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

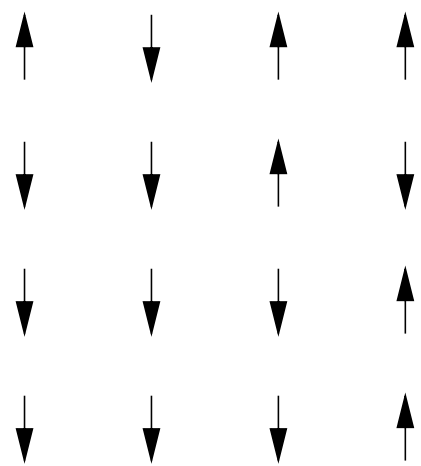
- **evolution**
  (to build the trajectory / the Markov chain)

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:

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

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:

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

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:

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

(see also: Ashcroft & Mermin, chap. 32,
"Spin hamiltonian and Heisemberg 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

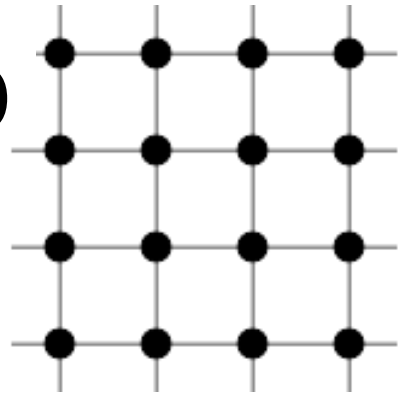
(choosing the kind of interaction, we specify the **energy model**)

Ising model on a lattice

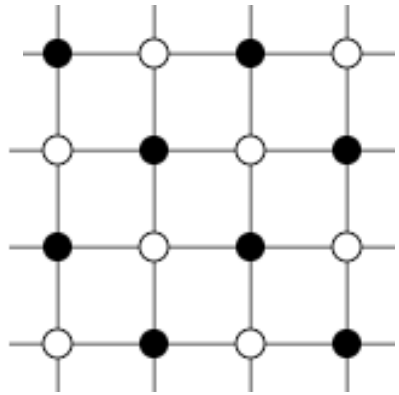
lattice containing N sites

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- average magnetization per spin:

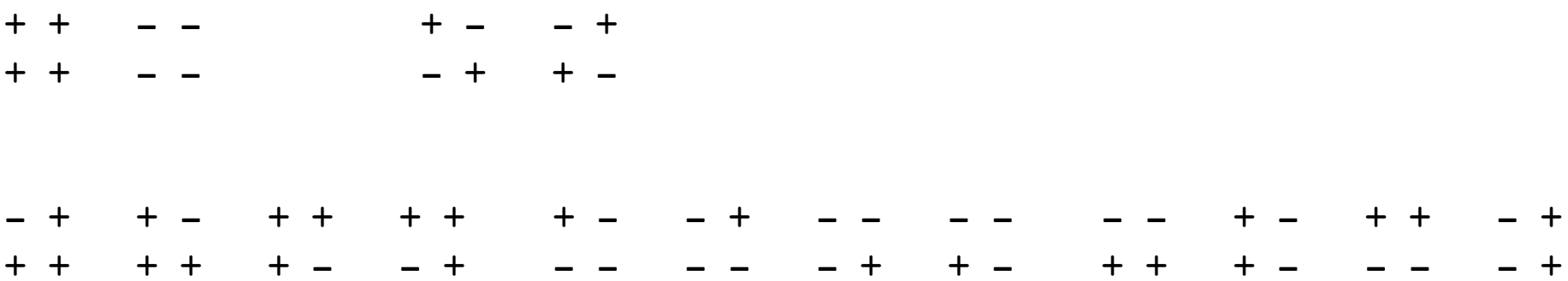
$$m = \frac{M}{N} = \frac{1}{N} \sum_{i=1}^{N} s_i$$

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

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:

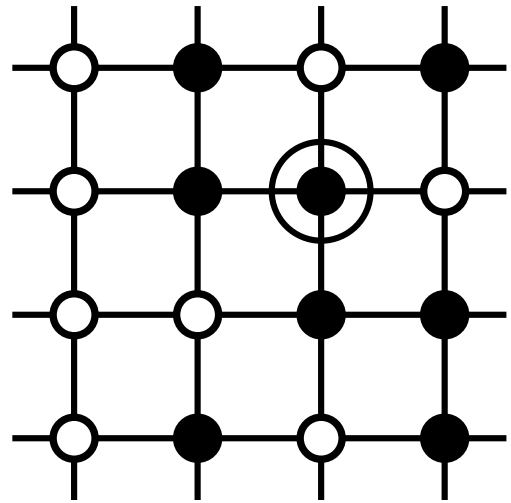
$$E_0/N = -\ 2J$$

Ising model: 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)

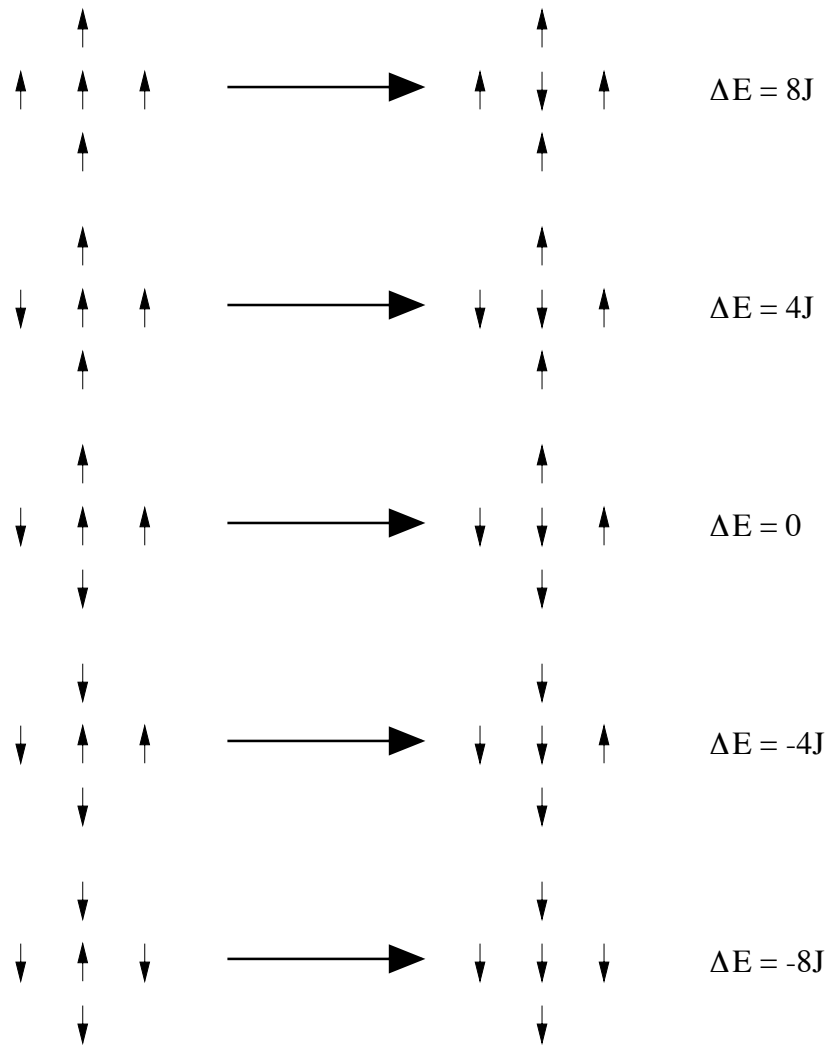


Apply **Metropolis Monte Carlo** method for evolution in the **canonical ensemble** (fix T).

