

Numerical methods for strongly correlated systems

Thereza Paiva



SCHOOL ON RECENT ADVANCES IN STRONGLY CORRELATED QUANTUM MATERIALS

October 5-9, 2026 ICTP-SAIFR

Summary

- 1 – Classical Monte Carlo**
- 2 – Quantum Monte Carlo Method**
- 3 – Measurements in QMC – I**
- 4 – Measurements in QMC – II**
- 5 – The Sign problem**

Before we start

**My main goal with this set of classes is to
be understood**

**My main goal with this set of classes is to
be understood**

Stop me at any time

Ask questions

Summary

1 – Classical Monte Carlo

2 – Quantum Monte Carlo

3 – Measurements in QMC – I

4 – Measurements in QMC – II

5 – The Sign problem

Summary of the first class

Why do we need numerical methods?

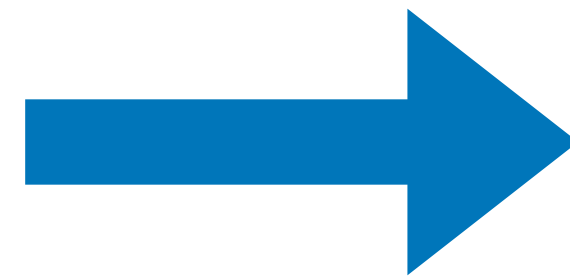
The Ising Model

Monte Carlo Method

Metropolis Algorithm

Monte Carlo time

Boundary conditions, size effects



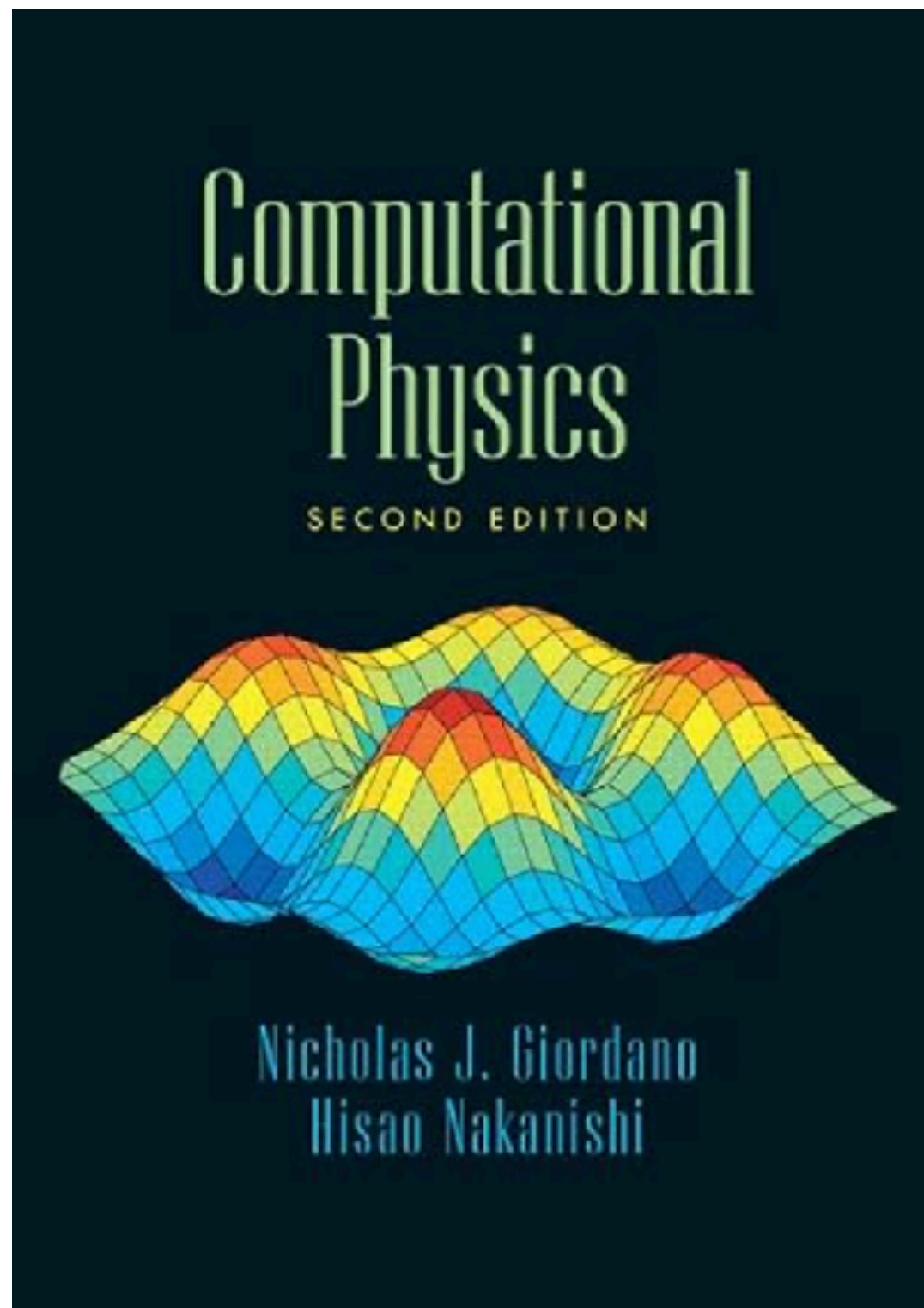
Importance sampling

Markovian processes

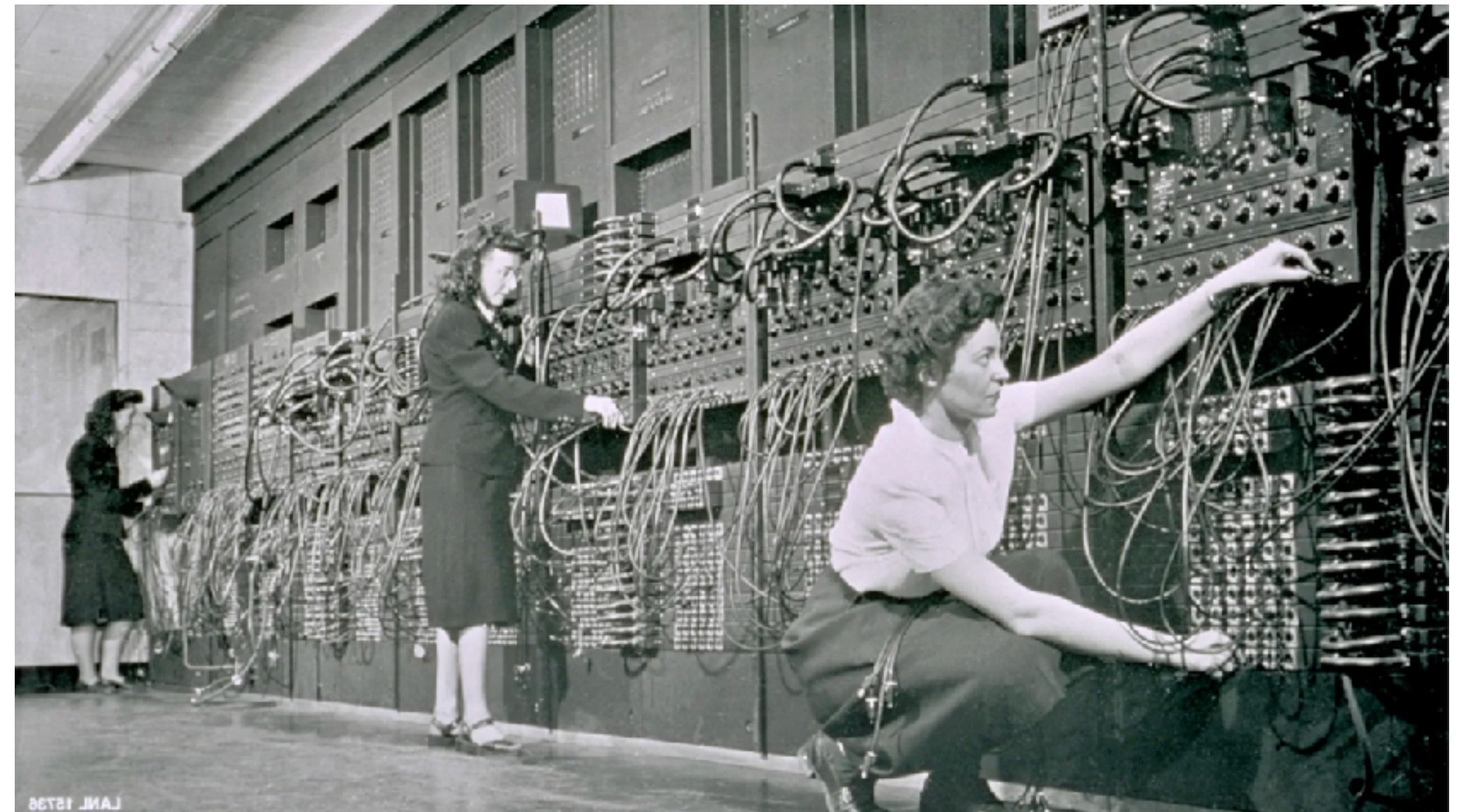
Ergodicity

Detailed balance

Suggested bibliography



**Why do we need numerical
methods?**



Getty images

Solve a quantum mechanics problem

$$H |\psi\rangle = E |\psi\rangle$$



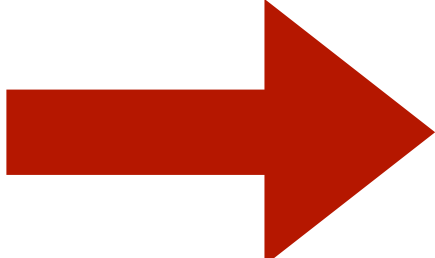
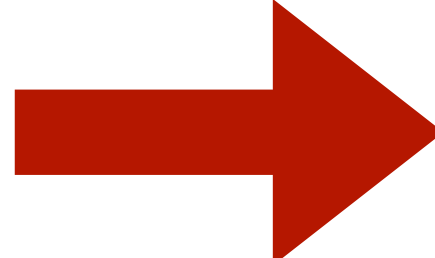
Solve a quantum mechanics problem

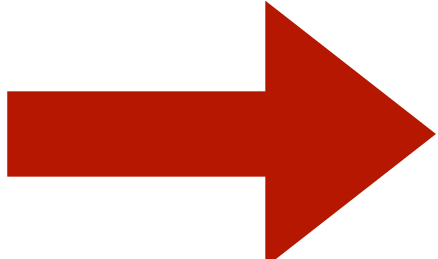
$$H|\psi\rangle = E|\psi\rangle$$



DONE

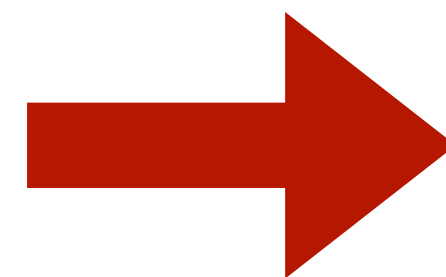
NOT SO EASY...

Write H  Diagonalize H  Find eigenvalues and eigenvectors

H  $N_M \times N_M$ Matrix

$N_M?$

Strongly interacting
systems



~~Independent electron
approximation~~

Number of states N_M

Depends on the size of the system N sites

Depends on the model

Heisenberg model $|\uparrow\rangle |\downarrow\rangle$ $N_M = 2^N$

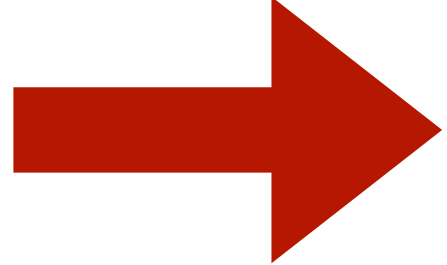
t-J model $|\uparrow\rangle |\downarrow\rangle |0\rangle$ $N_M = 3^N$

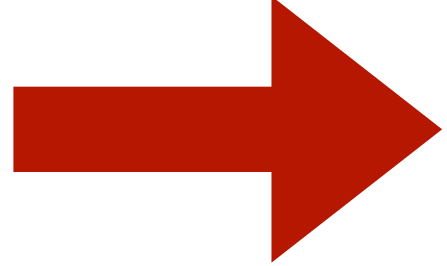
Hubbard model $|\uparrow\rangle |\downarrow\rangle |0\rangle |\uparrow\downarrow\rangle$ $N_M = 4^N$

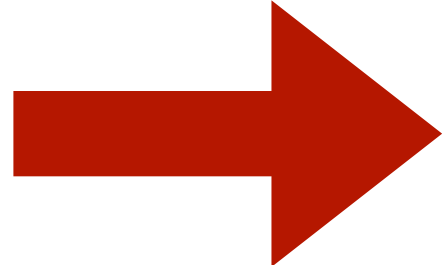
N_M grows fast with N

COMPLEXITY

Relation between T (computational time) and N (degrees of freedom)

$T \propto \mathcal{O}(N)$  Better: linear

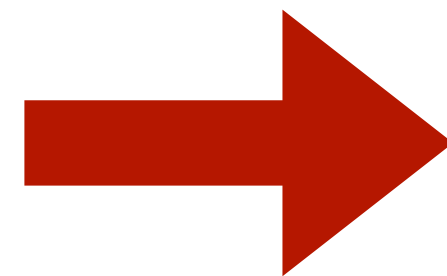
$T \propto \mathcal{O}(N^3)$  Matrix diagonalization and matrix inversion: quantum mechanics

$T \propto \mathcal{O}(e^N)$  "Naive methods" such as direct integration: scattering

