Micro- to Macroscopic Description of a Complex System

Chapter I

Monday April 8

Micro- to Macroscopic Description of a Complex System

Course Chapter I

Questions: Homework

Quiz 1 next week: Monday or Thursday?

Plan: **Lecture 1: From micro to macro:** brief review of equilibrium statistical physics for complex systems

Lecture 2: Example of the **Ising model**

Lecture 3: Example of the **percolation problems**

References: Book "Complexity and Criticality", K. Christensen, N. Moloney, Chapter 1 and 2

"Critical Phenomena in Natural Sciences Chaos, Fractals, Self-organization and Disorder", by D. Sornette

Before we begin: Focus on **Equilibrium Statistical Mechanics:**

attempts to derive thermodynamic **laws of macroscopic quantities from** a **microscopic description** of a system.

Lecture 1: From micro to macro: brief review of equilibrium statistical physics

Plan:

1) Connecting Micro to macro
2) Entropy thermodynamics and statistical
3) Boltzmann distribution
4) Free energy
5) Back to the Ising model

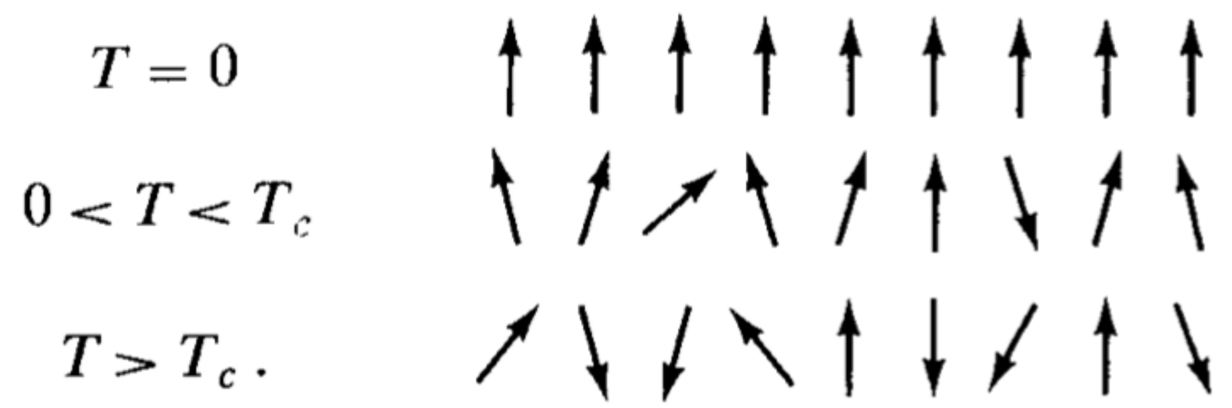
Expectations: Participate in the discussions, take notes, try to (re)-do the analytical calculations

Before we begin: Focus on **Statistical mechanics:**
attempts to derive thermodynamic **laws of macroscopic quantities from** a **microscopic description** of a system.

Part I.1

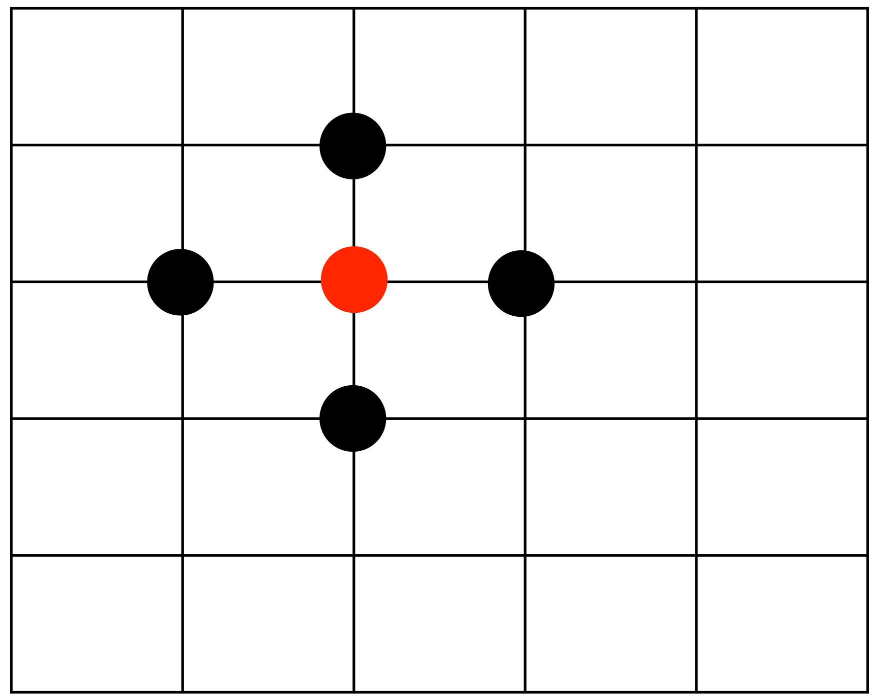
From Microscopic to Macroscopic description

Equilibrium Statistical Mechanics



Last week: Ising model

Ex. In 2D



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 $s_i = \pm 1$

Microscopic description

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

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

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

Contains all the information about the system!

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

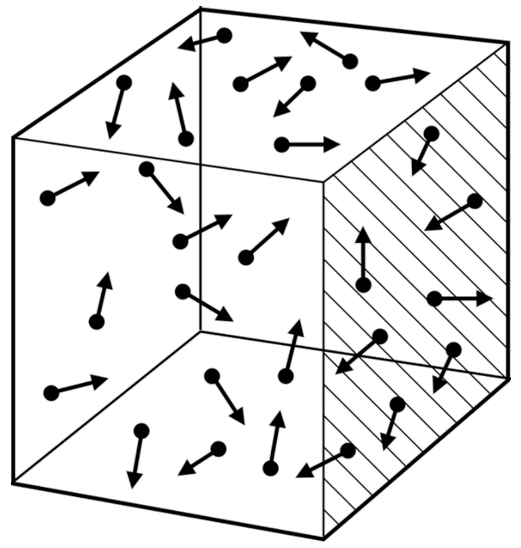
???

Micro to Macro with Statistical Mechanics

When observing physical systems, we don't see the system in all its little microscopic states,

instead we will see the system in a "macrostate", in which we measure macroscopic observables.

Ex. Gas in a box



Microstate

Macrostate

For complex systems, we may be able to see the microstates,

but we still want to understand properties of the system at a macroscopic level.

Ex. Voting

Microstate

Macrostate

We would like to understand **how the properties of the system at a microscopic level gives rise to its macroscopic properties.**

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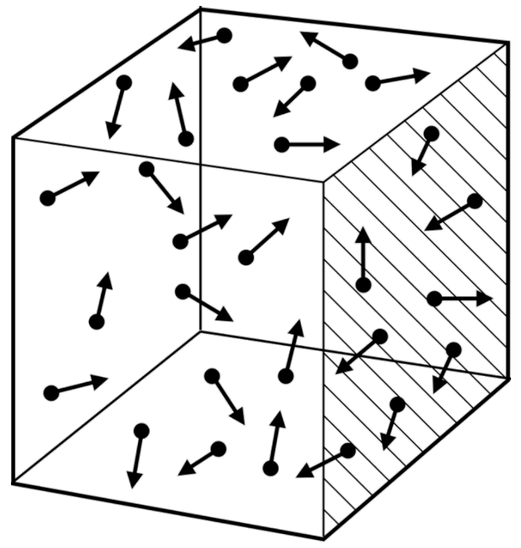

Microstate

Exact positions/speed of all the molecules of a gas

Macrostate ——>>>> **Thermodynamics**

Characterised by Pressure (P),
temperature (T) of the gas,
Average energy of the system (E)

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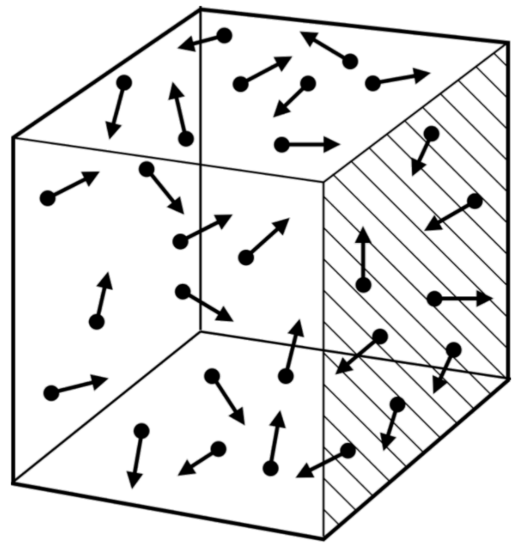

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Ex. Voting

Microstate

Result of a single vote (yes/no — liberal/conservative)
for all the persons in the poll

Macrostate

Average orientation of a person (liberal/conservative),
Average orientation of the group, correlation between
the people in the group

We would like to understand **how the properties of the system at a microscopic level**

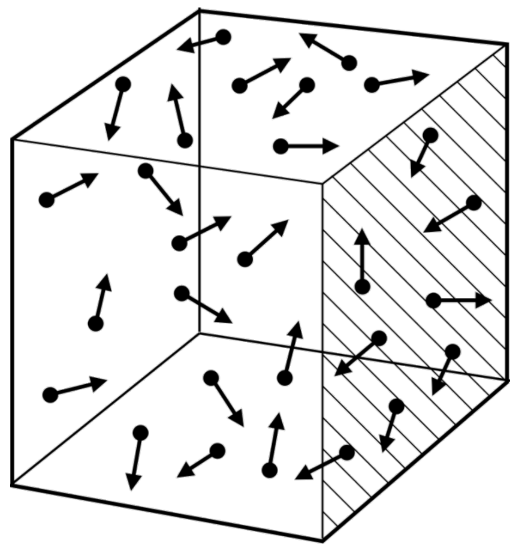
gives rise to its macroscopic properties.

Micro to Macro with Statistical Mechanics

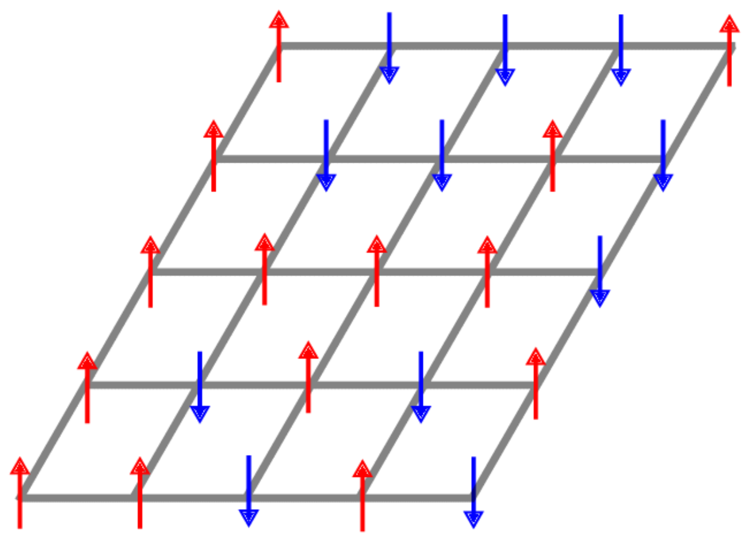
Statistical mechanics:

attempts to derive thermodynamic **laws of macroscopic quantities from** a **microscopic description** of a system.

Microstates State of a system at the level of its constituents.



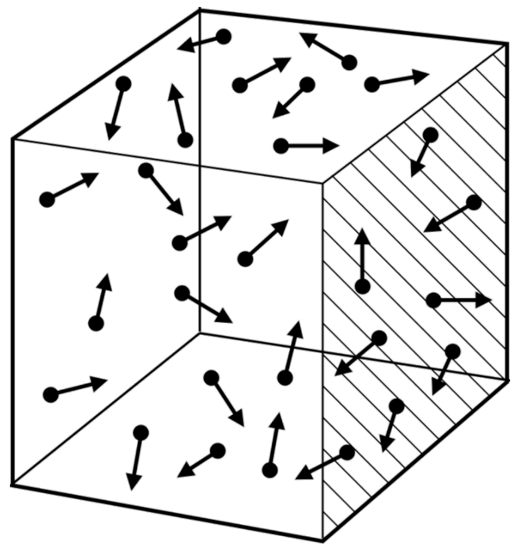
Ex. Exact positions/speed of all the molecules of a gas



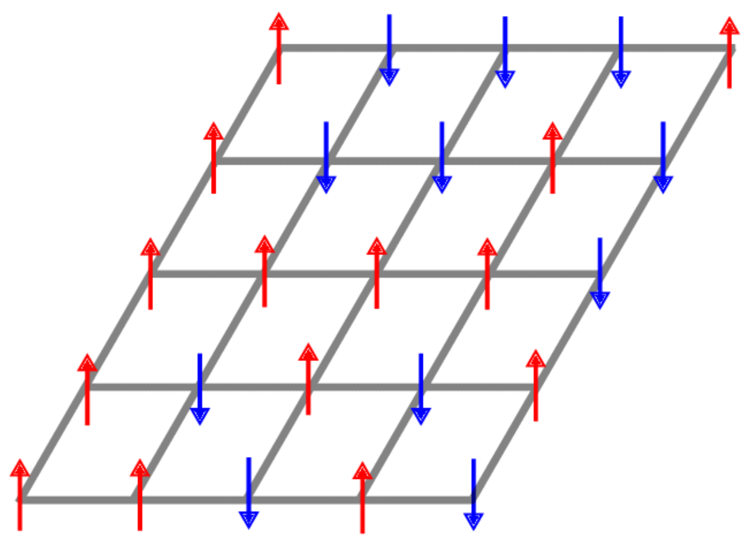
Ex. Exact positions (up/down) of all the spins of the system

Ex. Voting:
result of a single vote (yes/no — liberal/conservative) for all the persons in the poll

Macrostates State of a system at the macroscopic scale, characterised by **macroscopic observables**.



Ex. Characterised by Pressure (P), temperature (T) of the gas, Average energy of the system (E)



Ex. Average magnetisation, average energy of the system, correlation between the spins

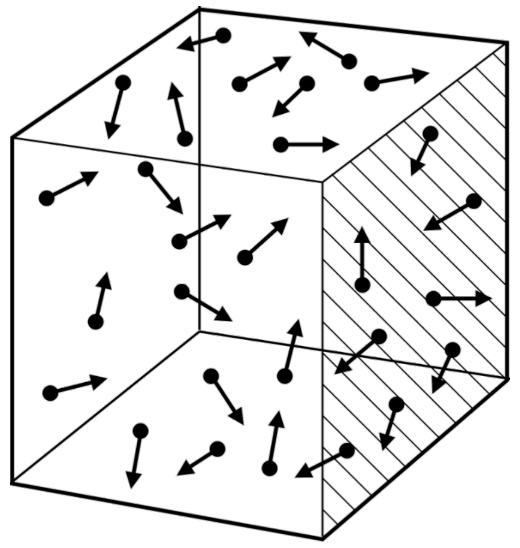
Ex. Average orientation of a person (liberal/conservative), Average orientation of the group, correlation between the people in the group

From Micro to Macro

Microstates $\vec{s}$ = Vector of all the characteristics of each constituents of the system.

