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:

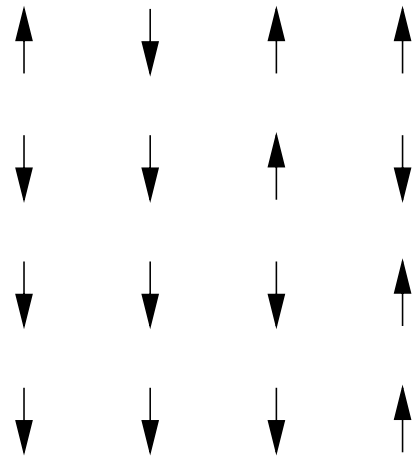- **energy** => Ising model

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

Ising model

the simplest model of interacting spin on a lattice

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

$$s_i = \pm 1$$

(next: 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 $|S, S_z>$ of the Hilbert space in the coupled representation, and a hamiltonian $\mathcal{H} = h_1 + h_2 + V_{12}$:

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

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

We have:

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

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:

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

which is diagonal on the coupled basis, with eigenvalues:

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

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

We have:

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

Heisemberg 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 (Es > Et) ⇈ spins favored => ferromagnetic case

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

Heisemberg hamiltonian

Extension to the case of several spins:

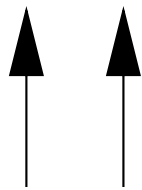$$\mathcal{H}^{spin} = -\sum_{\substack{i,j=1 \\ i \neq j}}^{N} J_{ij} \ \vec{s_i} \cdot \vec{s_j}$$

Ising model

Consider only the possibility : $s_i = \pm 1$ and nearest neighbor interaction only, with the same interaction constant J
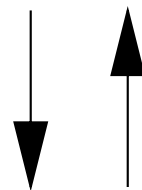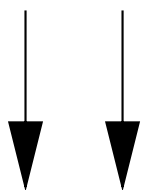
$$\mathcal{H}^{spin} = -J \sum_{i,j=1}^{N} s_i s_j$$

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

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

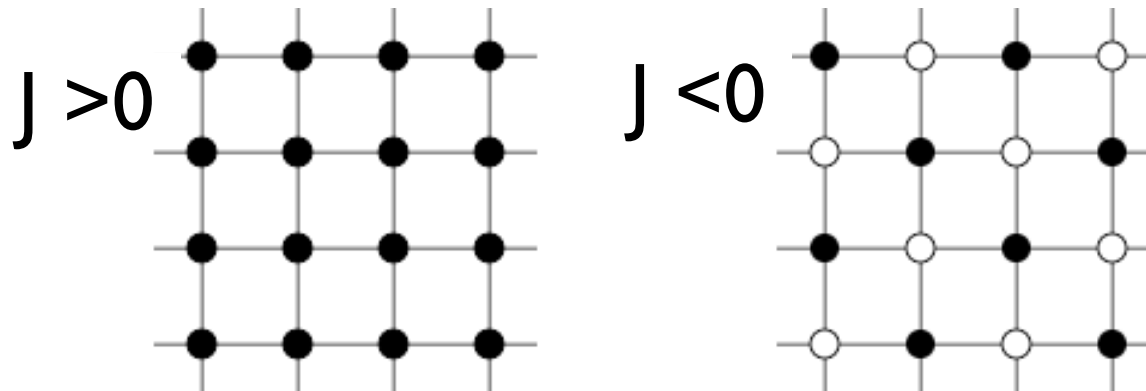E = -J   E = +J
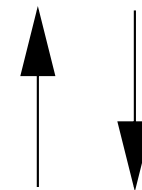
(choosing the kind of interaction, we specify the **energy model**)

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

J >0   J <0

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:

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

(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- 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 $2x2$ 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: 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)
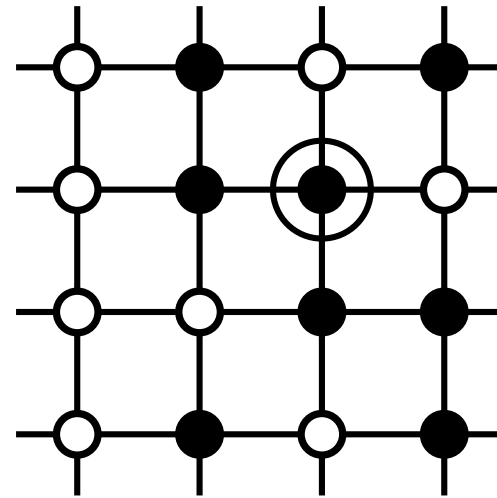
Apply **Metropolis Monte Carlo** method for evolution in the **canonical ensemble** (fix T).
Evolution is driven by the **energy change** between the old and the new configuration, ΔE .
Remark: Is it sufficient to calculate only ΔE , not E at each new configuration!

Ising model: spin flip dynamics
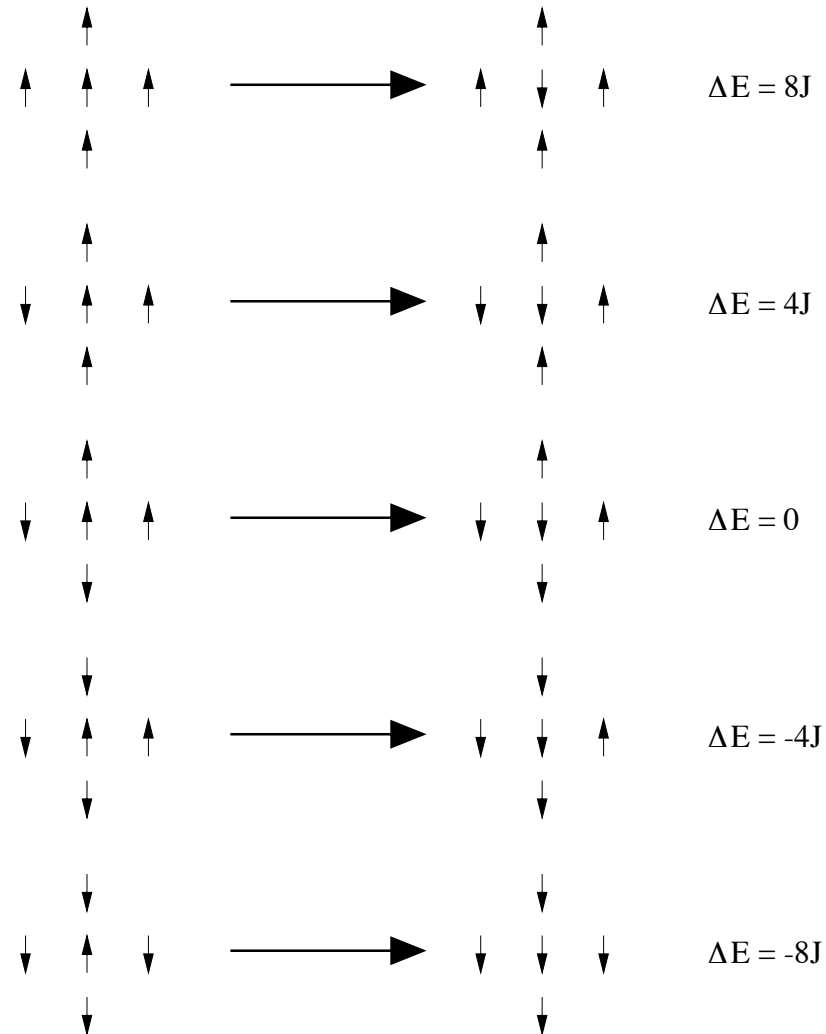
$\Delta E = 8J$

$\Delta E = 4J$

$\Delta E = 0$

$\Delta E = -4J$

$\Delta E = -8J$

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;
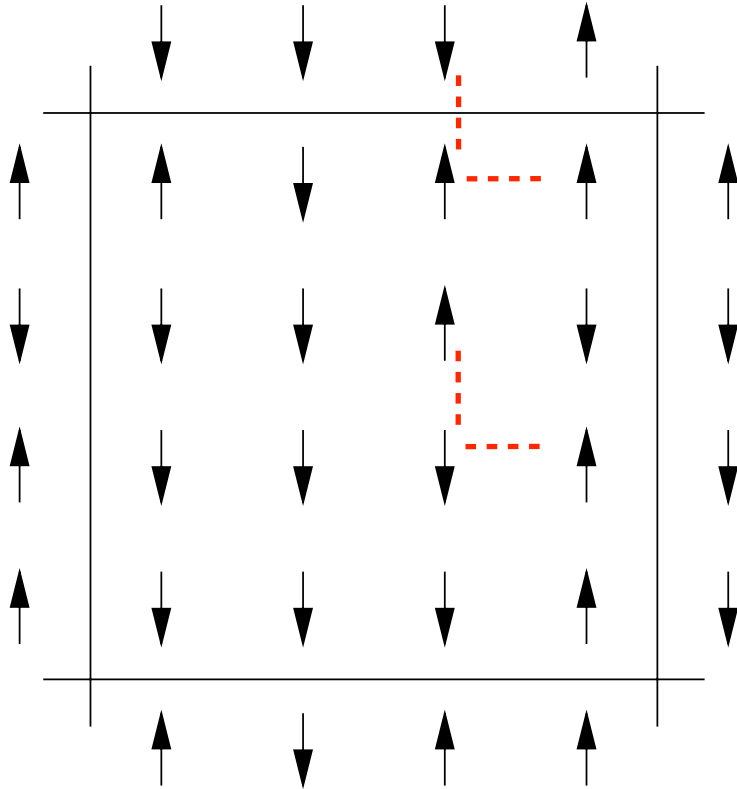for the ferromagnetic g.s. configuration, for instance, the energy is:

$$
\begin{array}{cccc}
 & & + & + & + & + \\
 & + & + & + & & + & + & + & + \\
+ & + & & + & + & + & & + & + & + & + \\
+ & + & & + & + & + & & + & + & + & +
\end{array}
$$

