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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

M. Peressi - UniTS - Laurea Magistrale in Physics
Laboratory of Computational Physics - Unit IX

(from lecture VII)

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 lecture VII)

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:

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

We can generate these m microstates:

- simply randomly, without any rule, and sum the values of A_s with the proper weight, or

- randomly but with a probability distribution $\pi_s = \frac{e^{-\beta E_s}}{\sum_{s=1}^m e^{-\beta E_s}}$ (Note : $\pi_s \neq P_s$!)
Here m , not M !

(from lecture VII)

Importance sampling in the canonical ensemble

Ensemble averages can be calculated as **simple** averages if microstates are generated according to the proper probability distribution:

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

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 lecture VII)

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)

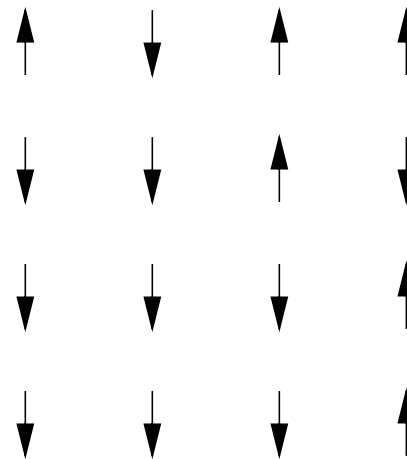
stochastic simulations of an interacting spin ensemble

We need a model for:

- **energy** => **Ising model**

- **evolution**

(to build the trajectory / the Markov chain)

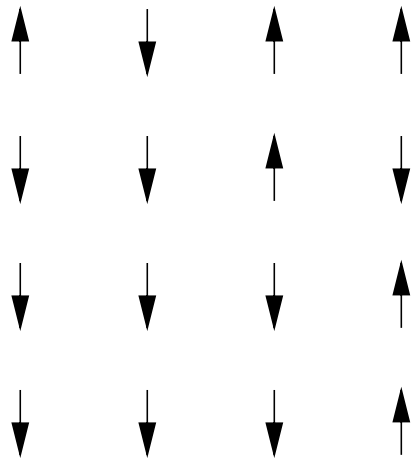


Ising model

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 ?

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

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

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

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

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:

$$\begin{aligned}J_{12} &= \langle \phi(1)\psi(2) | V_{12} | \phi(1)\psi(2) \rangle \\ K_{12} &= \langle \phi(1)\psi(2) | V_{12} | \phi(2)\psi(1) \rangle\end{aligned}$$

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

$$\begin{aligned}\langle S = 0 | \mathcal{H} | S = 0 \rangle &= E_s && \text{singlet} \\ \langle S = 1 | \mathcal{H} | S = 1 \rangle &= E_t && \text{triplet}\end{aligned}$$

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 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 \Rightarrow ferromagnetic case

$J < 0$ ($E_s < E_t$) $\uparrow\downarrow$ spins favored \Rightarrow 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”)

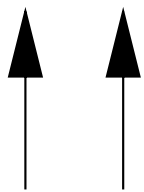
Ising model

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

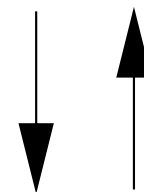
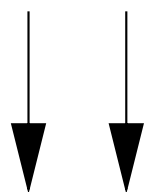
$$\mathcal{H}^{spin} = -J \sum_{i,j=1}^N s_i s_j$$

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

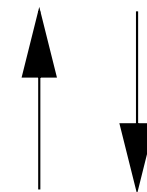
$J < 0$ ($E_s < E_t$) $\uparrow\downarrow$ spins favored \Rightarrow **antiferromagnetic case**



$$E = -J$$



$$E = +J$$

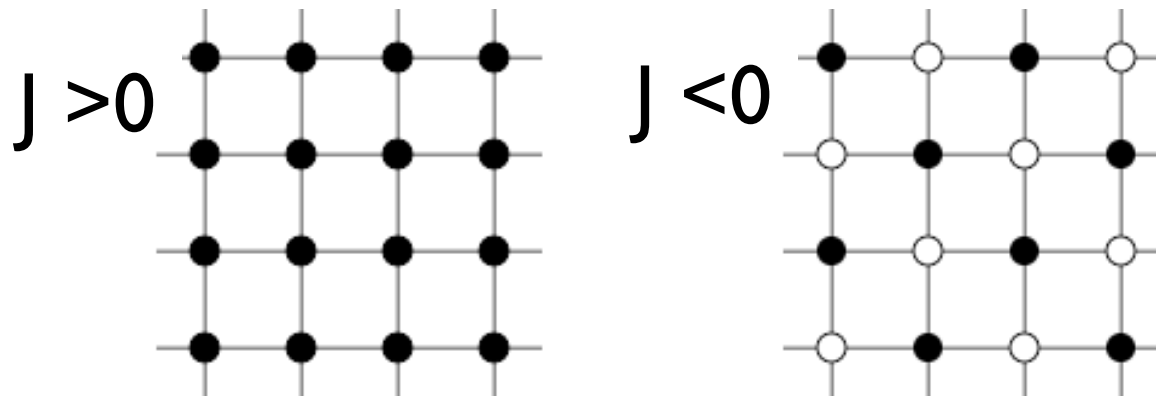


(choosing the kind of interaction, we specify the **energy model**)

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-
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 2×2 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:

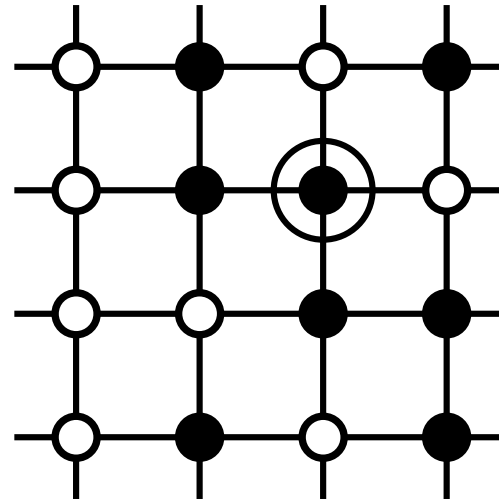
$$E_0/N = - 2J$$

Ising model: 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

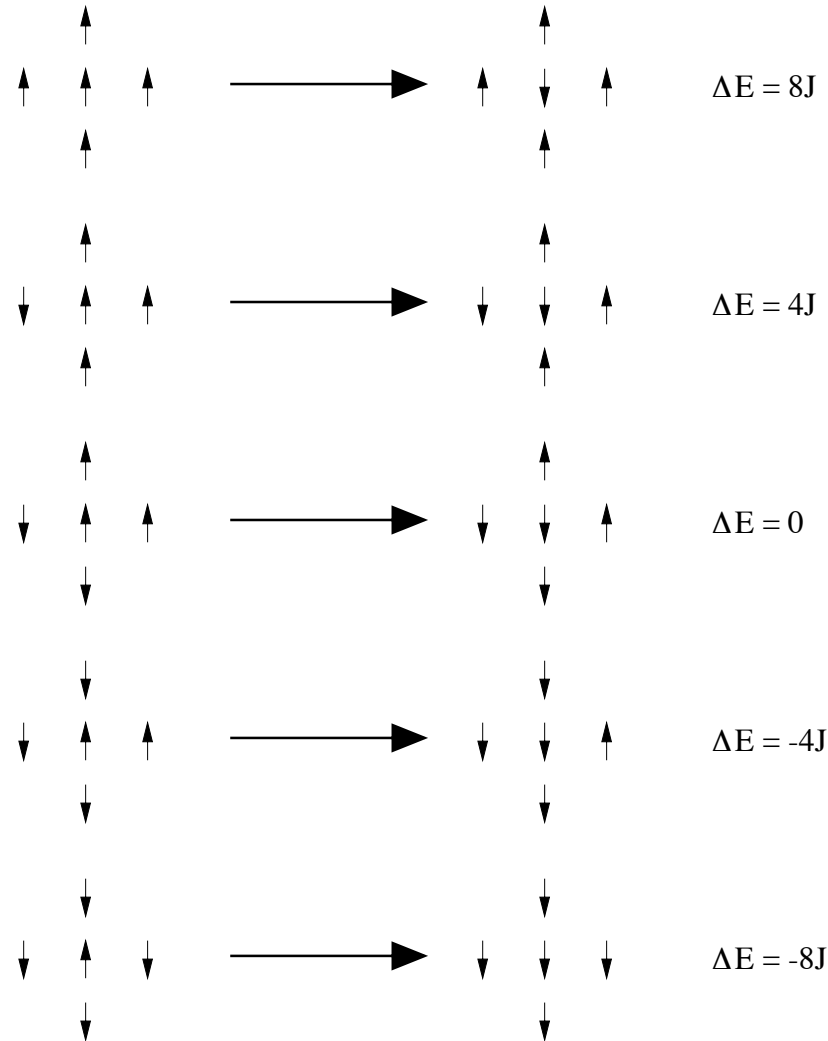
Consider nn interactions, choose a random spin and flip it: it's **a new configuration** (a microstate)



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

Ising model: boundary conditions

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

We have two choices for the simulation cell:

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

Ising model: free boundary conditions

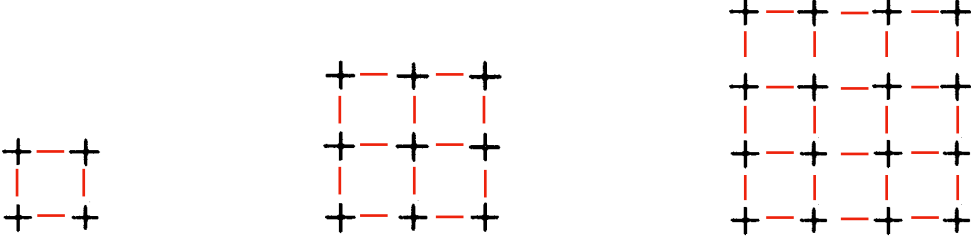
in a $N=L \times L$ spin lattice there are $2L(L-1)$ nn interactions;
for the ferromagnetic g.s. configuration, for instance, the energy is:

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

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:



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

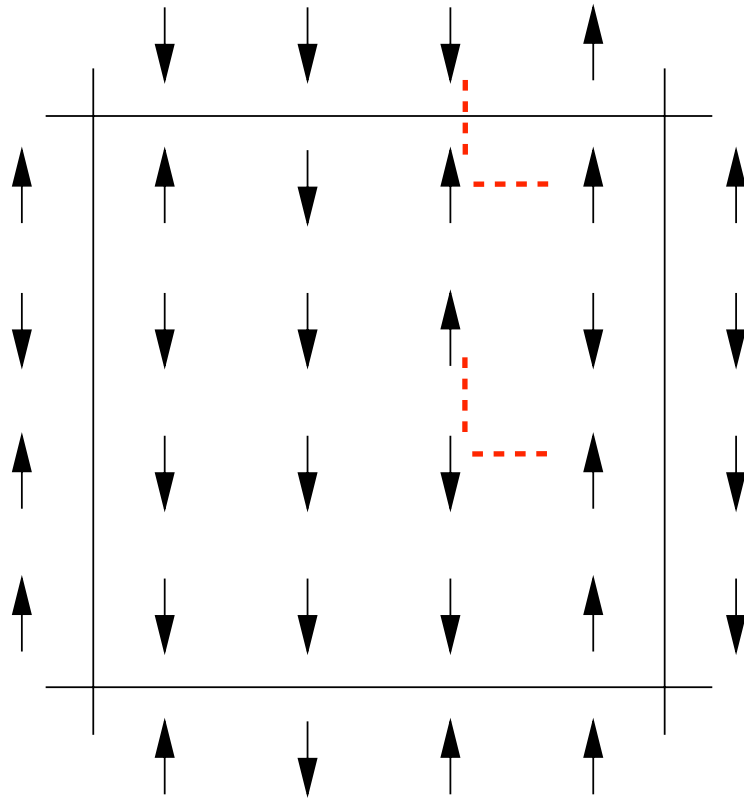
(volume term)
(surface term)

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

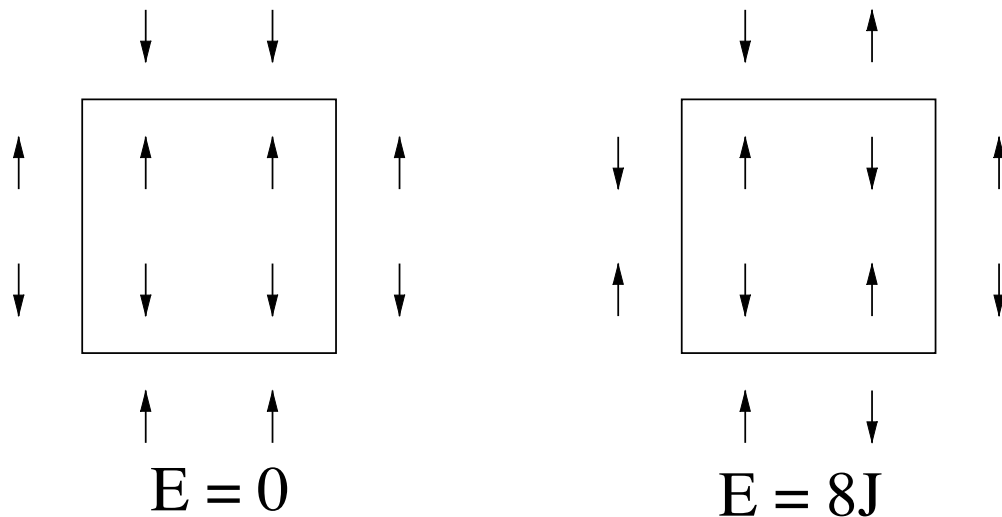
One of the 2^N possible configurations of a system of $N = 16$ Ising spins on a square lattice.
with periodic boundary conditions.