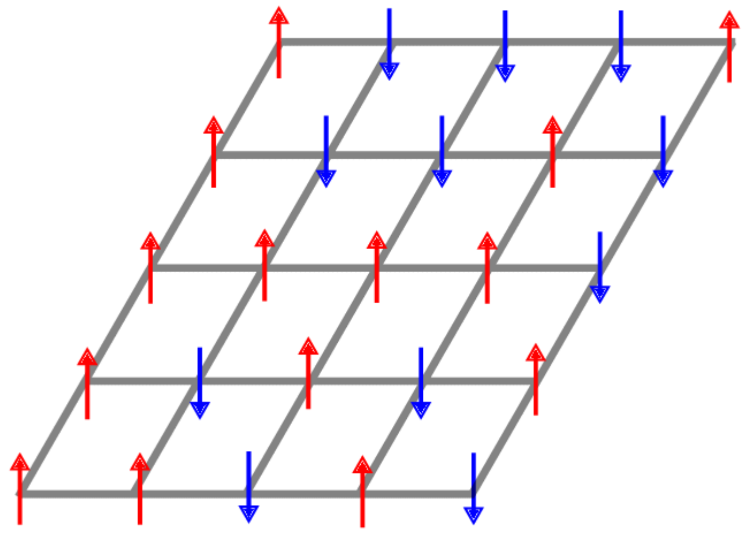
Characterised by $P(\vec{s})$ = probability to observe the system in state $\vec{s}$ at equilibrium.

Ex.



$\vec{s}$ = positions and speed of each molecule

$P(\vec{s})$



$\vec{s}$ = positions (+/- 1) of each spin

$P(\vec{s})$

Micro to Macro with Statistical Mechanics

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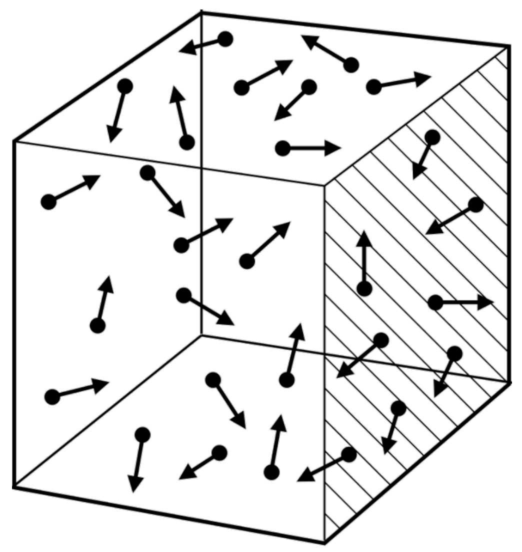

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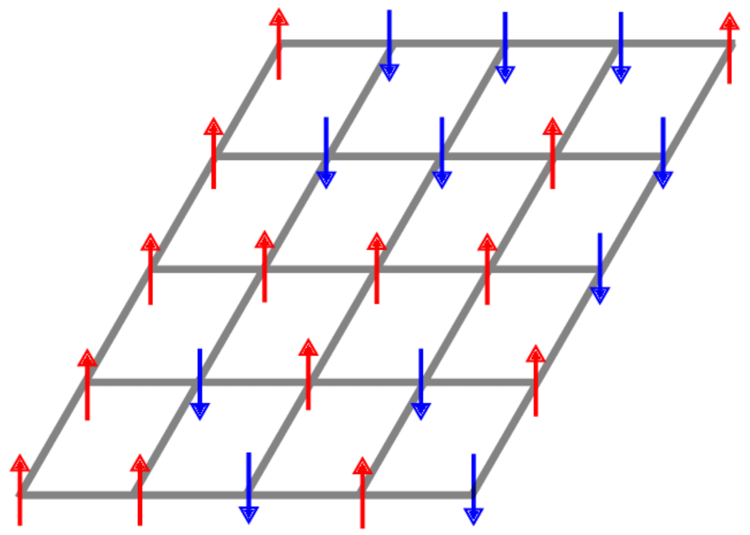

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Macrostates Composed of the most probable microstates. Characterised by macroscopic observables.

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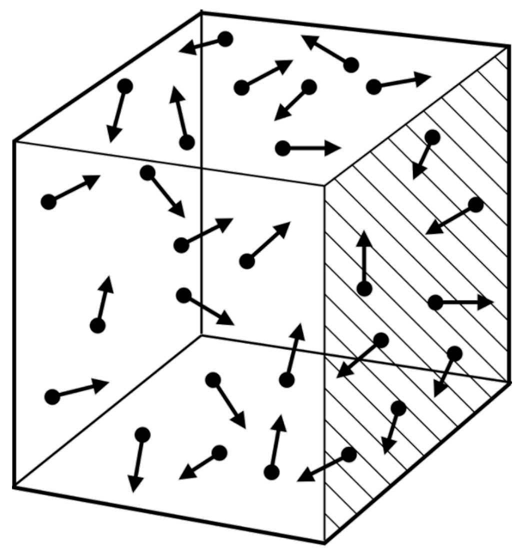

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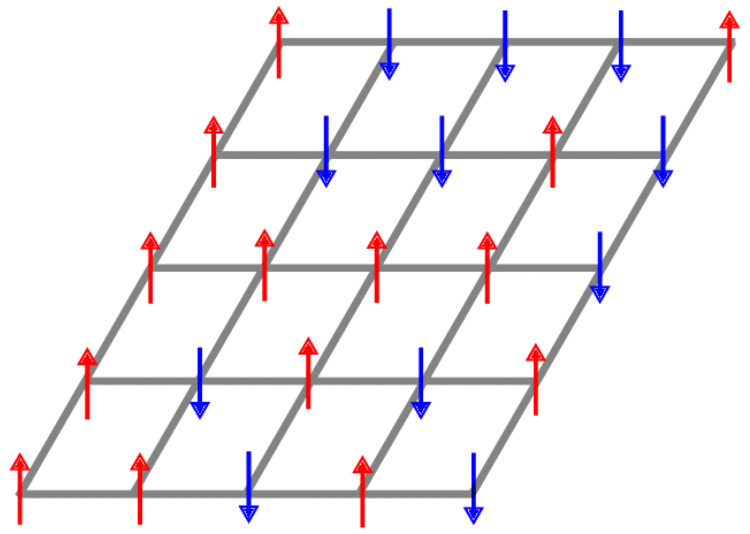

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Macroscopic observables: (**first postulate of statistical thermodynamics**)

At equilibrium, a macroscopic observable $\langle A \rangle$ is defined from the microscopic observable $A(\vec{s})$.

by the weighted ensemble **average over all possible microstates** of the system:

Macroscopic observables:

$$\langle A \rangle = \sum_{\vec{s}} A(\vec{s})\, P(\vec{s})$$

Sum over all the microstates

Observable at the microscopic level

Probability to observe the system in the microstate

Micro to Macro with Statistical Mechanics

Macroscopic observables: **(first postulate of statistical thermodynamics)**

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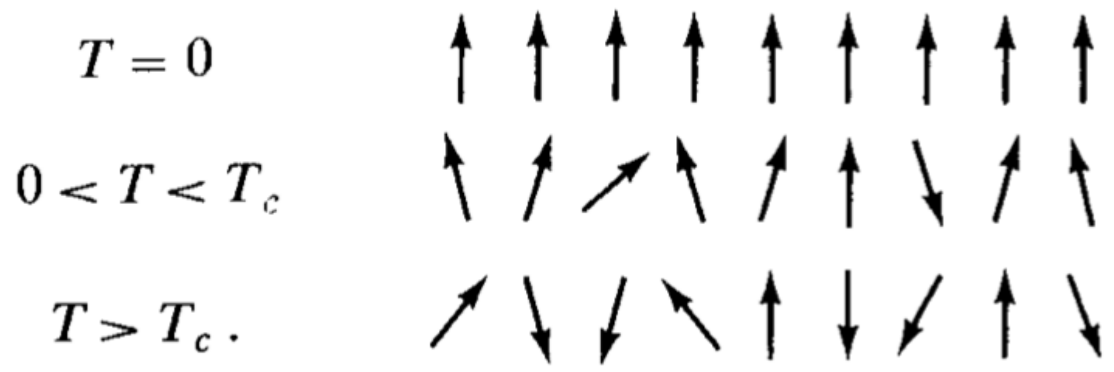
Macroscopic observables:
$$\langle A \rangle = \underbrace{\sum_{\vec{s}}}_{\text{Sum over all the microstates}} \underbrace{A(\vec{s})}_{\text{Observable at the microscopic level}} \underbrace{P(\vec{s})}_{\text{Probability to observe the system in the microstate}}$$

Gibbs' postulate:

$$\underbrace{U}_{\text{Thermodynamics}} = \underbrace{\langle E \rangle}_{\text{Statistical physics}}$$

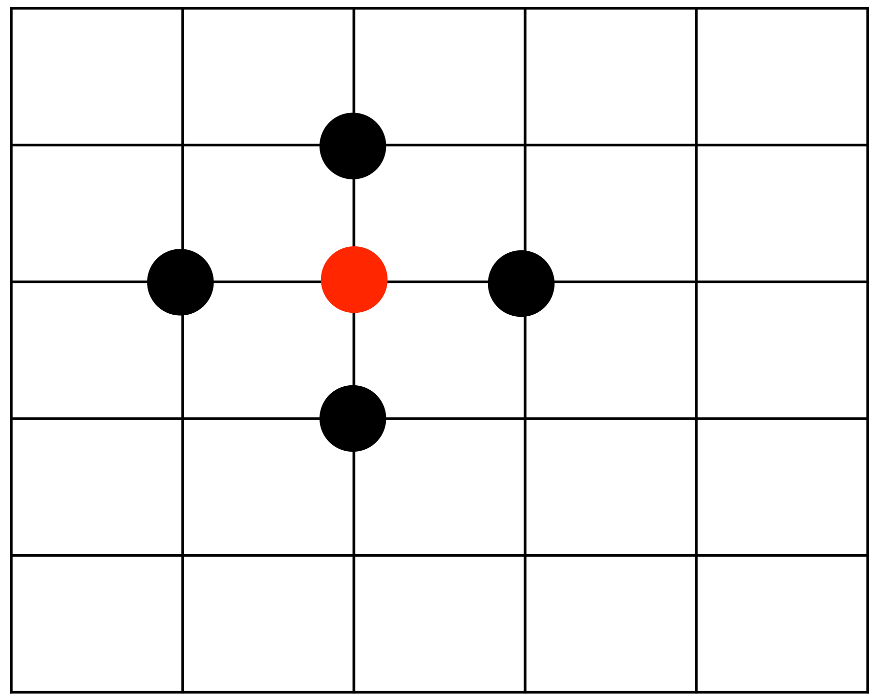
Thermodynamics:
Internal energy
of the system

Statistical physics:
Ensemble average
of the energy $E(\vec{s})$
over all microstates



Ex. Ising model

Ex. In 2D

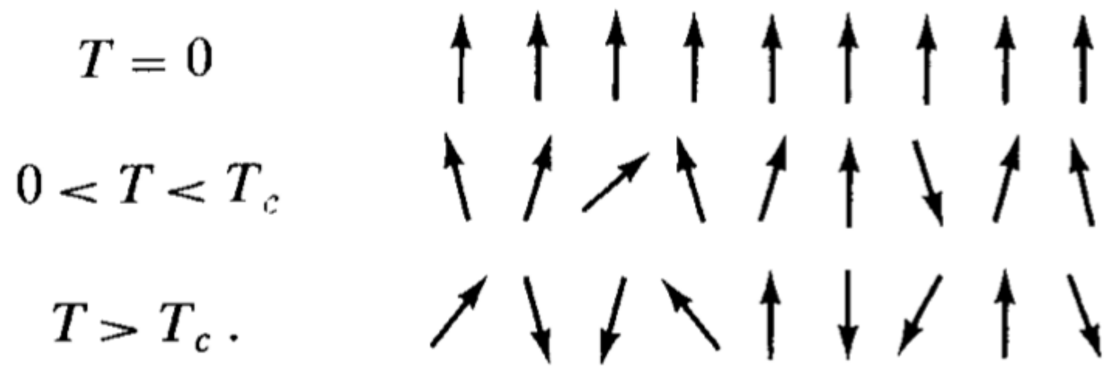


Microscopic observables:

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

Scalar spins: $s_i = \pm 1$

Sum over closest neighbours only



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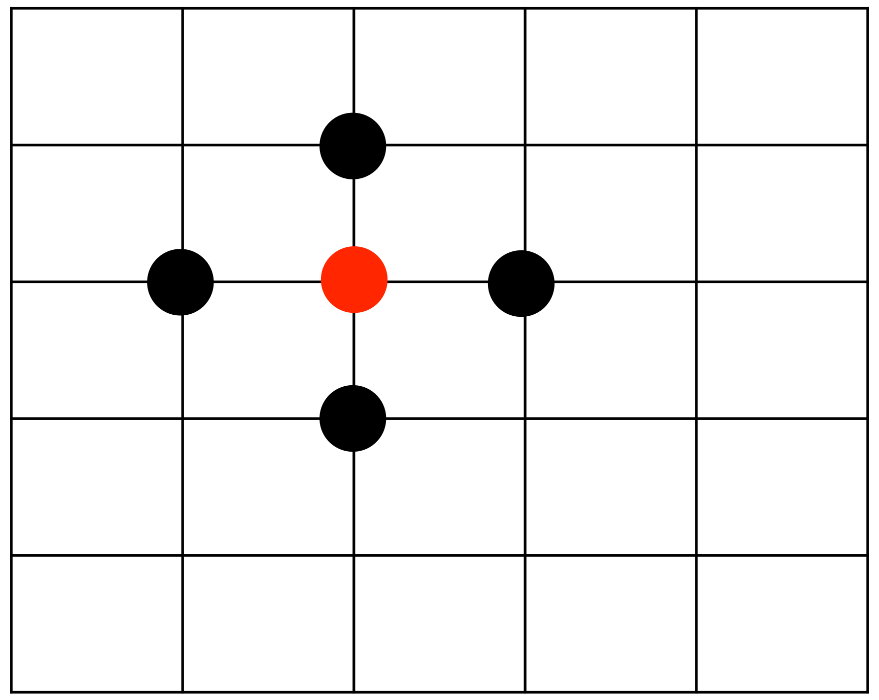

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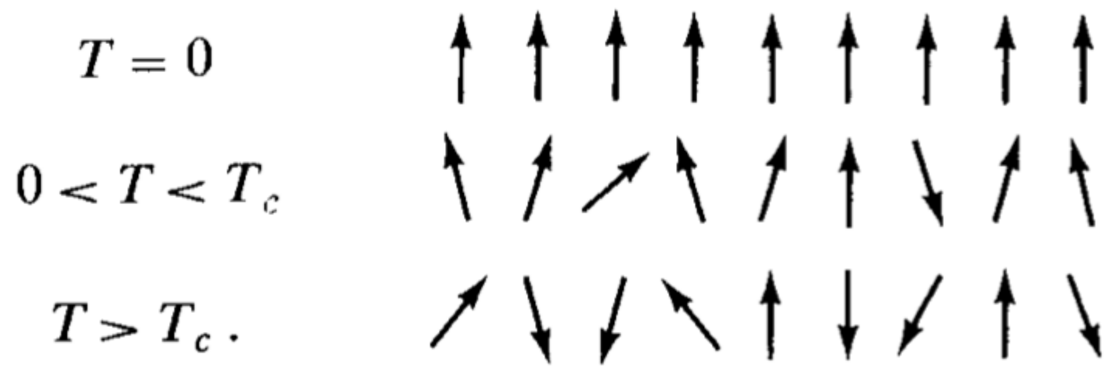
Total Magnetisation per spin: $M(\vec{s}) = \sum_{i=1}^{N} s_i$

