993SM - Laboratory of Computational Physics
Unit IX
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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.

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

(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:

$$< A > \approx \frac{1}{m} \sum_{s=1}^{m} A_s$$ with microstates s 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 π_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

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

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

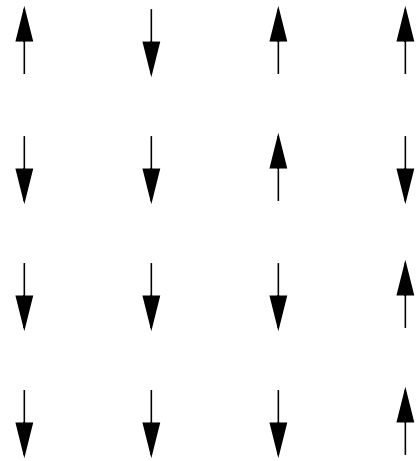
We need a model for:

- **energy**

- **evolution**
  (to build the trajectory / the Markov chain)

stochastic simulations of an interacting spin ensemble

We need a model for:



- **energy** => Ising model

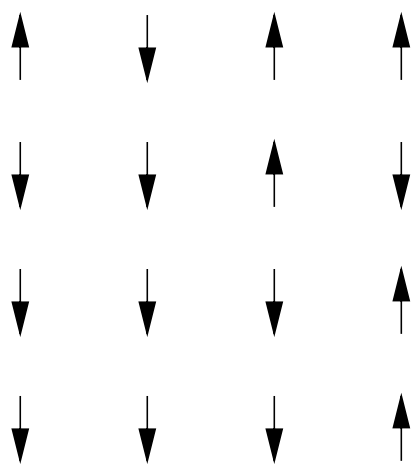
- **evolution**
  (to build the trajectory / the Markov chain)

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 $|S, S_z>$:

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

2 interacting spins

Eigenstates

$$\Psi^{orb}_{+,-}(1,2)|S,S_z>=(\phi(1)\psi(2)+(-)^S\phi(2)\psi(1))/\sqrt{2}\ \ |S,S_z>$$

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

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

$$\chi_{0,0}=\frac{1}{\sqrt{2}}\left[v_+(\sigma_1)v_-(\sigma_2)-v_-(\sigma_1)v_+(\sigma_2)\right]$$ Spin singlet: antisymmetric

2 interacting spins

Energy

$$< \Psi \quad _-|\mathcal{H}|\Psi \quad _- >=< \Psi^{orb}_{+,-}|\mathcal{H}|\Psi^{orb}_{+,-} >=< \phi|h|\phi > + < \psi|h|\psi > +J_{12}+(-1)^S K_{12}$$

$$= E_0 + J_{12} + (-1)^S K_{12}$$

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 => the energy is affected by spin even if $\mathcal{H}$ does not depend explicitly on it:

$$< S = 0|\mathcal{H}|S = 0 >= E_s \quad \text{singlet}$$
$$< S = 1|\mathcal{H}|S = 1 >= E_t \quad \text{triplet}$$

Hence:

$$< S = 0|\mathcal{H}|S = 0 > - < S = 1|\mathcal{H}|S = 1 >= E_s - E_t$$

$$= 2K_{12}$$

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:

$$\sum_{12} = \vec{s_1} \cdot \vec{s_2} = \frac{1}{2} S^2 - \frac{3}{4}$$

which is diagonal on the coupled basis, with eigenvalues:

$$< S = 0 | \Sigma_{12} | S = 0 > = -\frac{3}{4}, \qquad < S = 1 | \Sigma_{12} | S = 1 > = \frac{1}{4}$$

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

We have:

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

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 (Es > Et) ↑↑ spins favored => ferromagnetic case

J<0 (Es < Et) ↑↓ 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 (Es > Et) ↑↑ spins favored => ferromagnetic case

J<0 (Es < Et) ↑↓ spins favored => antiferromagnetic case

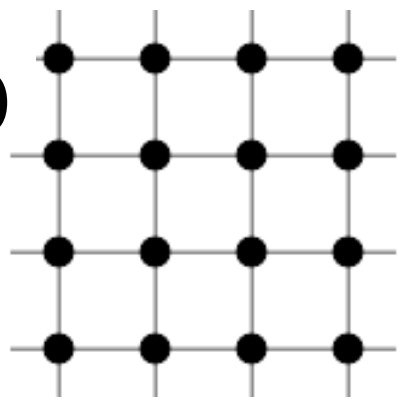
(choosing the kind of interaction, we specify the **energy model**)

Ising model on a lattice

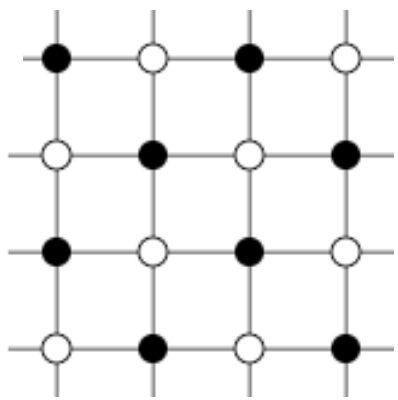
lattice containing N sites

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 $\{s_1, s_2, \ldots s_N\}$ for all lattice sites.

J >0



J <0



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:

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

(nn=nearest neighbor)

Energy in presence of an external magnetic field:

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

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:

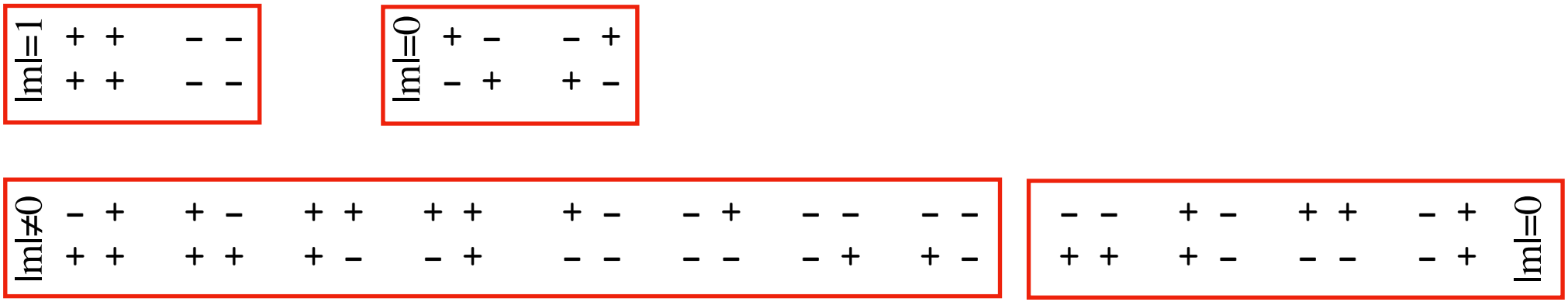
$$m = \frac{M}{N} = \frac{1}{N} \sum_{i=1}^{N} s_i$$

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

Ising model: configurations and energy

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

e.g. $2^4 = 16$ spin configurations for $2x2$ lattice



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:

$$E_0/N = -\ 2J$$

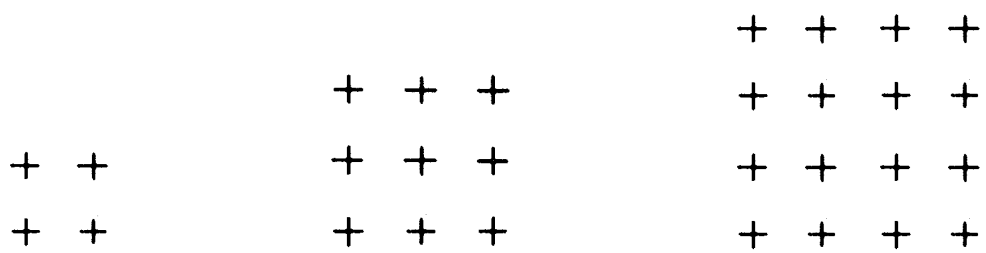
Ising model: boundary conditions

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

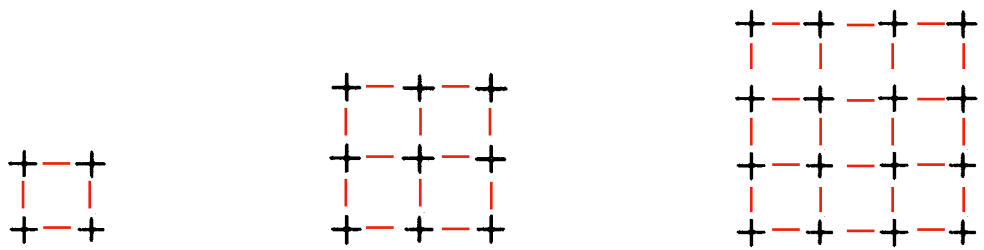
in a N=LxL spin lattice there are 2L(L-1) nn interactions;
for the ferromagnetic g.s. configuration, for instance, the energy is:



Let's count the interactions…

Ising model: open boundary conditions

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



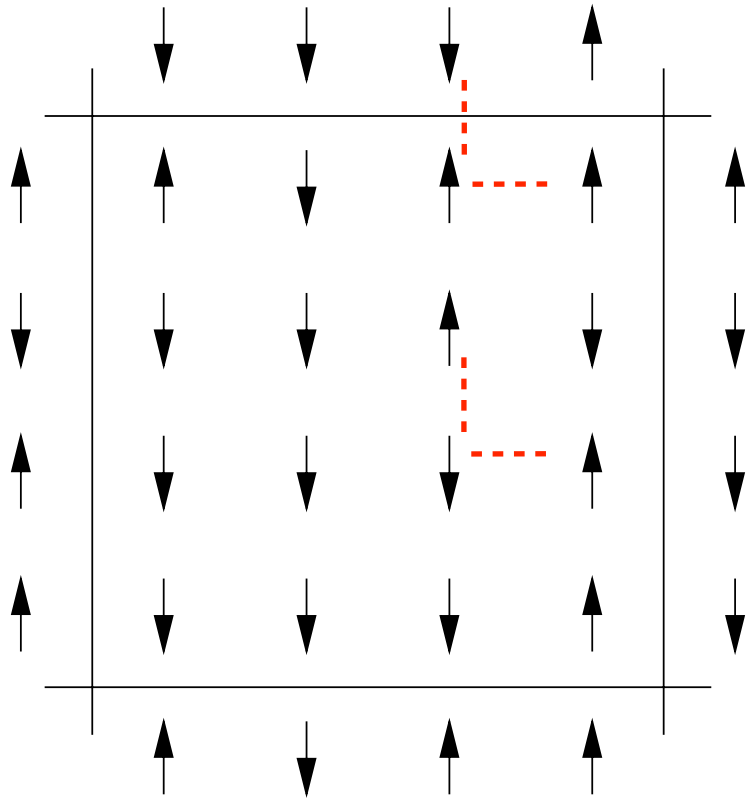
$E_0/N=-J$ $E_0/N=-(12/9)J$ $E_0/N=-(24/16)J$ ... $E_0/N = -J \times 2L(L-1)/L^2$

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

(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 ~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

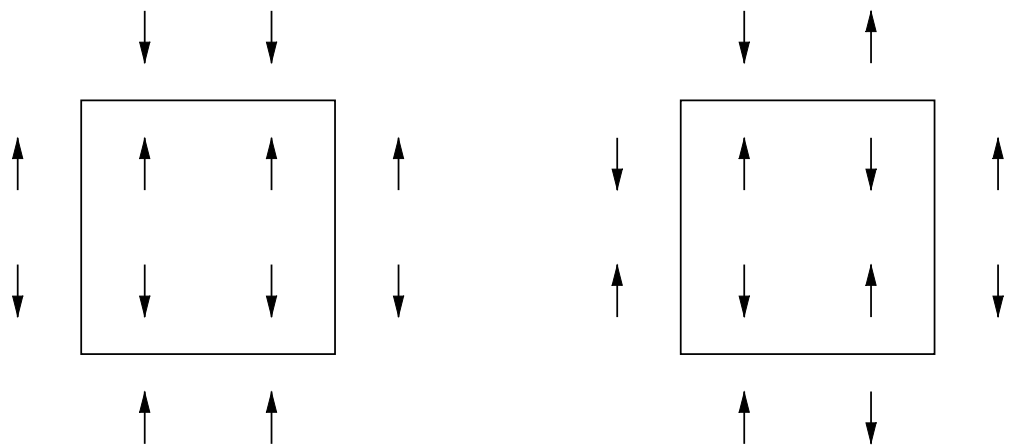
One of the 2^N possible configurations of a system of $N = 16$ Ising spins on a square lattice. with periodic boundary conditions.

Ising model: PBC

We have always:

$2^4 = 16$ spin configurations for $2x2$ 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

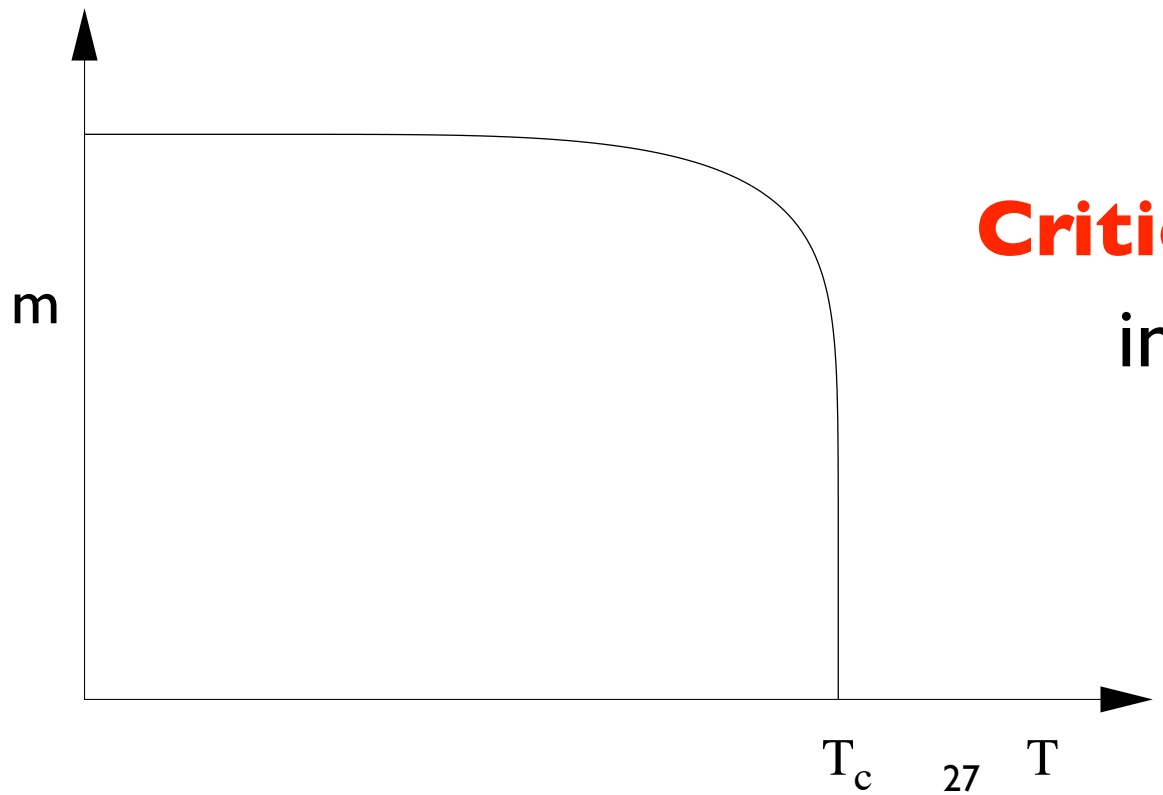
Energy and magnetization of 16 configurations of the 2×2 Ising model with PBC

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 => high (absolute) magnetization)

High T: spin configuration maximizes entropy
(=disorder) (spins tend to disalign => low magnetization)



existence of a
Critical temperature Tc

in 2D the model has an analytical solution:

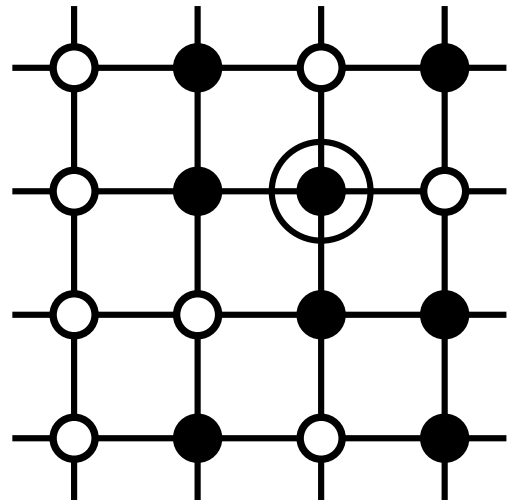
$T_c = 2.269\ J/k_B$

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)

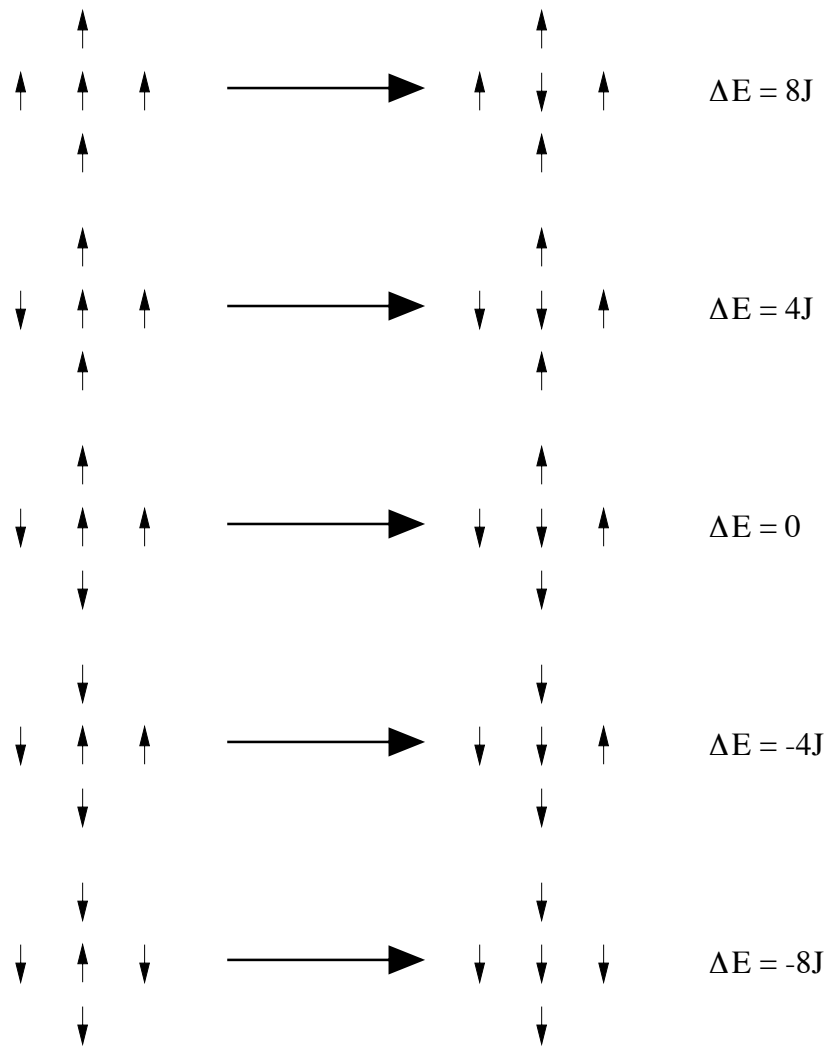


Apply **Metropolis Monte Carlo** method for evolution in the **canonical ensemble** (fix T).