COMPLEXITY

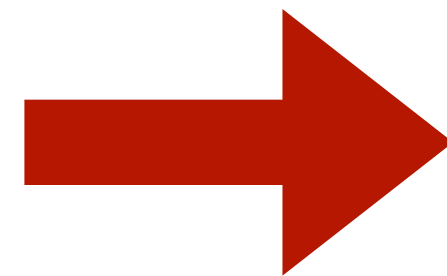
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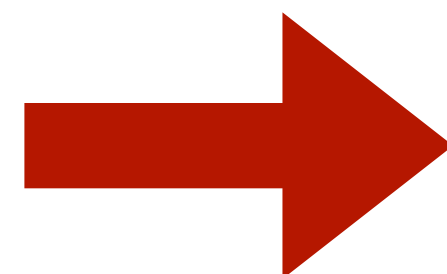
Better: linear

$$T \propto \mathcal{O}(N^3)$$



Matrix diagonalization and matrix inversion: quantum mechanics

$$T \propto \mathcal{O}(e^N)$$



"Naive methods" such as direct integration: scattering

Moore's Law

By Max Roser, Hannah Ritchie

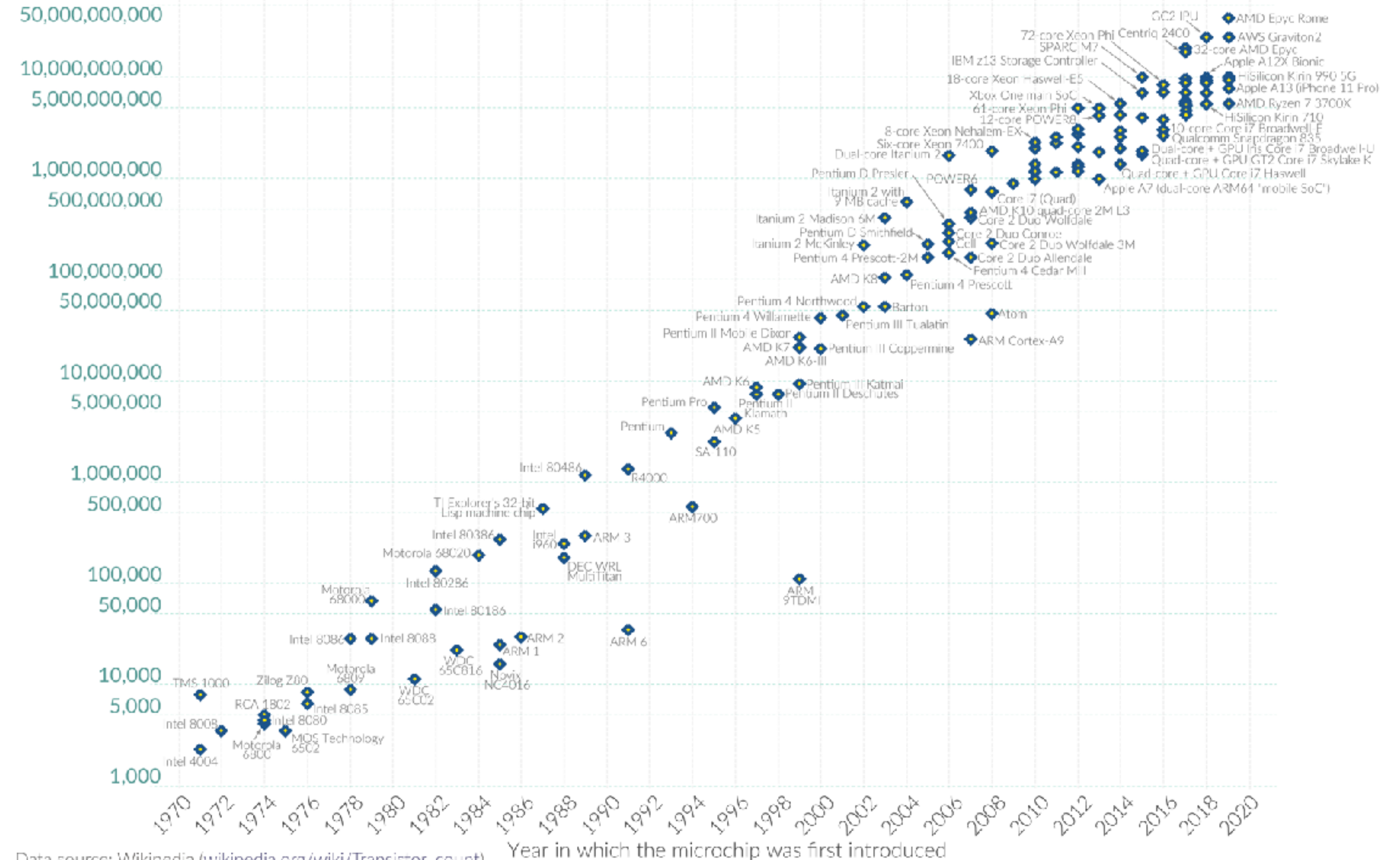
ourworldindata.org/uploads/2020/11/Transistor-Count-over-time.png, CC BY 4.0

Moore's Law: The number of transistors on microchips doubles every two years

Moore's law describes the empirical regularity that the number of transistors on integrated circuits doubles approximately every two years. This advancement is important for other aspects of technological progress in computing – such as processing speed or the price of computers.

Our World
in Data

Transistor count

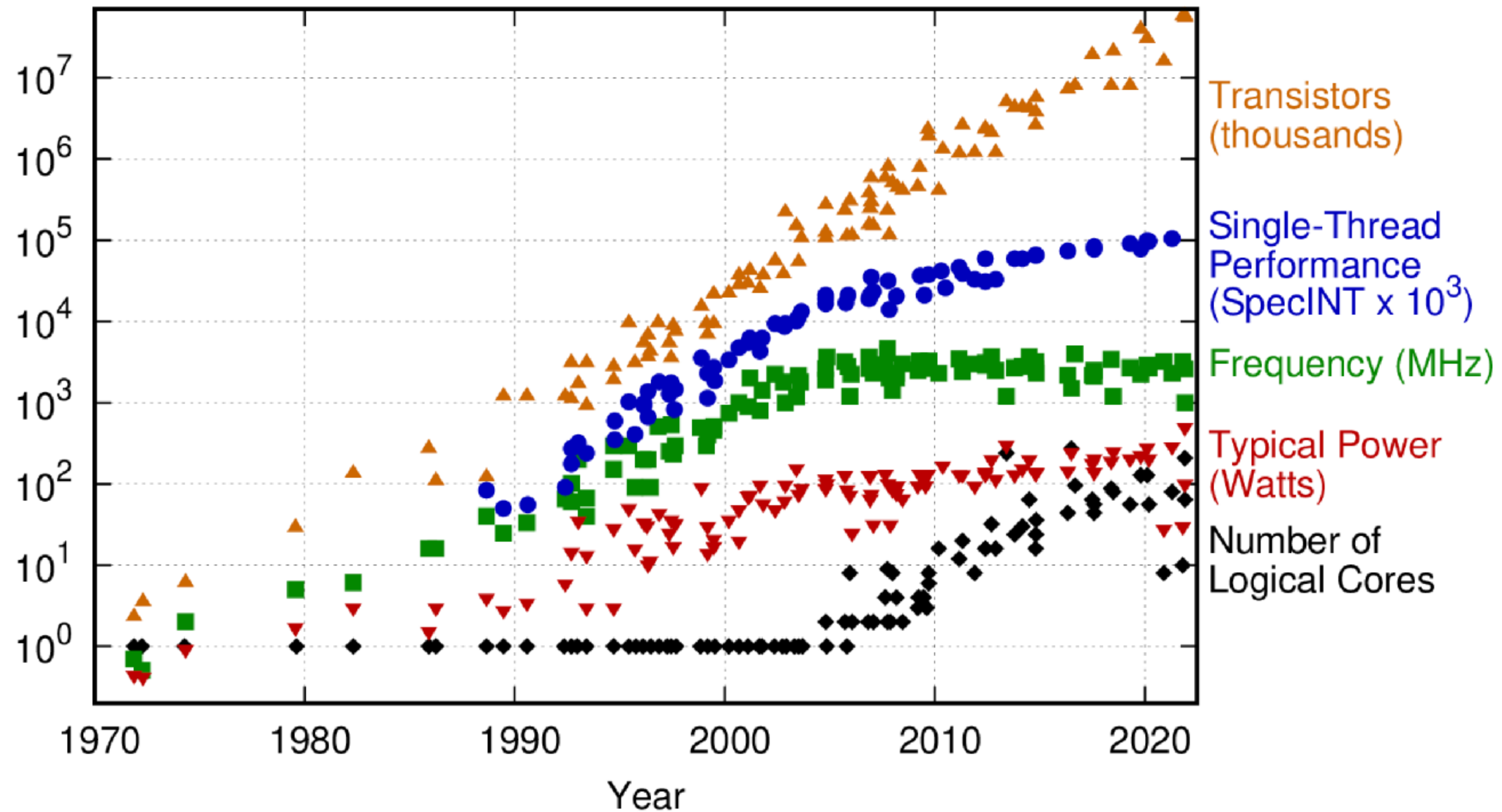


Data source: Wikipedia (wikipedia.org/wiki/Transistor_count)

OurWorldinData.org – Research and data to make progress against the world's largest problems.

Licensed under CC-BY by the authors Hannah Ritchie and Max Roser.

50 years of Microprocessor trend data



Original data up to the year 2010 collected and plotted by M. Horowitz, F. Labonte, O. Shacham, K. Olukotun, L. Hammond, and C. Batten
New plot and data collected for 2010-2021 by K. Rupp

But brute force diagonalization can only be applied to small system sizes

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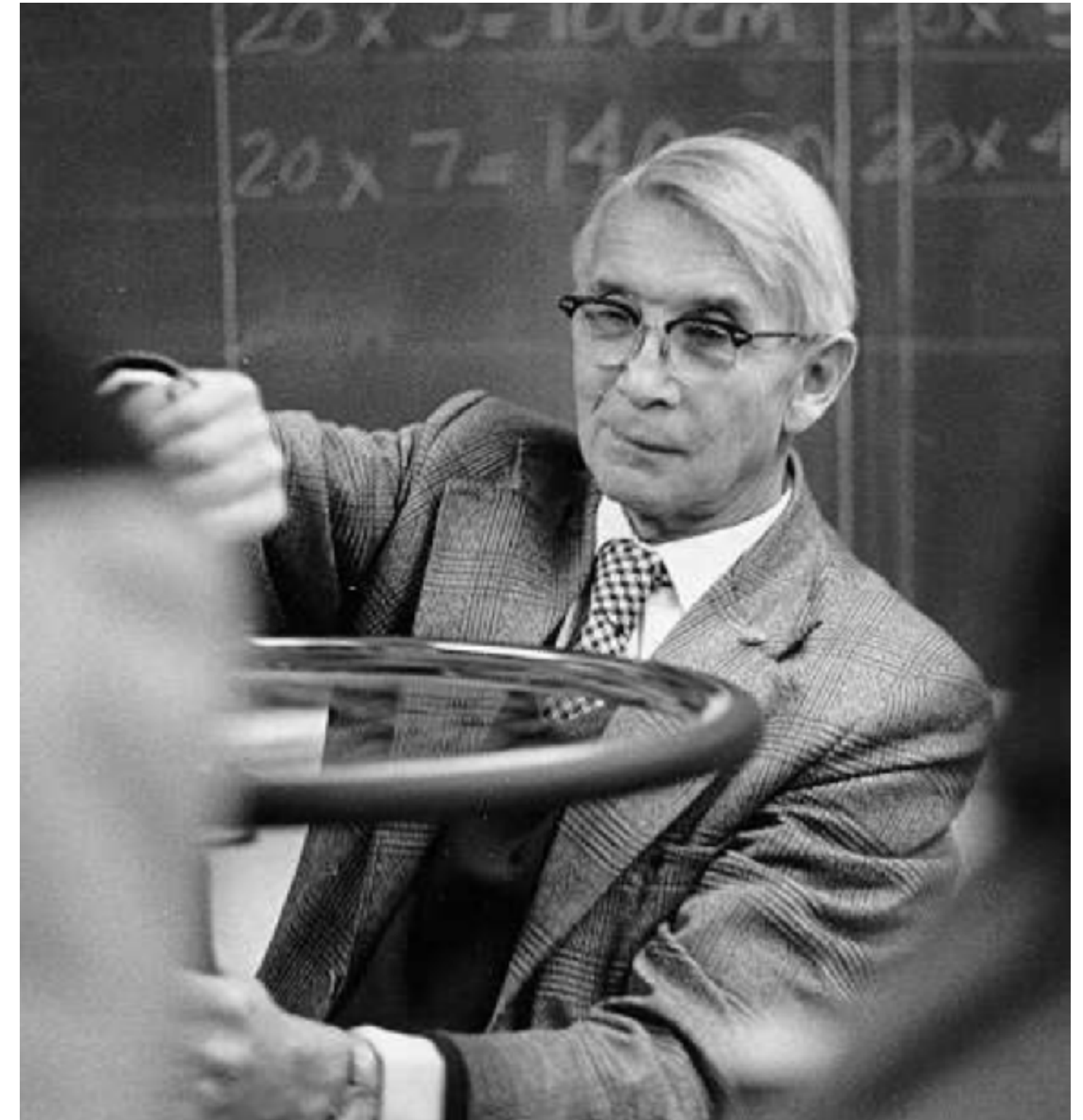
We need other methods...