Total number of spins

= number of spins up - number of spins down



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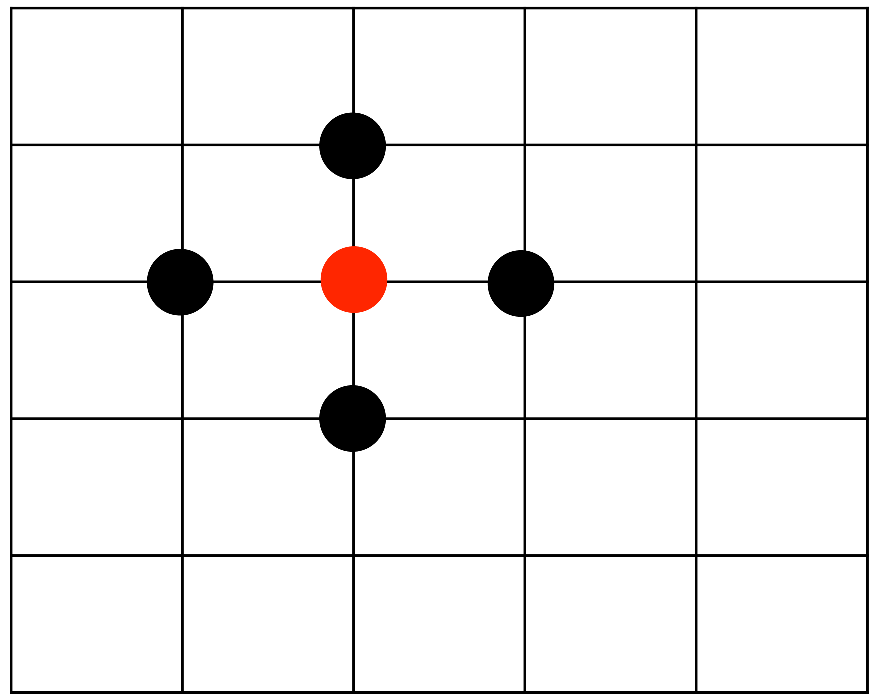

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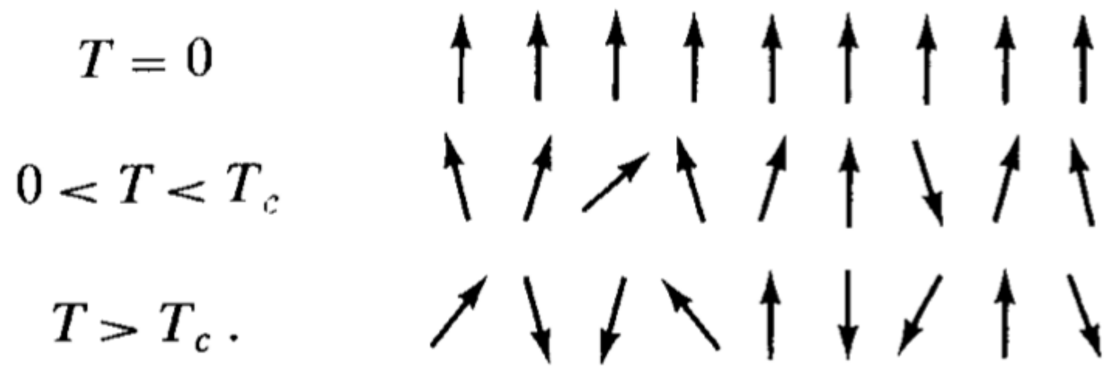

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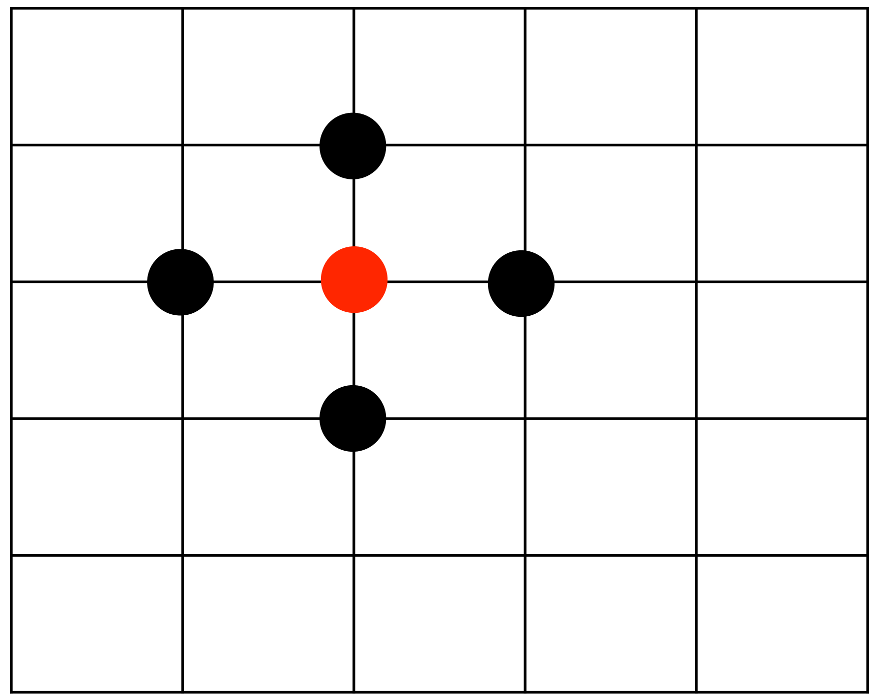

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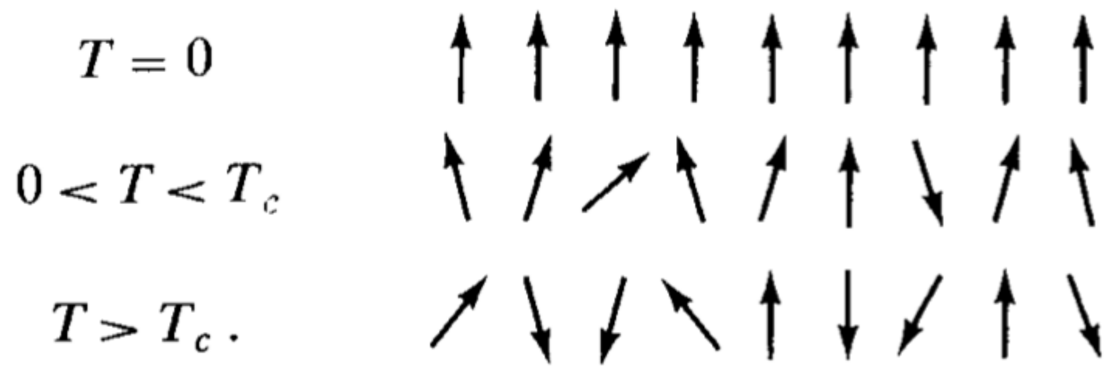
Gibbs' postulate:

$$U = \langle E \rangle$$

Thermodynamics: Internal energy of the system

Statistical physics: Ensemble average of the energy over all microstates



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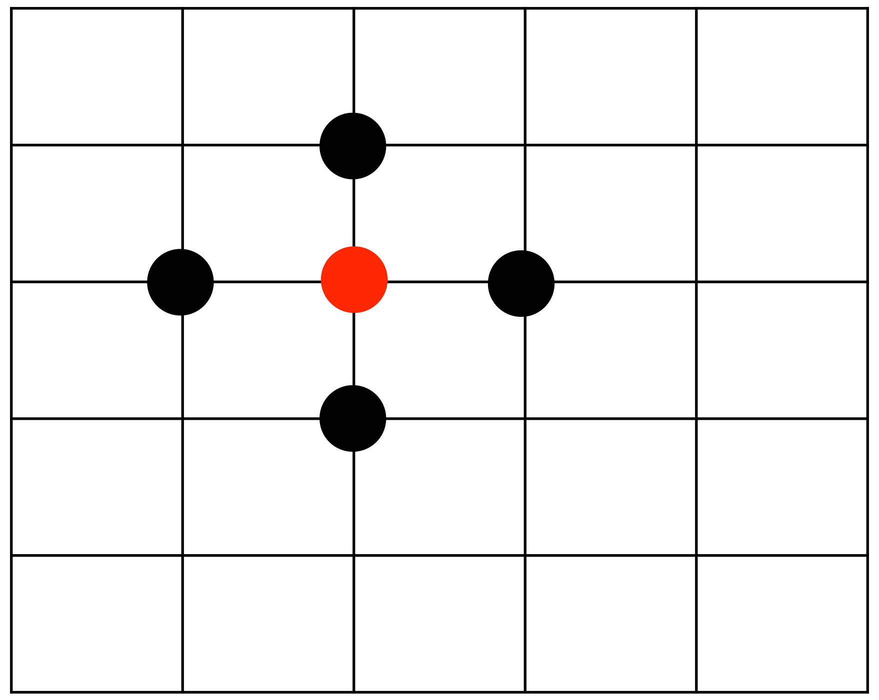

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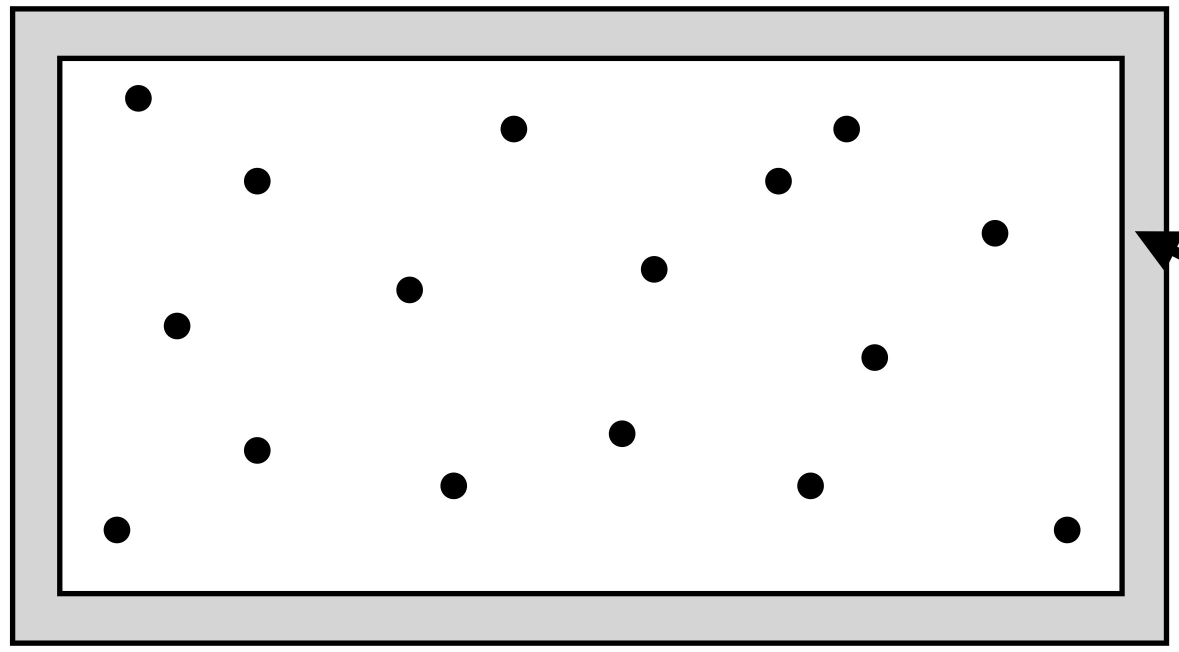
What is $P(\vec{s})$ **?**

Part I.2

Entropy:
thermodynamic and statistical

Micro to macro (again...)

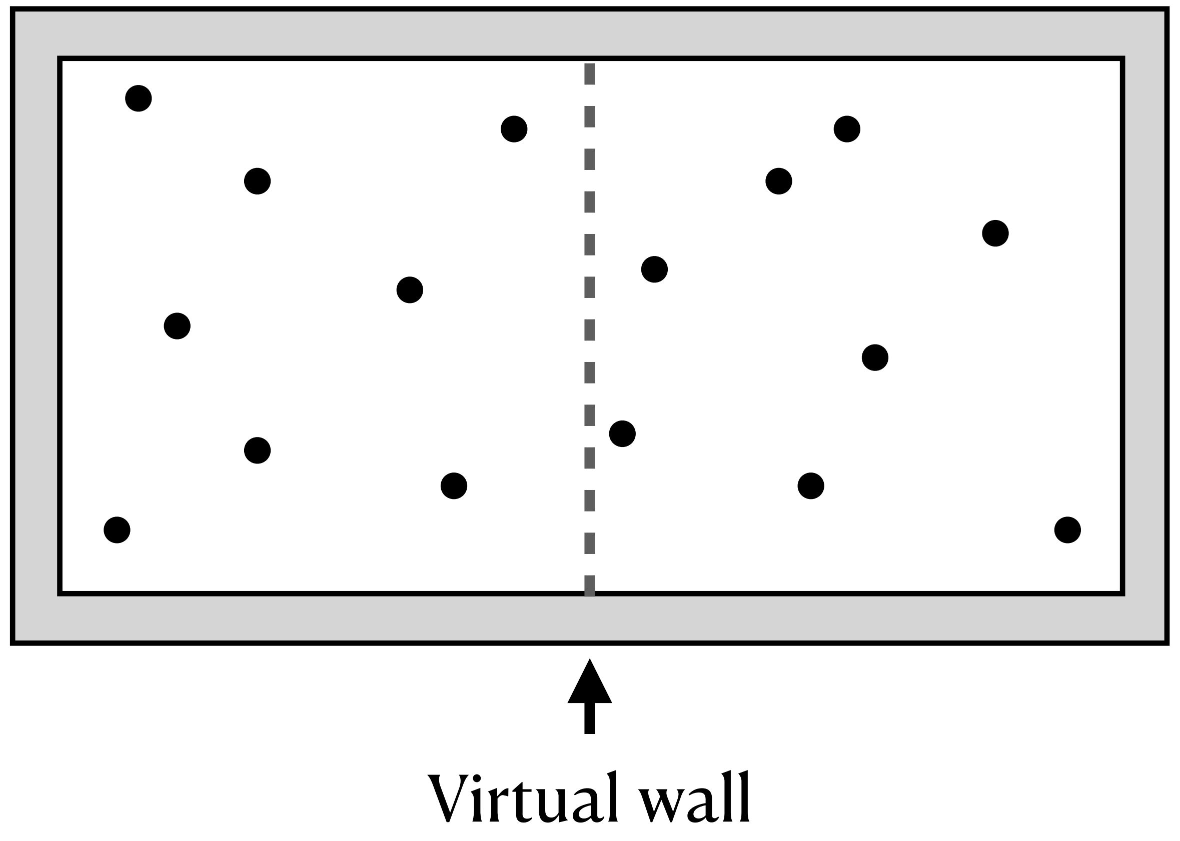


Isolated:

— V fixed
— N fixed = no exchange of particles
— no exchange of heat $\Delta Q = 0$

2nd postulate of statistical thermodynamics: In an isolate system, **all microstates are equiprobable**.

Micro to macro (again...)



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Each particle as a **probability 1/2** to be on the **left side**.