Ising model: PBC

We have always:

$2^4 = 16$ spin configurations for 2×2 lattice

but the energy for each configuration in case of free 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 equal to the value $E_0/N = -2J$ in the thermodynamic limit

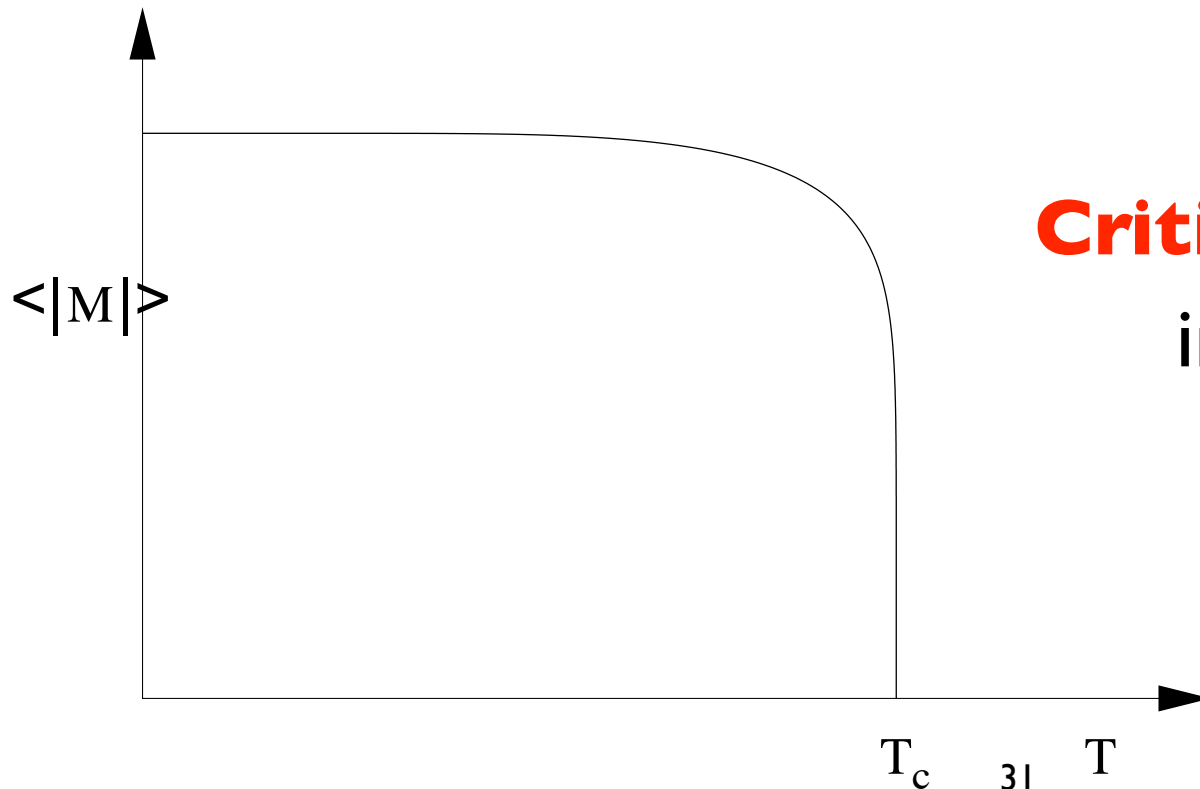
Ising model: phase transition

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**)



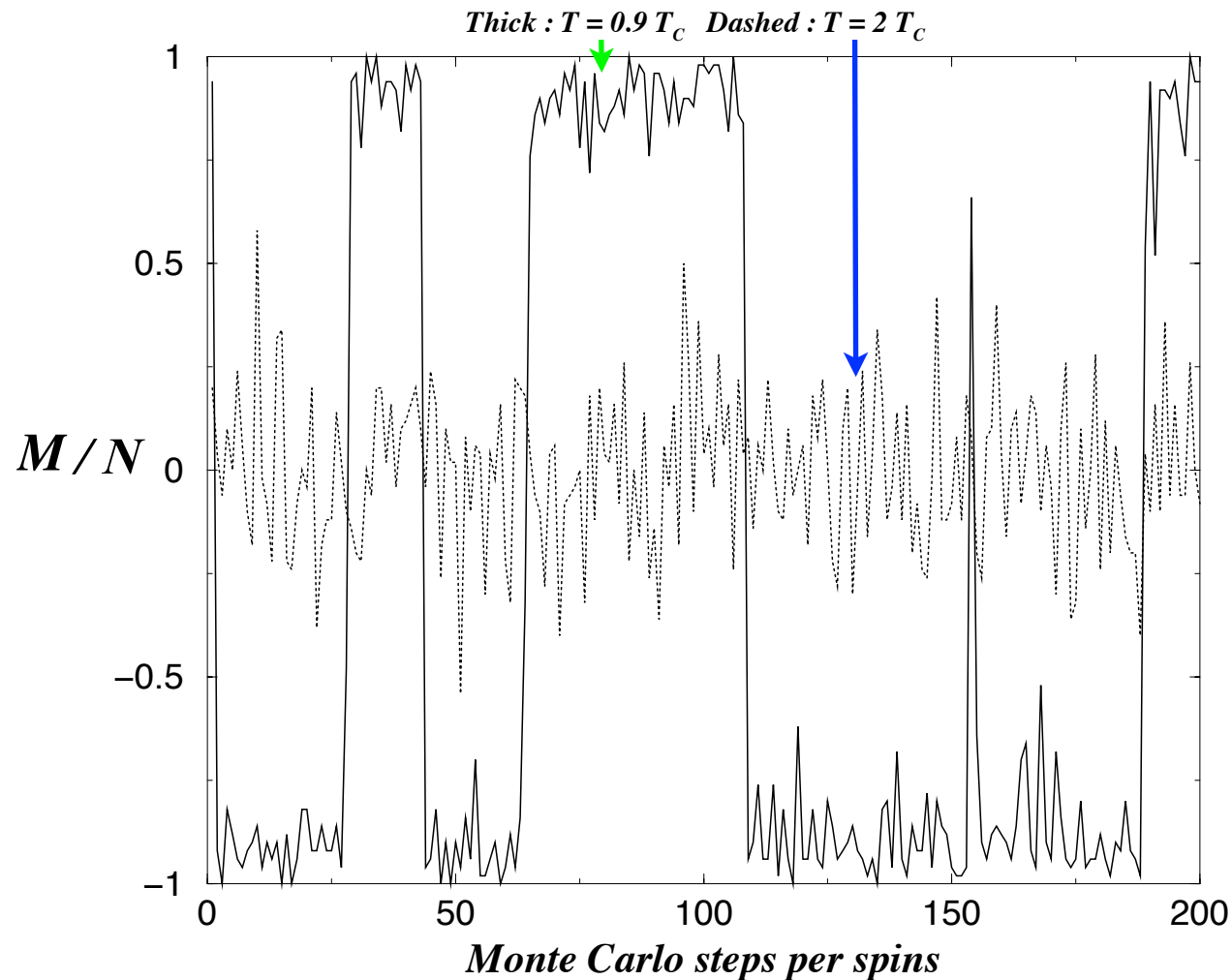
**existence of a
Critical temperature T_c**

in 2D the model has an
analytical solution:

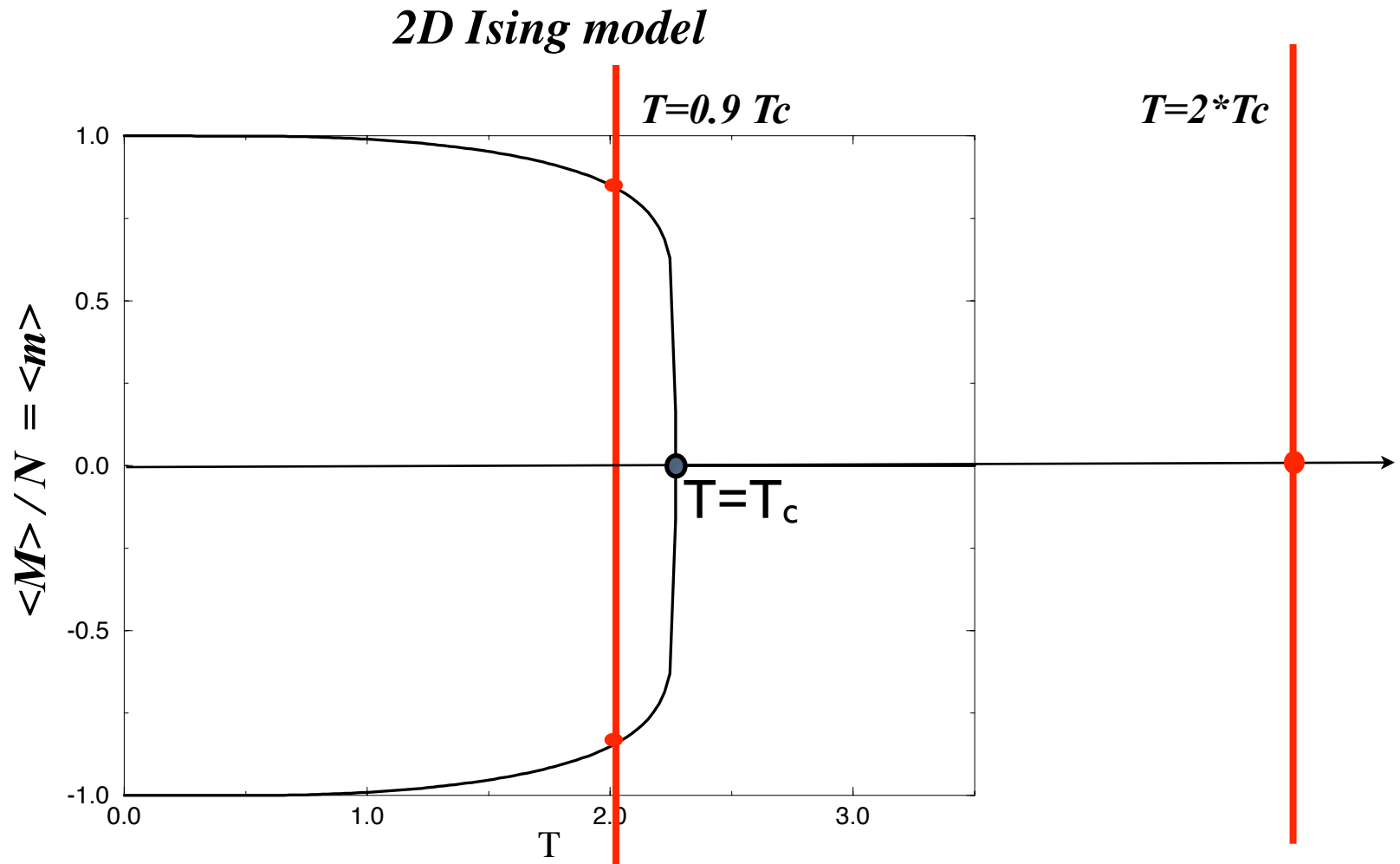
$$T_c = 2.269 J/k_B$$

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

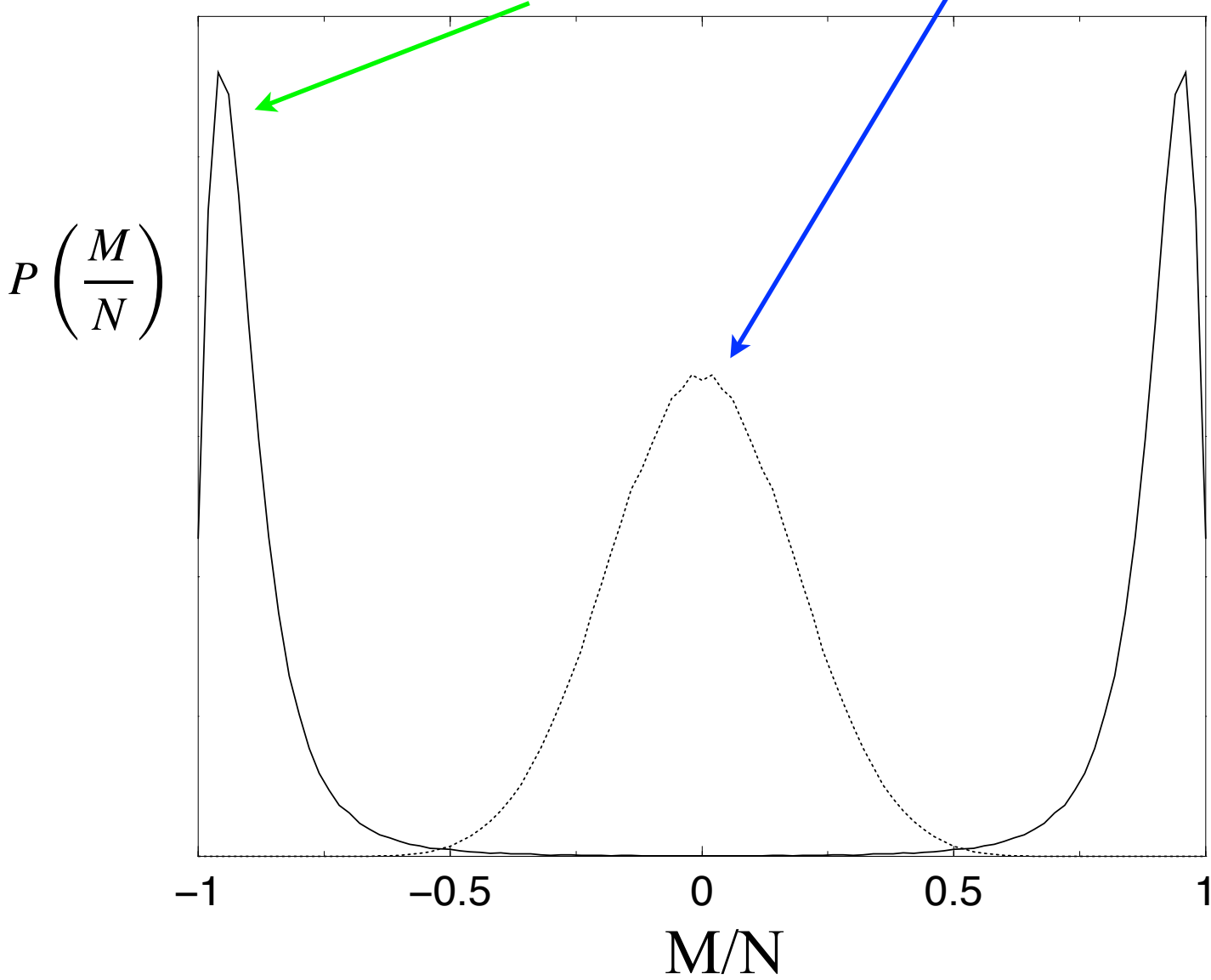


Fluctuations! do, as usual, **temporal averages**: $\langle M \rangle / N$, $\langle E \rangle / N$