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

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

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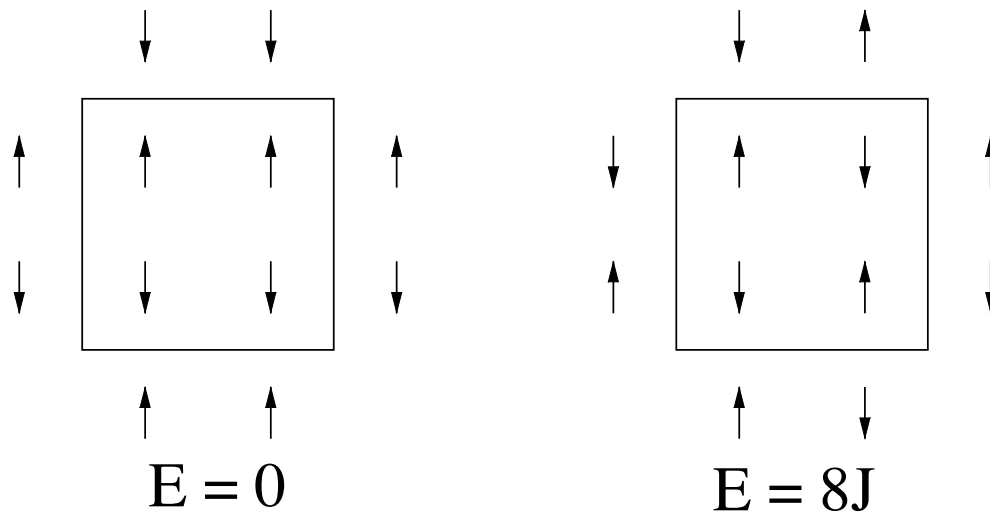
One of the 2^N possible configurations of a system of $N = 16$ Ising spins on a square lattice. with periodic boundary conditions.

Ising model: PBC

We have always:

$2^4 = 16$ spin configurations for *2x2* lattice$_N$

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

$E = 0$ $_N E = 8J$

Two different configurations with 2 spins up

♯ of spins UP	Degeneracy	Energy	Magnetisation
4	1	$-8\,J$	4
3	4	0	2
2	4	0	0
2	2	$8\,J$	0
1	4	0	-2
0	1	$-8\,J$	-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
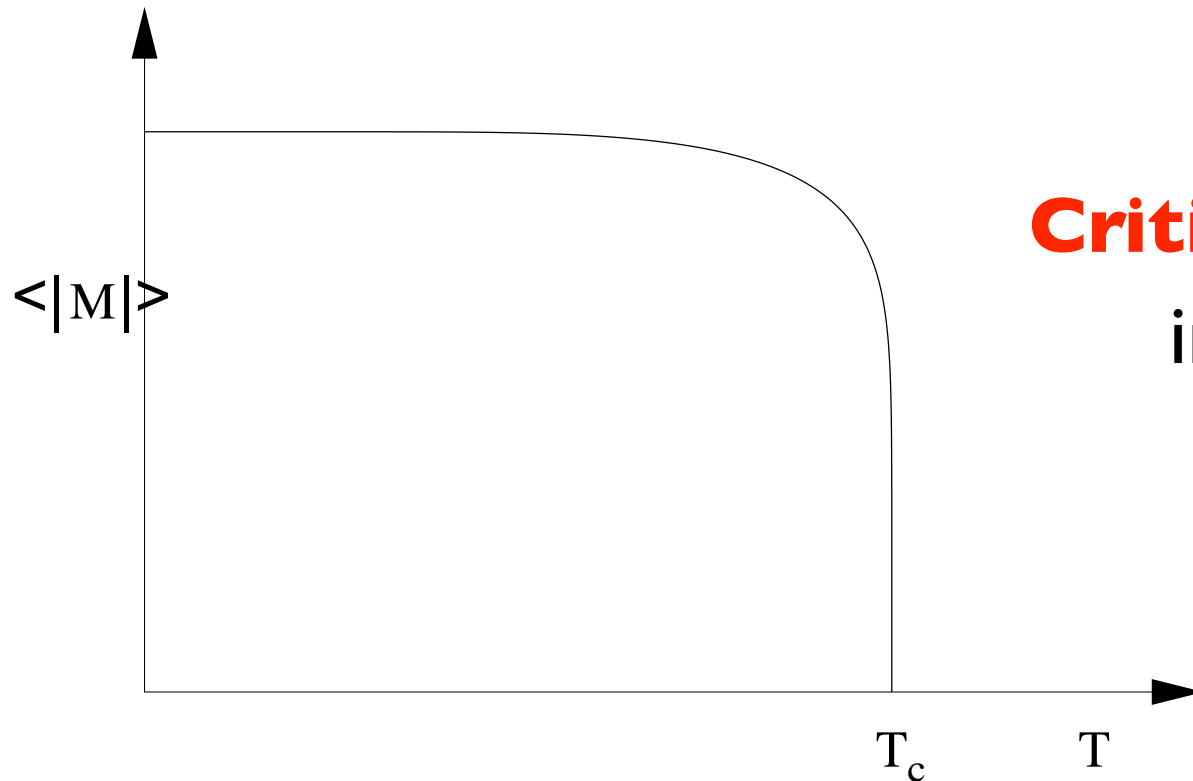
Ising model: phase transition

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)

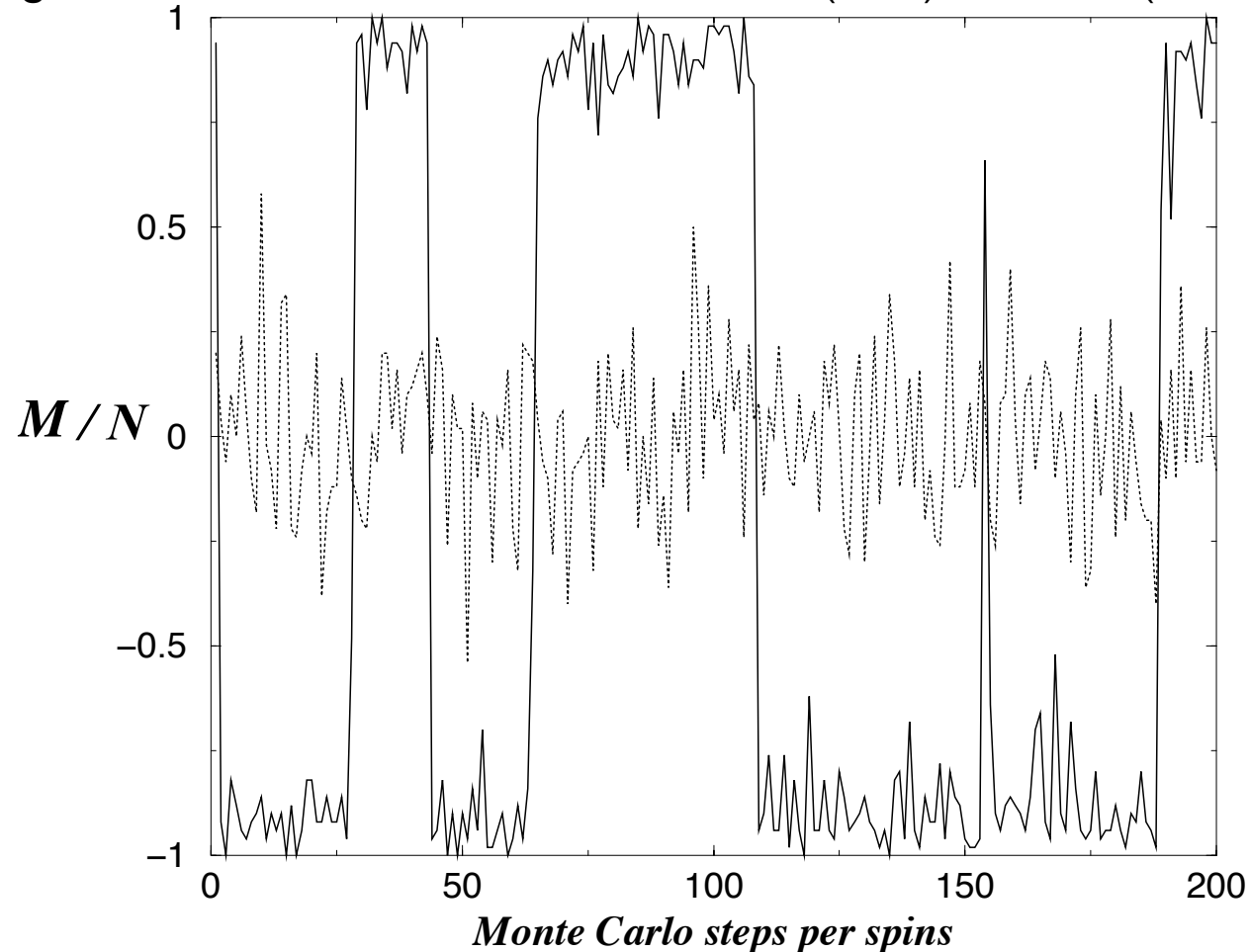**existence of a**
Critical temperature Tc