Evolution is driven by the **energy change** between the old and the new configuration, ΔE .

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

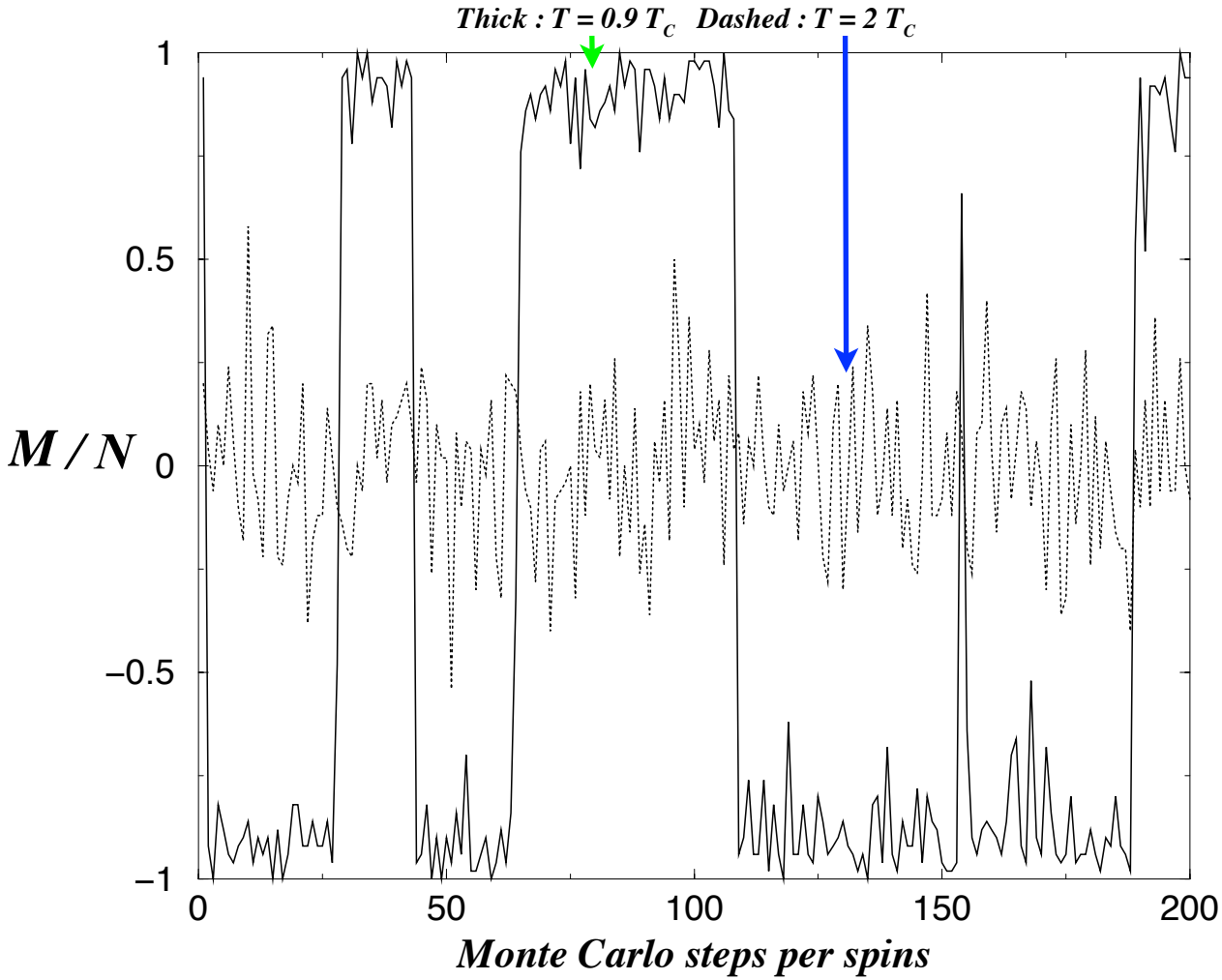
Ising model: spin flip dynamics



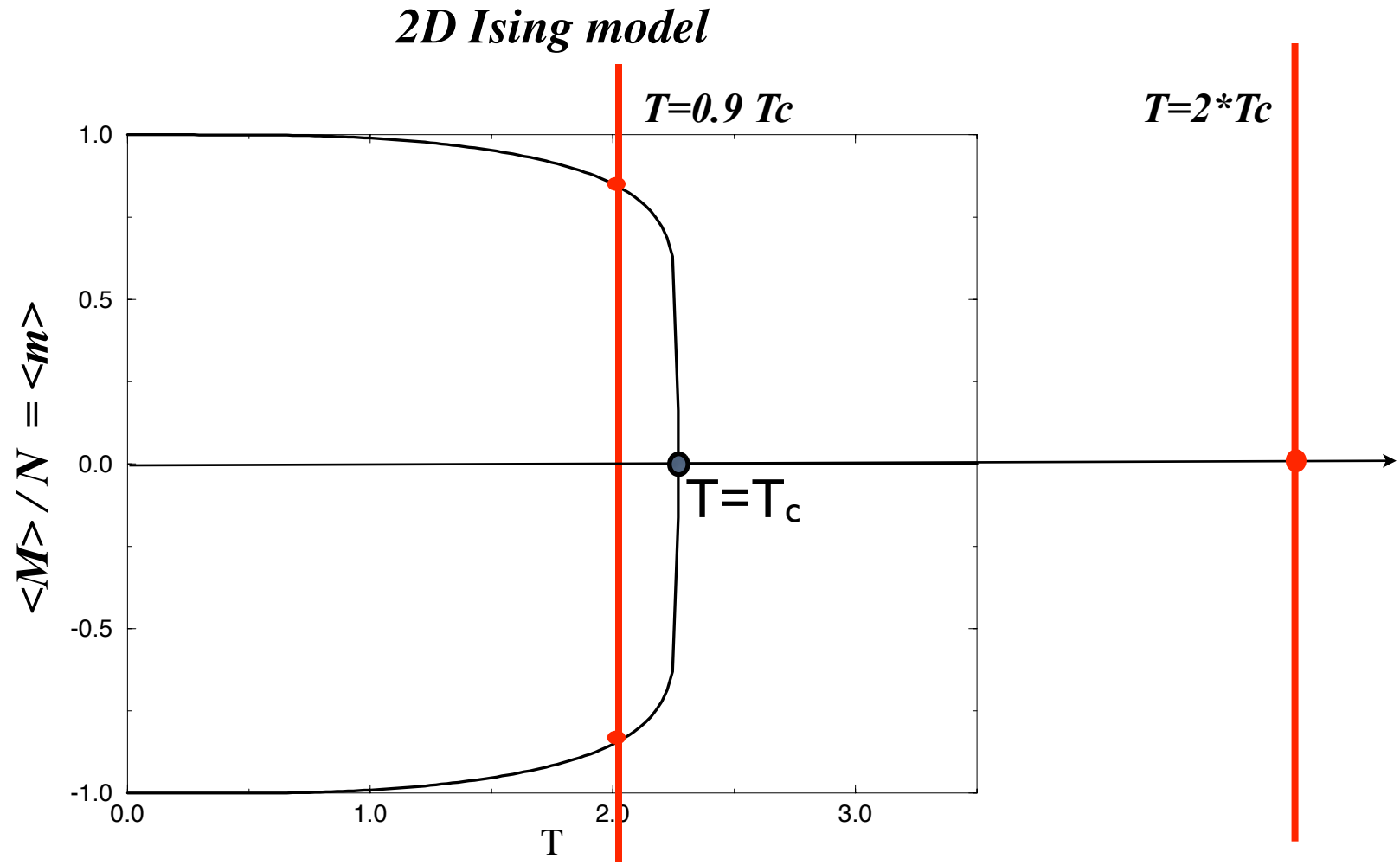
The five possible transitions of the Ising model on the square lattice with spin flip

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 10x10 and two different T



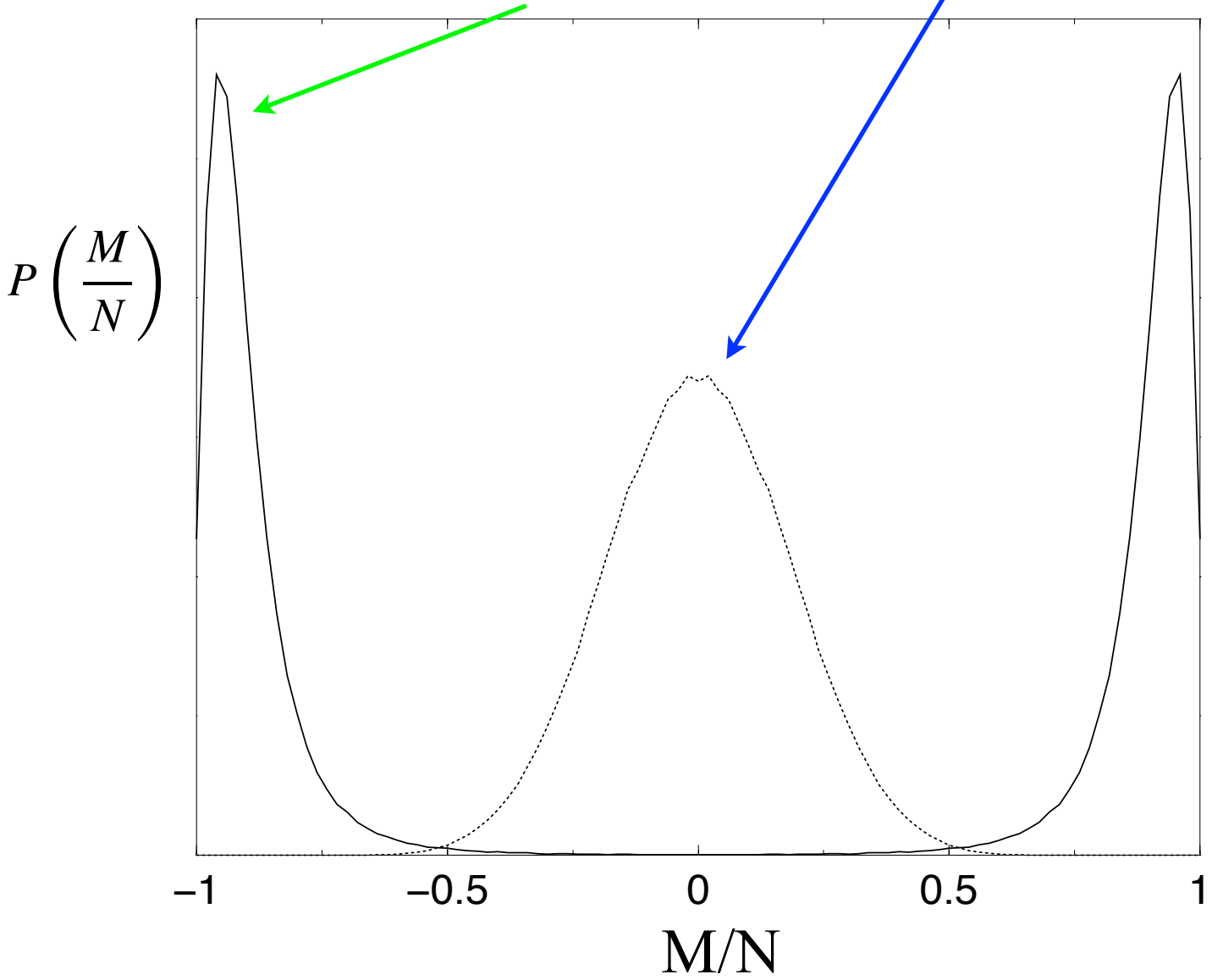
Fluctuations! do, as usual, temporal averages: $\langle M \rangle / N$, $\langle E \rangle / N$



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)

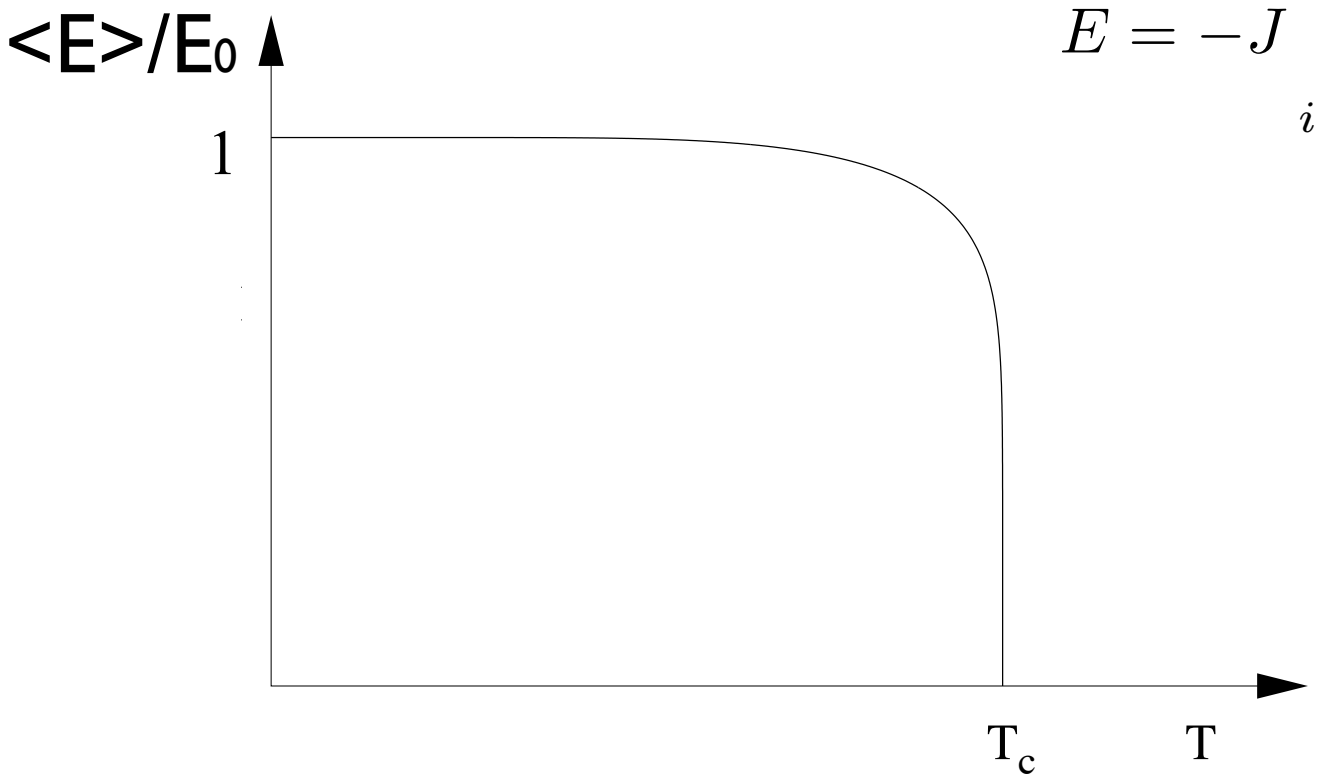


(data collected during time evolution, at equilibrium)

Ising model: phase transition

T_c also for energy, not only for magnetization:

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



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:

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

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

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

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: $E \to const.$, macro $\sim$ micro)

Ising model: fluctuations

Fluctuations are intrinsic to the system evolution and are important!

