

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

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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:

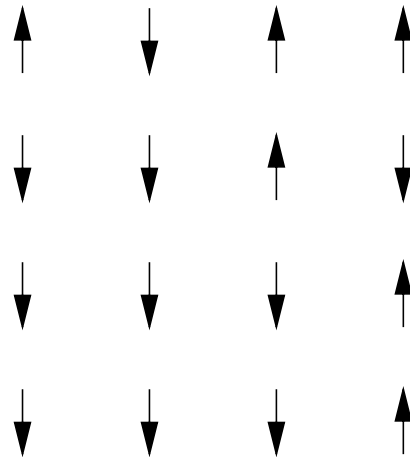
- energy => Ising model
- evolution
(to build the trajectory / the Markov chain)

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 spins $1/2$, \vec{s}_1 , \vec{s}_2 (e.g. electrons in He), their sum \vec{S} , the basis $|S, S_z\rangle$ of the Hilbert space in the coupled representation, and a hamiltonian $\mathcal{H} = h_1 + h_2 + V_{12}$:

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

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

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

We have:

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

2 interacting spins

Idea: write a model hamiltonian explicitly dependent on the spin giving the same energy difference between the 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 base, 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:

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

$J > 0$ ($E_s > E_t$) $\uparrow\uparrow$ 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:

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

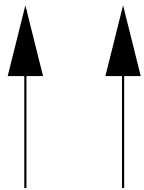
Ising model

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

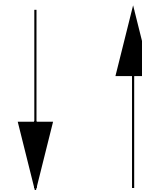
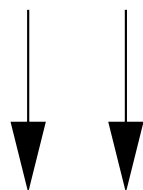
$$\mathcal{H}^{spin} = -J \sum_{i,j=1}^N s_i s_j$$

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

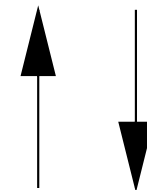
$J < 0$ ($E_s < E_t$) $\uparrow\downarrow$ spins favored \Rightarrow **antiferromagnetic case**



$$E = -J$$



$$E = +J$$

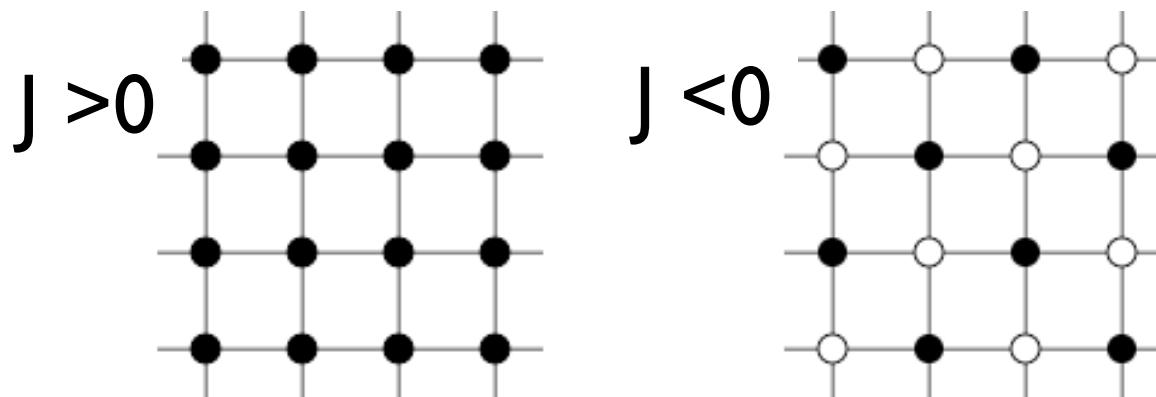


(choosing the kind of interaction, we specify the **energy model**)

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 states 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.

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:

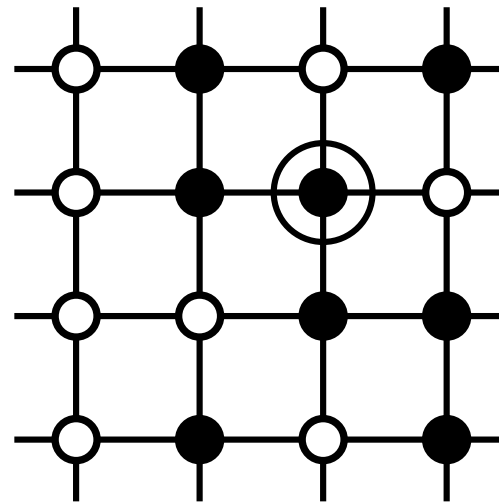
$$E_0/N = -2J$$

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

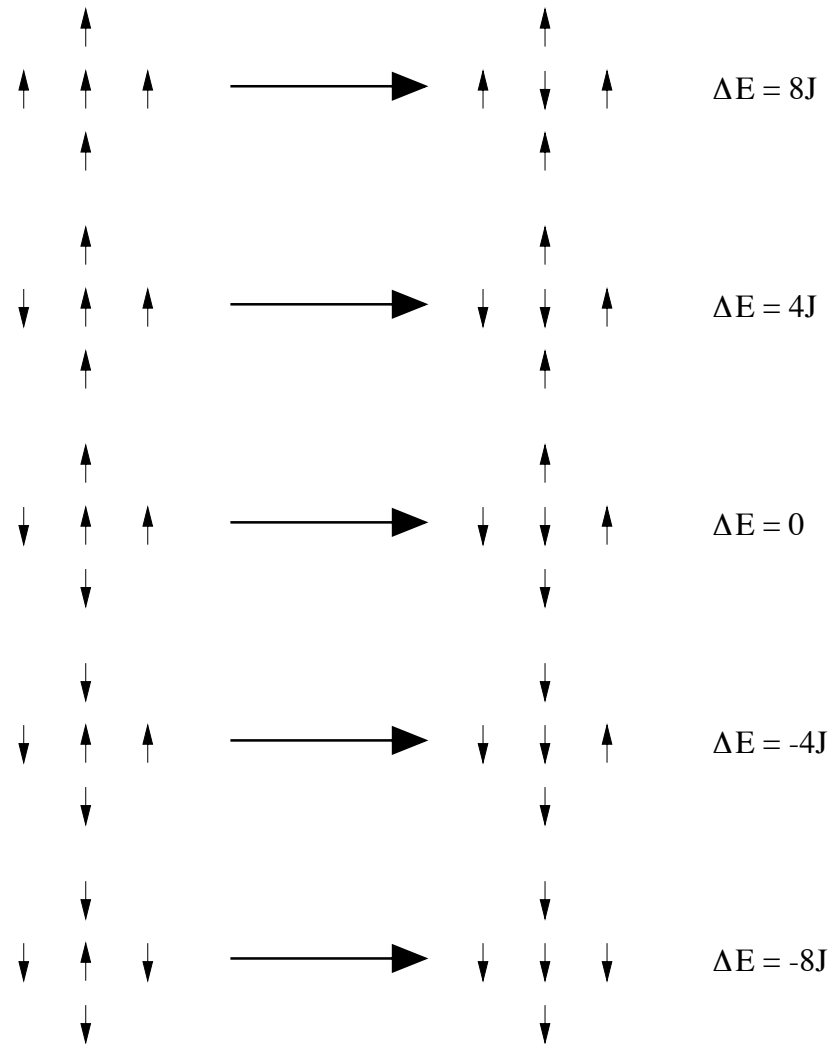
Consider nn interactions, choose a random spin and flip it: it's **a new configuration** (a microstate)



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:

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

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



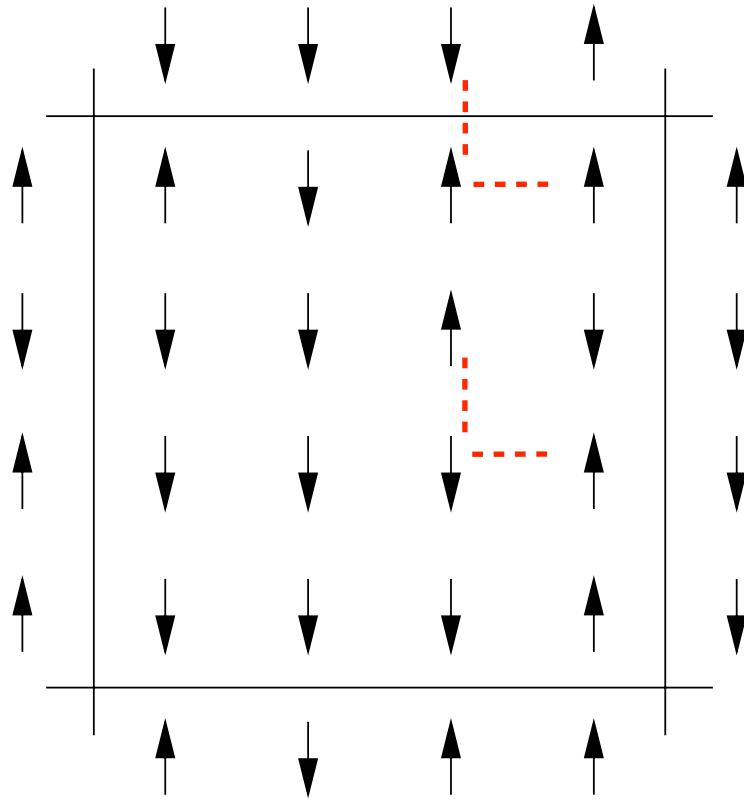
(volume term)



