993SM - Laboratory of Computational Physics
Unit VII
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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

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 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 $\pi_s = \dfrac{e^{-\beta E_s}}{\sum_{s=1}^{m} e^{-\beta E_s}}$

(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:

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

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 Unit VI)

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

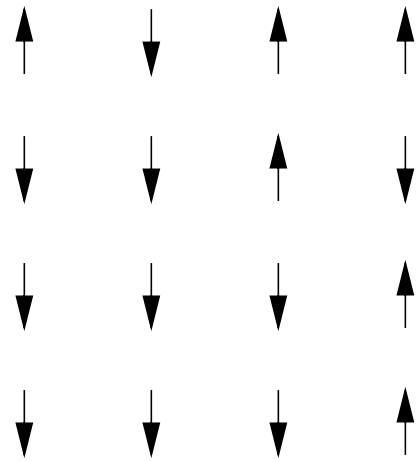
We need a model for:

- **energy**

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

stochastic simulations of an interacting spin ensemble

We need a model for:



- **energy** => Ising model

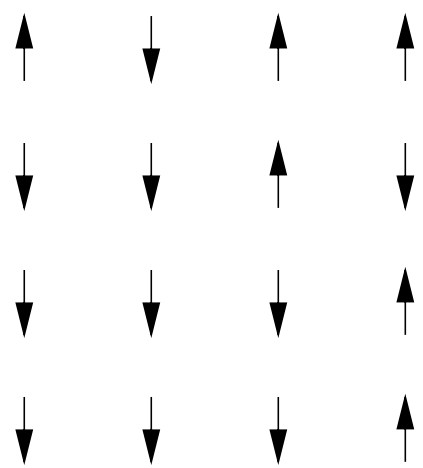
- **evolution**
  (to build the trajectory / the Markov chain)

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 10-16)

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:

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

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

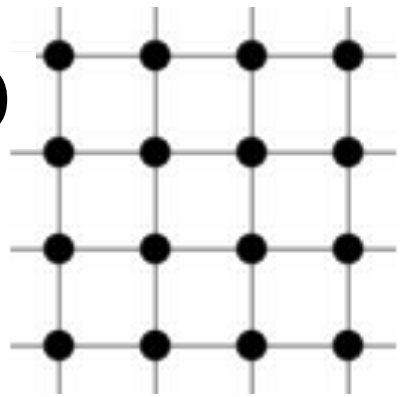
(choosing the kind of interaction, we specify the **energy model**)

Ising model on a lattice

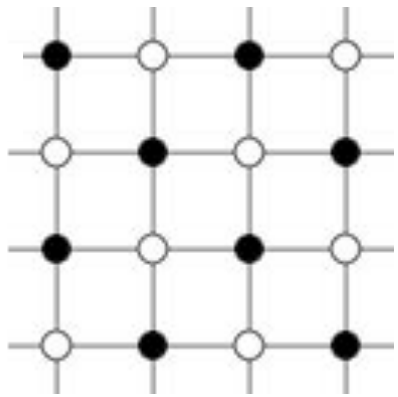
lattice containing N sites

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:

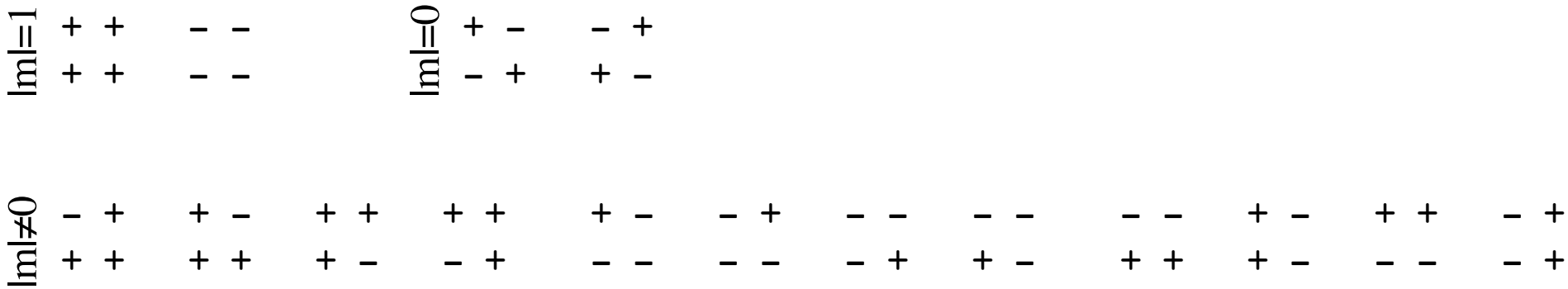
$$m = \frac{M}{N} = \frac{1}{N} \sum_{i=1}^{N} s_i$$

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

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)

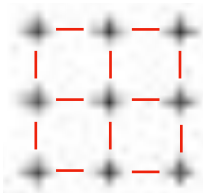
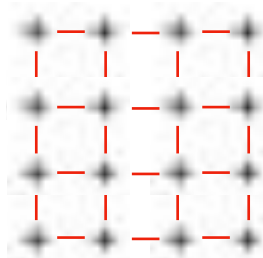
Ising model:
open boundary conditions

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:

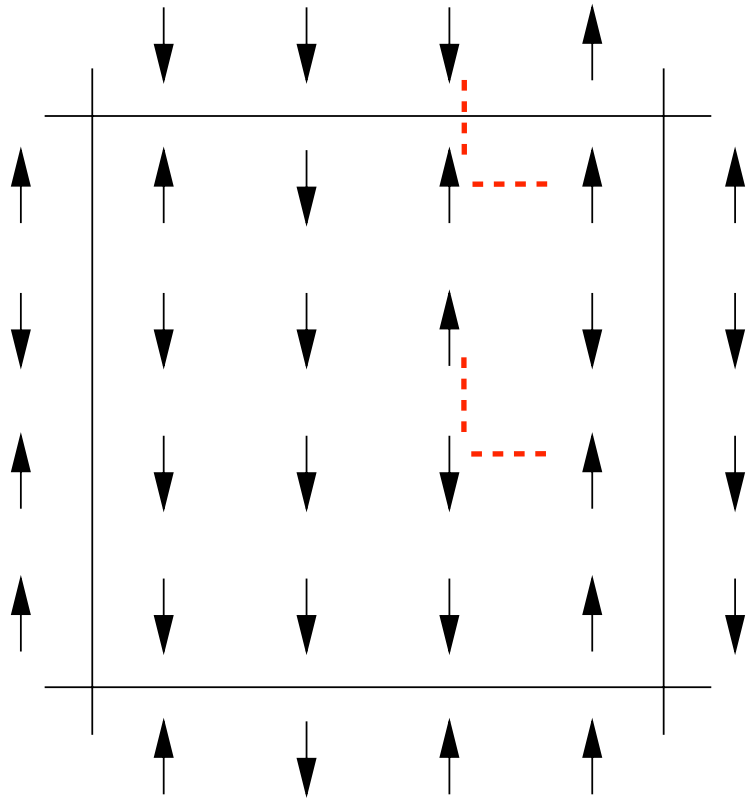
$E_0/N=-J$ $E_0/N=-(12/9)J$ $E_0/N=-(24/16)J$ ... $E_0/N = -J \times 2L(L-1)/L^2$

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

(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.

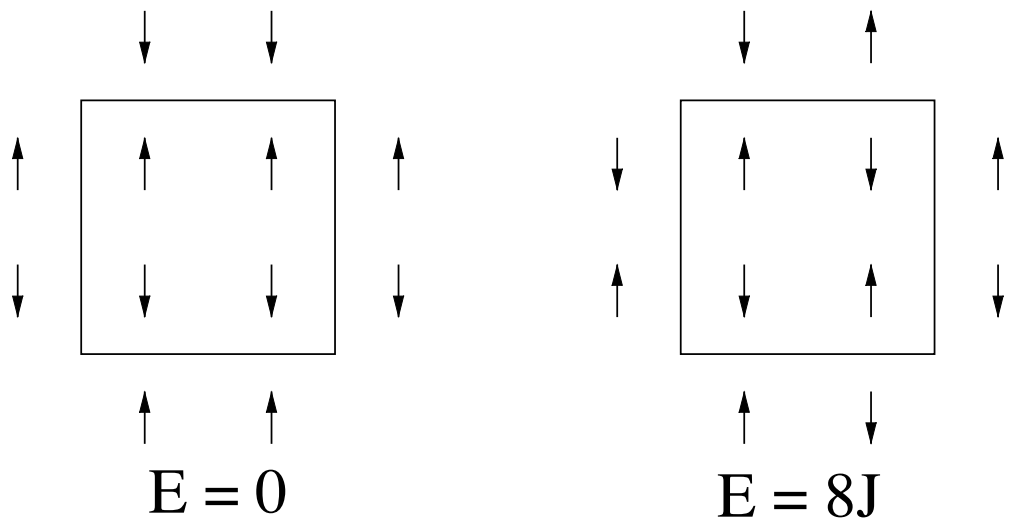
with periodic boundary conditions.

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

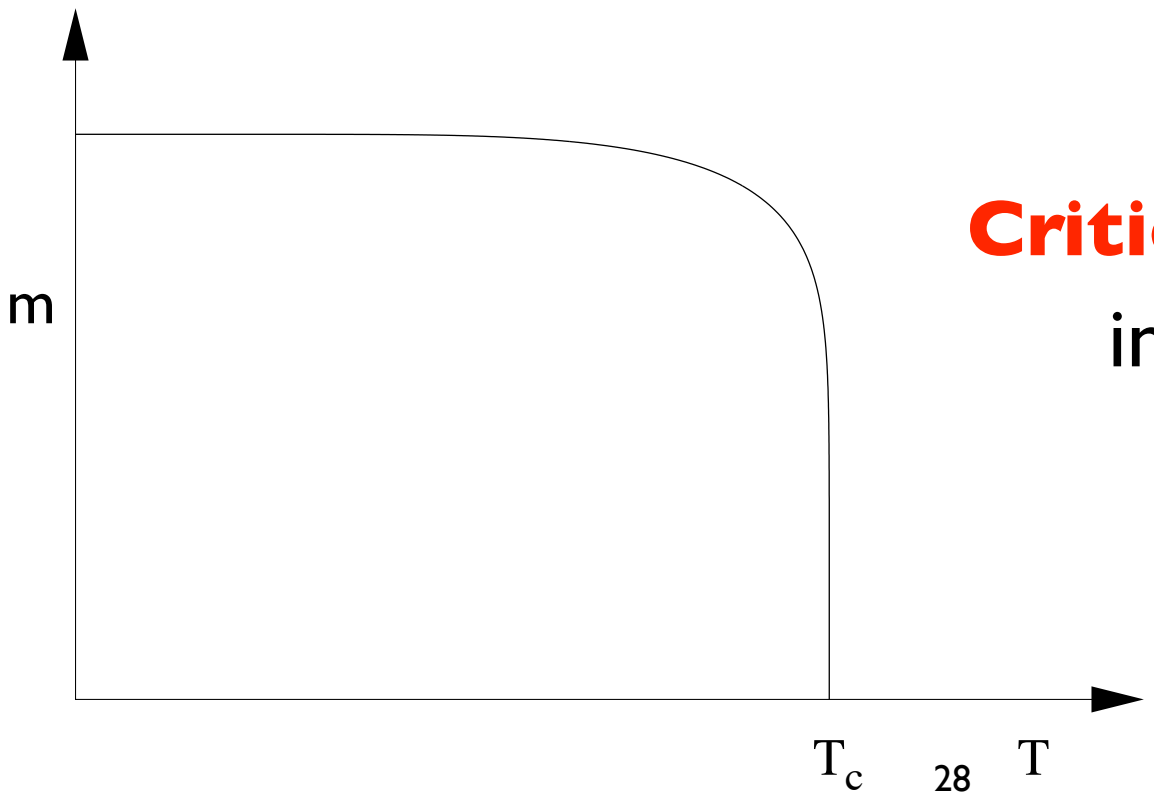
Energy and magnetization of 16 configurations of the 2×2 Ising model with PBC

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:

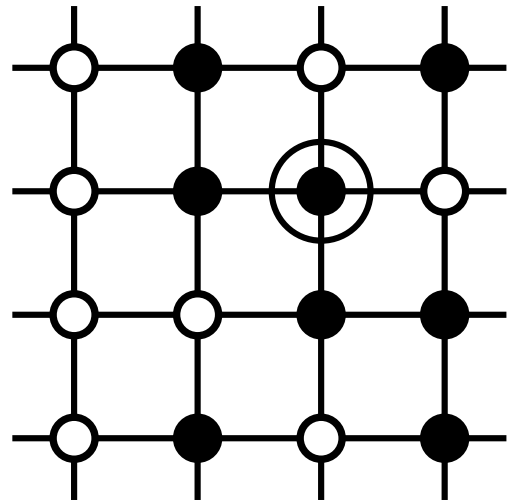
$T_c = 2.269\ J/k_B$

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)