Linear response functions are related to equilibrium fluctuations:

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

And

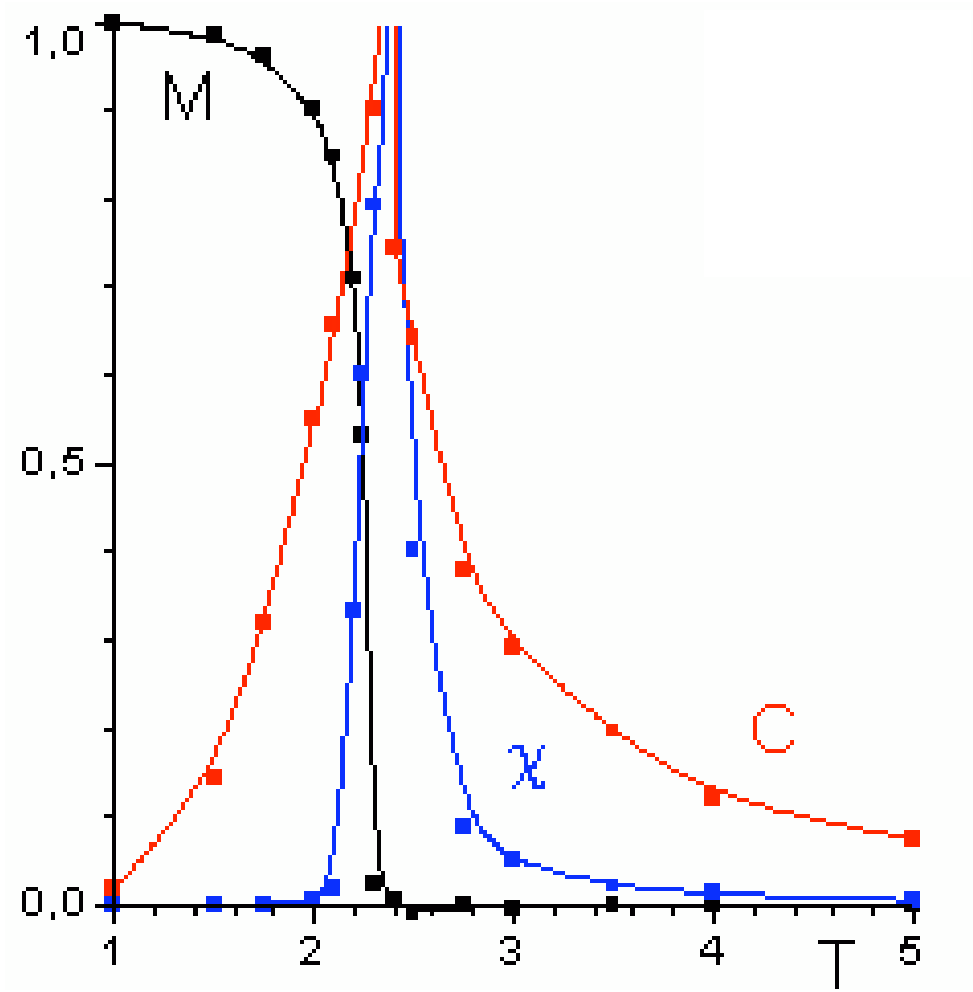
$$\chi = \lim_{H \to 0} \frac{\partial \langle M \rangle}{\partial H}\ , \quad \chi = \frac{1}{kT}\left(\langle M^2 \rangle - \langle M \rangle^2\right)$$

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

Ising model:

fluctuations and phase transition

Rapid change in <E> and <M> => singularities in C and χ



(Large fluctuations near the phase transition: Second Order phase transition)

specific heat:

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

magnetic susceptibility:

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

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

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

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:

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

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

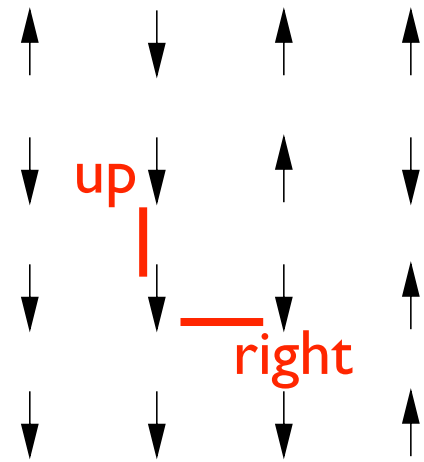
$$m = \frac{M}{N} = \frac{1}{N} \sum_{i=1}^{N} s_i$$

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

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

Ising model: energy

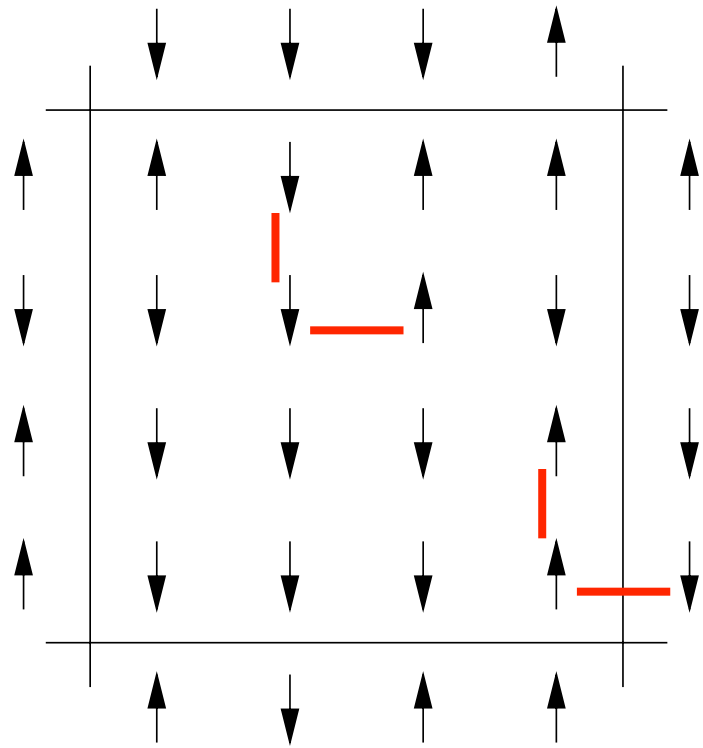
$$E = -J \sum_{i,j=\mathrm{nn}(i)}^{N} s_i s_j$$




```
!  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
! (gor 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
   call random_number(rnd)
   y = int(L*rnd) + 1
   .....
```

$1 \leq x \leq L$

$1 \leq y \leq L$

Flip is: `spin(x,y) = -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)
call random_number(rnd)
if (rnd <= w(dE)) then
   spin(x,y) = -spin(x,y)
   accept = accept + 1
   .....
   .....
```

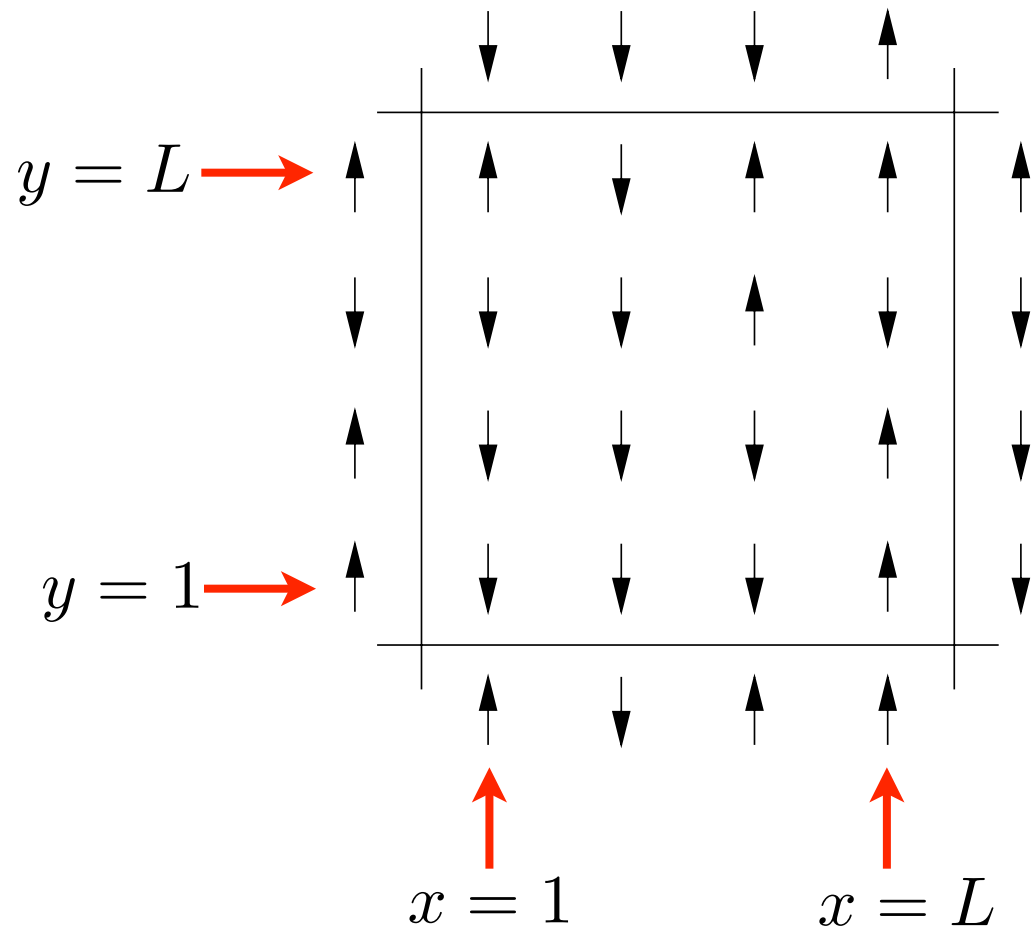
energy variation for `spin(x,y)` flip

`w(dE)` is $e^{-\Delta E/k_B T}$

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

Energy variations per spin flip with PBC

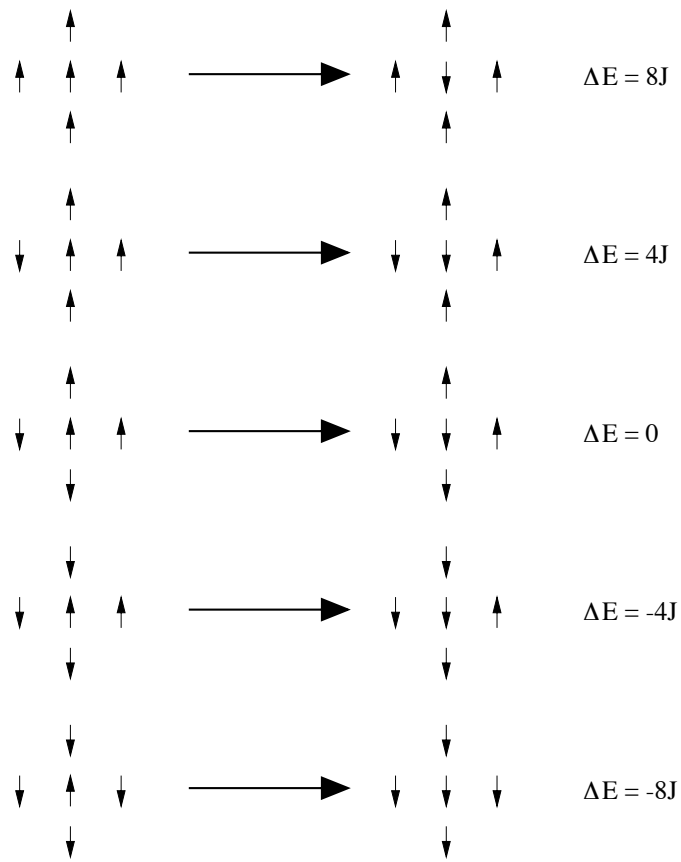
```
function DeltaE(x,y) result (DeltaE_result)
  !  periodic boundary conditions
.....
 if (x == 1) then
    left = spin(L,y)
    right = spin(2,y)
 else if (x == L) then
    left = spin(L-1,y)
    right = spin(1,y)
 else
    left = spin(x-1,y)
    right = spin(x+1,y)
 end if
 if (y == 1) then
    up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

ΔE 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
   call random_number(rnd)
   y = int(L*rnd) + 1
   .....
```

$\longleftarrow \quad 1 \leq x \leq L$

$\longleftarrow \quad 1 \leq y \leq L$

or ordered (sequential) ...

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

