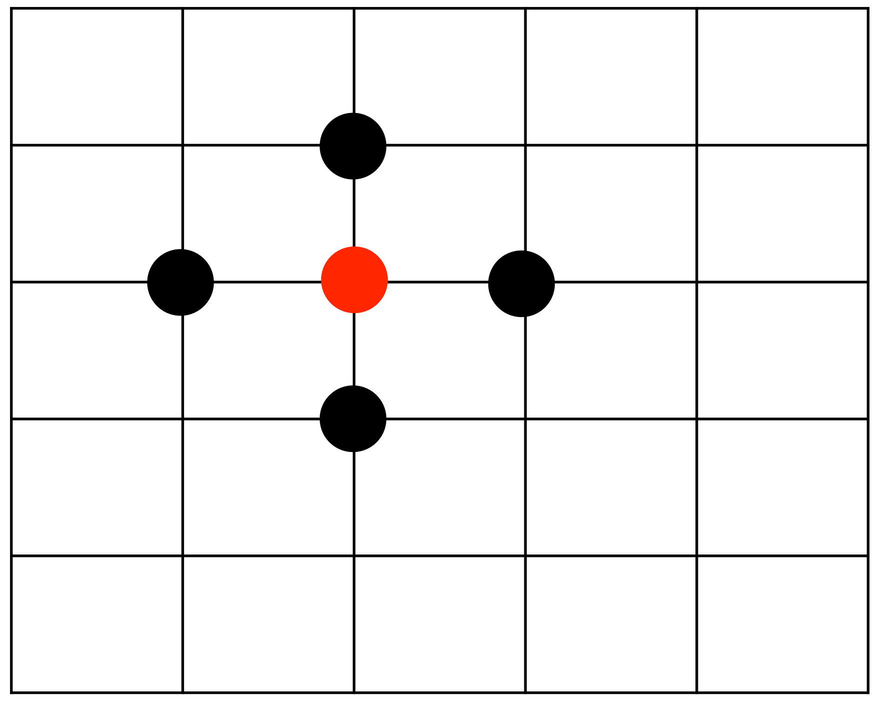

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Still too complicated....

For the Ising model: We replace the vectors by simple scalars spin, which can only take two values $s_i = +1$ and $s_i = -1$

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

Scalar spin $s_i = \pm 1$

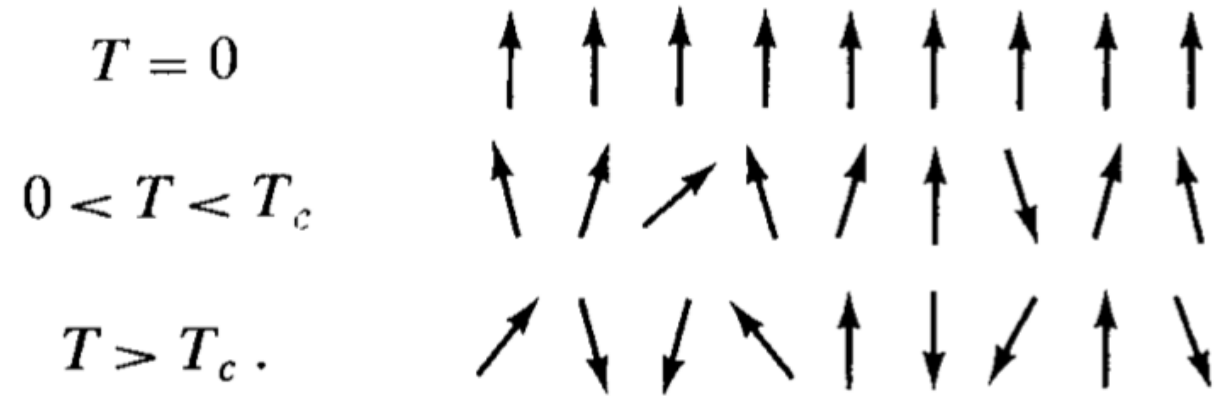
Sum over closest neighbours only

Between two neighbours: $E_{ij} = -J \, s_i \, s_j$ can only take two values: $-J$ if the spins are aligned ↑↑ ↓↓