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)

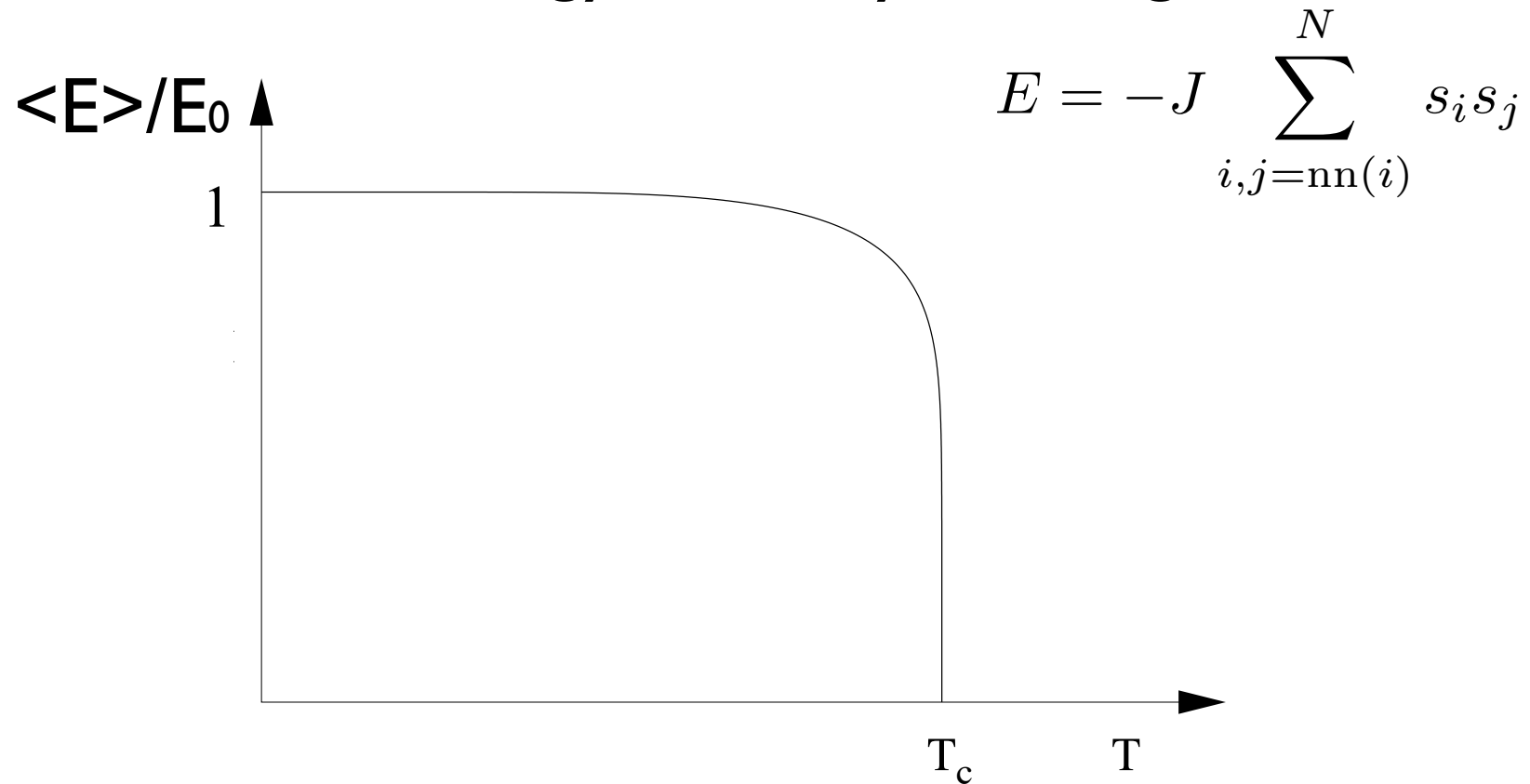
Magnetization distribution for $T < T_c$ (solid) and $T > T_c$ (dashed curve)



(data collected during time evolution, at equilibrium)

Ising model: phase transition

T_c also for energy, not only for magnetization:



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: $E \rightarrow const.$, 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 χ

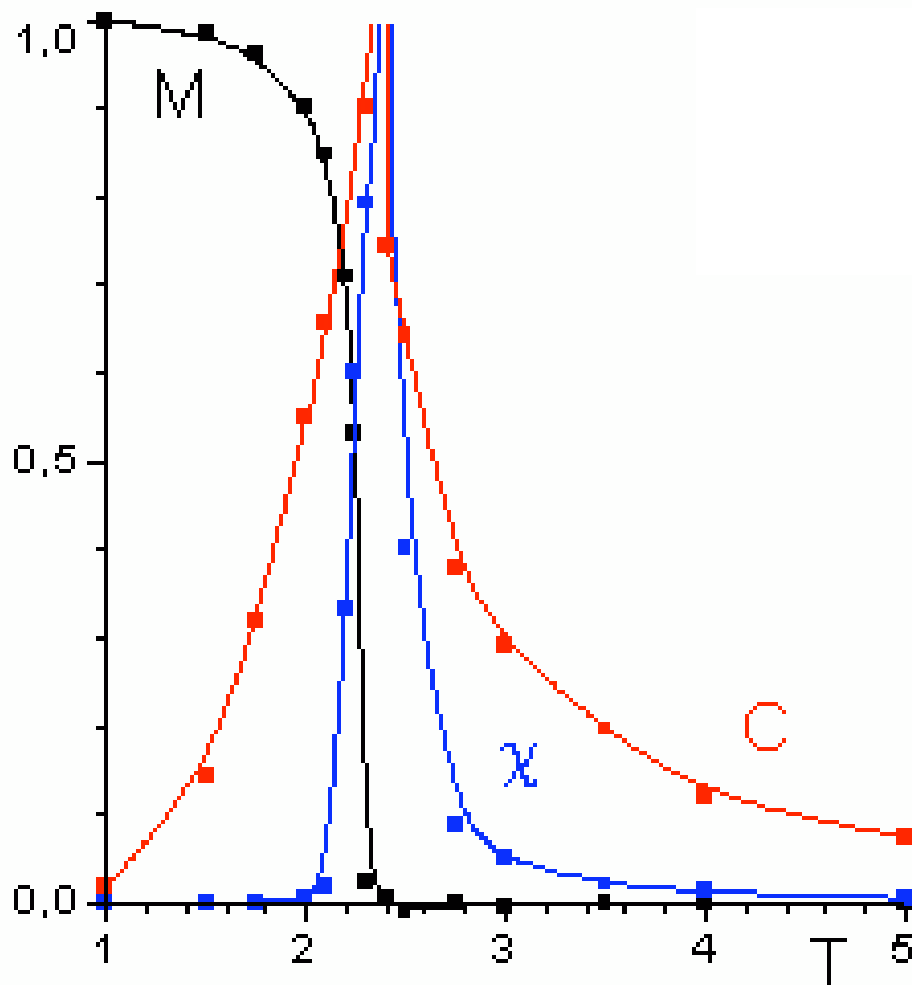
(Large fluctuations near the phase transition:
Second Order phase transition)

specific heat:

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

magnetic susceptibility:

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



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:

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

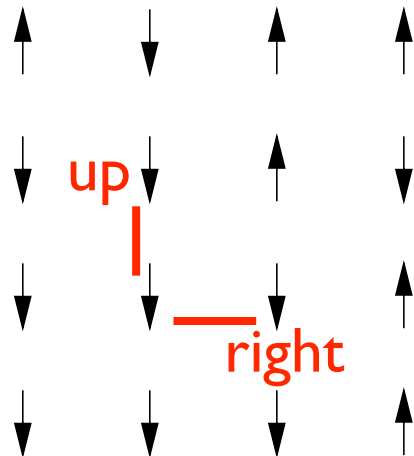
$$m = \frac{M}{N} = \frac{1}{N} \sum_{i=1}^N s_i$$

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

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

(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
```

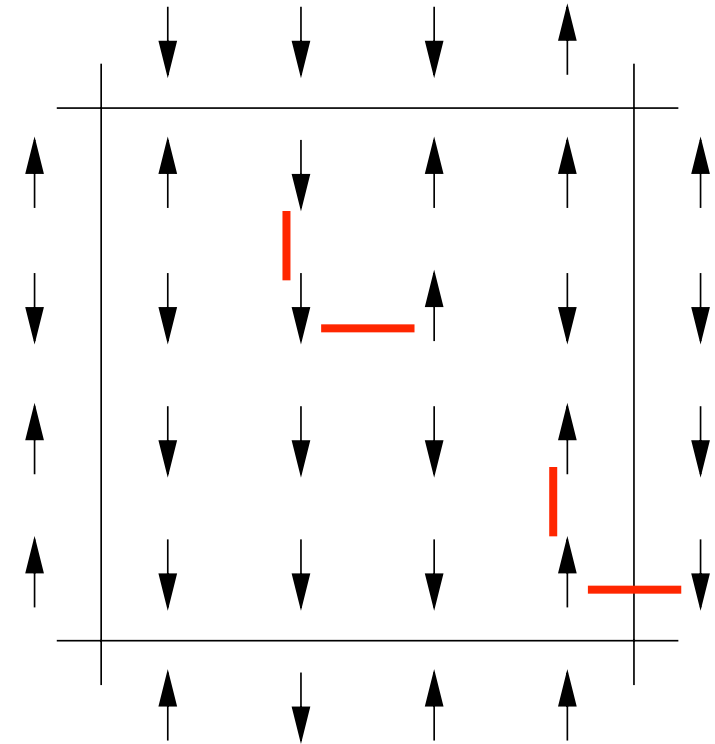
```
  E = E - spin(x,y)*sums
```

```
  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
    .....
```

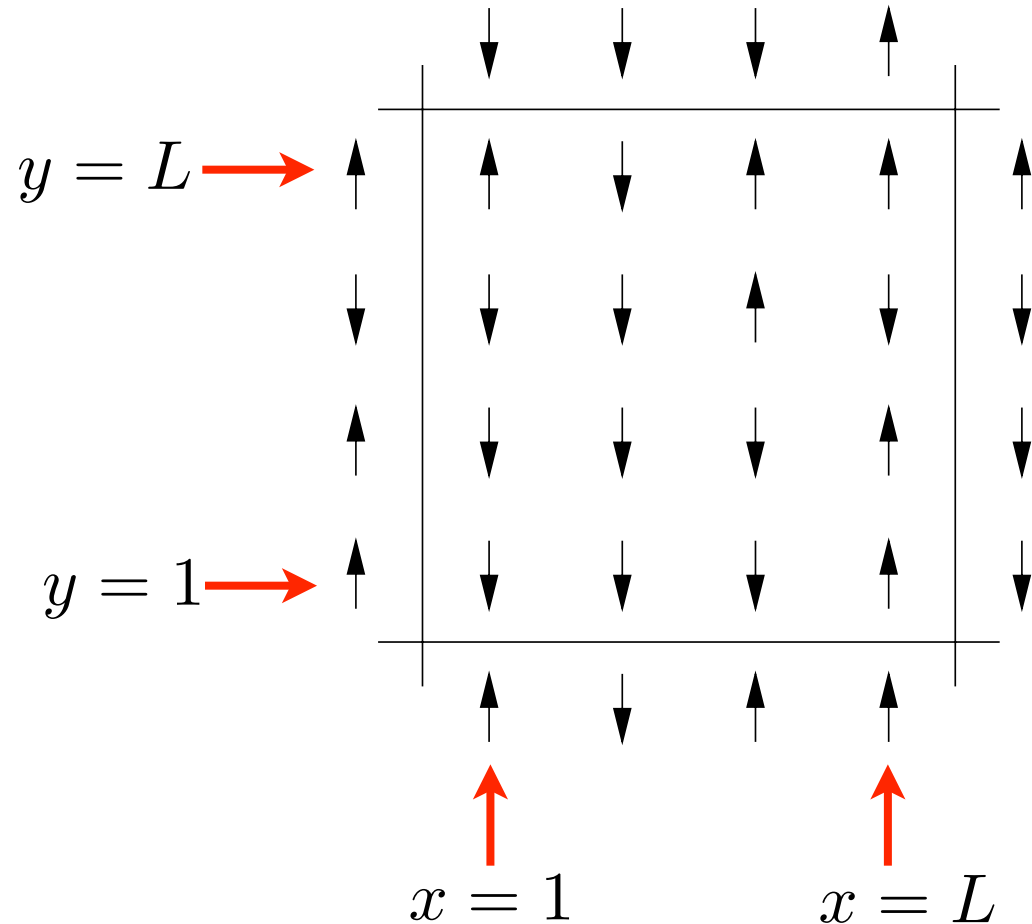
```
function DeltaE(x,y) result (DeltaE_result)
.....
DeltaE_result = 2*spin(x,y)*(left + right + up + down)
.....
```


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)
  .....