```
spin(x,y) = -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()
   call data(cum)
end do
```

contains the loop over all the spins

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:

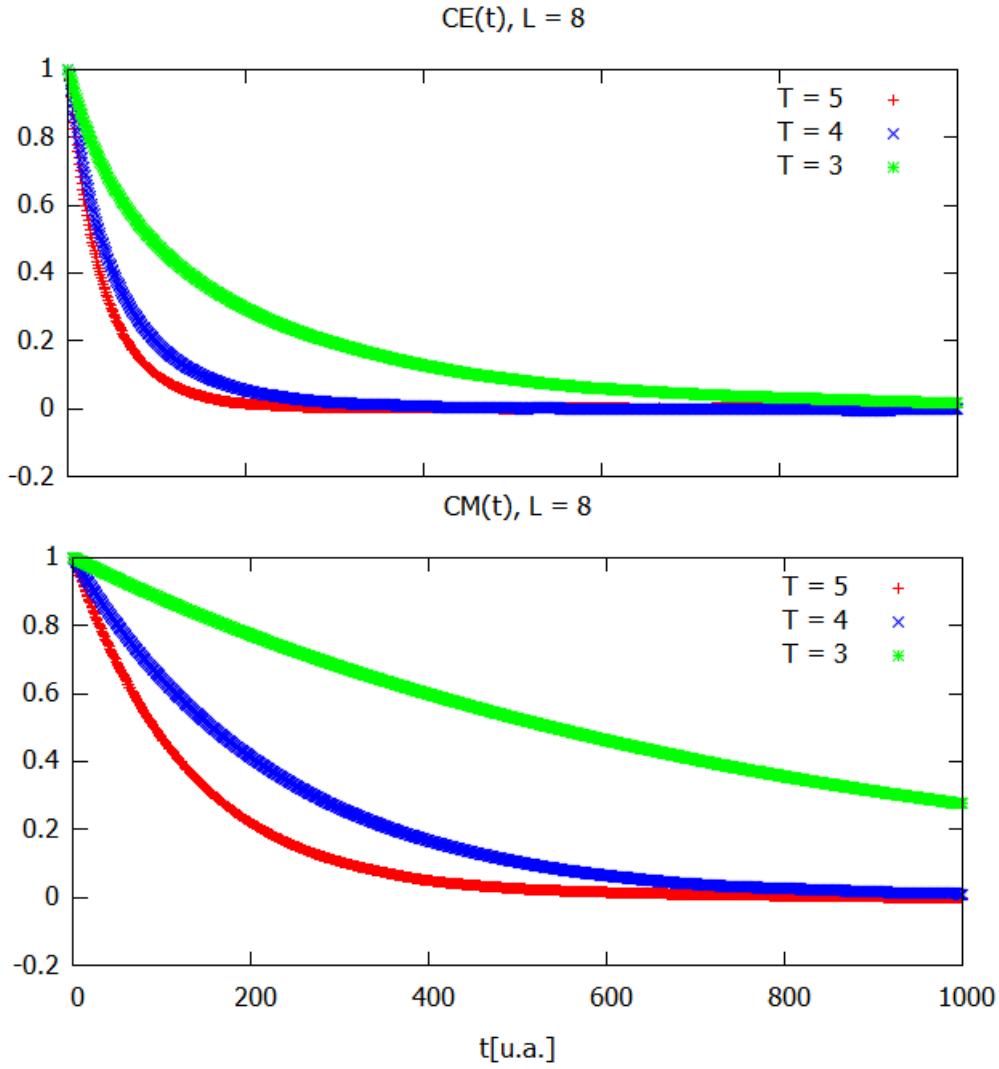
$$C_M(t) =< M(t)M(0) > - < M >^2, \quad C_E(t) =< E(t)E(0) > - < E >^2$$

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

$$C_M(t) \to 0 \text{ and } C_E(t) \to 0 \text{ exponentially for } t \to \infty$$

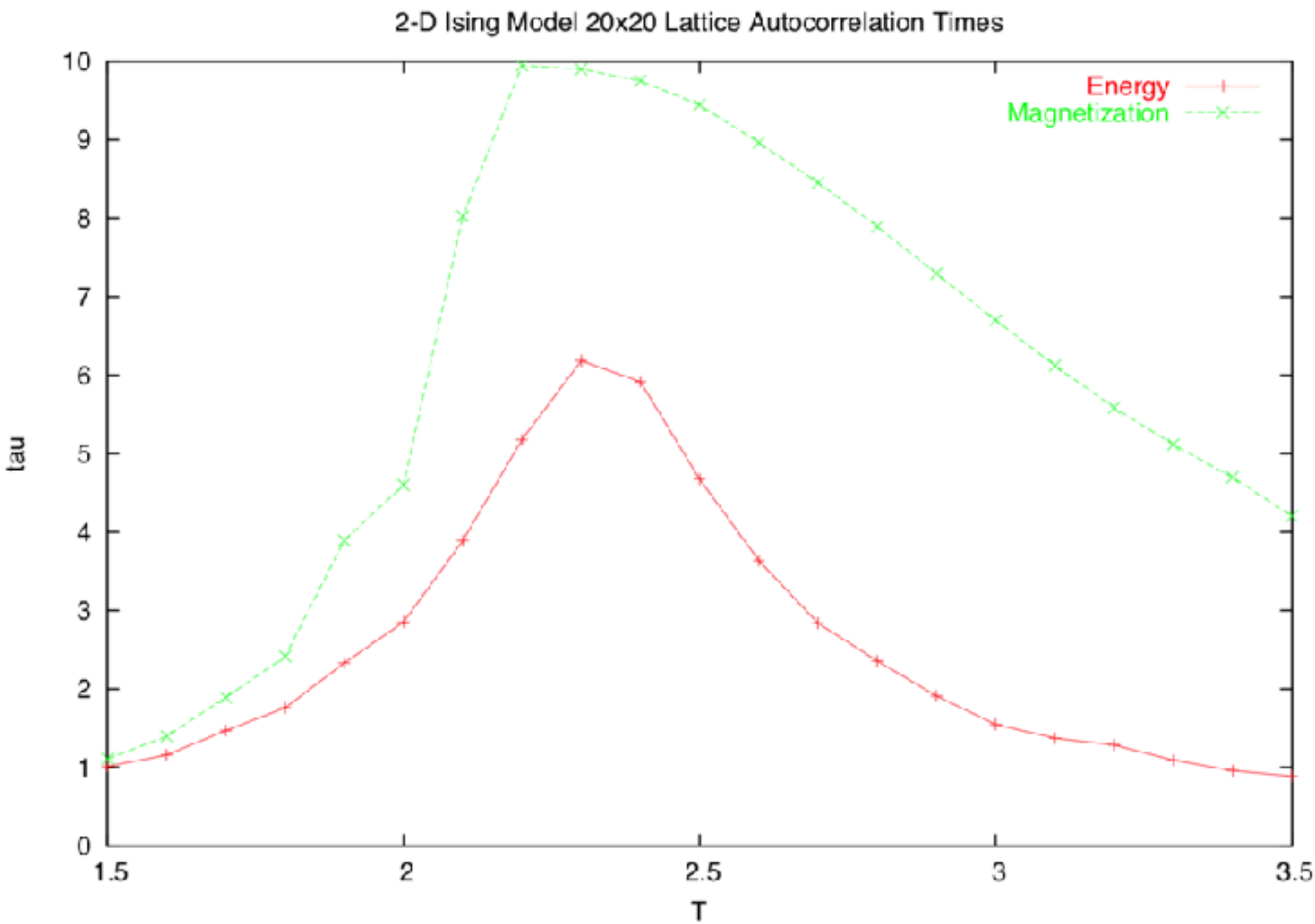
with a certain decay time τ: consider intervals longer than τ for statistical averages

Autocorrelation functions



(NOTE: "critical slowling down" for $T \to T_C$)

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


2-D Ising Model 20x20 Lattice Autocorrelation Times
Energy
Magnetization
tau
T
0
1
2
3
4
5
6
7
8
9
10
1.5
2
2.5
3
3.5

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

Program:

On moodle2:

ising.f90

993SM - Laboratory of Computational Physics
Unit X
November 27, 2023

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- more on Ising model

- Variational Monte Carlo

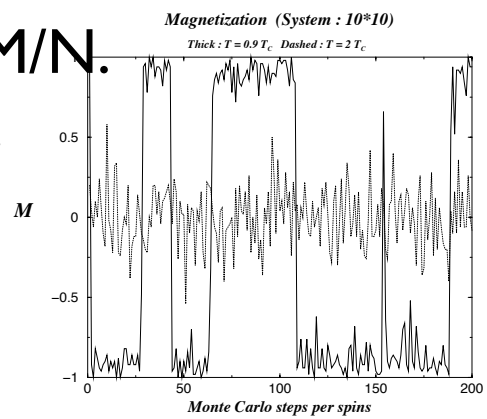
Exercise

(a) Choose L=30, T=2, and initially spin=±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 spin=±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 < E >/N and < M >/N; increasing the total *nmcs*, the two quantities should converge...

Exercise

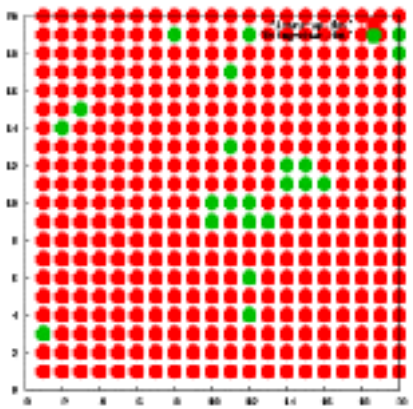
(a) Choose L=30, T=2, and initially spin=±1 randomly. ...

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

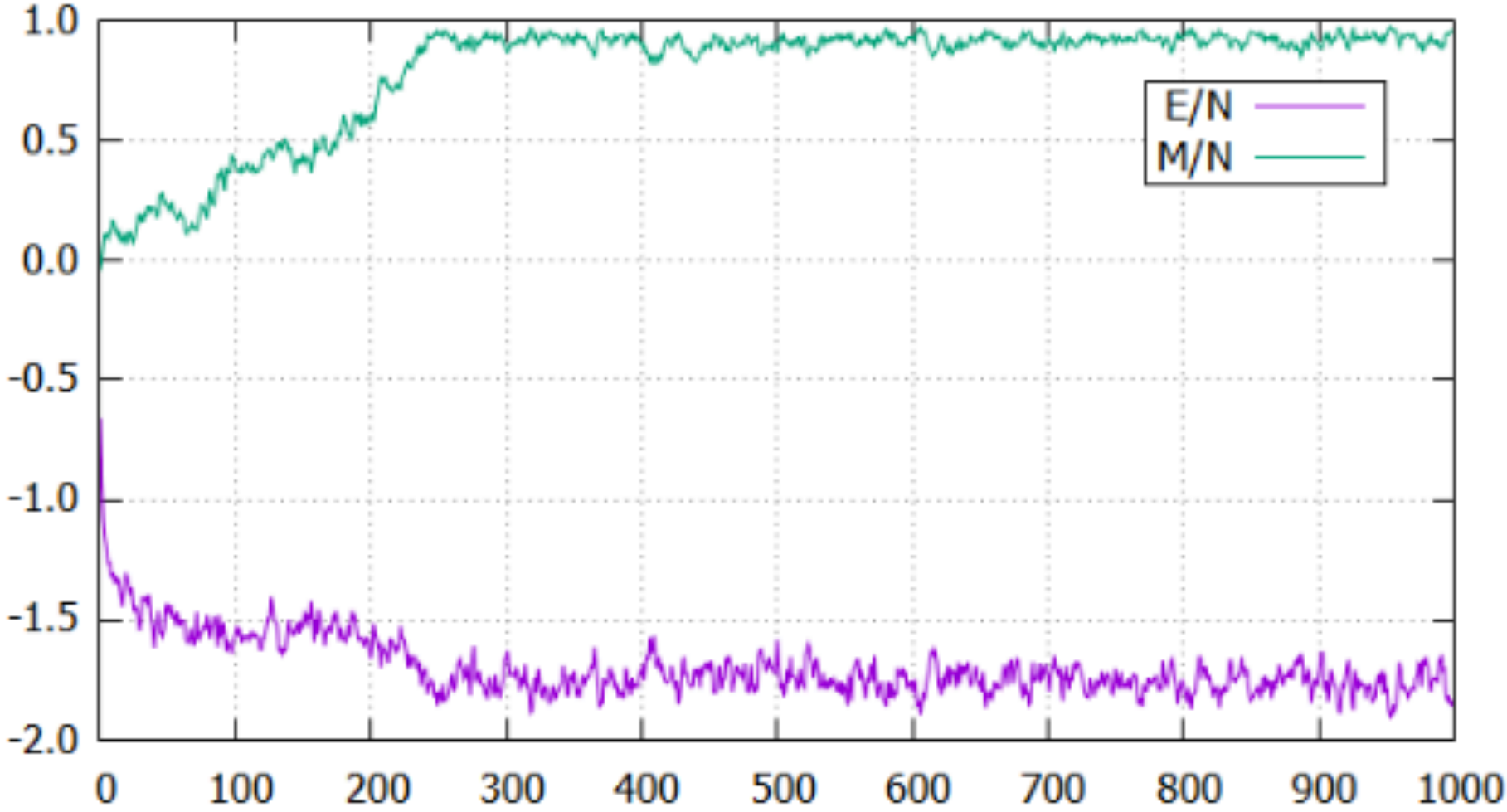
it should appear **ordered...**

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:



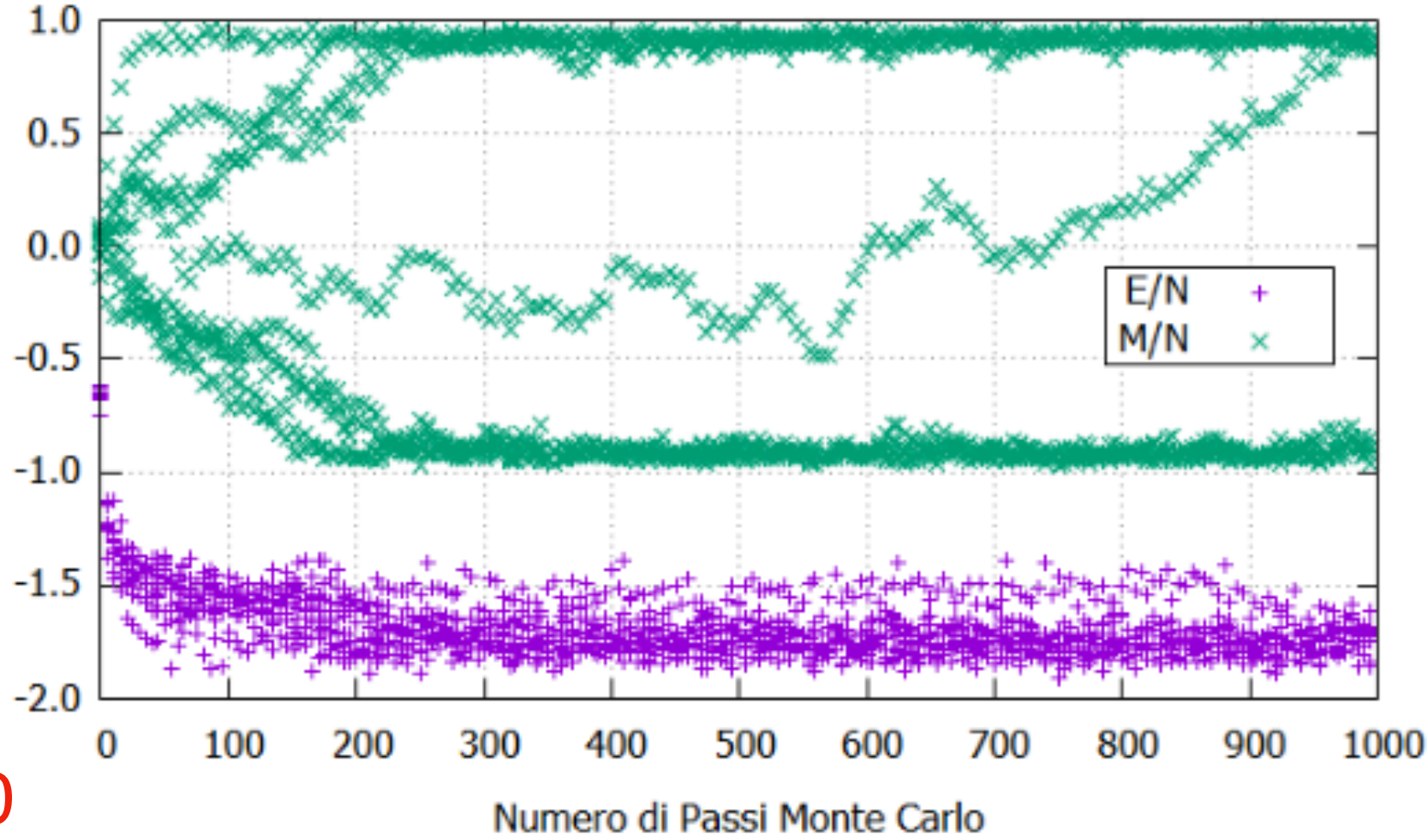
Some results that you should obtain…



L=30

(a) Energia media e magnetizzazione per spin al variare del tempo (ossia all'aumentare dei passi Monte Carlo svolti) per un sistema a temperatura $T = 2.0$.
Si noti che dopo circa 300 passi Monte Carlo il sistema sembra stabilizzarsi.

M. Dirindin, 2021