J if the spins are anti-aligned ↑↓ ↓↑

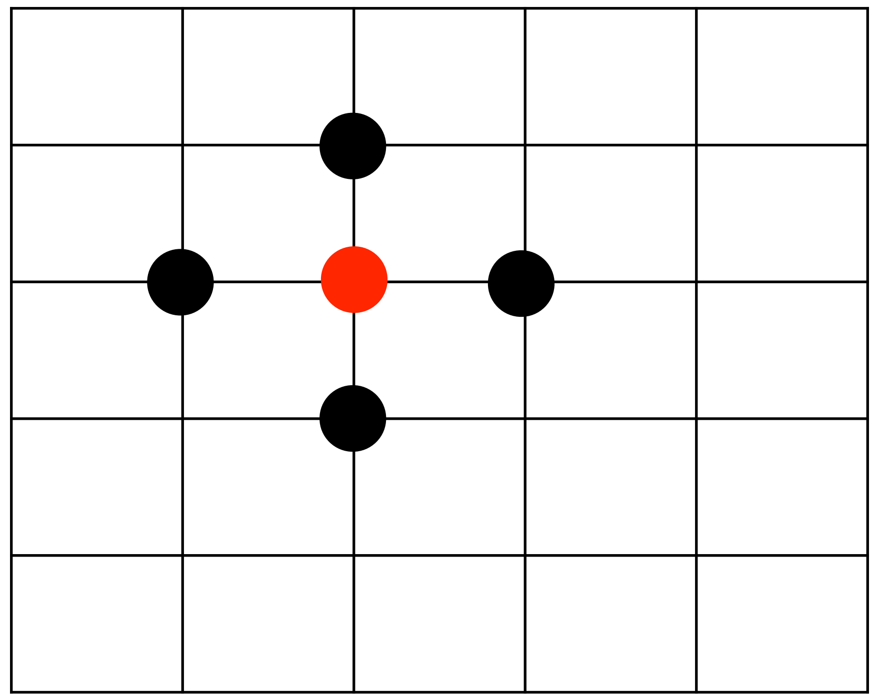
System is trying to go towards states of **lower energy**.

E_{ij} is smaller if the spin are aligned ==>> **spins tend to align**



Ising model

Ex. In 2D



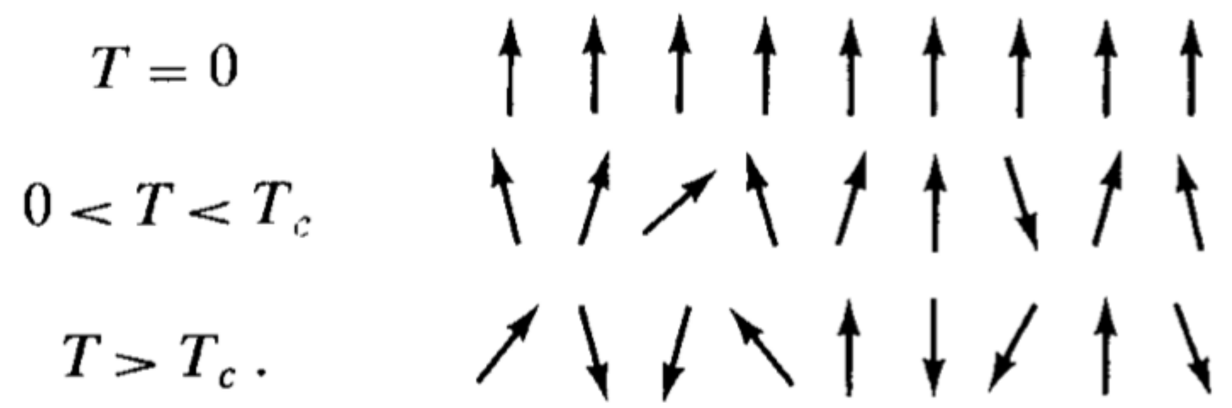
Energy of the system: $$H = -J \sum_{<i,j>} s_i\, s_j$$ with $J > 0$

Sum over closest neighbours only

Scalar spin $s_i = \pm 1$

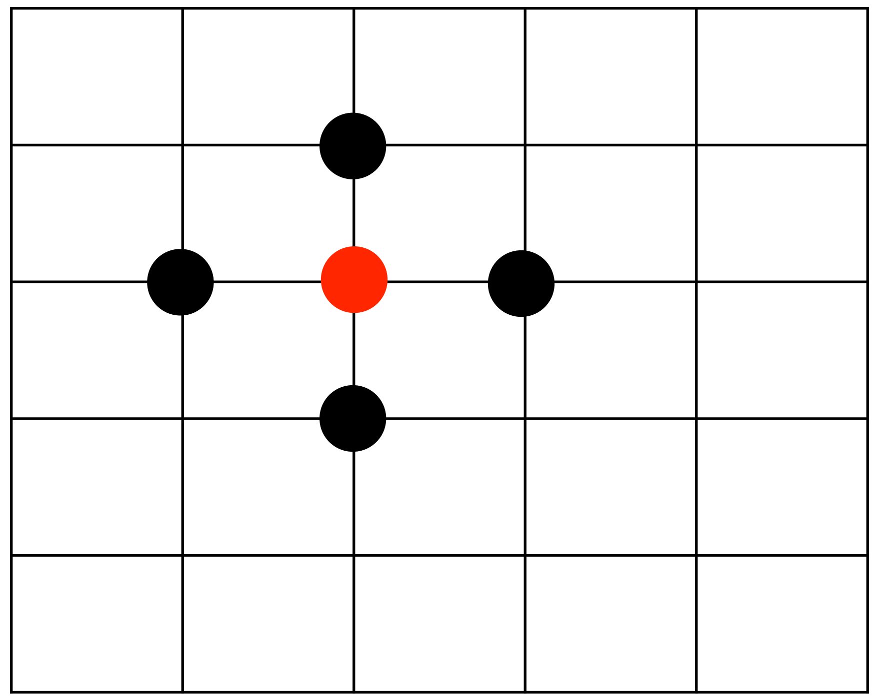
State probability: $$P(s_1, \cdots, s_N) = \frac{\exp(-\beta\, H)}{Z}$$