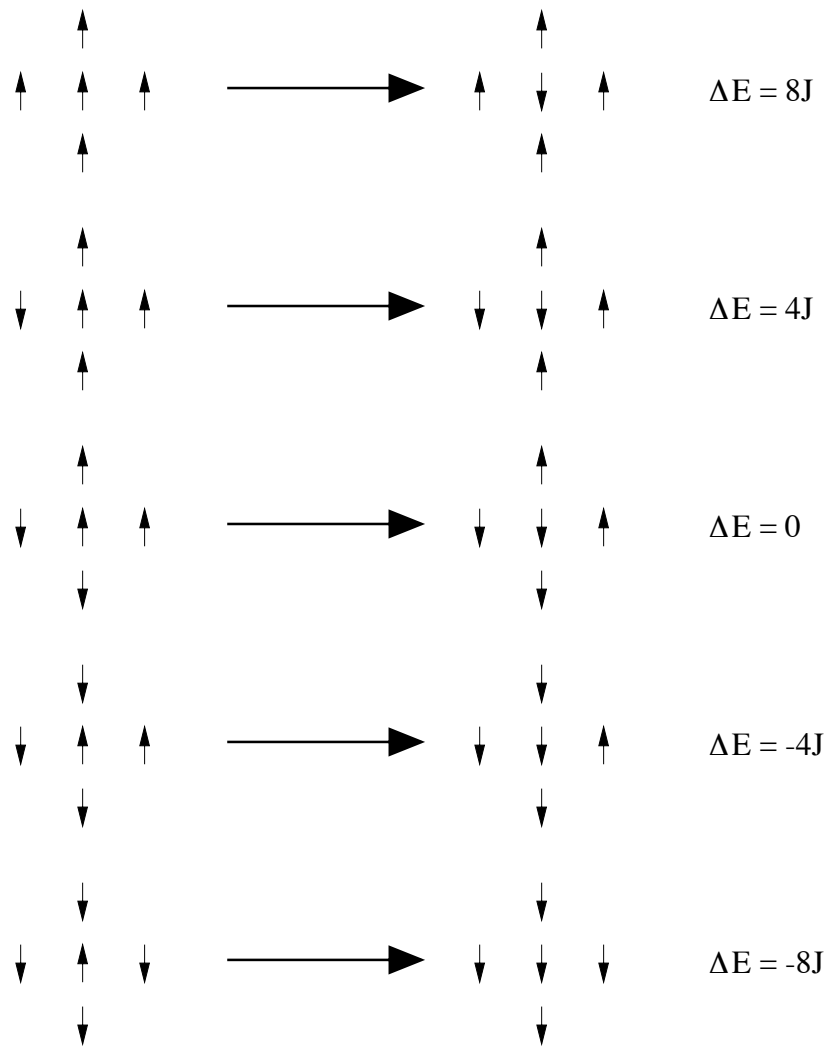


Apply **Metropolis Monte Carlo** method for evolution in the **canonical ensemble** (fix T).

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!

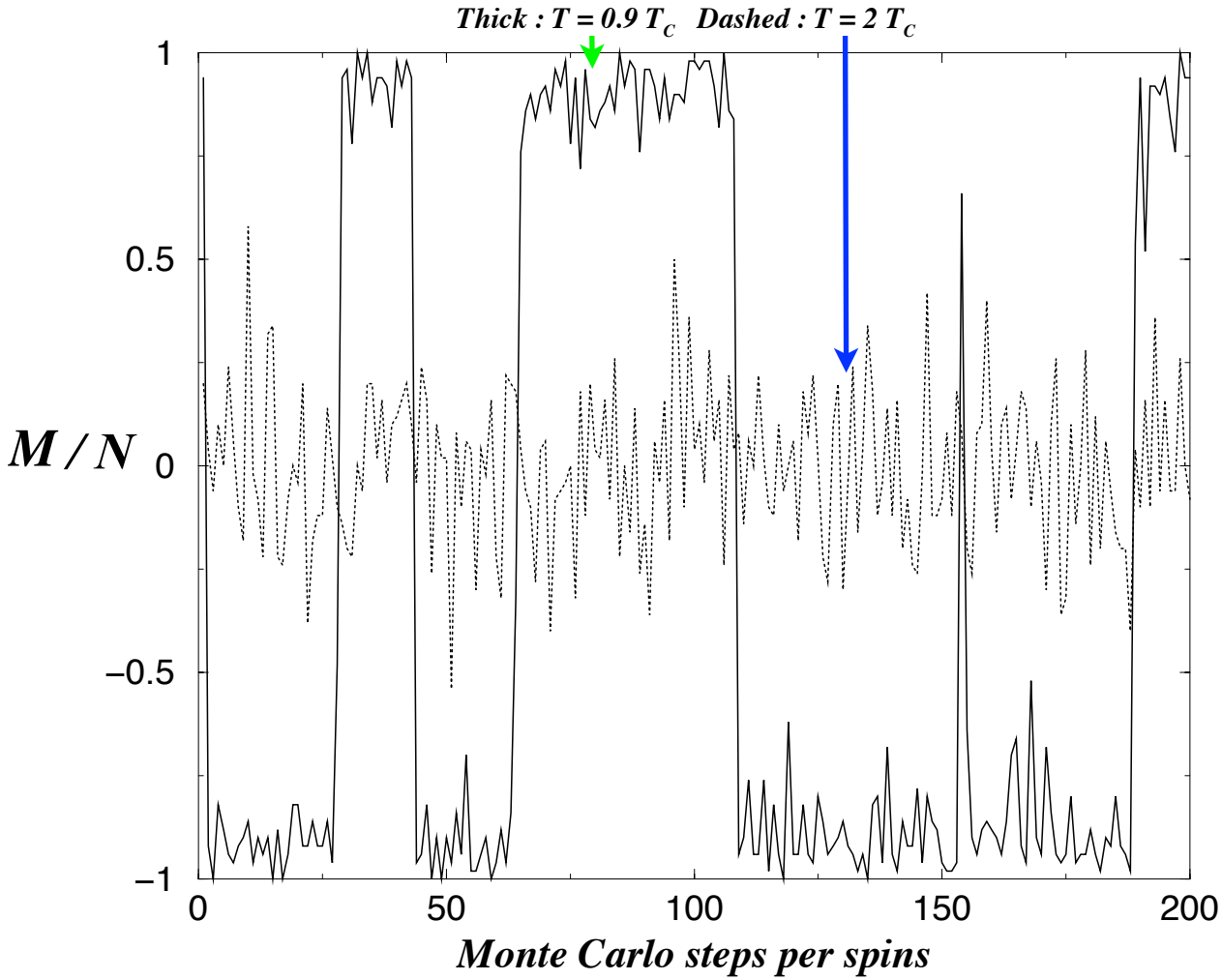
Ising model: spin flip dynamics



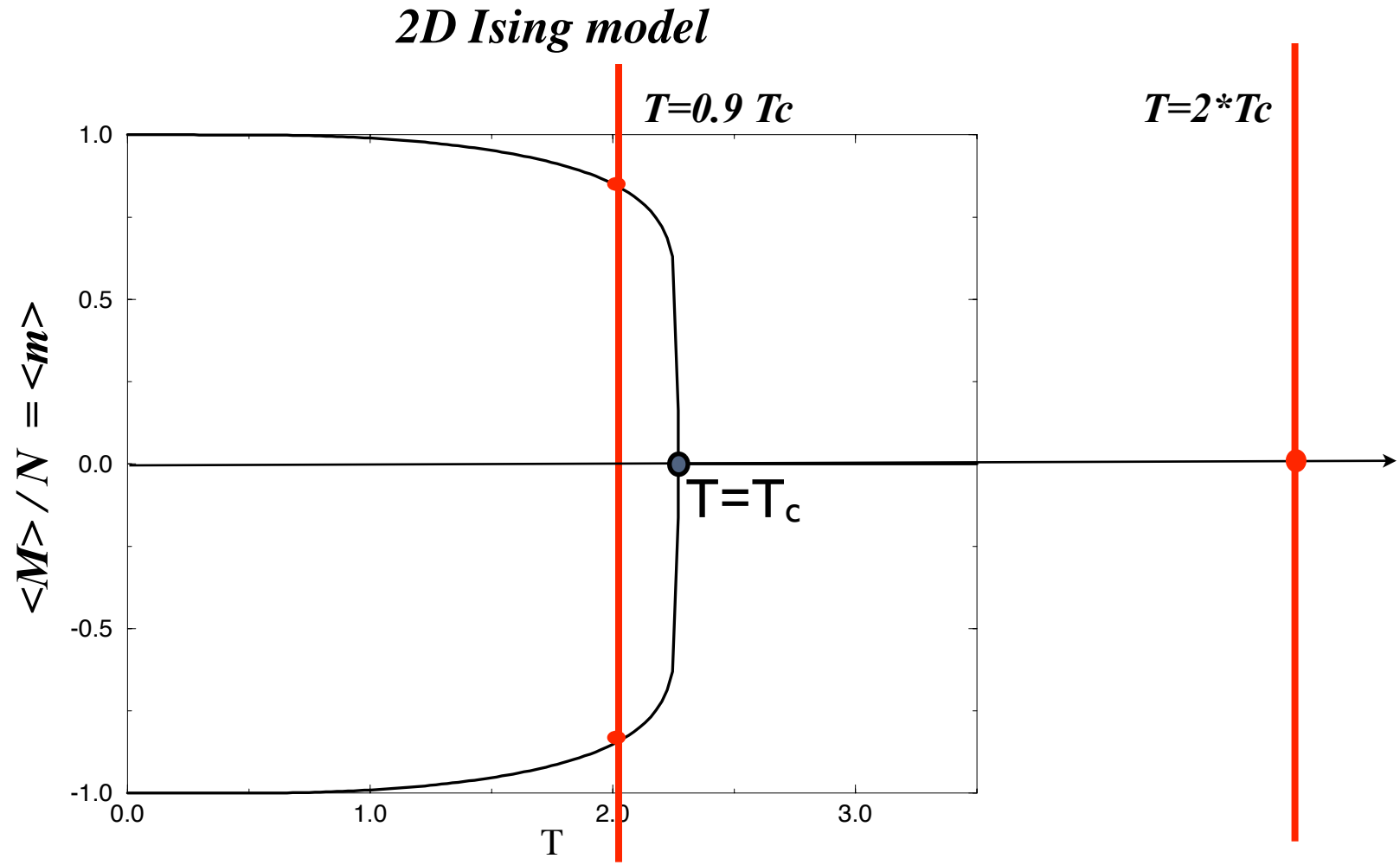
The five possible transitions of the Ising model on the square lattice with spin flip

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



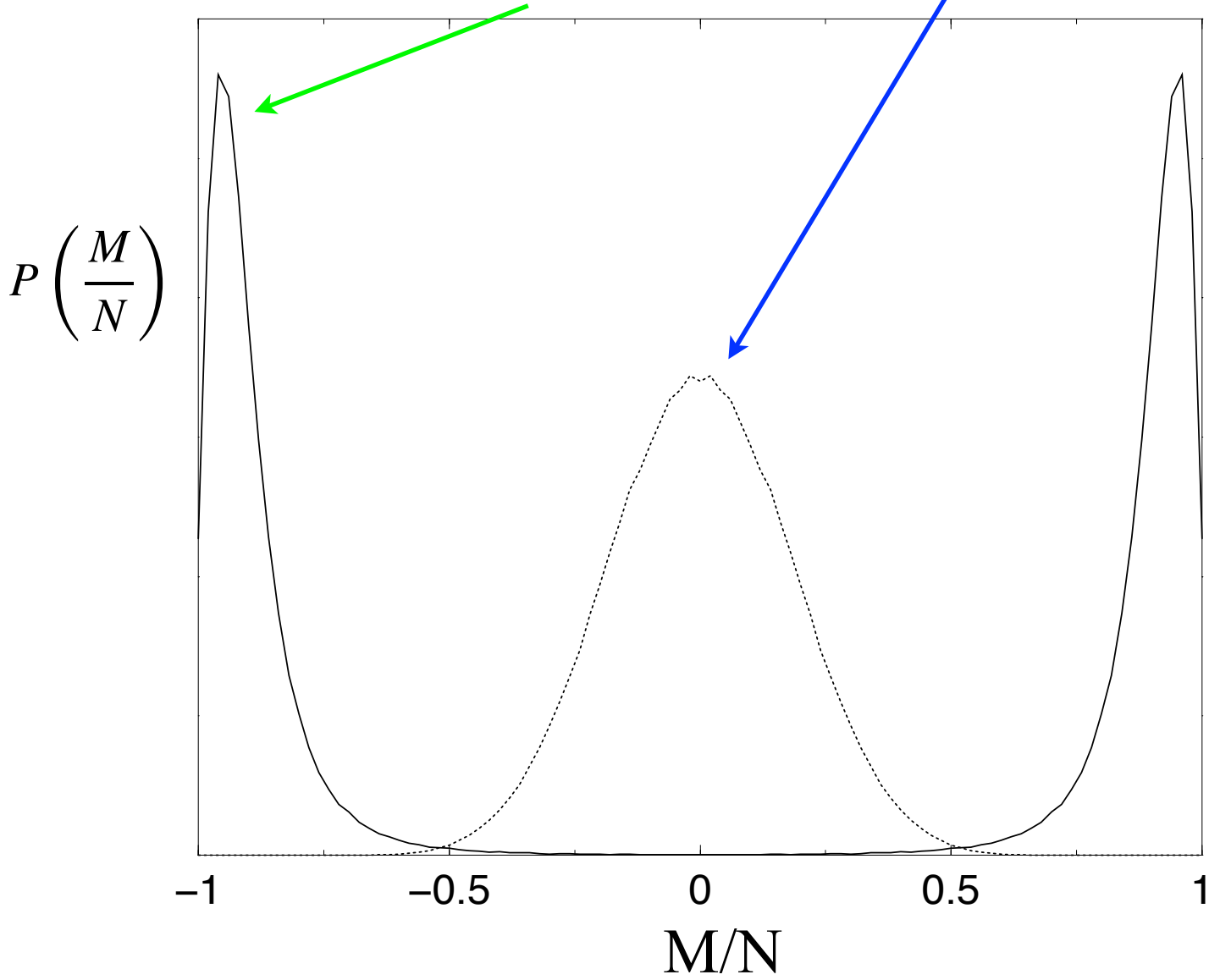
Fluctuations! do, as usual, temporal averages: $\langle M \rangle / N$, $\langle E \rangle / N$



