



# 993SM – Laboratory of Computational Physics Unit IX November 20, 2023

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# The Ising model in the canonical ensemble

- Introduction to the Ising model
- The Ising model in the canonical ensemble: application of Metropolis Monte Carlo Method
  - Implementation in a code

(from previous lecture)

# The canonical ensemble

**(N,V,T) fixed.** The probability that the system is in the microstate  $s$  with energy  $E_s$  is given by:

(here the energy identifies different microstates, it is not a characteristic of the macrostate)

$$P_s = \frac{1}{Z} e^{-\beta E_s}, \text{ (canonical distribution)}$$

where  $\beta = 1/kT$ , and  $Z$  is a normalization constant.

$$Z = \sum_{s=1}^M e^{-E_s/kT} \quad \text{partition function}$$

( $M$ : all accessible microstates of the system)  
characterized by different  $E_s$

(from previous lecture)

# Ensemble averages

To calculate the ensemble average of a physical quantity  $\langle A \rangle$  we work on a representative number  $m$  of the total number  $M$  of accessible microstates:

$$\langle A \rangle \approx A_m = \frac{\sum_{s=1}^m A_s e^{-\beta E_s}}{\sum_{s=1}^m e^{-\beta E_s}}$$

or, more conveniently:

$$\langle A \rangle \approx \frac{1}{m} \sum_{s=1}^m A_s \text{ with microstates } s \text{ generated according to } \pi_s = \frac{e^{-\beta E_s}}{\sum_{s=1}^m e^{-\beta E_s}}$$

Using Metropolis Monte Carlo,

The transition matrix that generates microstates  $s$  according to  $\pi_s$  is :

$$T_{old,new} = \min \left[ 1, \frac{\pi_{new}}{\pi_{old}} \right] = \min \left[ 1, \frac{p_{new}}{p_{old}} \right] = \min \left[ 1, \frac{e^{-\beta E_{new}}}{e^{-\beta E_{old}}} \right]$$



(from previous lecture)

# Metropolis algorithm in the canonical ensemble

$$T(i \rightarrow j) = \min(1, e^{-\beta \Delta E}) \quad (\text{Metropolis algorithm}),$$

where  $\Delta E = E_j - E_i$ .

1) always accept new configurations with lower energy

2) new configurations with higher energy are accepted with probability depending on T:

If  $E_j > E_i$ , accept the new (higher energy) configuration with probability  $p = \exp(-\Delta E/k_B T)$ . This means that when the temperature is high, we don't mind taking steps in the “wrong” direction.

# stochastic simulations of an interacting spin ensemble

We need a model for:

- **energy**

- **evolution**

(to build the trajectory / the Markov chain)

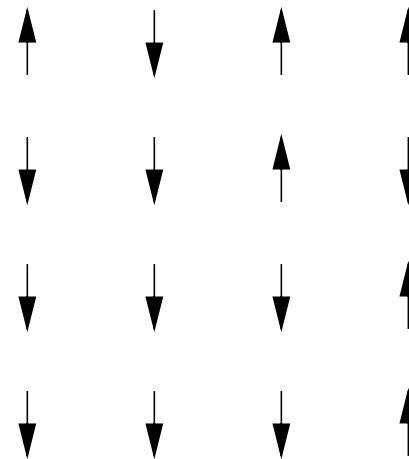
# stochastic simulations of an interacting spin ensemble

We need a model for:

- **energy** => Ising model

- **evolution**

(to build the trajectory / the Markov chain)

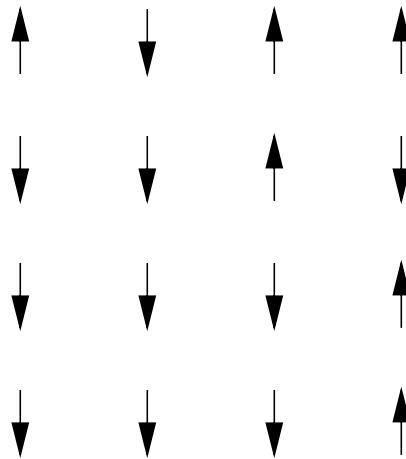


# Ising model

the simplest model of interacting spin on a lattice

$$\mathcal{H}^{spin} = -J \sum_{i,j=1}^N s_i s_j$$

$$s_i = \pm 1$$



But where does it come from ? (next slides 9-15)

# 2 interacting spins

Consider two fermions,  $\vec{s}_1, \vec{s}_2$  (e.g. electrons in He) described by a hamiltonian not depending explicitly on spin:

$$\mathcal{H} = h_1 + h_2 + V_{12}$$

=> the eigenstates can be in a factorized form (antisymmetric under particle exchange due to the Pauli exclusion principle):

$$\Psi_{-}(1,2) = \Psi_{+,-}^{orb}(1,2) \chi(1,2)$$

In the Hilbert **spin subspace** we can choose a **coupled representation**, referring to the spin sum  $\vec{S}$ , with eigenstates labeled by  $|S, S_z\rangle$ :

$$\Psi_{-}(1,2) = \Psi_{+,-}^{orb}(1,2) \chi_{S,S_z}(1,2) = \Psi_{+,-}^{orb}(1,2) |S, S_z\rangle$$

# 2 interacting spins

## Eigenstates

$$\Psi_{+,-}^{orb}(1,2)|S, S_z\rangle = (\phi(1)\psi(2) + (-)^S \phi(2)\psi(1))/\sqrt{2} \quad |S, S_z\rangle$$

where  $|S, S_z\rangle = \chi_{S,S_z}(\sigma_1, \sigma_2)$  have the explicit form:

$$\begin{aligned} \chi_{1,1} &= v_+(\sigma_1)v_+(\sigma_2) \\ \chi_{1,0} &= \frac{1}{\sqrt{2}} [v_+(\sigma_1)v_-(\sigma_2) + v_-(\sigma_1)v_+(\sigma_2)] \\ \chi_{1,-1} &= v_-(\sigma_1)v_-(\sigma_2) \end{aligned} \quad \left. \vphantom{\begin{aligned} \chi_{1,1} \\ \chi_{1,0} \\ \chi_{1,-1} \end{aligned}} \right) \text{Spin triplet: symmetric}$$
$$\chi_{0,0} = \frac{1}{\sqrt{2}} [v_+(\sigma_1)v_-(\sigma_2) - v_-(\sigma_1)v_+(\sigma_2)] \quad \text{Spin singlet: antisymmetric}$$

# 2 interacting spins

## Energy

$$\begin{aligned} \langle \Psi_- | \mathcal{H} | \Psi_- \rangle &= \langle \Psi_{+,-}^{orb} | \mathcal{H} | \Psi_{+,-}^{orb} \rangle = \langle \phi | h | \phi \rangle + \langle \psi | h | \psi \rangle + J_{12} + (-1)^S K_{12} \\ &= E_0 + J_{12} + (-1)^S K_{12} \end{aligned}$$

with the Hartree and the exchange terms:

$$J_{12} = \langle \phi(1)\psi(2) | V_{12} | \phi(1)\psi(2) \rangle$$

$$K_{12} = \langle \phi(1)\psi(2) | V_{12} | \phi(2)\psi(1) \rangle$$

The Pauli principle  $\Rightarrow$  the energy is affected by spin even if  $\mathcal{H}$  does not depend explicitly on it:

$$\langle S = 0 | \mathcal{H} | S = 0 \rangle = E_s \quad \text{singlet}$$

$$\langle S = 1 | \mathcal{H} | S = 1 \rangle = E_t \quad \text{triplet}$$

Hence:

$$\begin{aligned} \langle S = 0 | \mathcal{H} | S = 0 \rangle - \langle S = 1 | \mathcal{H} | S = 1 \rangle &= E_s - E_t \\ &= 2K_{12} \end{aligned}$$

# 2 interacting spins

## Energy

The relative order of  $E_s$ ,  $E_t$  depends on  $V_{12}$  ( $K_{12}$ )

In He, with  $V_{12}$ = repulsive Coulomb interaction,

$$E_s > E_t \quad (K > 0)$$

(a part from the ground state, when only singlet is allowed)

But the present discussion is independent on the sign of  $E_s - E_t$



# 2 interacting spins

**Idea: write a model hamiltonian explicitly dependent on spin (and only dependent on spin) which gives the same difference between the energy eigenvalues of its eigenstates as the original one.**

Consider the operator:

$$\Sigma_{12} = \vec{s}_1 \cdot \vec{s}_2 = \frac{1}{2}S^2 - \frac{3}{4}$$

which is diagonal on the coupled basis, with eigenvalues:

$$\langle S = 0 | \Sigma_{12} | S = 0 \rangle = -\frac{3}{4}, \quad \langle S = 1 | \Sigma_{12} | S = 1 \rangle = \frac{1}{4}$$

Consider then:

$$\mathcal{H}^{spin} = -(E_s - E_t)\Sigma_{12}$$

We have:

$$\langle S = 0 | \mathcal{H}^{spin} | S = 0 \rangle - \langle S = 1 | \mathcal{H}^{spin} | S = 1 \rangle = E_s - E_t$$

# Heisenberg hamiltonian

$$\mathcal{H}^{spin} = -(E_s - E_t)\Sigma_{12}$$

is therefore OK! Defining:  $J \equiv E_s - E_t$  , we have  
(going back to the individual basis representation):

$$\mathcal{H}^{spin} = -J\vec{s}_1 \cdot \vec{s}_2$$

$J > 0$  ( $E_s > E_t$ )  $\uparrow\uparrow$  spins favored => ferromagnetic case

$J < 0$  ( $E_s < E_t$ )  $\uparrow\downarrow$  spins favored => antiferromagnetic case

# Heisenberg hamiltonian

Extension to the case of several spins:

$$\mathcal{H}^{spin} = - \sum_{\substack{i,j=1 \\ i \neq j}}^N J_{ij} \vec{s}_i \cdot \vec{s}_j$$

(see also: Ashcroft & Mermin, chap. 32,  
“Spin hamiltonian and Heisenberg model”)

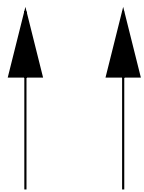
# Ising model

Consider only the possibility :  $s_i = \pm 1$  and **nearest neighbor interaction only**, with the same interaction constant  $J$

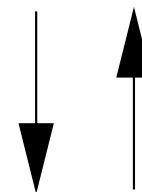
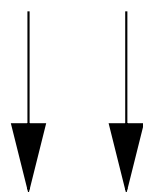
$$\mathcal{H}^{spin} = -J \sum_{i,j=1}^N s_i s_j$$

$J > 0$  ( $E_s > E_t$ )  $\uparrow\uparrow$  spins favored  $\Rightarrow$  **ferromagnetic case**

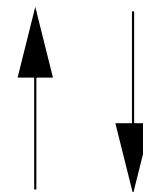
$J < 0$  ( $E_s < E_t$ )  $\uparrow\downarrow$  spins favored  $\Rightarrow$  **antiferromagnetic case**



$E = -J$



$E = +J$

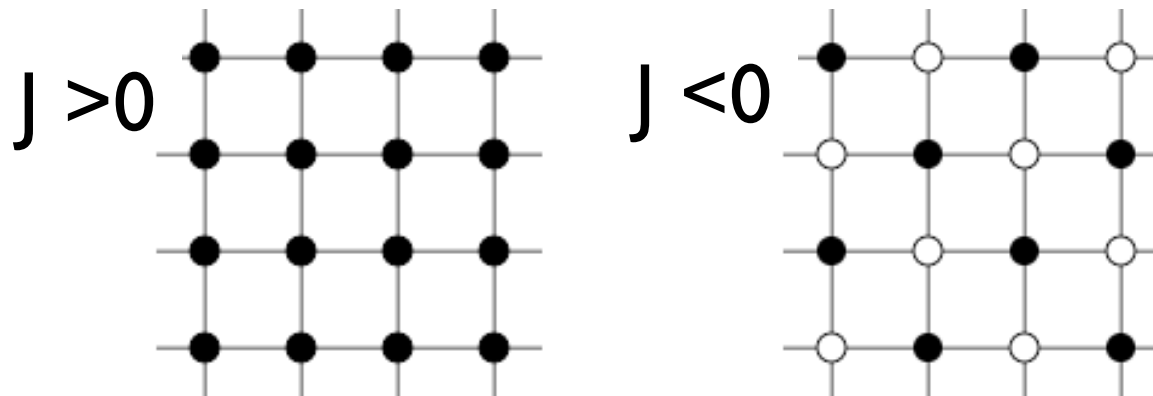


(choosing the kind of interaction, we specify the **energy model**)

# Ising model on a lattice

lattice containing  $N$  sites

lattice site  $i$  has associated with it a number  $s_i$ , where  $s_i = +1$  for an “up” ( $\uparrow$ ) spin and  $s_i = -1$  for a “down” ( $\downarrow$ ) spin. A particular configuration or **microstate** of the lattice is specified by the set of variables  $\{s_1, s_2, \dots, s_N\}$  for all lattice sites.



Lowest energy state of the 2D Ising model on a square lattice with ferromagnetic ( $J > 0$ ) and antiferromagnetic ( $J < 0$ ) interactions. Solid and open circles correspond to  $+1$  and  $-1$  spins, respectively.

# Ising model: interesting quantities

# Ising model: energy

lattice containing  $N$  sites  
No external magnetic field:

$$E = -J \sum_{i,j=\text{nn}(i)}^N s_i s_j$$

(nn=nearest neighbor)

Energy in presence of an external magnetic field:

$$E = -J \sum_{i,j=\text{nn}(i)}^N s_i s_j - H \sum_{i=1}^N s_i,$$

or, better, define an **average energy per spin**:  $E/N$

# Ising model: magnetization

$$M = \sum_{i=1}^N s_i$$

**“Order parameter”**: total magnetization,  
or -better- consider the average magnetization per spin:

$$m = \frac{M}{N} = \frac{1}{N} \sum_{i=1}^N s_i$$

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



# Ising model: configurations and energy

$2^n$  different configurations for  $n$  spins.  
(microstates)

e.g.  $2^4 = 16$  spin configurations for  $2 \times 2$  lattice

$ m =1$	+	+	-	-
	+	+	-	-

$ m =0$	+	-	-	+
	-	+	+	-

$ m  \neq 0$	-	+	+	-	+	+	+	+	+	-	-	+	+	-	-
	+	+	+	+	+	-	-	+	+	-	-	-	-	+	-

-	-	+	-	+	+	-	+	$ m =0$
+	+	+	-	-	-	-	+	

For  $J > 0$  the state of lowest energy is when all the spins are aligned.

The state has macroscopic magnetization (**ferromagnetic**).

The **ground state energy** per spin

(ferromagnetic case, thermodynamic limit ( $N$  large), no ext. field) is:

$$E_0/N = -2J$$

# Ising model: boundary conditions

Of course we cannot simulate an infinite system (the thermodynamic limit).

We have two choices for the simulation cell:

- free or open boundary conditions
- periodic boundary conditions (PBC)

# Ising model: open boundary conditions

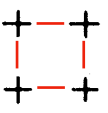
in a  $N=L \times L$  spin lattice there are  $2L(L-1)$  nn interactions;  
for the ferromagnetic g.s. configuration, for instance, the energy is:

			+	+	+	+
		+	+	+		
+	+	+	+	+	+	+
+	+	+	+	+	+	+

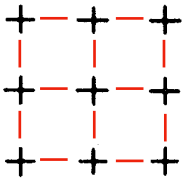
Let's count the interactions...

# Ising model: open boundary conditions

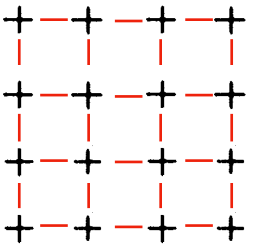
in a  $N=L \times L$  spin lattice there are  $2L(L-1)$  nn interactions;  
for the ferromagnetic g.s. configuration, for instance, the energy is:



$E_0/N = -J$



$E_0/N = -(12/9)J$



$E_0/N = -(24/16)J$

...