```

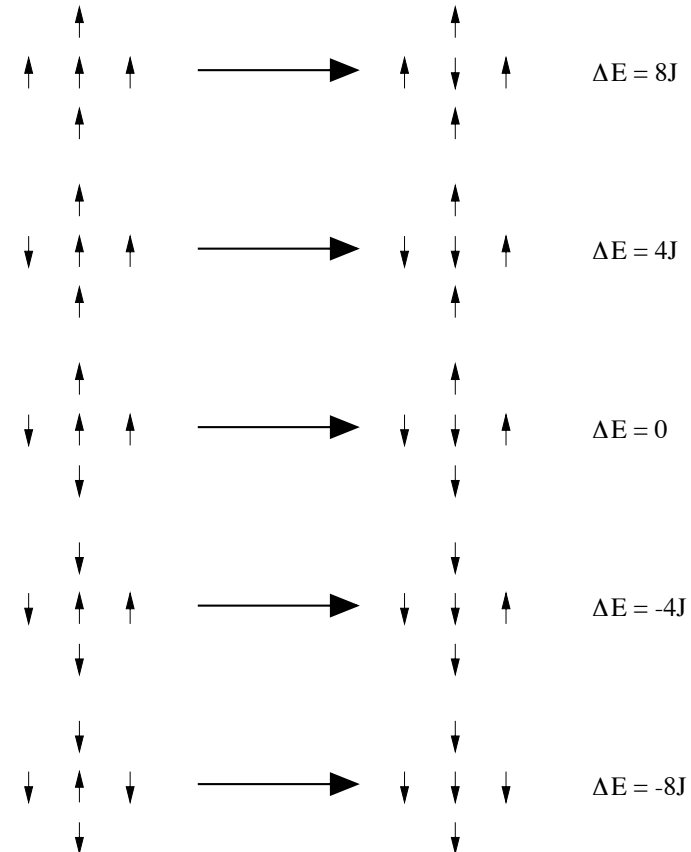


Ising model: storage of Boltzmann's coeff.

```
! 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!!**

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      ←  $1 \leq x \leq L$ 
  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**:

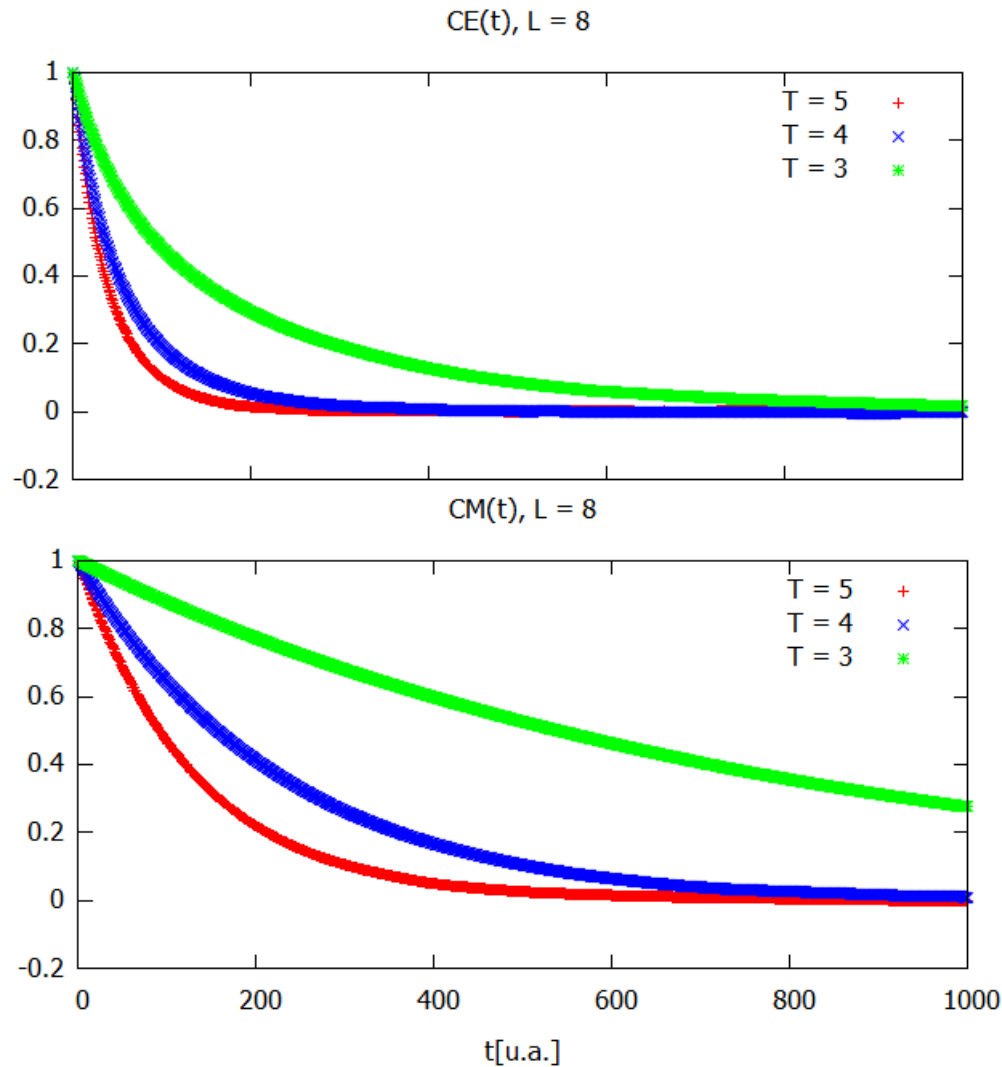
$$C_M(t) = \langle M(t)M(0) \rangle - \langle M \rangle^2, \quad C_E(t) = \langle E(t)E(0) \rangle - \langle E \rangle^2$$

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

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

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

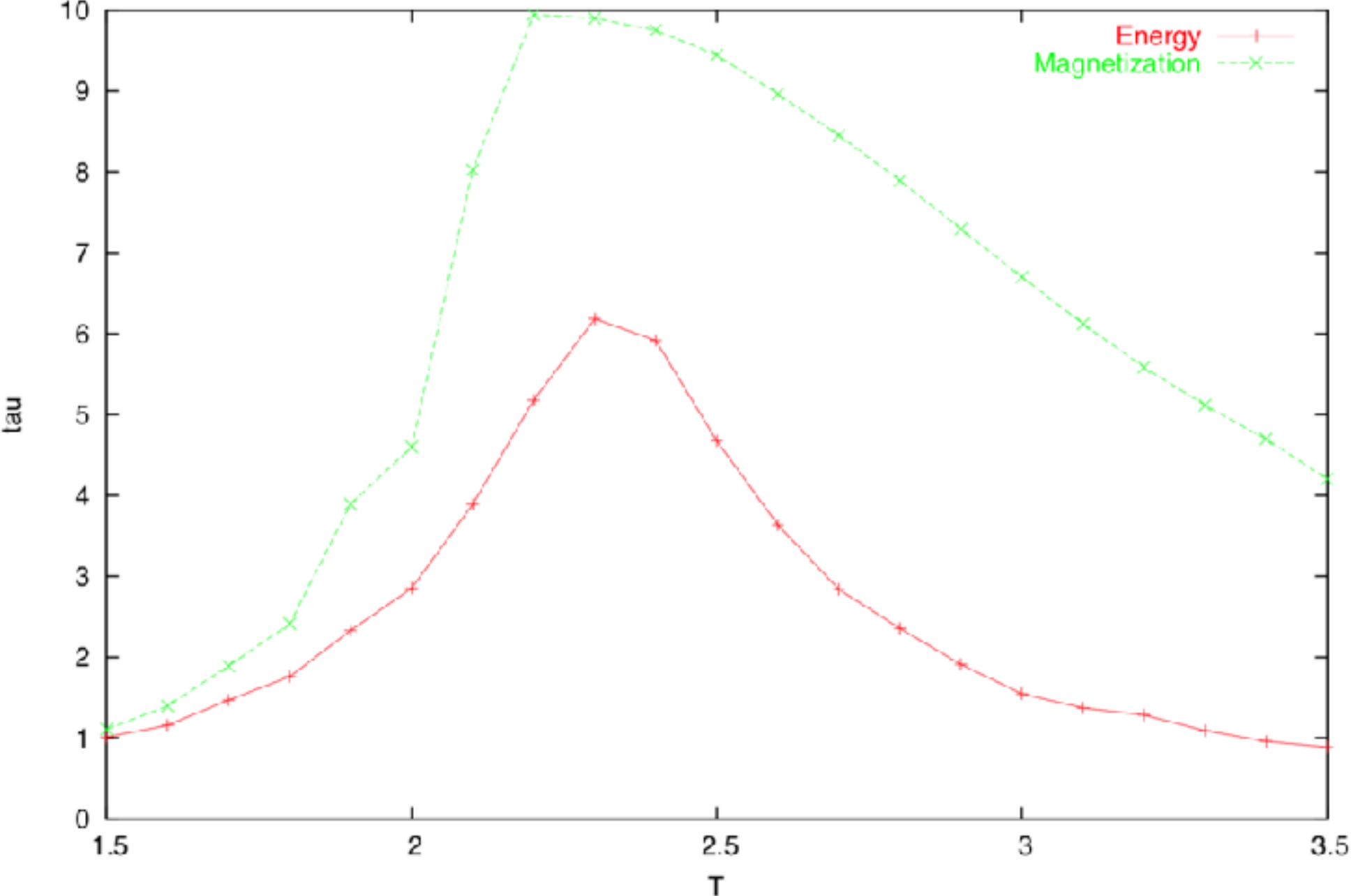
Autocorrelation functions



(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)

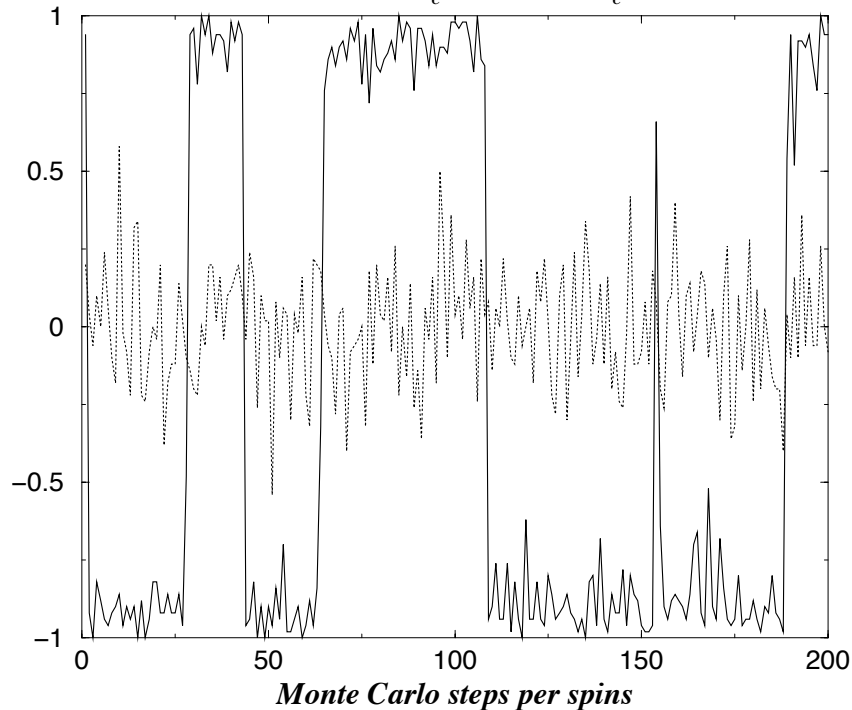
How to do efficiently simulations as a function of T ?

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

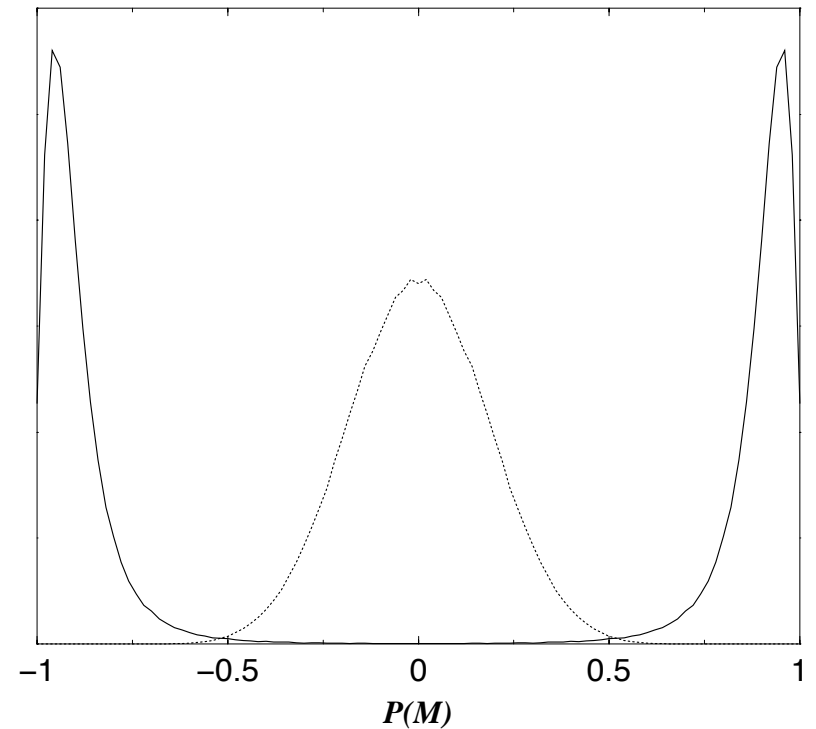
How to do efficiently simulations as a function of T ?

*Magnetization (System : 10*10)*

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

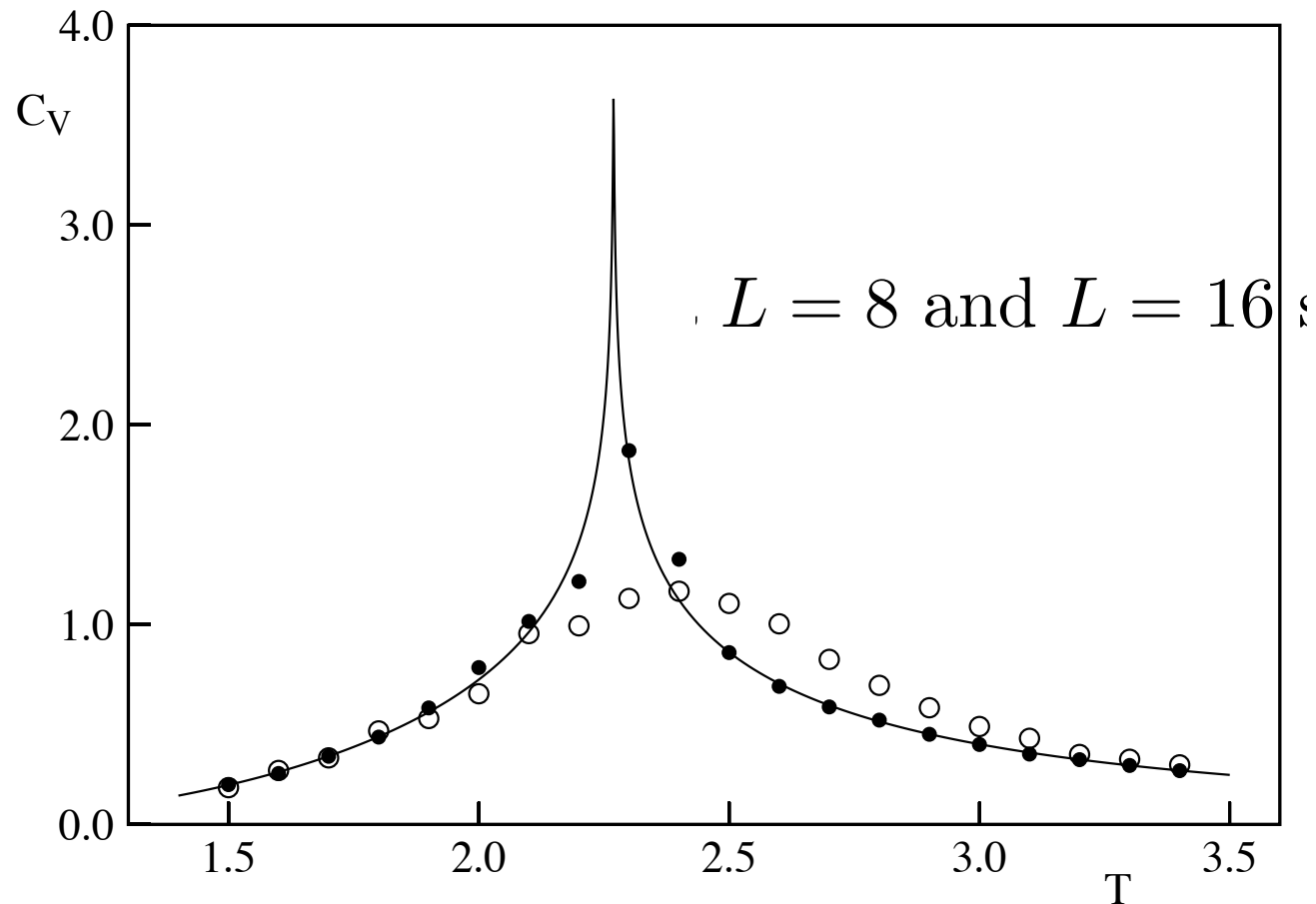


Magnetization distribution