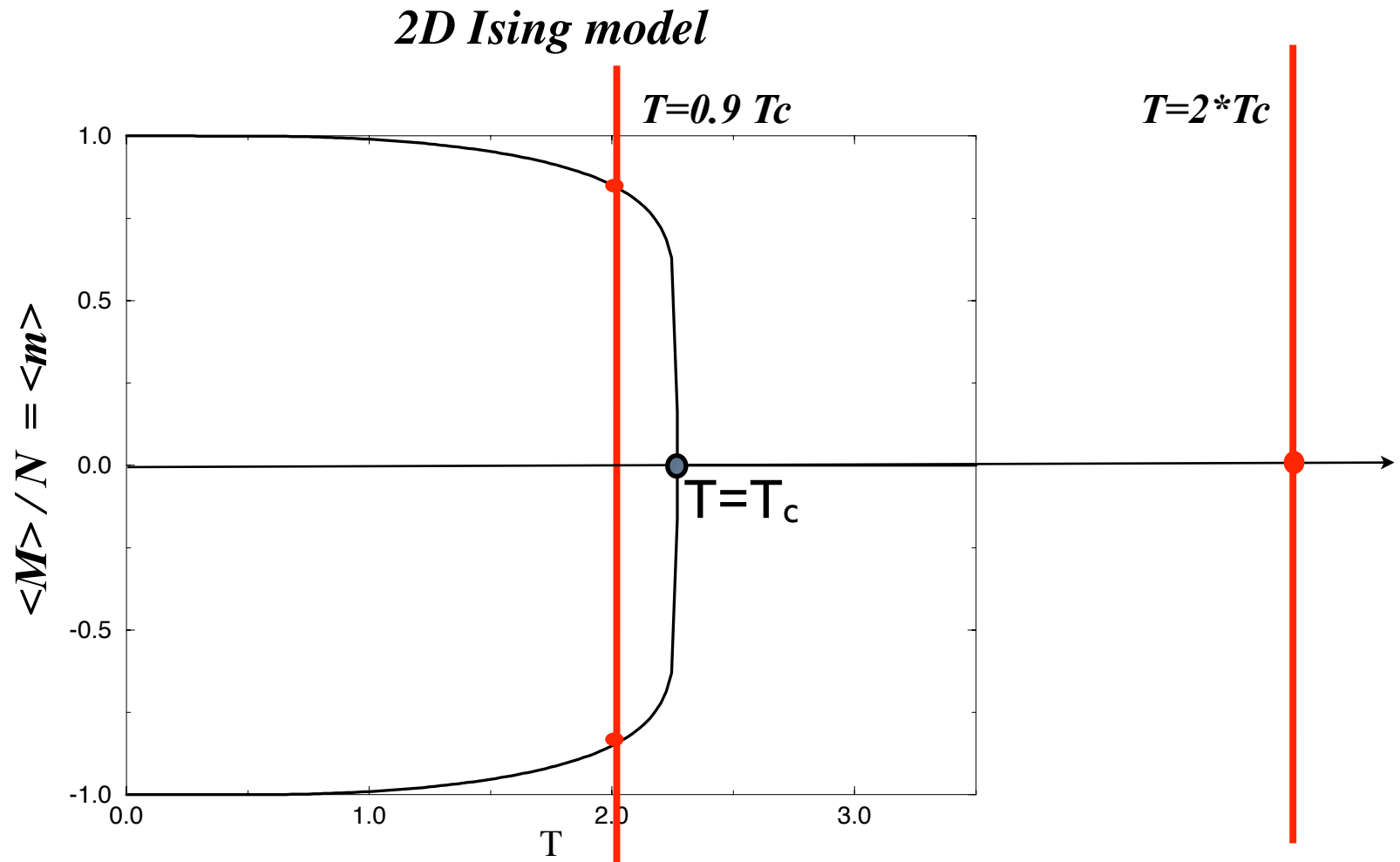in 2D the model has an analytical solution:

$T_c = 2.269 \, J/k_B$

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

*Magnetization (System : 10*10)*
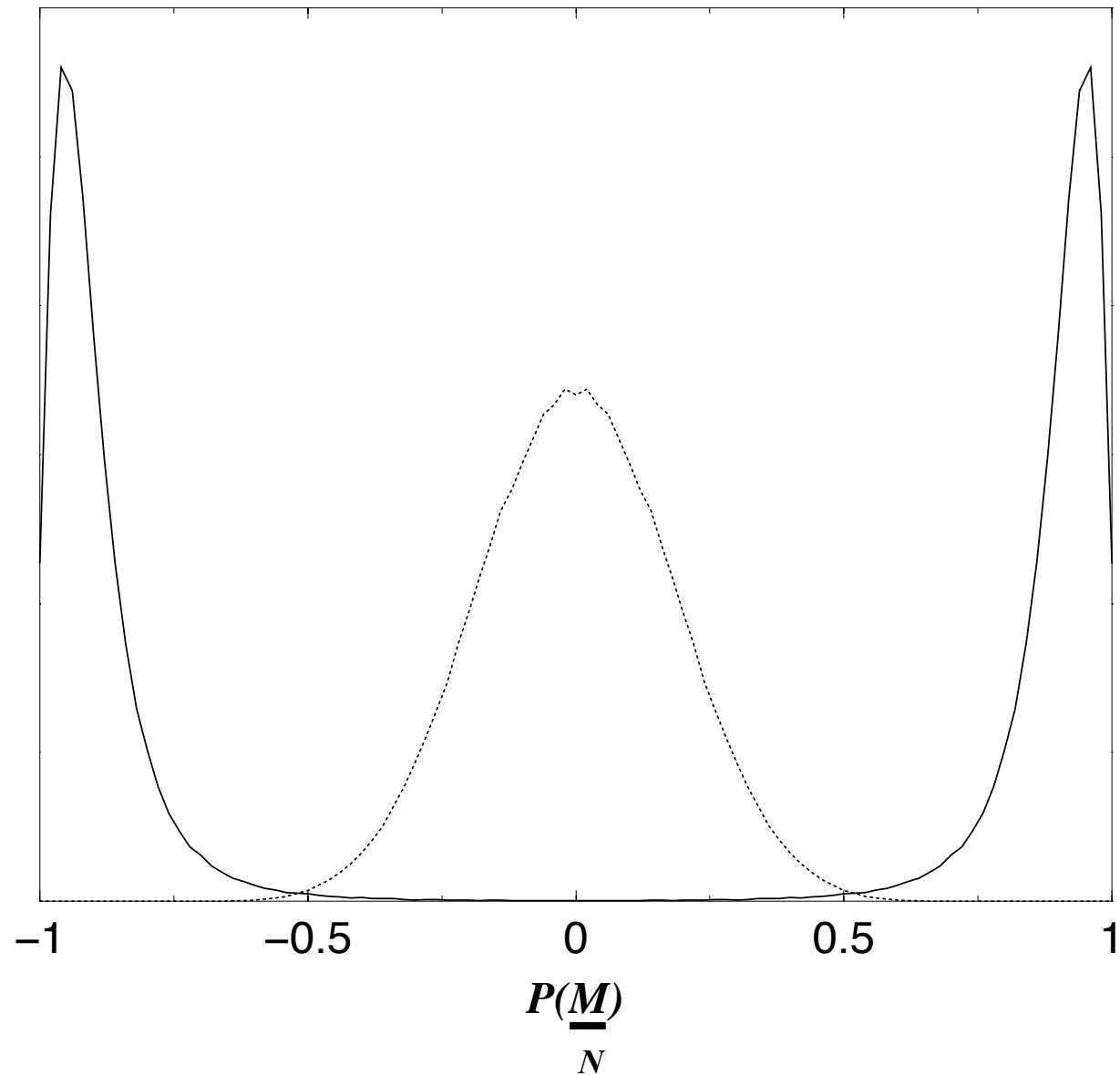Magnetization as a function of time for T<T_c (solid) and T>T_c (dashed curve)

Fluctuations! do, as usual, temporal averages: <M>/N, <E>/N

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)

$$\frac{P(\underline{M})}{N}$$

(data collected during time evolution, at equilibrium)

Ising model: phase transition

T_c also for energy, not only for magnetization:

$$E = -J \sum_{i,j=\mathrm{nn}(i)}^{N} s_i s_j$$
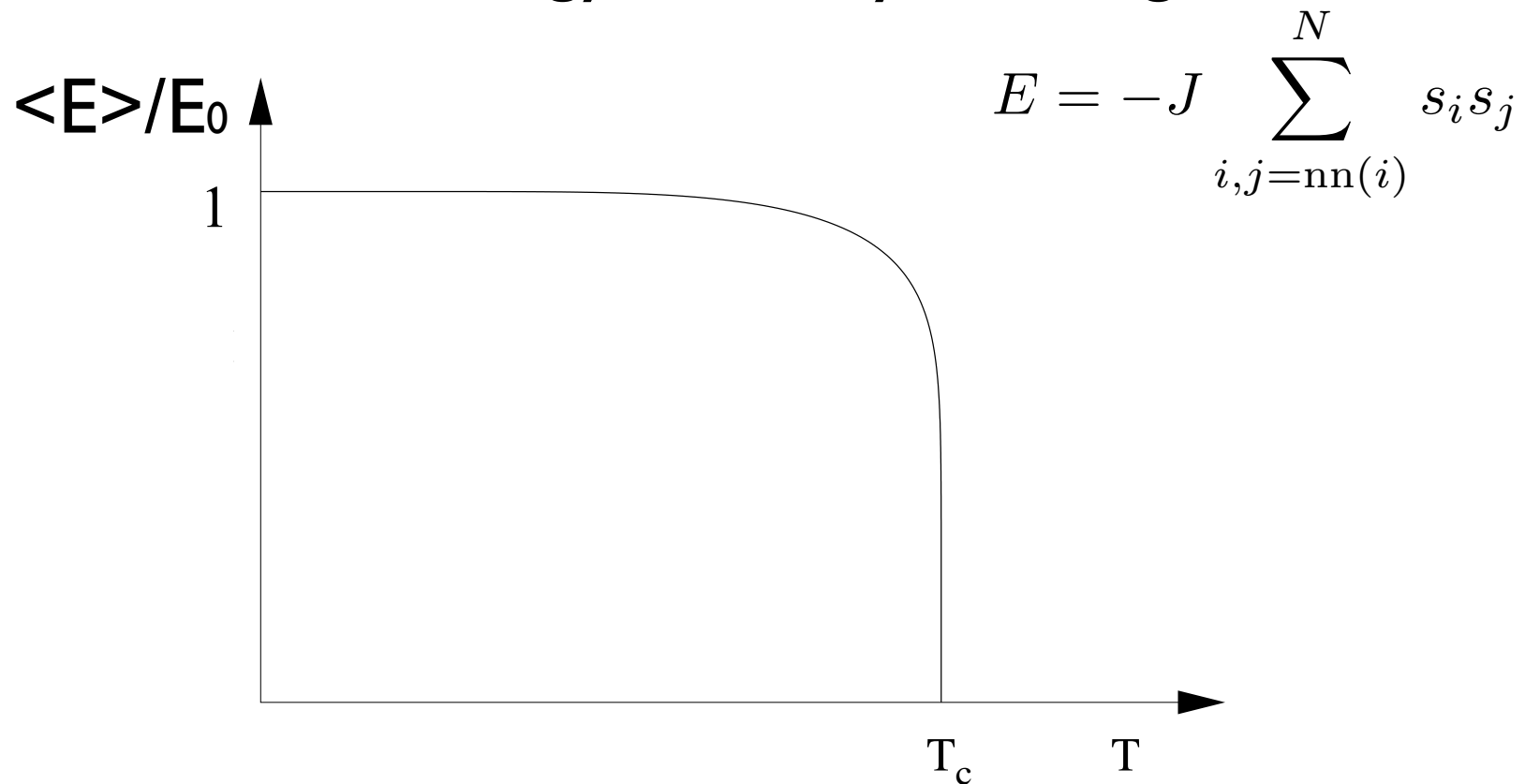
and also the energy fluctuates during time evolution...