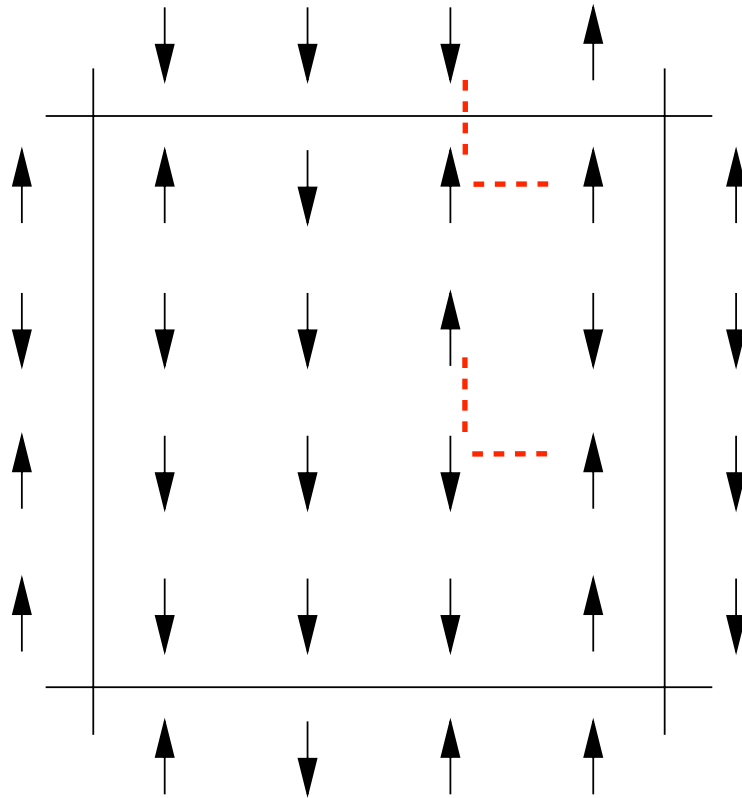
$E_0/N = -J \times 2L(L-1)/L^2$   
 $= -2J \times (1 - 1/L)$

(volume term)

(surface term)

Energy per spin in the ground state converges to the value  
 $E_0/N = -2J$  in the thermodynamic limit  
 (with deviations  $\sim 1/L$ )

# Ising model: PBC



The energy is a  $2N$ -term sum:  
each spin interacts with its NN  
within the simulation cell or  
with the NN images

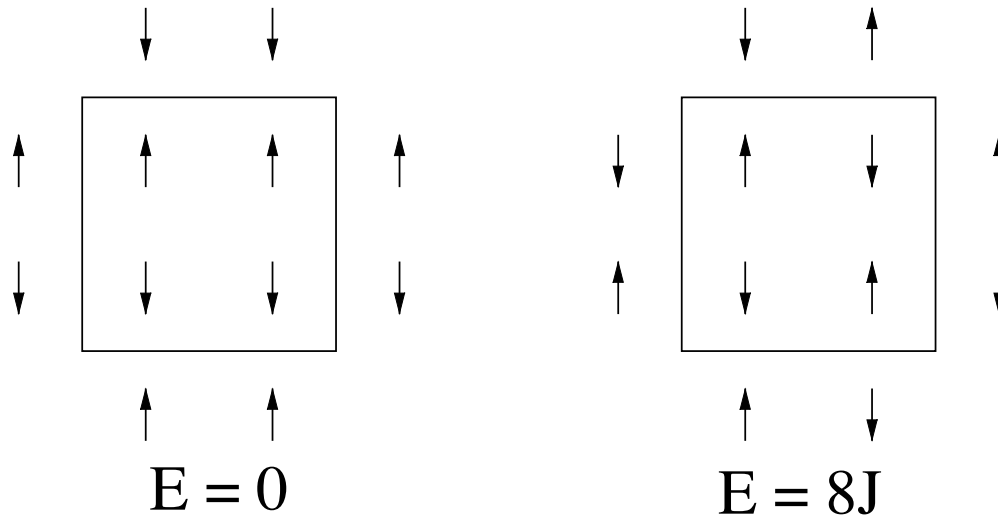
One of the  $2^N$  possible configurations of a system of  $N = 16$  Ising spins on a square lattice.  
with periodic boundary conditions.

# Ising model: PBC

We have always:

$2^4 = 16$  spin configurations for  $2 \times 2$  lattice

but the energy for each configuration in case of open boundary conditions and PBC is different:



Two different configurations with 2 spins up

# of spins UP	Degeneracy	Energy	Magnetisation
4	1	$-8J$	4
3	4	0	2
2	4	0	0
2	2	$8J$	0
1	4	0	-2
0	1	$-8J$	-4

Energy and magnetization of 16 configurations of the  $2 \times 2$  Ising model with PBC

Energy per spin in the ground state is always (also in small systems) equal to the value  $E_0/N = -2J$  of the thermodynamic limit

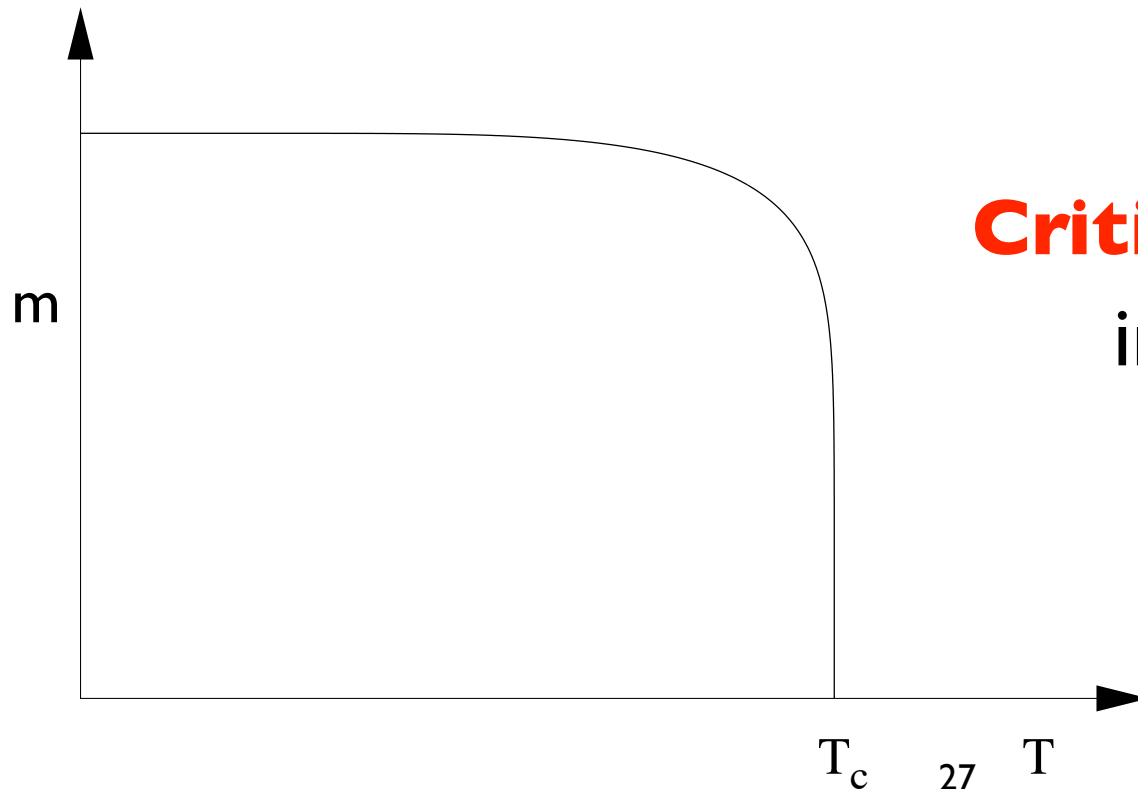
# Ising model: phase transition

**Low T: spin configuration minimizes energy**

(if  $J > 0$ : spins tend to align  $\Rightarrow$  **high (absolute) magnetization**)

**High T: spin configuration maximizes entropy**

(=disorder) (spins tend to disalign  $\Rightarrow$  **low magnetization**)



**existence of a  
Critical temperature  $T_c$**

in 2D the model has an  
analytical solution:

$$T_c = 2.269 J/k_B$$

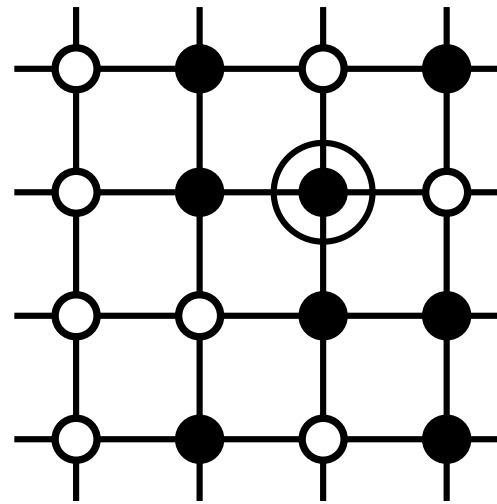
# Ising model: dynamics?

Beside an **energy model**, we must define a **dynamics** in order to simulate the evolution of the system (i.e. to generate the trajectory in the phase space, to generate the configurations of the Markov chain)



# Ising model: spin flip dynamics

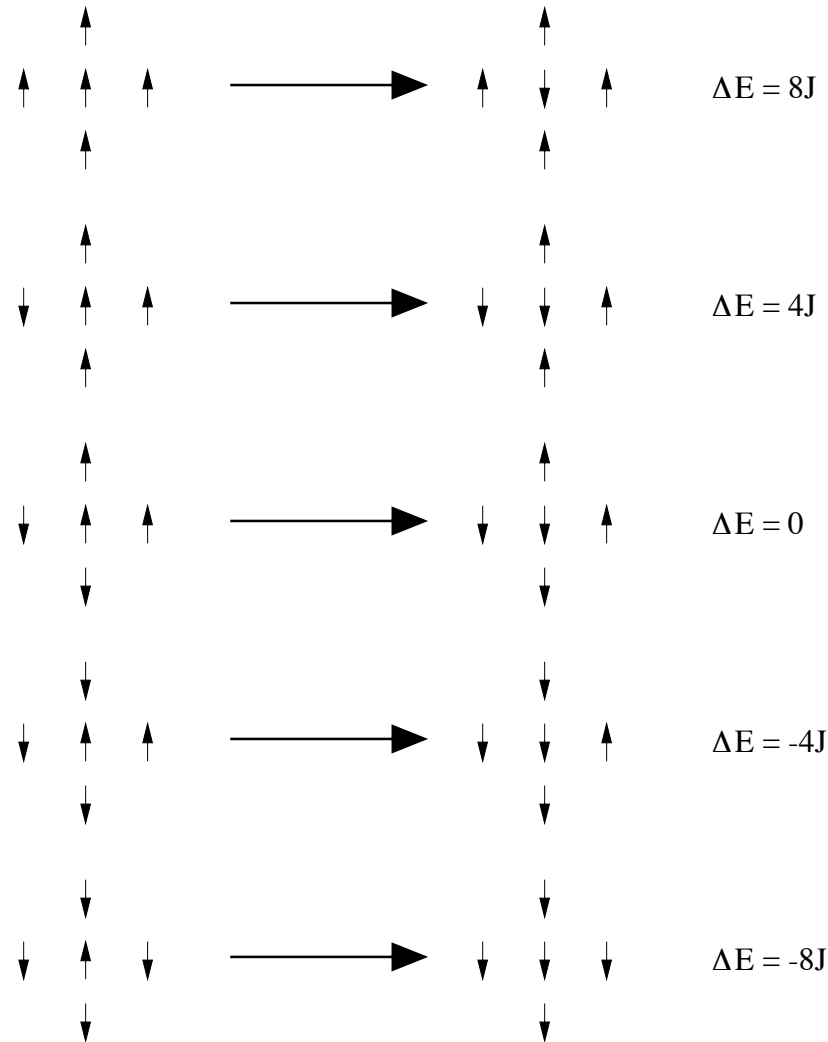
Consider  $nn$  interactions, choose a random spin and flip it: it's **a new configuration** (a microstate)



Apply **Metropolis Monte Carlo** method for evolution in the **canonical ensemble** (fix  $T$ ). Evolution is driven by the **energy change** between the old and the new configuration,  $\Delta E$ .

Remark: Is it sufficient to calculate only  $\Delta E$ , not  $E$  at each new configuration!

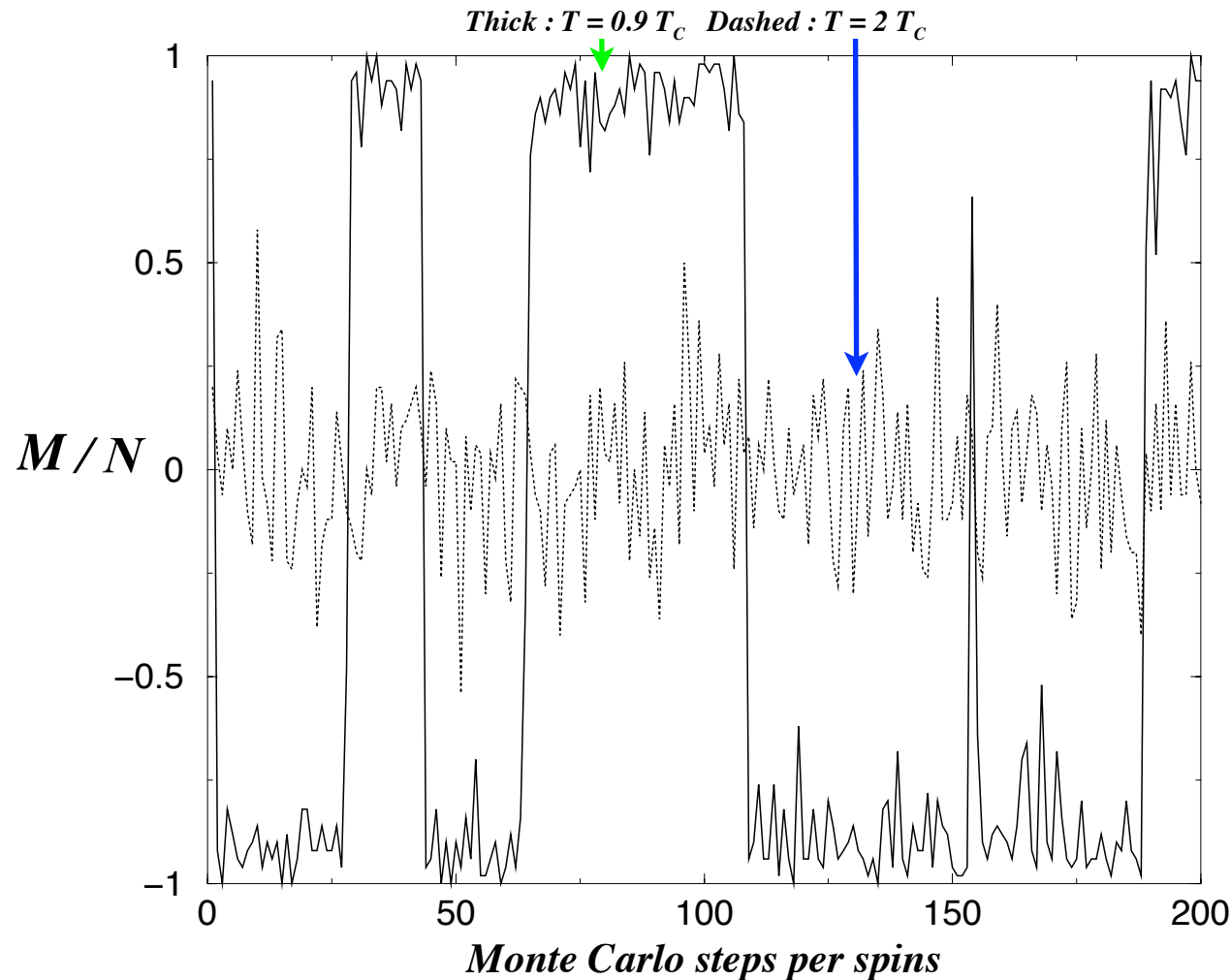
# Ising model: spin flip dynamics



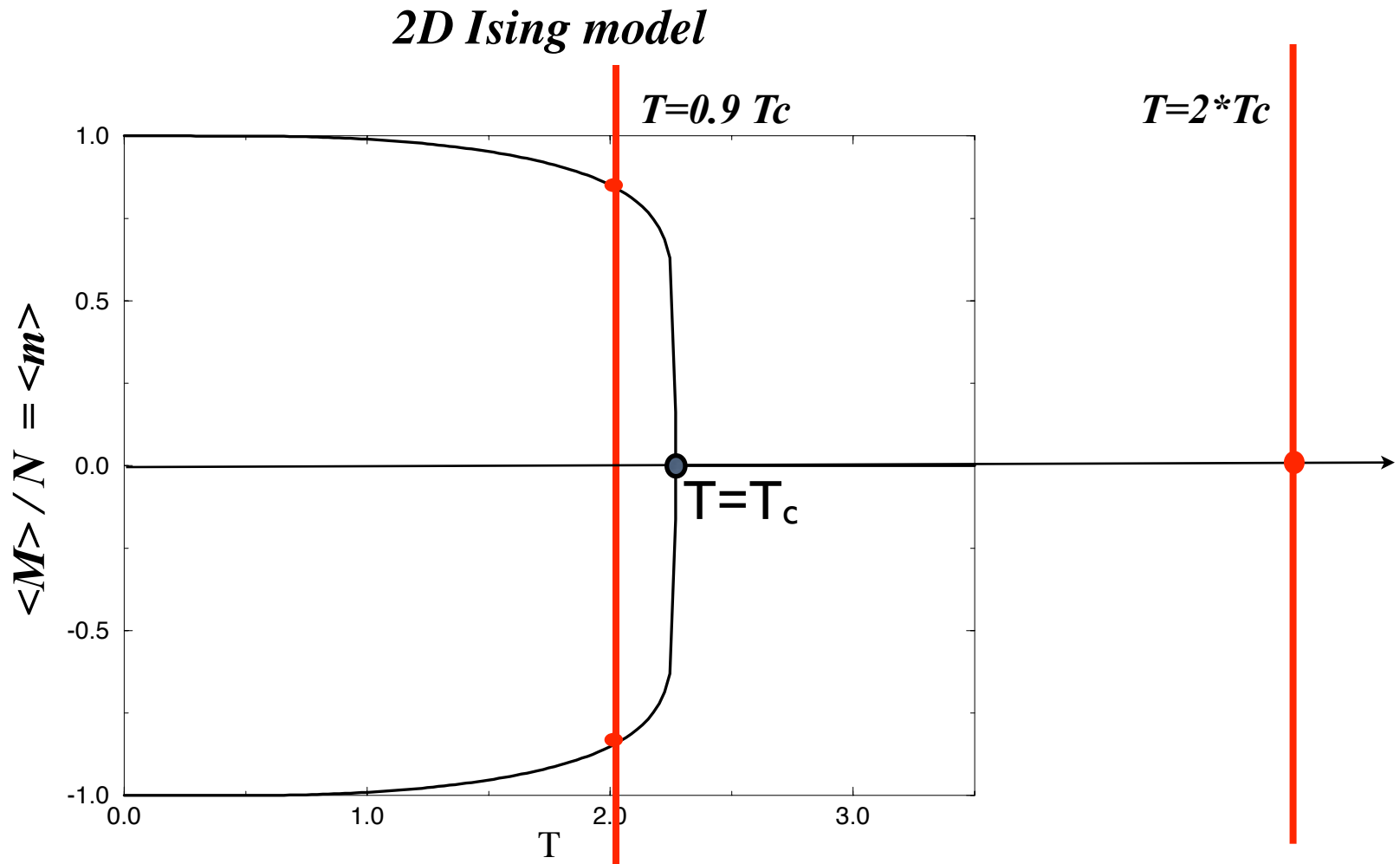
The five possible transitions of the Ising model on the square lattice with spin flip