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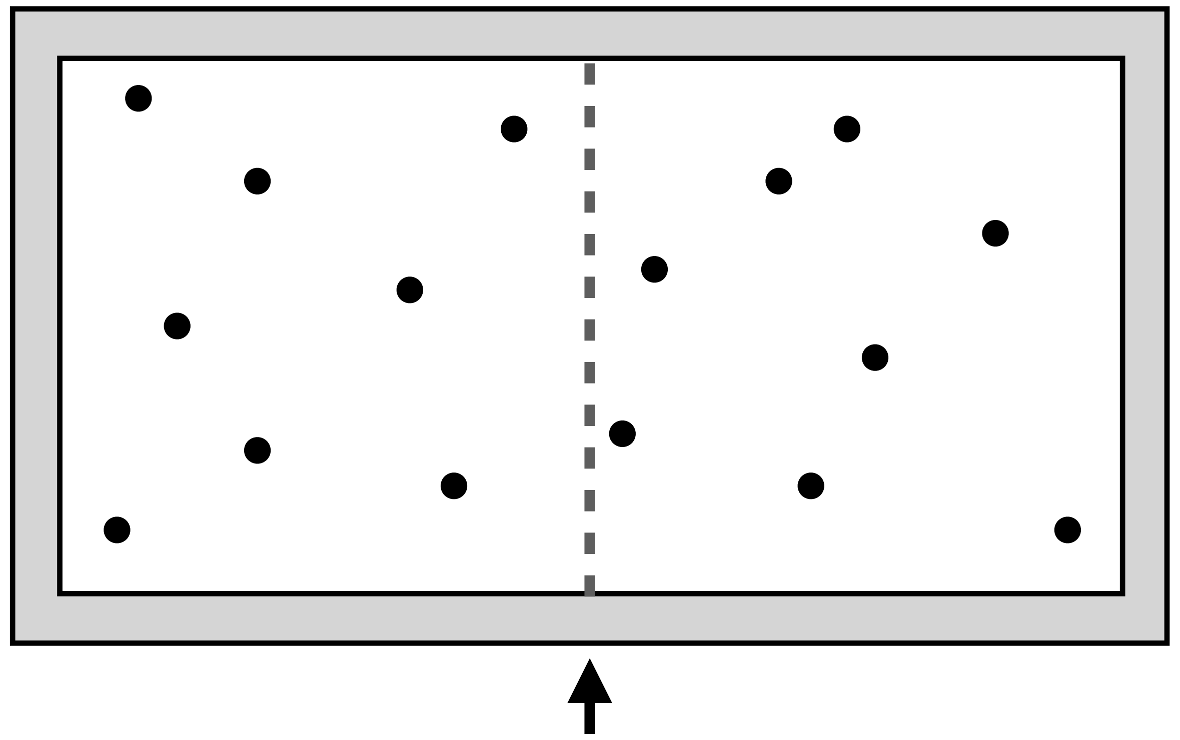
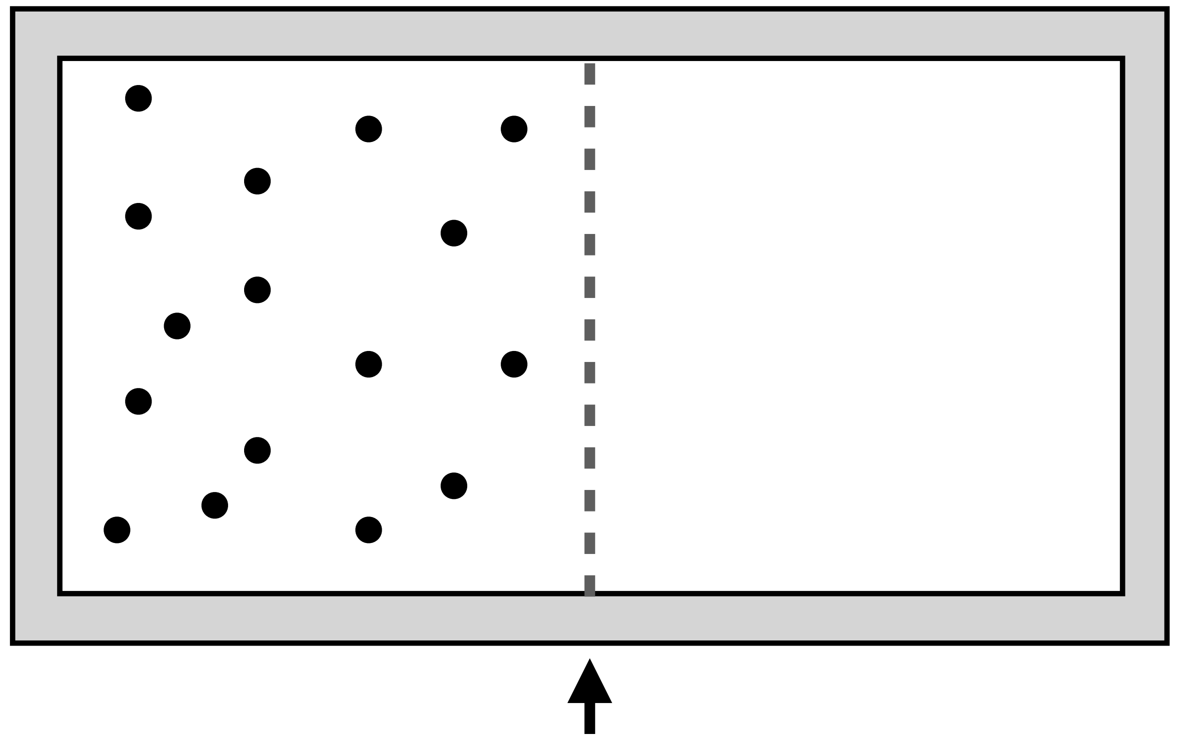
Micro to macro (again…)





Why is it unlikely to see this if N is very large?

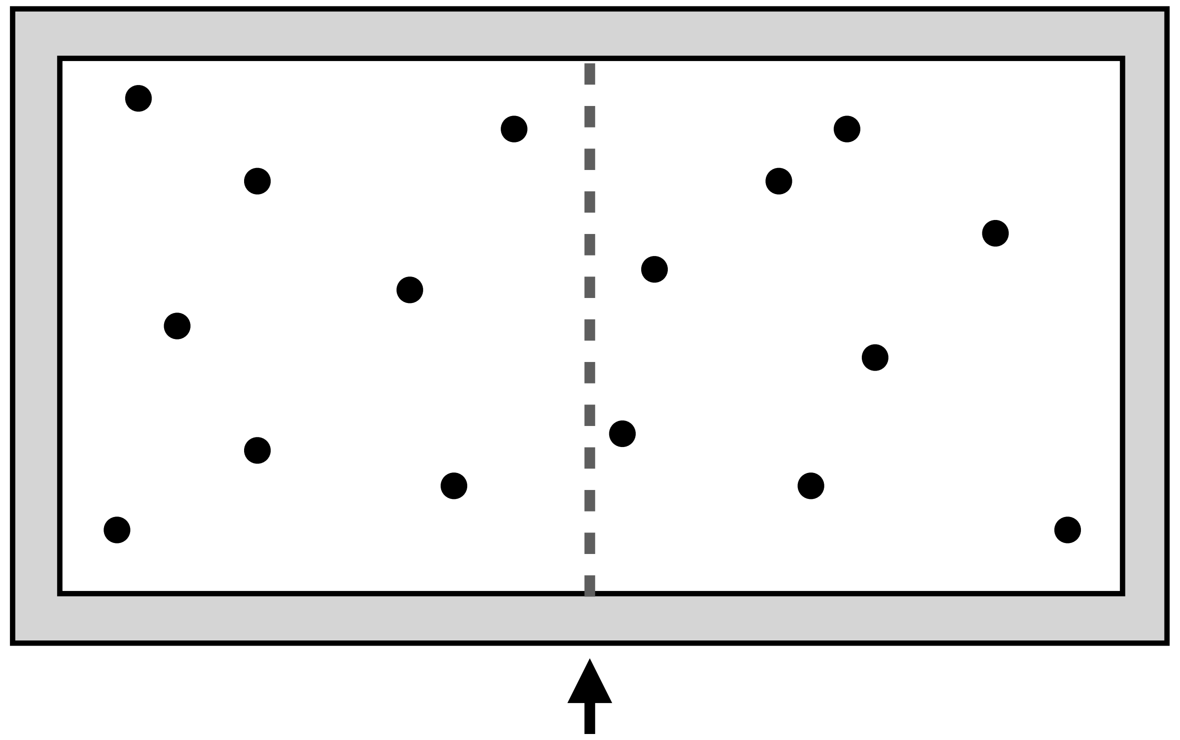
2nd postulate of statistical thermodynamics: In an isolate system, all microstates are equiprobable.

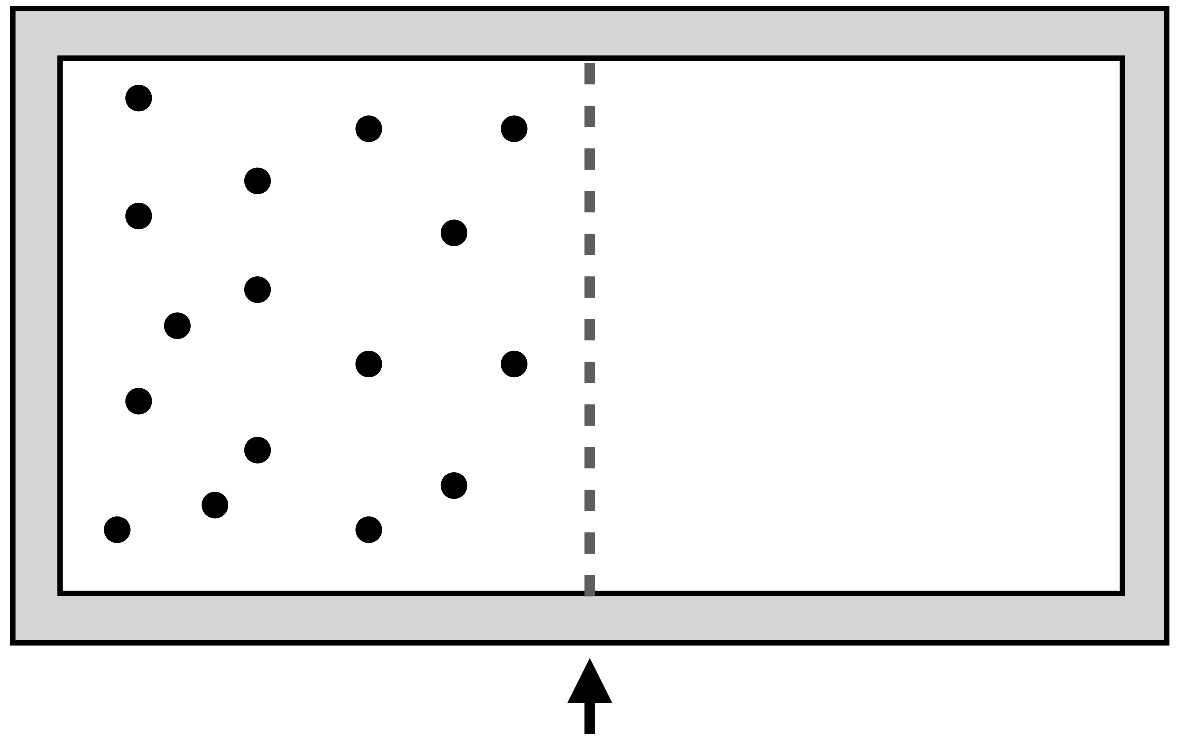
Each particle as a **probability 1/2** to be on the **left side**.

Probability that **all the particles** are **on the left**: $\dfrac{1}{2^N}$

= **probability of any other combination** of particles on the left or right. Ex. (L, R, L, L, R, ..., L)

Micro to macro (again...)





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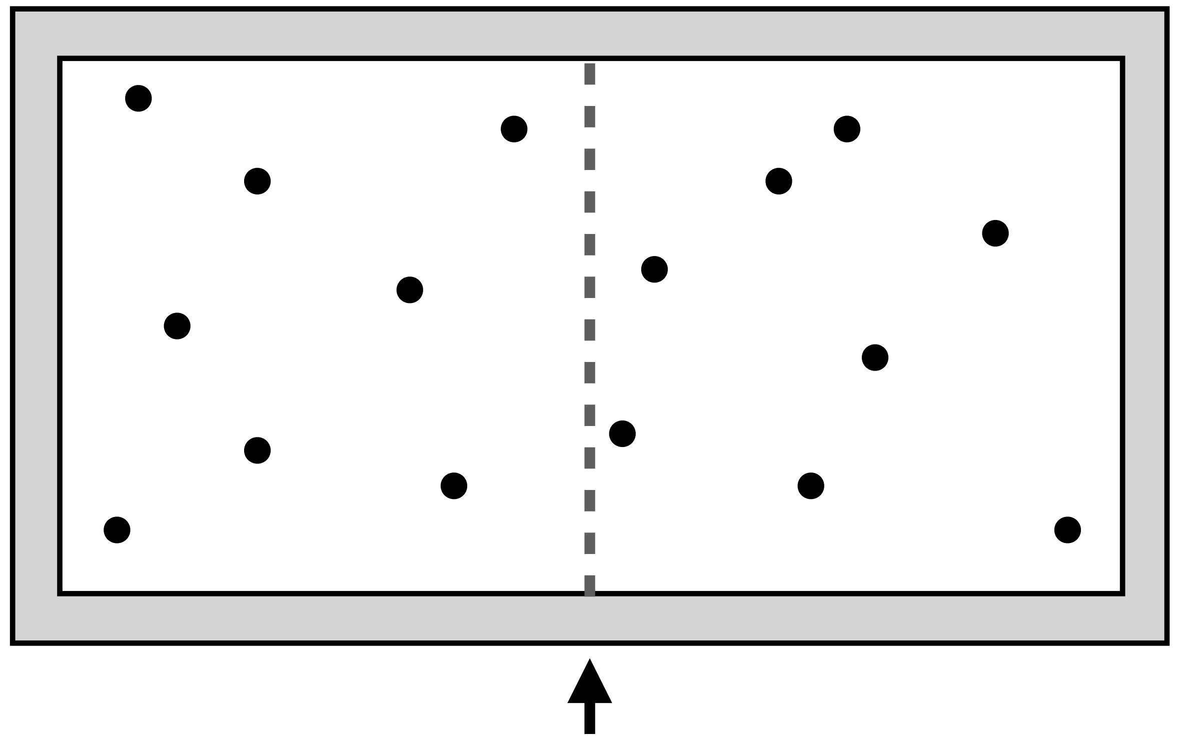
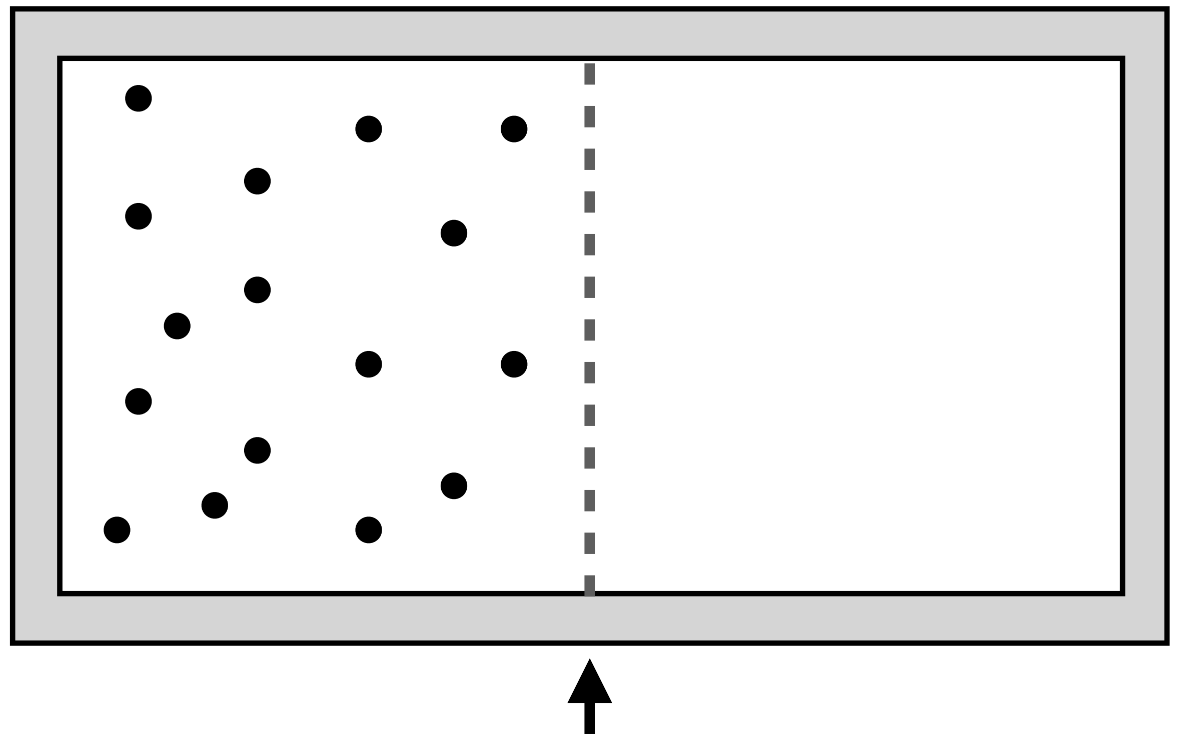
Micro to macro (again...)