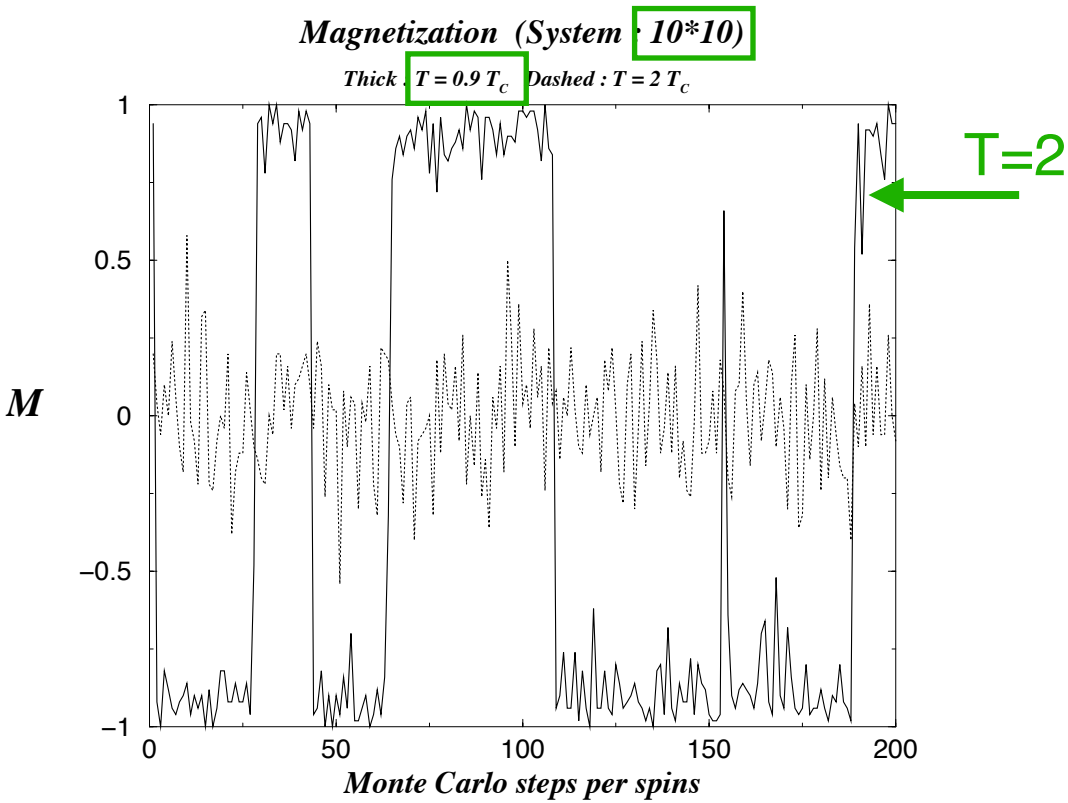


L=30

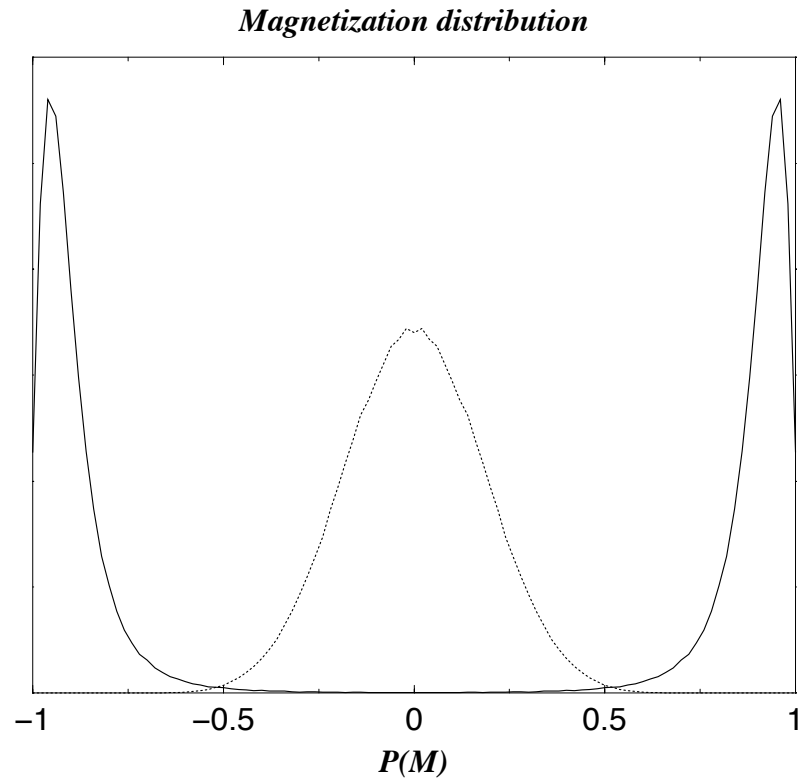
Figura 3: Energia e magnetizzazione per spin per 10 valori diversi di seed. Si noti come la maggior parte dei seed raggiunga l'equilibrio dopo circa 250 iterazioni, mentre un seed raggiunge l'equilibrio dopo appena 50 iterazioni ed un'altro lo raggiunge dopo 1000 passi Monte Carlo.

M. Dirindin, 2021

results for a smaller system:

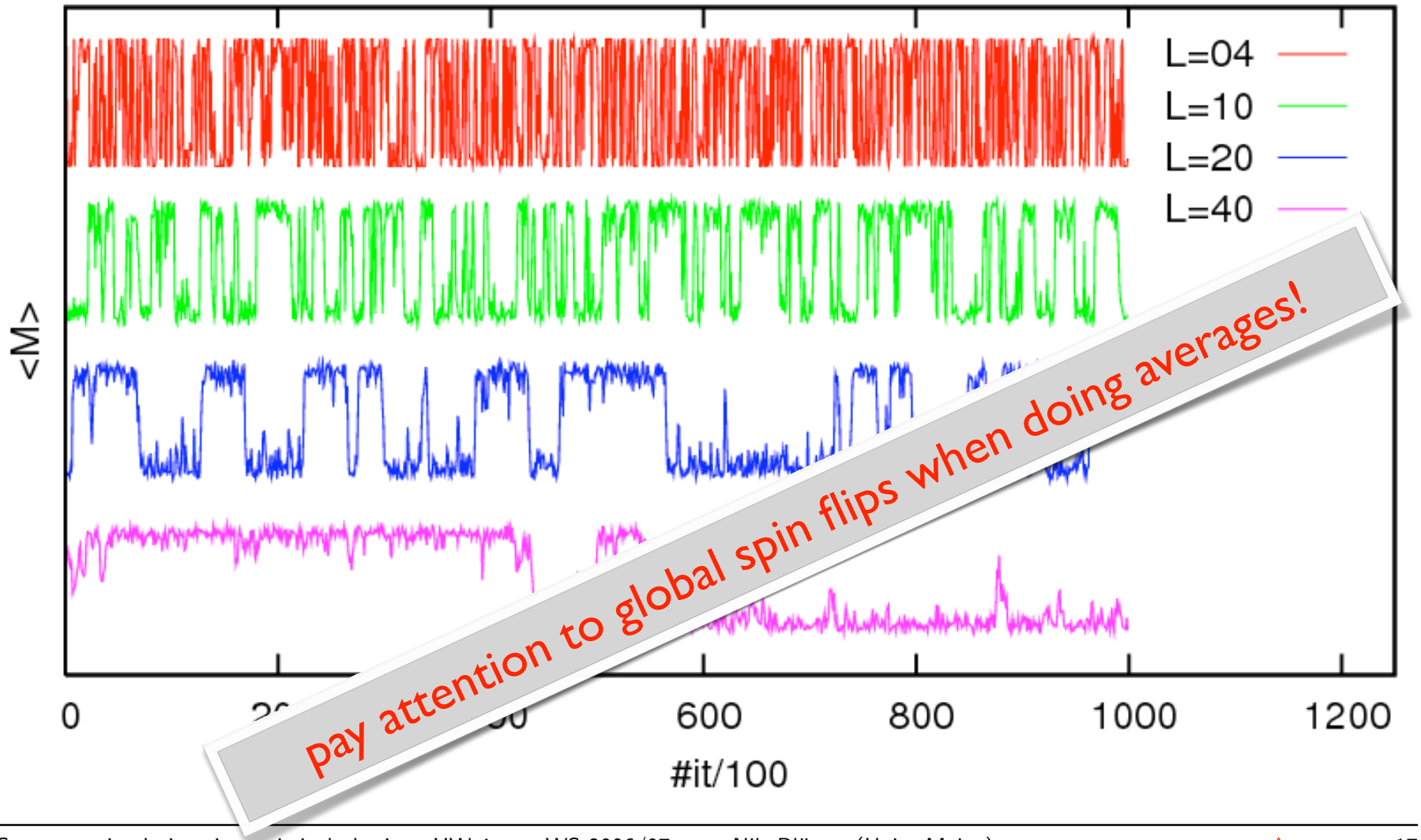


T=2



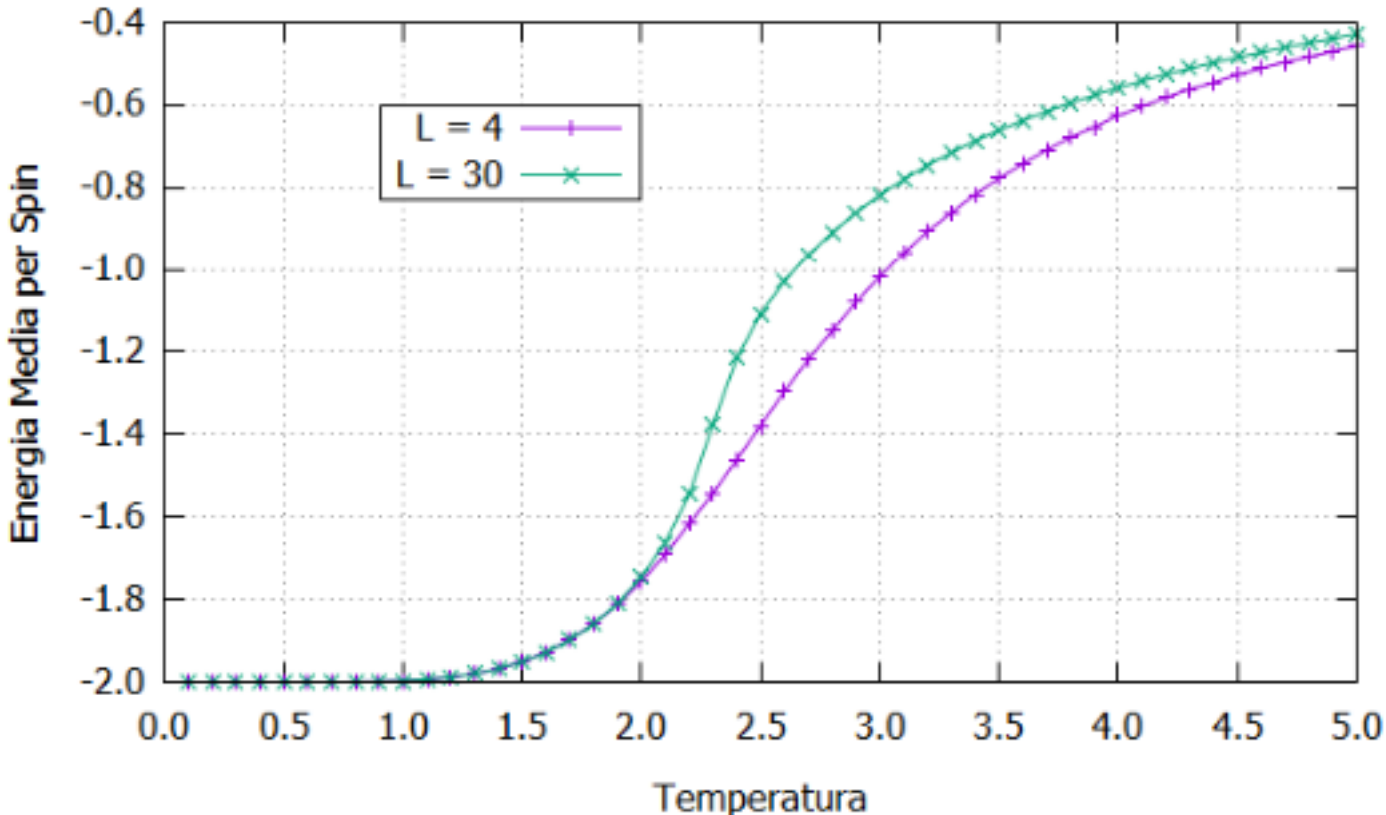
results for system of different size:

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



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



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)

(here K_{NN}=J)

D.P. Landau, PRB 13, 2997 (1976)

4x4

TABLE I. Comparison of Monte Carlo data and analytic values of the reduced internal energy per spin for an $N = 4$ square lattice with p.b.c.

kT/K_{nn}	$\langle U/U_0 \rangle_{anal}$	$\langle U/U_0 \rangle_A$ [a]	σ [b]	σ' [b]	$\langle U/U_0 \rangle_B$ [b]	σ [b]	σ' [b]
1.087	0.997 24	0.997 47	0.000 26	0.000 26	0.997 36	0.000 26	0.000 42
1.449	0.980 06	0.978 41	0.000 76	0.000 86	0.980 89	0.000 73	0.001 37
1.811	0.926 93	0.927 40	0.001 46	0.002 08	0.924 71	0.001 50	0.002 96
2.173	0.819 21	0.816 45	0.002 36	0.003 76	0.814 67	0.002 34	0.004 87
2.536	0.675 08	0.675 57	0.002 85	0.004 46	0.671 57	0.002 83	0.005 89
2.898	0.540 69	0.541 85	0.002 90	0.004 33	0.532 22	0.002 92	0.005 83
3.260	0.438 73	0.437 28	0.002 85	0.003 99	0.435 34	0.002 77	0.005 13
3.622	0.366 35	0.361 40	0.002 60	0.003 78	0.370 79	0.002 67	0.004 46

[a] Run A was made by going through the lattice in order. Run B was made by choosing the reference spin randomly.

[b] σ is the standard deviation of $\langle U/U_0 \rangle$ obtained assuming uncorrelated data. σ' is the standard deviation obtained using the coarse-grained technique described in the text. Values of the standard deviation which are too small to account for the discrepancy with the analytic values are underlined.