# Apply **Metropolis Monte Carlo** method for evolution in the **canonical ensemble** (fix $T$ ):

Average magnetization per spin as a function of time for a lattice  $10 \times 10$  and two different  $T$

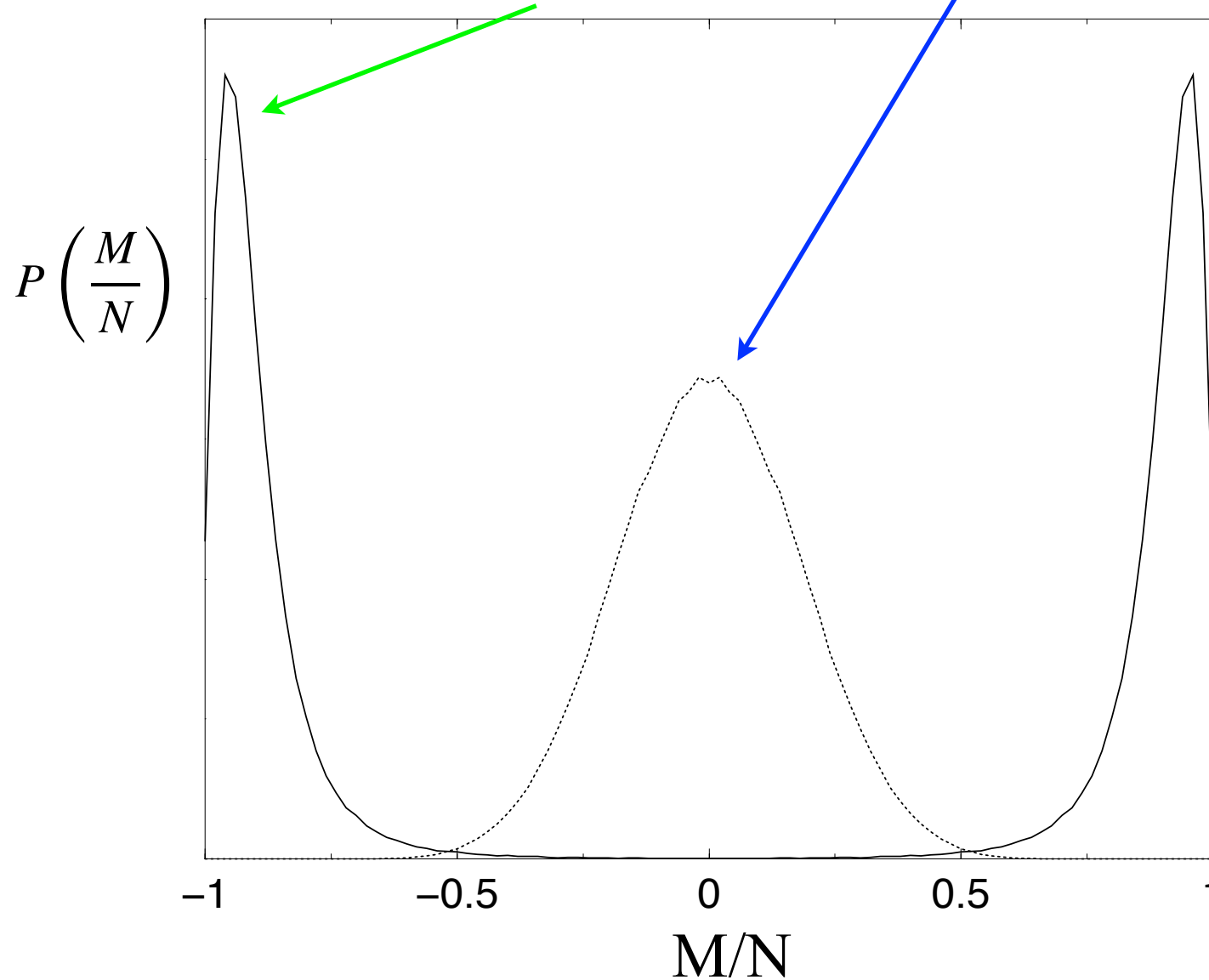


Fluctuations! do, as usual, **temporal averages**:  $\langle M \rangle / N$ ,  $\langle E \rangle / N$



Magnetisation as a function of the temperature for the 2D Ising model.  
(data averaged on time; red lines indicate the  $T$  values in the previous plot)

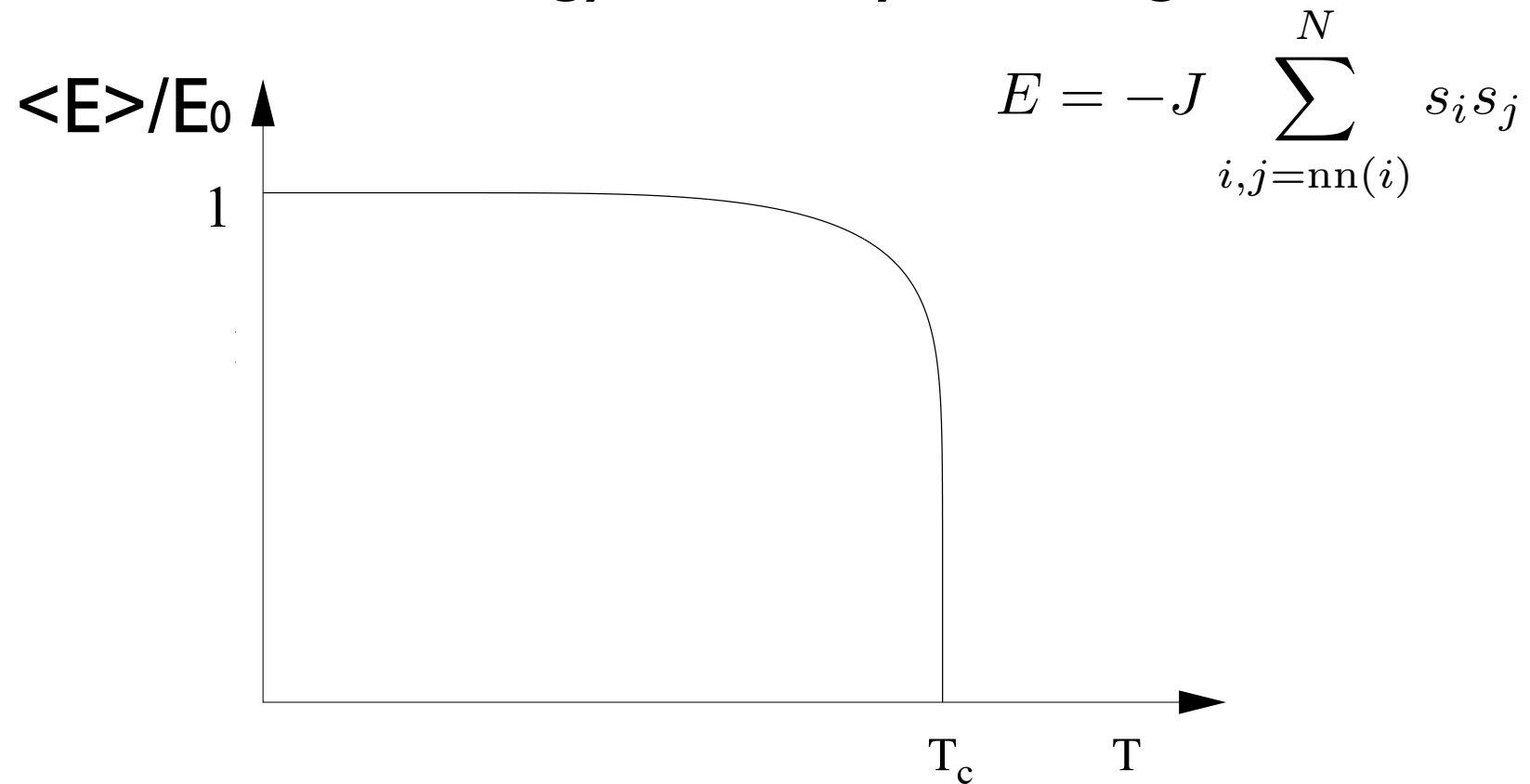
Magnetization distribution for  $T < T_c$  (solid) and  $T > T_c$  (dashed curve)



(data collected during time evolution, at equilibrium)

# Ising model: phase transition

$T_c$  also for energy, not only for magnetization:



and also the energy fluctuates during time evolution...

# Intrinsic energy fluctuations in the canonical ensemble - I

Remind:  $\langle E \rangle = \frac{1}{Z} \sum_s E_s e^{-\beta E_s}$  and  $Z = \sum_s e^{-\beta E_s}$ , therefore:  $\langle E \rangle = -\frac{\partial}{\partial \beta} \ln Z$

Consider the thermal capacity:

$$C_v = \frac{\partial \langle E \rangle}{\partial T} = \dots = -\frac{1}{kT^2} \frac{\partial \langle E \rangle}{\partial \beta}$$

we have

$$\frac{\partial \langle E \rangle}{\partial \beta} = -\frac{1}{Z^2} \frac{\partial Z}{\partial \beta} \sum_s E_s e^{-\beta E_s} - \frac{1}{Z} \sum_s E_s^2 e^{-\beta E_s} = \langle E \rangle^2 - \langle E^2 \rangle = -\langle (\delta E)^2 \rangle$$

where  $\delta E \equiv E - \langle E \rangle$

Result:

$$C_v = \frac{\langle (\delta E)^2 \rangle}{k_B T^2}$$

The thermal capacity (or specific heat if considered for each particle) is related to the intrinsic stochastic energy fluctuations

# Intrinsic energy fluctuations in the canonical ensemble - II

Since:

$$C_v = \frac{\langle (\delta E)^2 \rangle}{k_B T^2}$$

if  $N$  is the number of particles, we have:

$$\frac{\sqrt{\langle (\delta E)^2 \rangle}}{\langle E \rangle} = \frac{\sqrt{k_B T^2 C_v}}{\langle E \rangle} \propto \frac{\sqrt{N}}{N} \sim \frac{1}{\sqrt{N}}$$

i.e., the relative energy fluctuations reduce when  $N$  is large

(correct; in the thermodynamic limit:  $E \rightarrow \text{const.}$ , macro  $\sim$  micro)



# Ising model: fluctuations

Fluctuations are intrinsic to the system evolution  
and are important!

Linear response functions are related to  
equilibrium fluctuations:

$$C = \frac{\partial \langle E \rangle}{\partial T}, \quad C = \frac{1}{kT^2} (\langle E^2 \rangle - \langle E \rangle^2)$$

And

$$\chi = \lim_{H \rightarrow 0} \frac{\partial \langle M \rangle}{\partial H}, \quad \chi = \frac{1}{kT} (\langle M^2 \rangle - \langle M \rangle^2)$$

where  $\langle M \rangle$  and  $\langle M^2 \rangle$  are evaluated in zero magnetic fields.

# Ising model: fluctuations and phase transition

Rapid change in  $\langle E \rangle$  and  $\langle M \rangle \Rightarrow$  singularities in  $C$  and  $\chi$

(Large fluctuations near  
the phase transition:

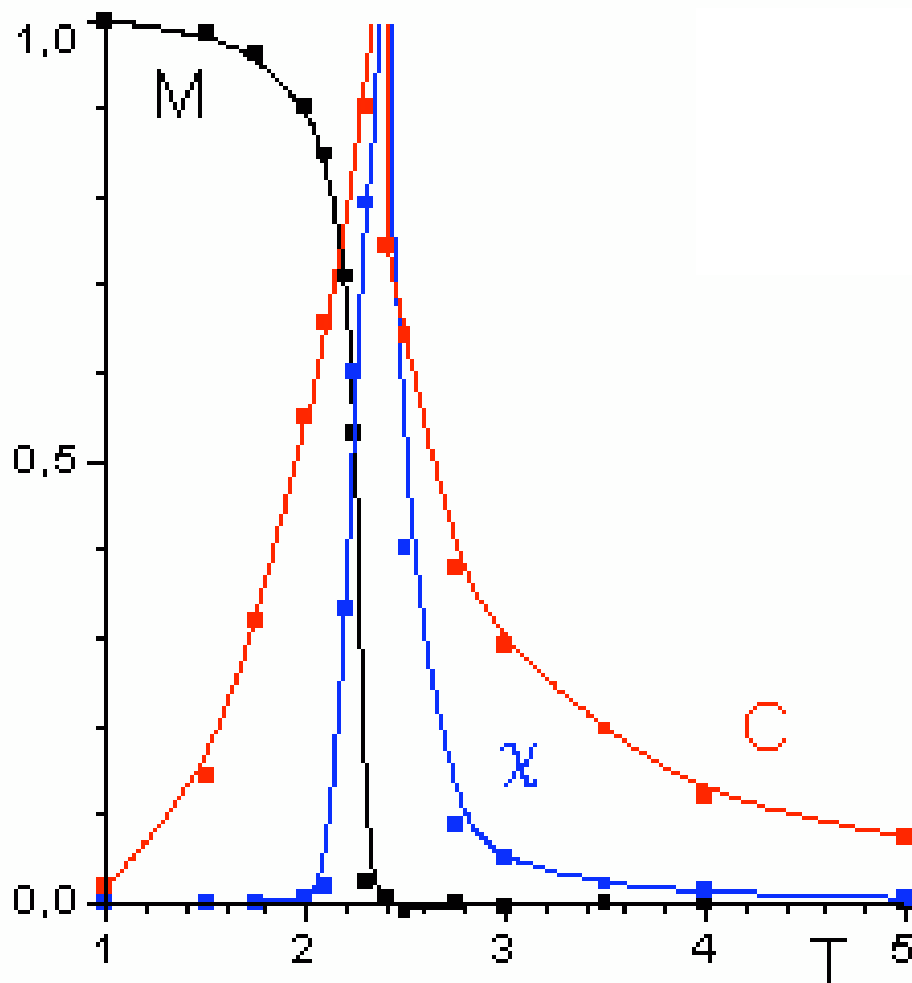
Second Order phase transition)

specific heat:

$$C = \frac{\partial \langle E \rangle}{\partial T}$$

magnetic susceptibility:

$$\chi = \lim_{H \rightarrow 0} \frac{\partial \langle M \rangle}{\partial H}$$



# Implementing the Ising model in the code

# Implementing the Ising model

on a 2D square lattice in the canonical ensemble

zero-field, nearest neighbor interactions only

$$\mathcal{H}^{spin} = -J \sum_{i,j=1}^N s_i s_j \quad s_i = \pm 1$$

Input parameters are:

- $L$  (linear lattice dimension, which gives the number of spins:  $N=L*L$ )
- *nmcs* (number of total MC steps per spin)
- *nequil* (number of equilibration MC steps per spin)
- $T$  (temperature of the thermal bath).