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)

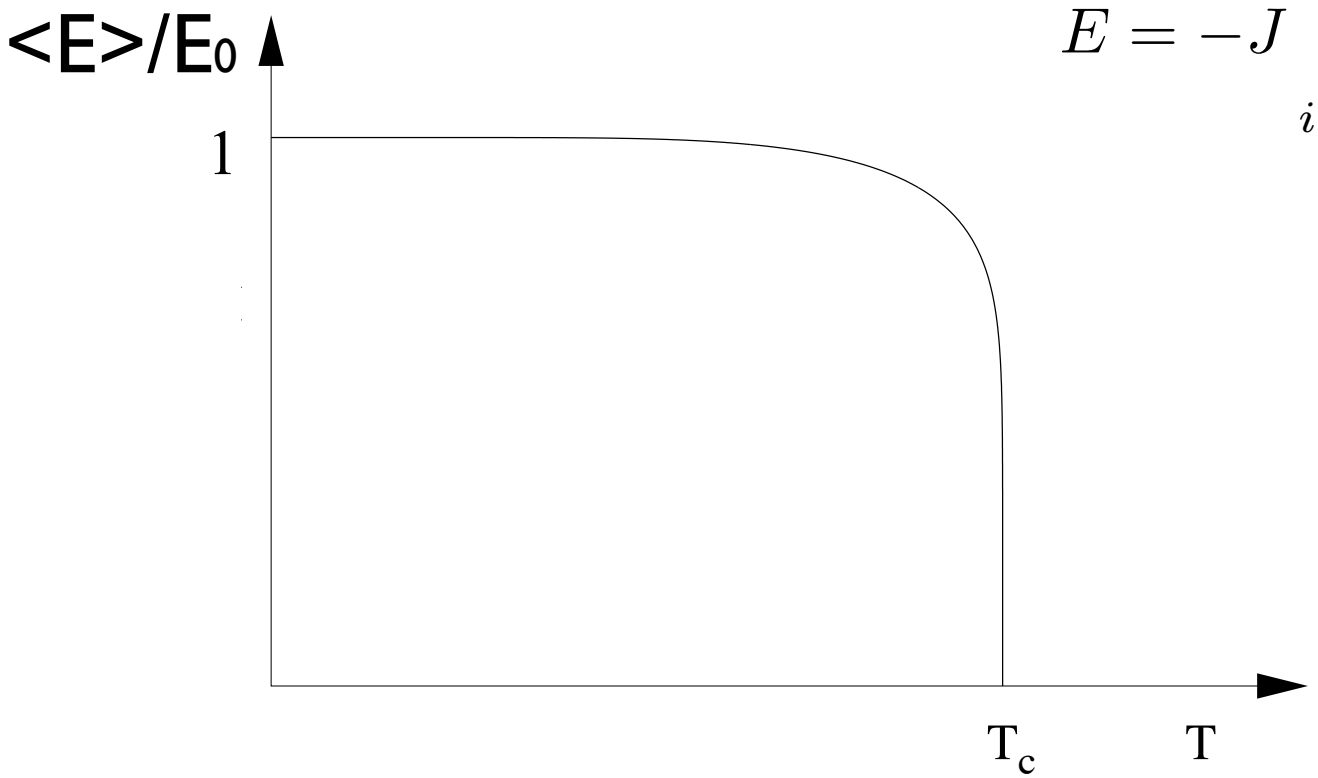


(data collected during time evolution, at equilibrium)

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

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

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

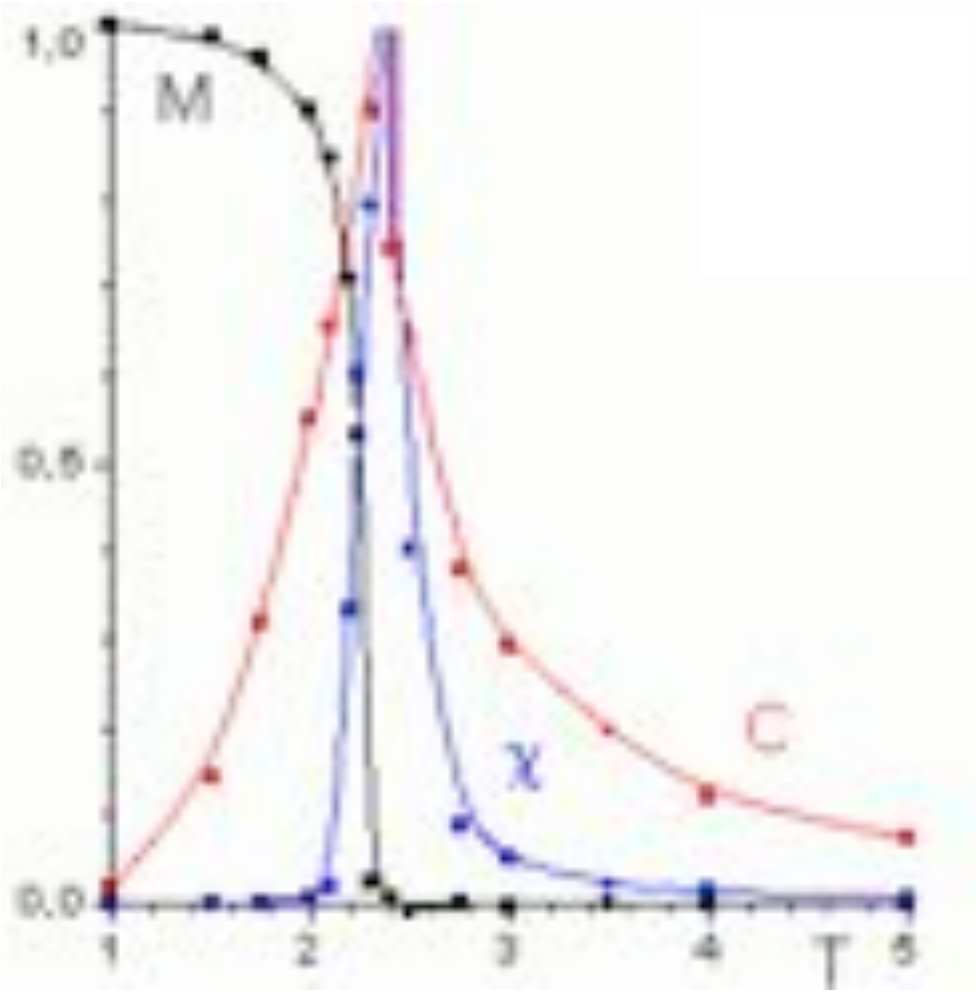
$$\chi = \lim_{H \to 0} \frac{\partial \langle M \rangle}{\partial H}\ , \quad \chi = \frac{1}{kT}\left(\langle M^2 \rangle - \langle M \rangle^2\right)$$

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
```

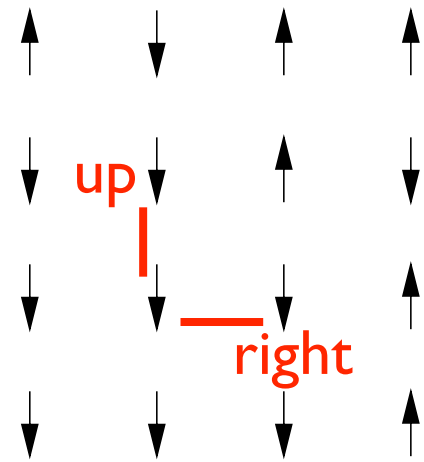
$$m = \frac{M}{N} = \frac{1}{N} \sum_{i=1}^{N} s_i$$

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

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

Ising model: energy

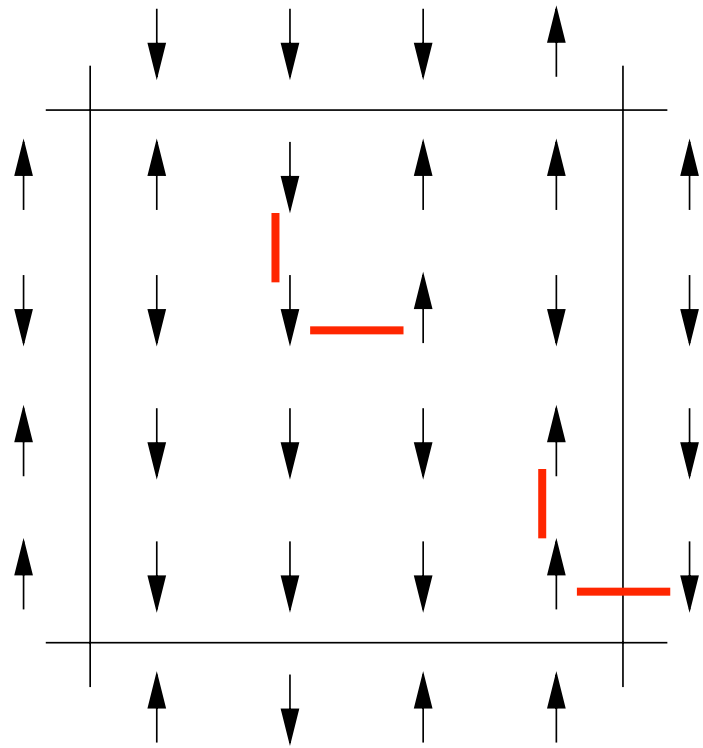
$$E = -J \sum_{i,j=\mathrm{nn}(i)}^{N} s_i s_j$$




```
!  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
   .....
   .....
```

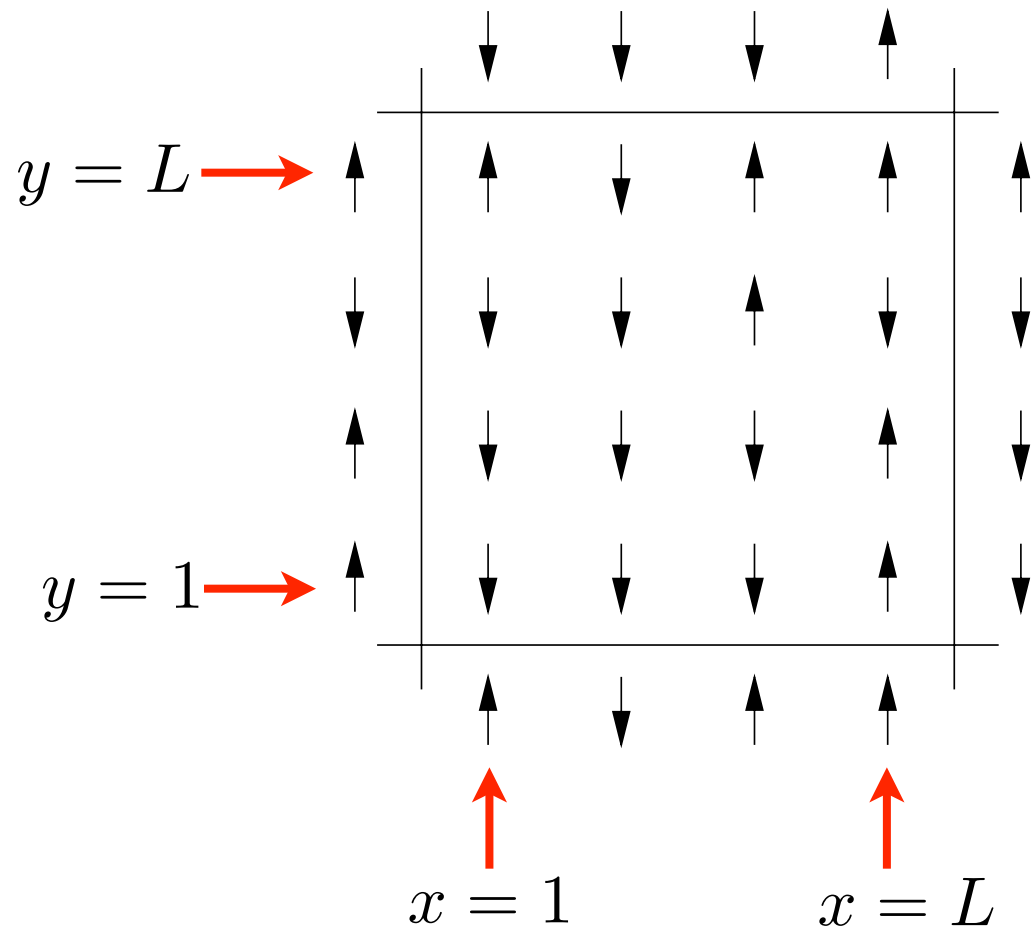
energy variation for `spin(x,y)` flip

`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

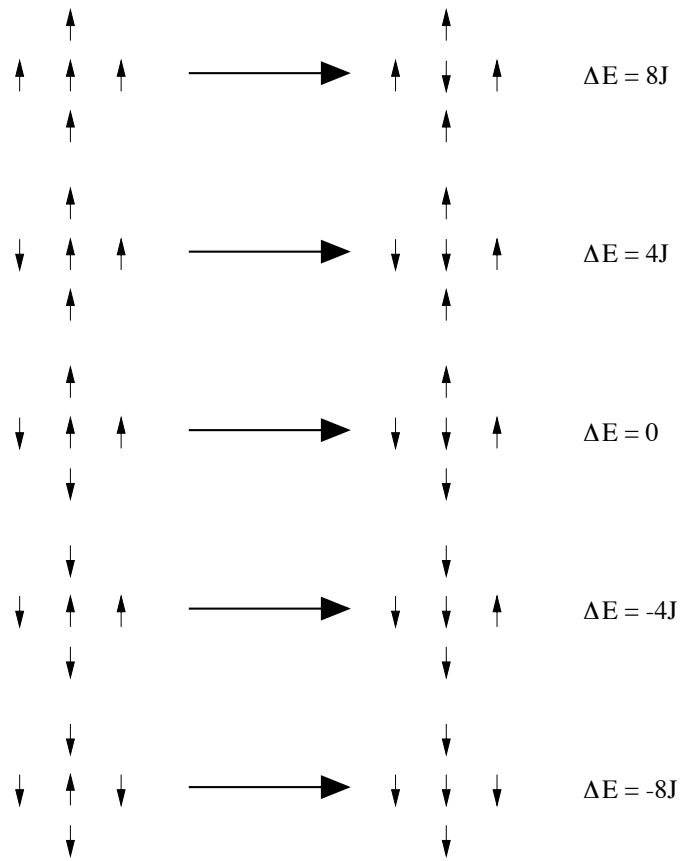
```
function DeltaE(x,y) result (DeltaE_result)
  !  periodic boundary conditions
.....
 if (x == 1) then
    left = spin(L,y)
    right = spin(2,y)
 else if (x == L) then
    left = spin(L-1,y)
    right = spin(1,y)
 else
    left = spin(x-1,y)
    right = spin(x+1,y)
 end if
 if (y == 1) then
    up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