(surface term)

Energy per spin in the ground state converges to the value
 $E_0/N = -2J$ in the thermodynamic limit
 with behavior $\sim 1/L$ in case of free boundaries

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

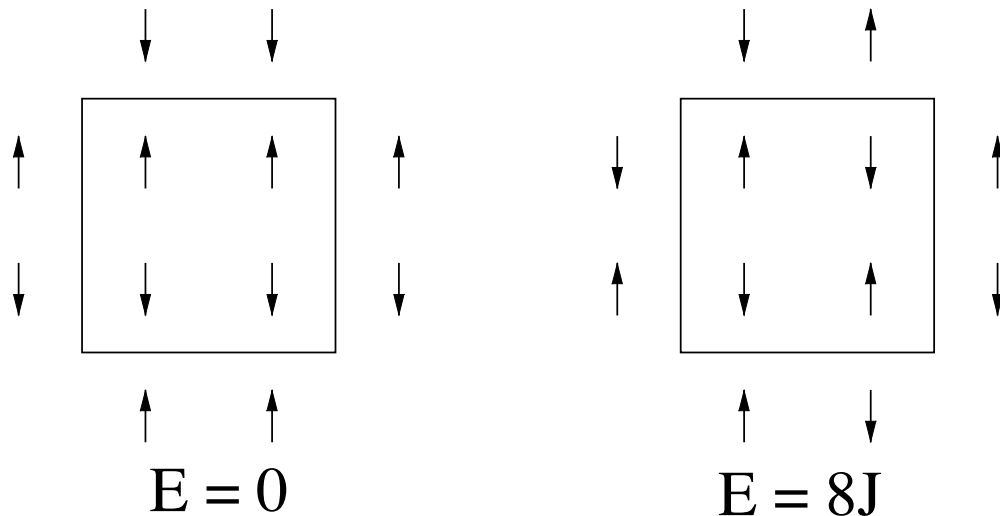
One of the 2^N possible configurations of a system of $N = 16$ Ising spins on a square lattice.
with periodic boundary conditions.

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

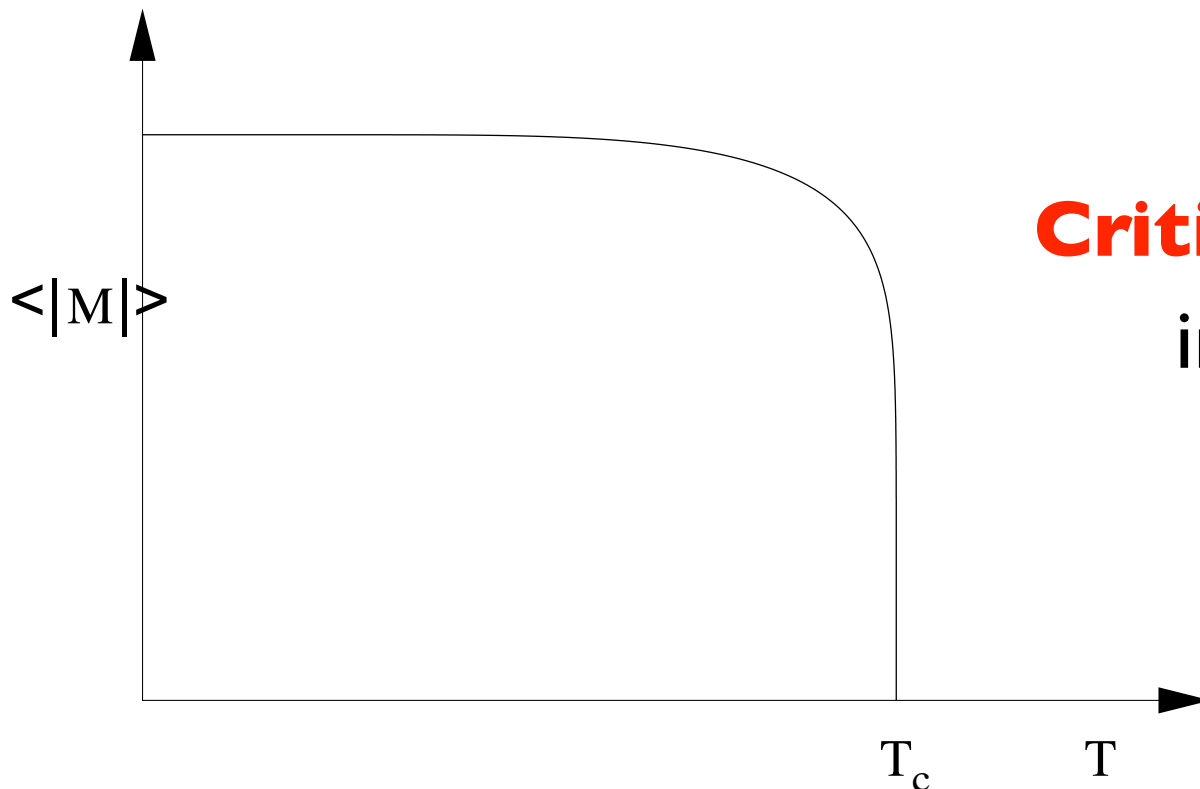
Ising model: phase transition

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**

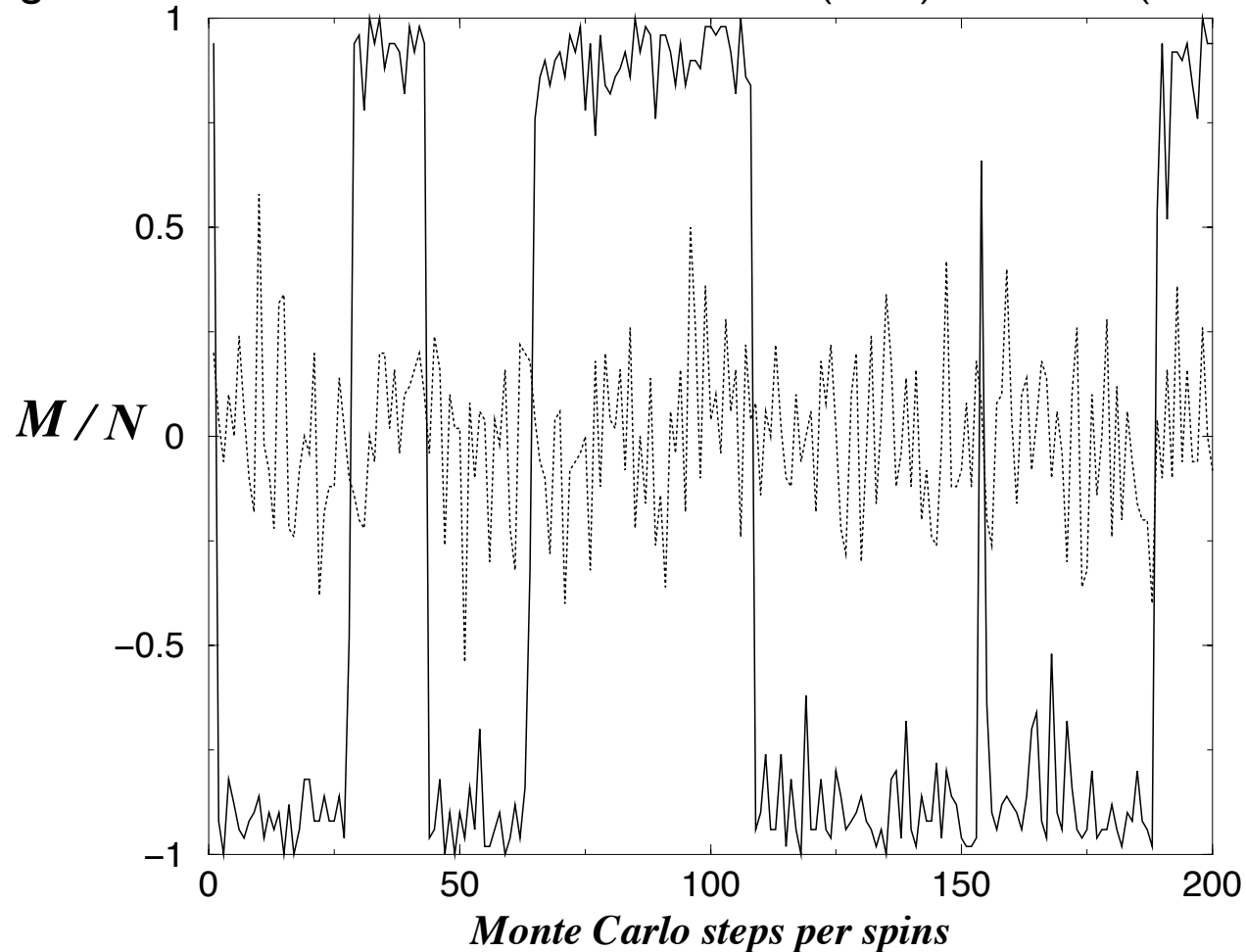
in 2D the model has an
analytical solution:

$$T_c = 2.269 J/k_B$$

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

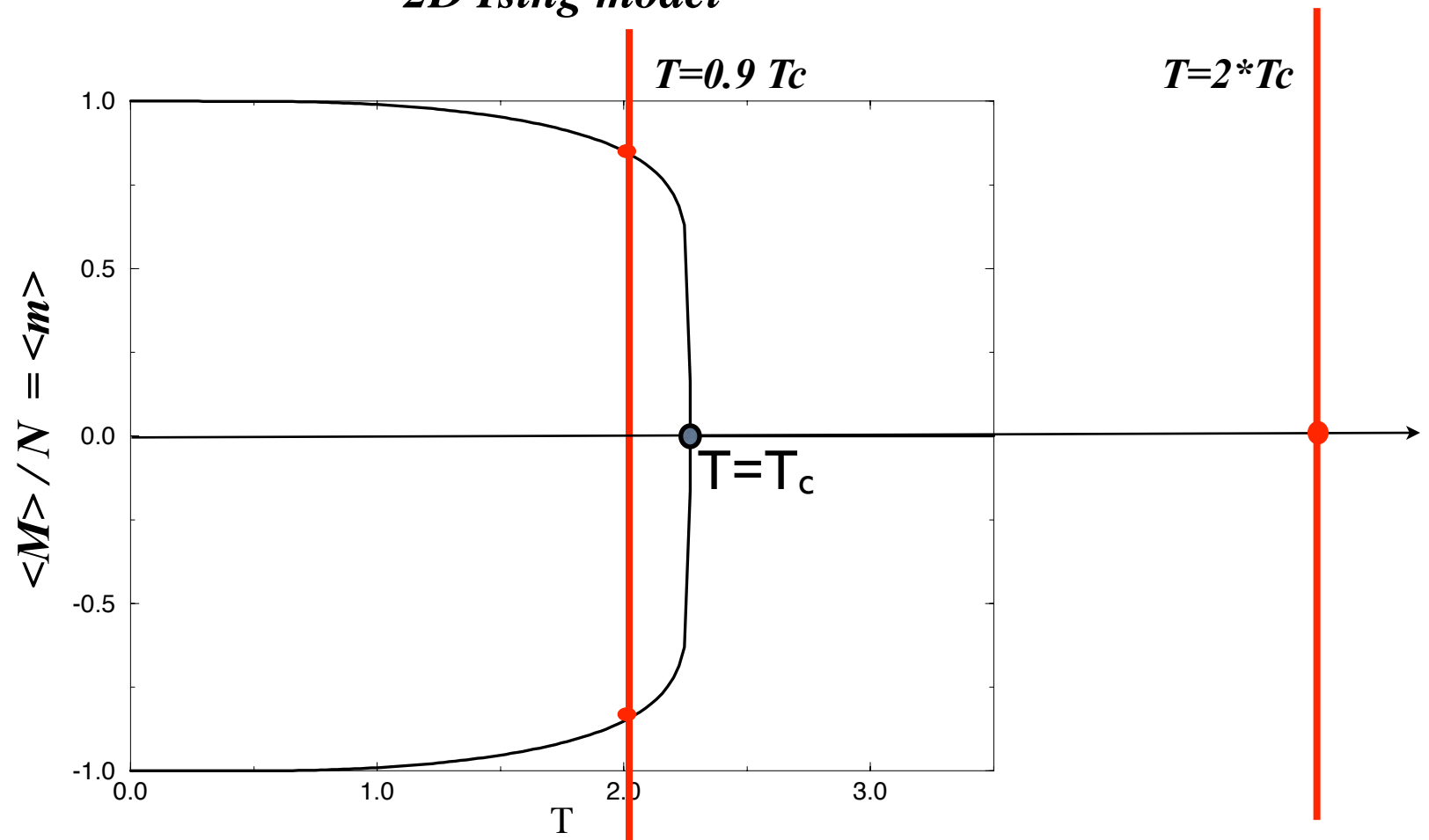
*Magnetization (System : 10*10)*

Magnetization as a function of time for $T < T_c$ (solid) and $T > T_c$ (dashed curve)



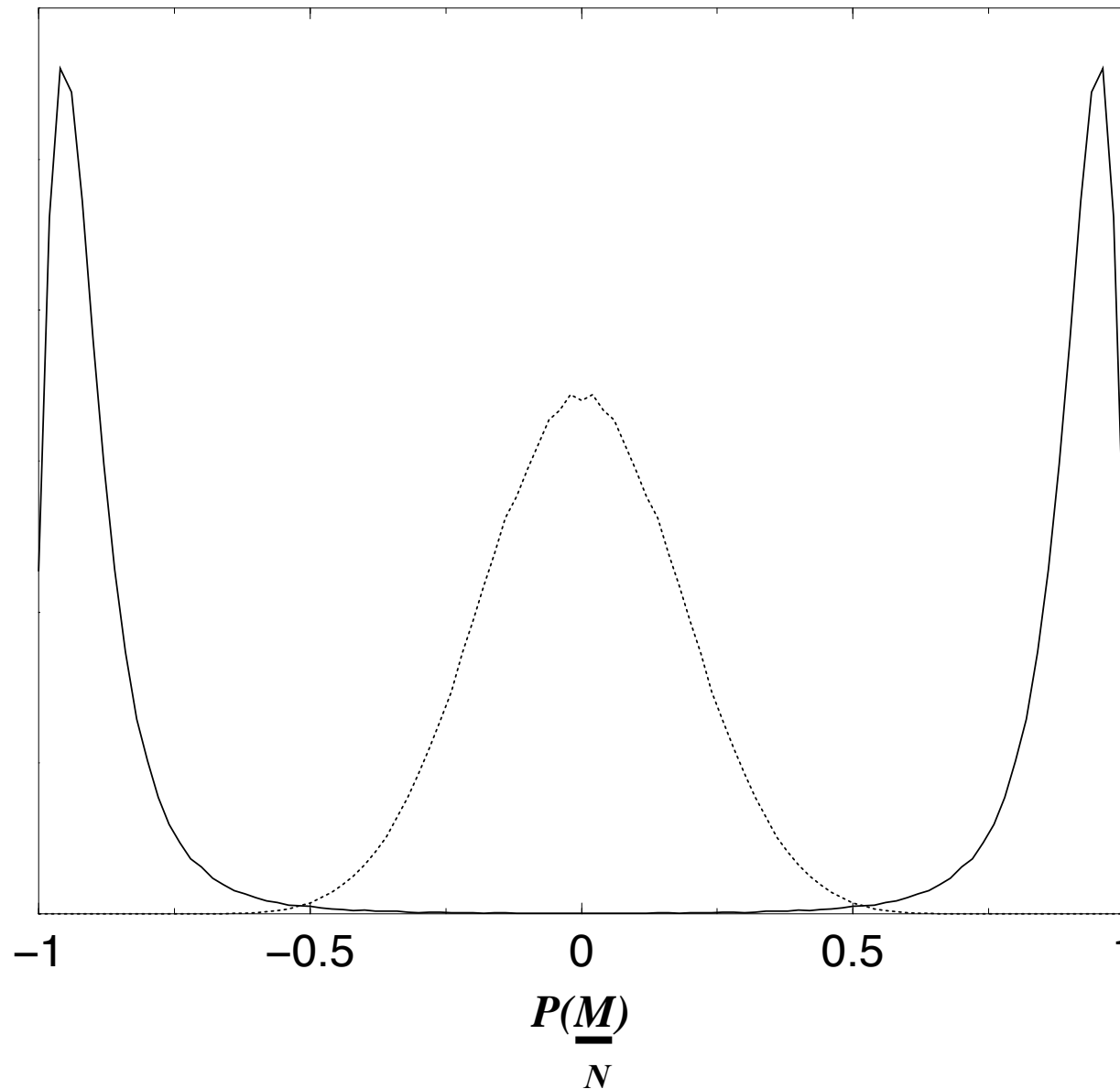
Fluctuations! do, as usual, **temporal averages**: $\langle M \rangle / N$, $\langle E \rangle / N$

2D Ising model



Magnetisation as a function of the temperature for the 2D Ising model.