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:

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

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

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

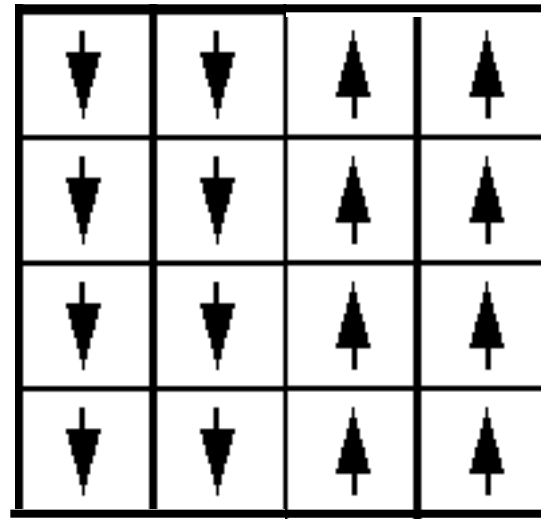
$$L=16 \quad E=-1.75$$

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

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

... 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 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?

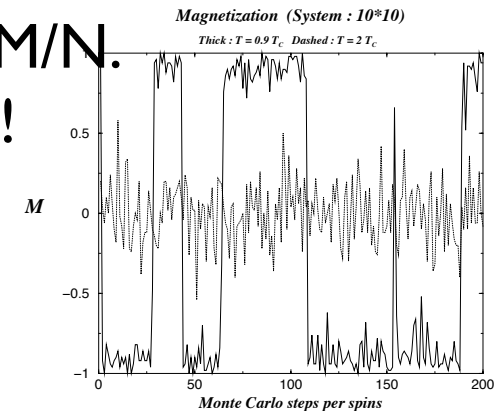
Hint:

- 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

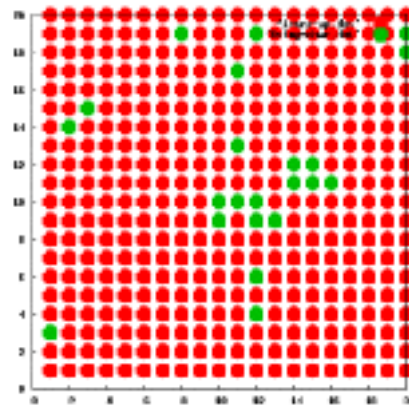
(a) Choose $L=30, T=2$, and initially $\text{spin}=\pm 1$ randomly. ...

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:



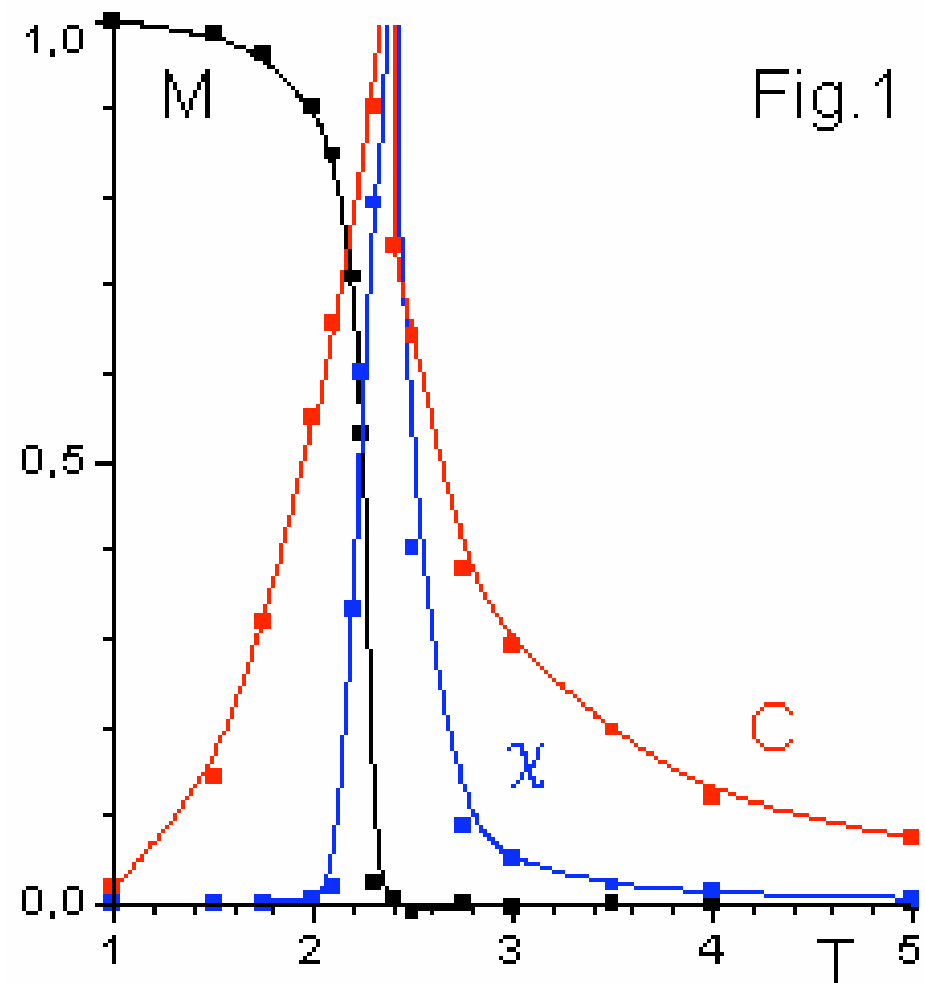
Calculate also c and χ .

Exercise

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

Calculate also c and χ .

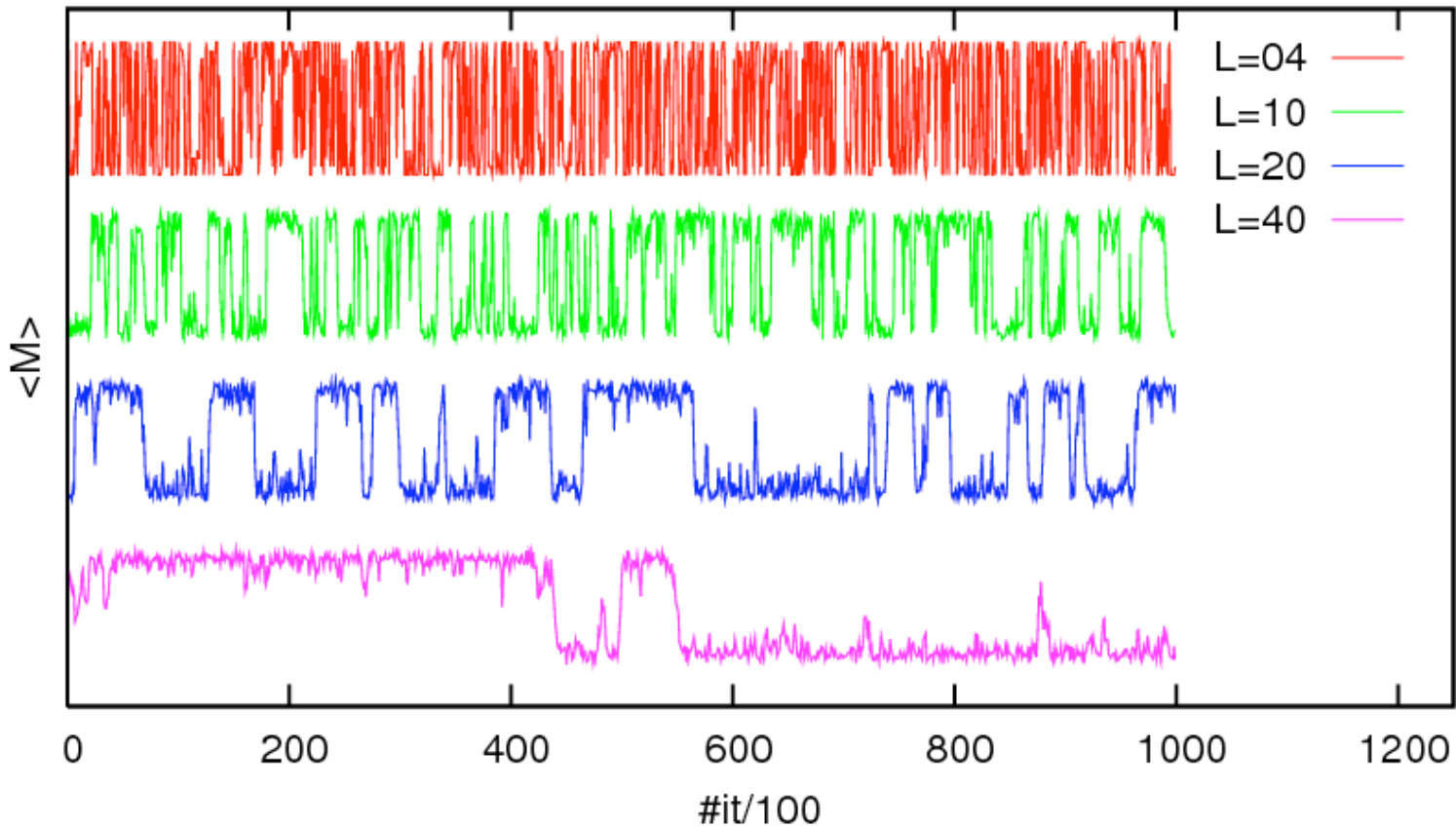
(b) Choose $T=I$ and repeat (a)...



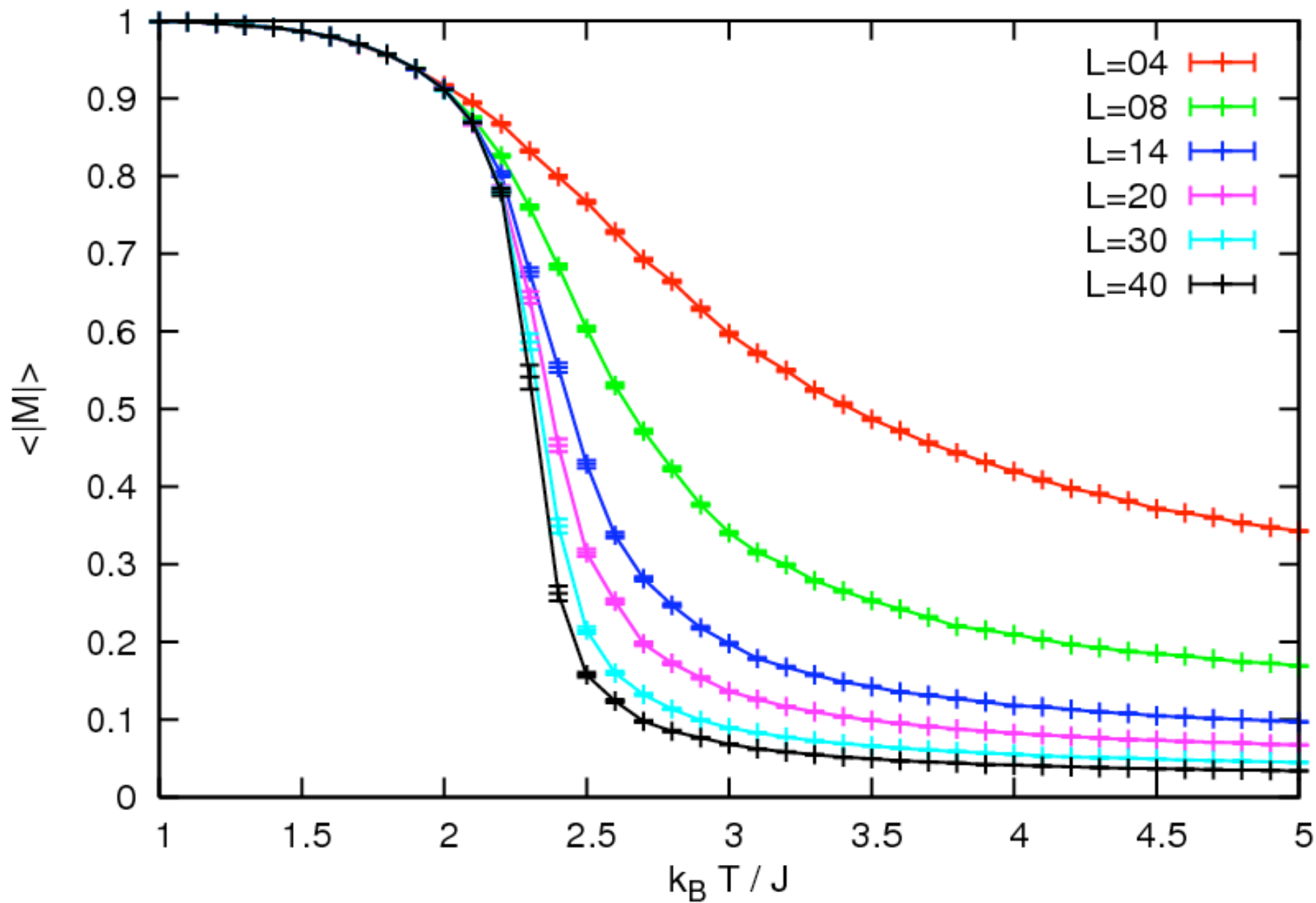
Some results that you should obtain...

Raw data: traces, covariance and autocorrelation time