Virtual wall



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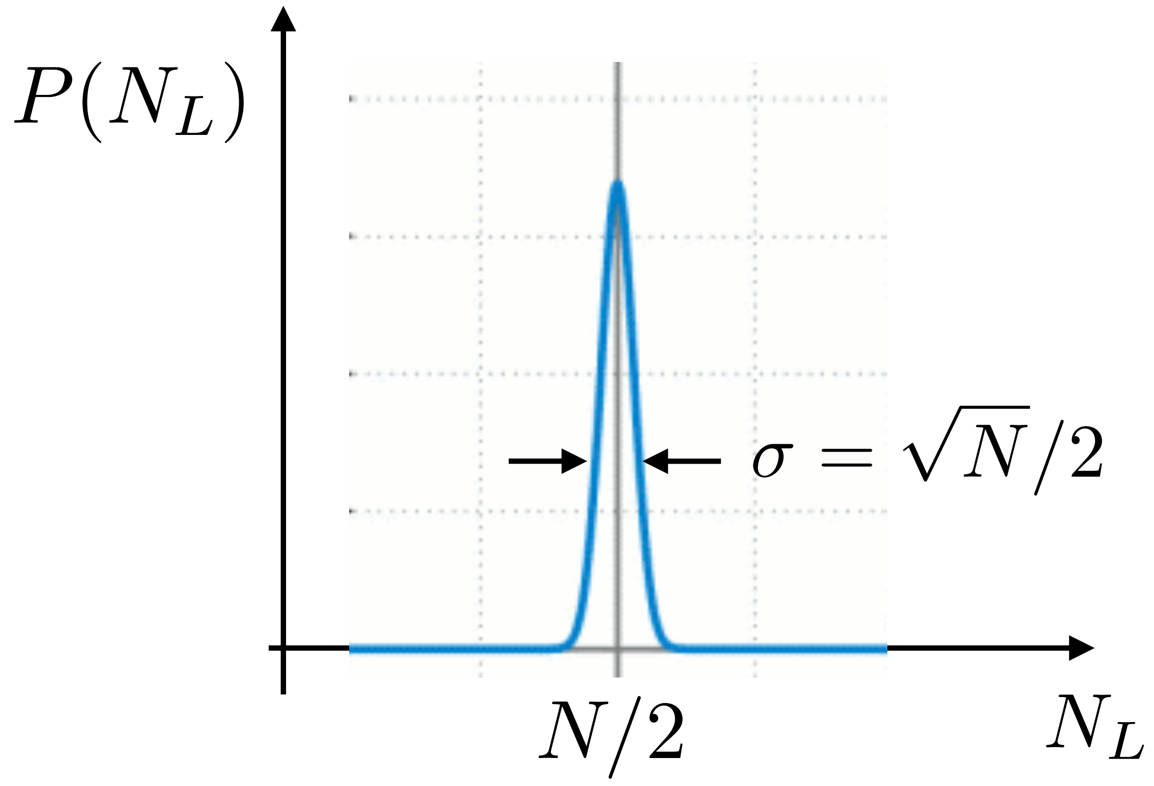
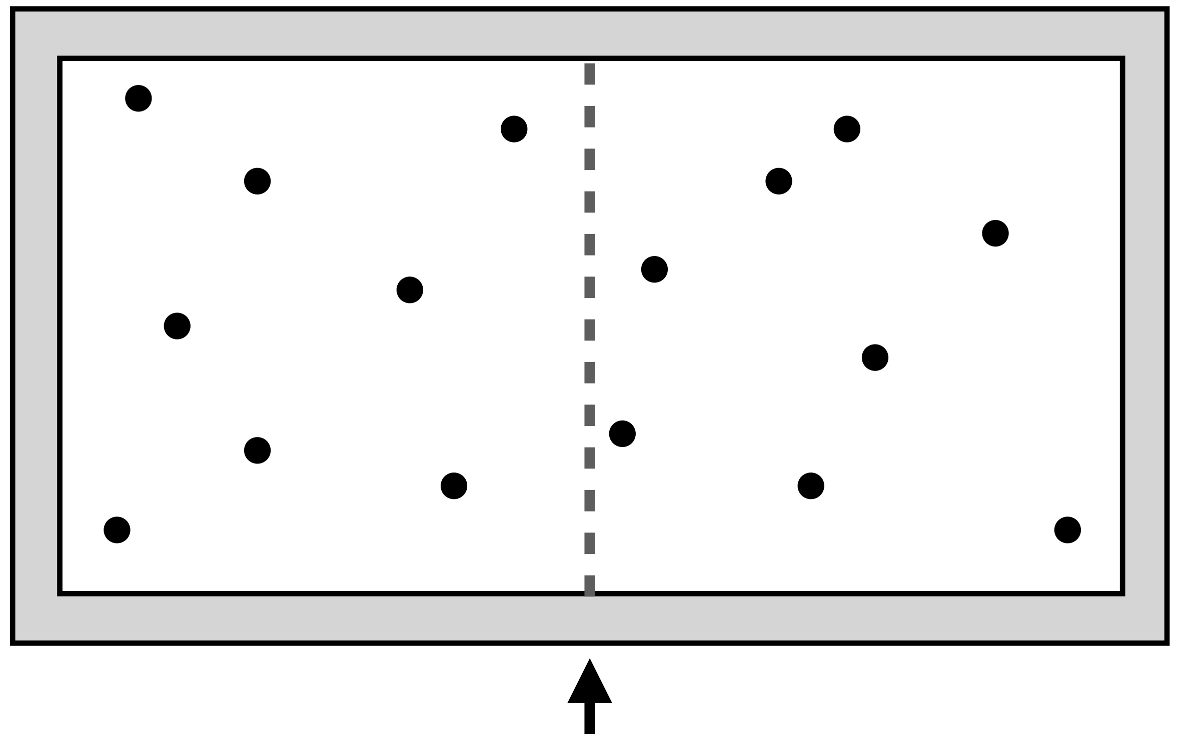


$$\frac{\sigma}{\mu} = \frac{\sqrt{N}}{N} = \frac{1}{\sqrt{N}}$$

As N becomes very large,

the fluctuation of N_L around N/2 become undetectable.

Micro to macro (again...)



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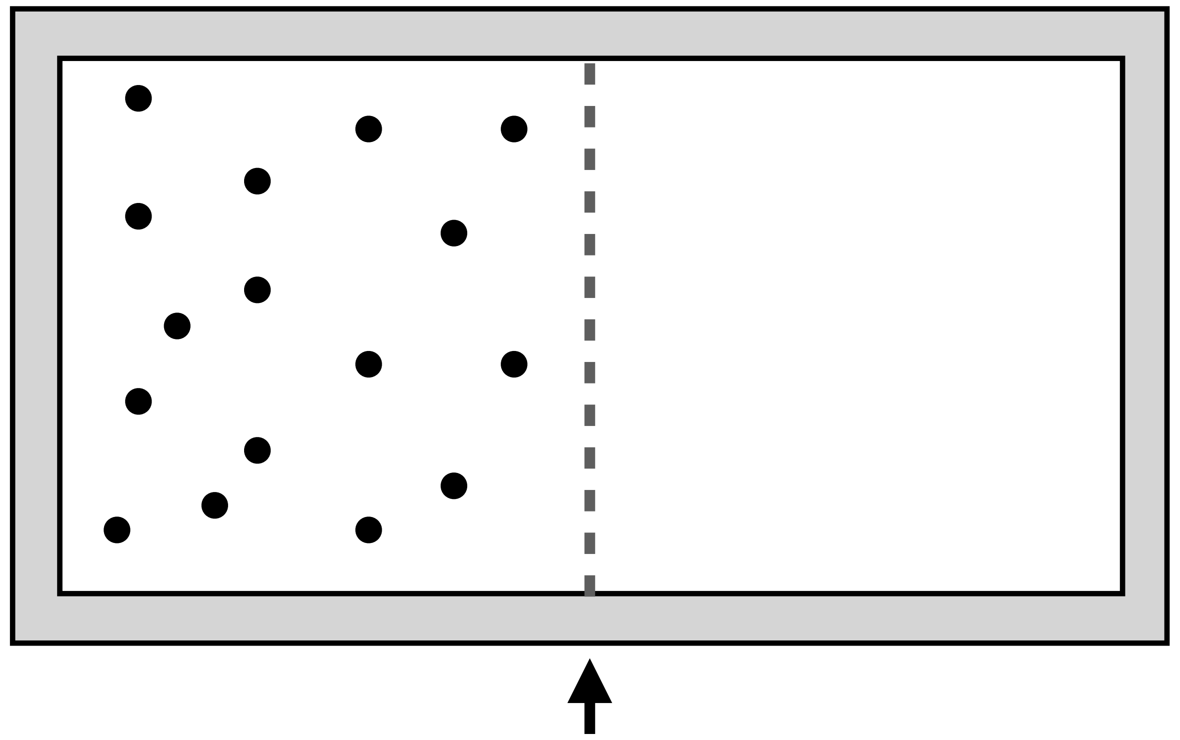

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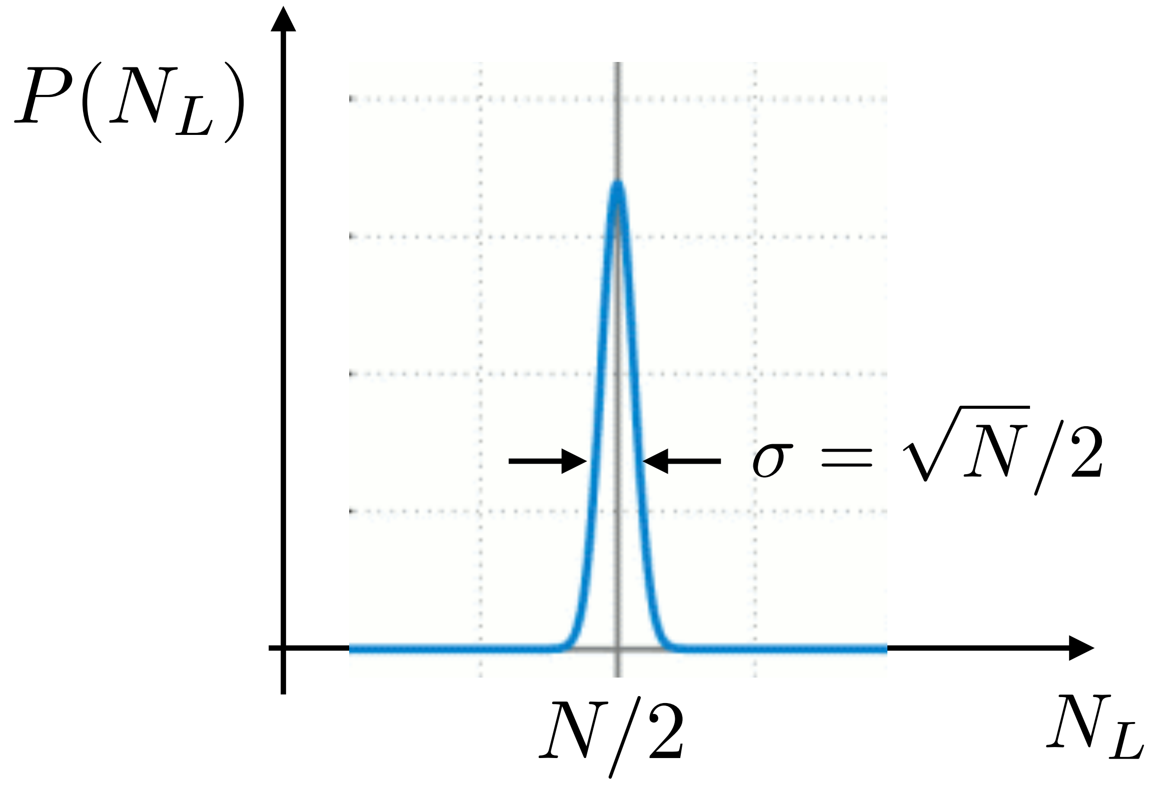
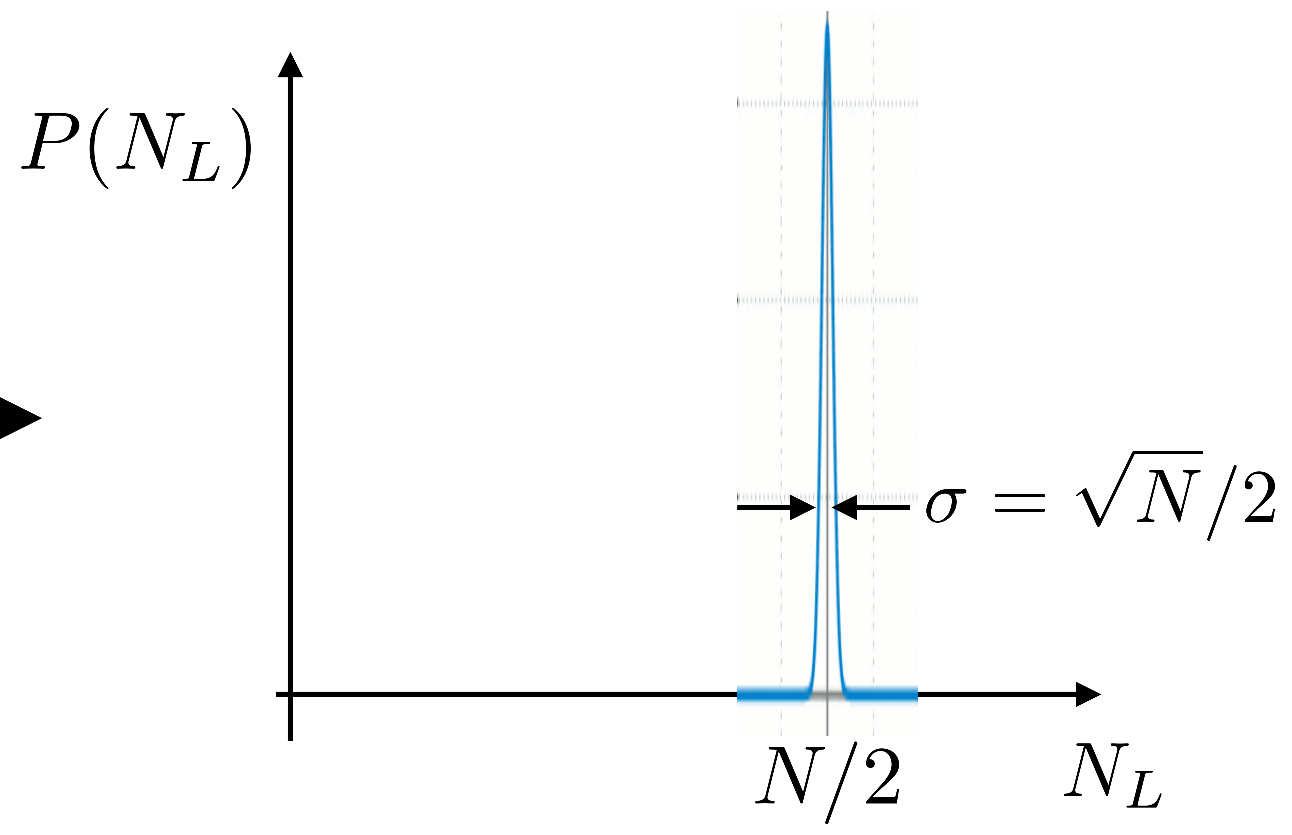