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

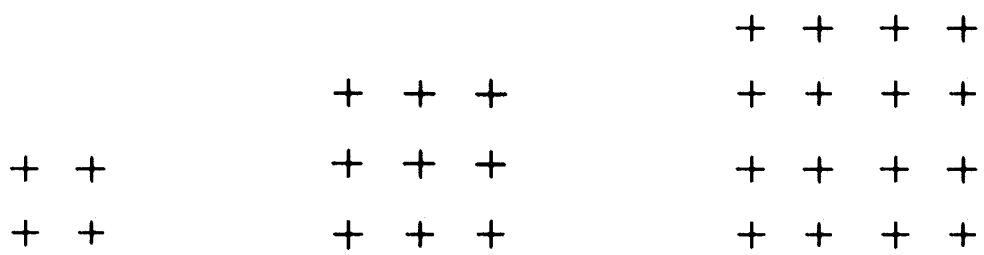
Ising model: boundary conditions

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



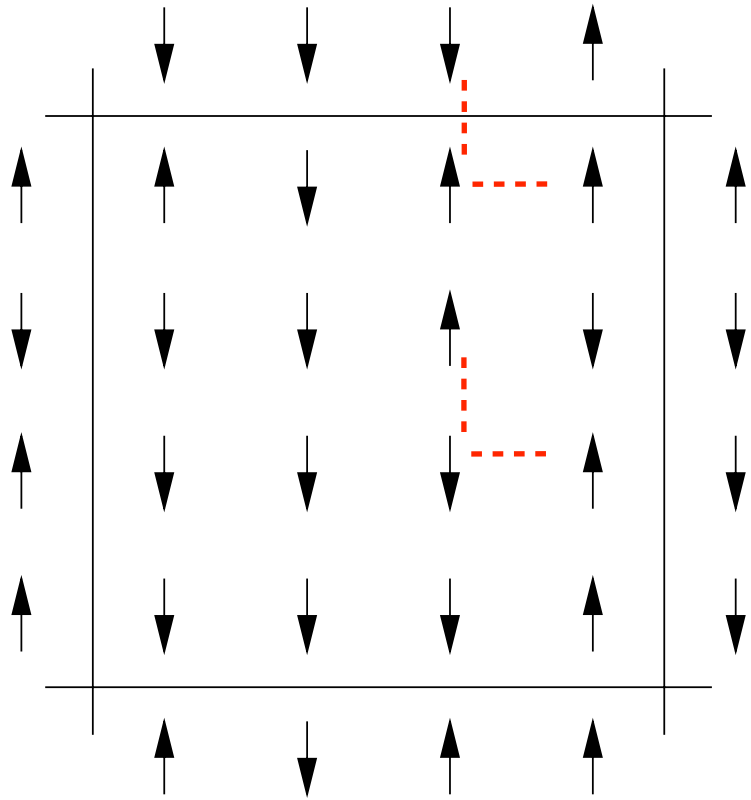
$E_0/N=-J$ $E_0/N=-(12/9)J$ $E_0/N=-(24/16)J$ ...

$$E_0/N = -J \times 2L(L-1)/L^2$$
$$= -2J \times (1-1/L)$$

(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.

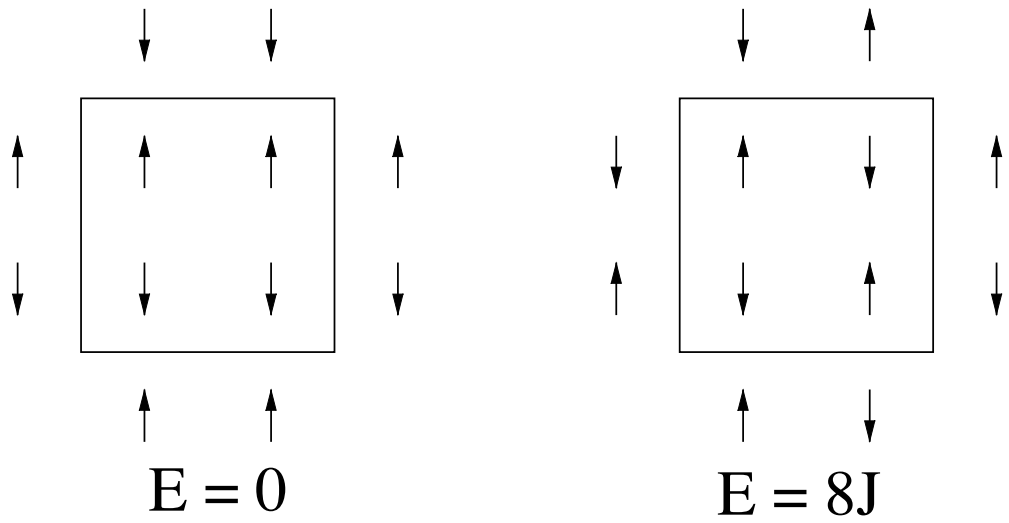
with periodic boundary conditions.