But brute force diagonalization can only be applied to small system sizes

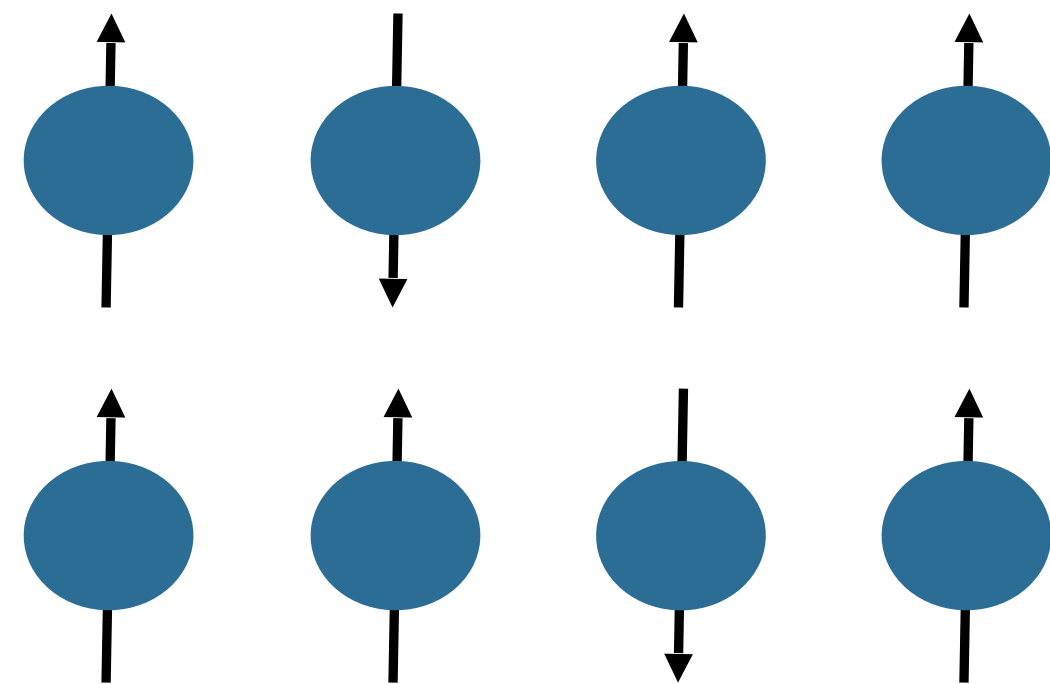
We need other methods...

Before discussing methods, let us discuss a model

The Ising Model



The Ising model – 1920



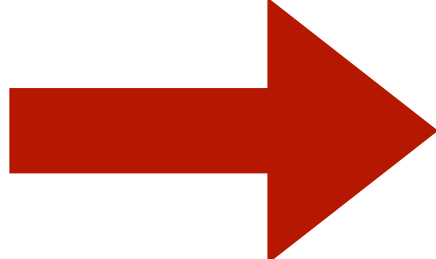
Collection of magnetic
moments **LOCALIZED** in a lattice

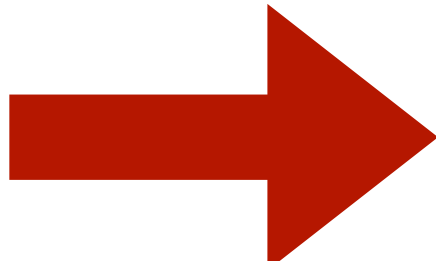
Magnetic moments = spin 1/2

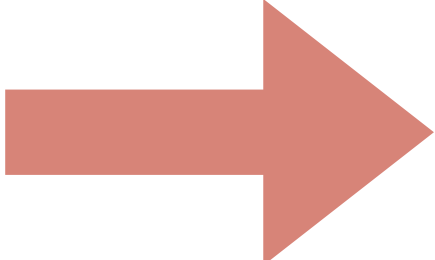
Can only point up or down

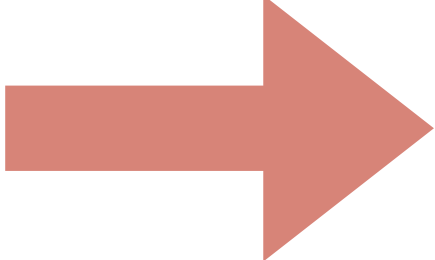
$$E = -J \sum_{\langle ij \rangle} S_i S_j \quad S_i = \pm 1$$

$$E = -J \sum_{\langle ij \rangle} S_i S_j$$

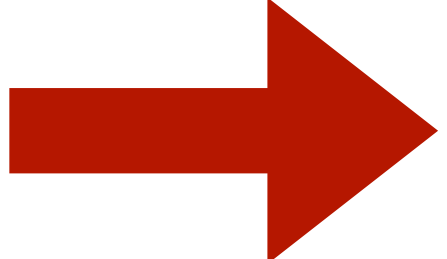
$\langle ij \rangle$  Nearest neighbors

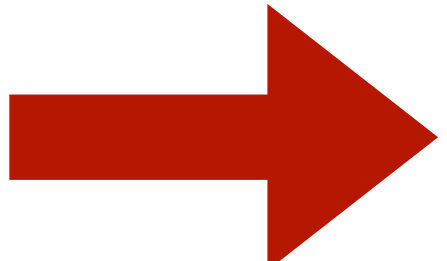
J  Exchange coupling

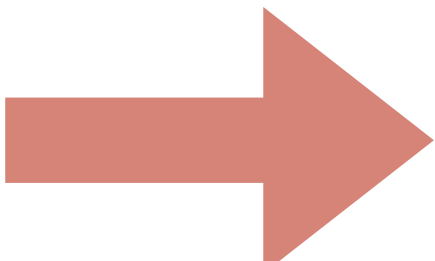
$J > 0$  Ferromagnetism

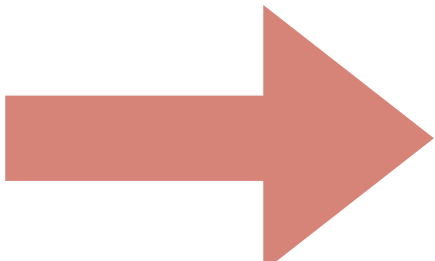
$J < 0$  Antiferromagnetism

$$E = -J \sum_{\langle ij \rangle} S_i S_j$$

$\langle ij \rangle$  Nearest neighbors

J  Exchange coupling

$J > 0$  Ferromagnetism

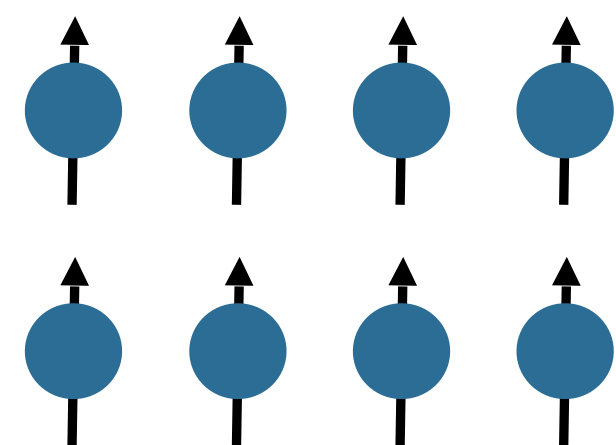
$J < 0$  Antiferromagnetism

Role of Temperature

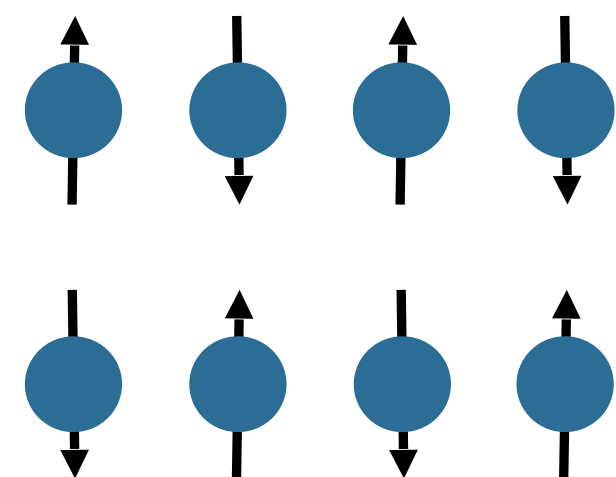
Low T - spins aligned

High T - disorder

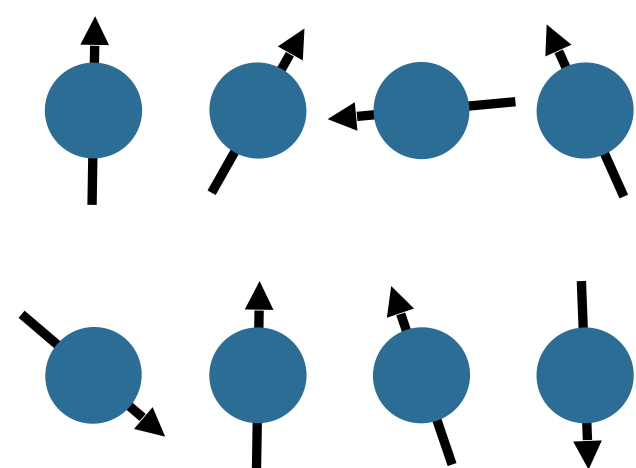
Magnetism



Ferromagnetism

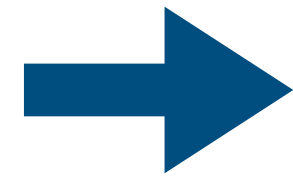


Antiferromagnetism



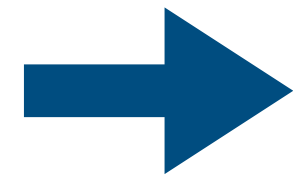
Paramagnetism

Microstate



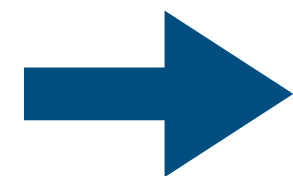
Spin configuration

N sites



$N_M = 2^N$ Number of microstates

E_α



Energy of the microstate α

An example: $N=4$ with periodic boundary conditions

α	microstate	E_α
1	↑ ↑ ↑ ↑	$E_1 = -4J$
2	↑ ↑ ↑ ↓	$E_2 = 0$
3	↑ ↑ ↓ ↑	$E_3 = 0$
4	↑ ↓ ↑ ↑	$E_4 = 0$
5	↓ ↑ ↑ ↑	$E_5 = 0$
6	↑ ↑ ↓ ↓	$E_6 = 0$
7	↑ ↓ ↑ ↓	$E_7 = 4J$
8	↑ ↓ ↓ ↑	$E_8 = 0$

α	microstate	E_α
9	↓ ↓ ↑ ↑	$E_9 = 0$
10	↓ ↑ ↓ ↑	$E_{10} = 4J$
11	↓ ↑ ↑ ↓	$E_{11} = 0$
12	↑ ↓ ↓ ↓	$E_{12} = 0$
13	↓ ↑ ↓ ↓	$E_{13} = 0$
14	↓ ↓ ↑ ↓	$E_{14} = 0$
15	↓ ↓ ↓ ↑	$E_{15} = 0$
16	↓ ↓ ↓ ↓	$E_{16} = -4J$

For a system in thermal equilibrium

Thermal bath at temperature T $P_\alpha \propto e^{-E_\alpha/k_B T}$

P_α $\longrightarrow$ Probability of finding the system in the microstate α

$$\sum_{\alpha=1}^{N_M} P_\alpha = 1$$

From a microscopic point of view: gaining or losing energy $\longrightarrow$ flipping a spin

For a system in thermal equilibrium

$$Z = \sum_{\alpha=1}^{N_M} e^{-E_{\alpha}/k_B T} \longrightarrow \text{Partition function}$$

$$P_{\alpha} = \frac{1}{Z} e^{-E_{\alpha}/k_B T}$$

$$M_{\alpha} = \sum_i S_i \longrightarrow \text{Magnetization of a microstate } \alpha$$

Measured magnetization

$$\langle M \rangle = \sum_{\alpha=1}^{N_M} M_{\alpha} P_{\alpha}$$

Measured Energy

$$\langle E \rangle = \sum_{\alpha=1}^{N_M} E_{\alpha} P_{\alpha}$$

For any given observable Q

$$\langle Q \rangle = \sum_{\alpha=1}^{N_M} P_{\alpha} Q_{\alpha} = \frac{1}{Z} \sum_{\alpha=1}^{N_M} e^{-E_{\alpha}/k_B T} Q_{\alpha}$$
$$P_{\alpha} = \frac{1}{Z} e^{-E_{\alpha}/k_B T}$$

N_M $\longrightarrow$ Number of micro states

N $\longrightarrow$ Number of sites

$$N_M = 2^N$$

Ising chain with $N=4$ sites $\longrightarrow N_M = 16$

3D Ising $10 \times 10 \times 10$ $\longrightarrow N_M = 2^{1000} \approx 10^{300}$ $\longrightarrow$ Too big!

Monte Carlo Method



As N_M can be too big

Choose a subset of M microstates **randomly**

$$\{\alpha_1, \alpha_2, \alpha_3, \dots, \alpha_M\}$$

With a given probability distribution p_α

Estimator Q_M

Best estimate for Q

$$\langle Q_M \rangle = \frac{\sum_{i=1}^M Q_{\alpha i} p_{\alpha, i}^{-1} e^{-\beta E_{\alpha i}}}{\sum_{i=1}^M p_{\alpha, i}^{-1} e^{-\beta E_{\alpha i}}}$$

$$\beta = \frac{1}{k_B T}$$

$$M \longrightarrow N_M$$

$$Q_M \longrightarrow Q$$

How do we choose the M microstates that enter in the sum?

or

How do we choose p_α ?