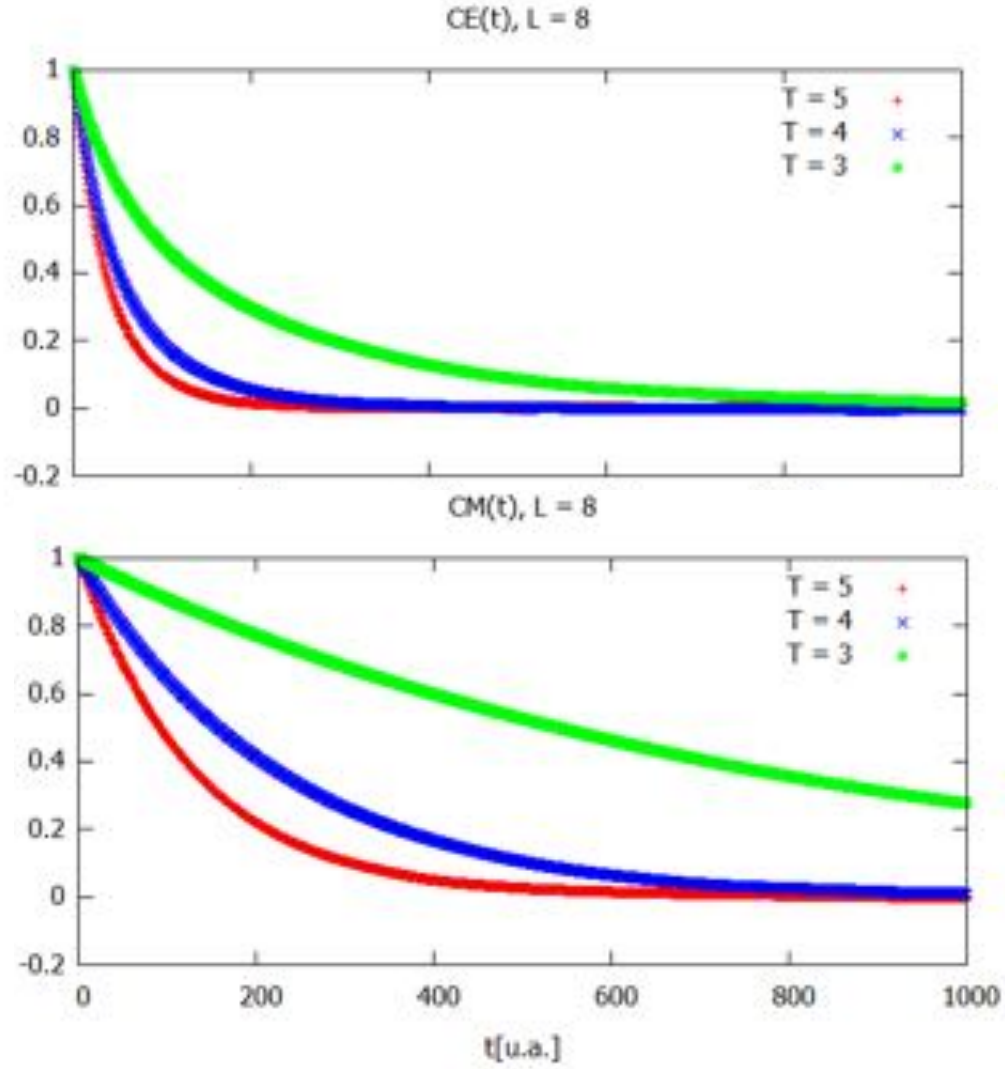
$$C_M(t) =< M(t)M(0) > - < M >^2, \quad C_E(t) =< E(t)E(0) > - < E >^2$$

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

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

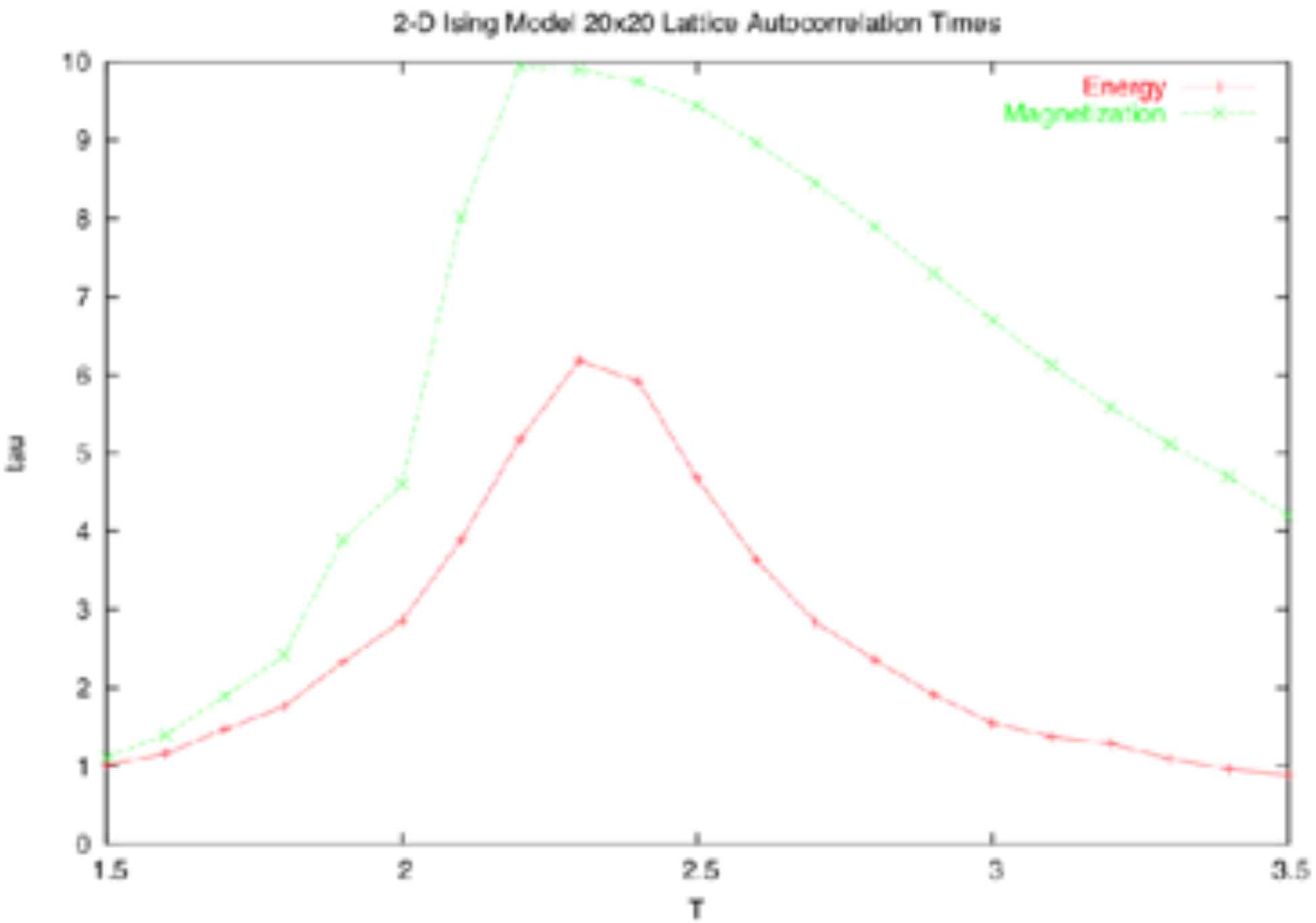
with a certain decay time τ: consider intervals longer than τ for statistical averages

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

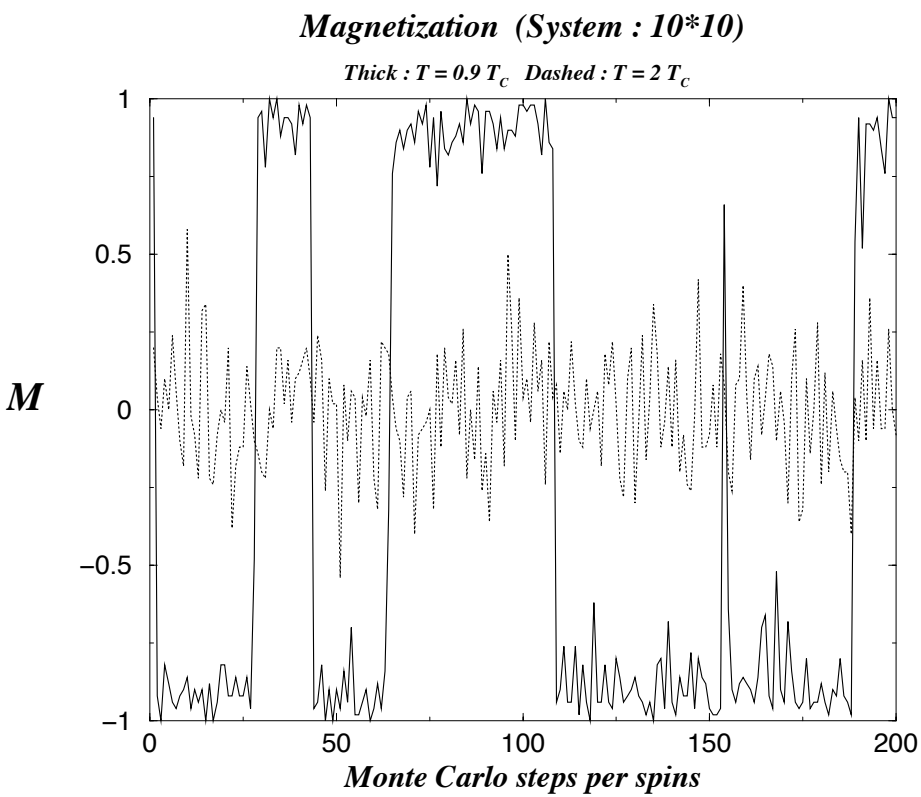
Measuring physical quantities: which errors?