# Implementing the Ising model

```
program ising
  ! metropolis algorithm for the ising model on a square lattice
  use common
  integer :: imcs, ispin, jspin
  real (kind = double), dimension(5) :: cum
  | call initial(nequil, cum)
  ! equilibrate system
  || do imcs = 1, nequil
  ||   call metropolis()
  || end do
  ! accumulate data while updating spins
  ||| do imcs = 1, nmcs
  |||   call metropolis()
  |||   call data(cum)
  ||| end do
  call output(cum)
  ....
  ....
end program ising
```

# Ising model on a lattice

L : linear lattice dimension

N = LxL : number of spins

**a configuration** (a microstate) is the whole sequence of spins, i.e. the LxL array spin(x,y)

```
module common
```

```
.....
```

```
integer, public, dimension(:, :), allocatable :: spin
```

```
subroutine initial(nequil,cum)
```

```
.....
```

```
allocate(spin(L,L))
```

```
.....
```

```
spin(x,y) = 1
```

```
else
```

```
spin(x,y) = -1
```

```
.....
```

$$S_i = \pm 1$$

# Ising model: magnetization

Total magnetization, or define an average magnetization per spin:

$$M = \sum_{i=1}^N s_i$$

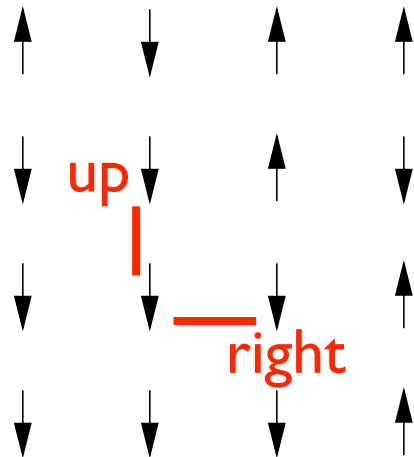
$$m = \frac{M}{N} = \frac{1}{N} \sum_{i=1}^N s_i$$

```
! compute initial magnetization
M = 0.0_double
do y = 1,L
  do x = 1,L
    ....
    ....
    M = M + spin(x,y)
  end do
end do
```

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

(Instead of the loop over x,y, write: `M=sum(spin)` )

# Ising model: energy

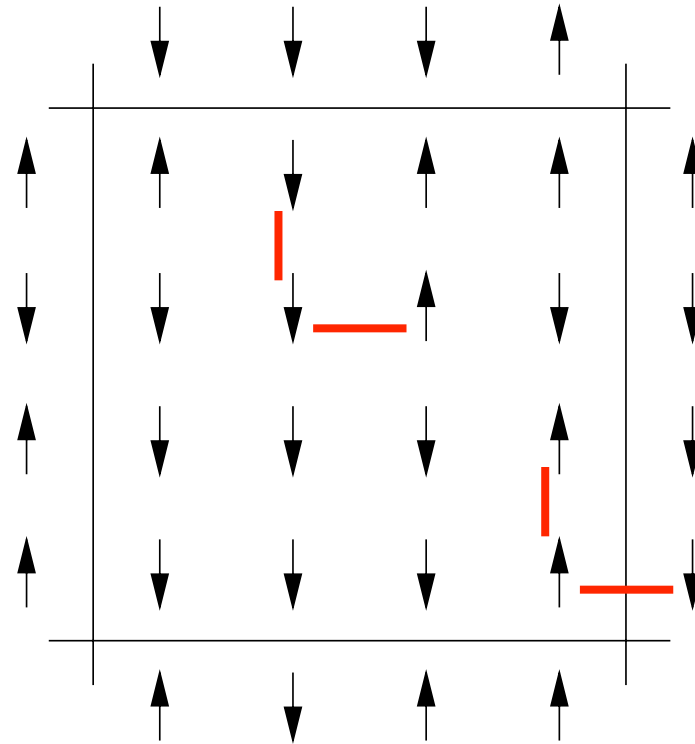
$$E = -J \sum_{i,j=\text{nn}(i)}^N s_i s_j$$


```
! compute initial energy
E = 0.0_double
do y = 1,L
.....
    do x = 1,L
        .....
        sums = spin(x,up) + spin(right,y)
! calculate the initial energy summing all over pairs
! (for a given spin, consider only the up NN and the right NN
! - NOT the down and the left NN - : each interaction is counted once
        E = E - spin(x,y)*sums
    end do
end do
```



# Ising model: energy with PBC

```
do y = 1,L
! periodic boundary conditions
if (y == L) then
  up = 1
else
  up = y + 1
end if
do x = 1,L
  if (x == L) then
    right = 1
  else
    right = x + 1
  end if
  sums = spin(x,up) + spin(right,y)
! calculate the initial energy summing all over pairs
! (for a given spin, consider only the up NN and the right NN
! - NOT the down and the left NN - : each interaction is counted once
  E = E - spin(x,y)*sums
end do
end do
```



# Ising model: spin flip dynamics

Choose a random spin and flip it:  
it's **a new configuration** (a microstate)

```
do ispin = 1,N
  !      random x and y coordinates for trial spin
  call random_number(rnd)
  x = int(L*rnd) + 1      ←  $1 \leq x \leq L$ 
  call random_number(rnd)
  y = int(L*rnd) + 1      ←  $1 \leq y \leq L$ 
  .....
```

Flip is:  $\text{spin}(x,y) = -\text{spin}(x,y)$

but do it later, only if you decide to accept the flip (according to Metropolis)

# Ising model: energy variations per spin flip

Evolution is driven by the **energy change** between the old and the new configuration (Metropolis MC)

```
dE = DeltaE(x,y) ← energy variation for spin(x,y) flip
call random_number(rnd)
if (rnd <= w(dE)) then ← w(dE) is  $e^{-\Delta E/k_B T}$ 
    spin(x,y) = -spin(x,y)
    accept = accept + 1
    .....
```

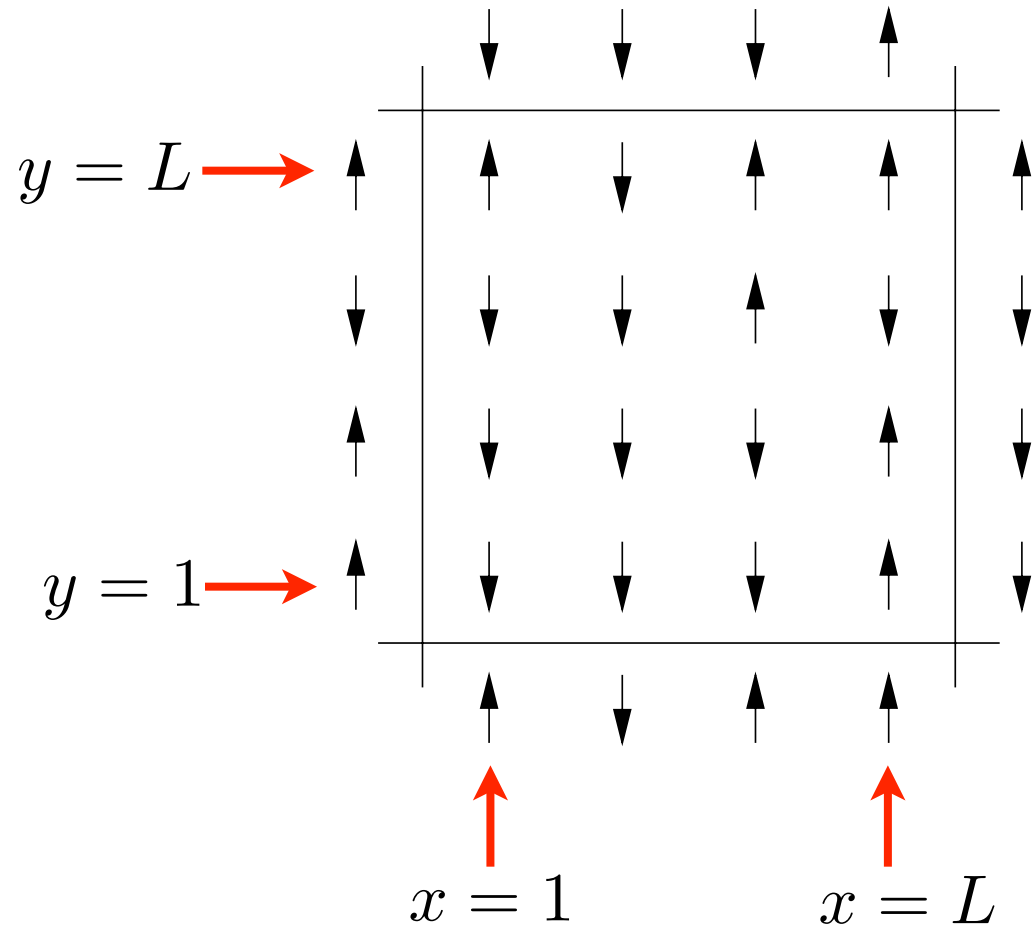
```
function DeltaE(x,y) result (DeltaE_result)
    .....
    DeltaE_result = 2*spin(x,y)*(left + right + up + down)
    .....
```

# Energy variations per spin flip with PBC

```

function DeltaE(x,y) result (DeltaE_result)
    ! periodic boundary conditions
    .....
    if (x == 1) then
        left = spin(L,y)
        right = spin(2,y)
    else if (x == L) then
        left = spin(L-1,y)
        right = spin(1,y)
    else
        left = spin(x-1,y)
        right = spin(x+1,y)
    end if
    if (y == 1) then
        up = spin(x,2)
        down = spin(x,L)
    else if (y == L) then
        up = spin(x,1)
        down = spin(x,L-1)
    else
        up = spin(x,y+1)
        down = spin(x,y-1)
    end if
    DeltaE_result = 2*spin(x,y)*(left + right + up + down)
    .....

```

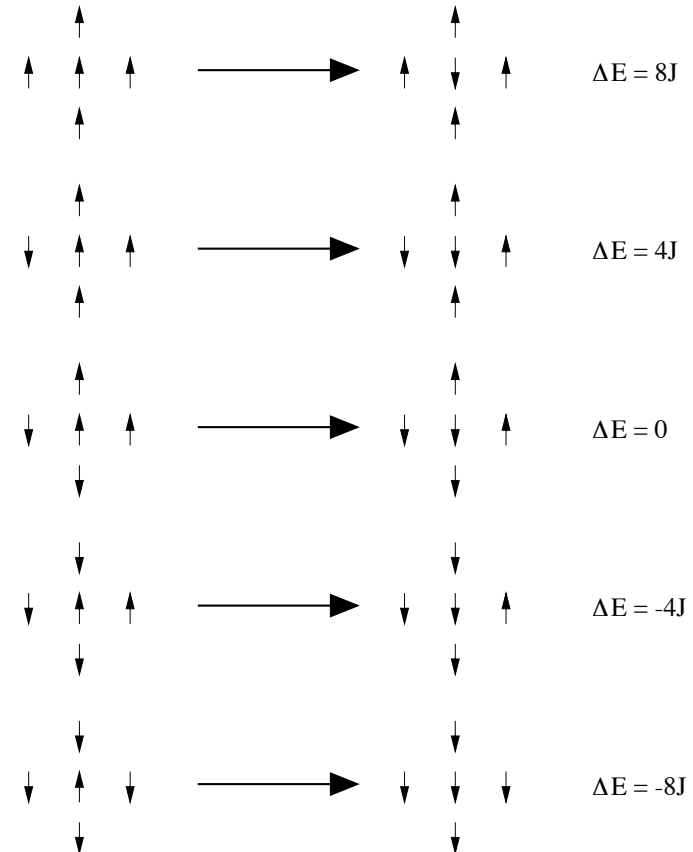


# Ising model: storage of Boltzmann's coeff.

```
! Choosing the interaction parameter J=1,  
! possible energy variations per spin flip are -8,-4,0,+4,+8:
```

```
  do dE = -8,8,4  
    w(dE) = exp(-dE/T)  
  end do  
  accept = 0  
  do i = 1,5  
    cum(i) = 0.0_double  
  end do
```

Convenient to store the  
Boltzmann's coefficient for  
these discrete values of  
energy variations



The five possible transitions of the Ising model on the square lattice with spin flip

# Ising model: updating energy and magnetization

```
subroutine metropolis()  
  ! one Monte Carlo step per spin  
  ....  
do ispin = 1,N  
  ....  
  dE = DeltaE(x,y)  
  call random_number(rnd)  
  if (rnd <= w(dE)) then  
    spin(x,y) = -spin(x,y)  
    accept = accept + 1  
    M = M + 2*spin(x,y) ! factor 2 is to account for the variation:  
    E = E + dE          ! (-(-)+(+))  
  end if  
end do  
end subroutine metropolis
```

DO NOT CALCULATE  
EVERYTHING FROM THE  
SCRATCH!!

$\Delta E$  is already a variation

# Spin flip dynamics: how to choose spin to flip?

## Random ...

```
do ispin = 1,N
  !      random x and y coordinates for trial spin
  call random_number(rnd)
  x = int(L*rnd) + 1      ←  $1 \leq x \leq L$ 
  call random_number(rnd)
  y = int(L*rnd) + 1      ←  $1 \leq y \leq L$ 
  ....
```

## or ordered (sequential) ...

```
do x = 1,L
do y = 1,L
  ...
```

$\text{spin}(x,y) = -\text{spin}(x,y)$

# Spin flip dynamics: how to choose spin to flip?

- ORDERED: in some cases, it could go more slowly towards equilibrium (see later: correlation time), but it depends...
- NO appreciable differences in the statistics at equilibrium



# Measuring physical quantities: how to accumulate data?

```
subroutine data(cum)
  ! accumulate data after every Monte Carlo step per spin
  real (kind = double), dimension(5), intent (inout) :: cum
  cum(1) = cum(1) + E
  cum(2) = cum(2) + E*E
  cum(3) = cum(3) + M
  cum(4) = cum(4) + M*M
  cum(5) = cum(5) + abs(M)
end subroutine data
```

After one MC step per spin for all spins:

```
do imcs = 1,nmcs
  call metropolis()           contains the loop over all the spins
  call data(cum)
end do
```

Alternatively, do it after each MC step per individual spin...

# Measuring physical quantities: how to accumulate data?

## Further remarks...

- Use statistically INDEPENDENT configurations
- Calculate therefore the CORRELATION TIME by considering the autocorrelation functions:

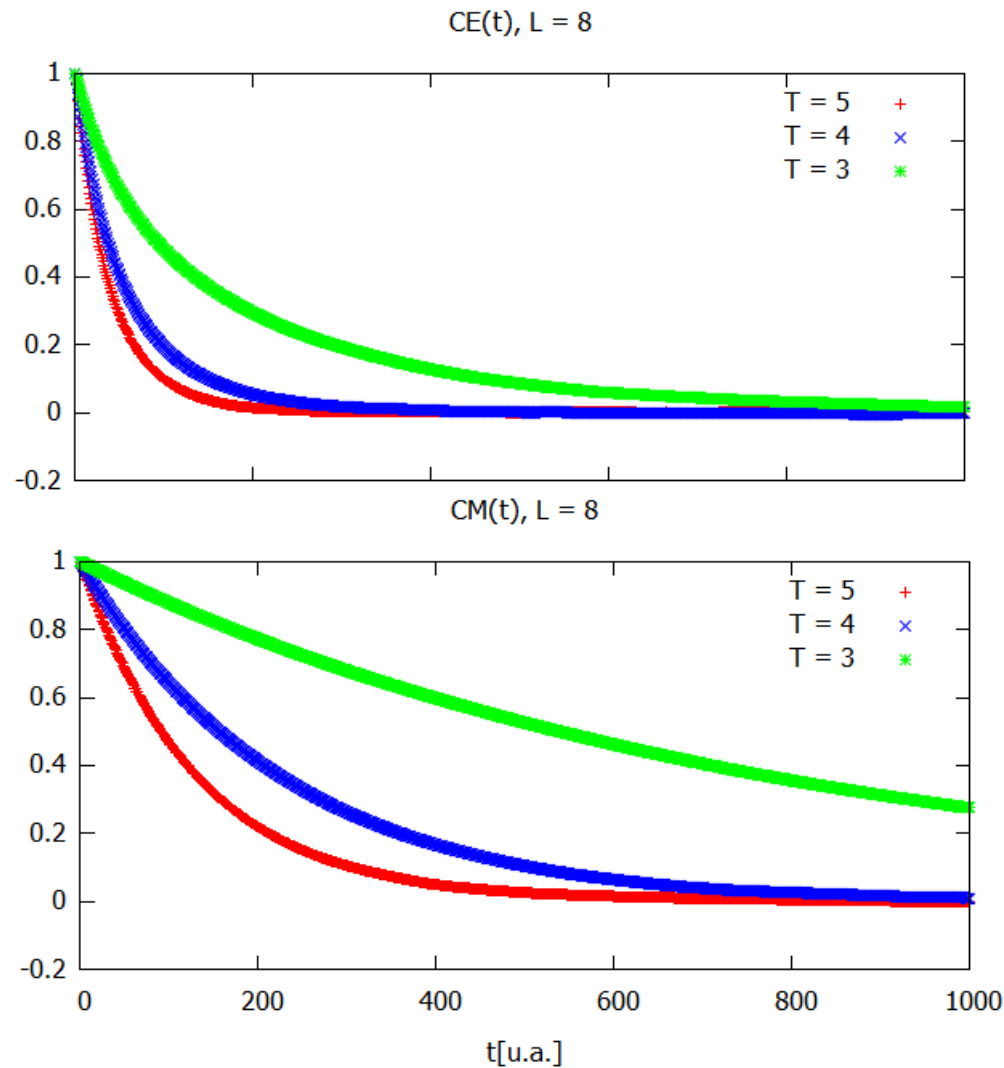
$$C_M(t) = \langle M(t)M(0) \rangle - \langle M \rangle^2, \quad C_E(t) = \langle E(t)E(0) \rangle - \langle E \rangle^2$$

$$(C_M(0) \propto \chi, \quad C_E(0) \propto C_V)$$

$C_M(t) \rightarrow 0$  and  $C_E(t) \rightarrow 0$  exponentially for  $t \rightarrow \infty$

with a certain decay time  $\tau$ : consider intervals longer than  $\tau$  for statistical averages