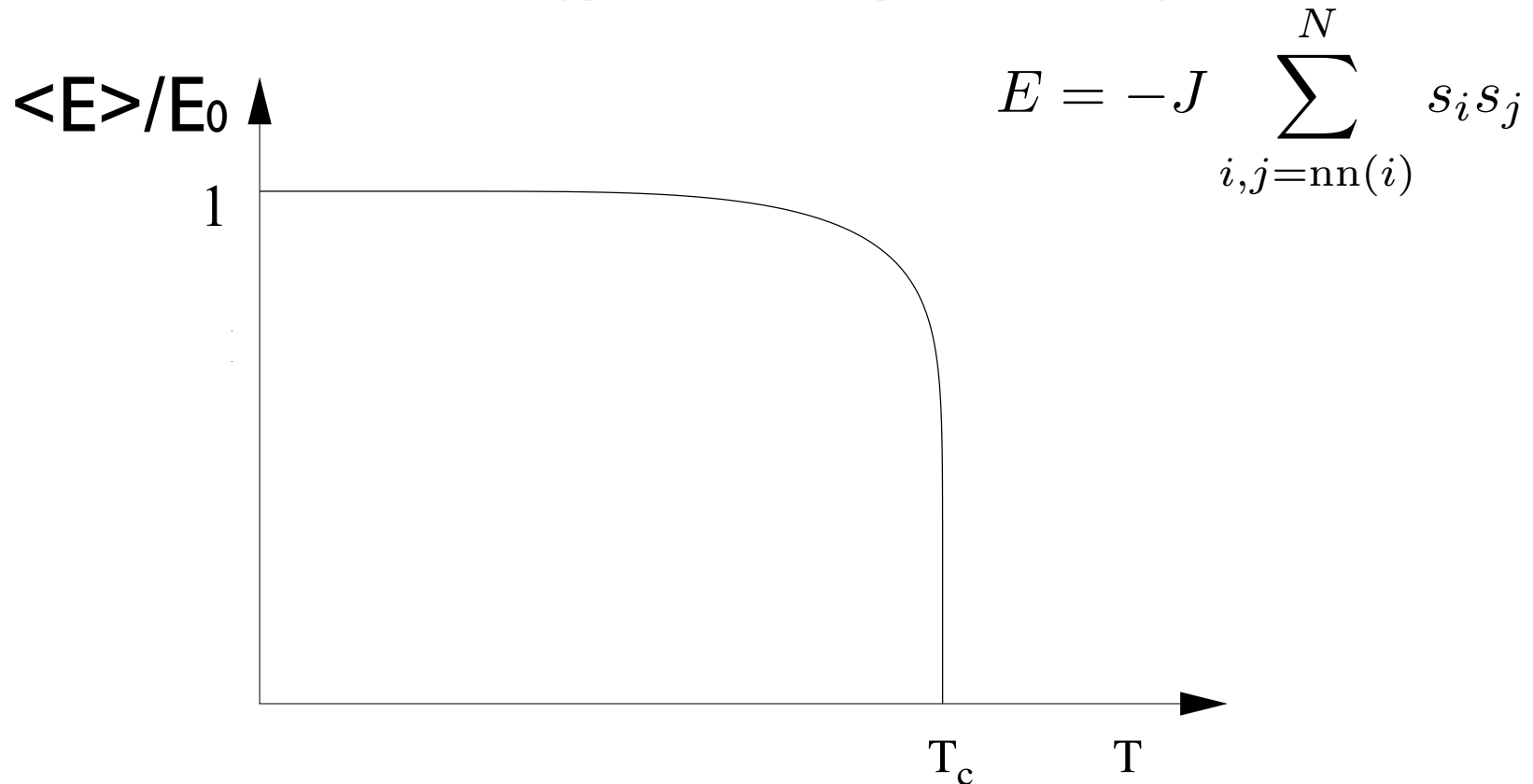
Magnetization distribution for $T < T_c$ (solid) and $T > T_c$ (dashed curve)



(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...

Ising model: fluctuations

Fluctuations are intrinsic to the system evolution
and are important!

Linear response functions are related to
equilibrium fluctuations:

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

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

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

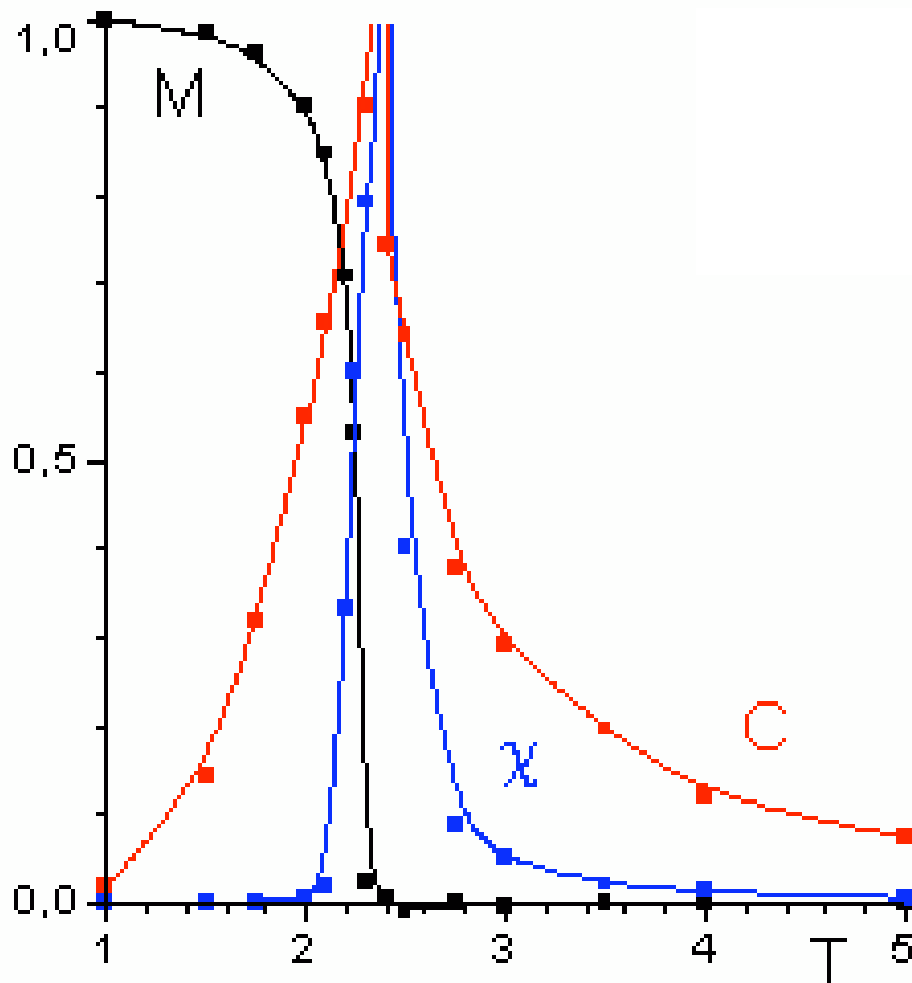
(Large fluctuations near the phase transition:
Second Order phase transition)

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, do also simply: `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
```

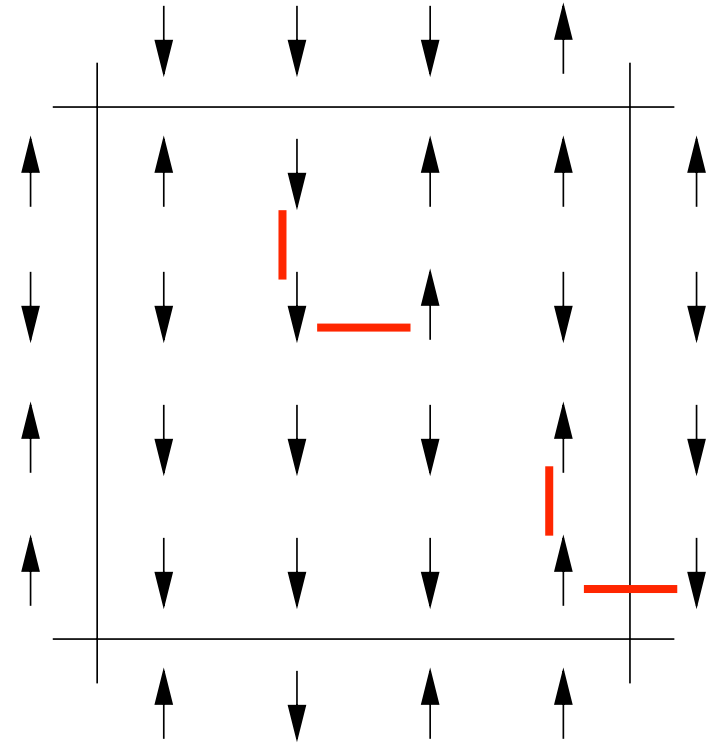
```
E = E - spin(x,y)*sums
```

```
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

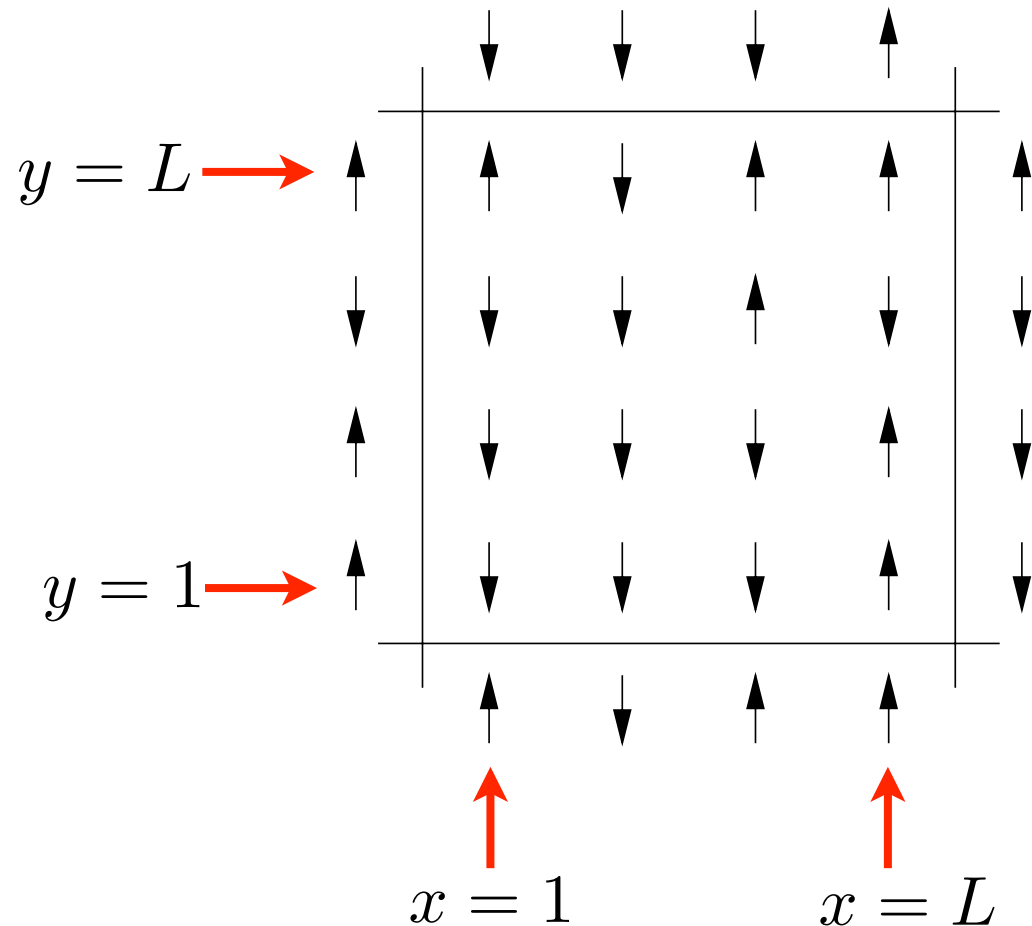
Evolution is driven by the **energy change** between the old and the new configuration (Metropolis MC)

```
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)
  .....
```