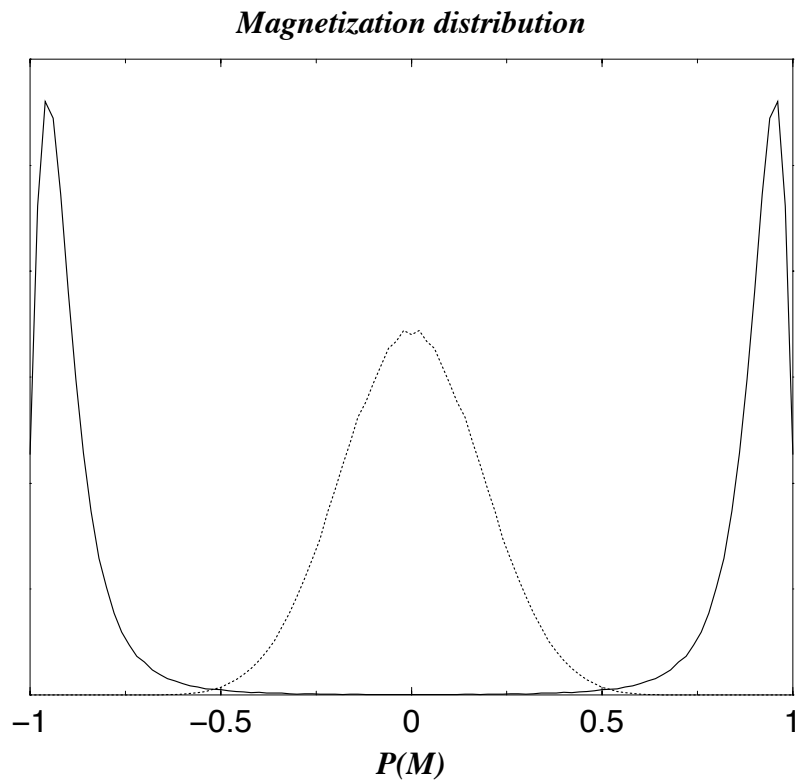
- necessary to give the ERROR ESTIMATE corresponding to the measured physical quantity !!!
- (see Tab. I of D.P. Landau, PRB 13, 2997 (1976), "Finite size behavior of the Ising square lattice")
- do also BLOCKING (called "coarse grained technique" in that paper)

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

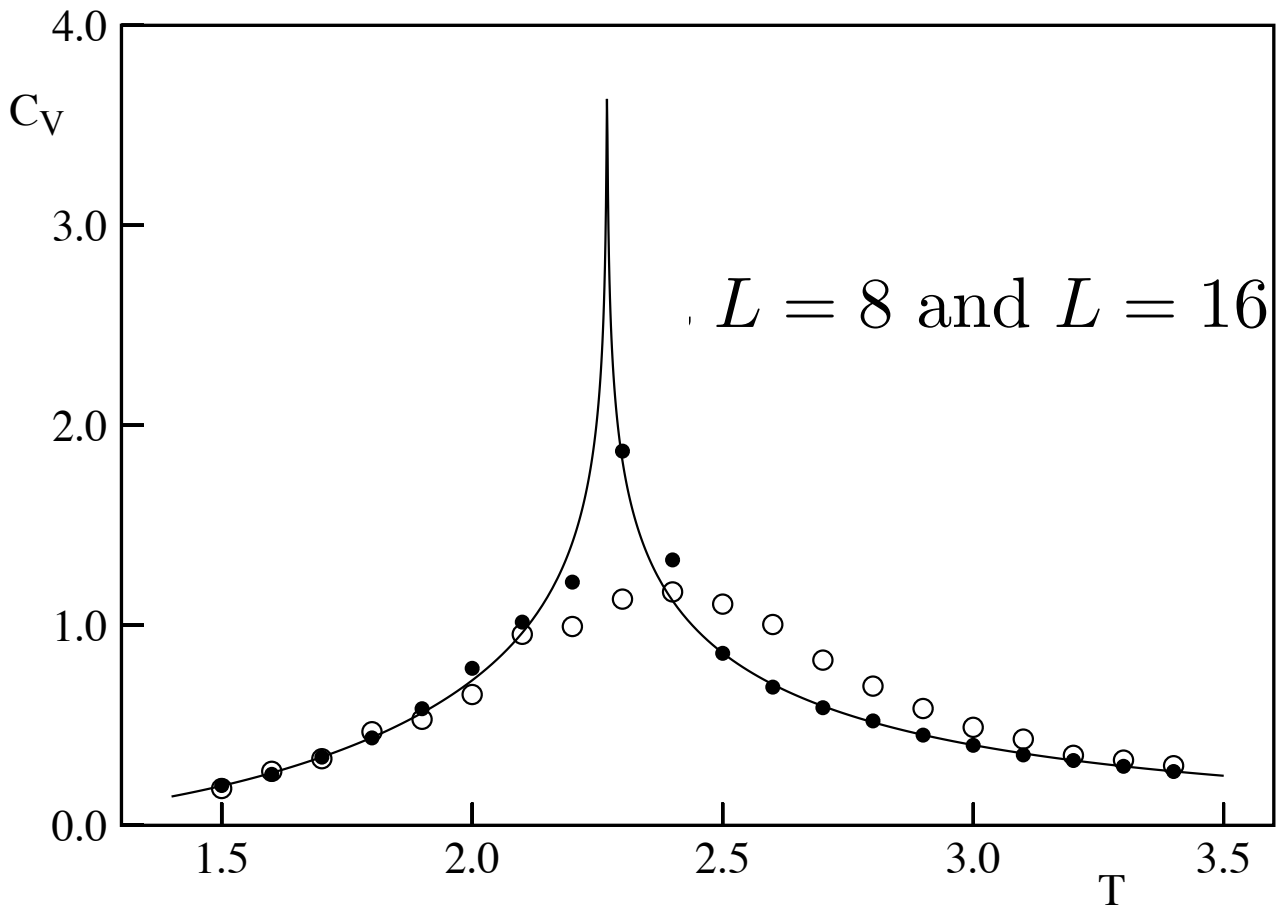
How to do efficiently simulations as a function of T?





Ising model: size problems

We cannot simulate an INFINITE system!

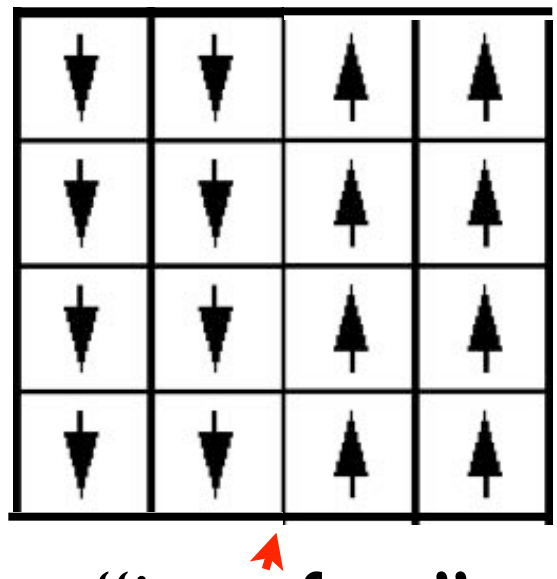


The temperature dependence of the specific heat C (per spin) of the Ising model

Ising model: size problems

INTERFACE EFFECTS:
example of energy for HALF UP/HALF DOWN configurations:

L=2	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



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

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

Program:

On moodle2:

ising.f90

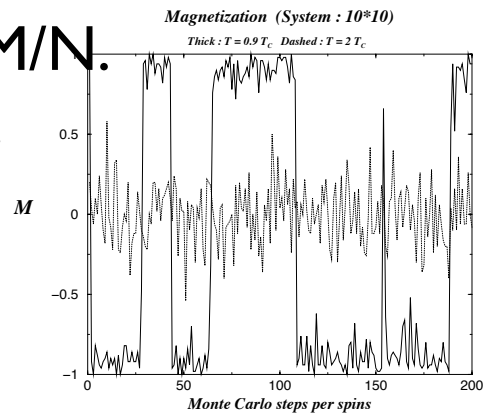
Exercise

(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

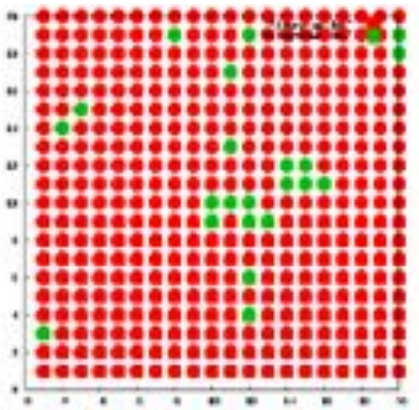
(a) Choose L=30, T=2, and initially spin=±1 randomly. ...

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:



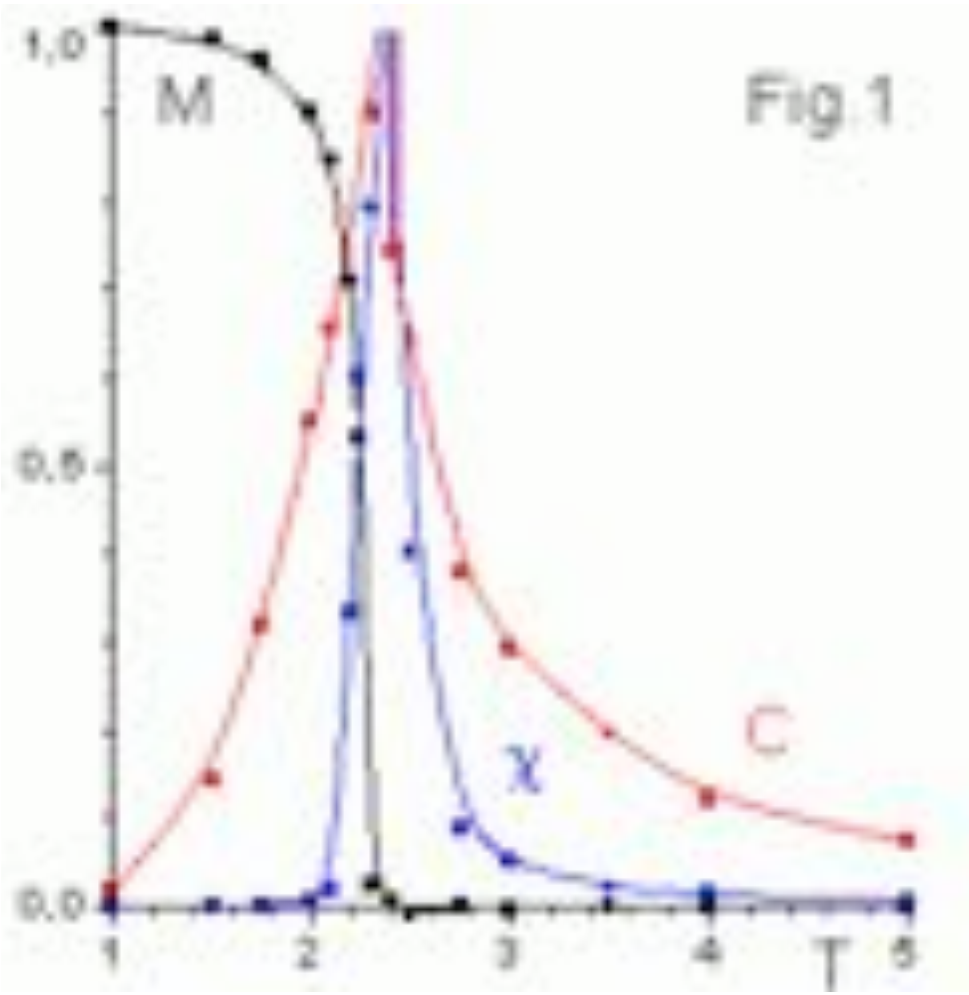
Calculate also c and χ.

Exercise

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

Calculate also c and χ.

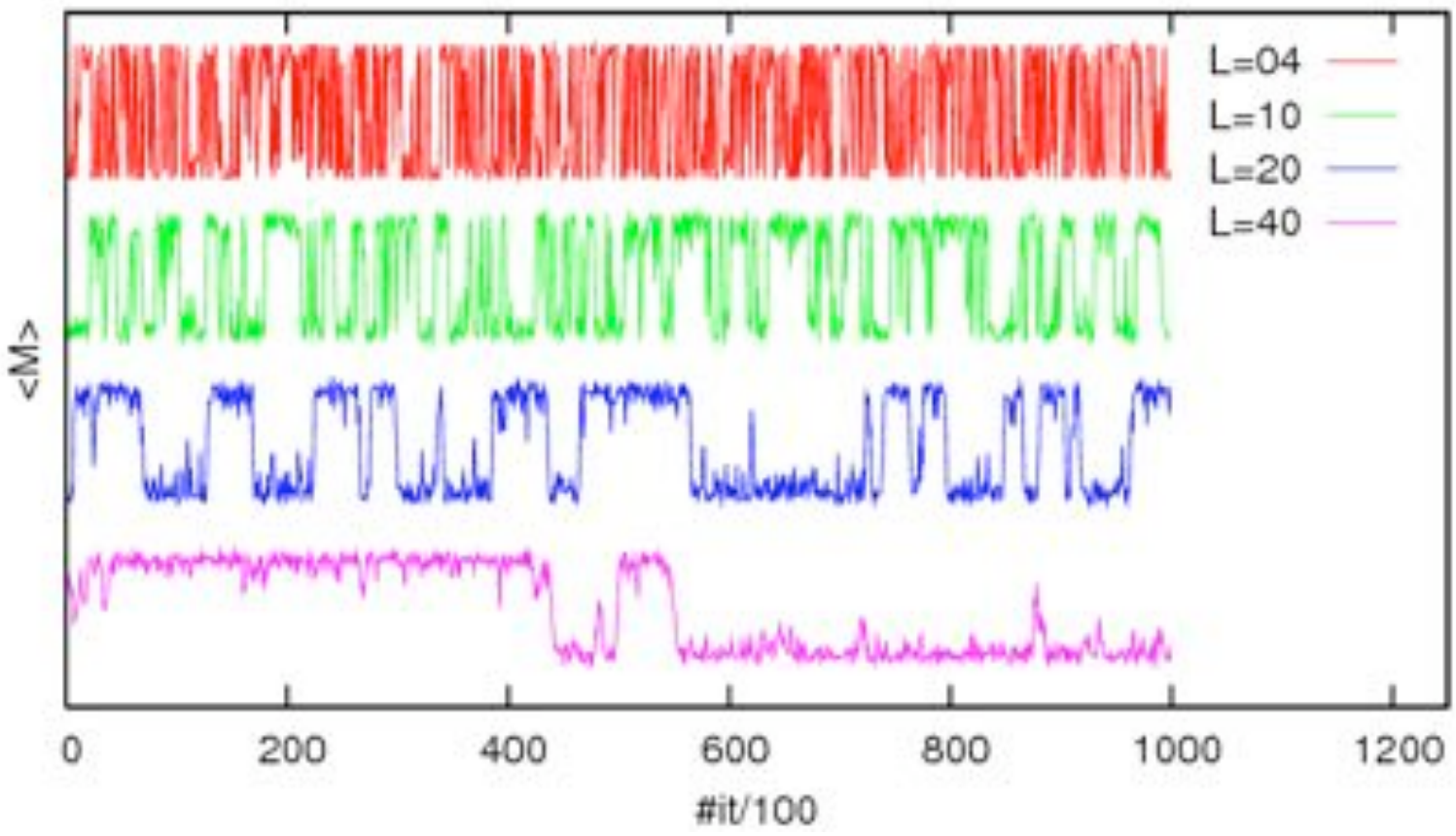
(b) Choose T=1 and repeat (a). ..