Easier choice: all the states with equal probability

$$\text{3D Ising } 10 \times 10 \times 10 \longrightarrow N_M = 2^{1000} \approx 10^{300}$$

$$\text{A couple of hours} \longrightarrow 10^8 \longrightarrow 10^{-292} N_M \longrightarrow \text{Too small}$$

Low T: few microstates contribute

The probability of one of them be chosen is 10^{-292}

Essence of the Monte Carlo Method

How do we choose the most important states
among the large number of accessible states?

Importance sampling

Importance sampling

What happens when a measurement is made in a real system?

The system does not visit all microstates...

→ **Narrow energy band**

→ **Boltzmann factor**

Importance sampling

Probability of choosing a state α

$$p_{\alpha} = \frac{1}{Z} e^{-\beta E_{\alpha}}$$

The Boltzmann weights cancel

$$\langle Q_M \rangle = \frac{1}{M} \sum_{i=1}^M Q_{\alpha i}$$

A practical problem:

How do we choose the states so that we have

$$p_{\alpha} = \frac{1}{Z} e^{-\beta E_{\alpha}}$$

Markovian processes

Markovian processes

Given a state μ  Generates a state ν

MARKOV CHAIN

$$\mu \rightarrow \nu \rightarrow \lambda \rightarrow \dots$$

RULES

(1) $P(\mu \rightarrow \nu)$ does not change with time

(2) $P(\mu \rightarrow \nu)$ depends only on μ and ν , not on other states that might have been visited

$$(3) \sum_{\nu} P(\mu \rightarrow \nu) = 1$$

$$(4) P(\mu \rightarrow \mu) \neq 0$$

Markovian processes

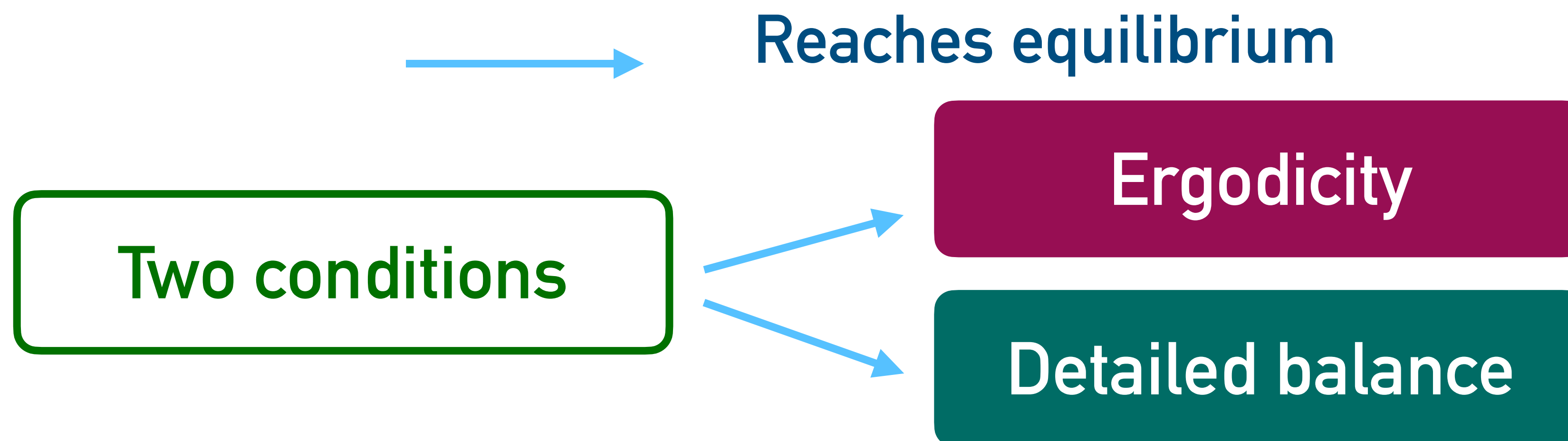
The markovian process is such that, when it runs for a sufficiently long time, starting from any initial state, the visited states are chosen according the Boltzmann weight



Reaches equilibrium

Markovian processes

The markovian process is such that, when it runs for a sufficiently long time, starting from any initial state, the visited states are chosen according the Boltzmann weight



Ergodicity

$p(\nu)$ $\longrightarrow$ Probability of finding the system in state ν

$$p(\nu) \neq 0 \quad \forall \nu$$

Starting from any state it must be possible to arrive at any other state if we wait long enough

Detailed balance

$$p(\mu)P(\mu \rightarrow \nu) = p(\nu)P(\nu \rightarrow \mu)$$

Recall that $\sum_{\nu} P(\mu \rightarrow \nu) = 1$

$$p(\mu) = \sum_{\nu} p(\nu)P(\nu \rightarrow \mu)$$

After equilibrium is reached the states are chosen according to the Boltzmann distribution

So far

Importance sampling

Markovian processes

Ergodicity

Detailed balance

Metropolis Algorithm

Illustration by Heinz Schulz-Neudamm
en.wikipedia.org/w/index.php?curid=63350586



Equation of State Calculations by Fast Computing Machines

NICHOLAS METROPOLIS, ARIANNA W. ROSENBLUTH, MARSHALL N. ROSENBLUTH, AND AUGUSTA H. TELLER,
Los Alamos Scientific Laboratory, Los Alamos, New Mexico

AND

EDWARD TELLER,* *Department of Physics, University of Chicago, Chicago, Illinois*

(Received March 6, 1953)

A general method, suitable for fast computing machines, for investigating such properties as equations of state for substances consisting of interacting individual molecules is described. The method consists of a modified Monte Carlo integration over configuration space. Results for the two-dimensional rigid-sphere system have been obtained on the Los Alamos MANIAC and are presented here. These results are compared to the free volume equation of state and to a four-term virial coefficient expansion.

Detailed balance

One possibility

(Not the only one!)

$$P(\mu \rightarrow \nu) = \min \left[1, \frac{p(\nu)}{p(\mu)} \right]$$

Where

$$\frac{P(\mu \rightarrow \nu)}{P(\nu \rightarrow \mu)} = \frac{p(\nu)}{p(\mu)} = e^{\beta(E_\nu - E_\mu)}$$

Metropolis algorithm

$$P(\mu \rightarrow \nu) = \min \left[1, e^{-\beta \Delta E} \right]$$

Metropolis algorithm for the Ising model

- Choose an initial configuration of the spins
- Choose one spin and propose a flip
- Calculate $\Delta E = E_{after\ flip} - E_{before\ flip}$

Metropolis algorithm for the Ising model

- Choose an initial configuration of the spins Randomly?
- Choose one spin and propose a flip Randomly?
- Calculate $\Delta E = E_{after\ flip} - E_{before\ flip}$

Metropolis algorithm for the Ising model

- Choose an initial configuration of the spins
- Choose one spin and propose a flip
- Calculate $\Delta E = E_{after\ flip} - E_{before\ flip}$
 - If $\Delta E < 0$ $\longrightarrow$ Accept the change

- If $\Delta E < 0$ $\longrightarrow$ Accept the change
- If $\Delta E > 0$ $\longrightarrow$ Accept with probability $e^{-\beta\Delta E}$

Pick a random number $r = [0,1]$

If $r \leq e^{-\beta\Delta E}$ $\longrightarrow$ Accept the change

If $r > e^{-\beta\Delta E}$ $\longrightarrow$ Does not accept

Why do we accept changes when $\Delta E > 0$?

Why do we accept changes when $\Delta E > 0$?

If not the system would always flow to the ground state

Curiosity

Metropolis algorithm for the Ising model at high temperature, starting with all the spins aligned

$$T \rightarrow \infty \quad P(\mu \rightarrow \nu) \rightarrow 1$$

Curiosity

Metropolis algorithm for the Ising model at high temperature, starting with all the spins aligned

$$T \rightarrow \infty$$

$$P(\mu \rightarrow \nu) \rightarrow 1$$



All flips accepted!

Curiosity

Metropolis algorithm for the Ising model at high temperature, starting with all the spins aligned

$$T \rightarrow \infty$$

$$P(\mu \rightarrow \nu) \rightarrow 1$$



All flips accepted!

Wrong!

Heat bath algorithm

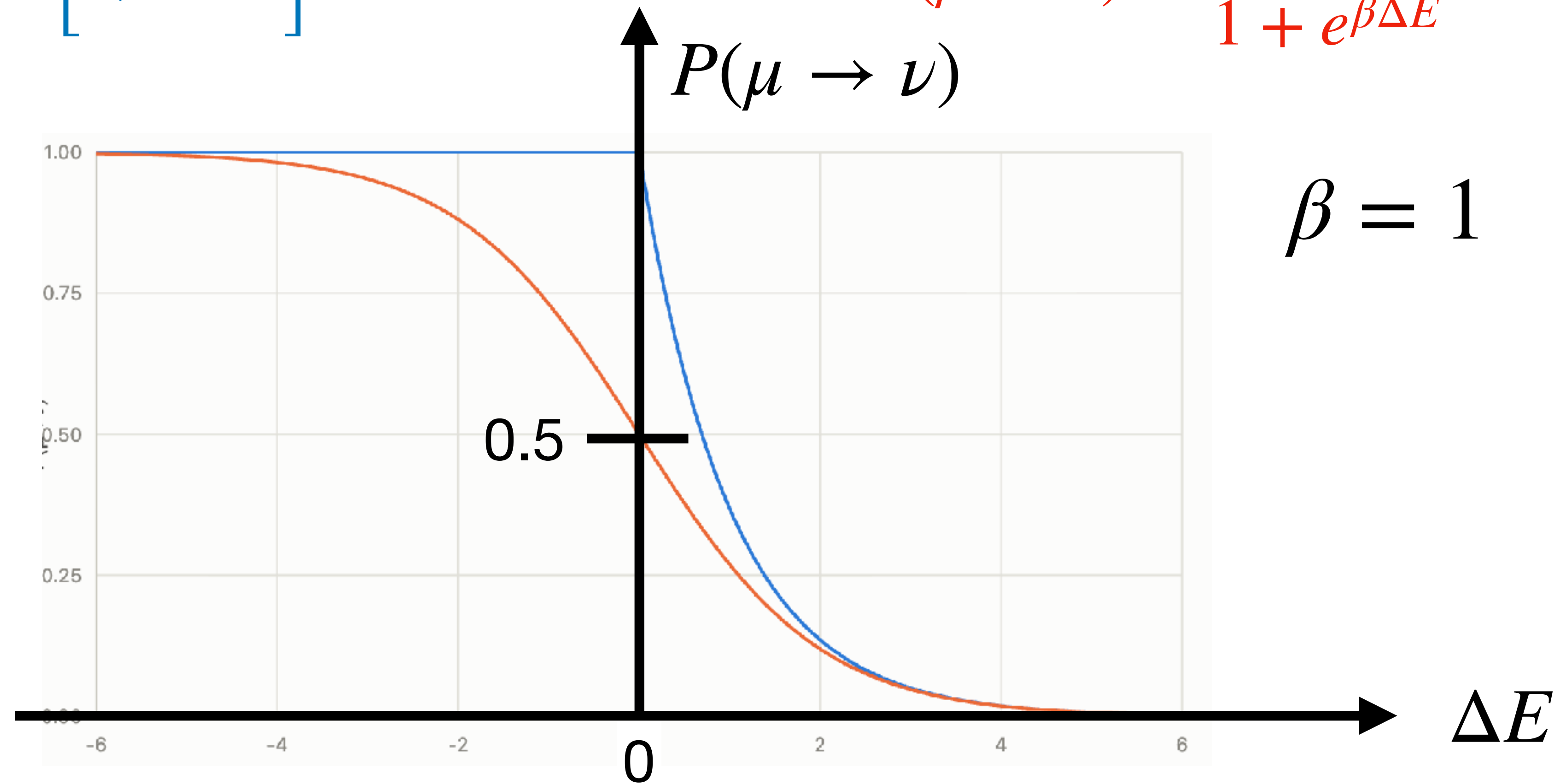
$$P(\mu \rightarrow \nu) = \frac{e^{-\beta E_\nu}}{e^{-\beta E_\nu} + e^{-\beta E_\mu}} = \frac{1}{1 + e^{-\beta \Delta E}}$$