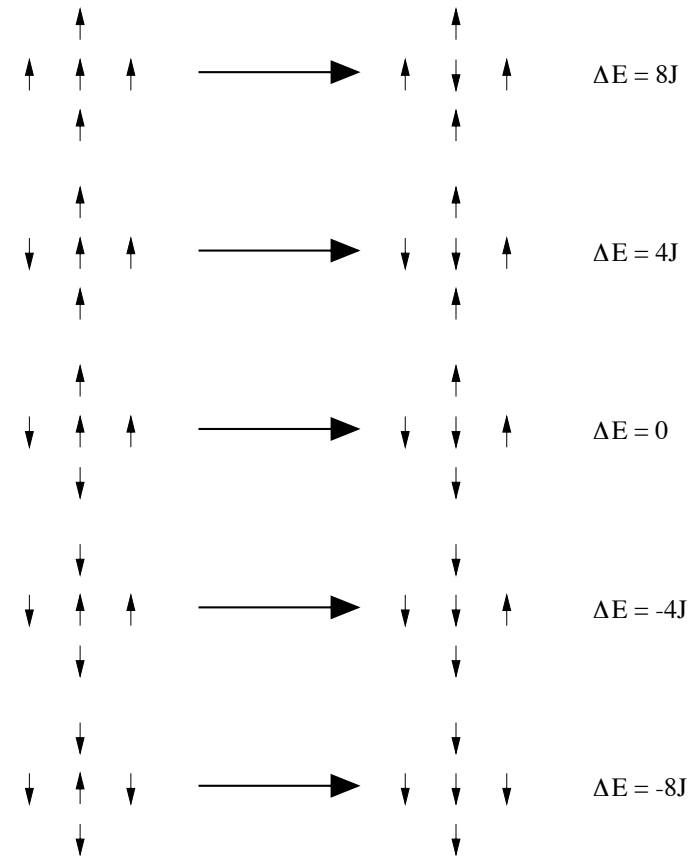


Ising model: storage of Boltzmann's coeff.

! 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

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

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?

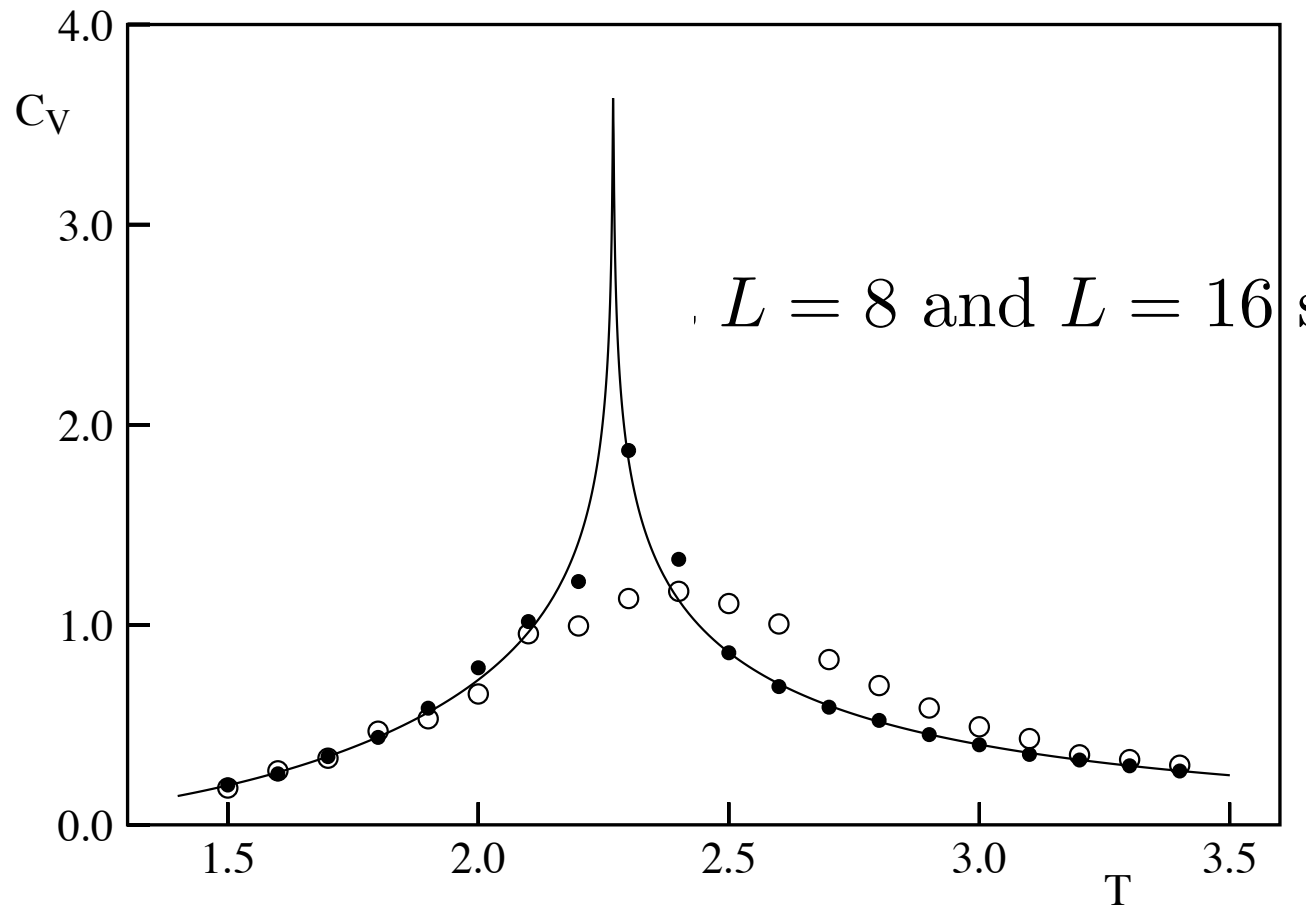
- necessary to give the **ERROR ESTIMATE** corresponding to the measured physical quantity !!!
- (see Tab. I of D.P. Landau, PRB 13, 2997 (1976), “Finite size behavior of the Ising square lattice”)
- do also **BLOCKING** (called “coarse grained technique” in that paper)

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

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

SURFACE EFFECTS:

example of energy for HALF UP/HALF DOWN configurations:

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

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

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

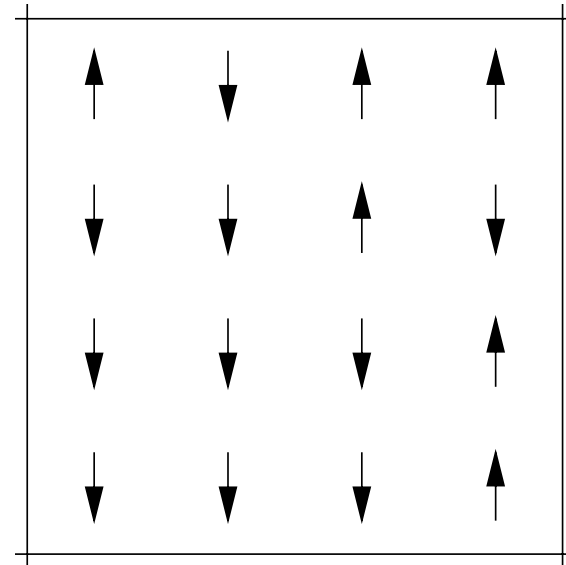
$$L=16 \quad E=-1.75$$

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

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

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

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



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



Ising model: other generalizations

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

Universality and critical exponents

Reduced temperature : $\Delta T = (T - T_c)/T_c$

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

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

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

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

Program:

on

`$/home/peressi/comp-phys/IX-ising/`

`[do: $cp /home/peressi/.../IX-ising/* .]`

ising.f90

Exercise

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

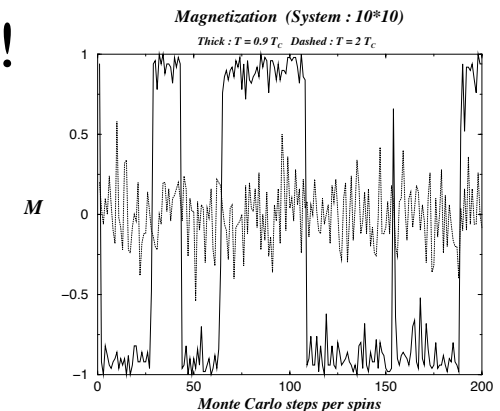
Hint:

- 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

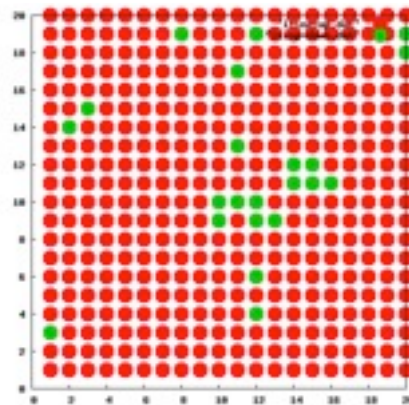
(a) Choose $L=30, T=2$, and initially $\text{spin}=\pm 1$ randomly. ...