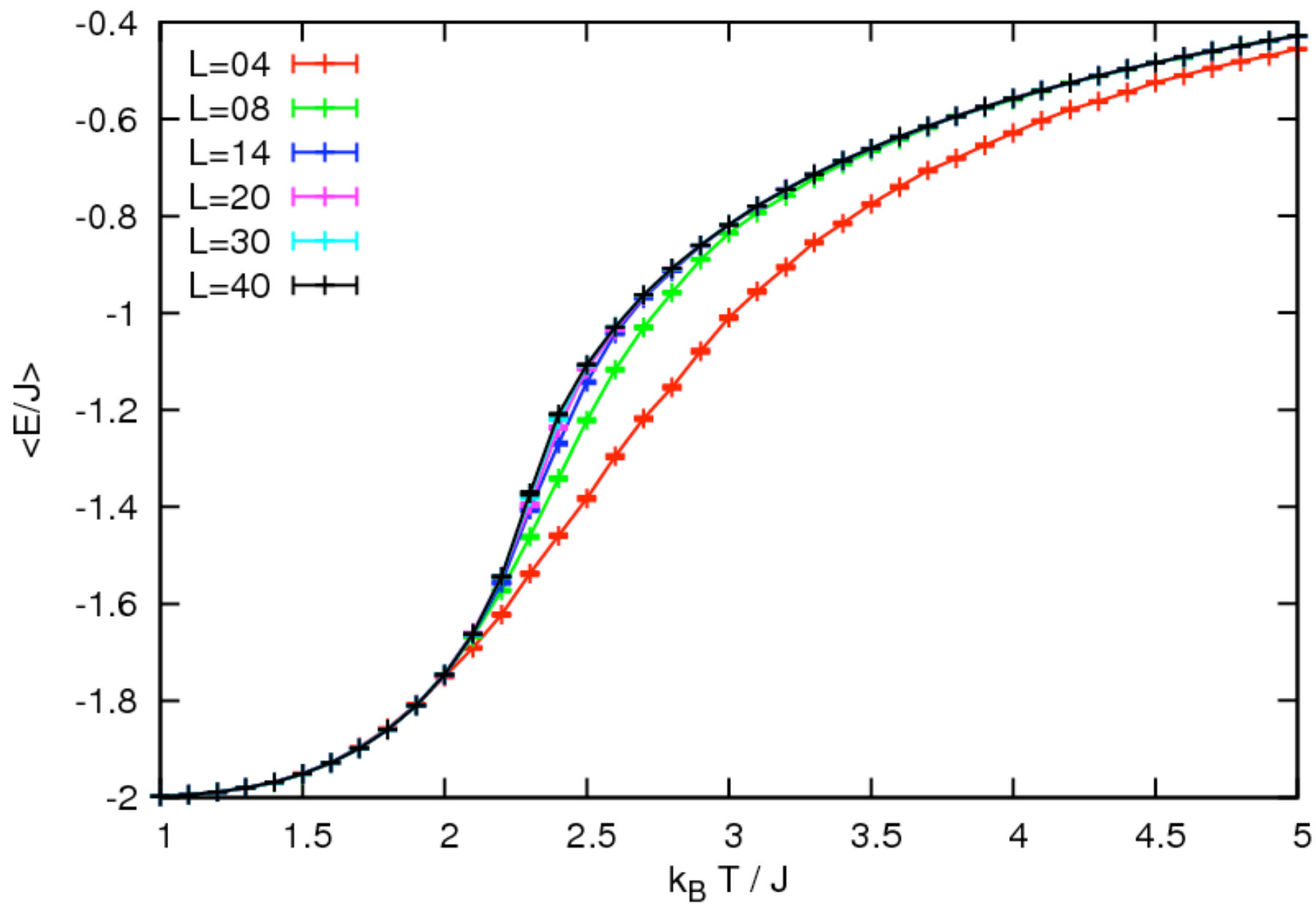
Trace: magnetization for $T = 2.27J/k_B \approx T_C$ (10^5 sweeps)



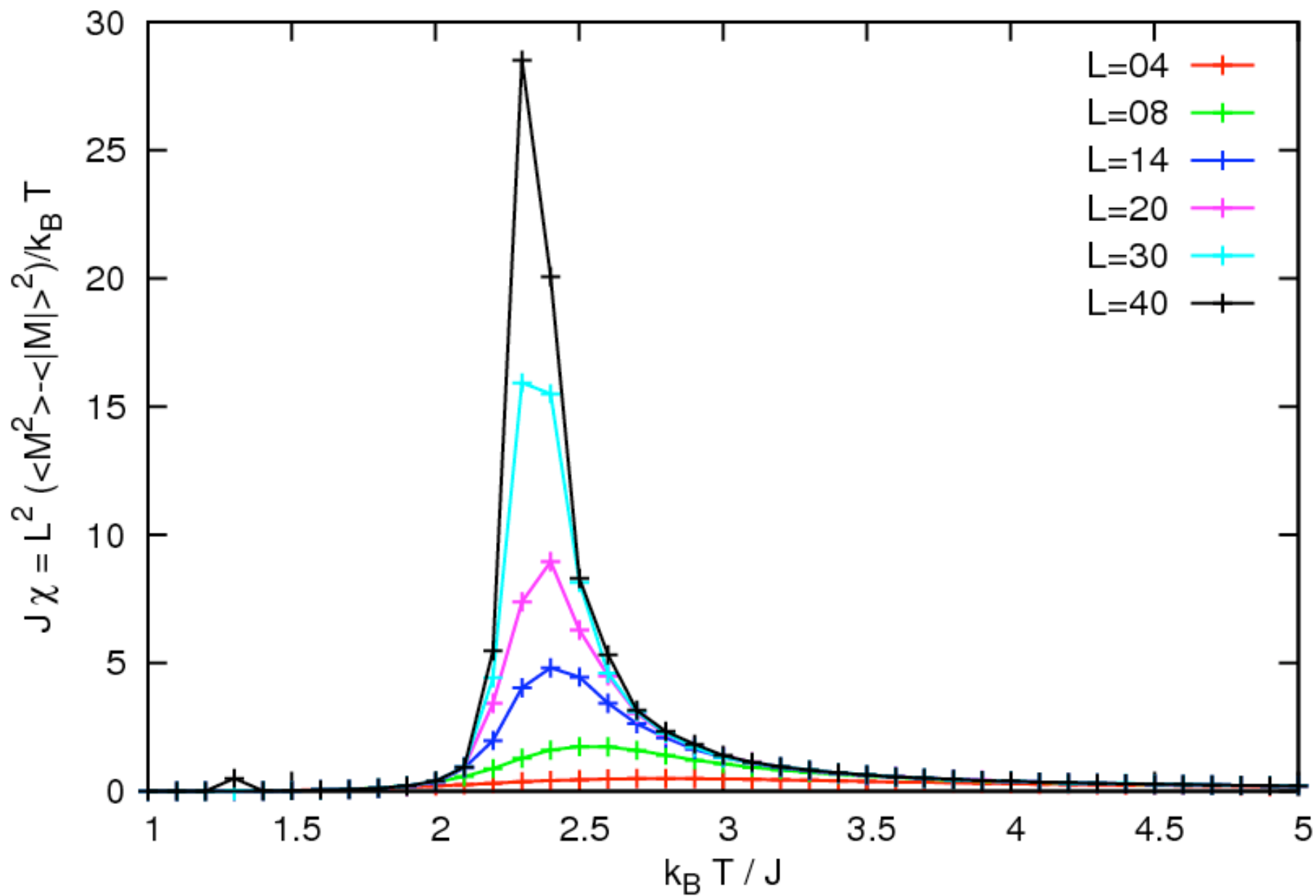
Magnetization (10^5 sweeps)



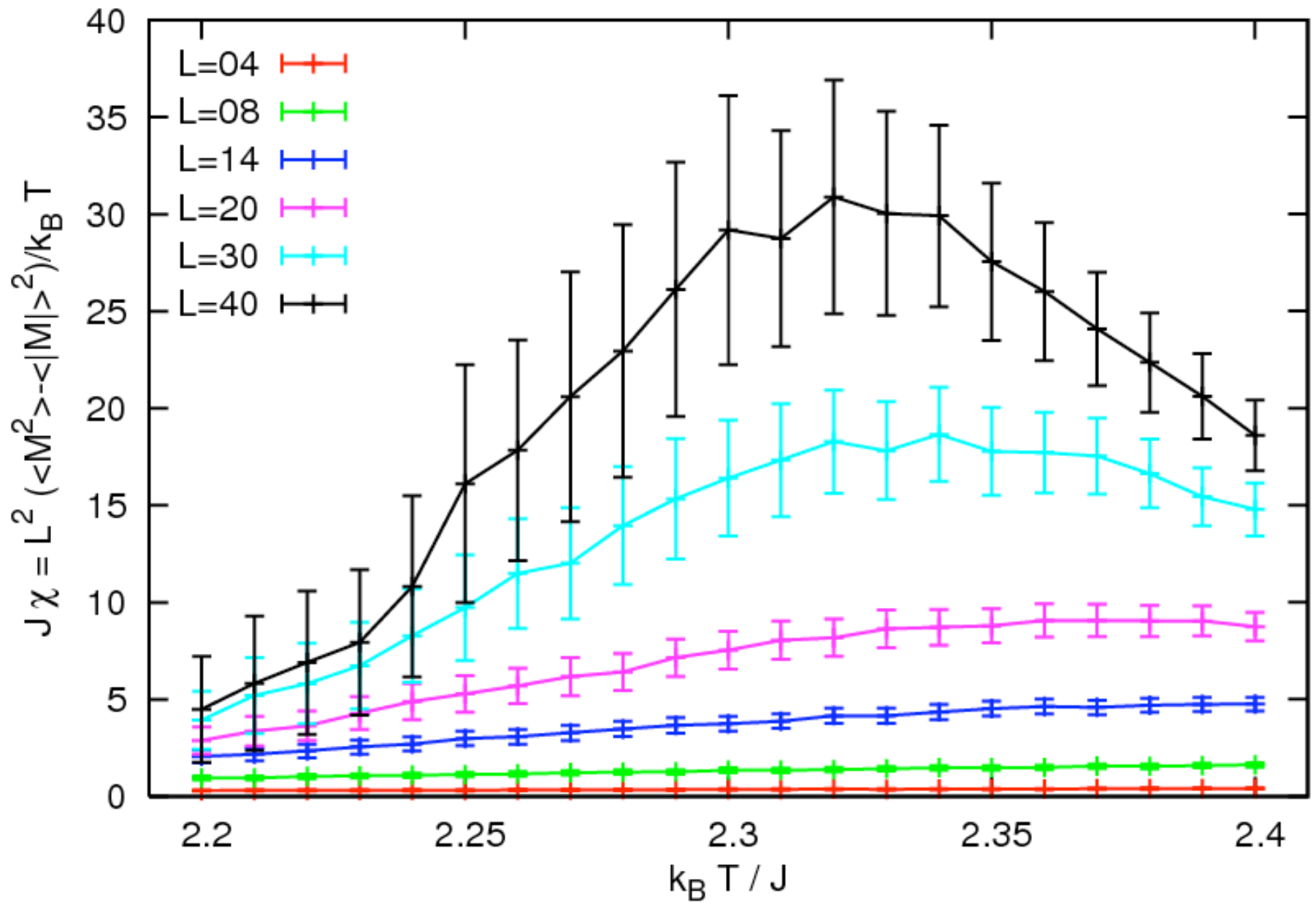
Energy (10^5 sweeps)



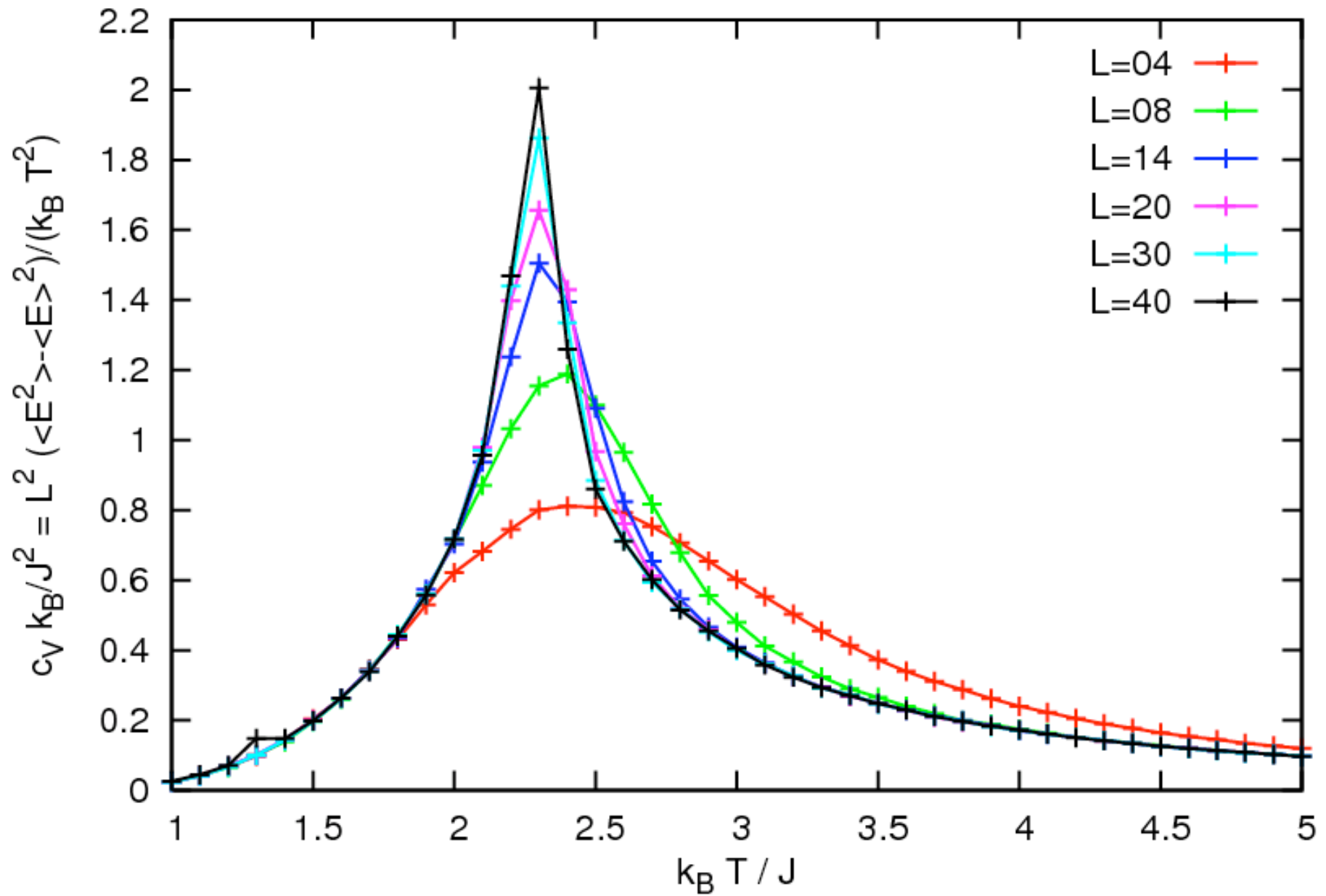
Magnetic susceptibility (10^5 sweeps)



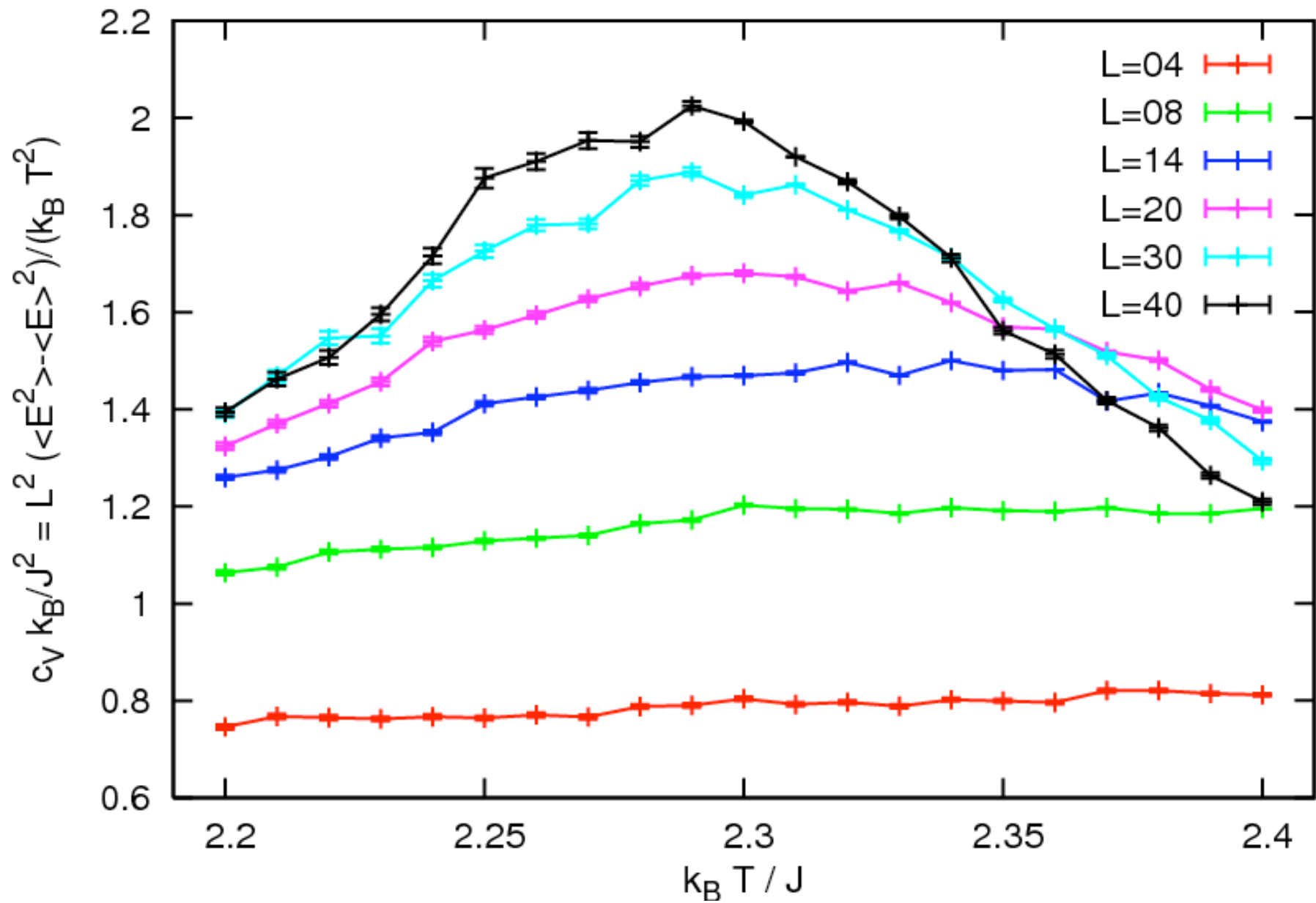
Magnetic susceptibility near T_c (10^6 sweeps)



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 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

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

and

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

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 :

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

Universality and critical exponents

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

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

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

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:

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 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 α , ν , β , 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 χ with respect to the critical temperature corresponding to the thermodynamic limit is described by: $T_c(L) - T_c(\infty) \propto L^{-\lambda}$

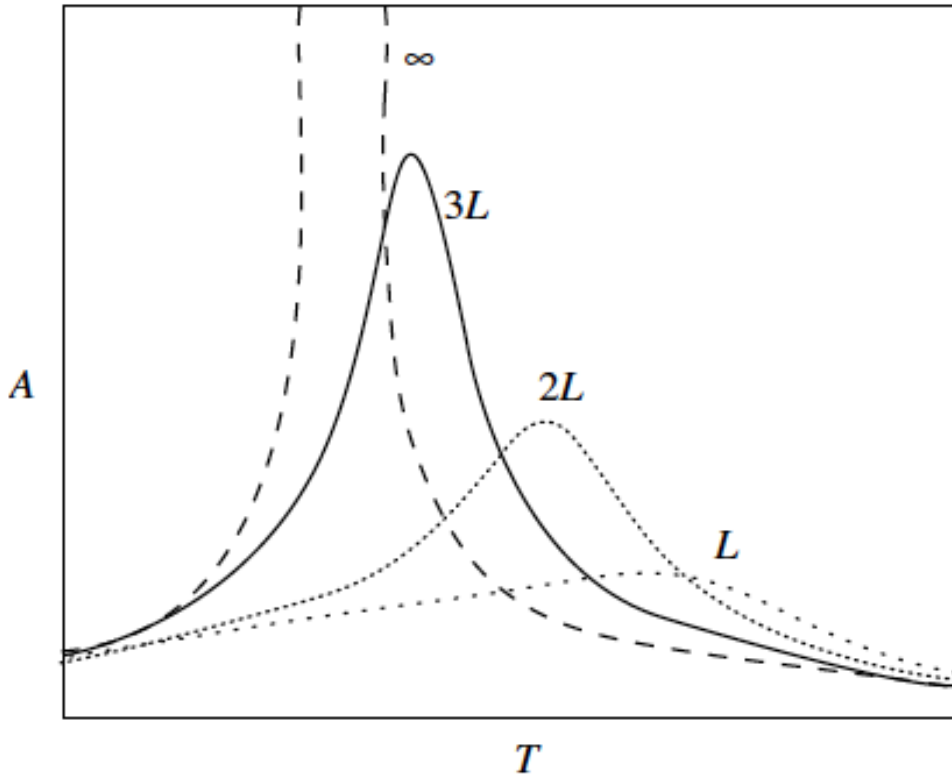


FIG. 1. Typical behaviour of a physical quantity A vs temperature close to the critical point for various system sizes. Figure taken from Thijsen⁸.

[Thijsen, Computational Physics (Cambridge University Press)]

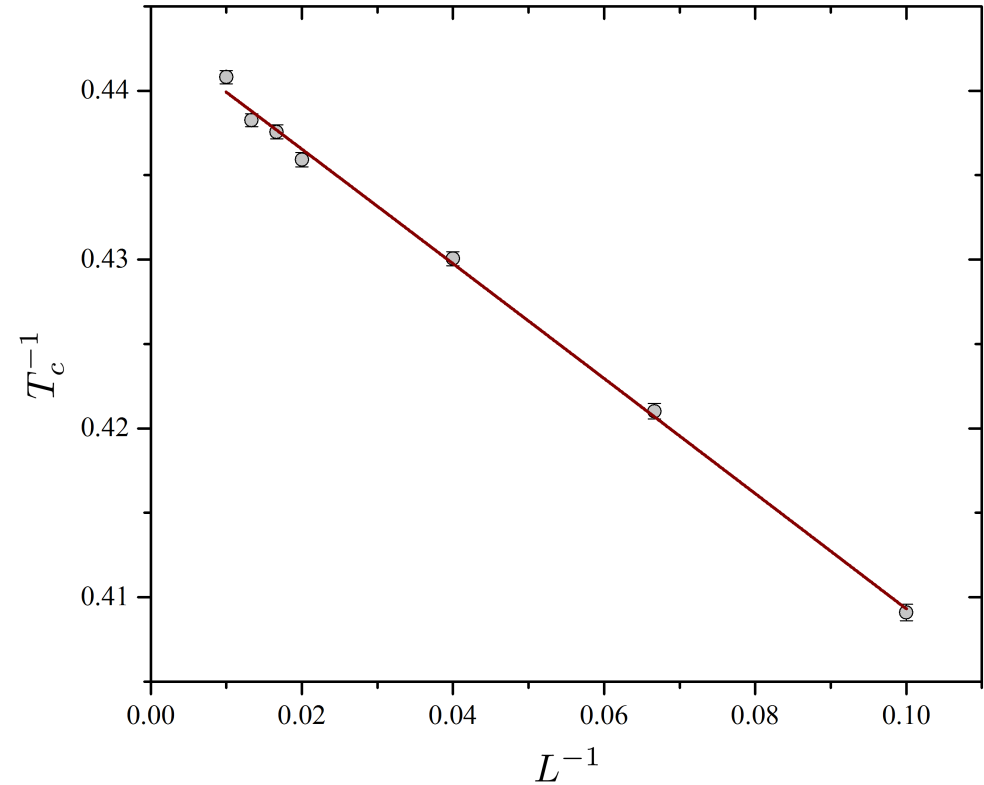


FIG. 9. (Color online) Inverse of the critical temperature T_c^{-1} vs inverse of lattice size L^{-1} for the 2D Ising model. The curve was fitted with a power law $T_c^{-1} = T_c^{-1} - bL^{-1/\nu}$, and the critical exponent ν was determined.

- 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 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 $L \rightarrow \infty$. 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 ν is defined in (17.25). The finite size of the lattice is important when the correlation length

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

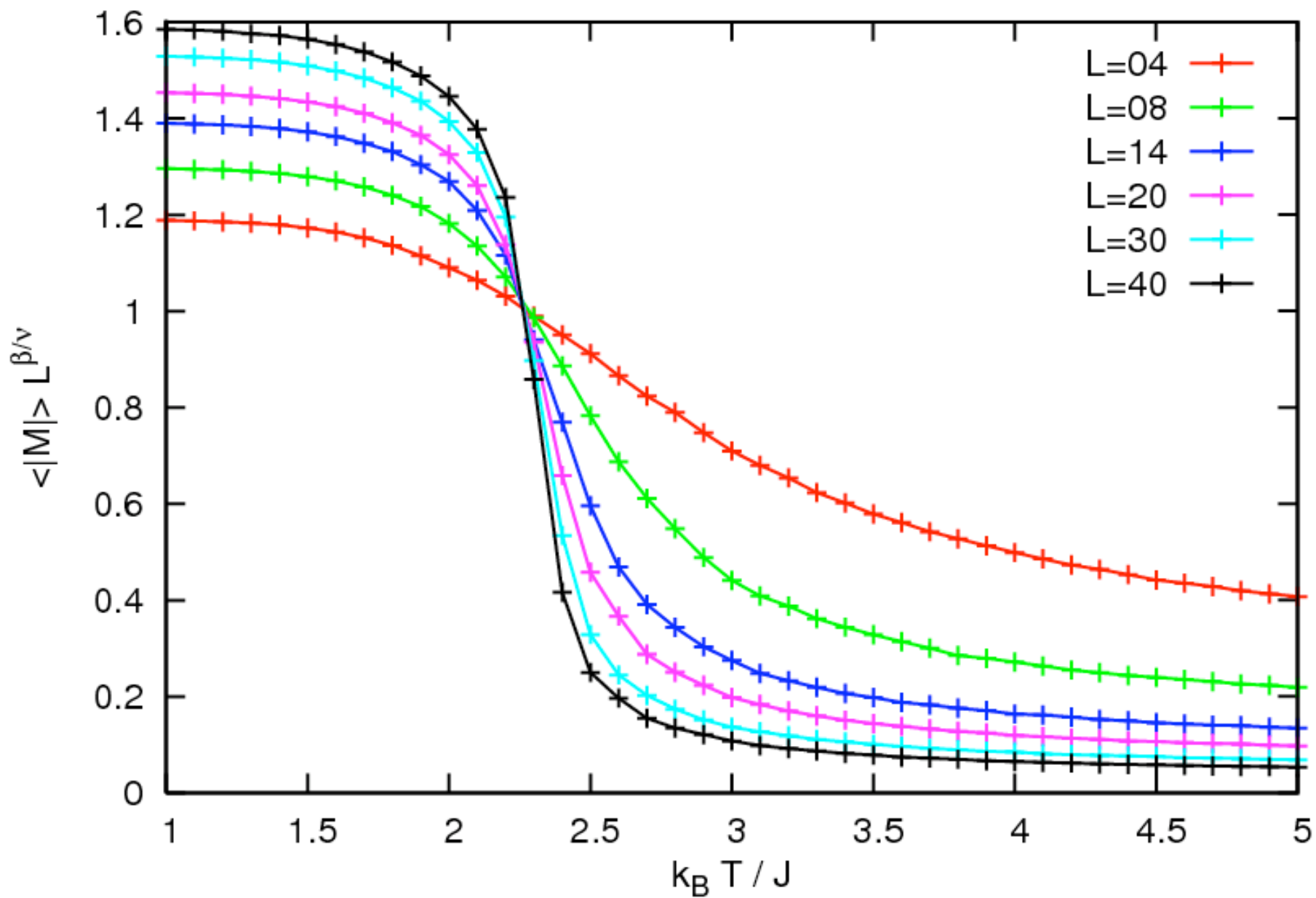
As in Section 13.4, we can set $T = T_c$ and consider the L -dependence of M , C , and χ :