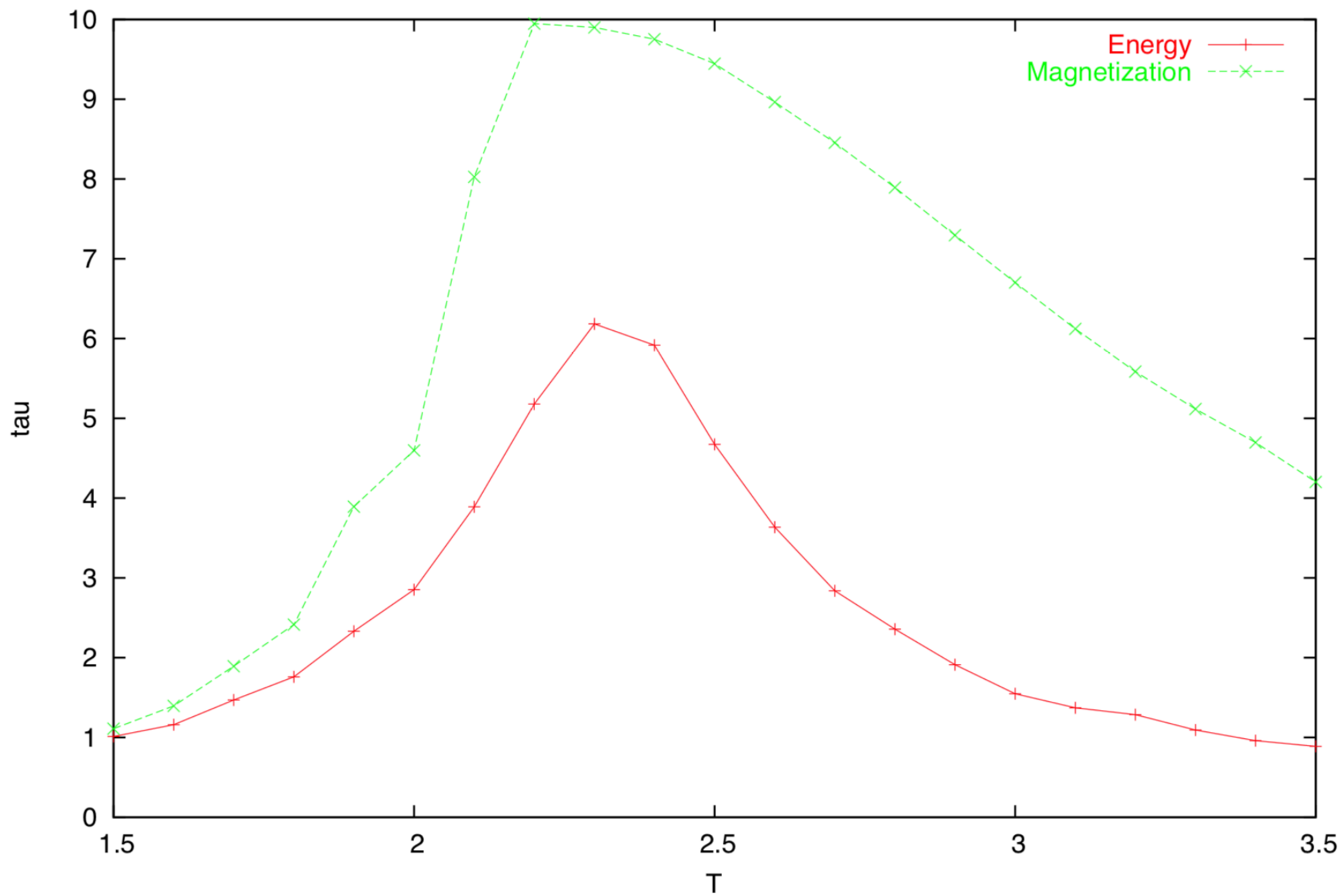
# Autocorrelation functions



(NOTE: "critical slowing down" for  $T \rightarrow T_C$ )

=> configurations change very slowly, and it is difficult to sample enough configurations

2-D Ising Model 20x20 Lattice Autocorrelation Times



# Measuring physical quantities: how to accumulate data?

## Further remarks...

- see also CORRELATION LENGTH between magnetic domains,  $\zeta(T)$
- close to  $T_c$ , also the correlation length increases (spin alignments are more correlated), up to divergence

# Measuring physical quantities: which errors?

- necessary to give the ERROR ESTIMATE corresponding to the measured physical quantity !!!
- (see Tab. I of D.P. Landau, PRB 13, 2997 (1976), “Finite size behavior of the Ising square lattice”)
- do also BLOCKING (called “coarse grained technique” in that paper)

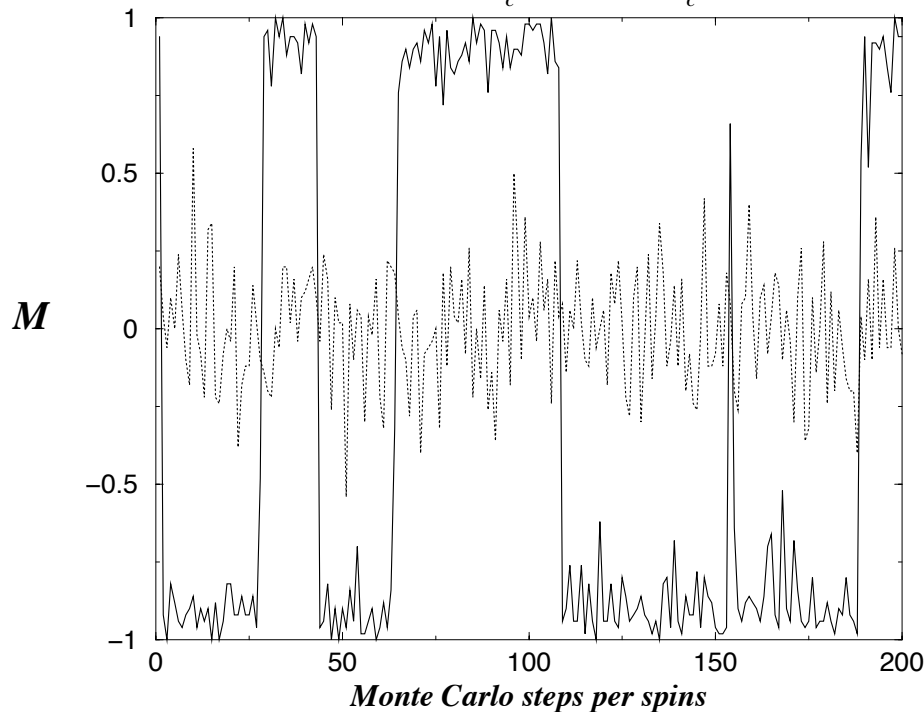
# How to do efficiently simulations as a function of $T$ ?

- Sometimes EQUILIBRATION time is long...
- IDEA: for  $T'$  close to  $T$ , choose as starting point the equilibrated output of  $T$

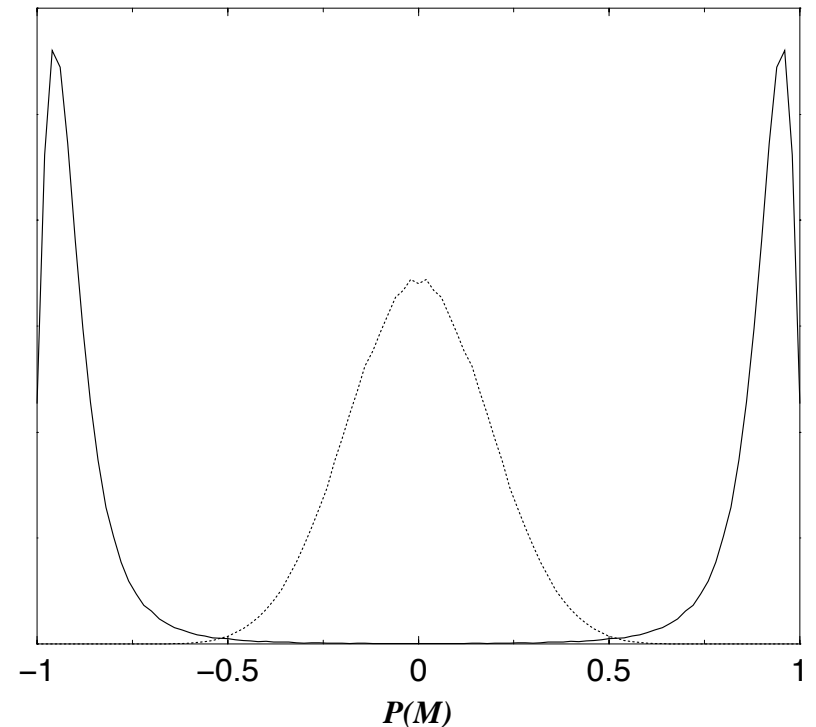
# How to do efficiently simulations as a function of $T$ ?

**Magnetization (System :  $10 \times 10$ )**

Thick :  $T = 0.9 T_c$  Dashed :  $T = 2 T_c$



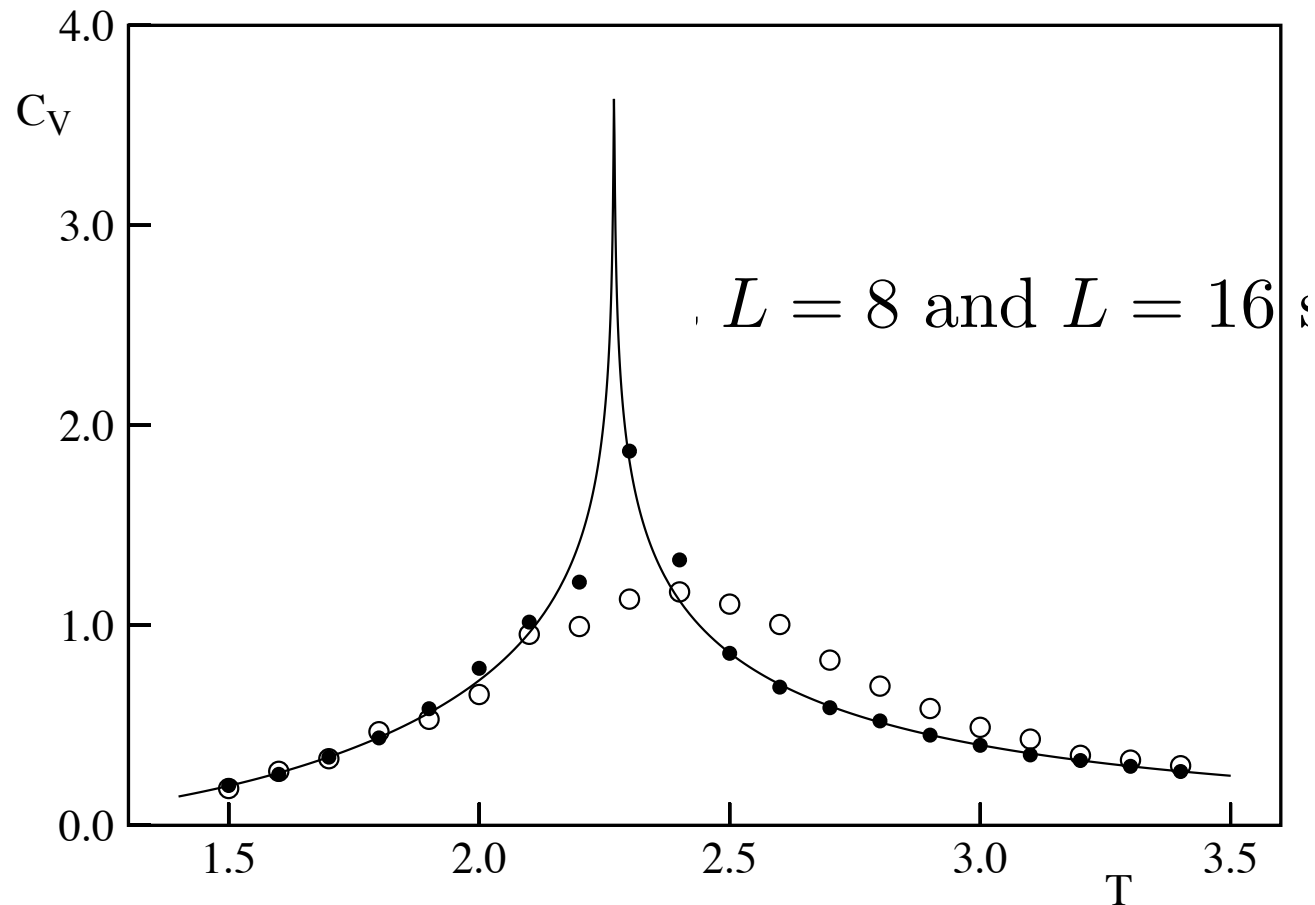
**Magnetization distribution**





# Ising model: size problems

We cannot simulate an INFINITE system!



The temperature dependence of the specific heat  $C$  (per spin) of the Ising model

# Ising model: size problems

## INTERFACE EFFECTS:

example of energy for HALF UP/HALF DOWN configurations:

$$L=2 \quad E=0$$

$$L=4 \quad E=-1$$

$$L=8 \quad E=-1.5$$

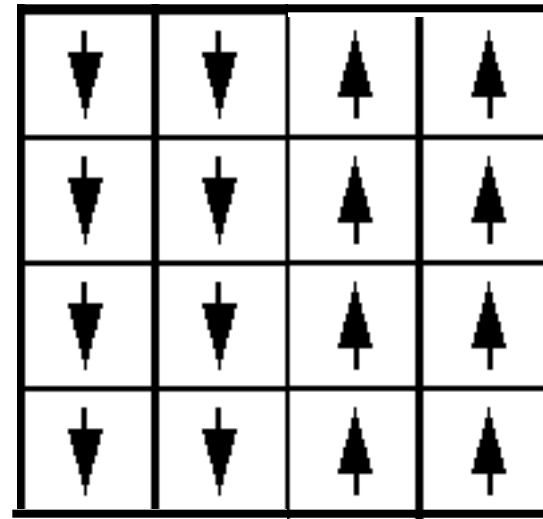
$$L=16 \quad E=-1.75$$

$$L=20 \quad E=-1.8$$

$$L=32 \quad E=-1.875$$

... for an infinite system:  $E=-2$

We have a (“interface”) term proportional to  $1/L$



“interface”

# Program:

On moodle2:

**ising.f90**

# Exercise

(a) Choose  $L=30, T=2$ , and initially  $\text{spin}=\pm 1$  randomly. Calculating and plotting the instantaneous values of the energy  $E/N$  and (together!) the magnetization  $M/N$  per spin (averaged over the lattice) as a function of Metropolis-MC steps, how much time (i.e. how many *nequil* MC steps) is it necessary to equilibrate the system?

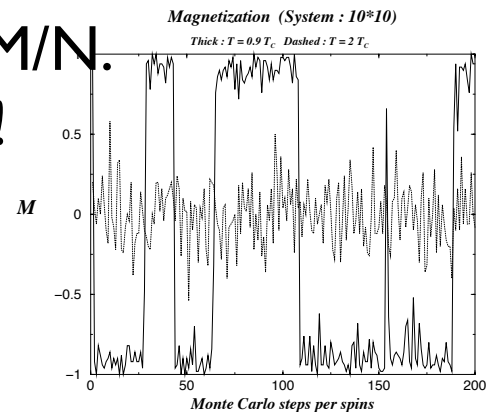
Hint:

- Since initially  $\text{spin}=\pm 1$  randomly,  $E/N$  and  $M/N$  initially will be far from the expected equilibrium average value.

First, set *nequil*=0 and plot instantaneous values of  $E/N$  and  $M/N$ .

Estimate *nequil* from that plot!!! Visualization is important!!!!

*nequil* of course depends on  $T$  and on the initial situation



Then, set *nequil* not zero and calculate the time average  $\langle E \rangle/N$  and  $\langle M \rangle/N$ ; increasing the total *nmcs*, the two quantities should converge...

# Exercise

(a) Choose  $L=30, T=2$ , and initially  $\text{spin}=\pm 1$  randomly. ...

Plot a snapshot of the spin pattern: does the system appear ordered or disordered?

it should appear **ordered**...