Ising model: fluctuations

Fluctuations are intrinsic to the system evolution
and are important!
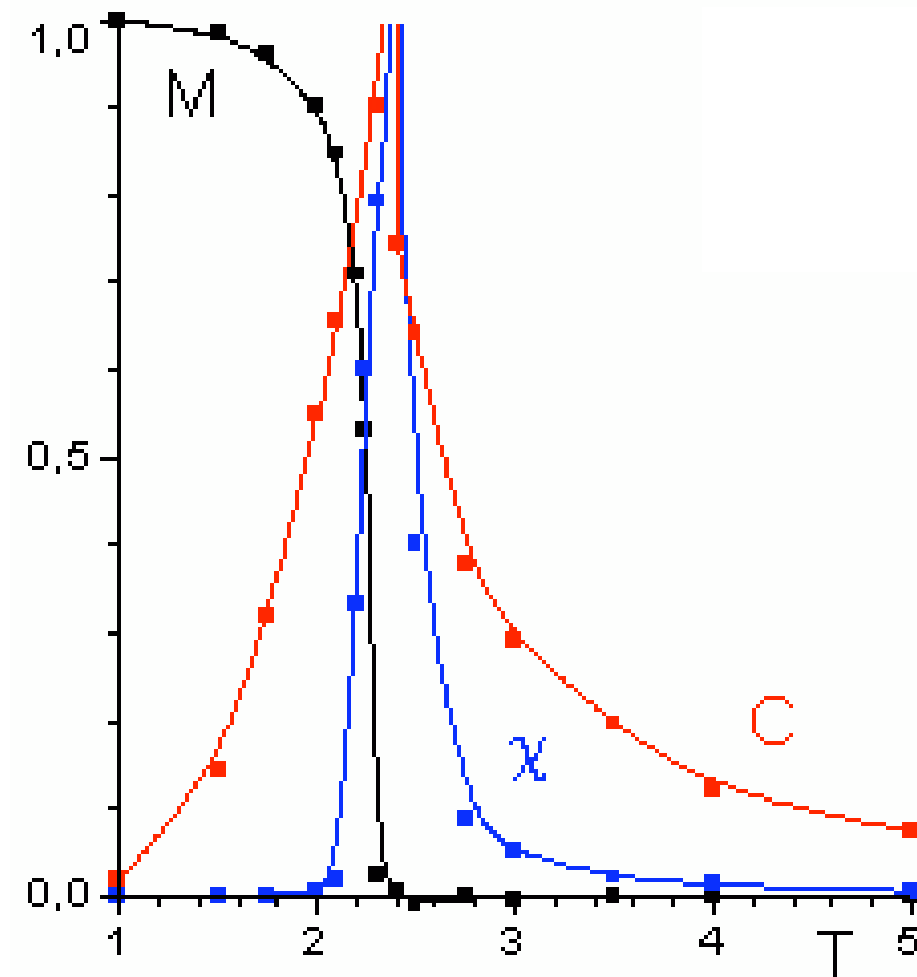Linear response functions are related to
equilibrium fluctuations:

(already proved): $\quad C = \dfrac{\partial \langle E \rangle}{\partial T} \; , \; C = \dfrac{1}{kT^2}\left(\langle E^2 \rangle - \langle E \rangle^2\right)$

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

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

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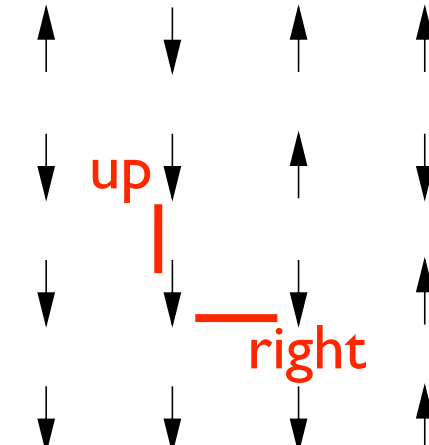
$$m = \frac{M}{N} = \frac{1}{N} \sum_{i=1}^{N} s_i$$

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

(Instead of the loop over x,y, 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
```
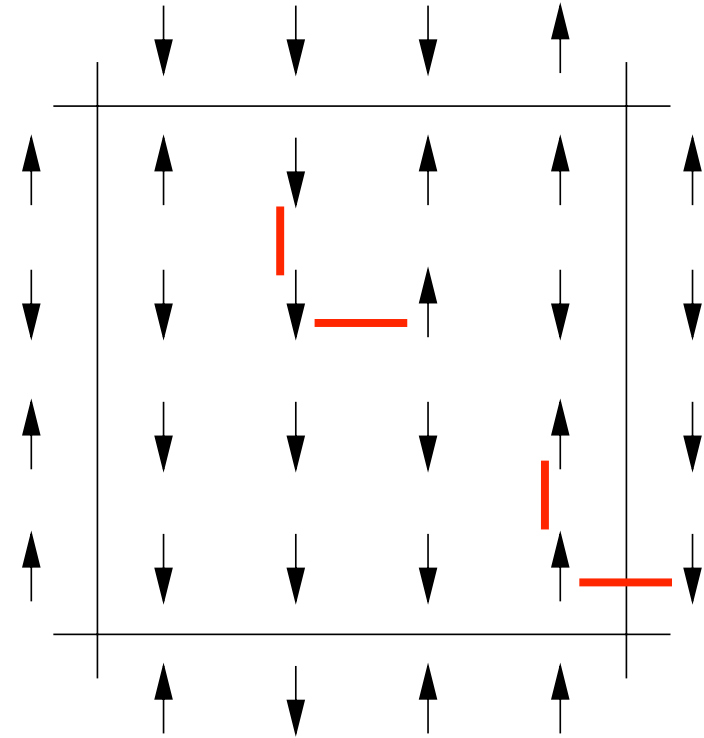
Ising model: energy with PBC

```
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
! (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)              ←——— energy variation for spin(x,y) flip
call random_number(rnd)
if (rnd <= w(dE)) then        ←——— w(dE) is e^{-ΔE/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)
.....
```

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

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)
.....
```
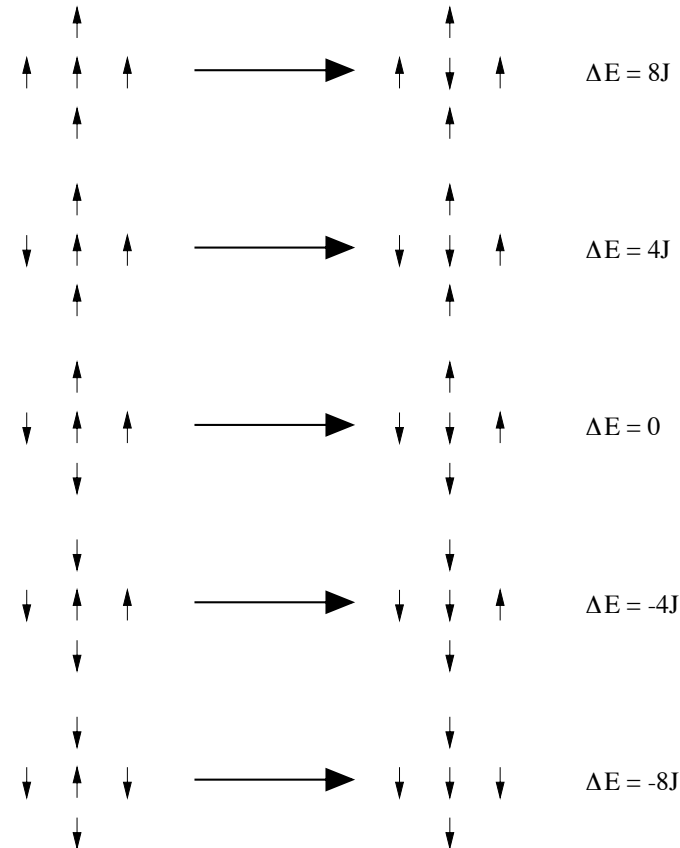
$y = L$