Ising model: PBC

We have always:

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

but the energy for each configuration in case of 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

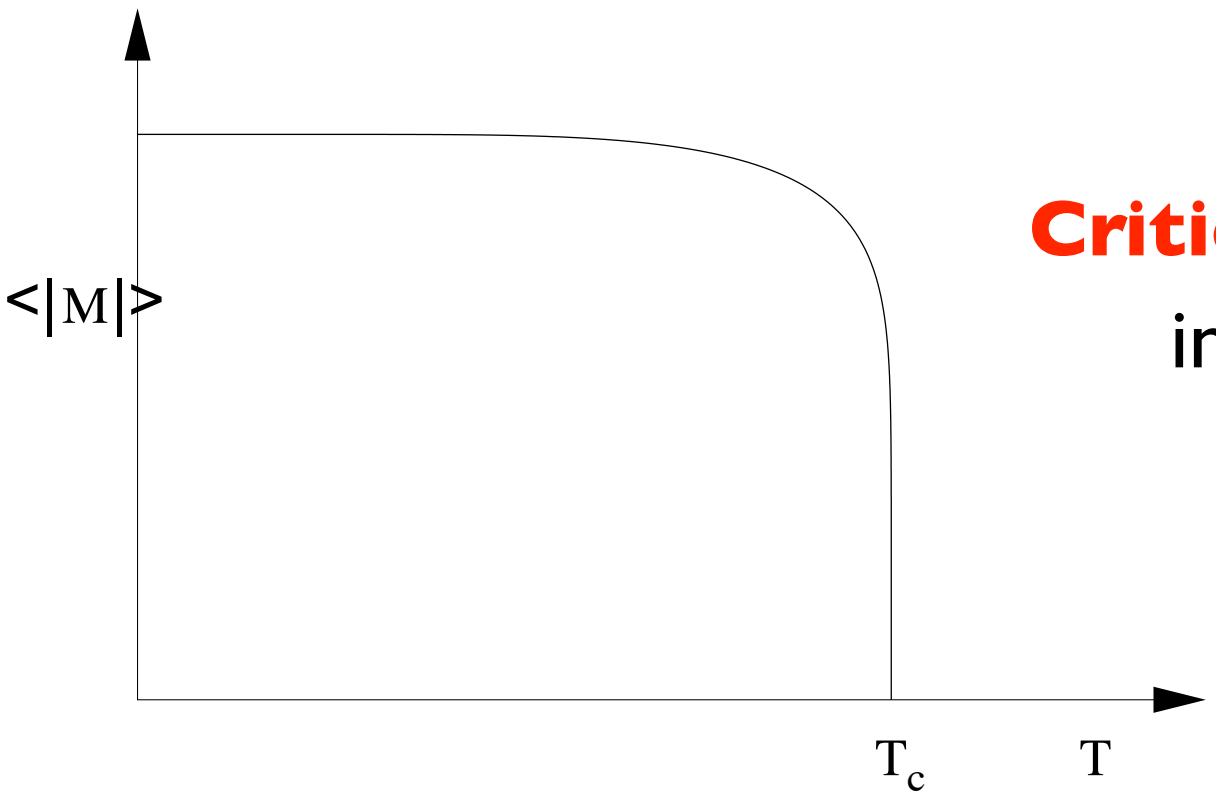
Energy and magnetization of 16 configurations of the 2×2 Ising model with PBC