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:



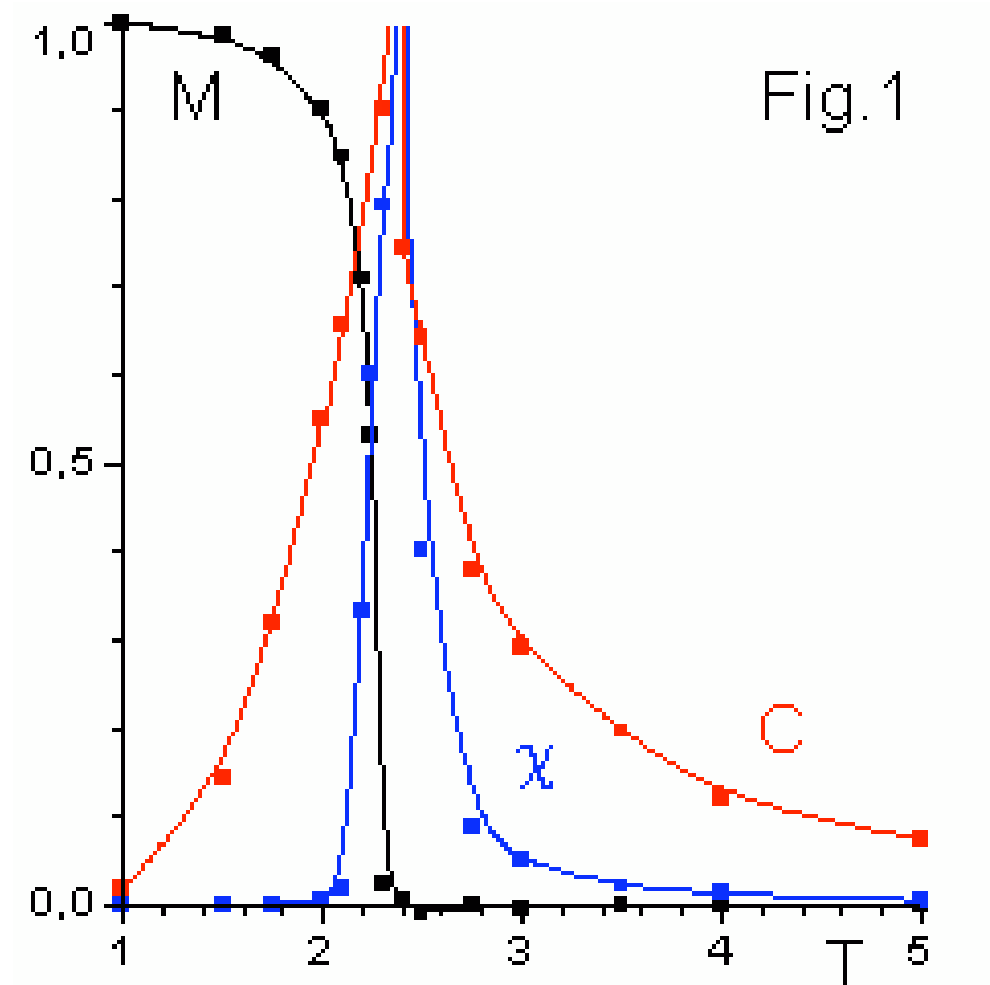
Calculate also c and χ .

Exercise

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

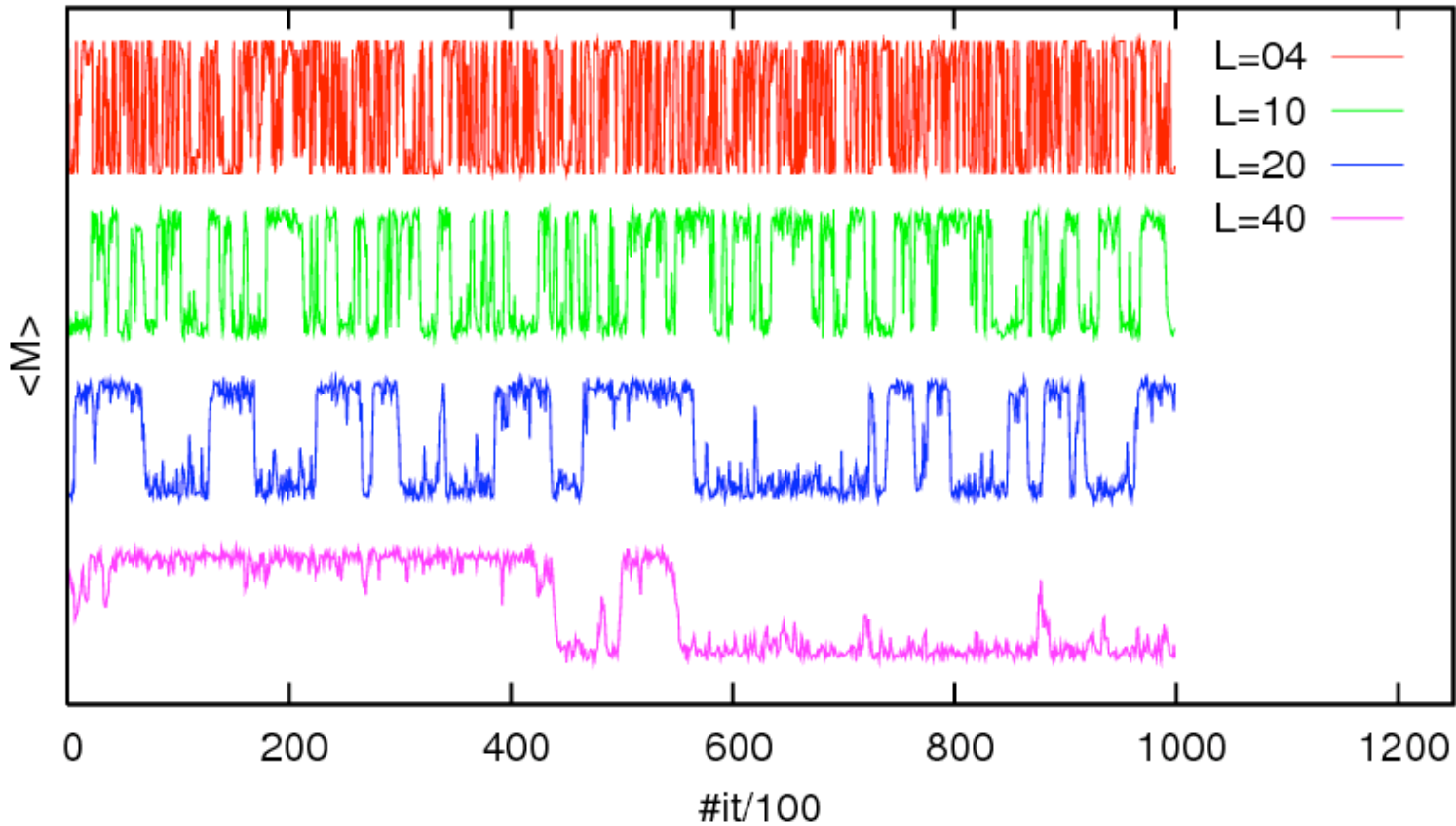
Calculate also c and χ .