Where $\beta = \dfrac{1}{k_b\, T}$ = inverse temperature. Control the **level of "noise"** in the system.



Ising model

Ex. In 2D



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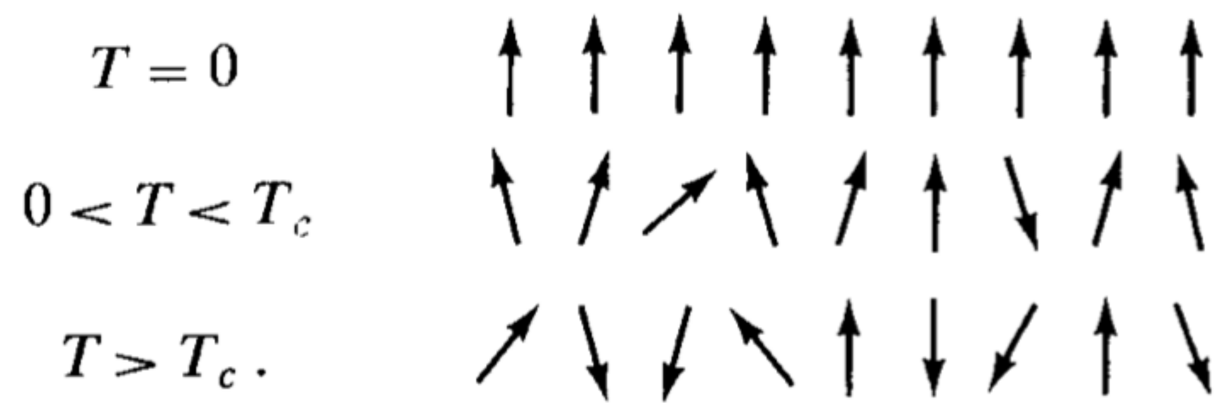
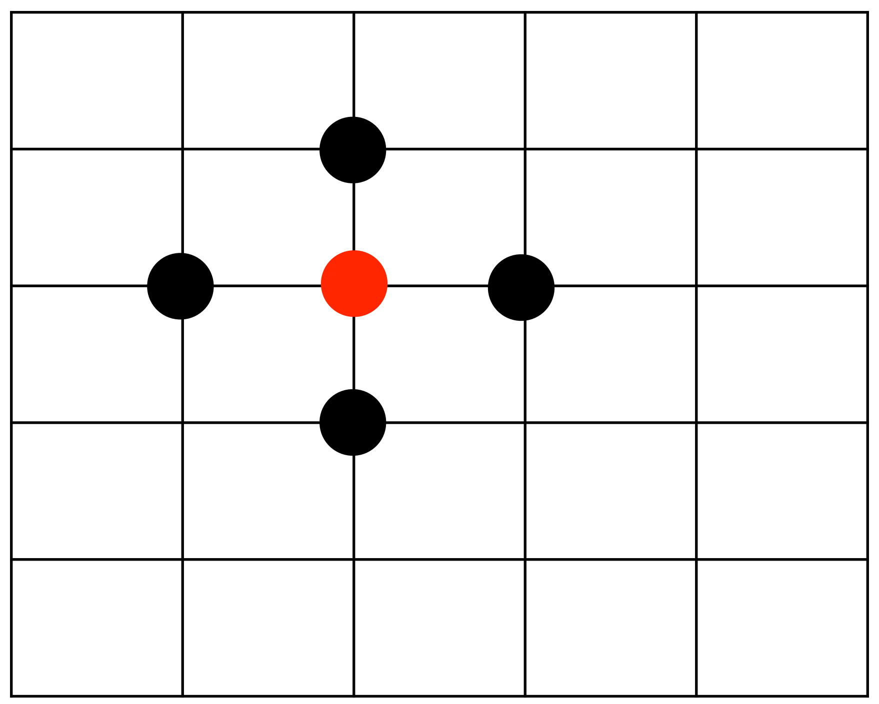
Normalisation

Contains all the information about the system!