choice of the reference spin:

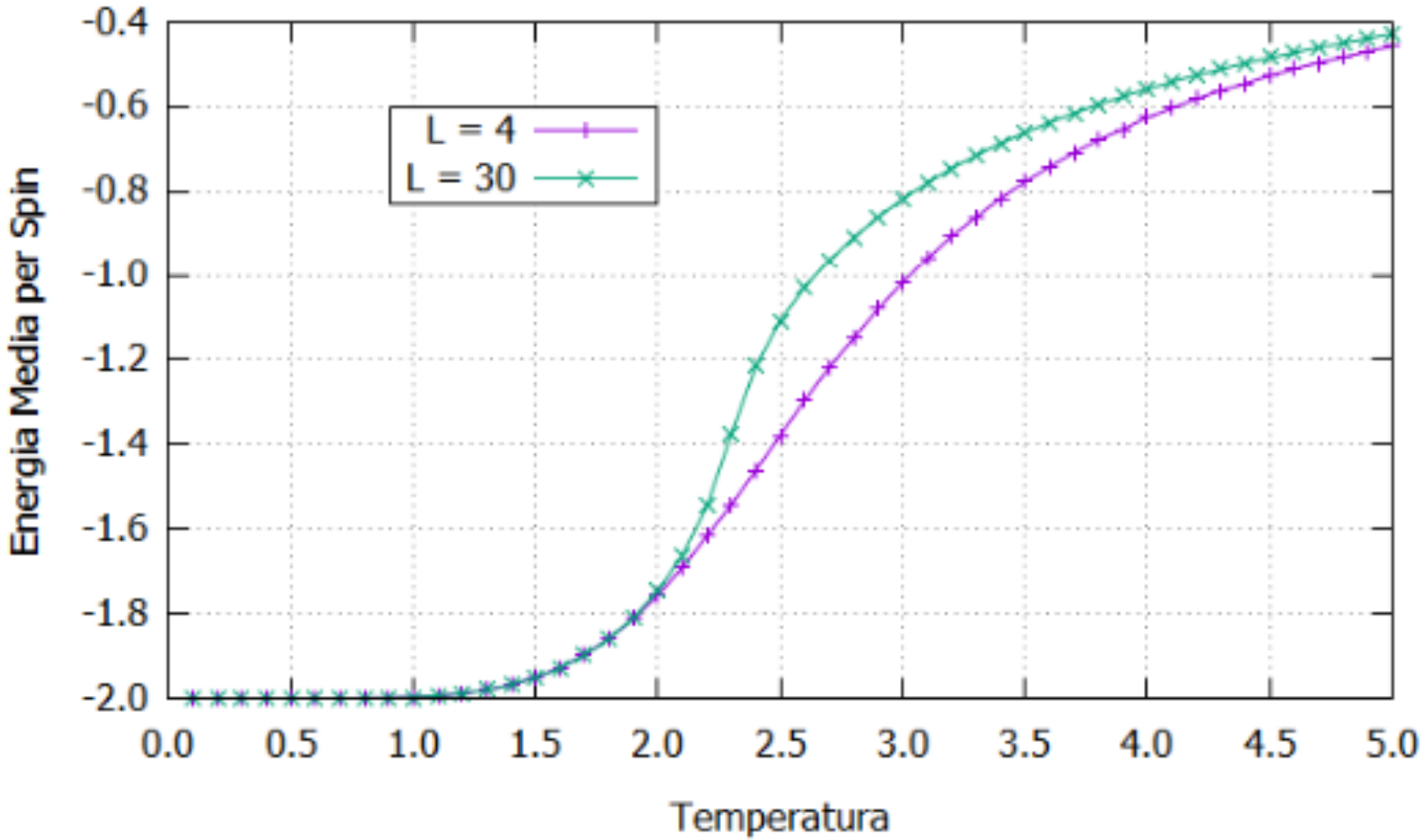
in order

randomly

Ising model: size problems

We cannot simulate an INFINITE system!

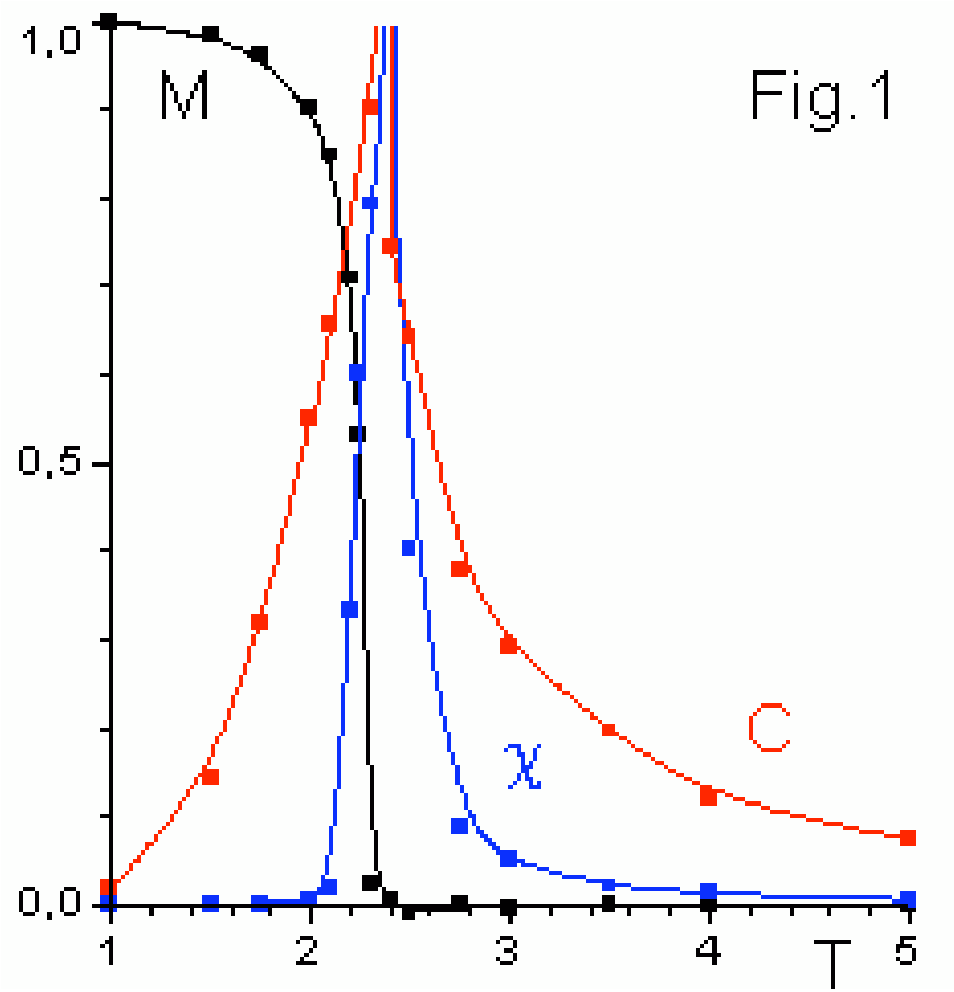
size effects with PBC on E(T):



Exercise

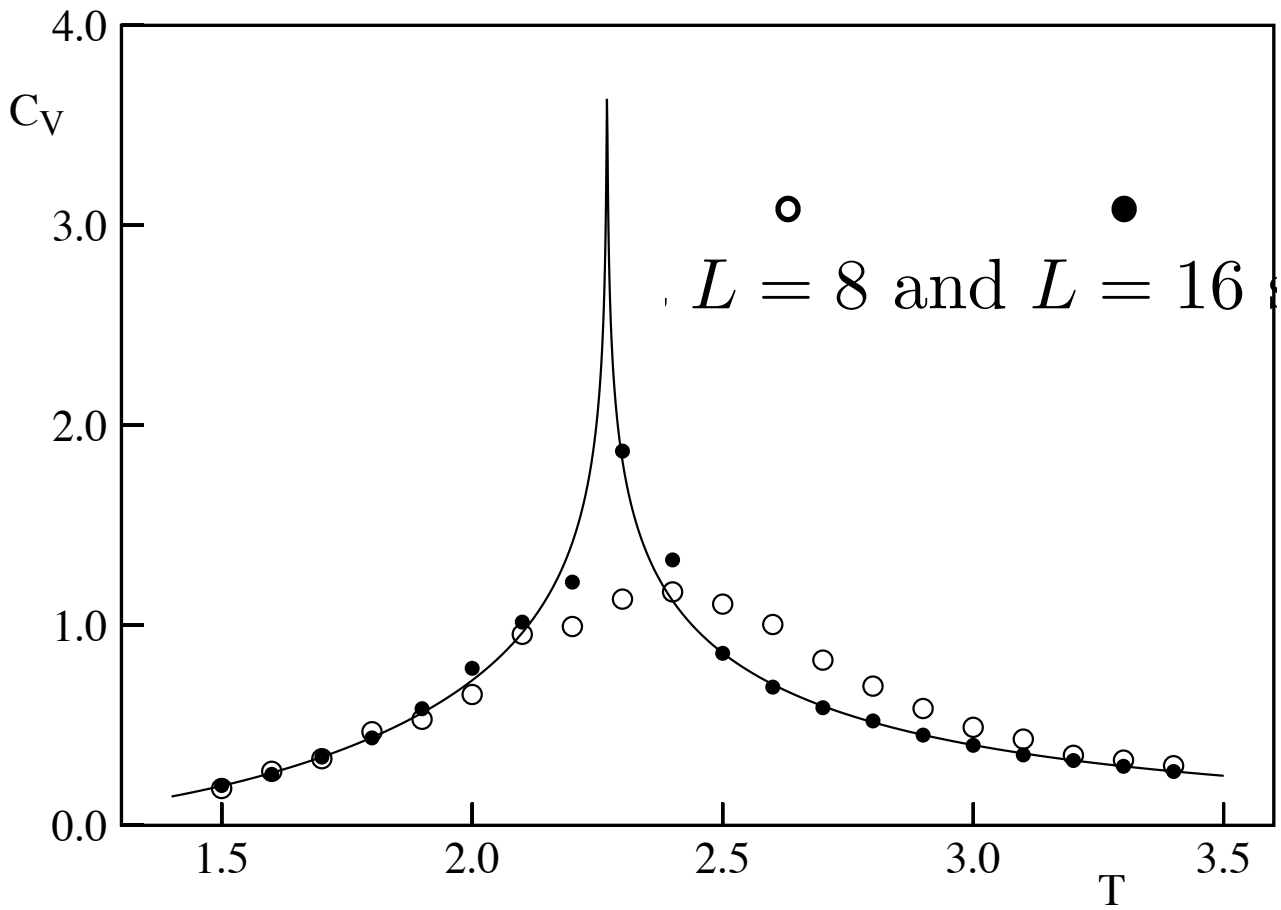
(a) Choose L=30, T=2, and initially spin=±1 randomly. ...

Calculate also c and χ.



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

We cannot simulate an INFINITE system!

INTERFACE EFFECTS: example of energy (units of J) for HALF UP/HALF DOWN configurations:

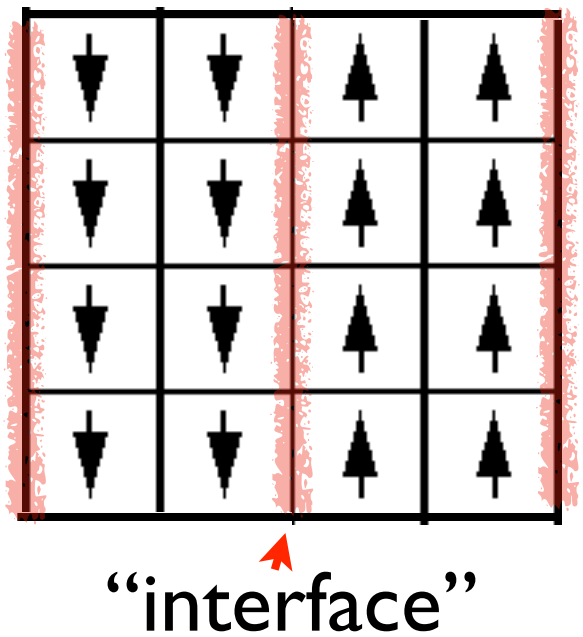
L=2	E= 0
L=4	E=-1
L=8	E=-1.5
L=16	E=-1.75
L=20	E=-1.8
L=32	E=-1.875

32 pairs, 4 of them with "wrong" intractions

=>

E = (-32 +8 +8) /16 = -1

2 x L x L. 2 x L



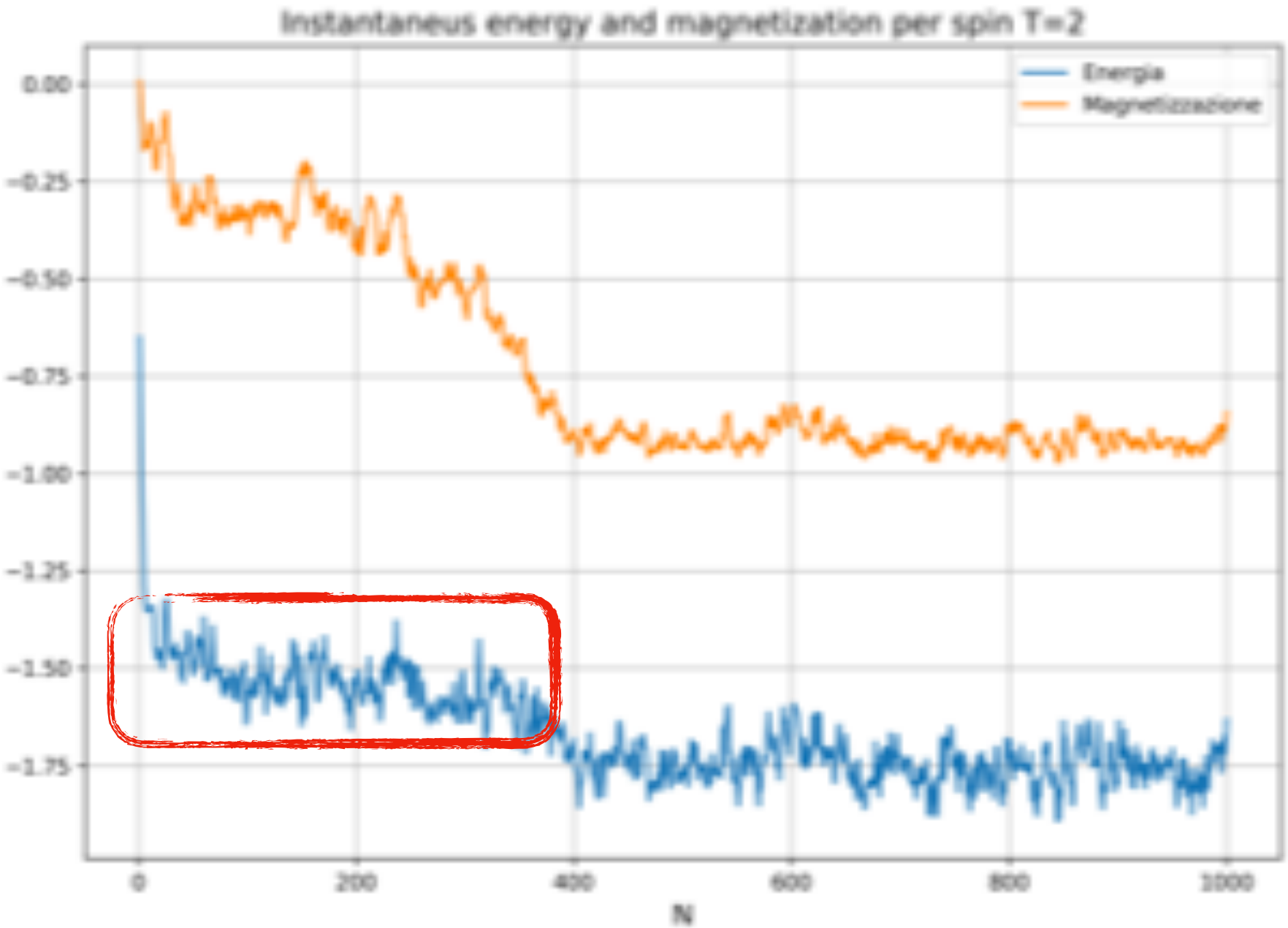
with PBC

"interface"

···· for an infinite system: E=-2

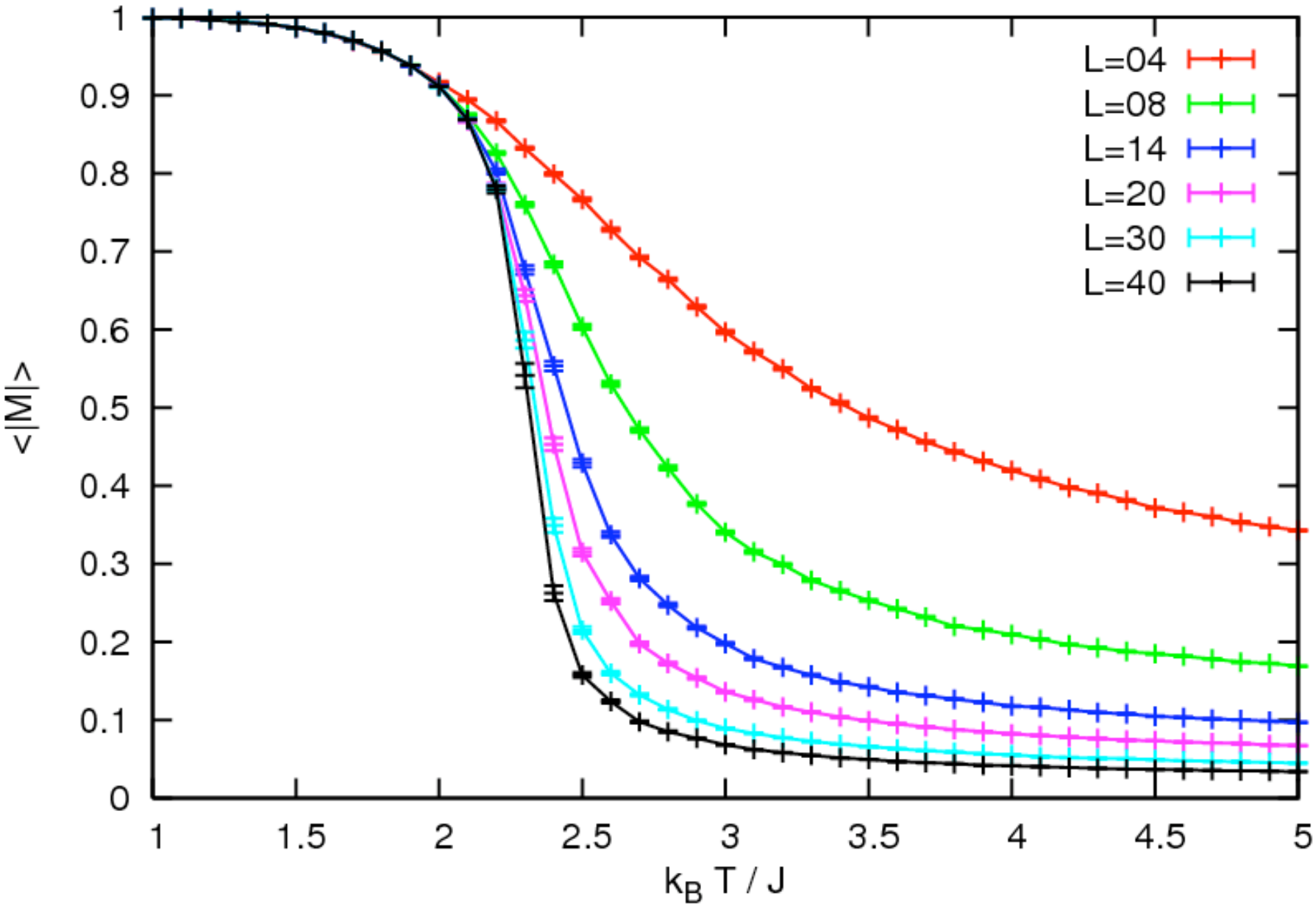
We have a ("interface") term proportional to 1/L

important monitoring E(t) and M(t) at the same time to identify possible metastable states

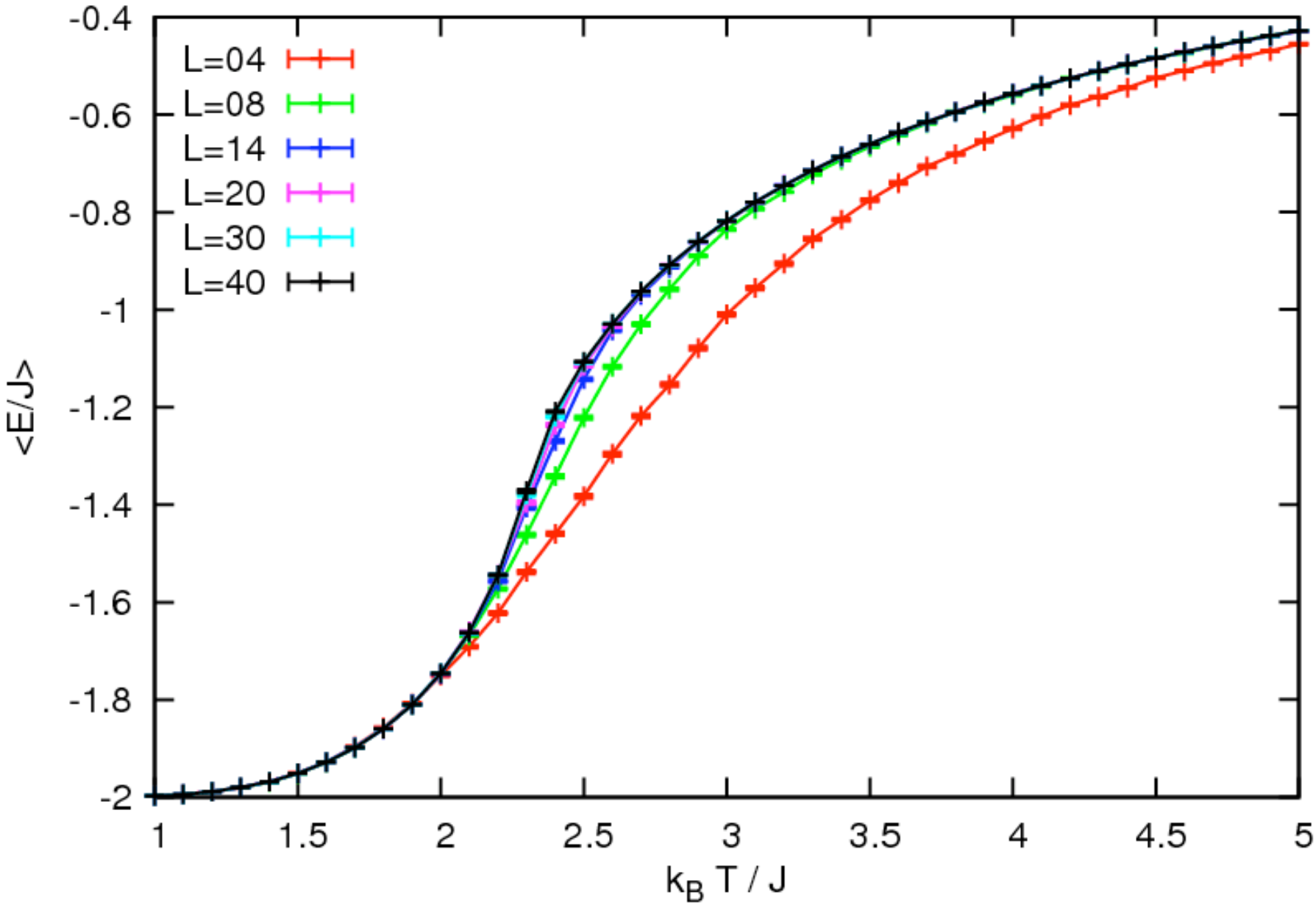


more on size effects…

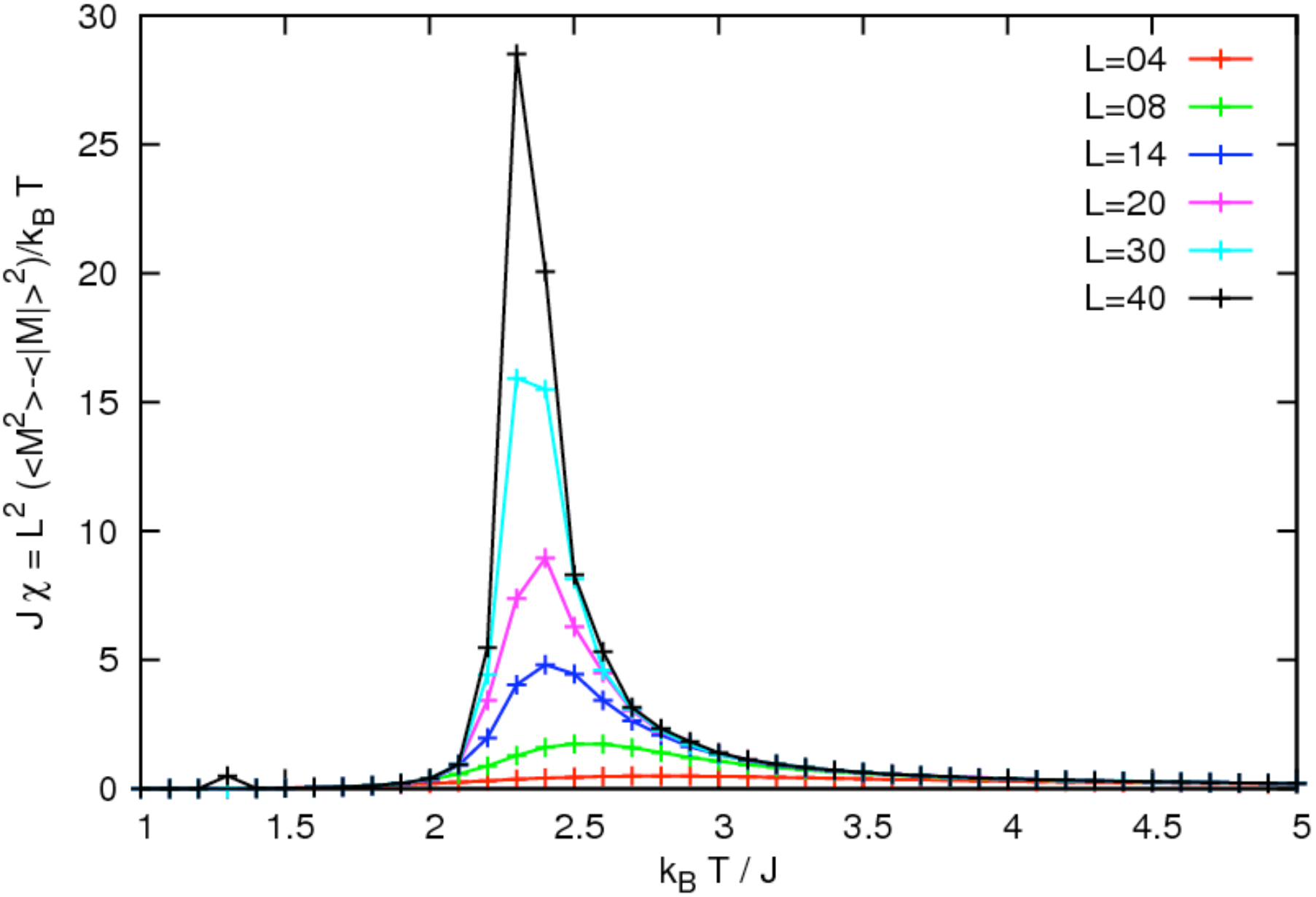
Magnetization (10^5 sweeps)



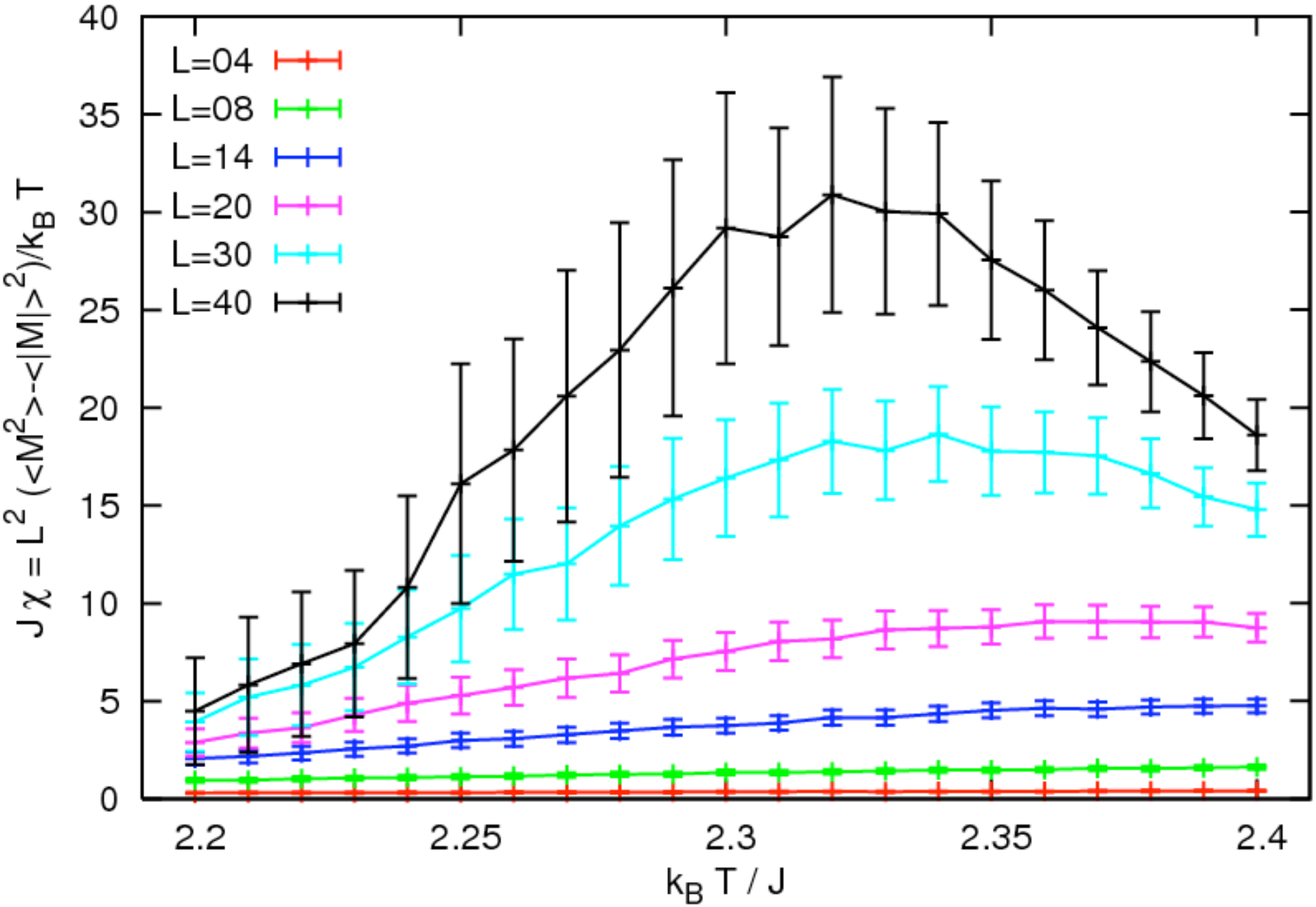
Energy (10^5 sweeps)



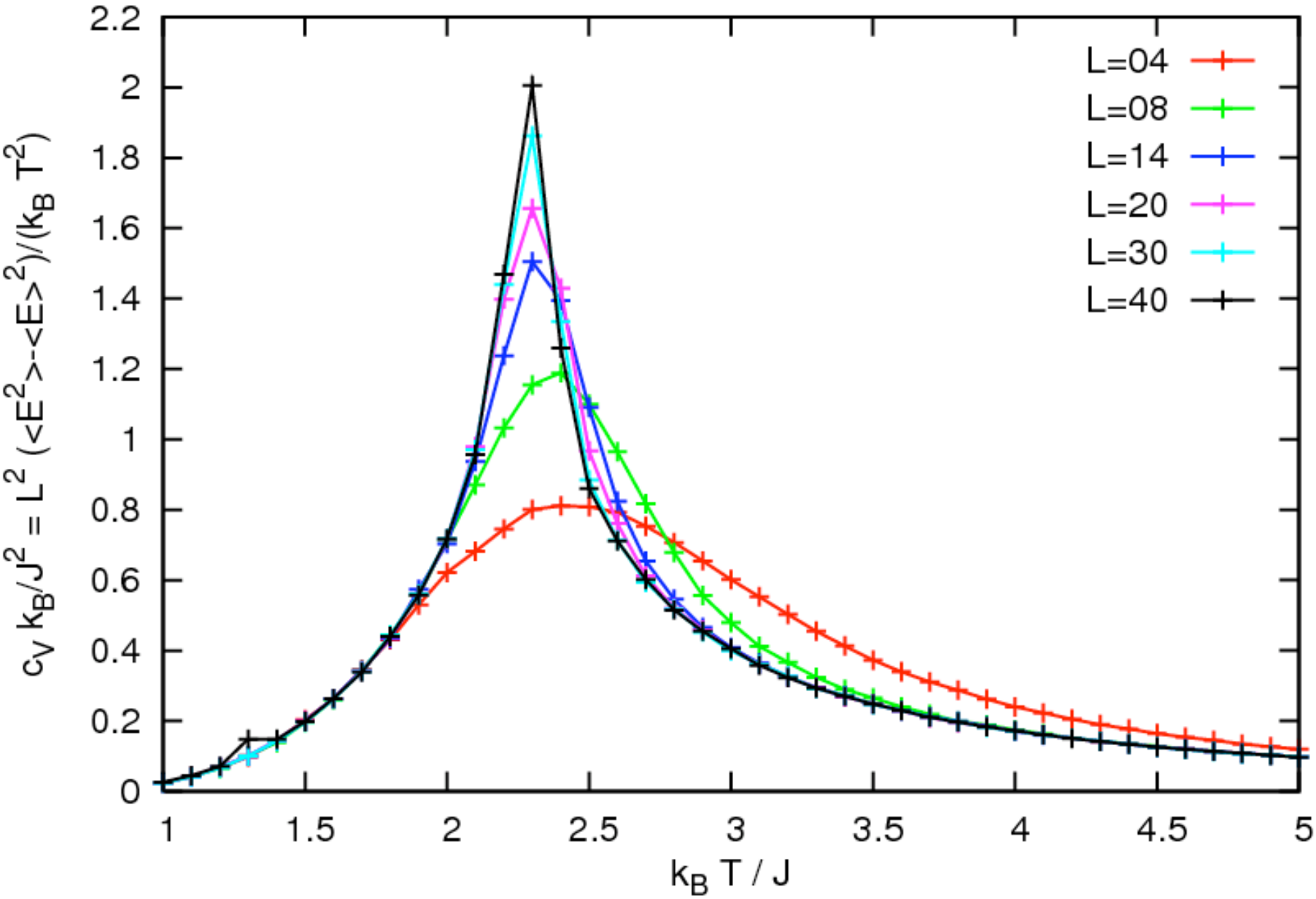
Magnetic susceptibility (10^5 sweeps)



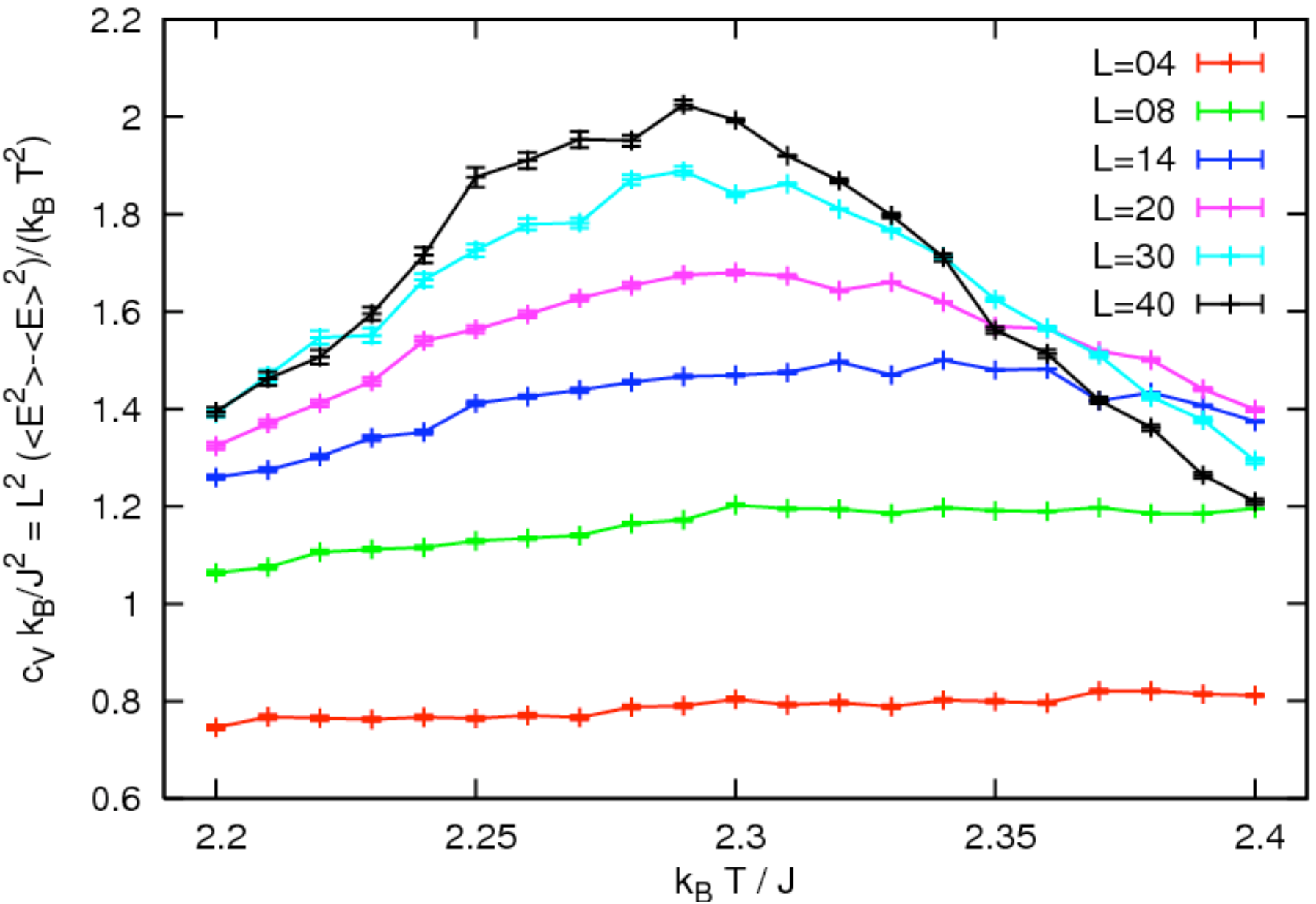
Magnetic susceptibility near T_c (10^6 sweeps)



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 . For example, we can write m near T_c as

$$m(T) \sim (T_c - T)^{\beta}, \tag{17.22}$$

where β 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

$$\chi \sim |T - T_c|^{-\gamma} \tag{17.23}$$

and

$$C \sim |T - T_c|^{-\alpha}. \tag{17.24}$$

We have assumed that χ 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 ν:

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

From: Gould-Tobochnich

Universality and critical exponents

More precisely, the magnetisation follow a power law close to the transition only approaching T_c 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 : $\Delta T = (T - T_c)/T_c$