$y = 1$

$x = 1$

$x = L$
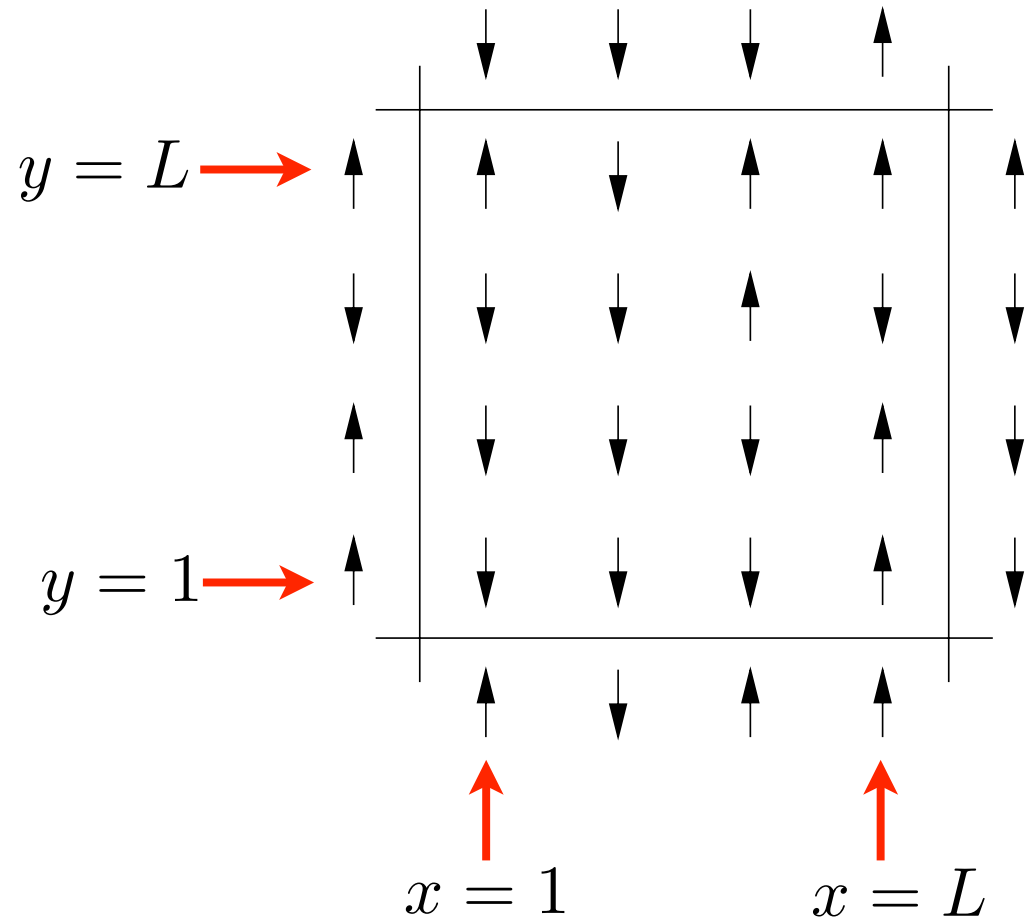
Ising model: storage of Boltzmann's coeff.

```
! 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

$\Delta E = 8J$

$\Delta E = 4J$

$\Delta E = 0$

$\Delta E = -4J$

$\Delta E = -8J$

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

Ising model:
updating energy and magnetization

```fortran
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
    .....
```

$$1 \leq x \leq L$$

$$1 \leq y \leq L$$

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?