Metropolis algorithm

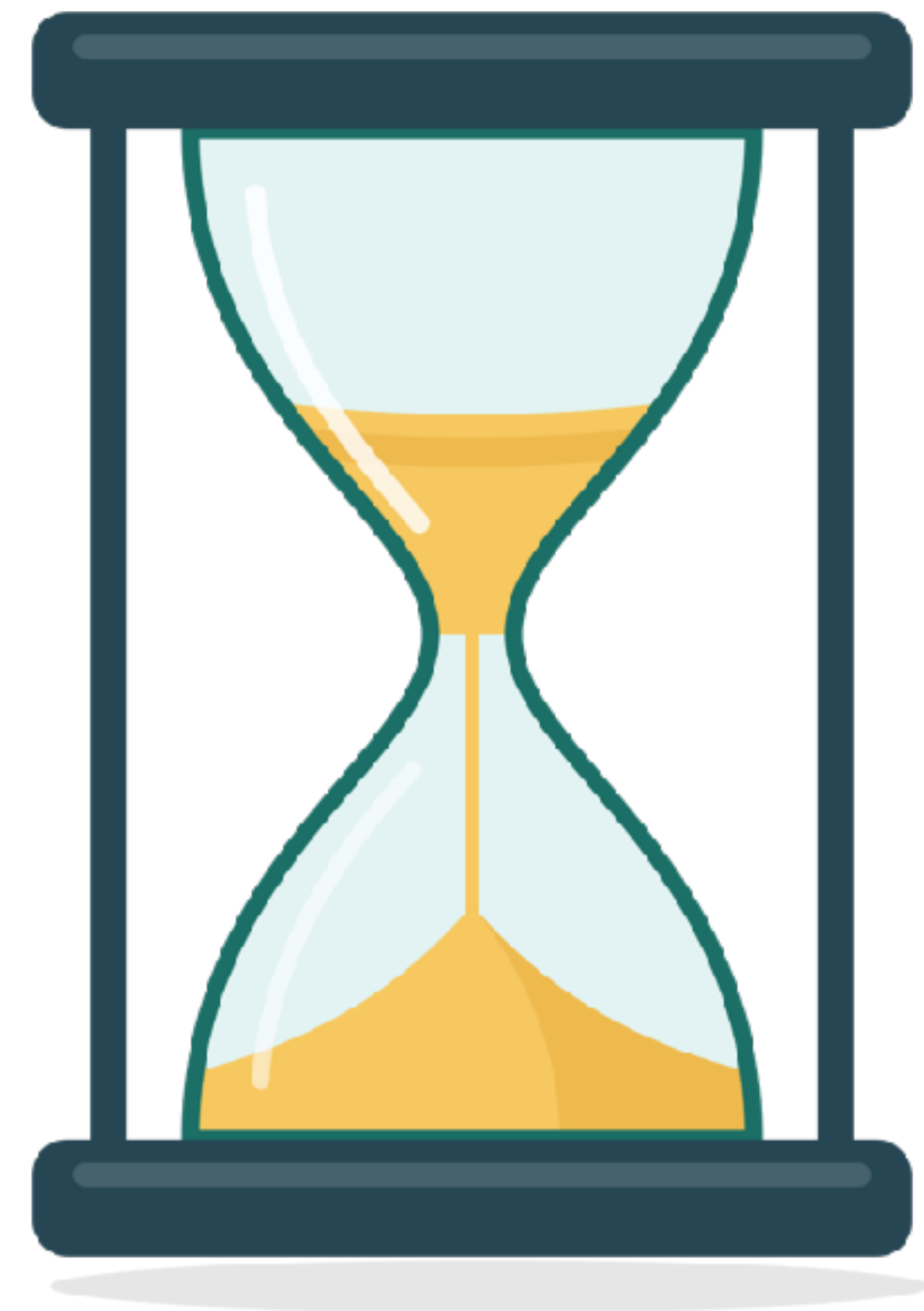
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Heat bath algorithm

$$P(\mu \rightarrow \nu) = \frac{1}{1 + e^{\beta\Delta E}}$$



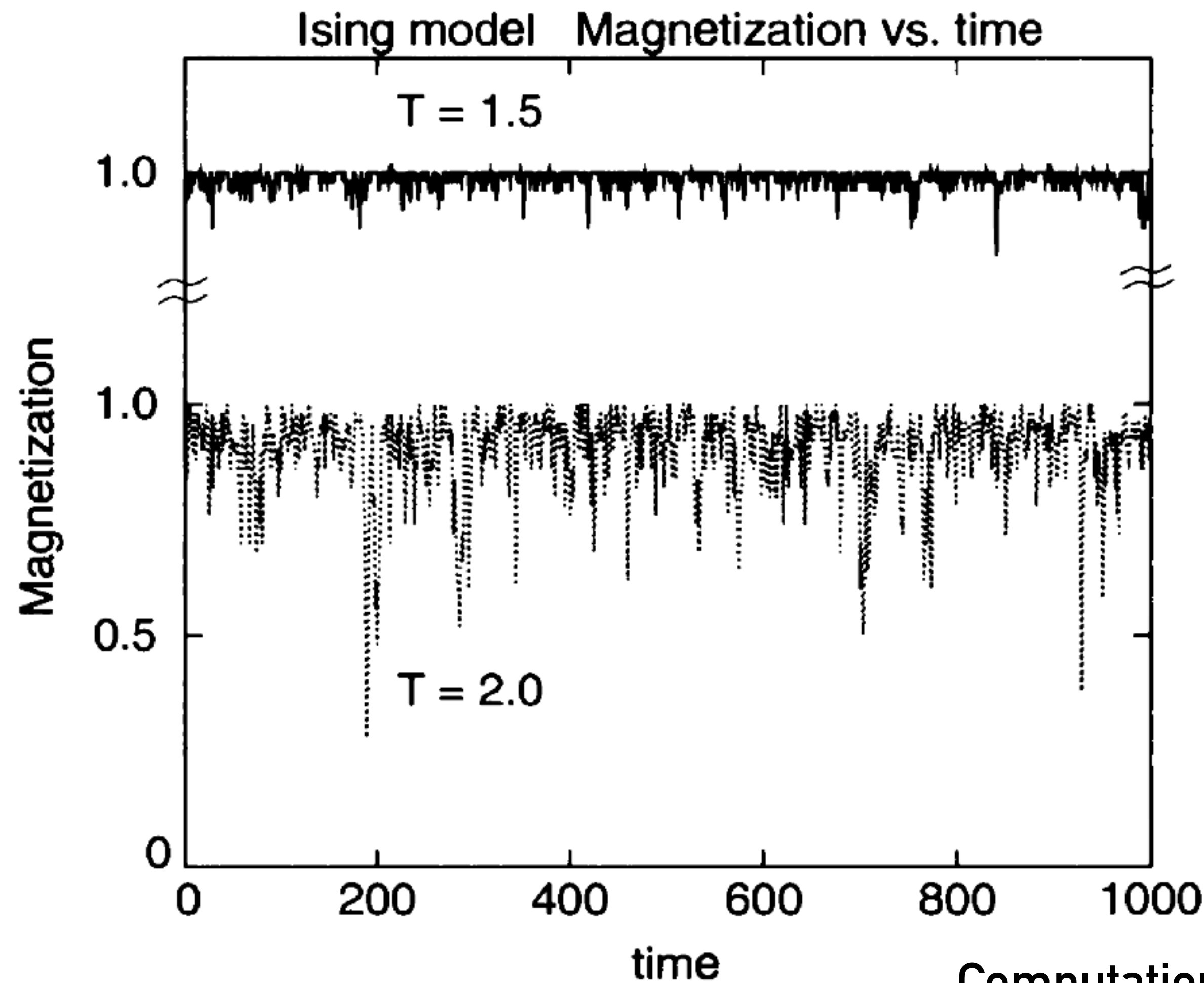
Monte Carlo time



Monte Carlo time

- Not real time
- One sweep through the lattice  one unit of time
- Not completely disconnected from real time

Magnetization as a function of Monte Carlo time

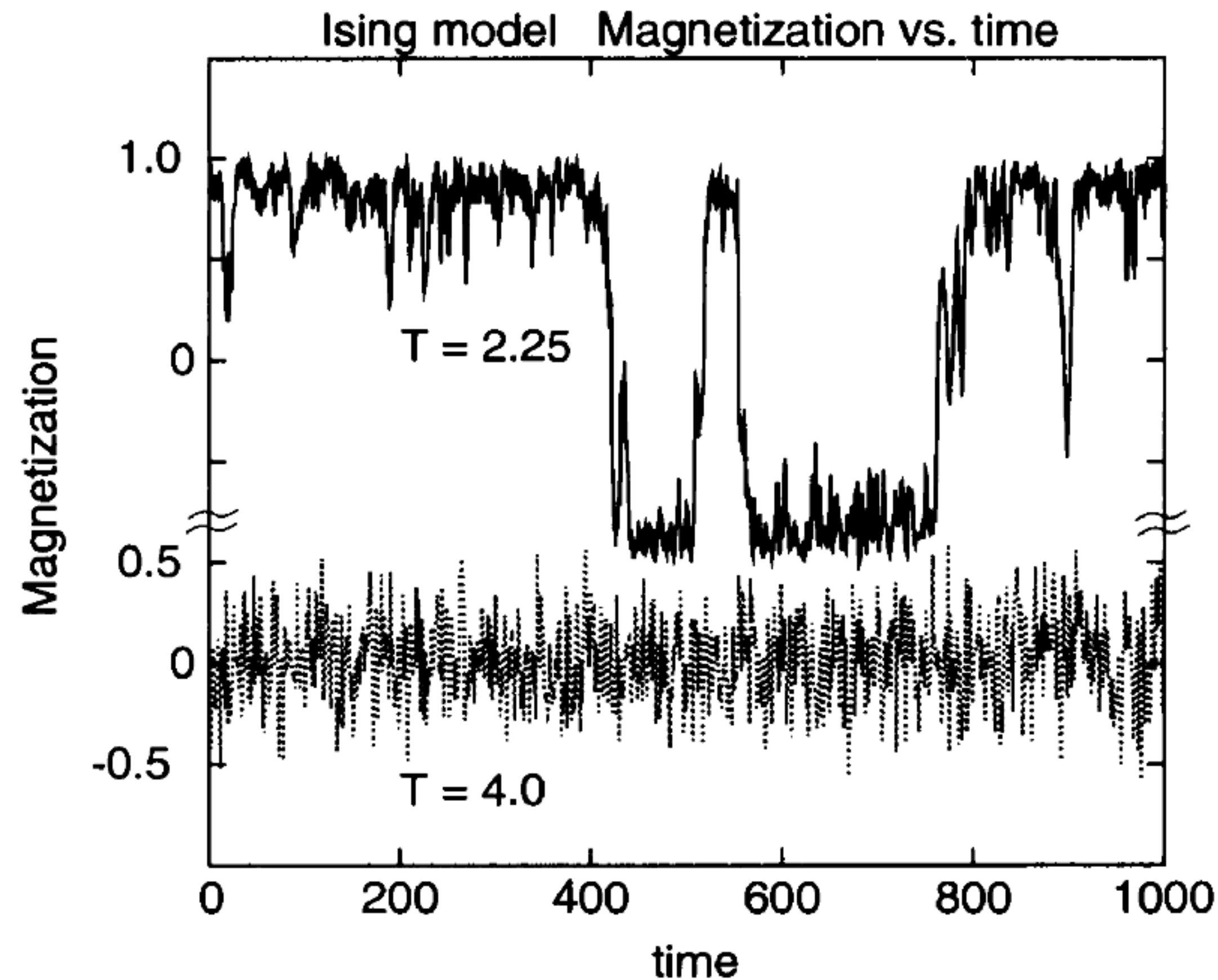


10 x 10 lattice, $J=1$

$T=1.5$ $M \sim 1$ $\longrightarrow$ small fluctuations

$T=2.0$ $M \sim 0.9$ $\longrightarrow$ fluctuations increase

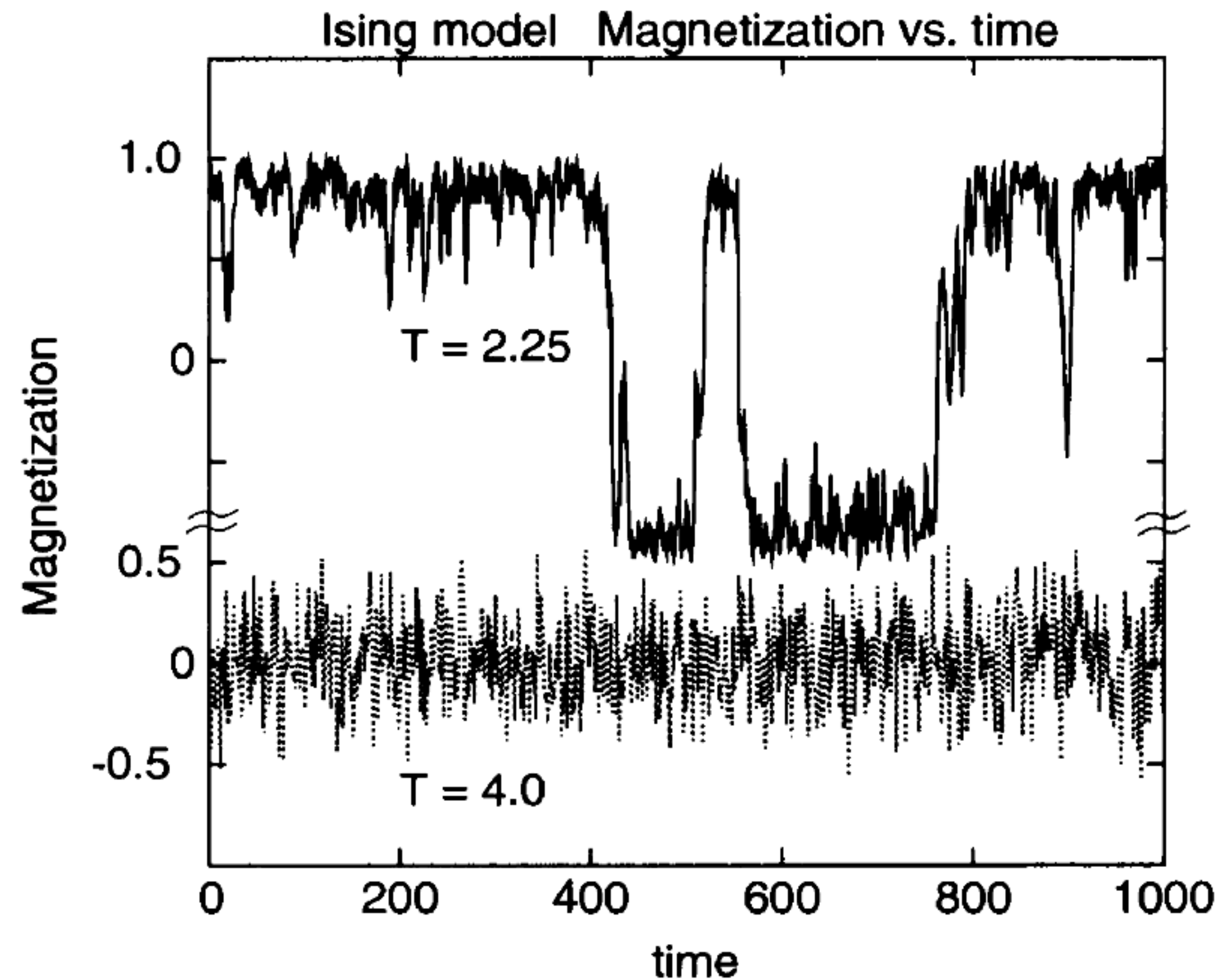
Magnetization as a function of Monte Carlo time