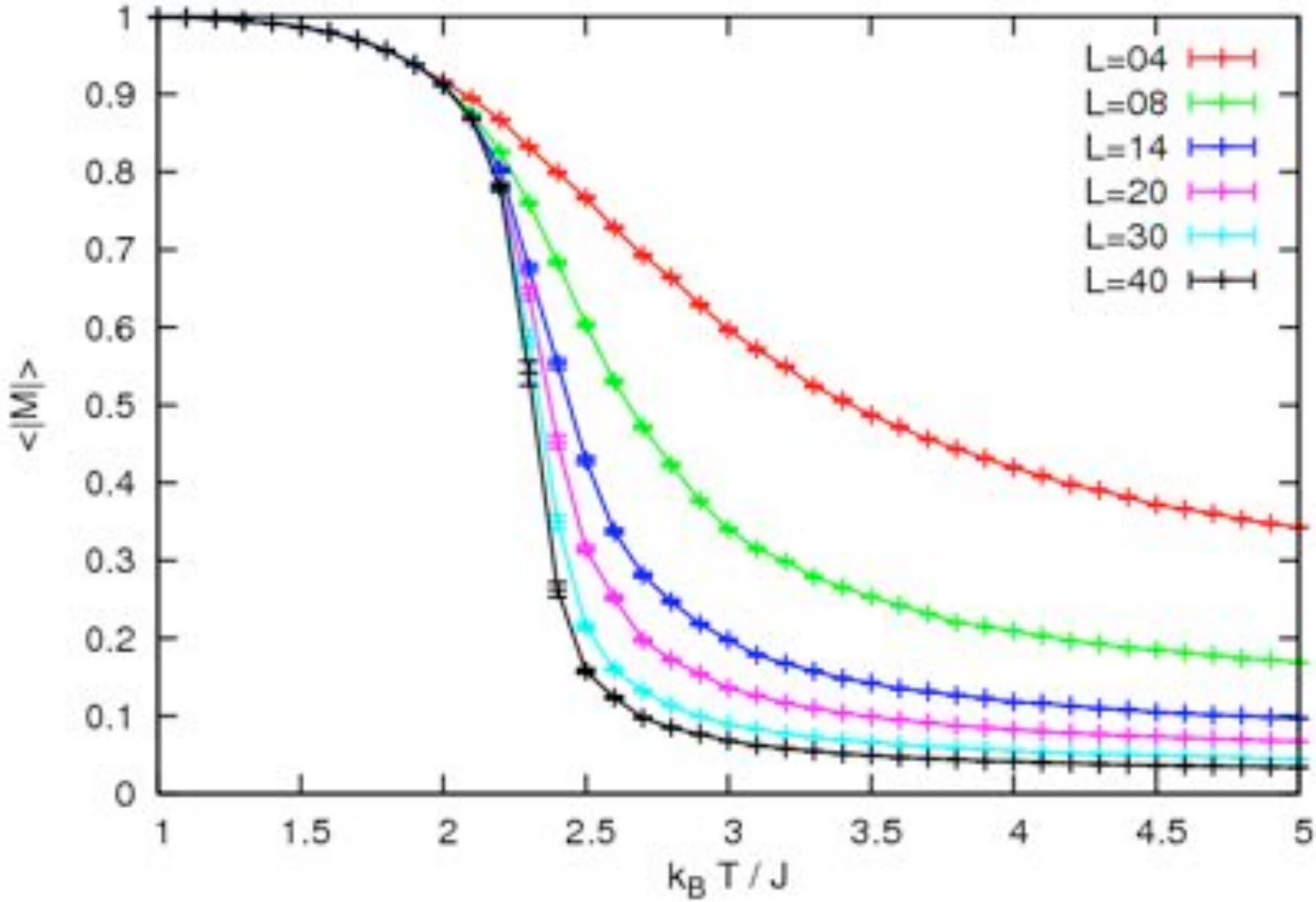
Some results that you should obtain...

Raw data: traces, covariance and autocorrelation time

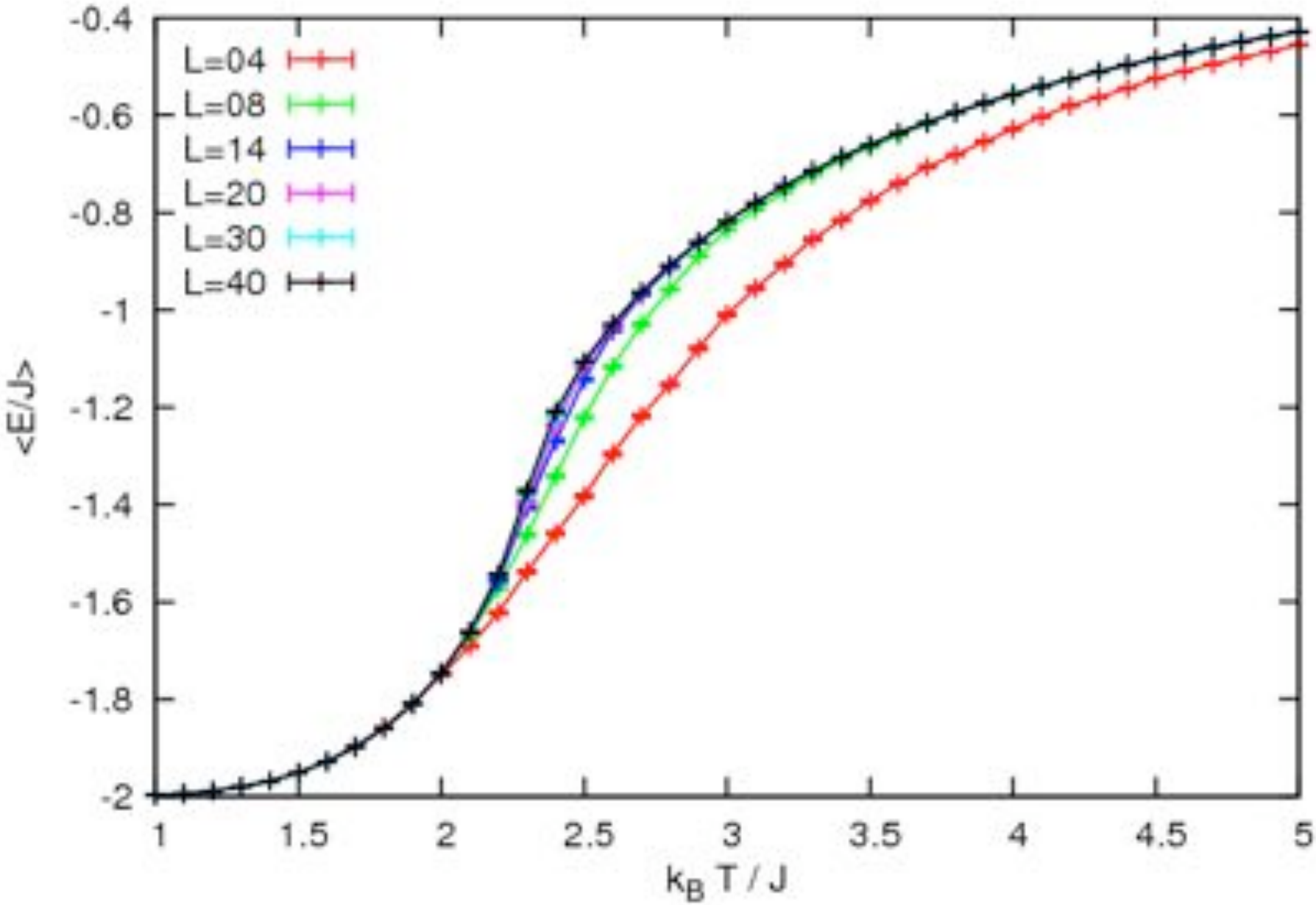
Trace: magnetization for $T = 2.27 J/k_B \approx T_C$ (10^5 sweeps)



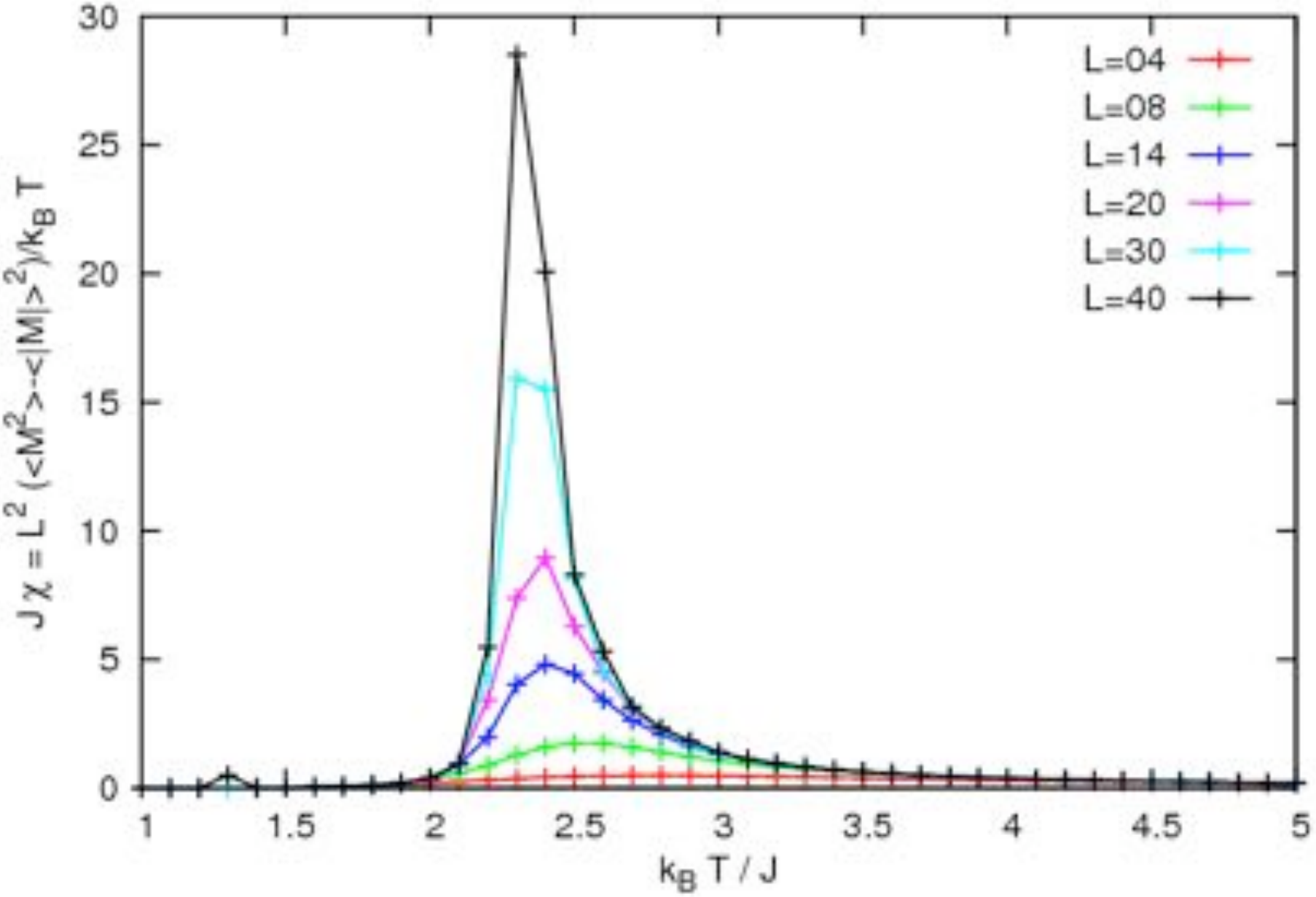
Magnetization (10^5 sweeps)