**p 'ising-up.dat' ps 3 pt 7, 'ising-down.dat' ps 3 pt 7**

Plotting “ising-up.dat” and “ising-down.dat” which contain the coordinates of spin up and down respectively, one should get something like that:



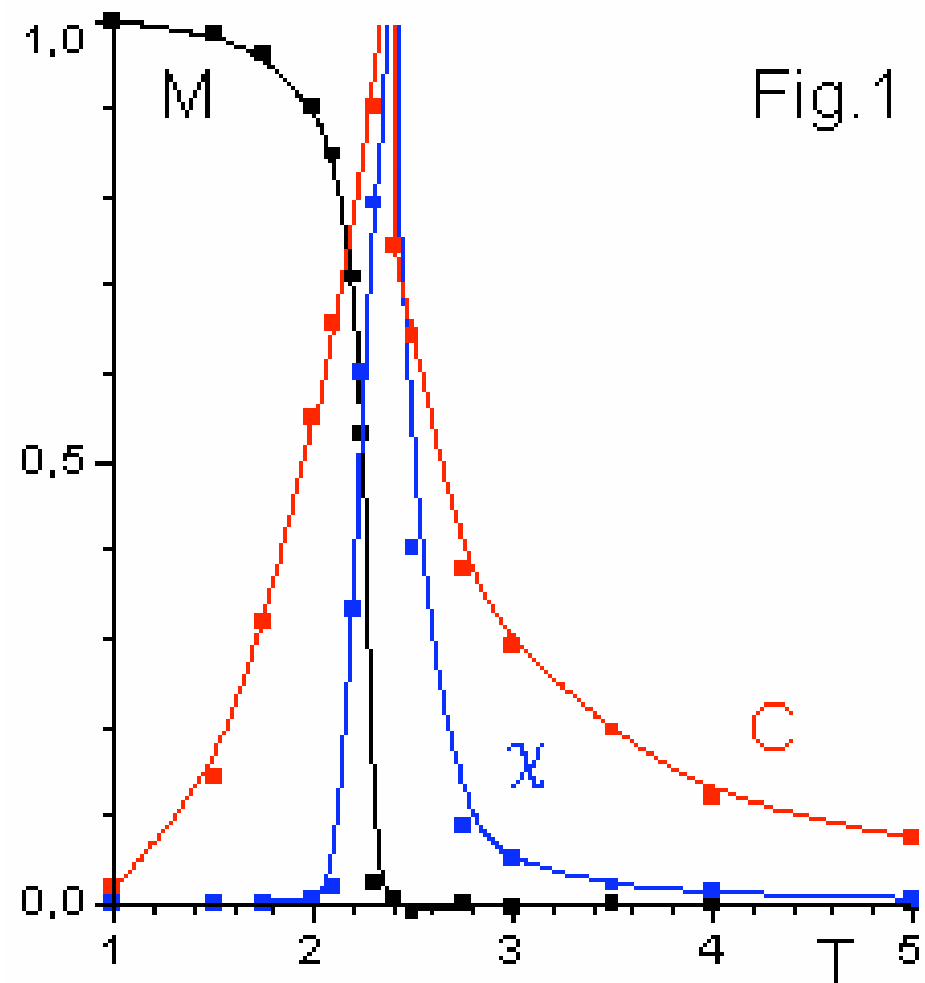
Calculate also  $c$  and  $\chi$ .

# Exercise

(a) Choose  $L=30, T=2$ , and initially  $\text{spin}=\pm 1$  randomly. ...

Calculate also  $c$  and  $\chi$ .

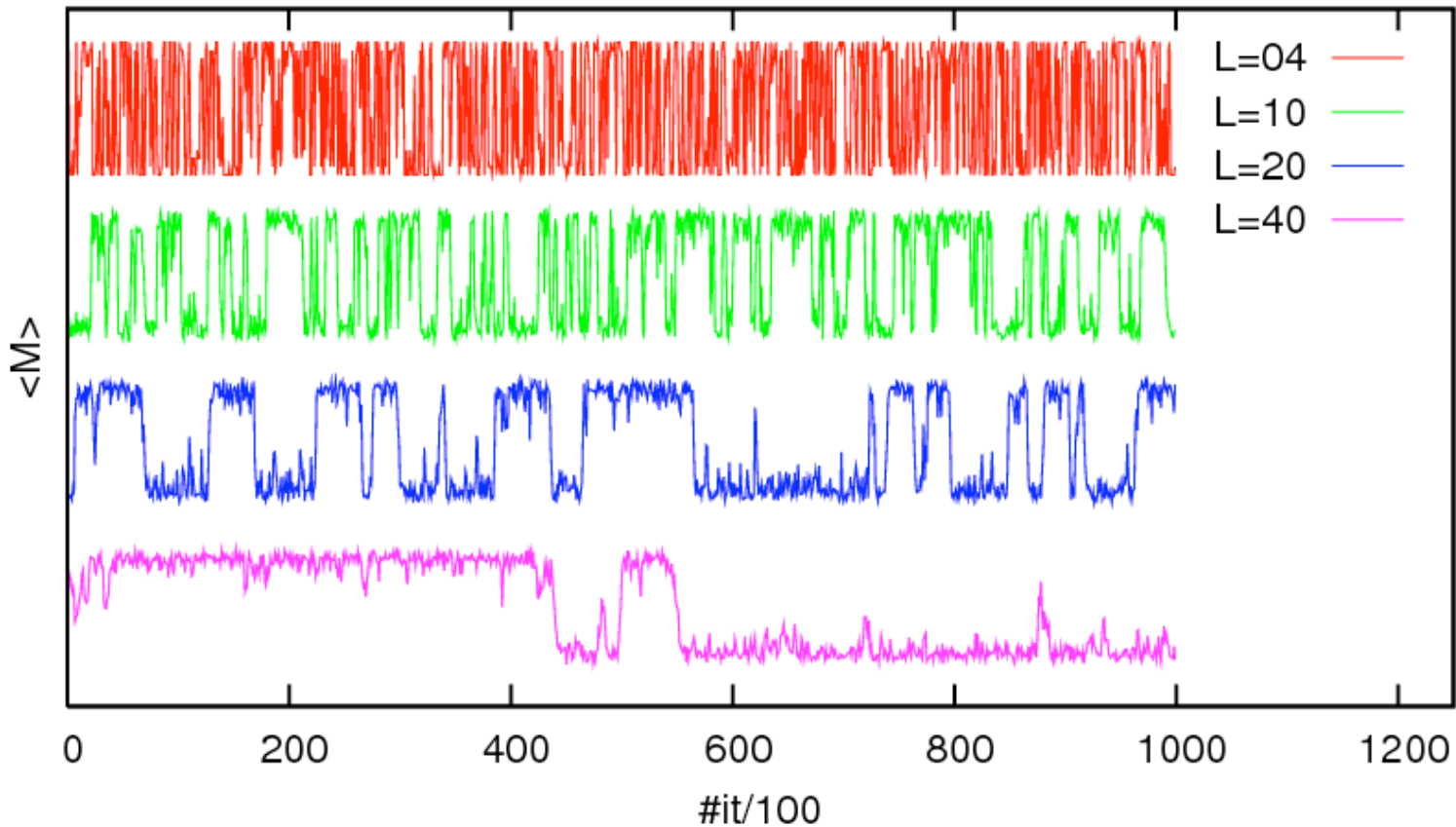
(b) Choose  $T=1$  and repeat (a)...



**Some results that you should obtain...**

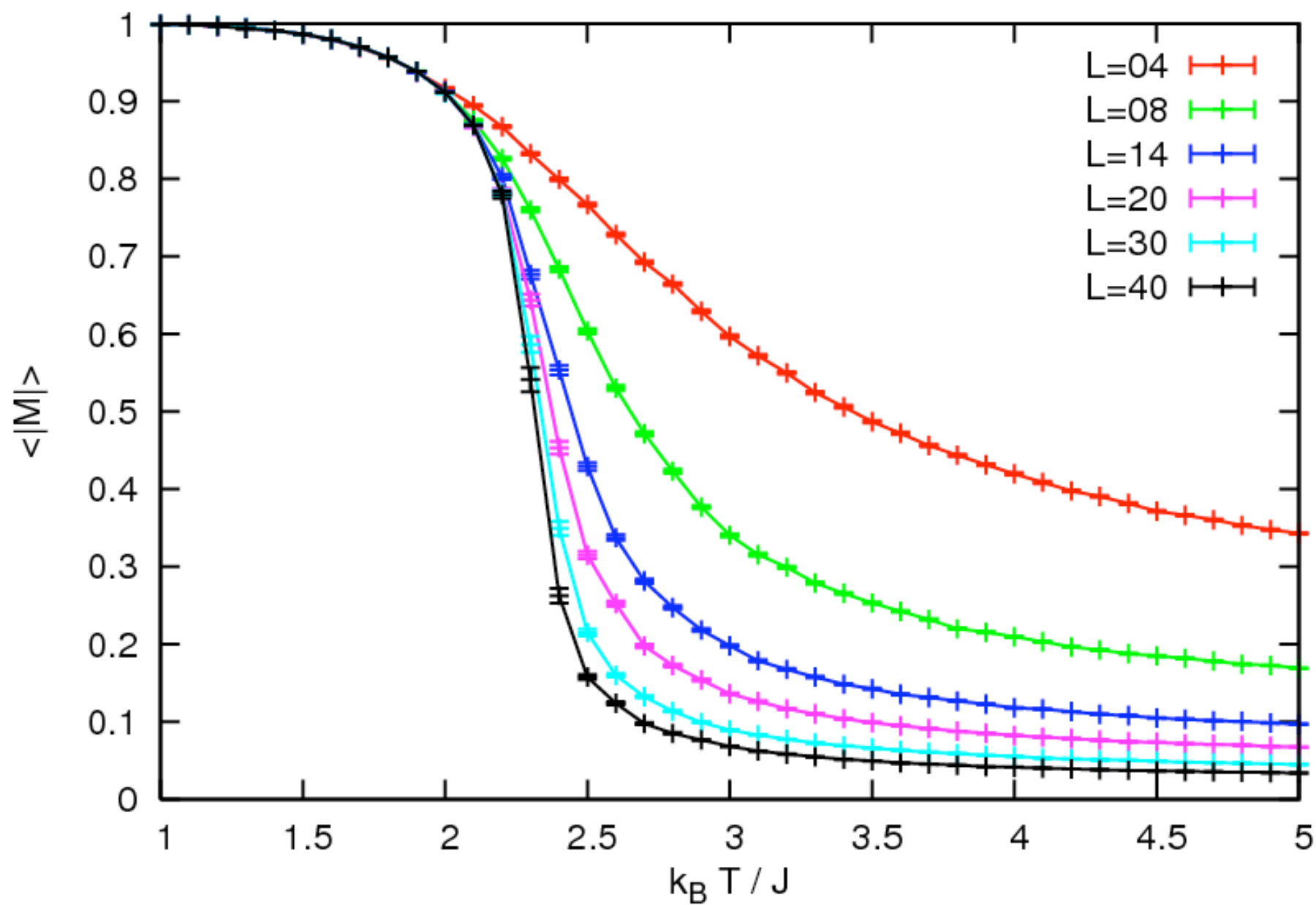
## Raw data: traces, covariance and autocorrelation time

Trace: magnetization for  $T = 2.27J/k_B \approx T_C$  ( $10^5$  sweeps)

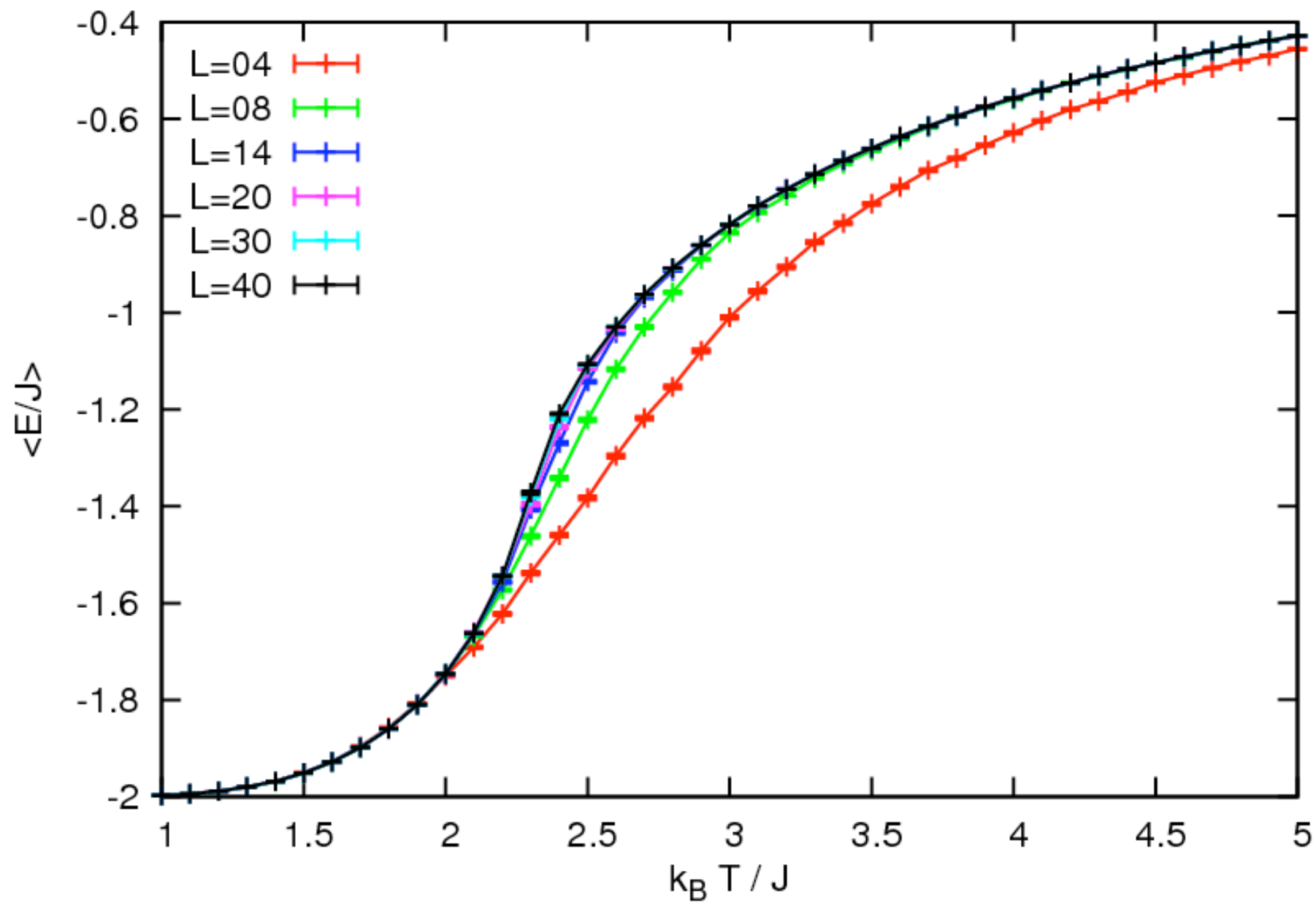




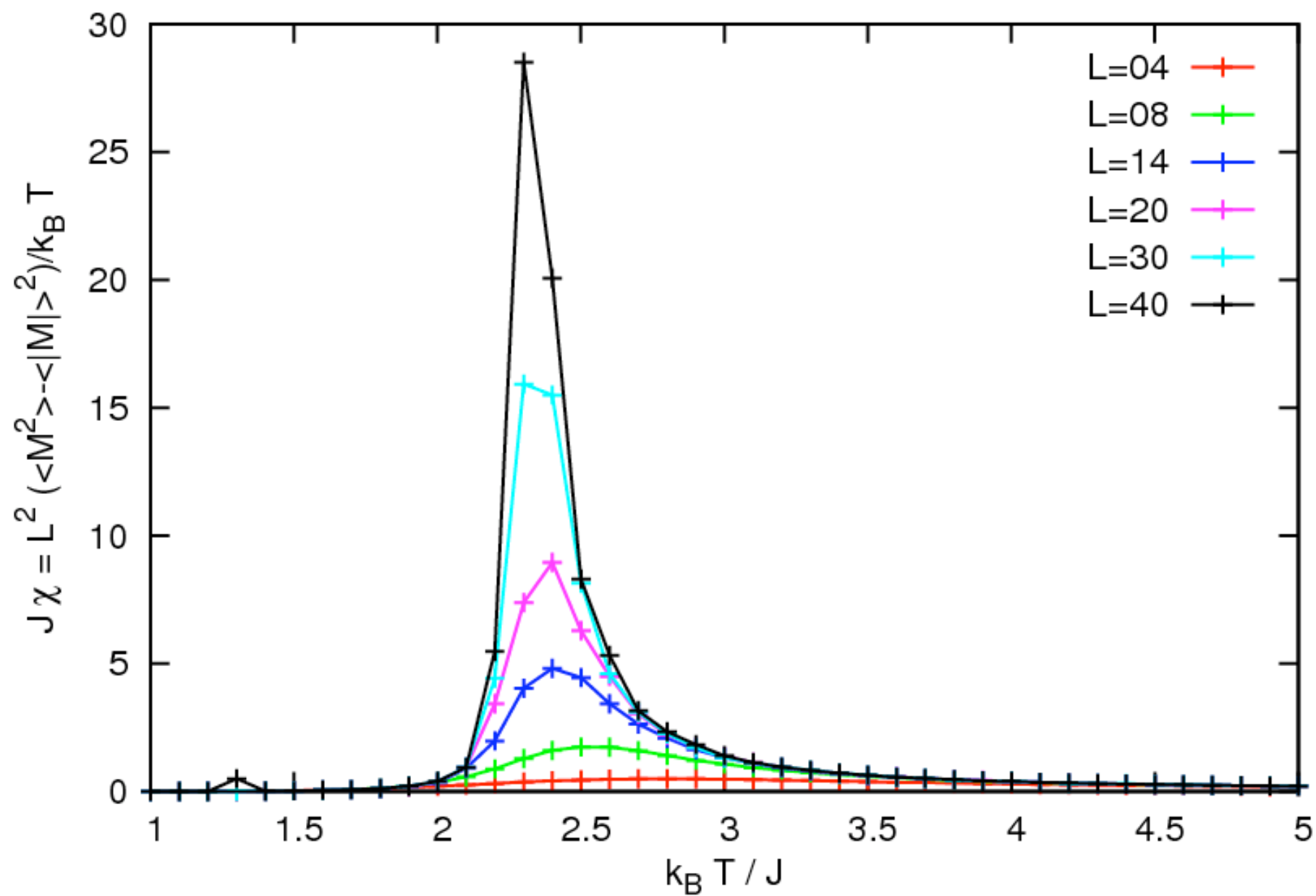
## Magnetization ( $10^5$ sweeps)