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

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

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

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)

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:

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

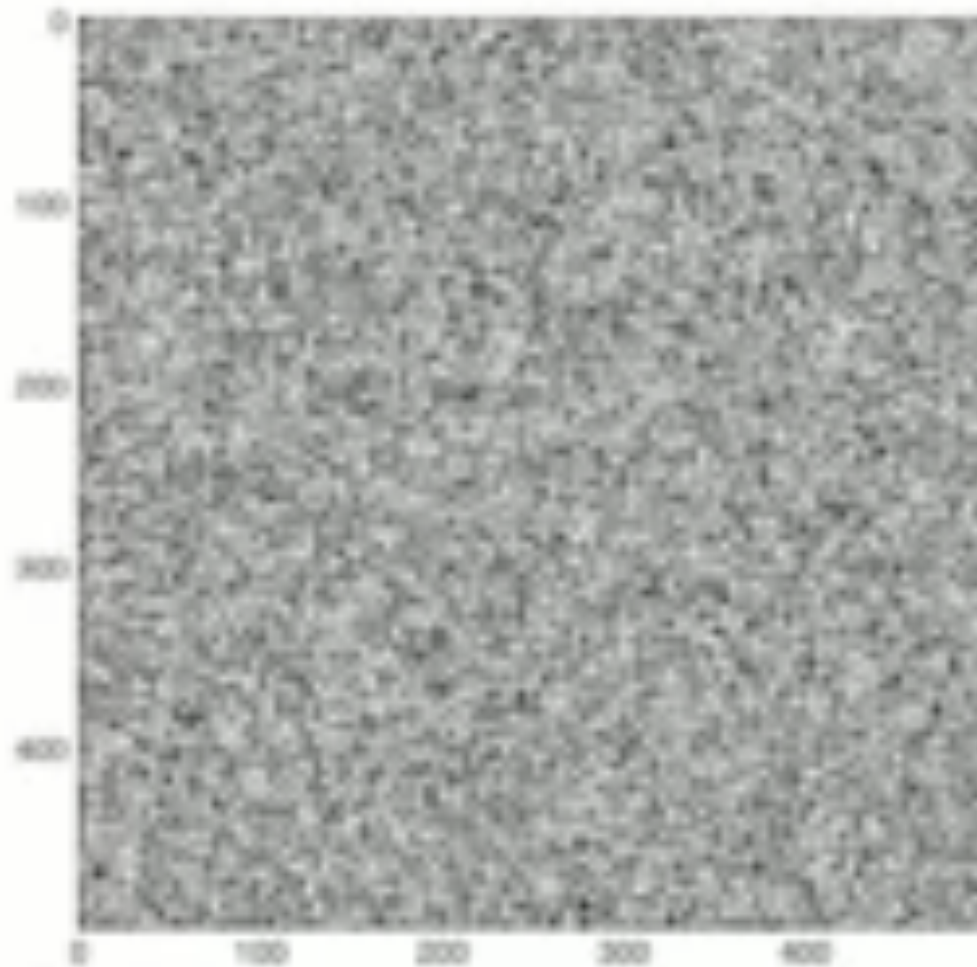
=> Trend to aggregation (diffusive behavior is limited to a transient)

- 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

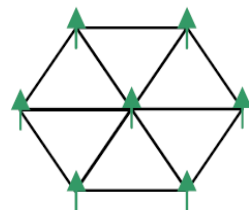


T=10, starting from random configuration

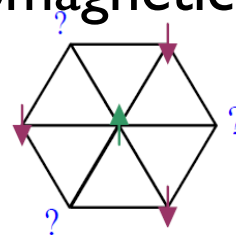
Ising model: other generalizations

- 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:



FM



AFM

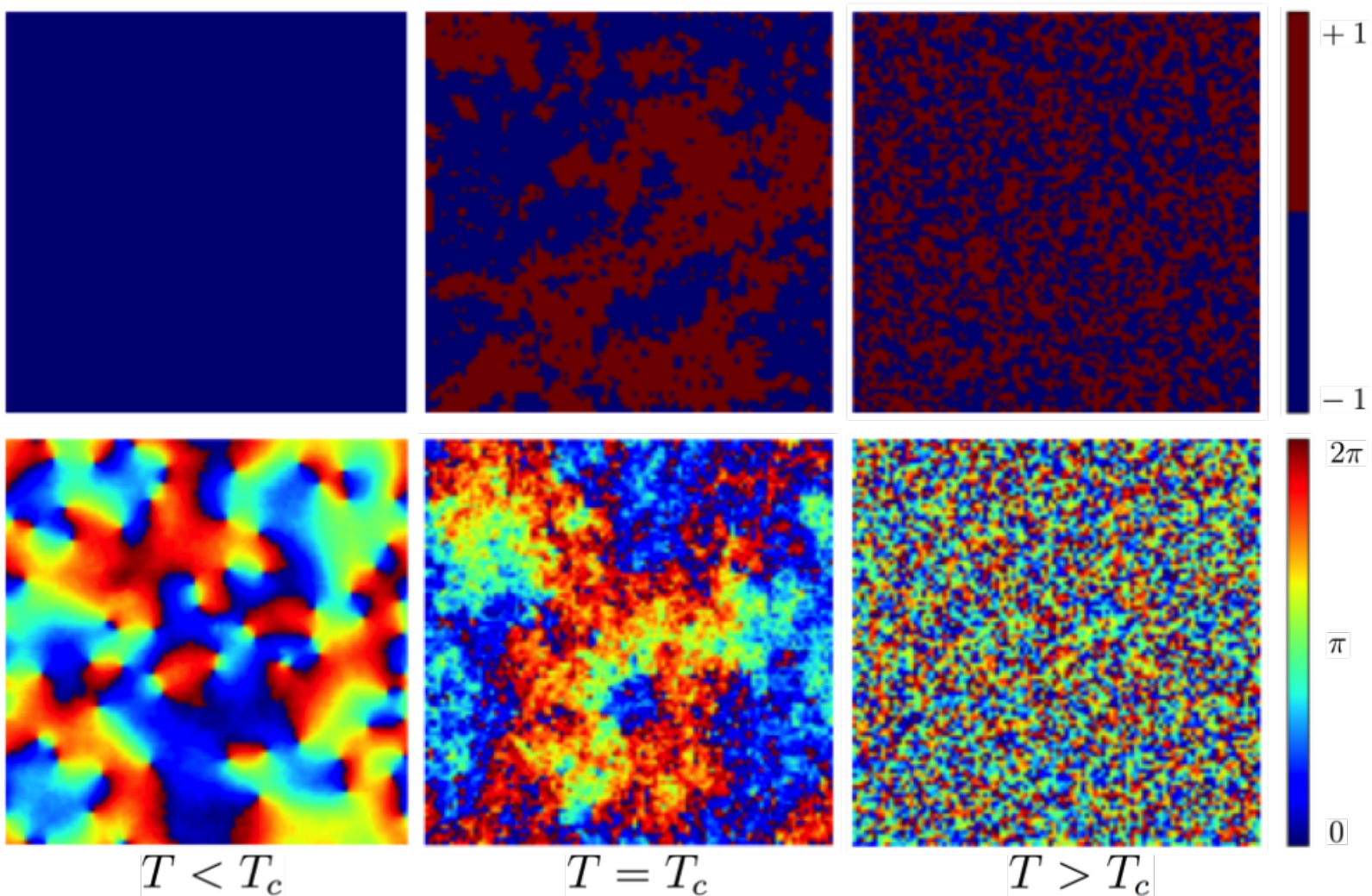


FIG. 15. (Color online) Behavior of the two dimensional Ising model (top) and XY model (bottom) at $T < T_c$, $T = T_c$ and $T > T_c$. For the Ising model, an \uparrow spin ($s_i = 1$) is represented by red and a \downarrow spin ($s_i = -1$) is represented by blue. For the XY model, because every spin is determined by 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).