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)

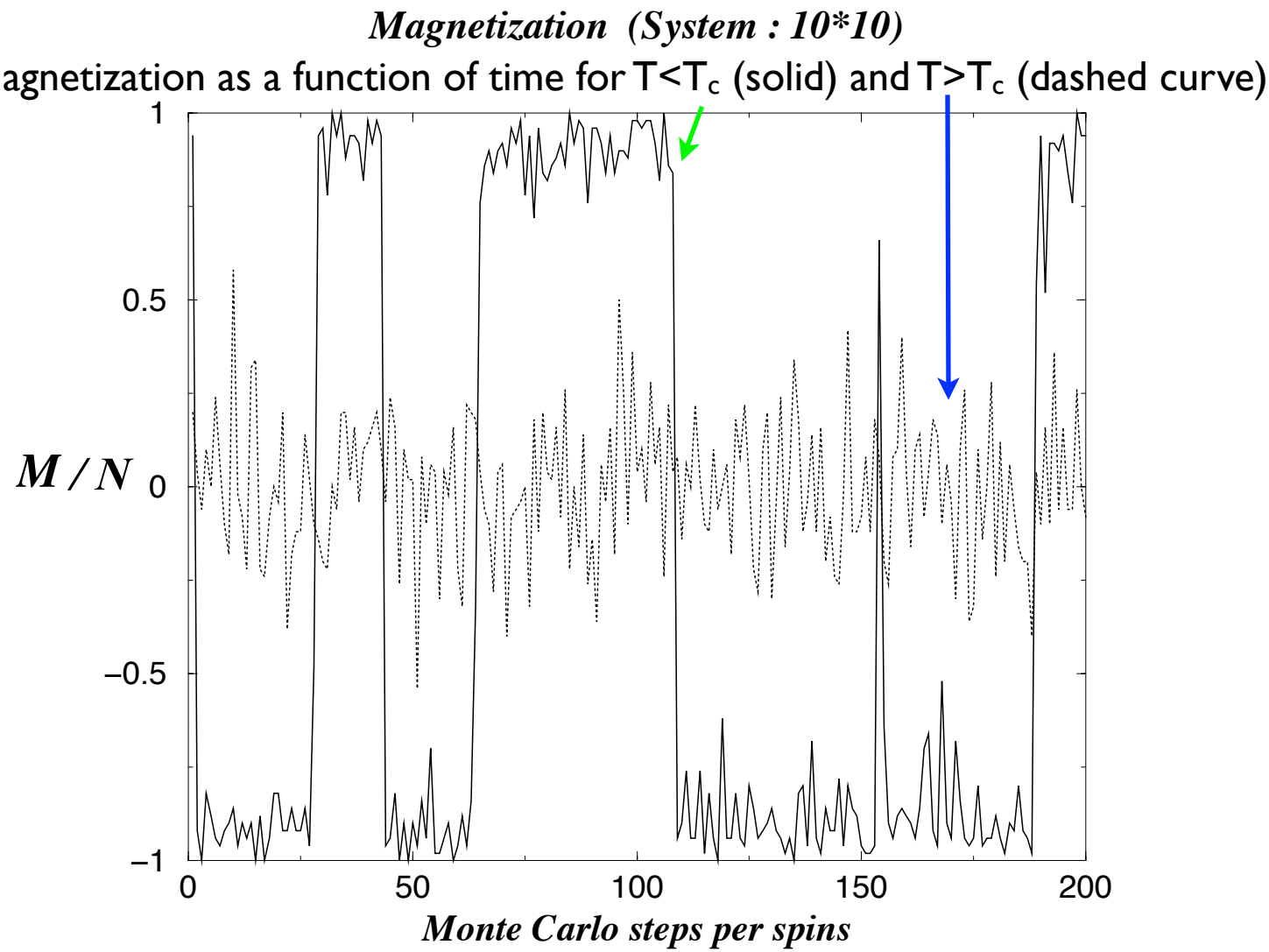


existence of a
Critical temperature Tc