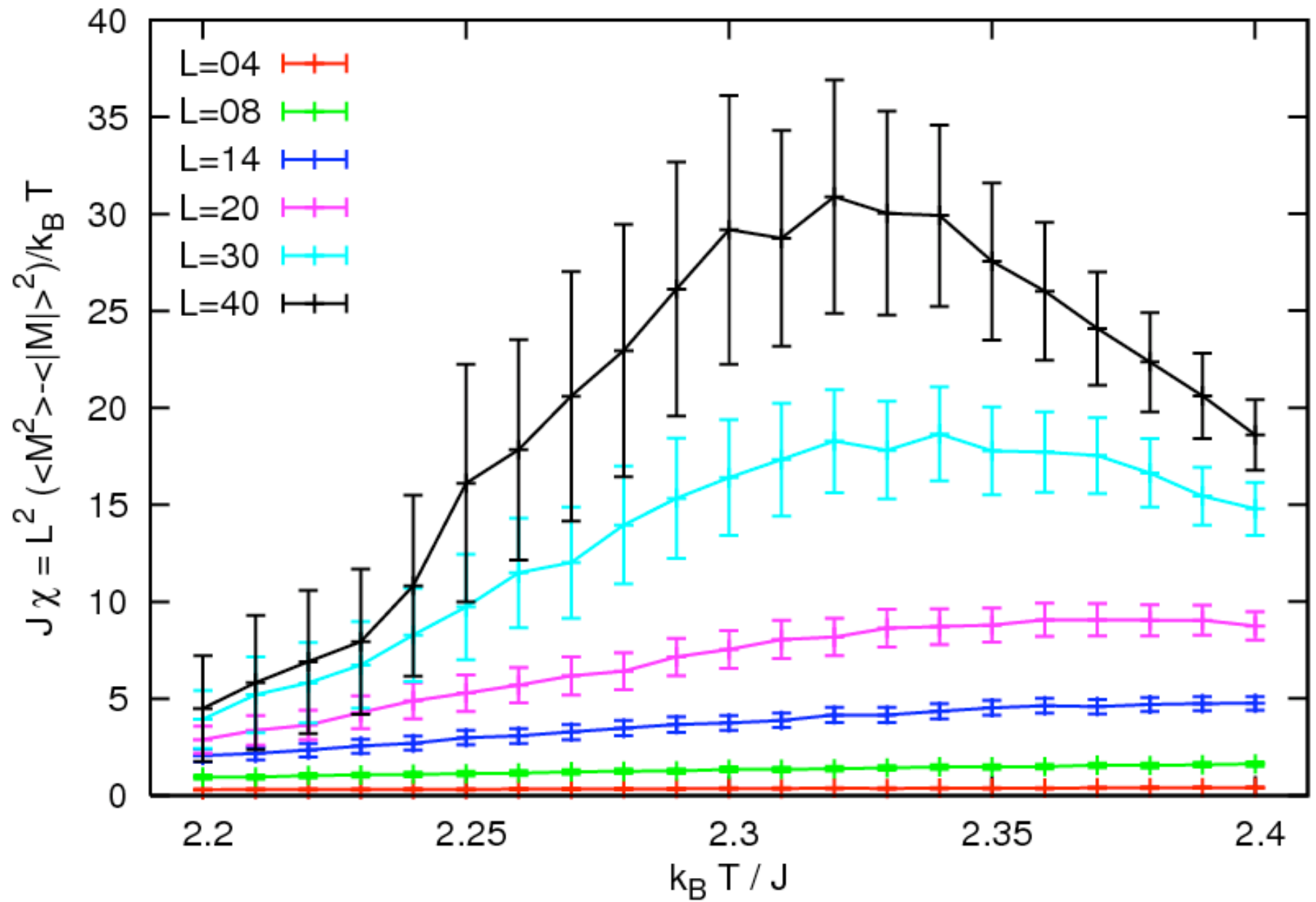
Energy ( $10^5$  sweeps)



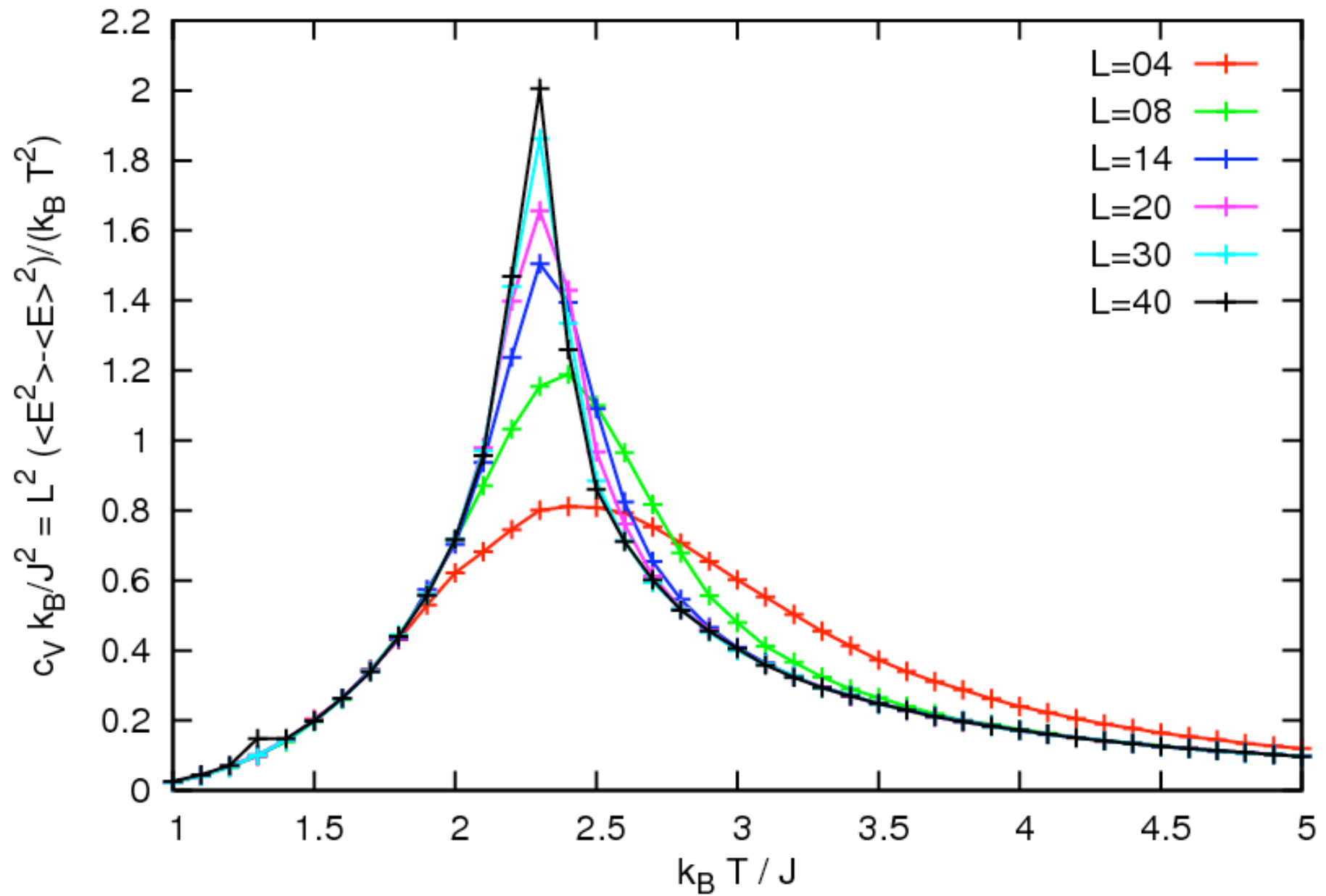
## Magnetic susceptibility ( $10^5$ sweeps)



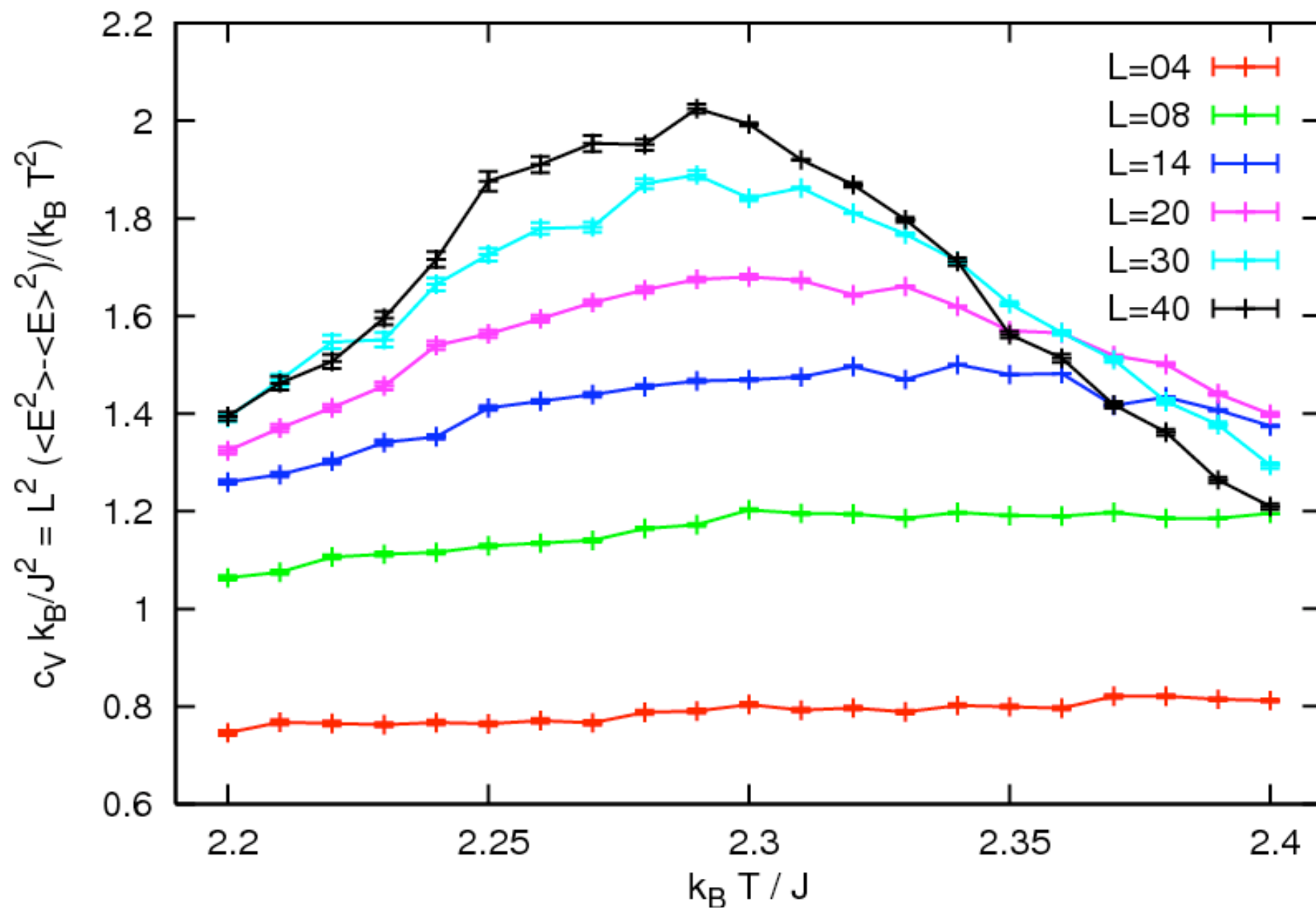
## Magnetic susceptibility near $T_c$ ( $10^6$ sweeps)



## Specific heat ( $10^5$ sweeps)



## Specific heat near $T_c$ ( $10^6$ sweeps)



# extra:

- References
- More on finite size effects: finite size analysis and critical exponents
- Alternative dynamics
- Other interactions
- Other lattices
- Other models

# A few references

Ising E 1925 Zeitschrift fur Physik 31 253–258

Bethe H 1931 Zeitschrift fur Physik 71 205

Heisenberg W 1928 Zeitschrift fur Physik 49 205



# Universality and critical exponents

Near  $T_c$ , we can characterize the behavior of many physical quantities by power law behavior just as we characterized the percolation threshold (see Table 13.1). For example, we can write  $m$  near  $T_c$  as

$$m(T) \sim (T_c - T)^\beta, \quad (17.22)$$

where  $\beta$  is a critical exponent (not to be confused with the inverse temperature). Various thermodynamic derivatives such as the susceptibility and heat capacity diverge at  $T_c$ . We write

$$\chi \sim |T - T_c|^{-\gamma} \quad (17.23)$$

and

$$C \sim |T - T_c|^{-\alpha}. \quad (17.24)$$

We have assumed that  $\chi$  and  $C$  are characterized by the same critical exponents above and below  $T_c$ .

Another measure of the magnetic fluctuations is the linear dimension  $\xi(T)$  of a typical magnetic domain. We expect the *correlation length*  $\xi(T)$  to be the order of a lattice spacing for  $T \gg T_c$ . Because the alignment of the spins becomes more correlated as  $T$  approaches  $T_c$  from above,  $\xi(T)$  increases as  $T$  approaches  $T_c$ . We can characterize the divergent behavior of  $\xi(T)$  near  $T_c$  by the critical exponent  $\nu$ :

$$\xi(T) \sim |T - T_c|^{-\nu}. \quad (17.25)$$

# Universality and critical exponents

More precisely, the magnetisation follow a power law close to the transition only approaching from smaller  $T$ :

$$M = 0 \qquad T \geq T_c$$

$$M \sim |1 - T/T_c|^\beta \qquad T < T_c$$

If we use the Reduced temperature :  $\Delta T = (T - T_c)/T_c$

$$C \sim |\Delta T|^{-\alpha}$$

$$M \sim |\Delta T|^\beta \quad \text{for } \Delta T < 0$$

$$\chi \sim |\Delta T|^{-\gamma}$$

$$\xi \sim |\Delta T|^{-\nu}$$

# Universality and critical exponents

the critical exponents are not independent from each other, because of the following scaling laws (●):

$$\begin{aligned}\gamma &= \nu(2 - \eta), \\ 2 &= \alpha + 2\beta + \gamma, \\ \nu d &= 2 - \alpha, \\ \gamma &= \beta(\delta - 1),\end{aligned}$$

so it is only necessary to know two of them to determine the others.

For the 2D Ising model:

$\alpha$	0
$\beta$	0.125
$\gamma$	1.750
$\nu$	1

- Kerson Huang, Introduction to Statistical Physics (CRC Press)

# Universality and critical exponents

If the heat capacity goes like:  $C(T) \propto |T - T_c|^{-\alpha}$

we could plot  $\frac{1}{C(T)}$  as a function of  $T$  and make a linear fit:

$$\frac{1}{C(T)} = a + bT$$

and similarly for the other quantities.