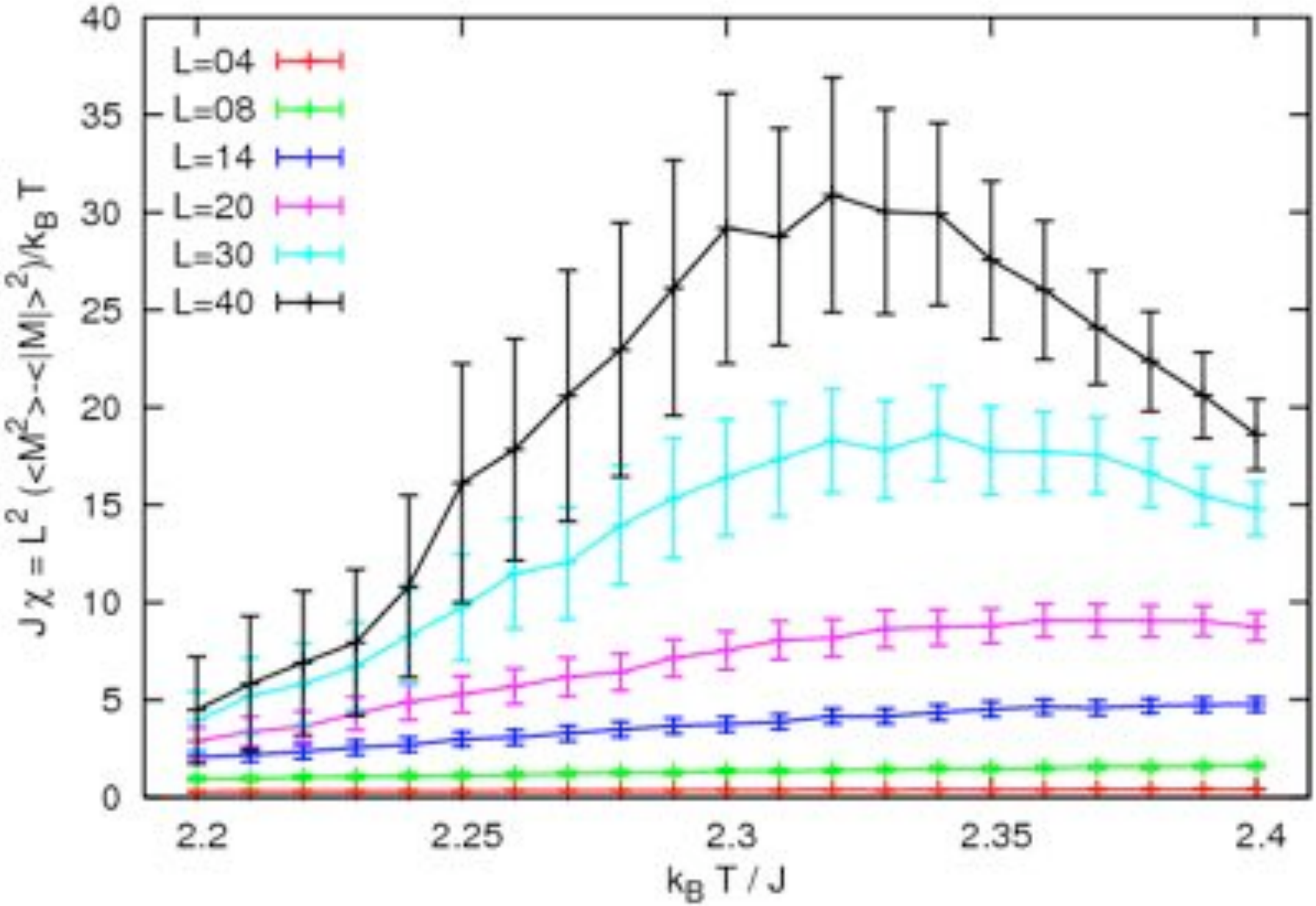
Energy (10^5 sweeps)



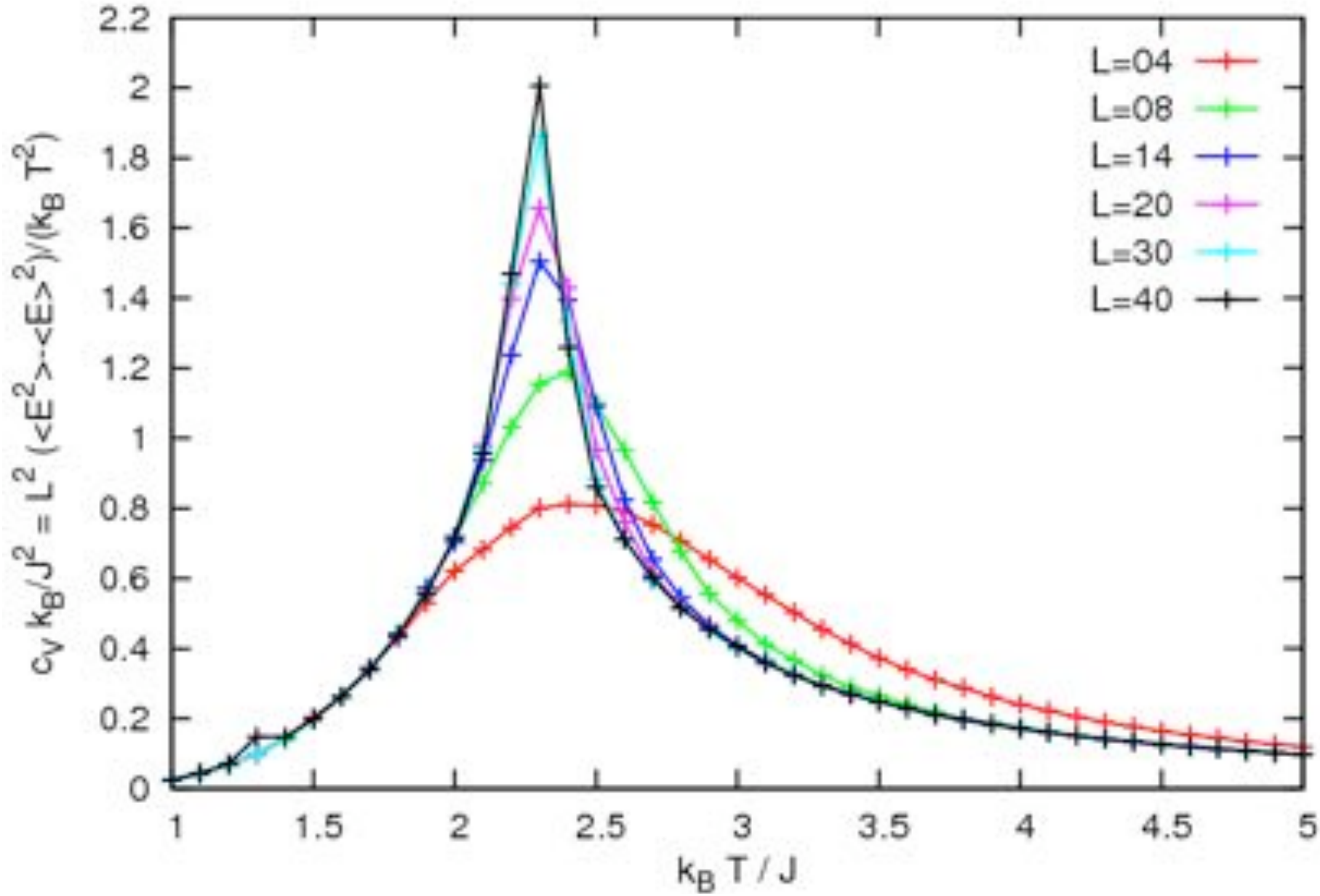
Magnetic susceptibility (10^5 sweeps)



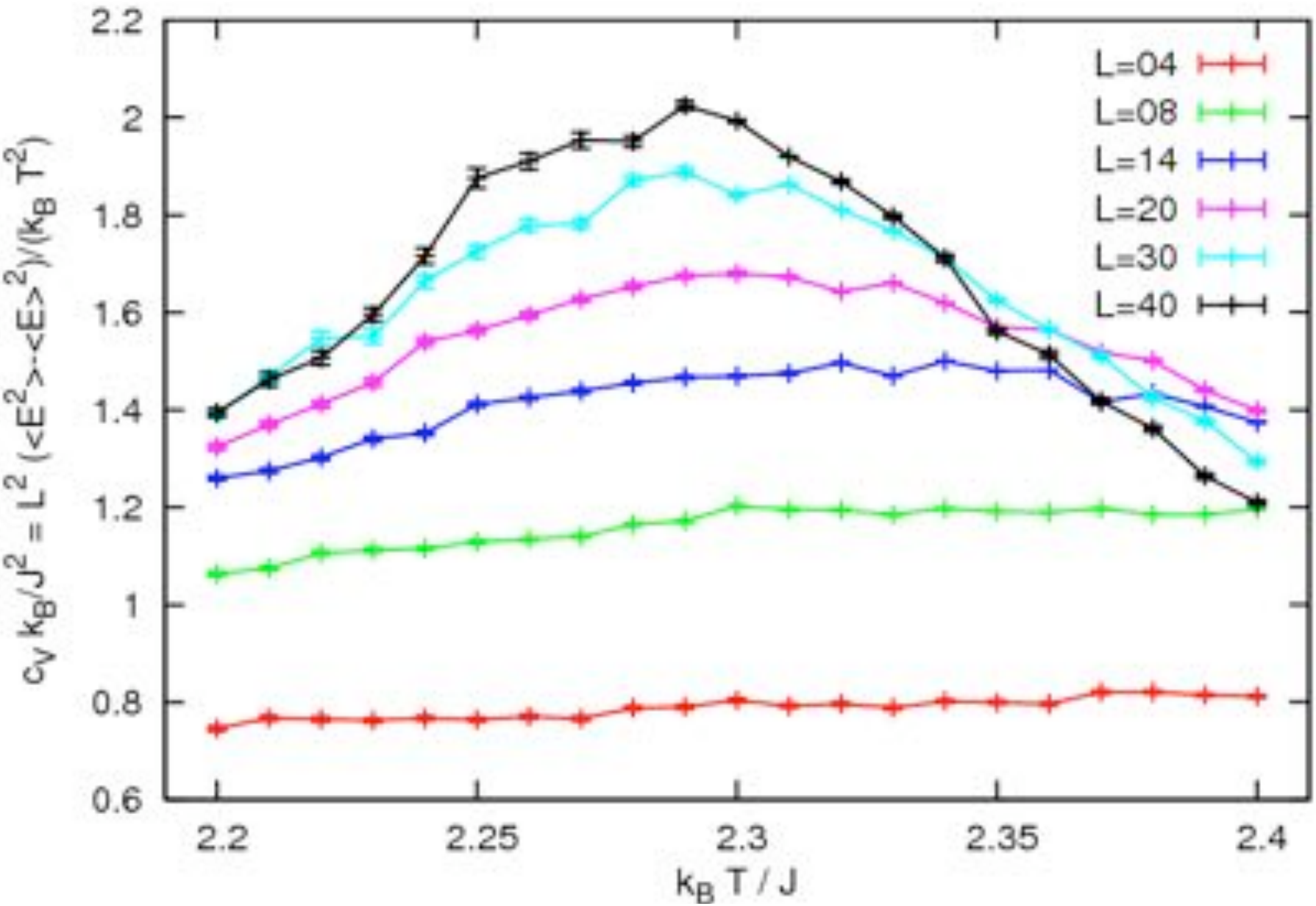
Magnetic susceptibility near T_c (10^6 sweeps)



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

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

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 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 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 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: $T_c(L) - T_c(\infty) \propto L^{-\lambda}$

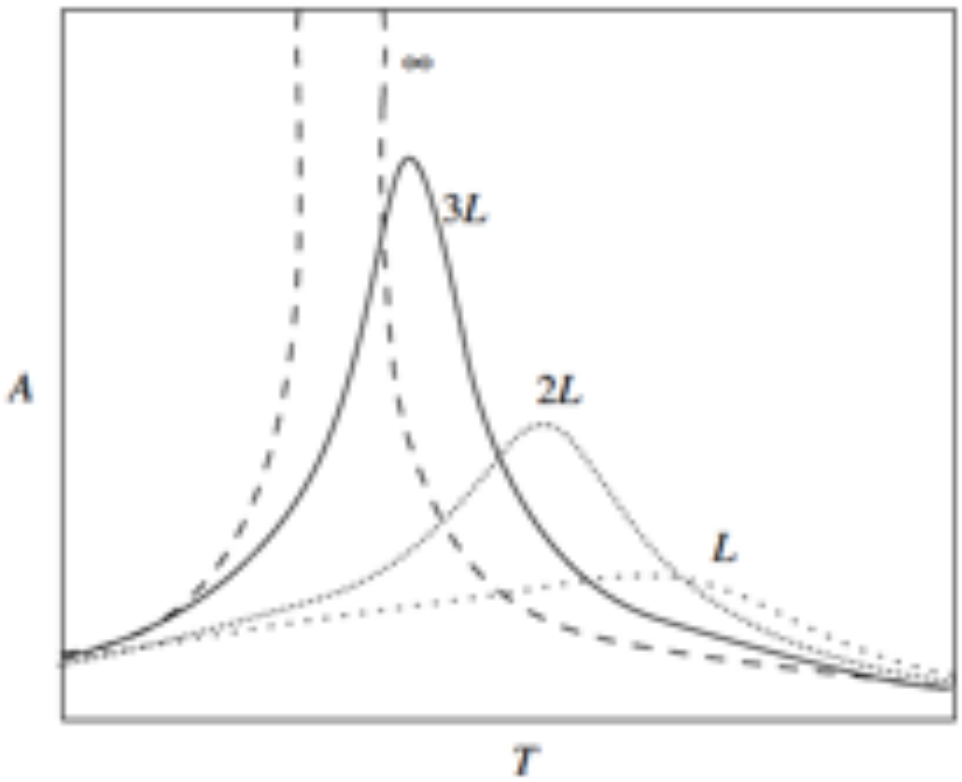


FIG. 1. Typical behaviour of a physical quantity A vs temperature close to the critical point for various system sizes. Figure taken from Thiissen[8].