$T=4.0$ $M \sim 0$ $\longrightarrow$ small fluctuations

$T=2.25$ $\longrightarrow$ very large fluctuations

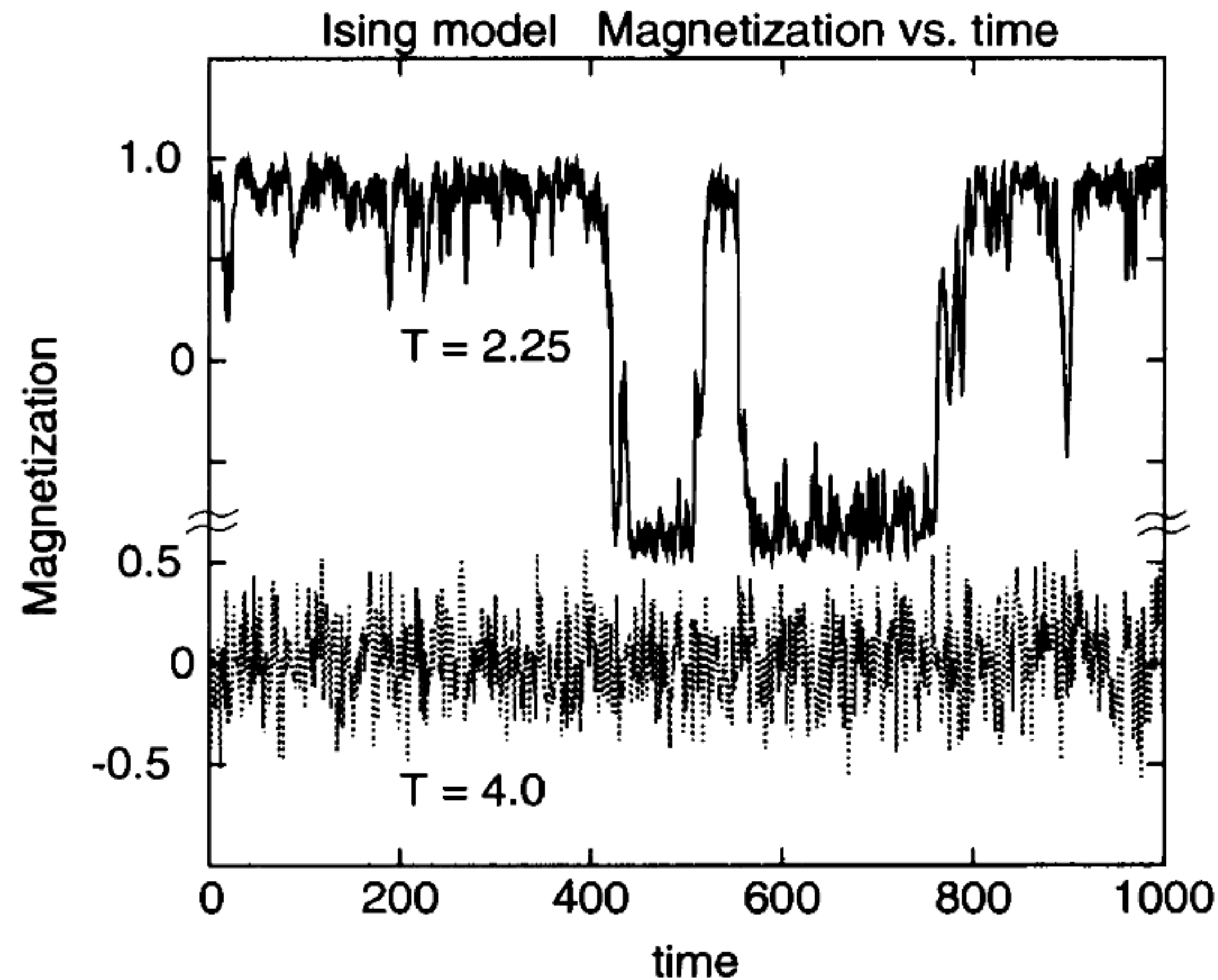
Magnetization as a function of Monte Carlo time



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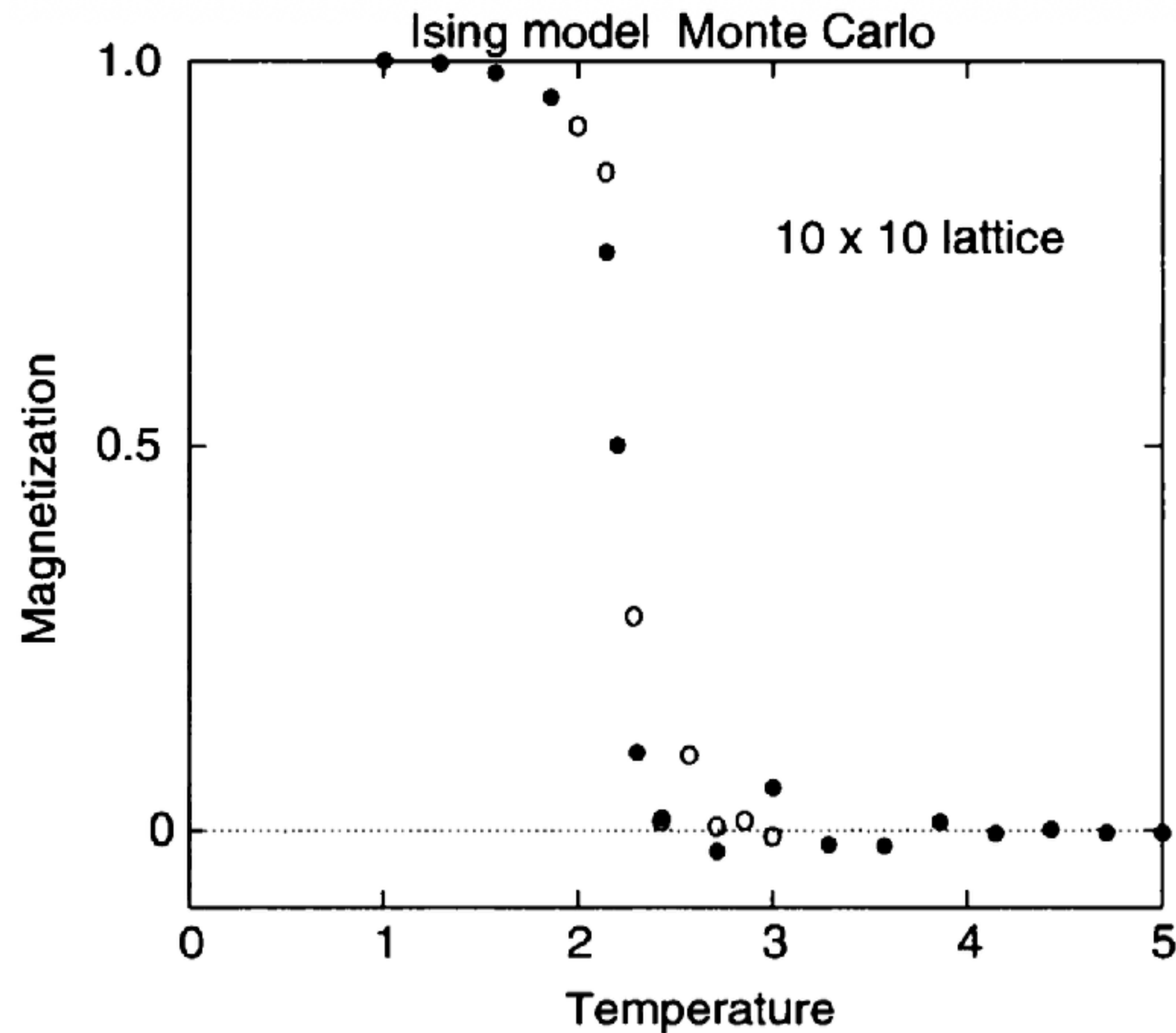
Magnetization as a function of Monte Carlo time



Critical slowing down

Large fluctuations signal that we are in the vicinity of a 2nd order phase transition

Fluctuation-dissipation theorem



Onsager's exact solution

$$T_C = \frac{2}{\ln(1 + \sqrt{2})} \simeq 2.27$$

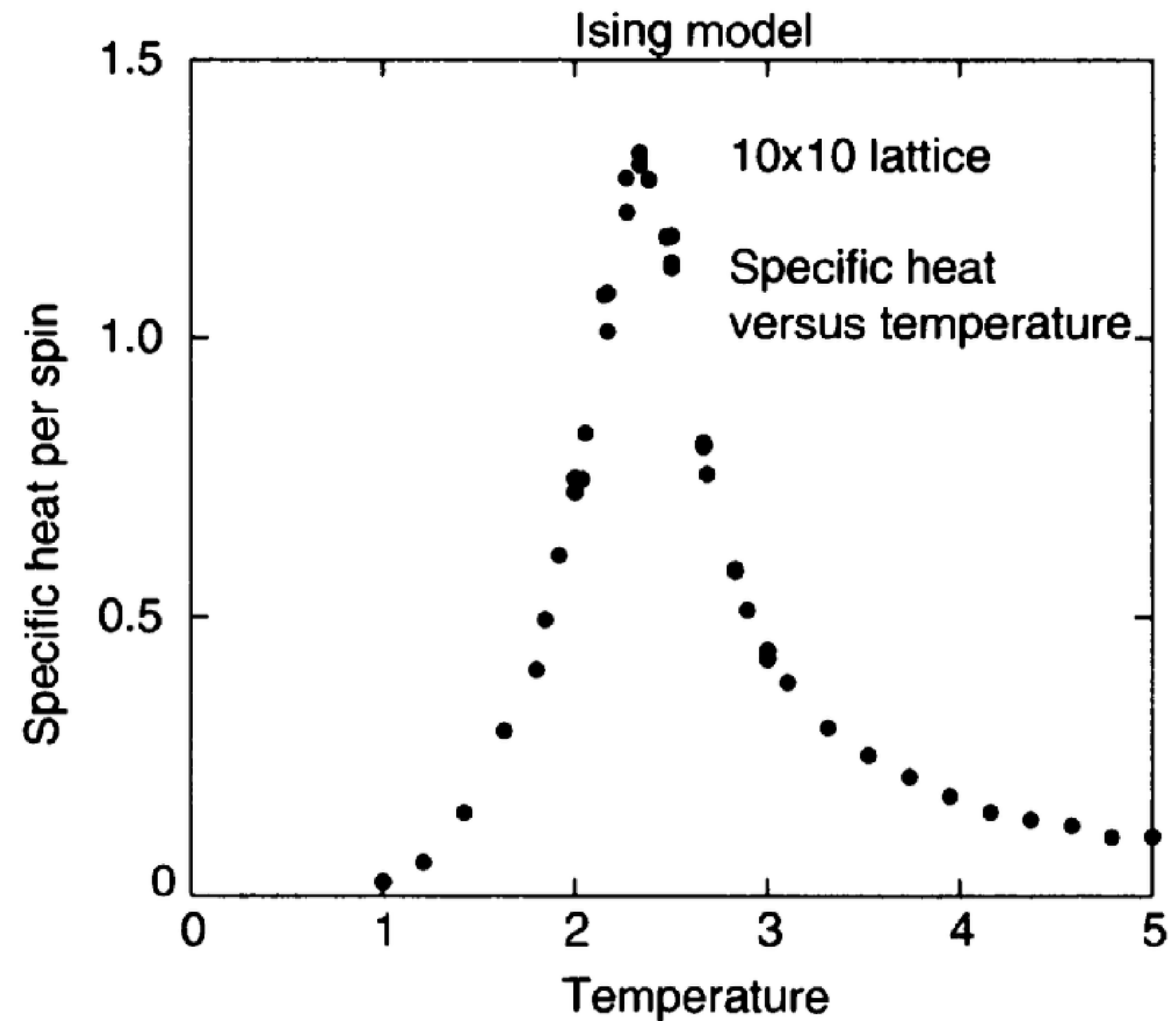
Opened and closed circles: different realizations