$\xrightarrow{\text{larger } N}$



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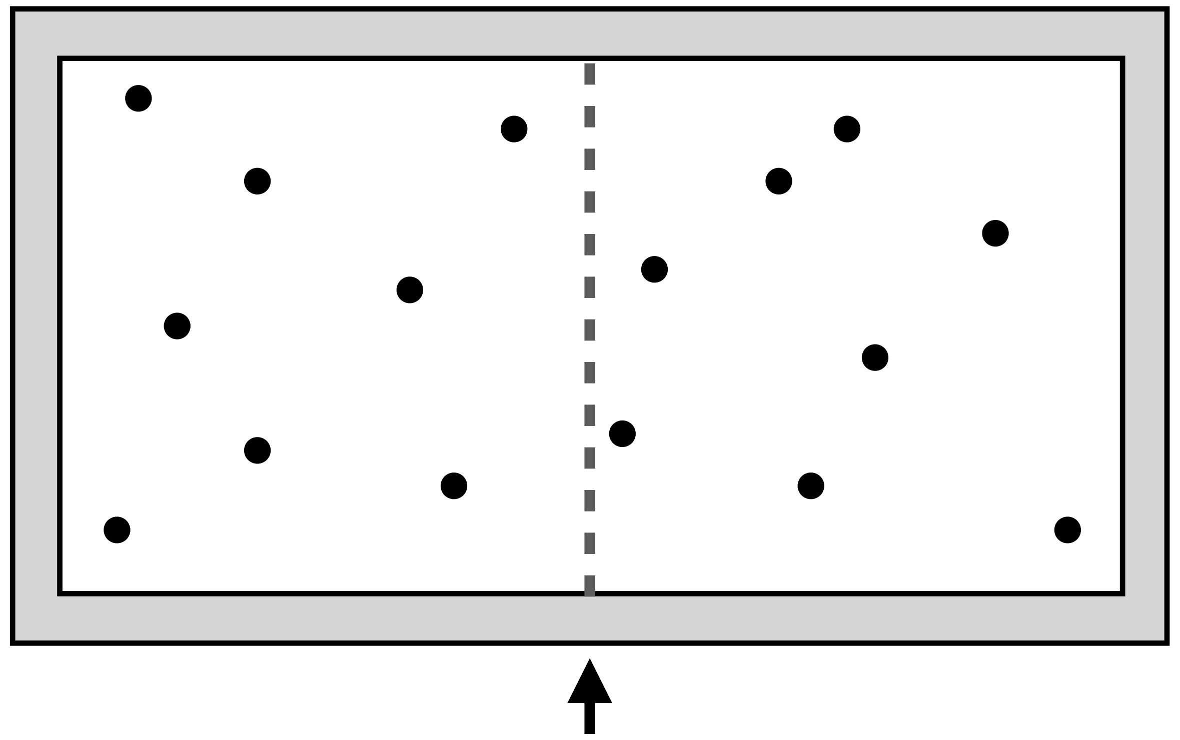

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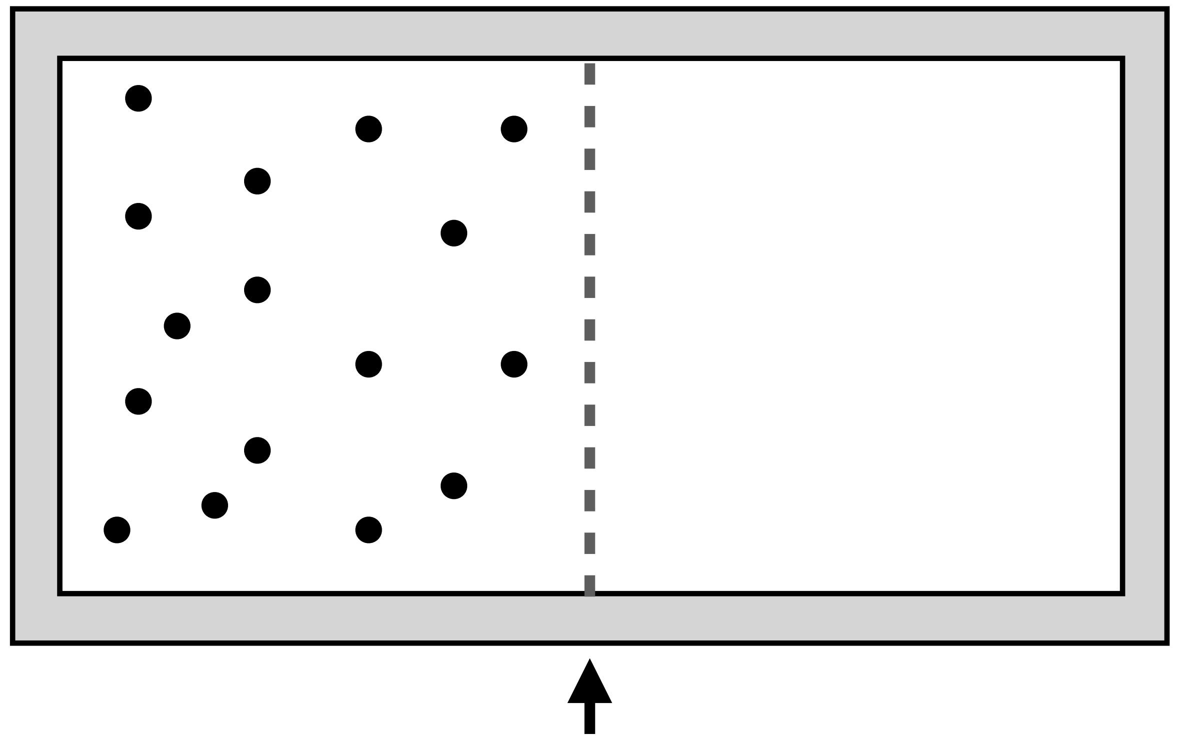

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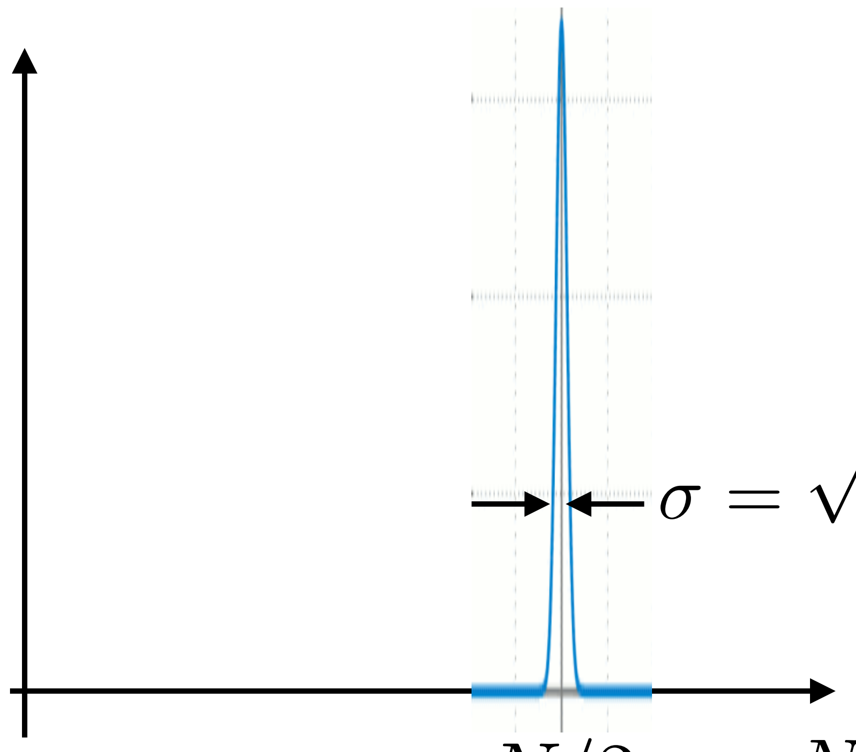
Probability that **all the particles** are **on the left**: $\dfrac{1}{2^N}$

Probability that N_L are on the left: $P(N_L) = \dfrac{1}{2^N}\dbinom{N}{N_L} \xrightarrow{N \text{ large}} \mathcal{N}\left(\mu = \dfrac{N}{2}, \sigma^2 = \dfrac{N}{4}\right)$



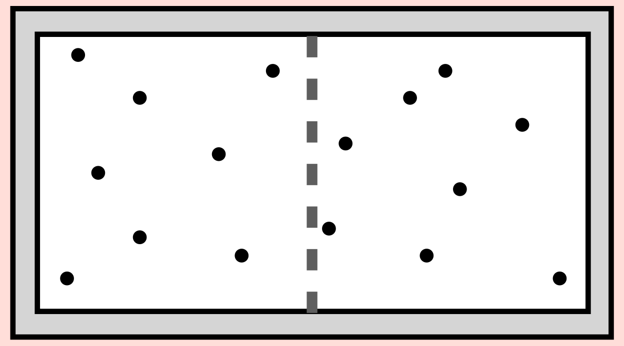
Conclusion in this case (isolated system):

Microscopic: All the microstates are equiprobable

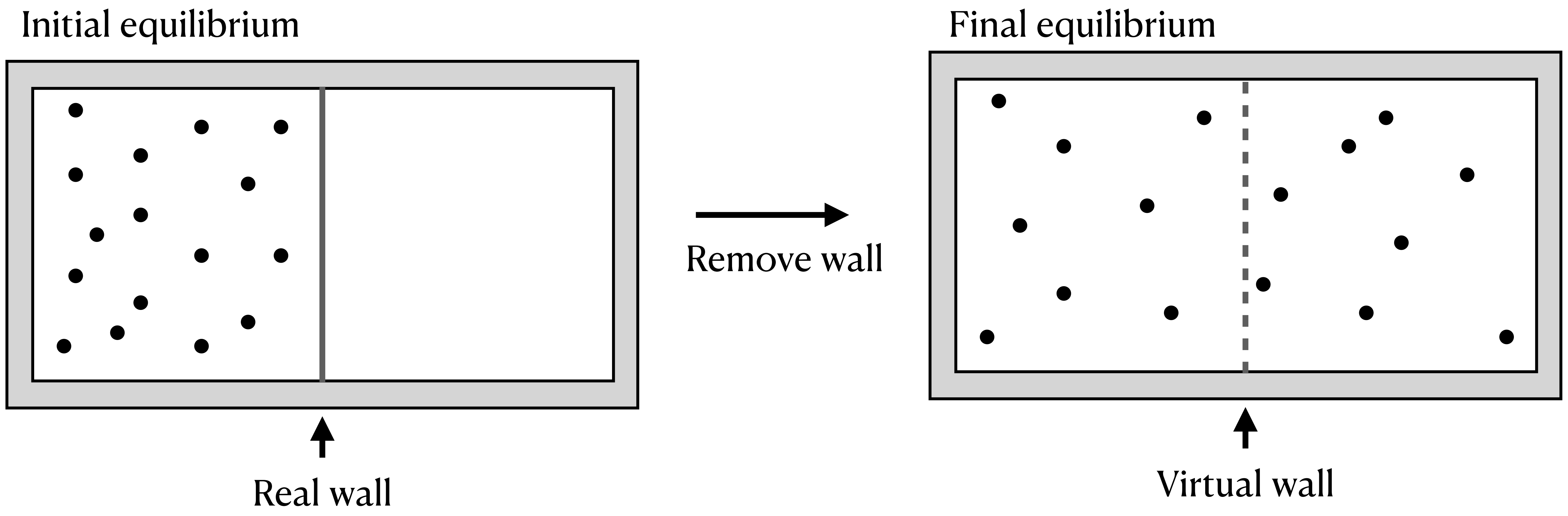
Macroscopic: As N becomes very large,

the fluctuation of N_L around N/2 become undetectable.

We mainly see:



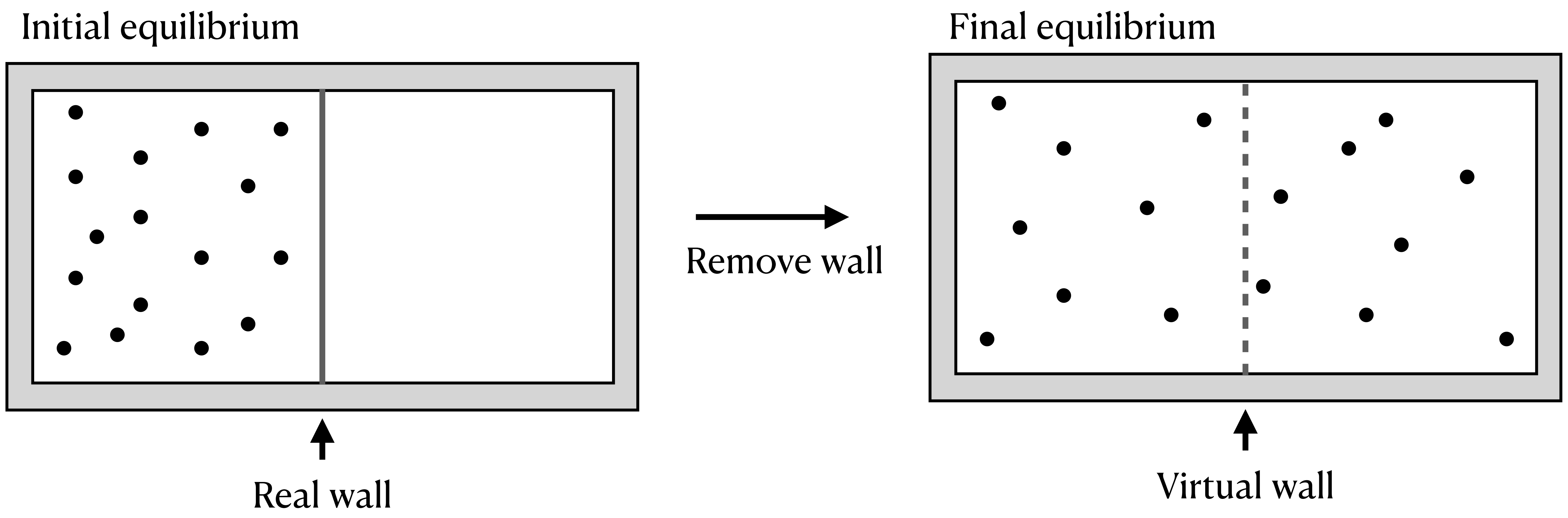
Macroscopic irreversibility



Macroscopic: If this happens, it is so fast that it is undetectable. . —>> **“Macroscopic irreversibility”**

Thermodynamics Entropy increases: $S_F > S_I$

Macroscopic irreversibility



Macroscopic: If this happens, it is so fast that it is undetectable. . —>> **"Macroscopic irreversibility"**