Ising model

Ex. In 2D



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Partition function: $$Z = \sum_{s_1, \cdots, s_N} \exp(-\beta \, H)$$

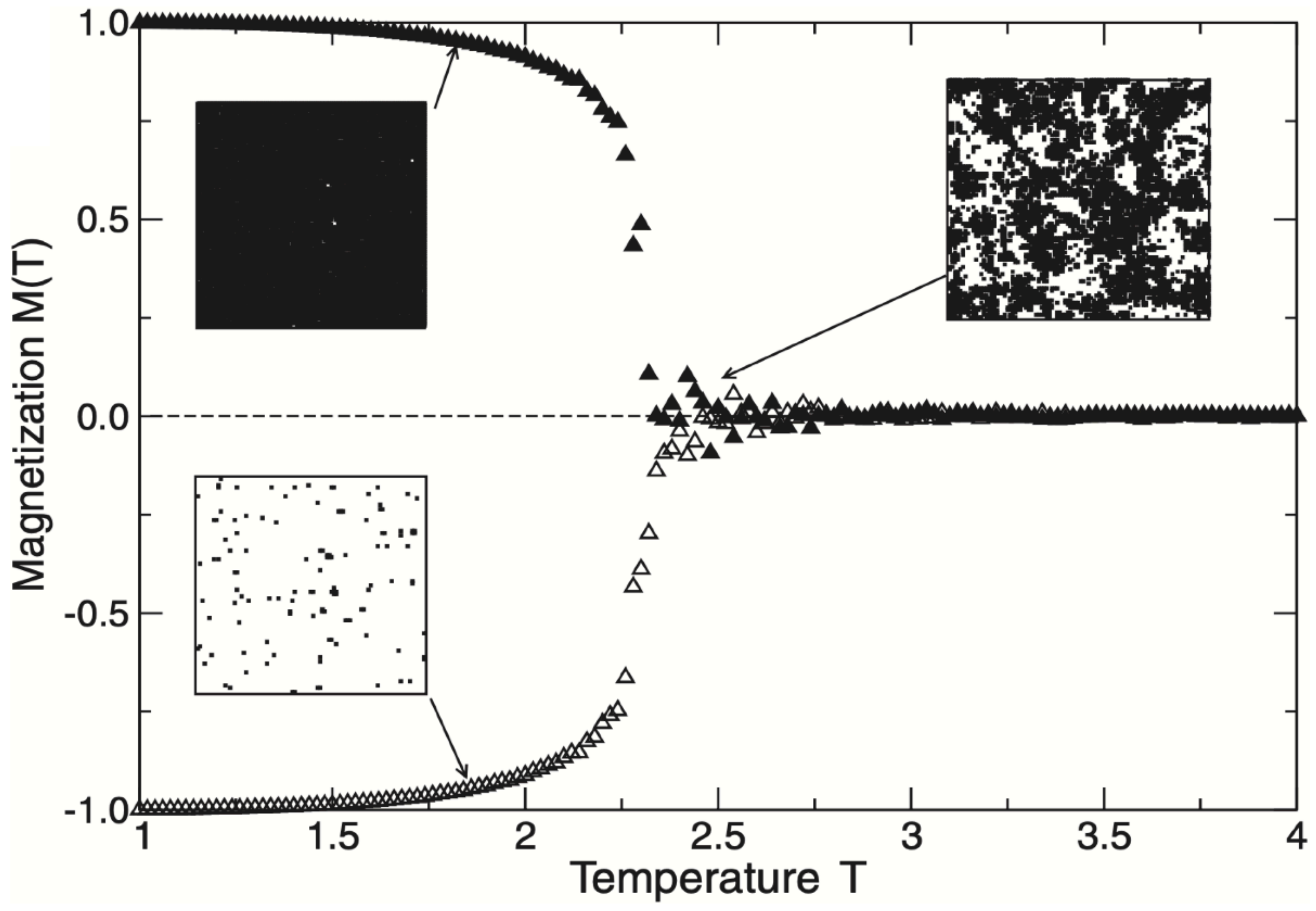
Normalisation

Contains all the information about the system!

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

Ising model: Coming up

Coming tutorial: We will see how we can simulate this system, to study numerically the phase transition.



[Link to Metropolis simulation of the Ising model]()

Coming lectures: We will see what can be done analytically…

The Ising model: has been used to model a broad range of systems,

social systems, neuronal activity, financial markets, psychological states, …