Specific heat

$$(\Delta E)^2 = \langle E^2 \rangle - \langle E \rangle^2$$

Fluctuation-dissipation theorem

$$C = \frac{(\Delta E)^2}{k_B T^2}$$



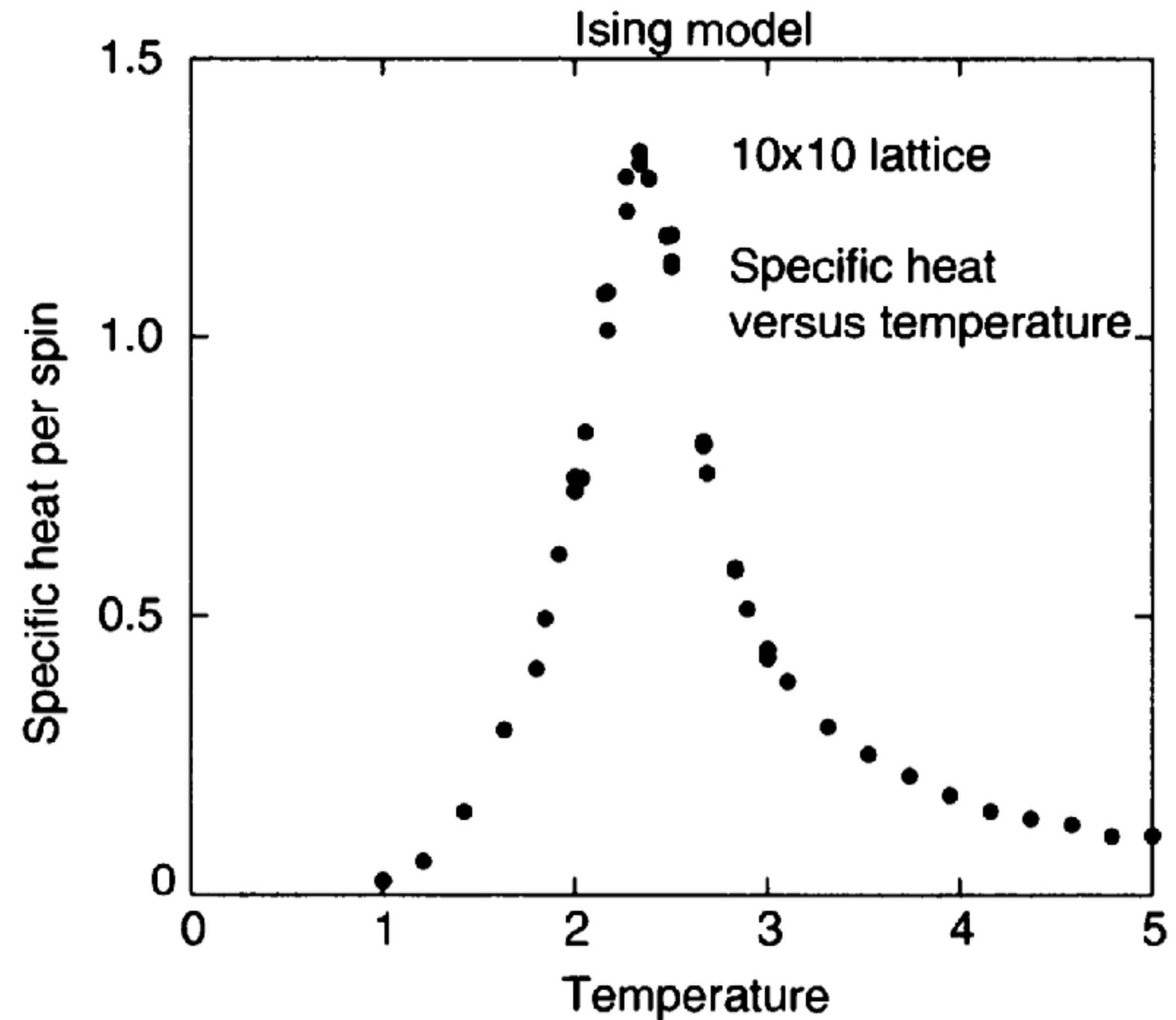
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No divergence for a finite system



Specific heat

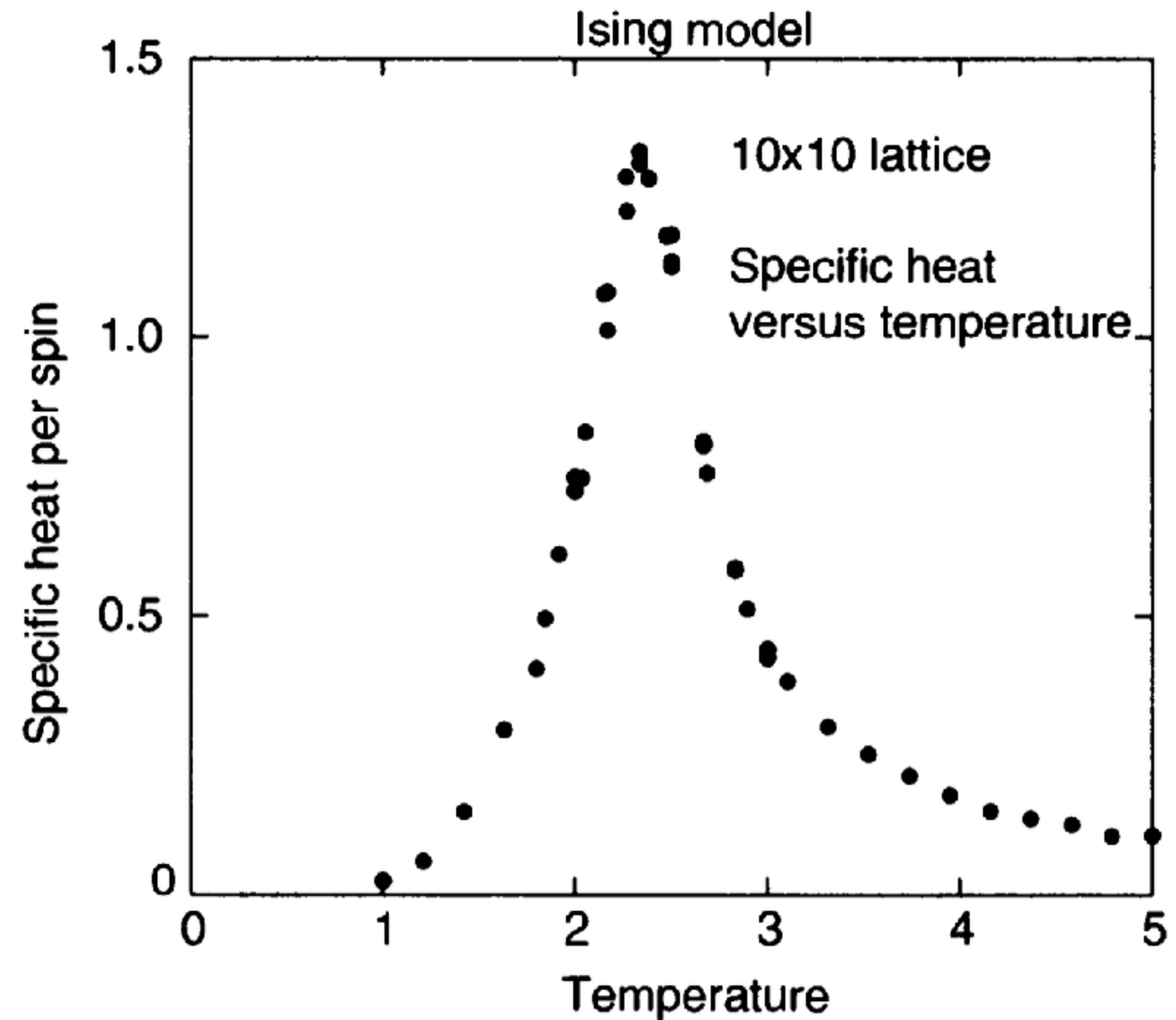
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Fluctuation-dissipation theorem

$$C = \frac{(\Delta E)^2}{k_B T^2}$$

No divergence for a finite system

Finite size effects



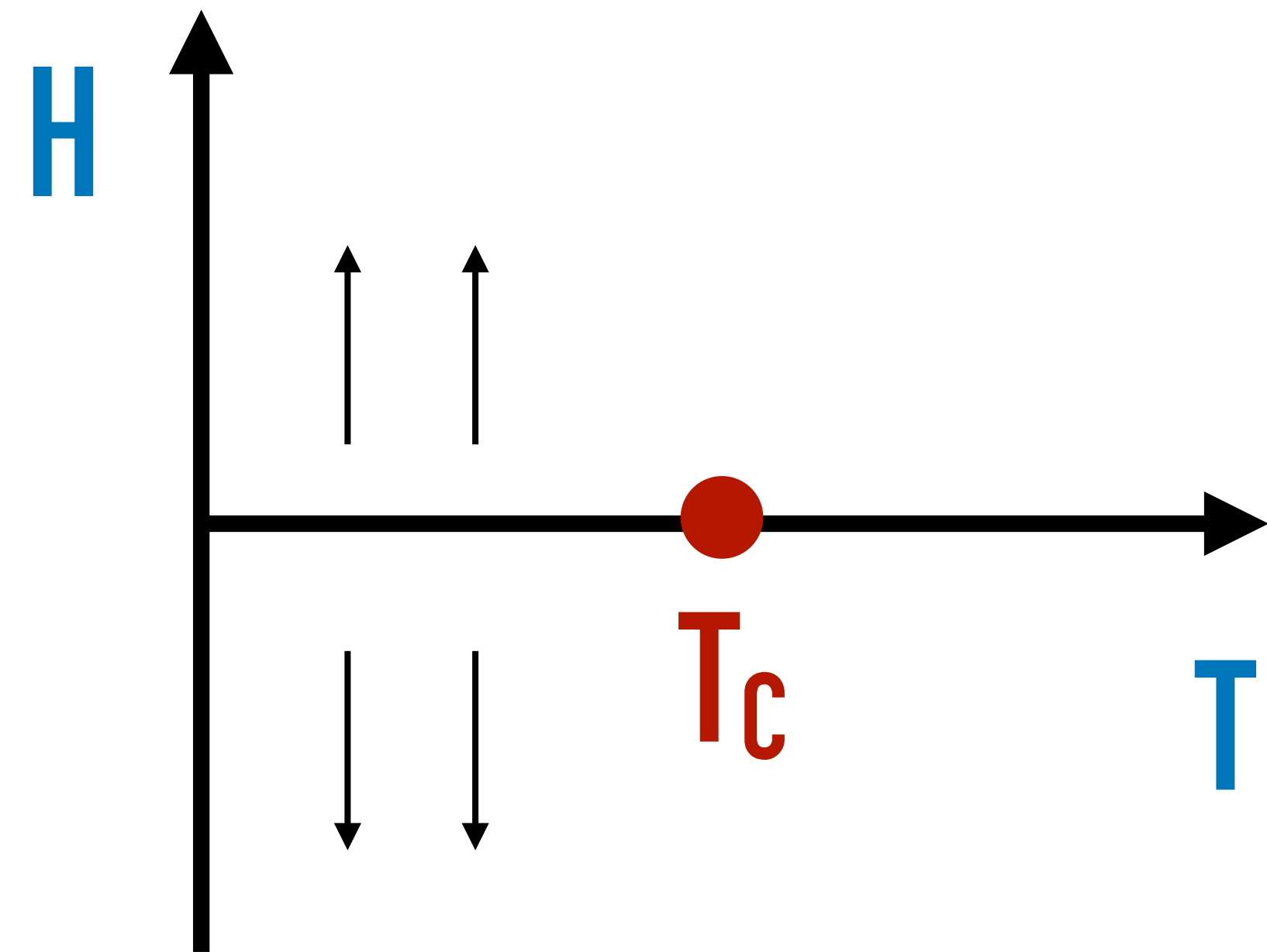
Boundary conditions

- Free
- Fixed
- Closed: periodic, antiperiodic, twisted

First-order phase transitions

Ising model with a magnetic field

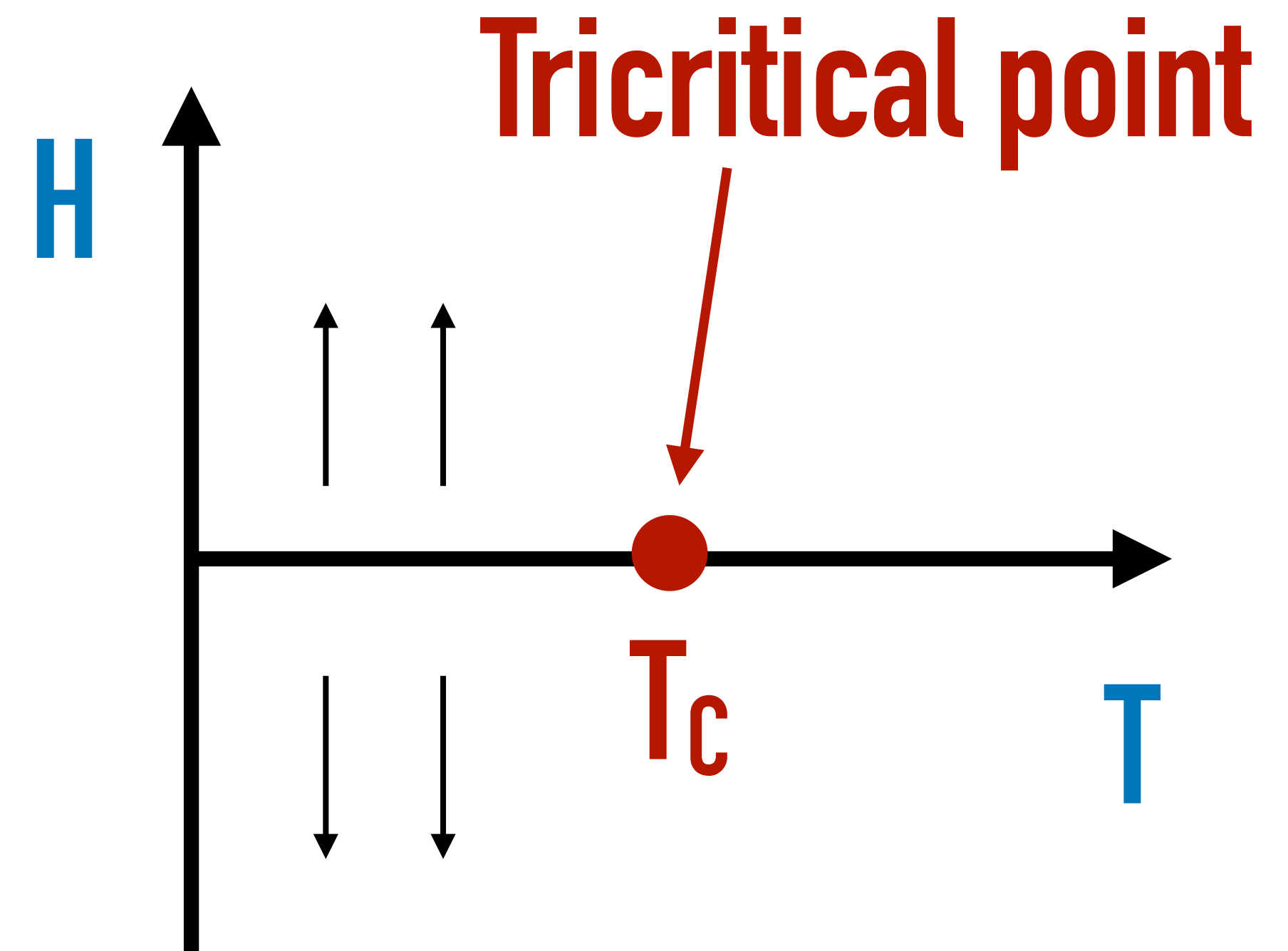
$$E = -J \sum_{\langle ij \rangle} S_i S_j - H \sum_i S_i$$