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

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

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

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

Universality and critical exponents

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

$$\gamma = \nu(2 - \eta),$$
$$2 = \alpha + 2\beta + \gamma,$$
$$\nu d = 2 - \alpha,$$
$$\gamma = \beta(\delta - 1),$$

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

For the 2D Ising model:

α	0
β	0.125
γ	1.750
ν	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 fit,

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 α, ν, β, and γ => we have to take into account the finite size of the system

=> **finite size scaling**

Universality and critical exponents

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

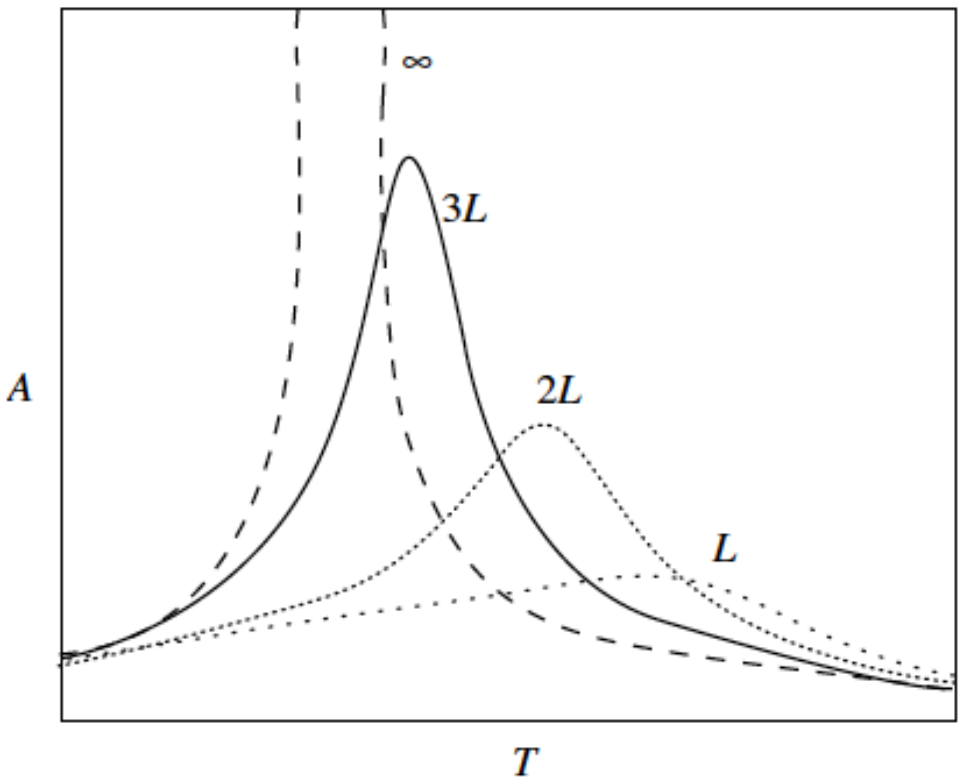


FIG. 1. Typical behaviour of a physical quantity A vs temperature close to the critical point for various system sizes. Figure taken from Thiissen[8].

[Thijssen, Computational Physics (Cambridge University Press)]

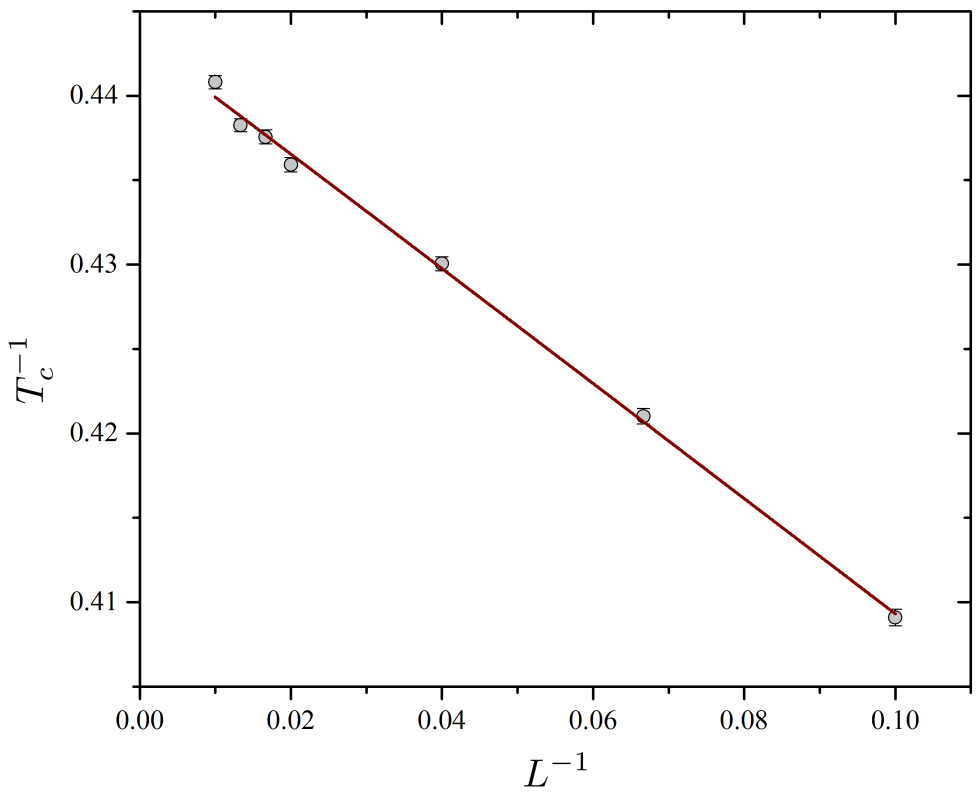


FIG. 9. (Color online) Inverse of the critical temperature T_c^{-1} vs inverse of lattice size L^{-1} for the 2D Ising model. The curve was fitted with a power law $T_c^{-1} = T_{c\infty}^{-1} - bL^{+1/\nu}$, and the critical exponent ν was determined.

$(L^{-1})^{-1/\nu}$

- From: E. Ibarra-Garcia-Padilla et al., European Journal of Physics 37(6):065103 DOI: 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 α, β, and γ 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 $L \to \infty$. 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

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

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

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

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

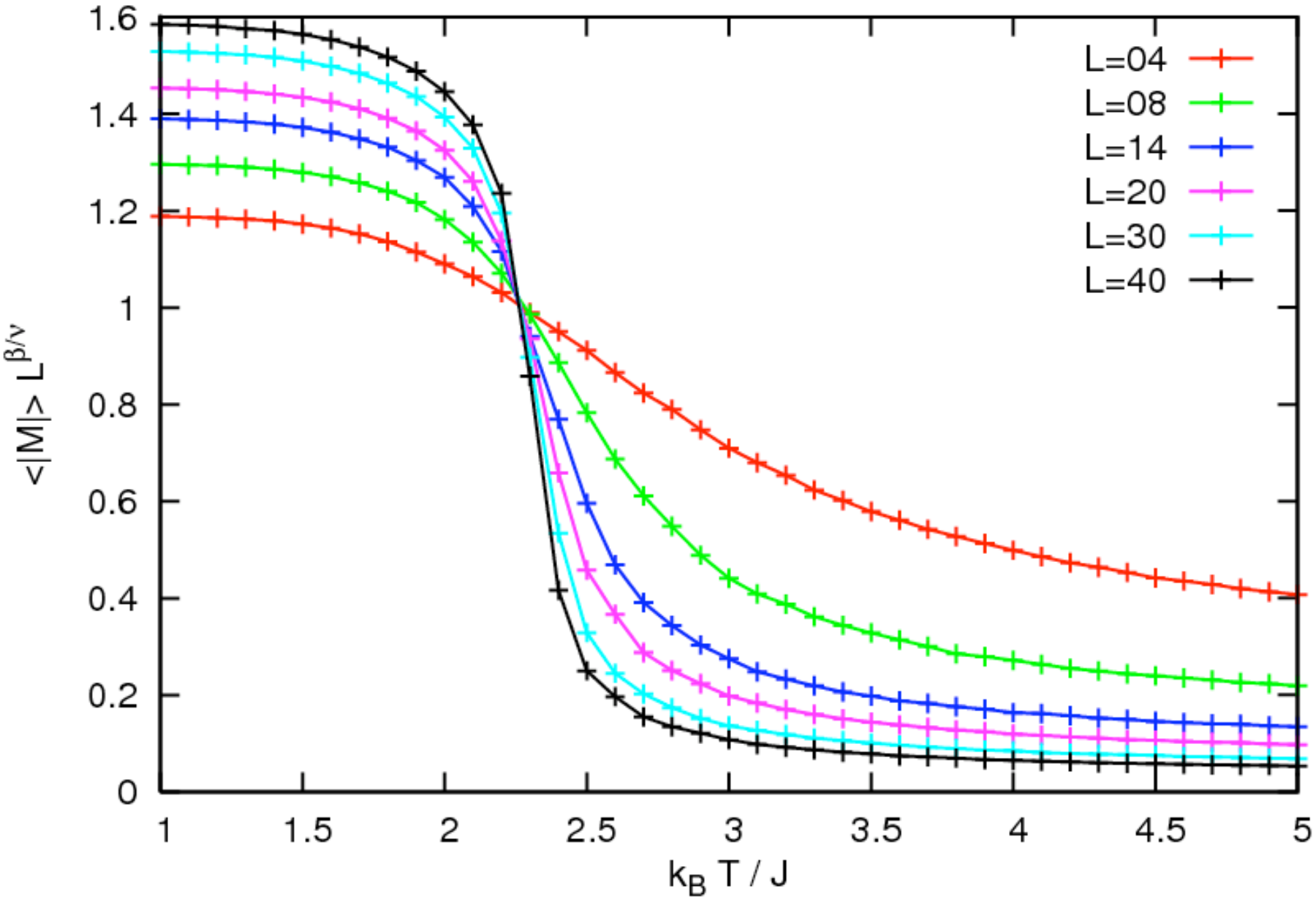