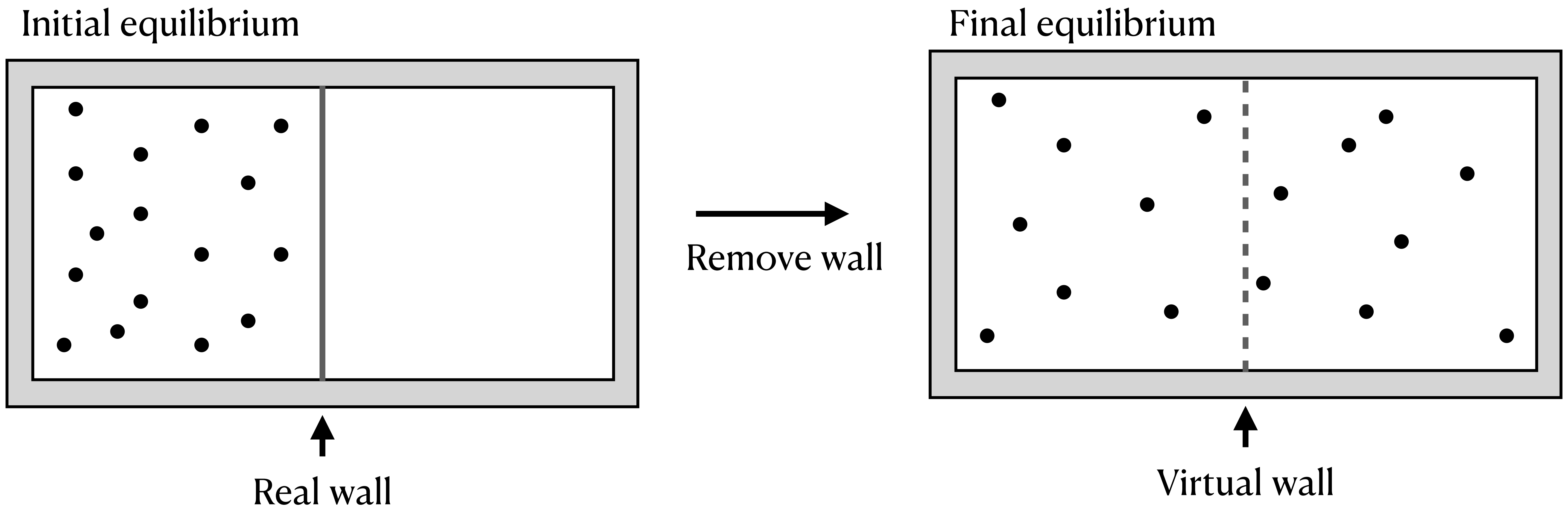
Thermodynamics Entropy increases: $S_F > S_I$

Microscopic: There is a very tiny probability that all particles come all back to the left. —>> **"Microscopic reversibility"**

Statistical definition of Entropy????

What can be at the origin of the increase of entropy at the microscopic level?

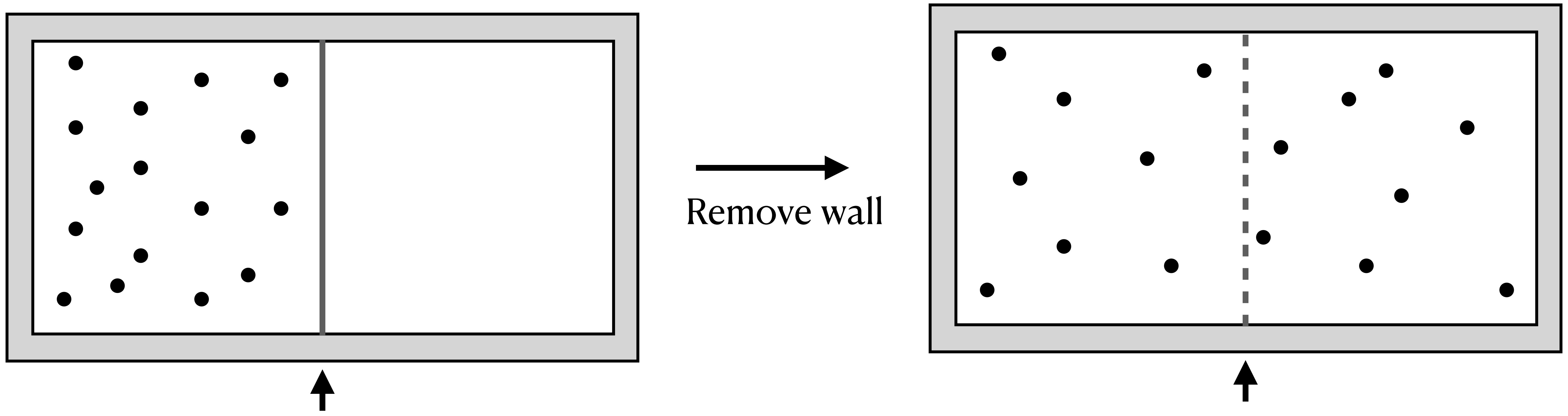
Statistical definition of Entropy



Microscopic: Big increase in volume ==> Huge increase in the number of microstates: $\Omega \propto V^N$ ==> Origin of increase in entropy?

$$S = f(\Omega)$$

Statistical definition of Entropy



Microscopic: Big increase in volume ==> Huge increase in the number of microstates: $\Omega \propto V^N$ ==> Origin of increase in entropy?

$$S = f(\Omega)$$

Boltzmann's entropy formula: $S = k \log \Omega$ for an isolated system

Statistics:

$$\Delta S = k \log\left(\frac{\Omega_F}{\Omega_I}\right) = Nk \log\left(\frac{V_F}{V_I}\right)$$

Thermodynamics:

$$\Delta S = Nk_B \log\left(\frac{V_F}{V_I}\right)$$

$$dS = \frac{P}{T}dV = Nk_B\frac{dV}{V}$$

Entropy statistics = Entropy thermodynamics

If $k = k_B = 1.38 \cdot 10^{-23}\, J.K^{-1}$

Boltzmann constant

Shannon Entropy

Shannon Entropy: $S = -k_B \sum_{\vec{s}} P(\vec{s}) \log P(\vec{s})$ where $k_B = 1.38 \cdot 10^{-23}\, J.K^{-1}$ Boltzmann constant

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- **minimal** when **one microstate has probability 1** and all the others have probability **0**

  $S = 0$ **no incertainty at all** (Observing that state doesn't provide any information about the system)

- **maximal** when **all the microstates have the same probability**: $P(\vec{s}) = \frac{1}{\Omega}$ where Ω = total number of microstates

  $S = k_B \log \Omega$ **maximum incertainty**

- **Other distributions** $P(\vec{s})$ give entropy between these two values.

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For an isolated system: All the microstates have the same probability: $P(\vec{s}) = \frac{1}{\Omega}$ where Ω = total number of microstates

Boltzmann's entropy formula: $S = k_B \log \Omega$ Maximal entropy!

Part I.3

Boltzmann distribution

What is $P(\vec{s})$? For system with T and V fixed

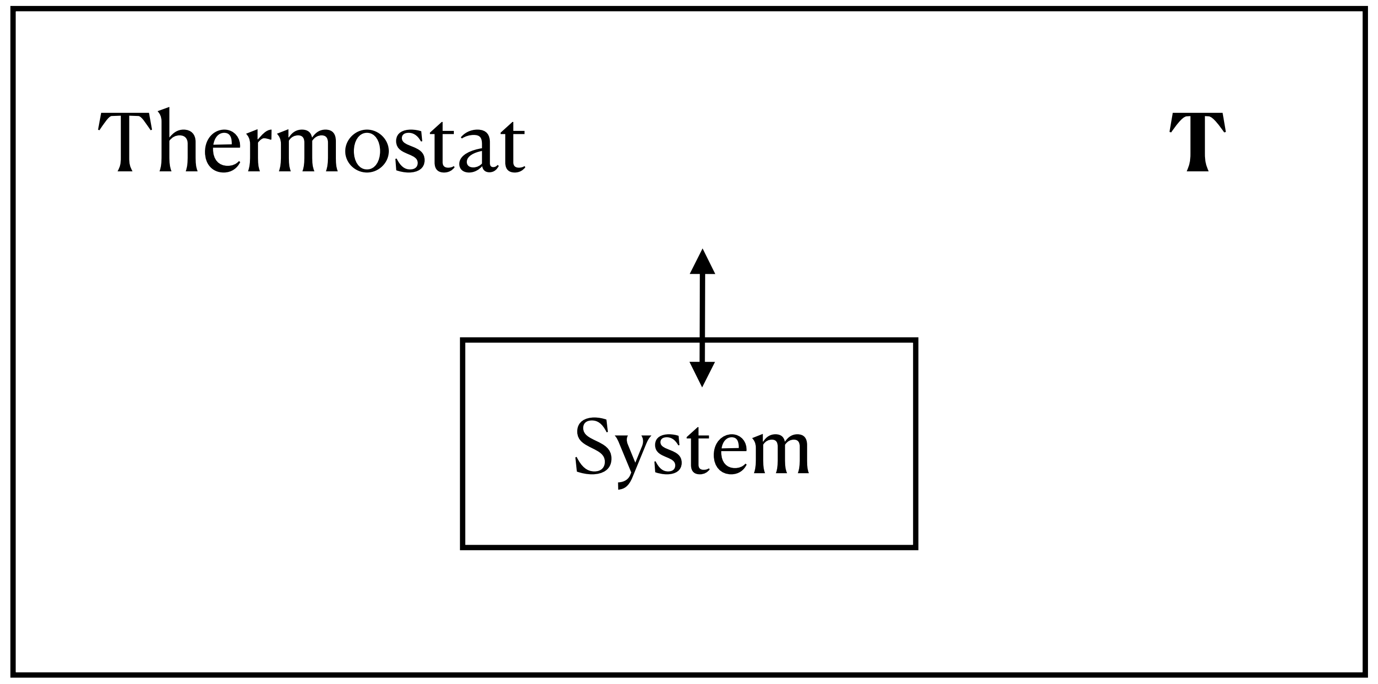
Boltzmann Distribution

Thermostat: We will often consider systems in contact with a thermostat at fixed temperature **T**.

The system exchanges energy with the thermostat.

The thermostat is a constant source of energy,

which allows to **control** the temperature, or **“noise” level,** of the system.



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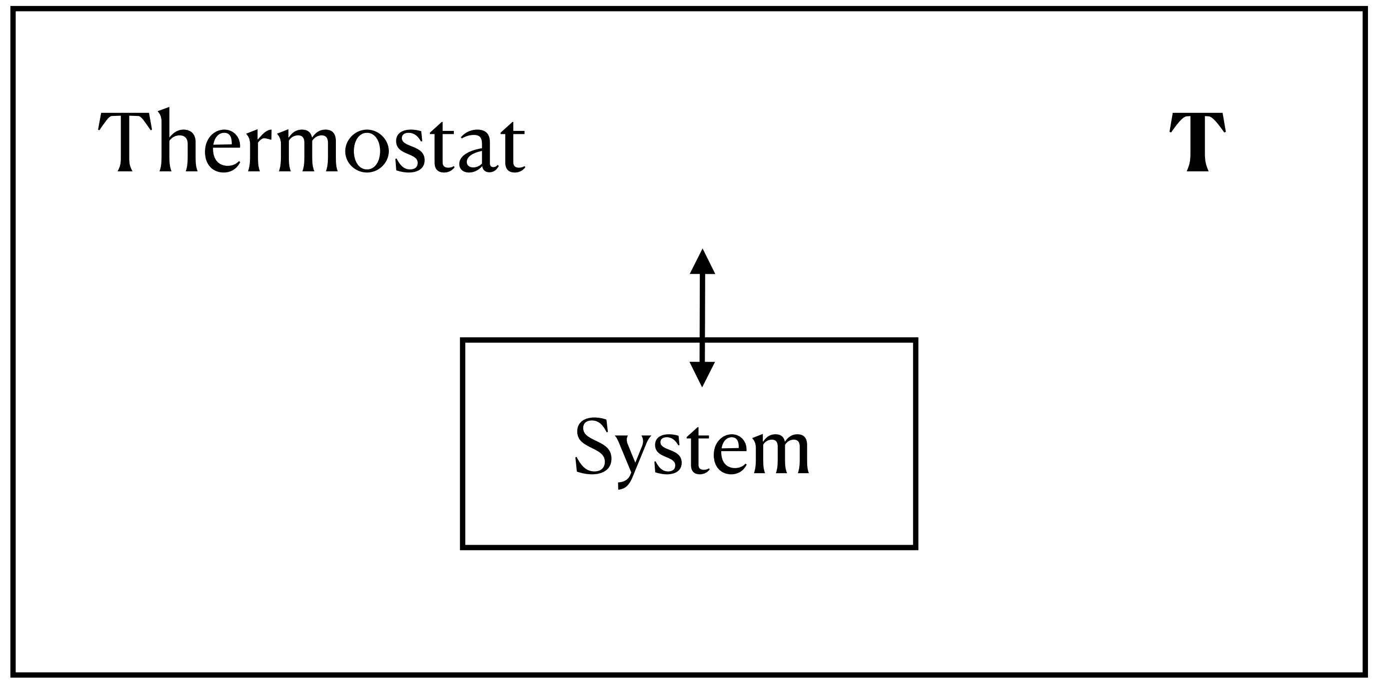


In this case, the **state probabilities** $P(\vec{s})$ are given by

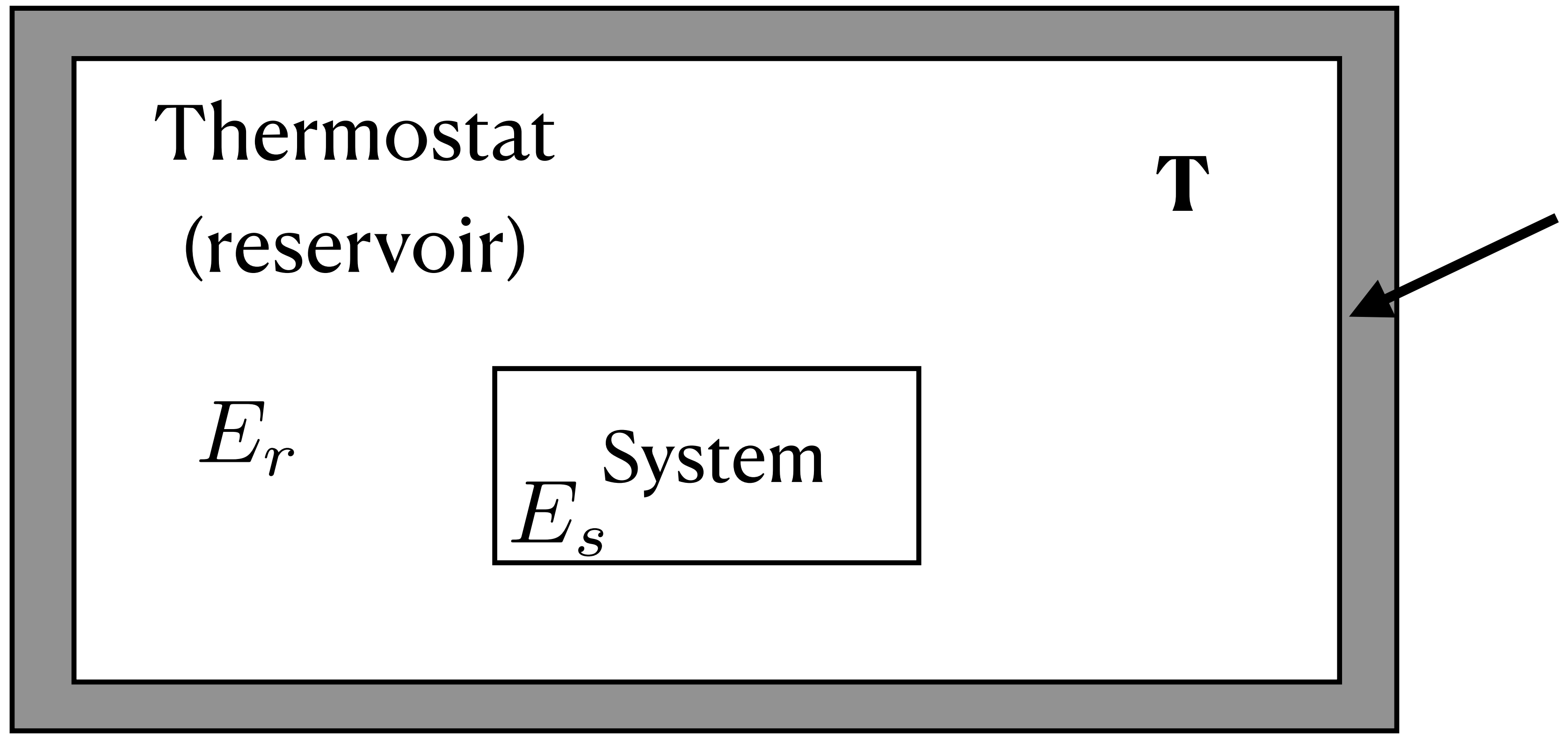
the **Boltzmann distribution**:
$$P(\vec{s}) = \frac{\mathrm{e}^{-\beta E(\vec{s})}}{Z}$$

where $E(\vec{s})$ = energy of the system in the microstate $\vec{s}$

$\beta = \frac{1}{k_b T}$ = inverse temperature. Control **noise level** in the system.