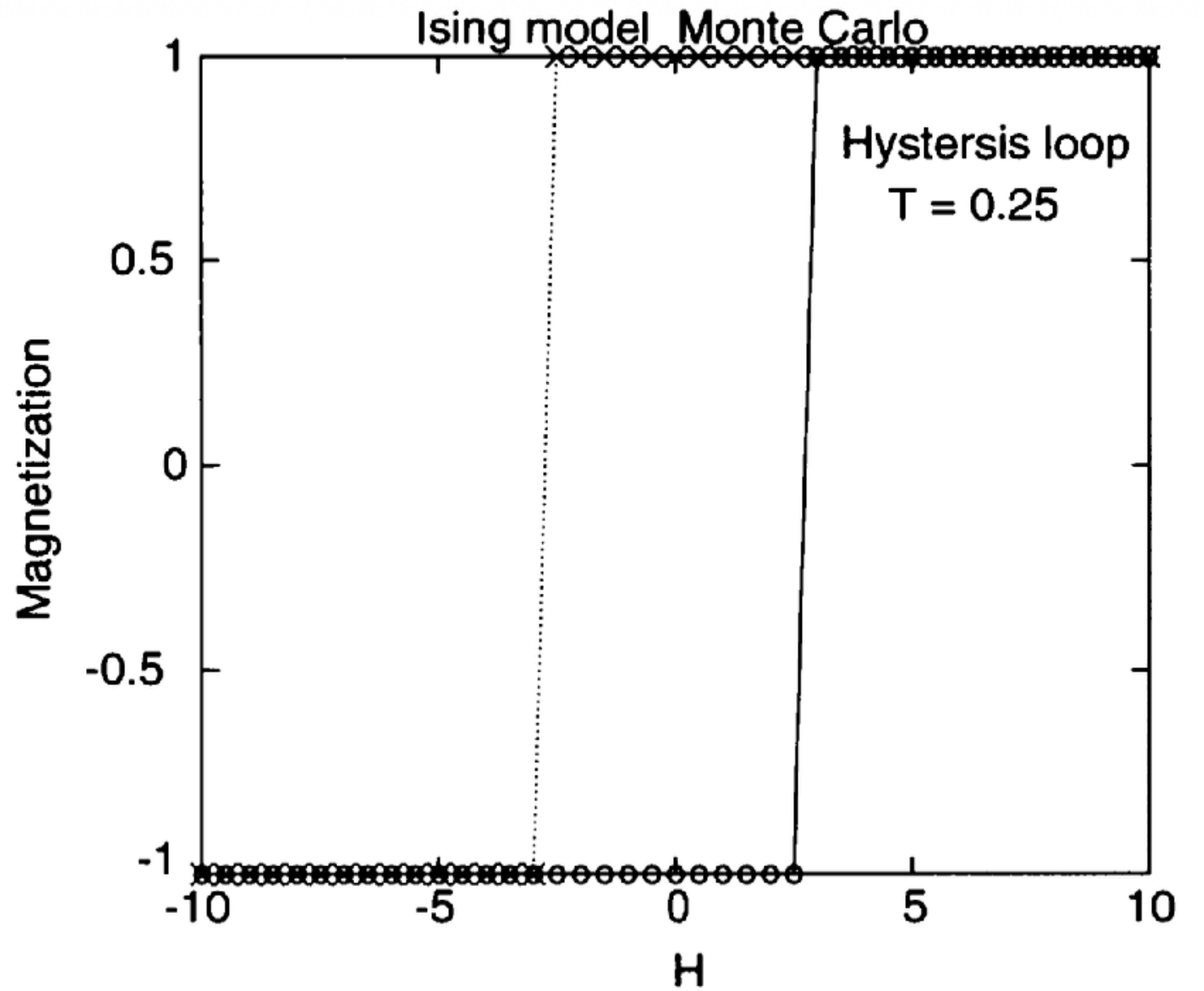
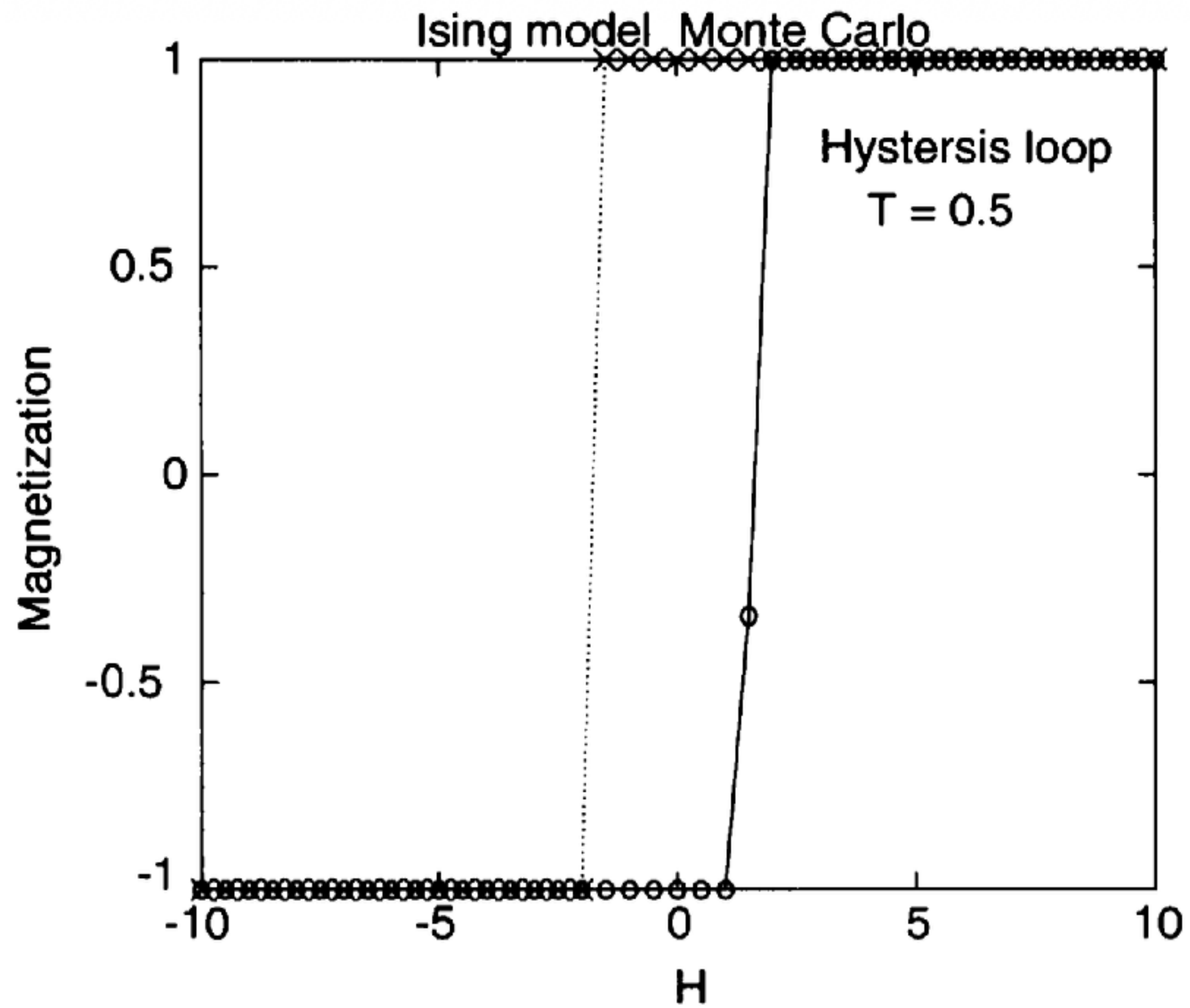
First-order phase transitions

Ising model with a magnetic field

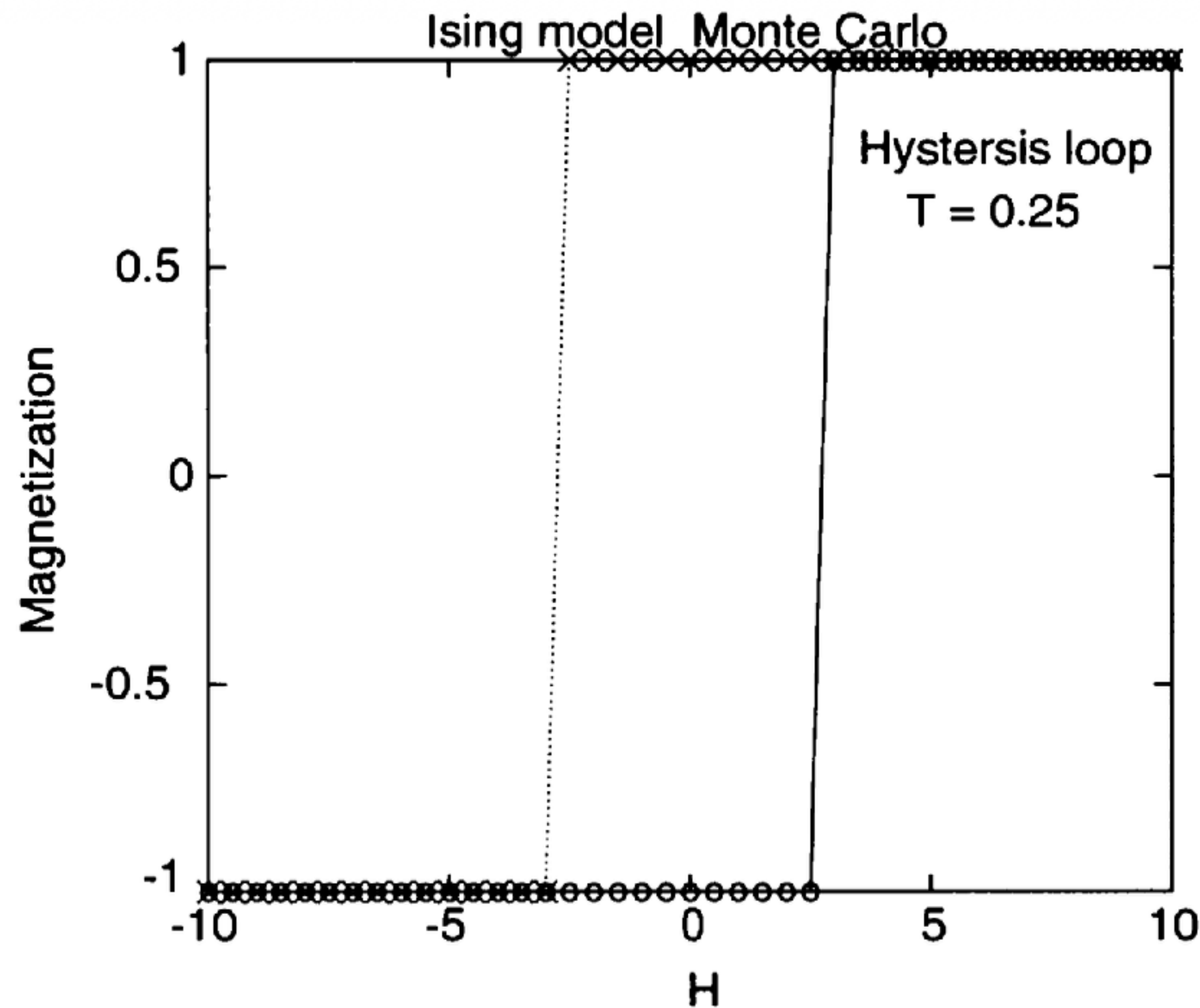
$$E = -J \sum_{\langle ij \rangle} S_i S_j - H \sum_i S_i$$



Hysteresis loop



Hysteresis loop



Configurations before and after the transition are very different

Monte Carlo flips one spin at a time

The state of the system depends on the history of the system

Monte Carlo Method

Importance sampling

Markovian processes

Ergodicity

Detailed balance

Monte Carlo Method

Measurements

Finite size scaling

End of first class