```fortran
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:

```fortran
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:

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

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

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

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

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

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. 1 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!

$L = 8$ and $L = 16$
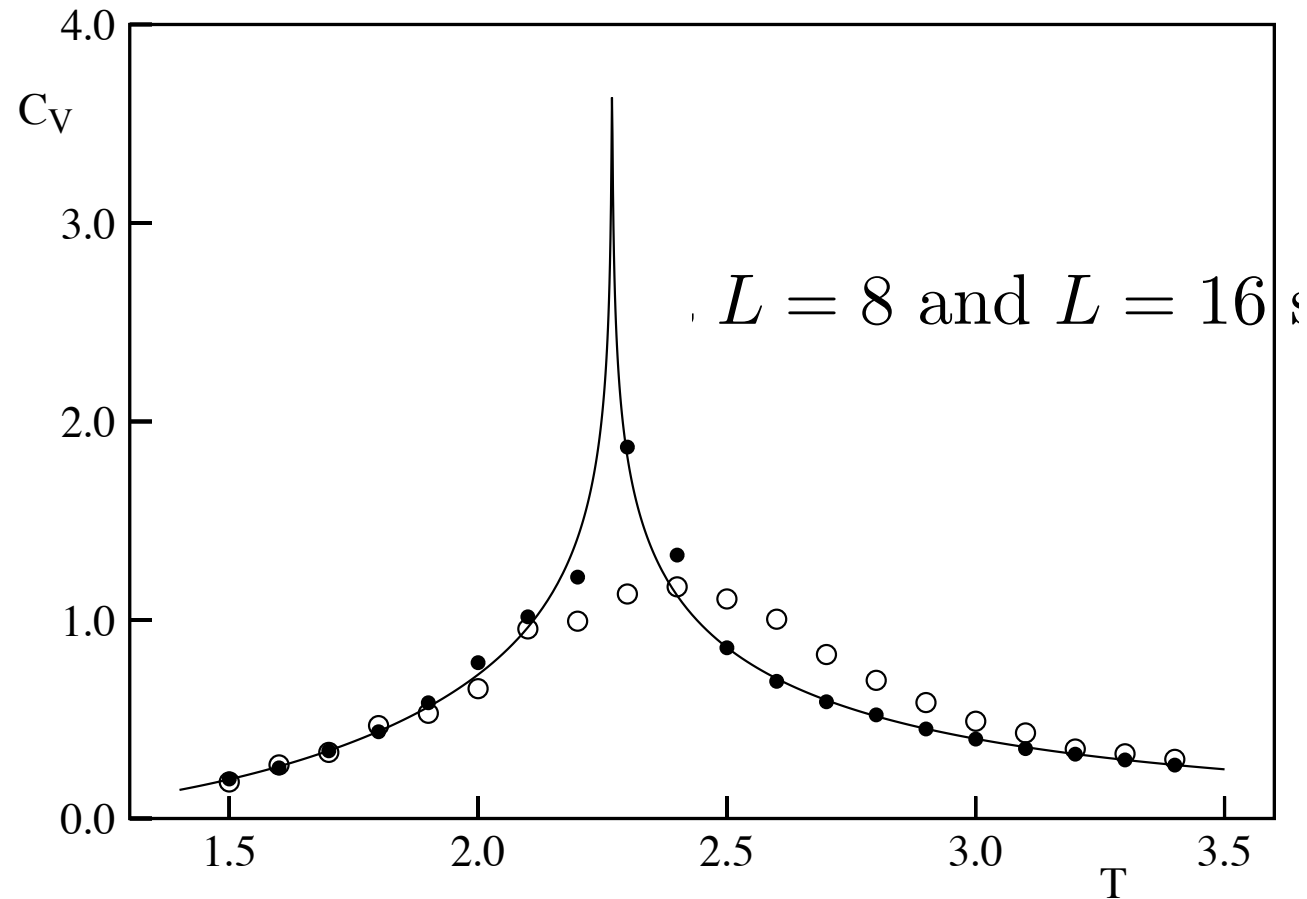
The temperature dependence of the specific heat C (per spin) of the Ising model

Ising model: size problems

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

L=2   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 ("surface") term proportional to 1/L