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

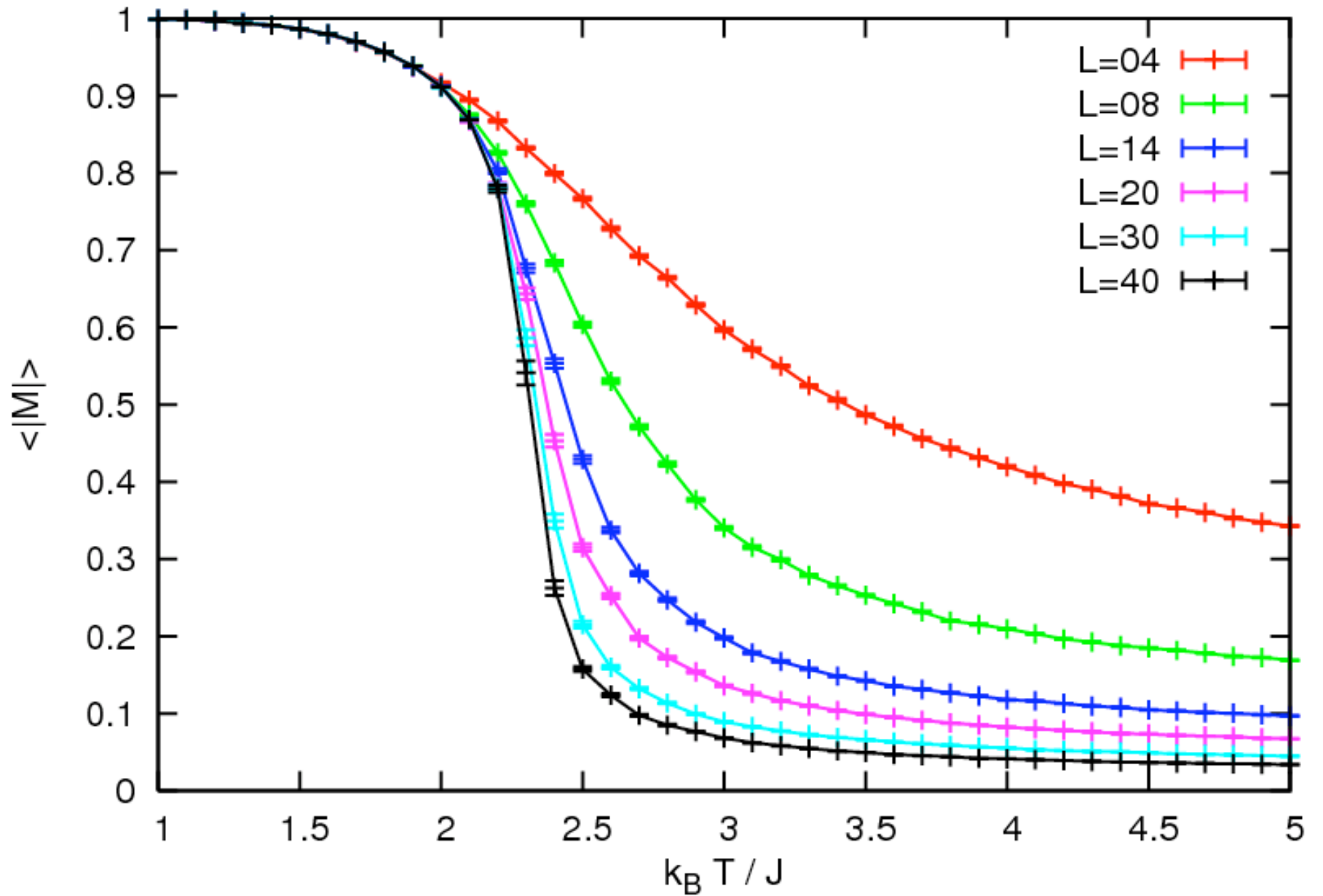


Raw data: traces, covariance and autocorrelation time

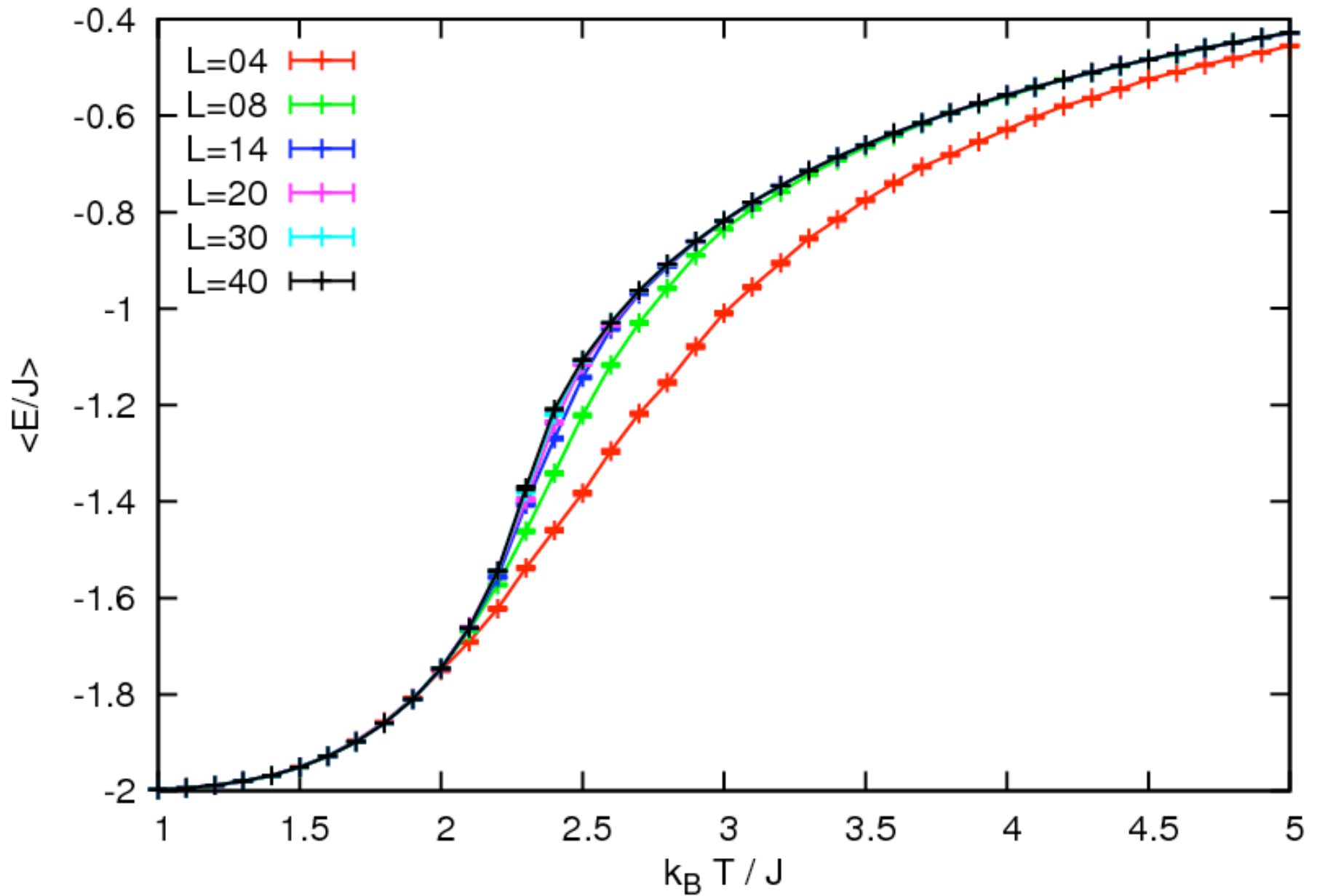
Trace: magnetization for $T = 2.27J/k_B \approx T_C$ (10^5 sweeps)



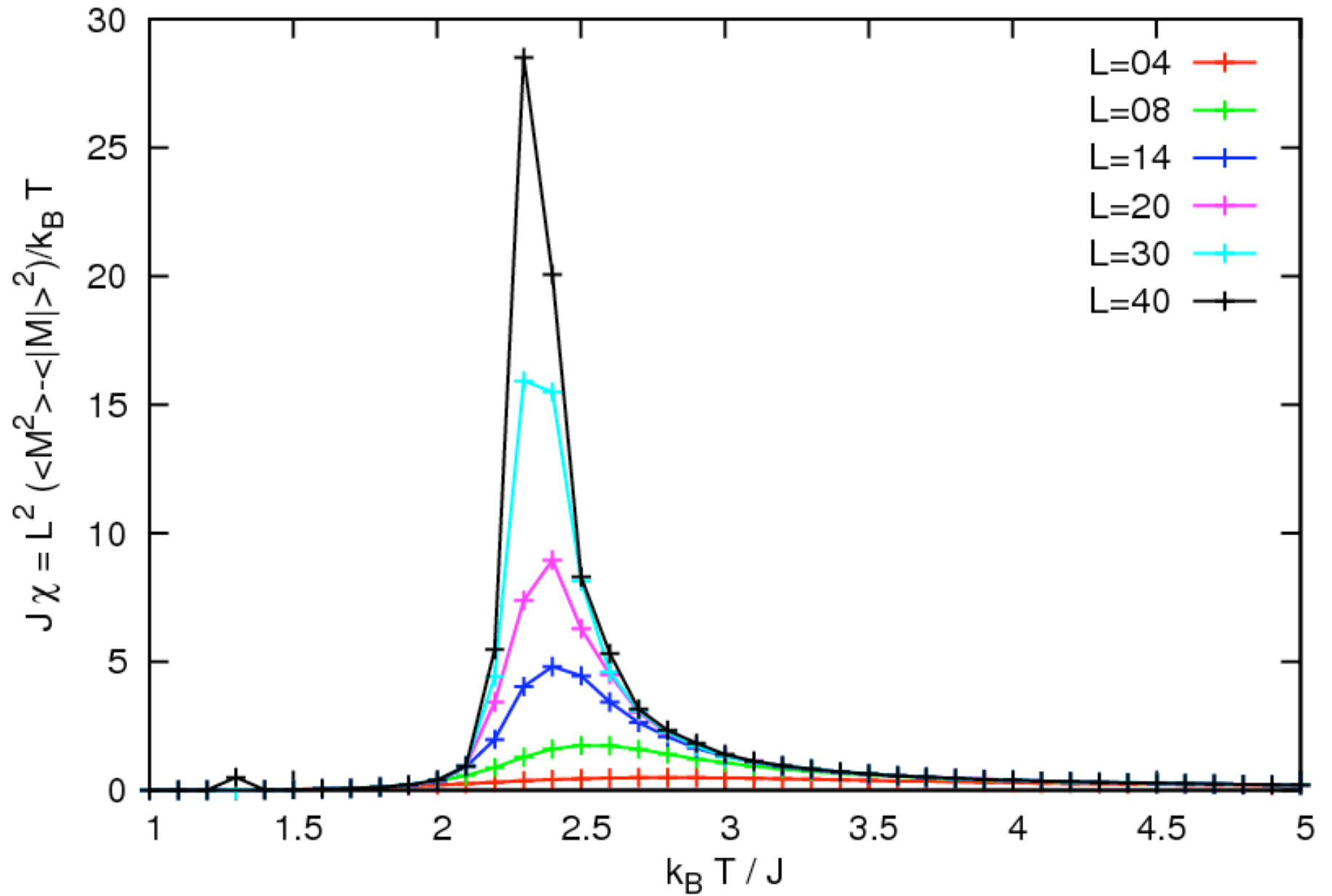
Magnetization (10^5 sweeps)