Z = normalisation factor

Why Boltzmann Distribution?



Isolation: $E_{tot} = E_r + E_s = \text{constant}$

Reservoir: Very big compared to the system: $E_r \gg E_s$

Competition between order and disorder

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

where $E(\vec{s})$ = energy of the system in the microstate $\vec{s}$

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Comments:

— States with the **same energy** have the **same probability** to occur;

— System has a **larger probability** to be in states with **lower energy**;

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- **Limit** $T \to 0$ **:** $\mathrm{e}^{-\beta E(\vec{s})}$ is governed by the minimal $E(\vec{s})$

  Order: the system minimises its energy

The system takes the microstates with minimal energy.
All the other states are infinitely less probables.

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  The system takes the microstates with minimal energy. All the other states are infinitely less probables.

- **Limit** $T \to +\infty$ **:** $\mathrm{e}^{-\beta E(\vec{s})} \to 1$ for all the states

  "Infinite" disorder: no interaction is able to order the system

  All the states have the same probability independently of their energy.

Competition between order and disorder

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

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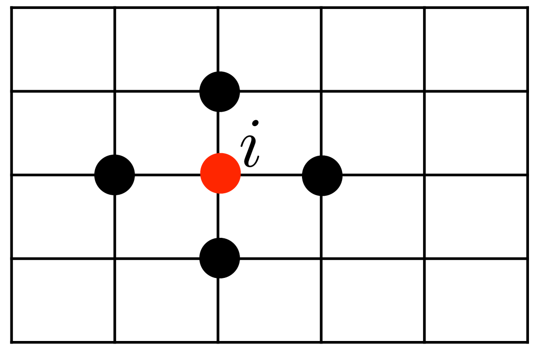
Ex. Ising model: $$E(\vec{s}) = -J \sum_{<i,j>} s_i \, s_j$$



● = neighbours j of i

Minimal energy?

Competition between order and disorder

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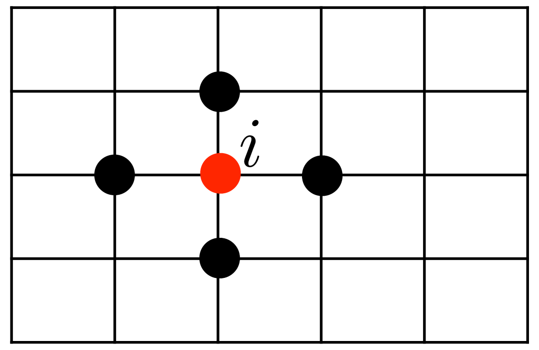

● = neighbours j of i

Minimal energy: $E_{\text{min}} = -J\, N_{\text{pairs}}$ Reached when all the spins are aligned: either **ALL UP** or **ALL DOWN**

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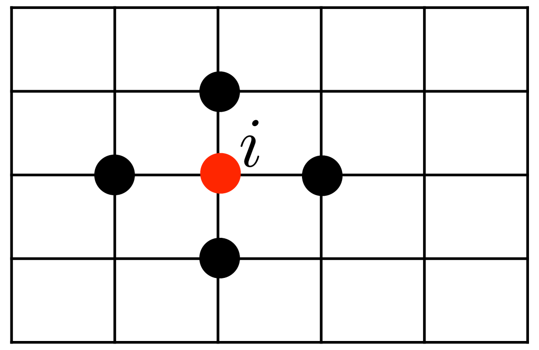

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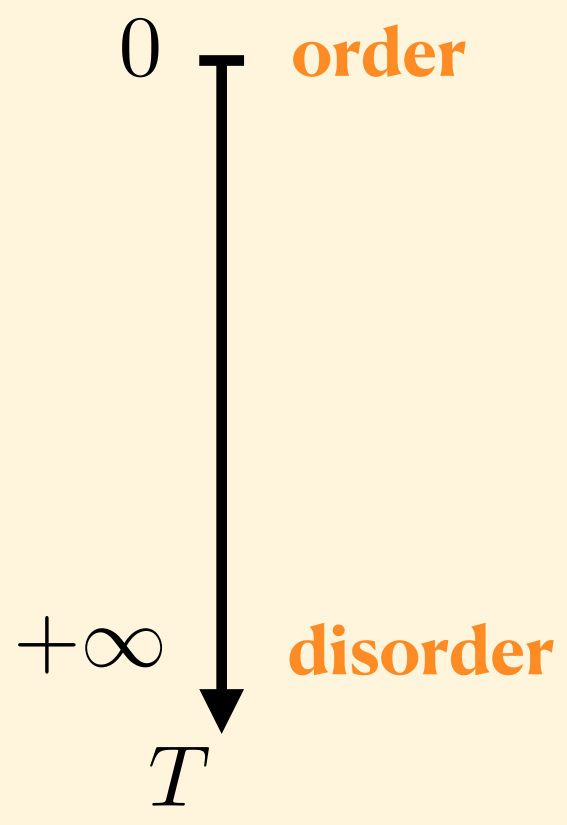
Minimal energy: $E_{\text{min}} = -J\, N_{\text{pairs}}$ Reached when all the spins are aligned: either **ALL UP** or **ALL DOWN**

Competition: $$\frac{E(\vec{s})}{k_B\, T}$$

$E(\vec{s}) = -J \sum_{<i,j>} s_i\, s_j$ **Energy of interaction** between the spins: **tend to align** them —> Wins at small temperatures

$k_B\, T$ **Thermal noise** that has a **disordering effect** —> Wins at large temperatures / noise



Part I.4

Statistical description of the Free energy

$$F = U - TS \quad = ?$$

Free energy

Thermodynamics: $F = U - TS$ Potential thermodynamics for system with V and T constant

Statistical description of F ?

Free energy

Thermodynamics: $F = U - TS$ Potential thermodynamics for system with V and T constant

1) **Gibb's postulate:** $$U = \langle E \rangle = \sum_{\vec{s}} E(\vec{s})\, P(\vec{s})$$

2) **Shannon entropy:** $$S = -k_B \sum_{\vec{s}} P(\vec{s}) \log P(\vec{s})$$

3) **Boltzmann distribution:** $$\log P(\vec{s}) = -\beta E(\vec{s}) - \log Z$$

Free energy

Thermodynamics: $F = U - TS$ Potential thermodynamics for system with V and T constant

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3) **Boltzmann distribution:** $$\log P(\vec{s}) = -\beta E(\vec{s}) - \log Z$$

Statistical description: $F = -k_B T \log Z$ All the properties of the system are encoded in Z

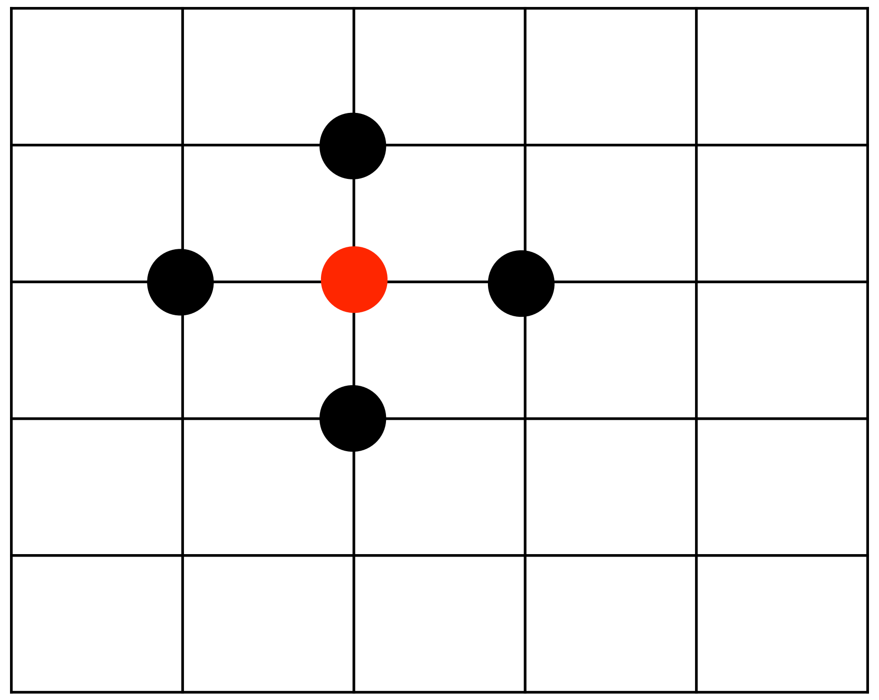
One can obtain all the thermodynamic quantities of interest from Z:

Ex. Internal energy: $$U = \langle E \rangle = -\frac{\partial \log Z}{\partial \beta}$$

Back to the Ising model

Last week: Ising model

Ex. In 2D



Microscopic description:

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

Scalar spin $s_i = \pm 1$

Sum over closest neighbours only

Microscopic description

From Microscopic to macroscopic description:

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

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

Contains all the information about the system!

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

Thermodynamic potential — **Macroscopic description**

Partition function — **Statistical (microscopic) description**

OK!

Ising model: Quantities of interest

More general version of the Ising model

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

Coupling parameter

"External field"

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

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

Contain all the information about the system

Internal energy: $$U = \langle E \rangle = -\frac{\partial \log Z}{\partial \beta} \quad = \beta \frac{\partial F}{\partial \beta}$$

Entropy: $$S = -\left(\frac{\partial F}{\partial T}\right)_H$$

Average magnetisation: $$\langle M \rangle = \frac{1}{\beta}\left(\frac{\partial \log Z}{\partial H}\right)_T = -\left(\frac{\partial F}{\partial H}\right)_T$$

Susceptibility: $$\chi = \left(\frac{\partial M}{\partial H}\right)_T = -\left(\frac{\partial^2 F}{\partial H^2}\right)_T$$

Coming up

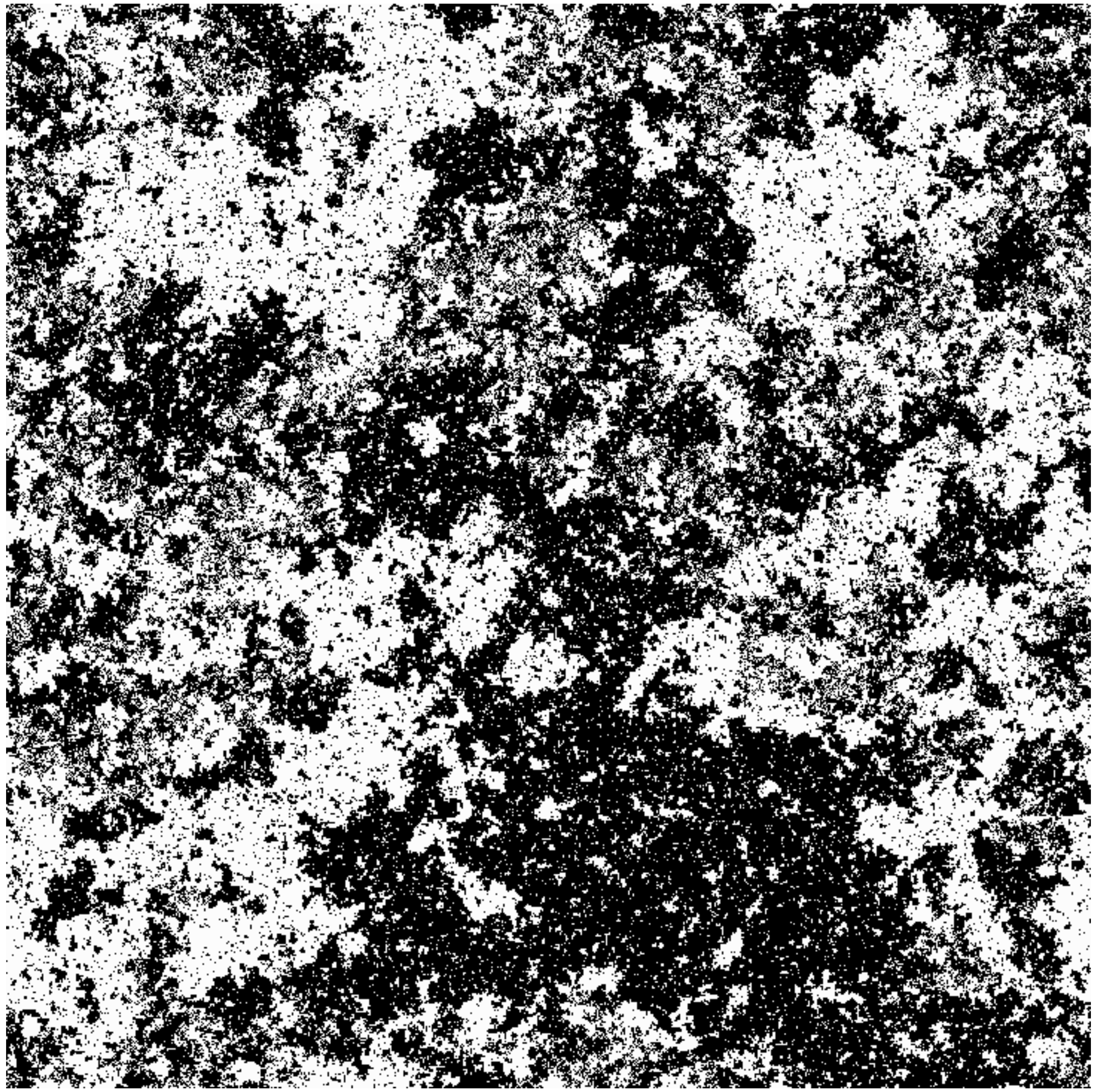
Coming tutorial: Metropolis algorithm:
How to sample stationary states from the Ising model?

Homework: The Inverse problem:

Inferring the microscopic interactions based on macroscopic observables computed from data/experimental observations.

Coming lecture:

Is there a phase transition in the Ising model?
Is this a critical phase transition?



2D Ising model
at T ~ 2.27