[Thijssen, Computational Physics (Cambridge University Press)]

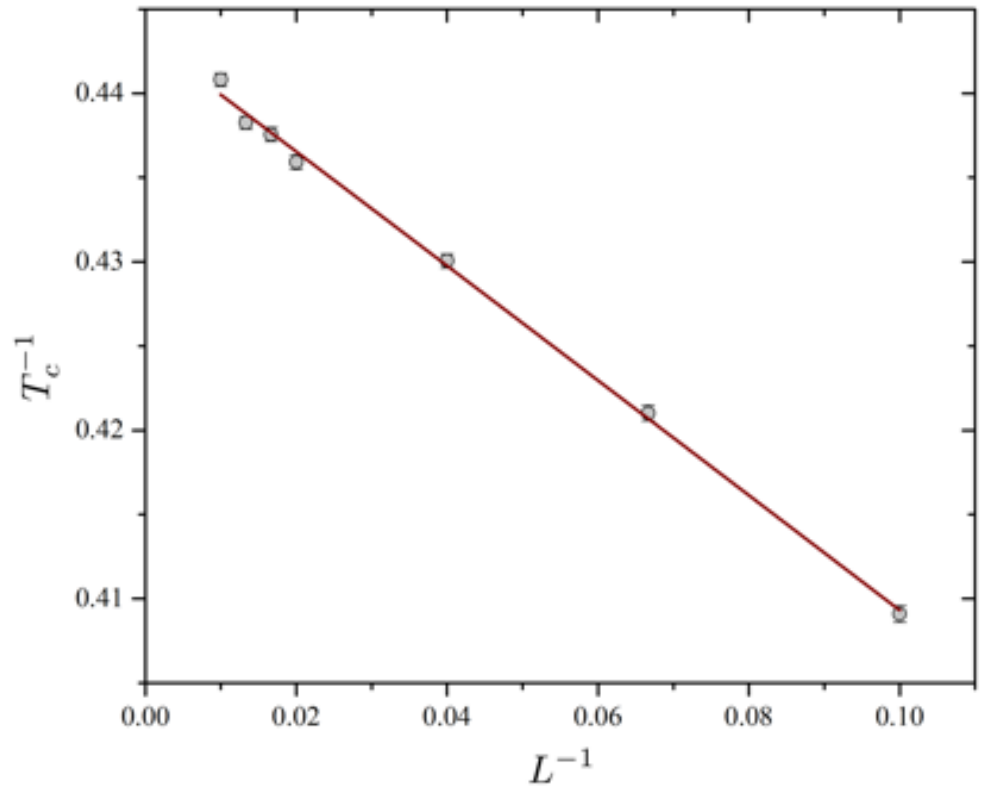


FIG. 9. (Color online) Inverse of the critical temperature T_c^{-1} vs inverse of lattice size L^{-1} for the 2D Ising model. The curve was fitted with a power law $T_c^{-1} = T_{c\infty}^{-1} - bL^{-1/\nu}$, and the critical exponent ν was determined.

- 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:

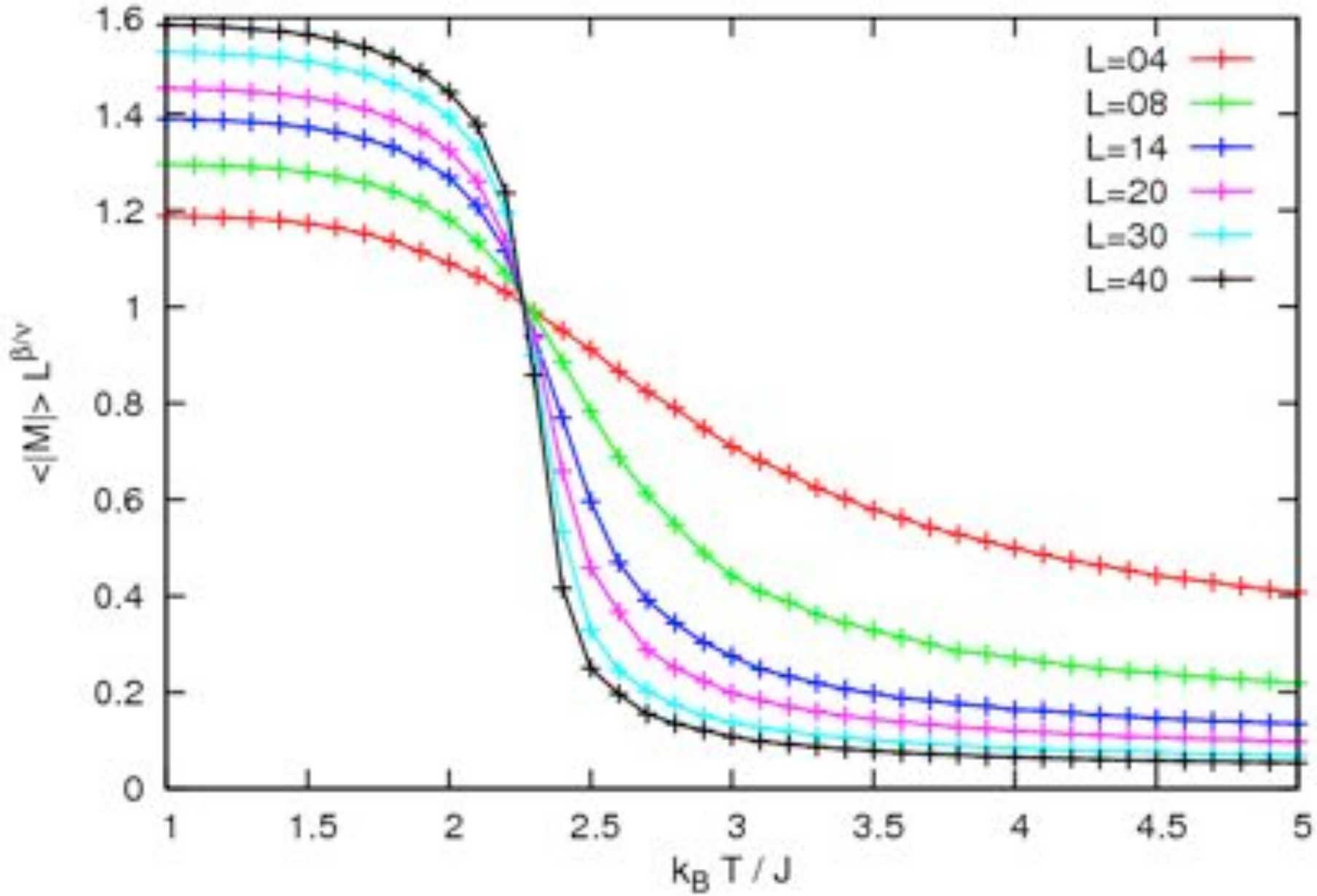
$$m(T) \sim (T_c - T)^{\beta} \to L^{-\beta/\nu} \tag{17.29}$$

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

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

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)

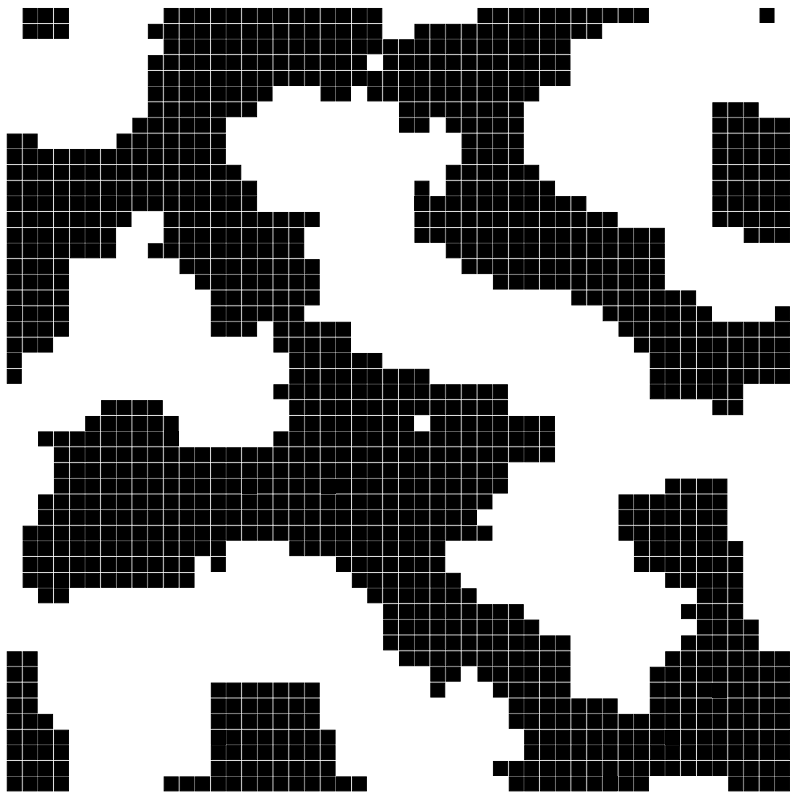
see e.g.: https://mattbierbaum.github.io/ising.js

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

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:

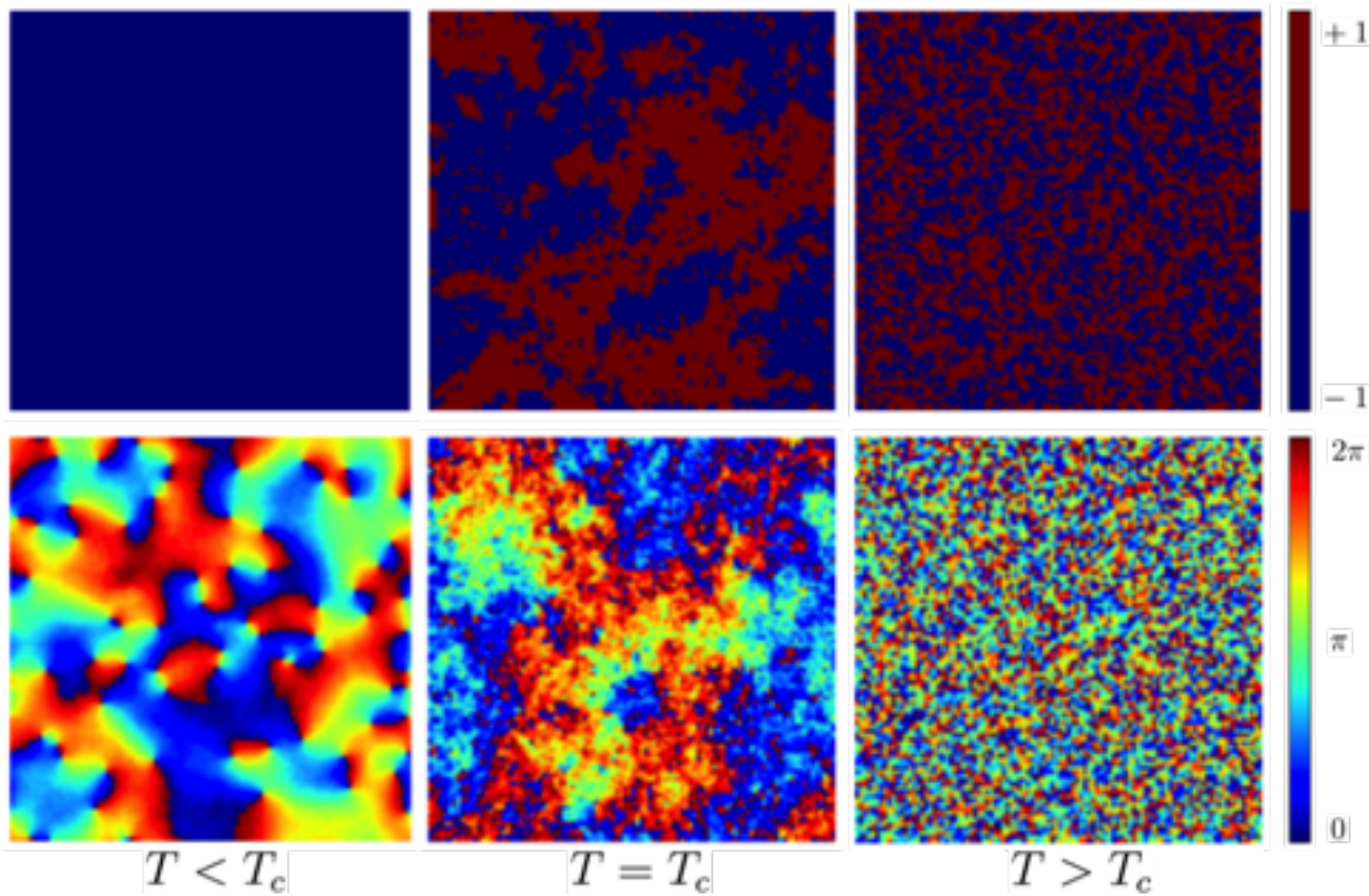


FIG. 15. (Color online) Behavior of the two dimensional Ising model (top) and XY model (bottom) at $T < T_c$, $T = T_c$ and $T > T_c$. For the Ising model, an $\uparrow$ spin ($s_i = 1$) is represented by red and a $\downarrow$ spin ($s_i = -1$) is represented by blue. For the XY model, because every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