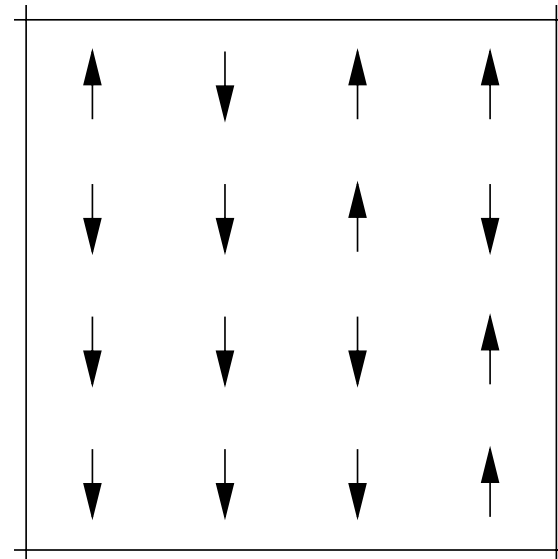
Ising model: alternative dynamics

- 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
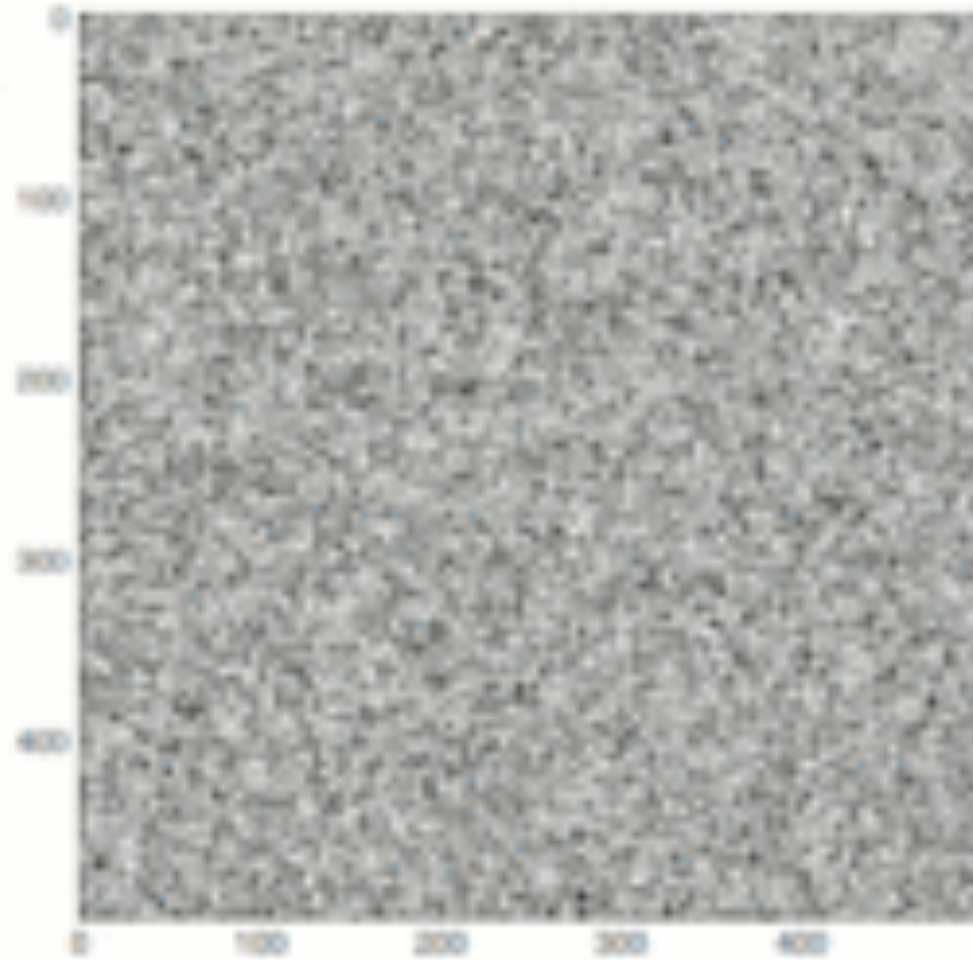
T=10, starting from random configuration

Ising model:
other generalizations

- SPINS: XY, Heisenberg, Potts...

- LATTICES: Square, Triangle, Cubic,
  Honeycomb, Kagome....

- INTERACTIONS: Magn. Field, Antiferrom.,
  Next Nearest Neighbor (NNN)....

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 spin=±1 randomly. Calculating and plotting the energy < E >/N and the magnetization < M >/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 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
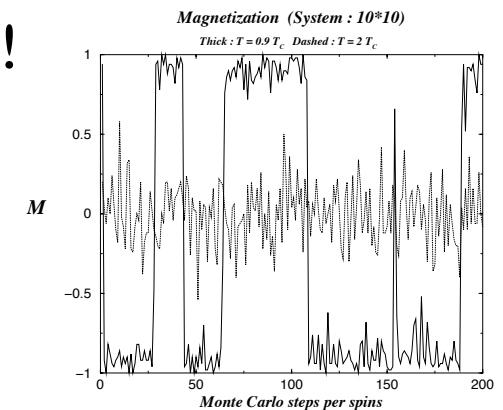
Then, set *nequil* not zero and calculate the time average < E >/N and < M >/N; increasing the total *nmcs*, the two quantities should converge…