BUT: Because we can simulate only finite lattices, a direct fit of the measured quantities does not yield good estimates for the corresponding exponents  $\alpha$ ,  $\nu$ ,  $\beta$ , and  $\gamma \Rightarrow$  we have to take into account the finite size of the system

**$\Rightarrow$  finite size scaling**

# Universality and critical exponents

The shift in the peak position of  $C$  and  $\chi$  with respect to the critical temperature corresponding to the thermodynamic limit is described by:  $T_c(L) - T_c(\infty) \propto L^{-\lambda}$

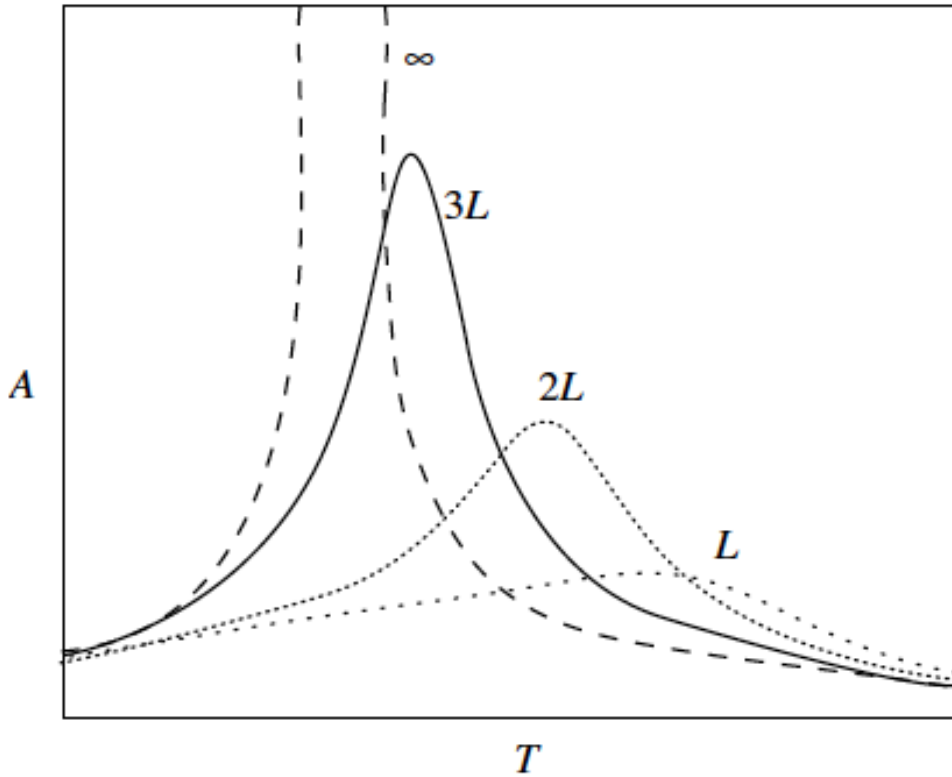


FIG. 1. Typical behaviour of a physical quantity  $A$  vs temperature close to the critical point for various system sizes. Figure taken from Thijsen<sup>8</sup>.

[Thijsen, Computational Physics (Cambridge University Press)]

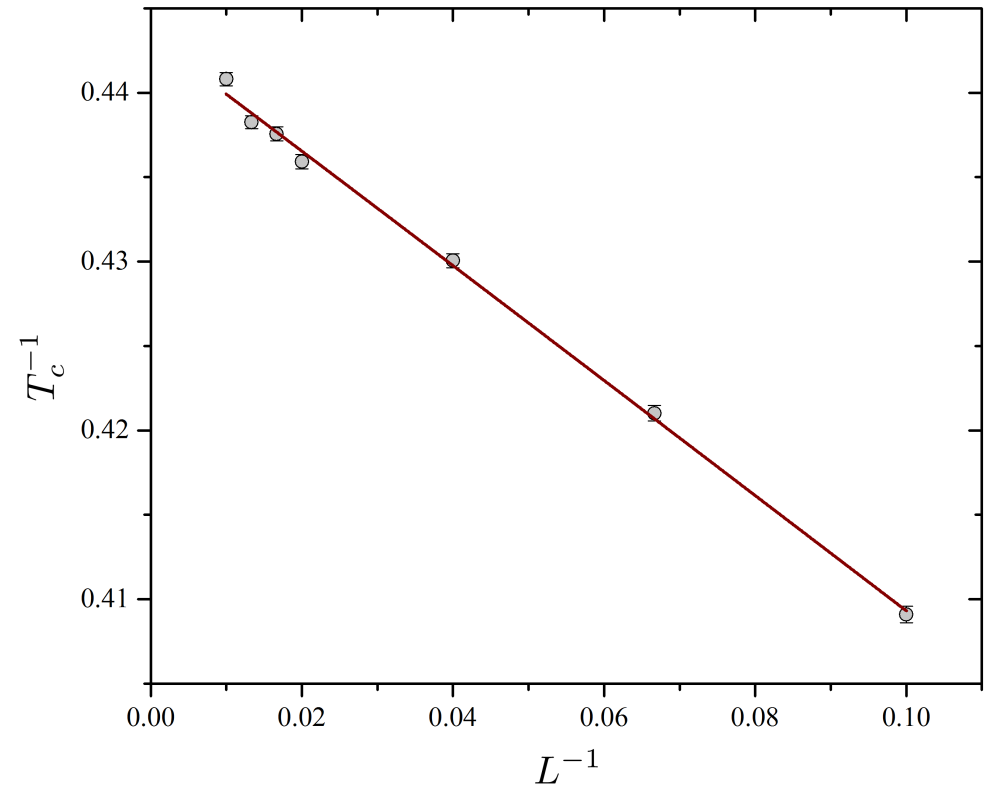


FIG. 9. (Color online) Inverse of the critical temperature  $T_c^{-1}$  vs inverse of lattice size  $L^{-1}$  for the 2D Ising model. The curve was fitted with a power law  $T_c^{-1} = T_{c\infty}^{-1} - bL^{-1/\nu}$ , and the critical exponent  $\nu$  was determined.

- From: E. Ibarra-Garcia-Padilla et al., European Journal of Physics 37(6):065103 DOI: [10.1088/0143-0807/37/6/065103](https://doi.org/10.1088/0143-0807/37/6/065103)

# Universality and critical exponents

(This is referred to percolation)

Because we can simulate only finite lattices, it is difficult to obtain estimates for the critical exponents  $\alpha$ ,  $\beta$ , and  $\gamma$  by using the definitions (17.22)–(17.24) directly. We learned in Section 13.4, we can do a *finite size scaling analysis* to extrapolate finite  $L$  results to  $L \rightarrow \infty$ . For example, from Fig. 17.2 we see that the temperature at which  $C$  exhibits a maximum becomes better defined for larger lattices. This behavior provides a simple definition of the transition temperature  $T_c(L)$  for a finite system. According to finite size scaling theory,  $T_c(L)$  scales as

$$T_c(L) - T_c(L = \infty) \sim aL^{-1/\nu}, \quad (17.27)$$

where  $a$  is a constant and  $\nu$  is defined in (17.25). The finite size of the lattice is important when the correlation length

$$\xi(T) \sim L \sim |T - T_c|^{-\nu}. \quad (17.28)$$

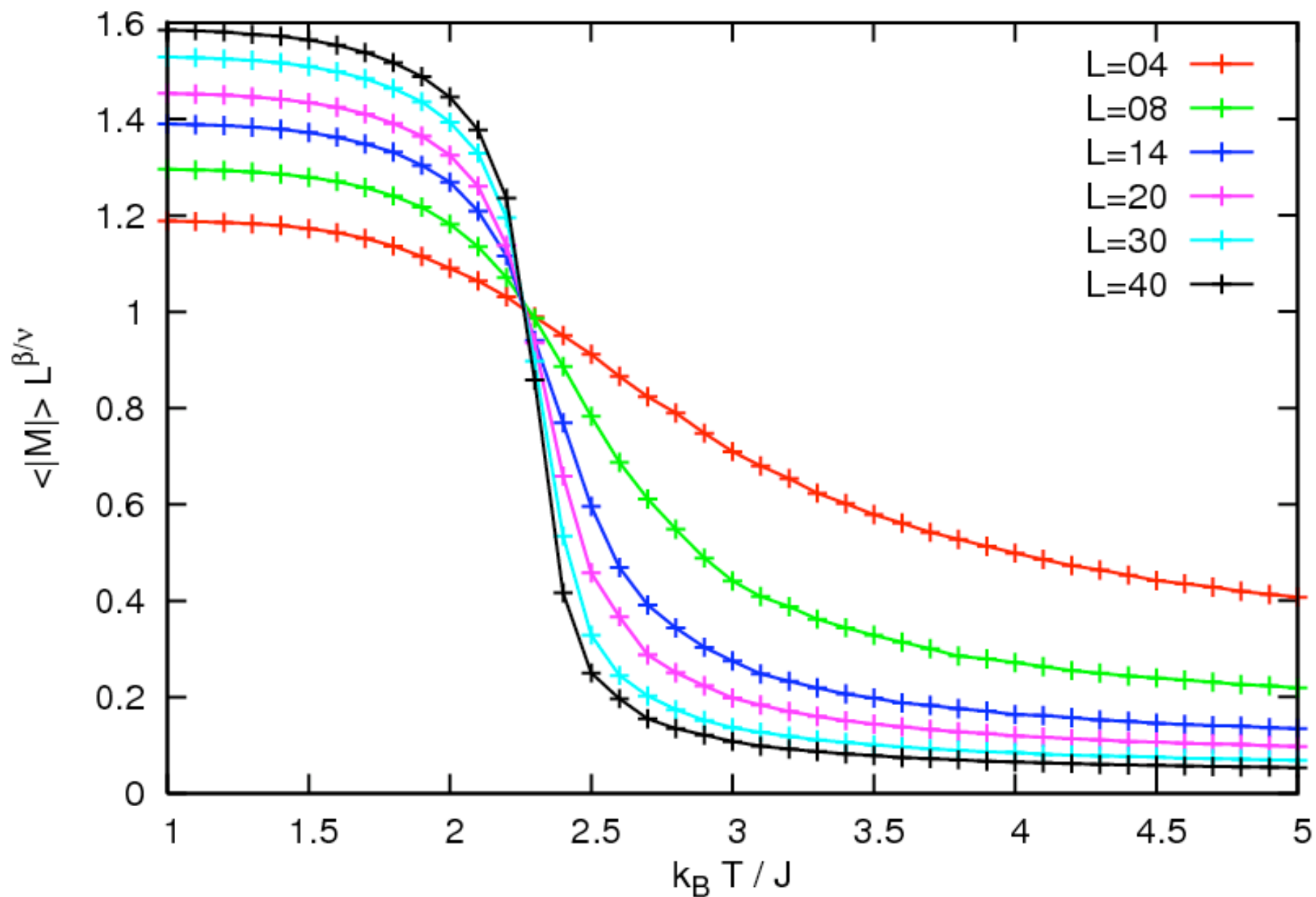
As in Section 13.4, we can set  $T = T_c$  and consider the  $L$ -dependence of  $M$ ,  $C$ , and  $\chi$ :

$$m(T) \sim (T_c - T)^\beta \rightarrow L^{-\beta/\nu} \quad (17.29)$$

$$C(T) \sim |T - T_c|^{-\alpha} \rightarrow L^{\alpha/\nu} \quad (17.30)$$

$$\chi(T) \sim |T - T_c|^{-\gamma} \rightarrow L^{\gamma/\nu}. \quad (17.31)$$

## Scaled magnetization vs unscaled $T$ ( $10^5$ sweeps)



# Ising model: alternative dynamics

- in the **SPIN FLIP dynamics** the order parameter is not conserved (**M changes** during evolution)
- alternative: **NN spin exchange (Kawasaki dyn.)**  
(exchange two NN spins picked at random;  
**M is conserved**; this is equivalent to LATTICE  
GAS MODELS with fixed number of particles)
- another alternative: **flip a cluster of spins (Wolff dynamics)**

see e.g.: <https://mattbierbaum.github.io/ising.js>



# Ising model: Kawasaki dynamics

Fixed magnetization : change of thermodynamical ensemble

No modification of the equilibrium properties  
except phase separation



# Addition of further interactions

- Attractive ( $J>0$ ) nearest-neighbor (NN) interaction only:  
total energy of the system:

$$E = -\frac{J}{2} \sum_{\langle ij \rangle} n_i n_j$$

=> Trend to aggregation (diffusive behavior is limited to a transient)

- Add a repulsive ( $J<0$ ) next-nearest-neighbor (NNN) interaction: total energy of the system:

$$E = -\frac{1}{2} \sum_{\langle ij \rangle} J_{ij} n_i n_j$$

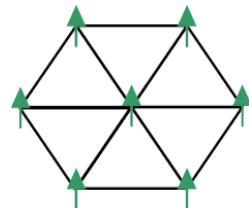
=> The behavior depends on the ratio  $R = J_{NNN}/J_{NN}$

- With finite NN and/or NNN interactions, temperature plays a role

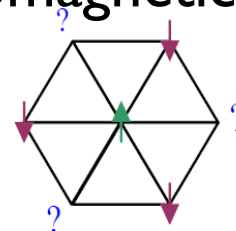
# Ising model: other generalizations

- SPINS: XY, Heisenberg, Potts...
- LATTICES: Square, Triangle, Cubic, Honeycomb, Kagome....
- INTERACTIONS: Magn. Field, Antiferrom., Next Nearest Neighbor (NNN)....

Different behaviour according to the geometry and the kind of interactions.  
Example: frustration in the triangular antiferromagnetic Ising model:



FM



AFM

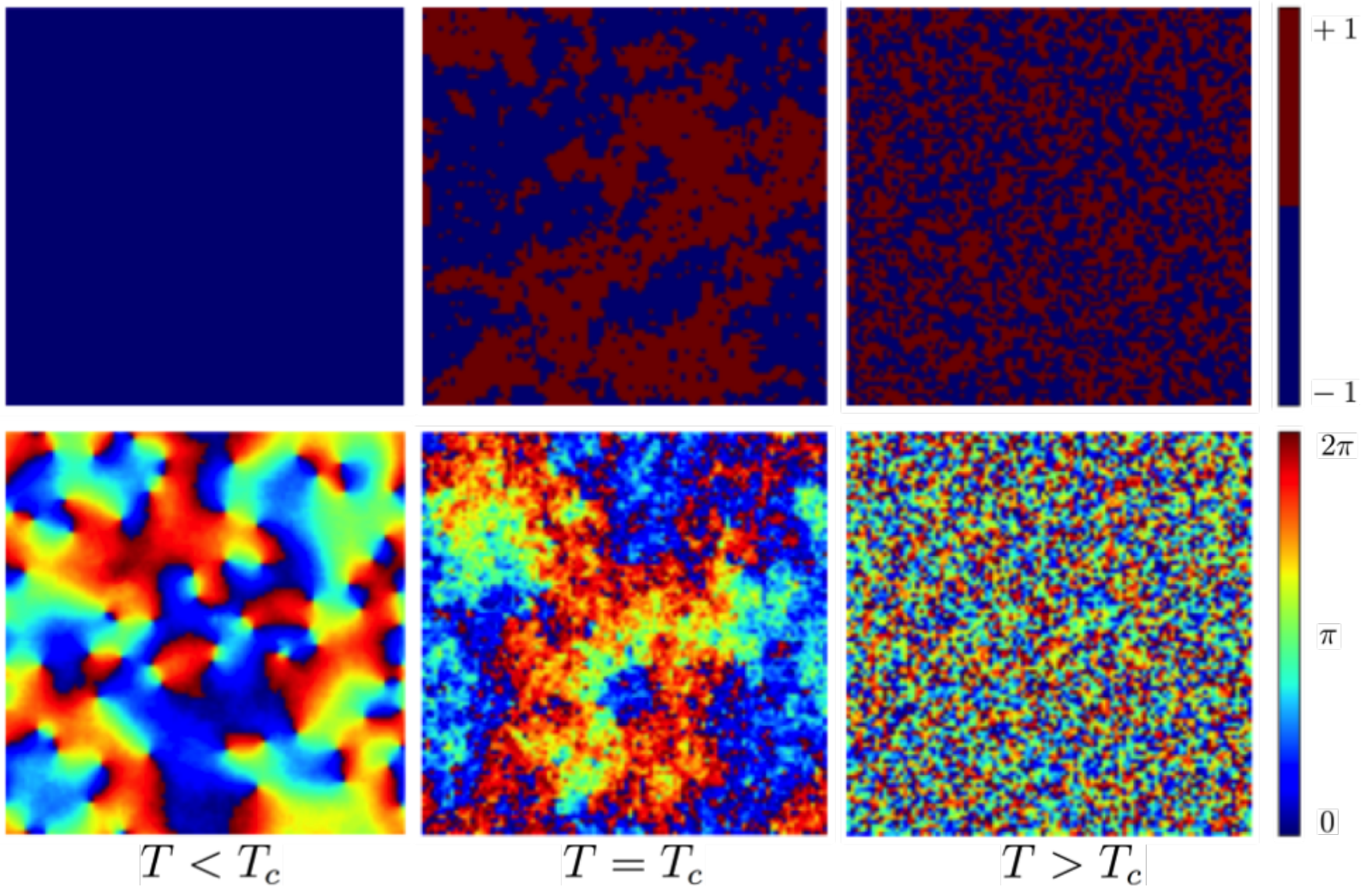


FIG. 15. (Color online) Behavior of the two dimensional Ising model (top) and XY model (bottom) at  $T < T_c$ ,  $T = T_c$  and  $T > T_c$ . For the Ising model, an  $\uparrow$  spin ( $s_i = 1$ ) is represented by red and a  $\downarrow$  spin ( $s_i = -1$ ) is represented by blue. For the XY model, because every spin is determined by  $\theta$ , so  $\mathbf{s}_i = (\cos \theta, \sin \theta)$ , an angle of  $2\pi$  is represented by red and an angle of 0 by blue. In the low-temperature phase, the Ising model exhibits spontaneous magnetization while in the XY model, vortex buddies appear (characterized by points where a continuum from blue to red, or viceversa, circle the point. It is worth to notice that these points are present by pairs with opposite circulation).