$$m(T) \sim (T_c - T)^{\beta} \to L^{-\beta/\nu} \tag{17.29}$$

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

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

From: Gould-Tobochnich

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)

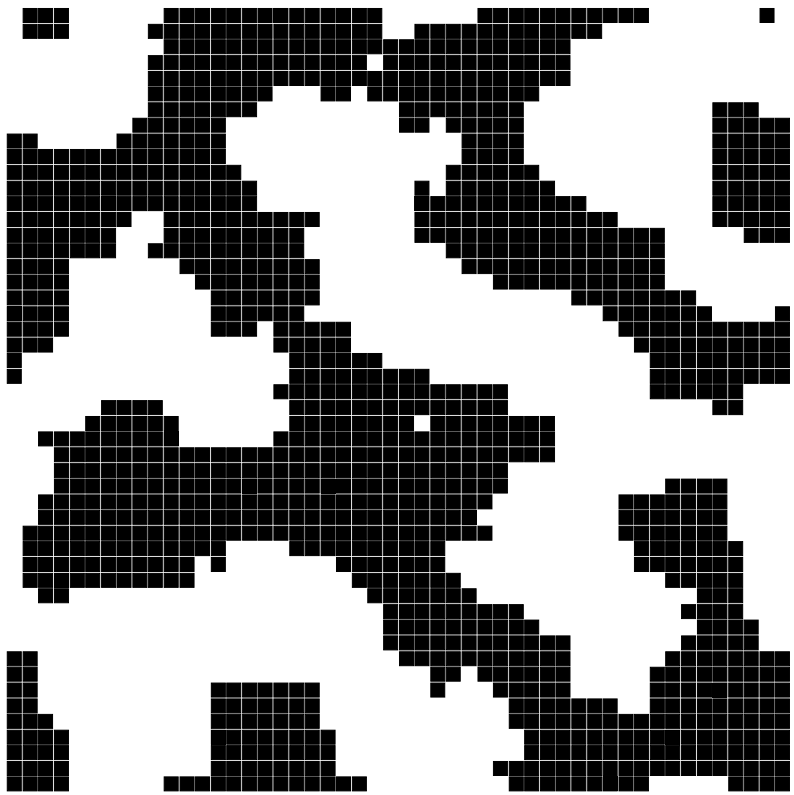
see e.g.: https://mattbierbaum.github.io/ising.js

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:

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

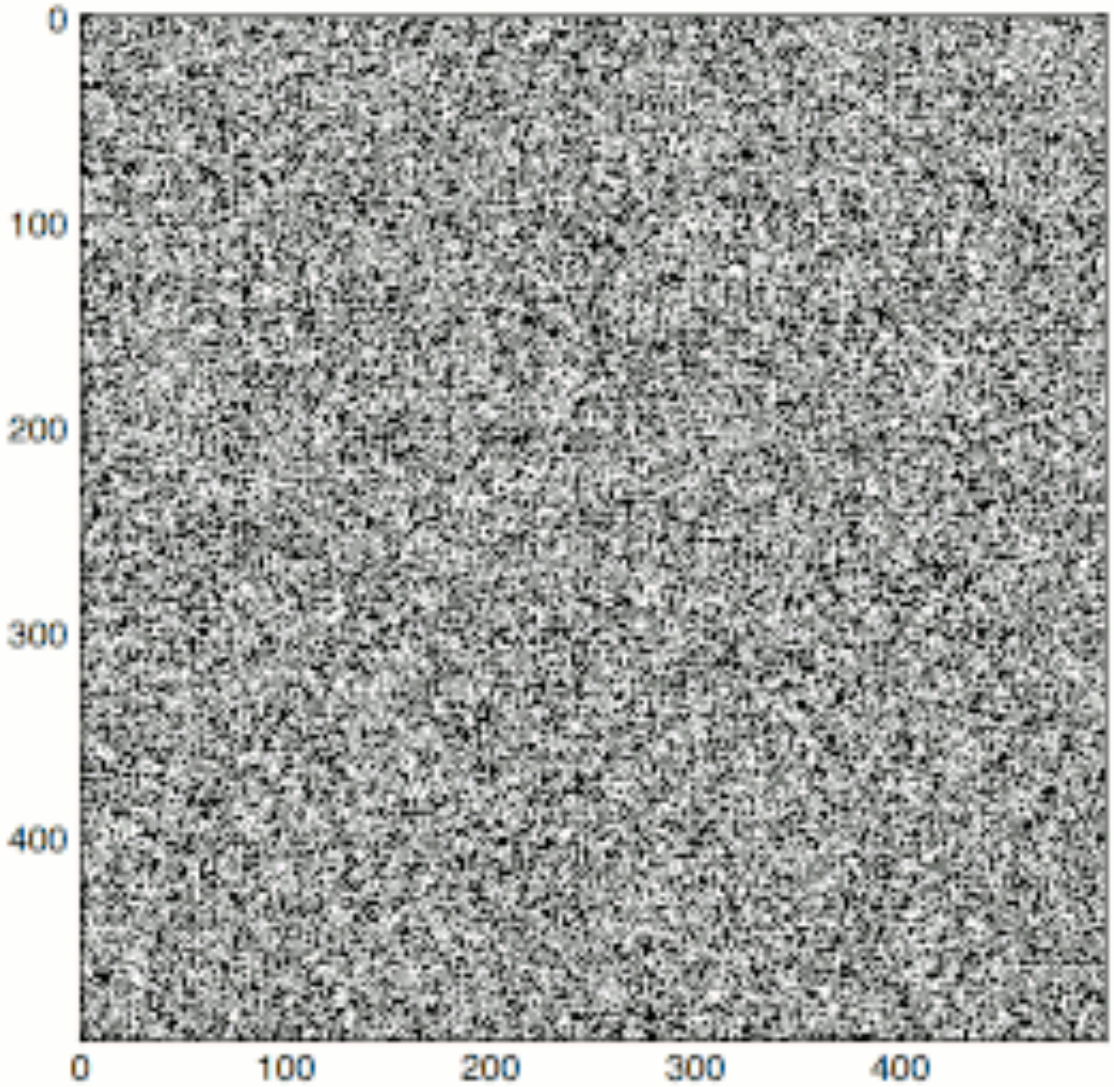
=> Trend to aggregation (diffusive behavior is limited to a transient)

- 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



500 x 500

parla di “inverse temperature beta” ???

T=?0, starting from random configuration

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:

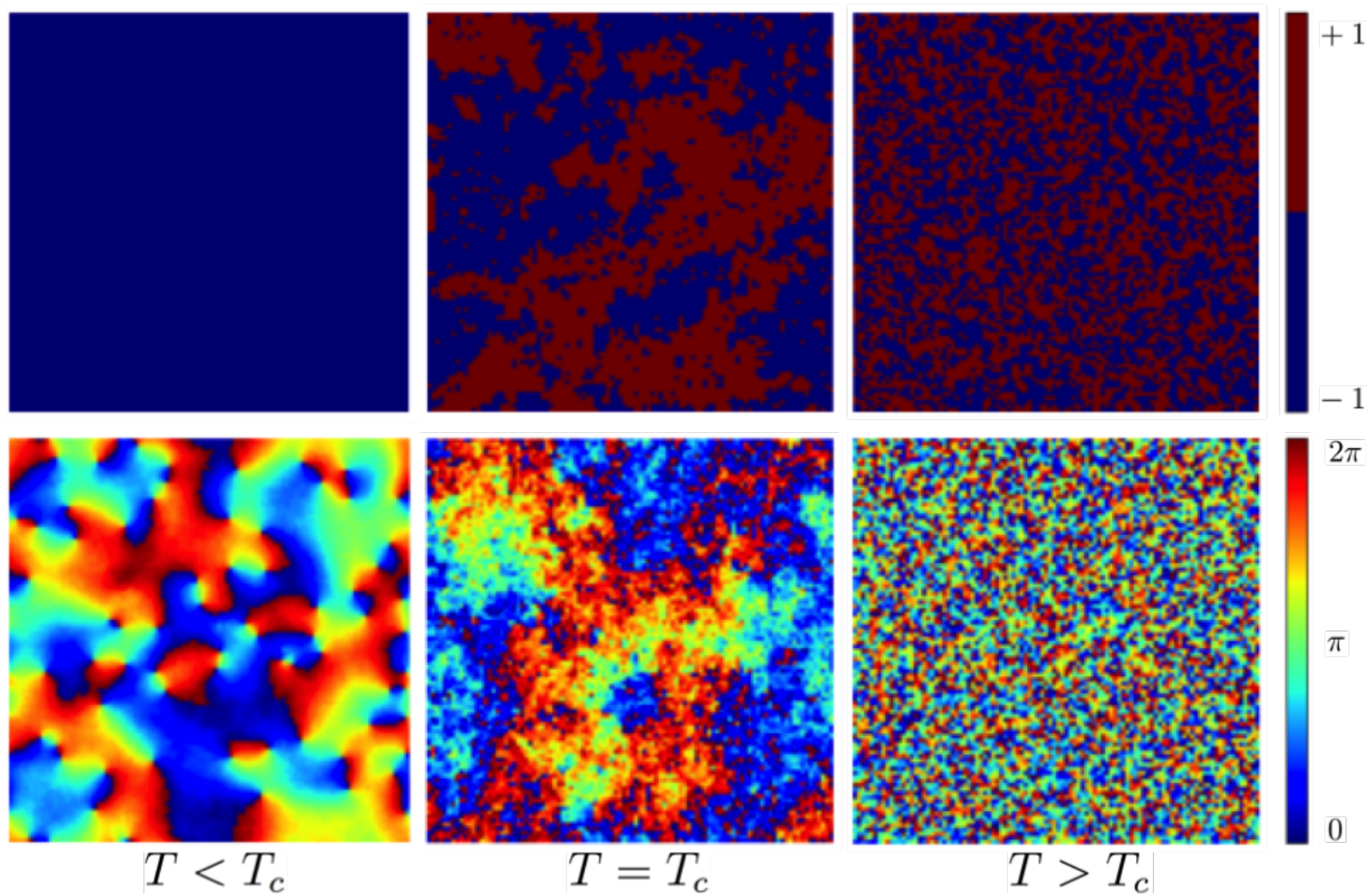
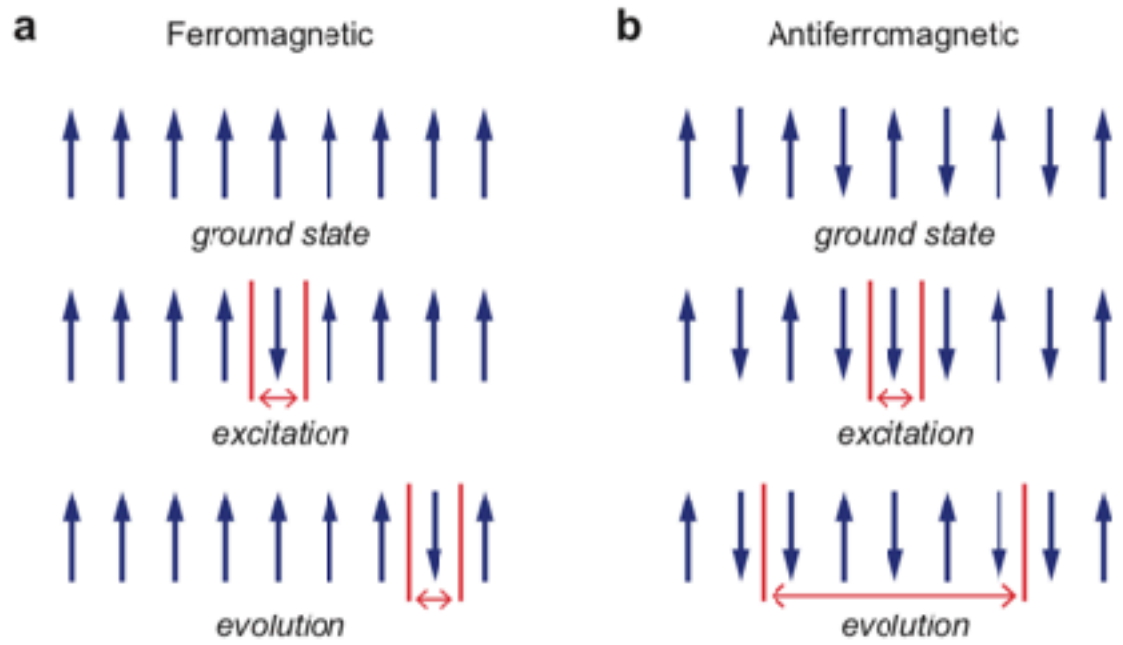


FIG. 15. (Color online) Behavior of the two dimensional Ising model (top) and XY model (bottom) at $T < T_c$, $T = T_c$ and $T > T_c$. For the Ising model, an $\uparrow$ spin ($s_i = 1$) is represented by red and a $\downarrow$ spin ($s_i = -1$) is represented by blue. For the XY model, because every spin is determined by θ, so $\mathbf{s}_i = (\cos\theta, \sin\theta)$, an angle of 2π 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).



a collective excitation of the spin structure in the lattice

With Spin exchange dynamics

Figure 1. (a) Magnon excitation and its evolution inside a ferromagnetic chain. In the ground state all the spins are in parallel alignment within each other. A magnon can be represented as a single reversed spin surrounded by two domain walls. It can propagate along the chain, but the domain walls will stay bounded to each other. (b) Same as (a) but for an antiferromagnetic chain, in the Ising limit. In the ground state, the spins are in antiparallel alignment. An excitation is achieved by creating two domain walls that separate two different AFM phases. Those two fractional excitations can independently propagate along the chain.