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:
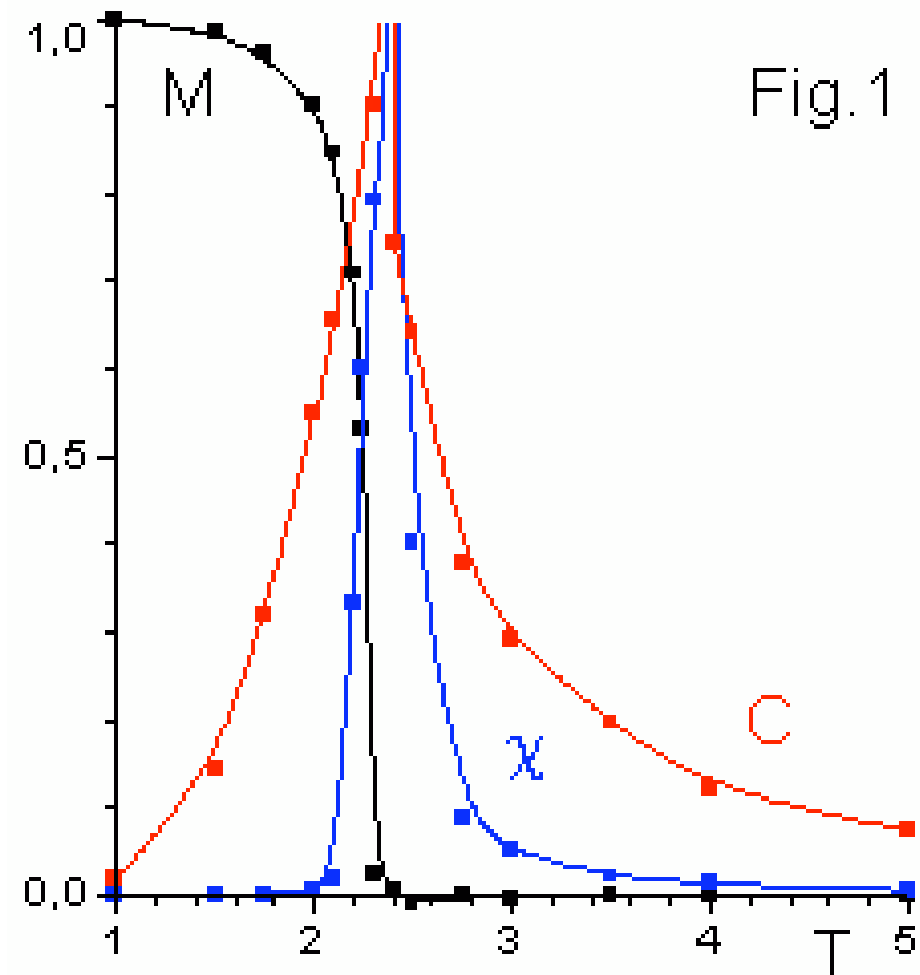

Calculate also c and χ.

Exercise

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

Calculate also c and χ.

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

Fig.1

Raw data: traces, covariance and autocorrelation time

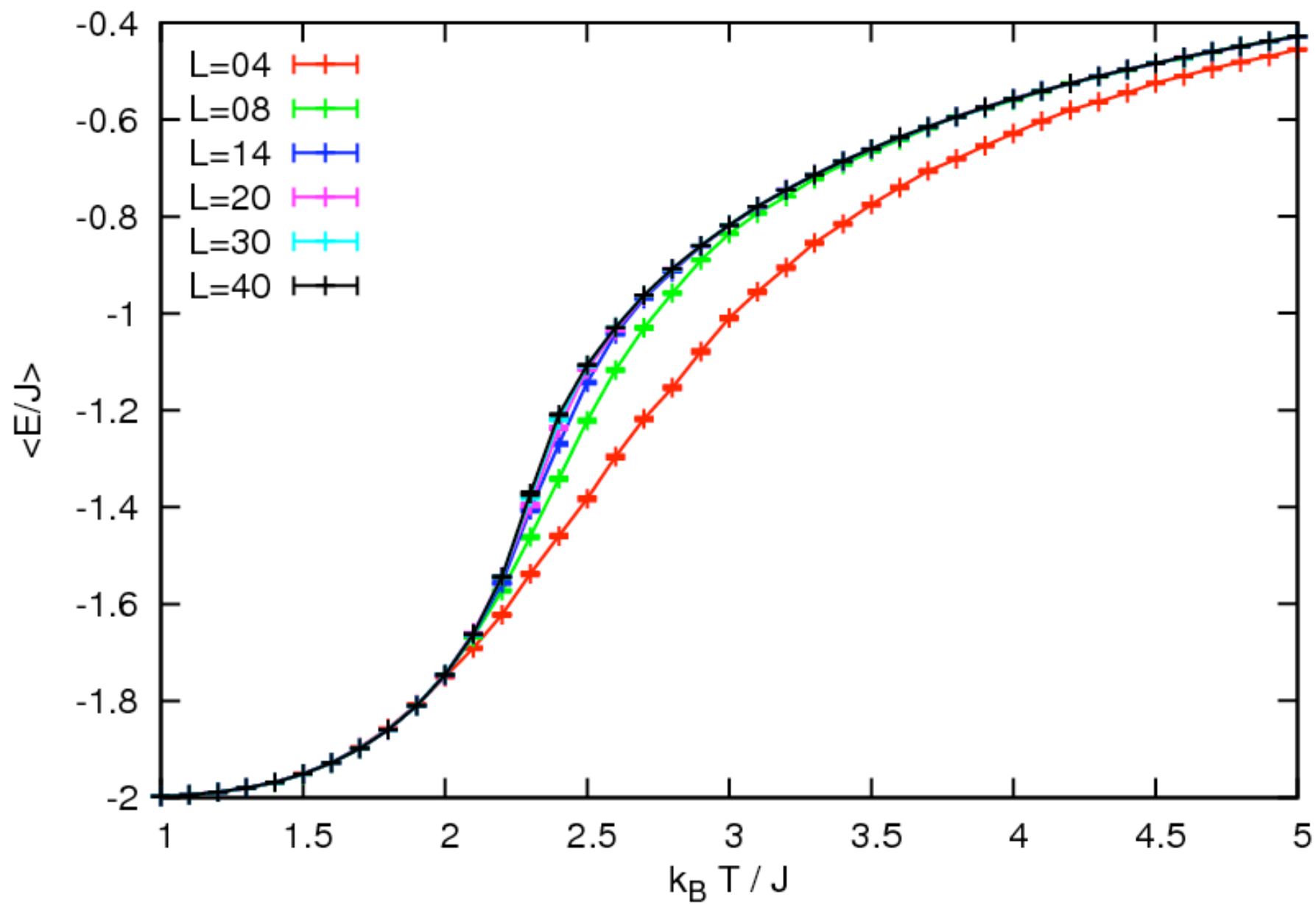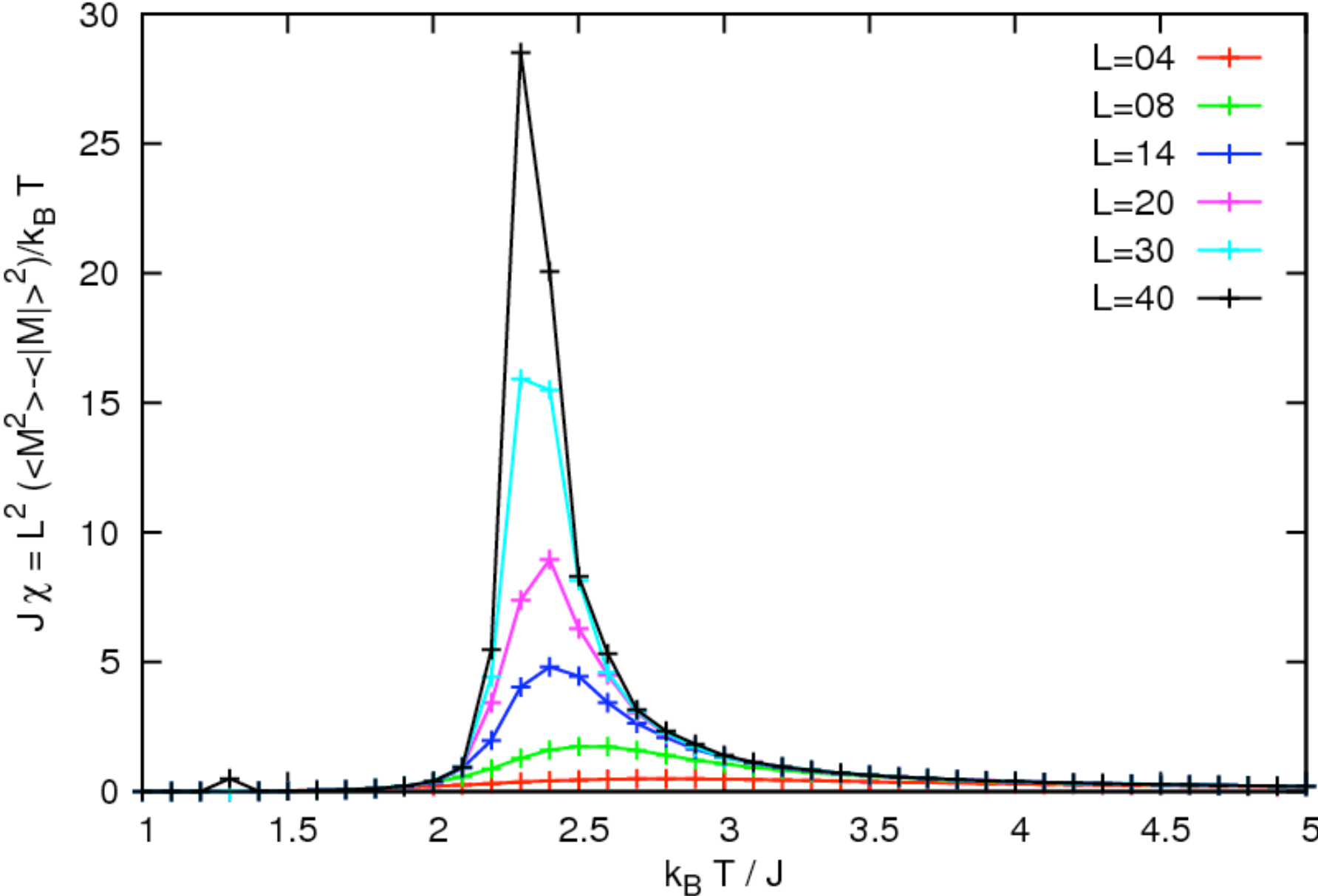**Trace: magnetization for $T = 2.27 J/k_B \approx T_C$ $\left(10^5 \text{ sweeps}\right)$**
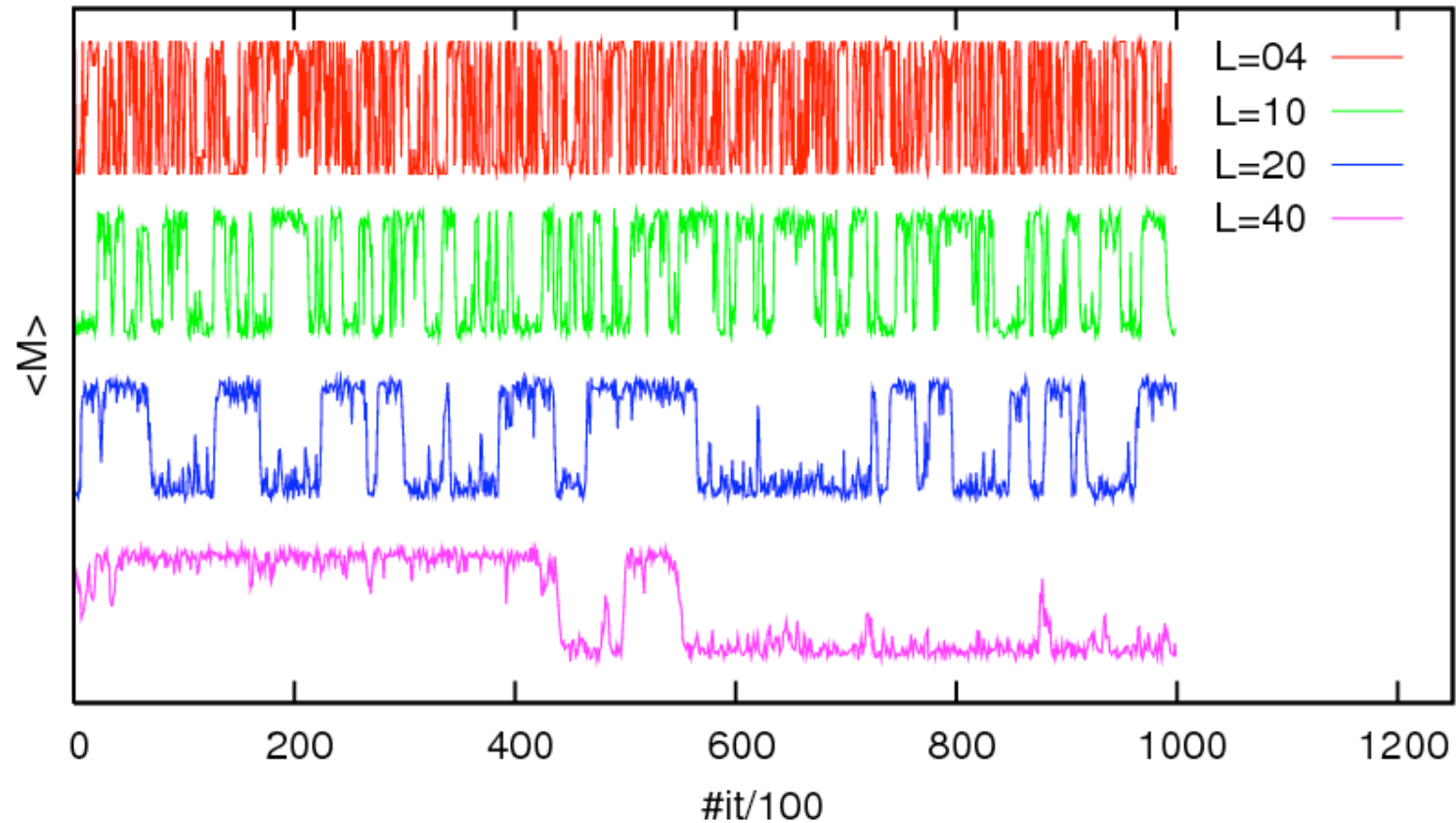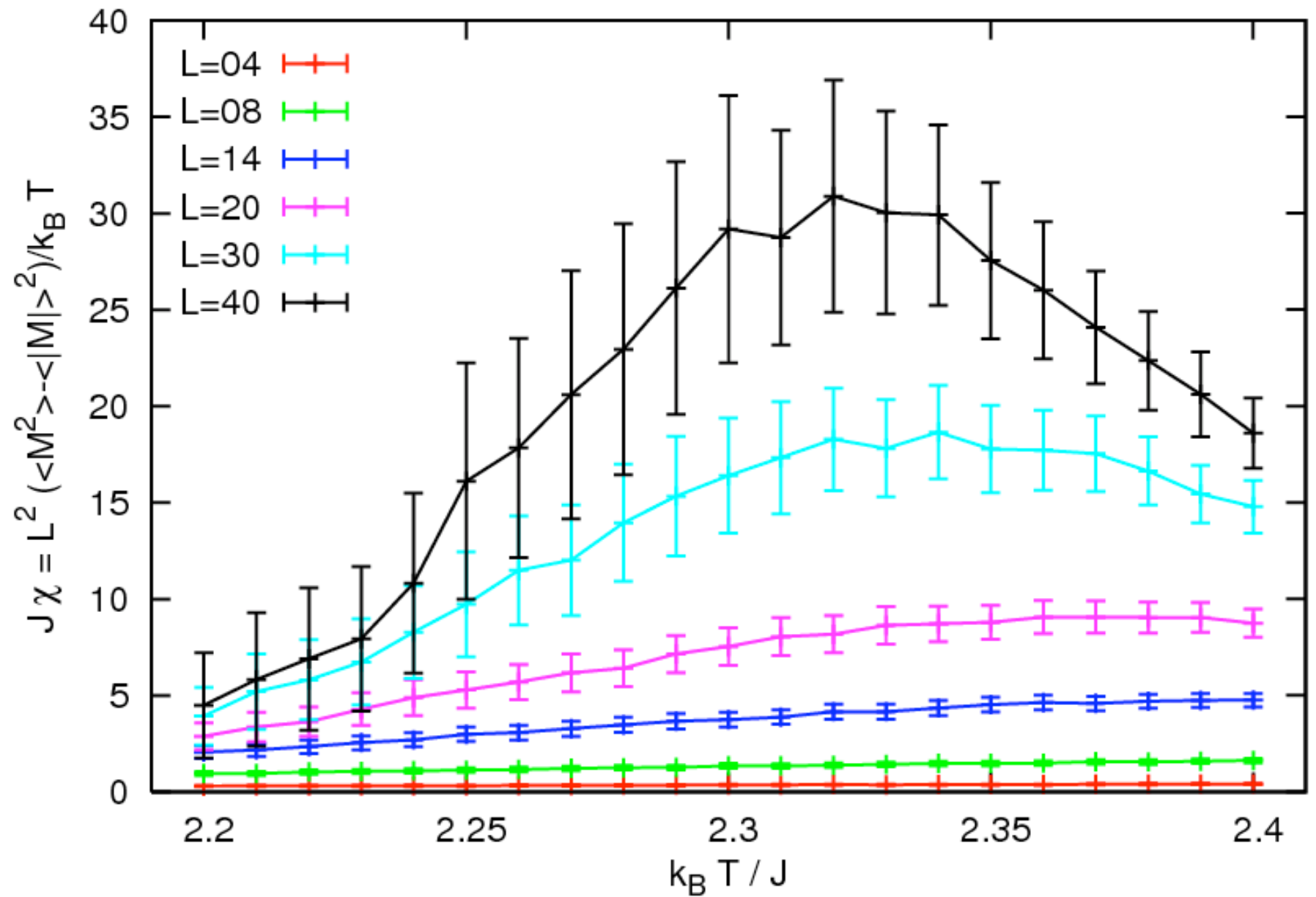
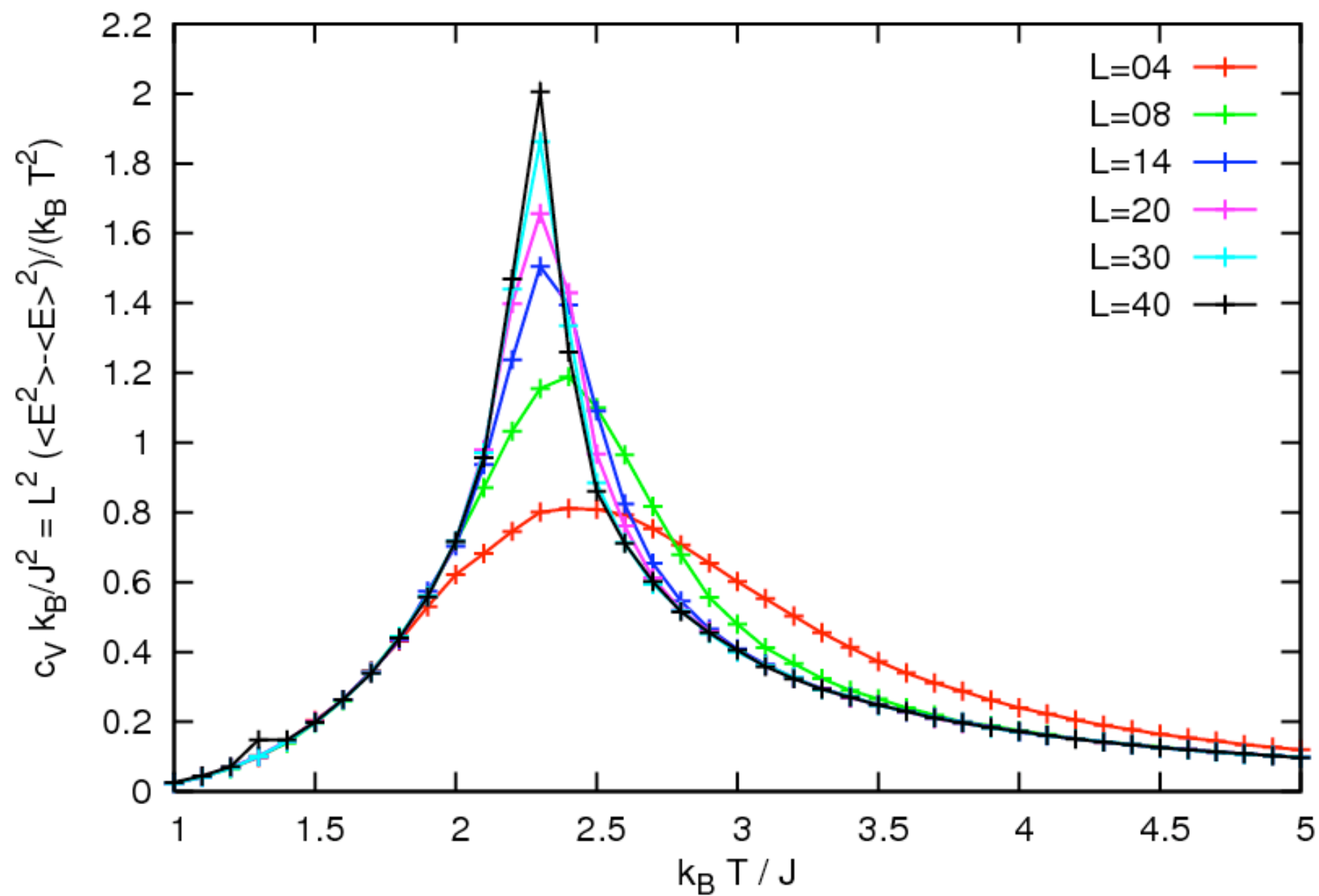**Magnetization (10^5 sweeps)**
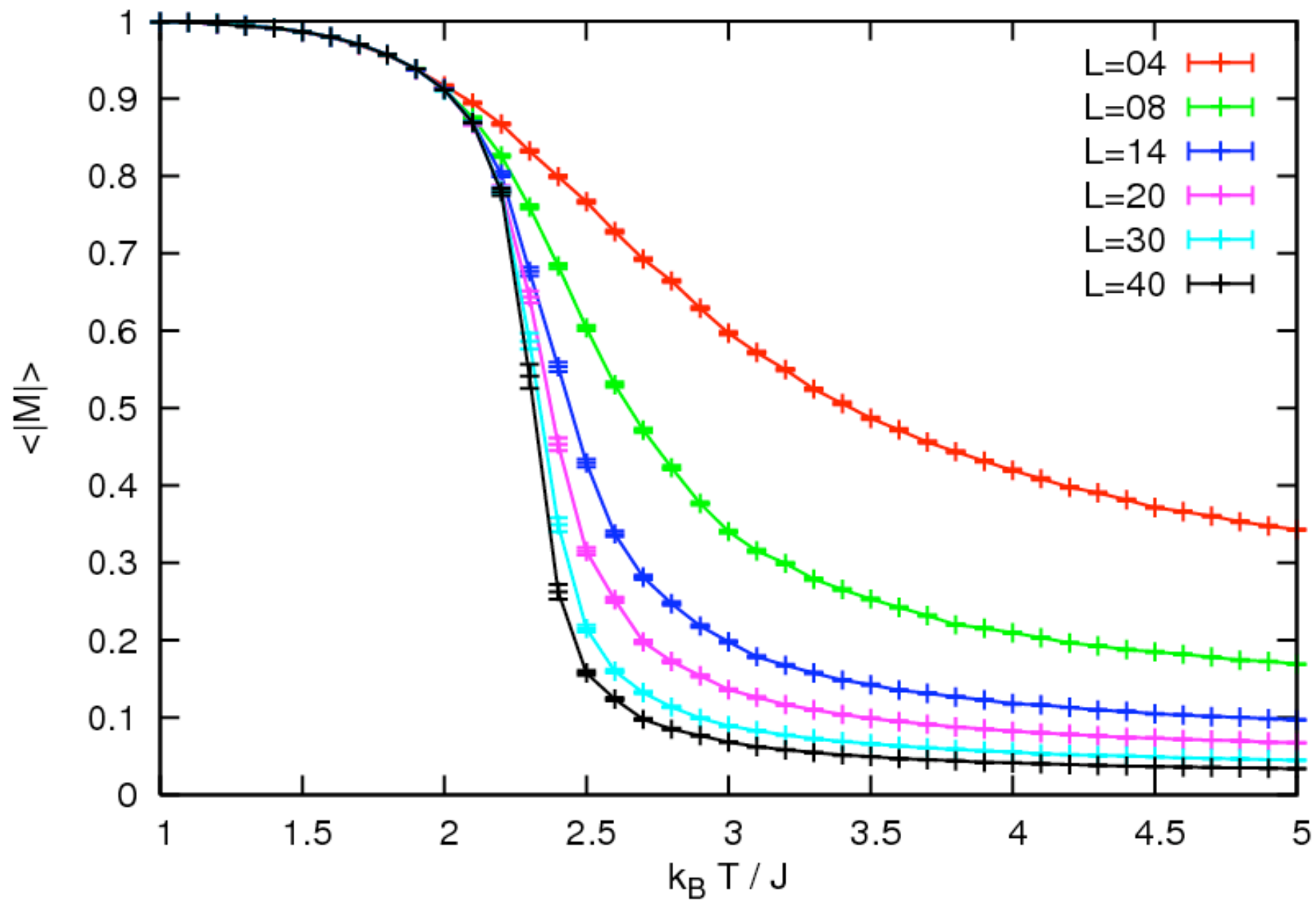
Energy (10^5 sweeps)

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)