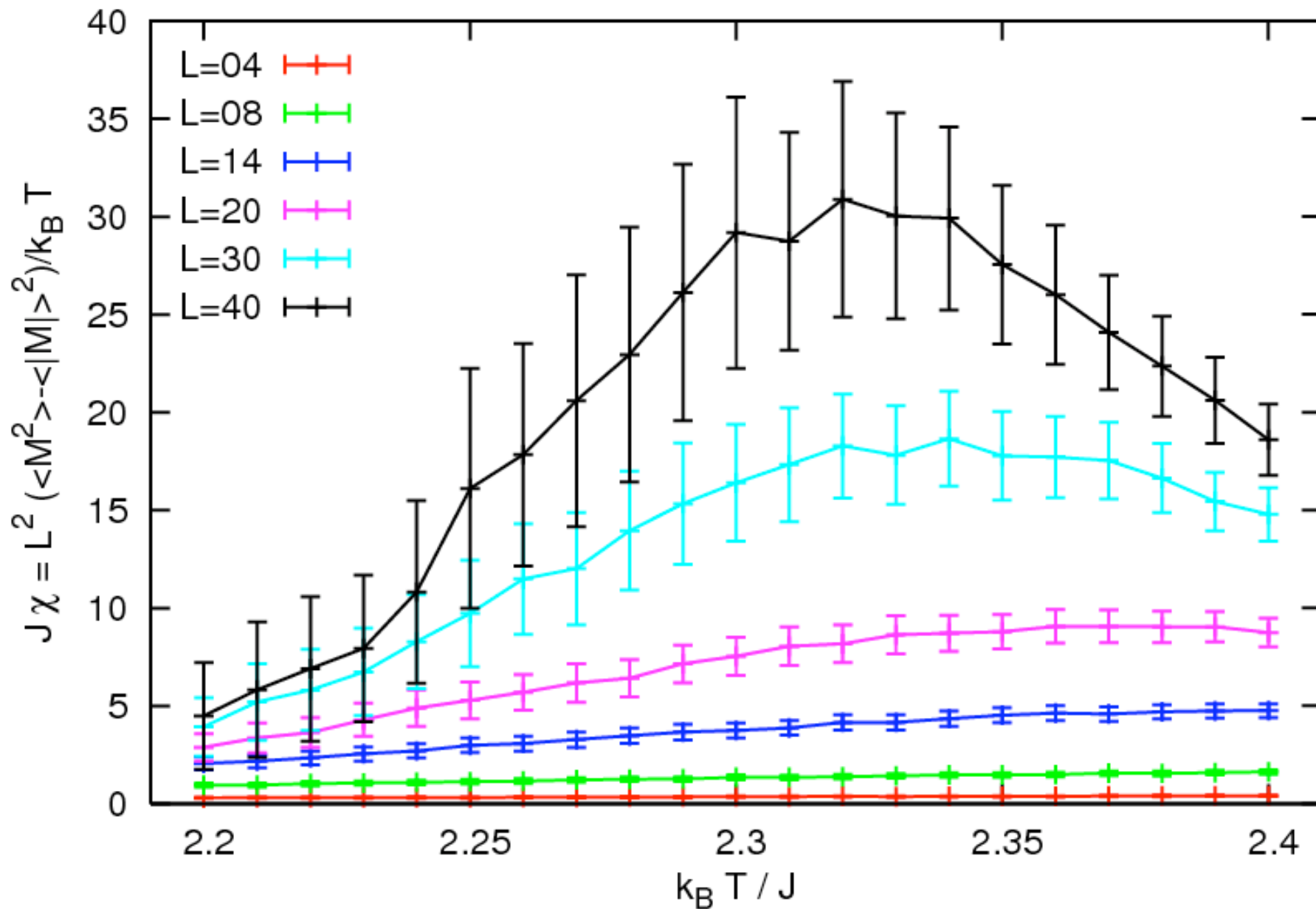
Energy (10^5 sweeps)



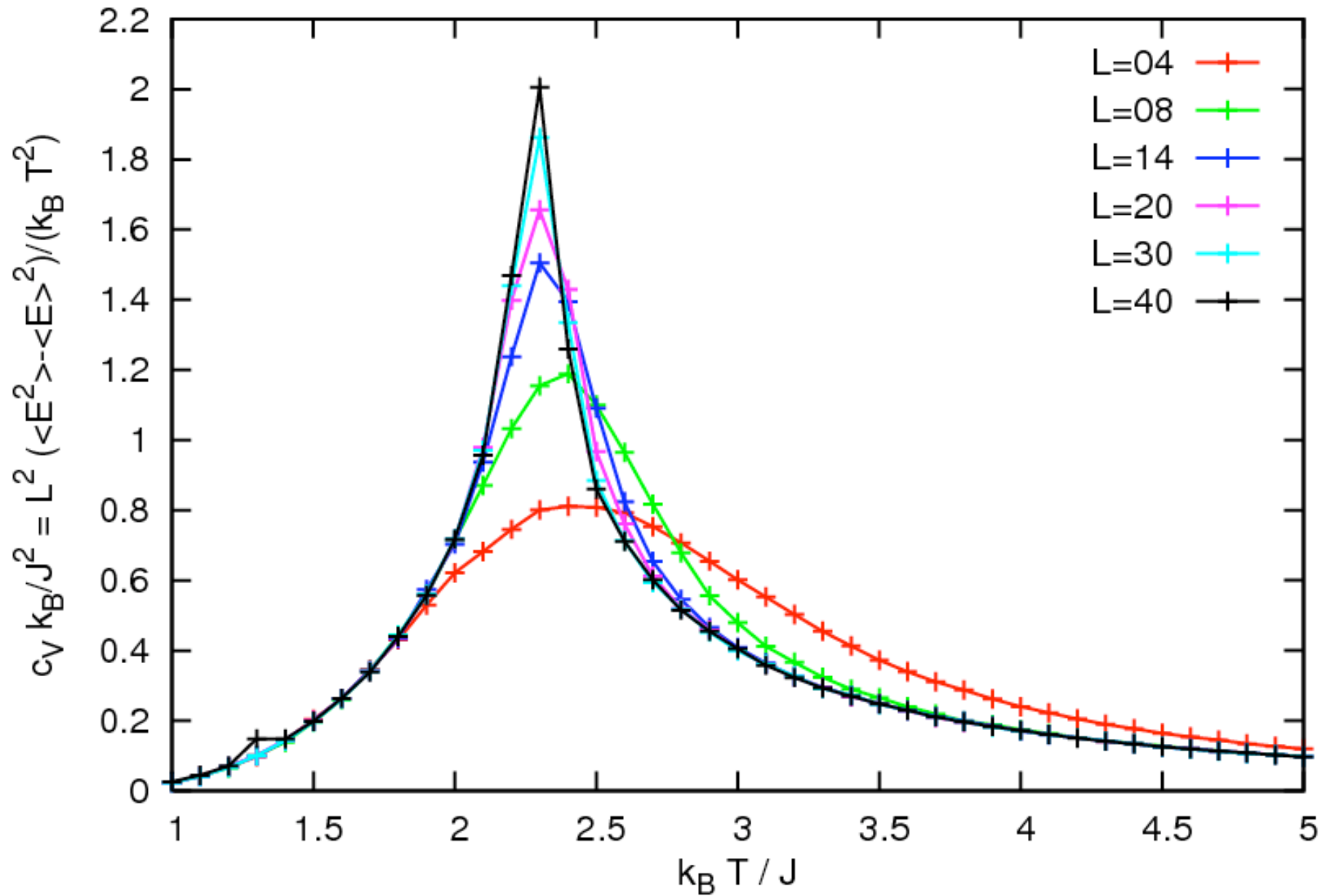
Magnetic susceptibility (10^5 sweeps)



Magnetic susceptibility near T_c (10^6 sweeps)



Specific heat (10^5 sweeps)



Specific heat near T_c (10^6 sweeps)