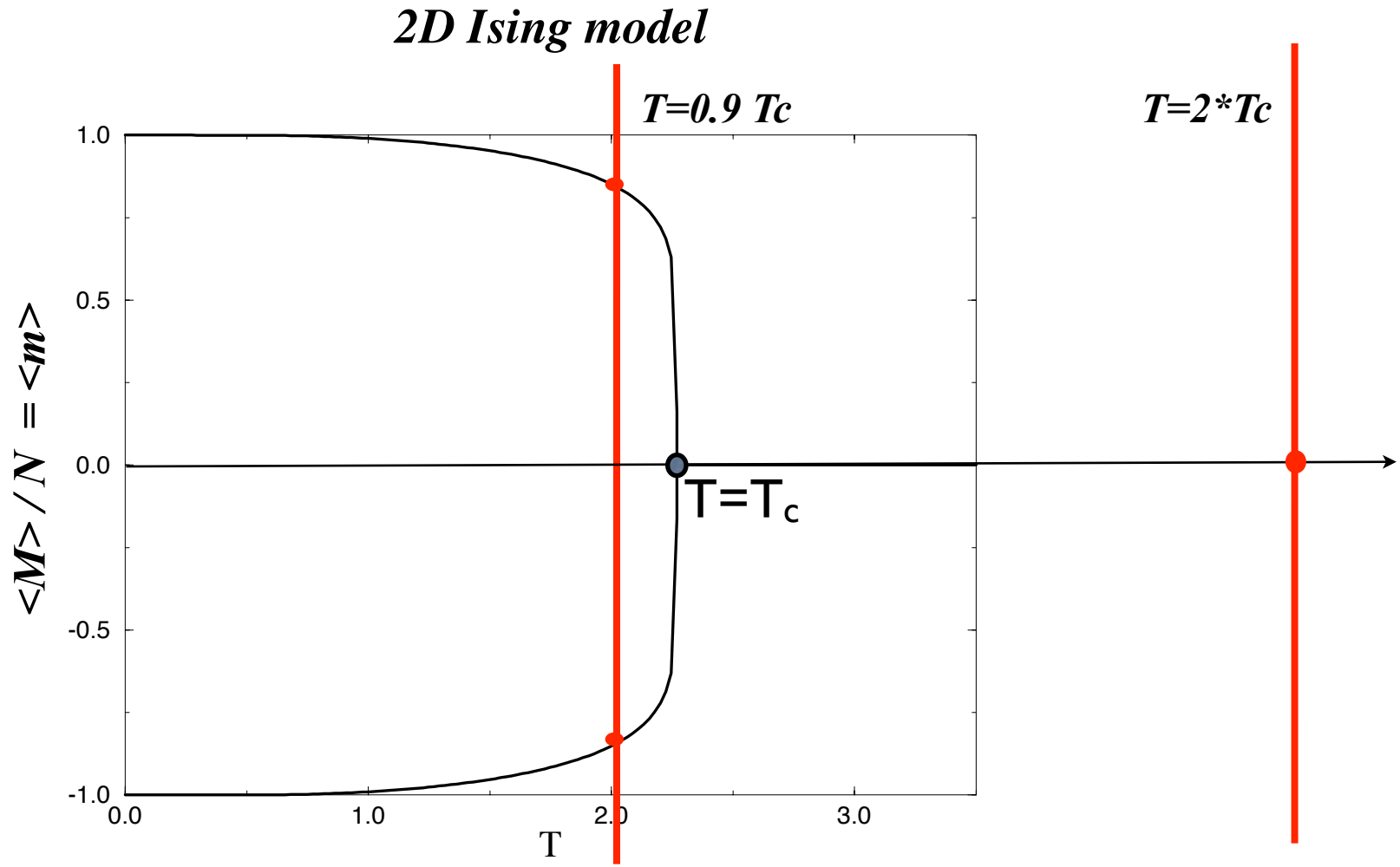
in 2D the model has an analytical solution:

$T_c = 2.269\ J/k_B$

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

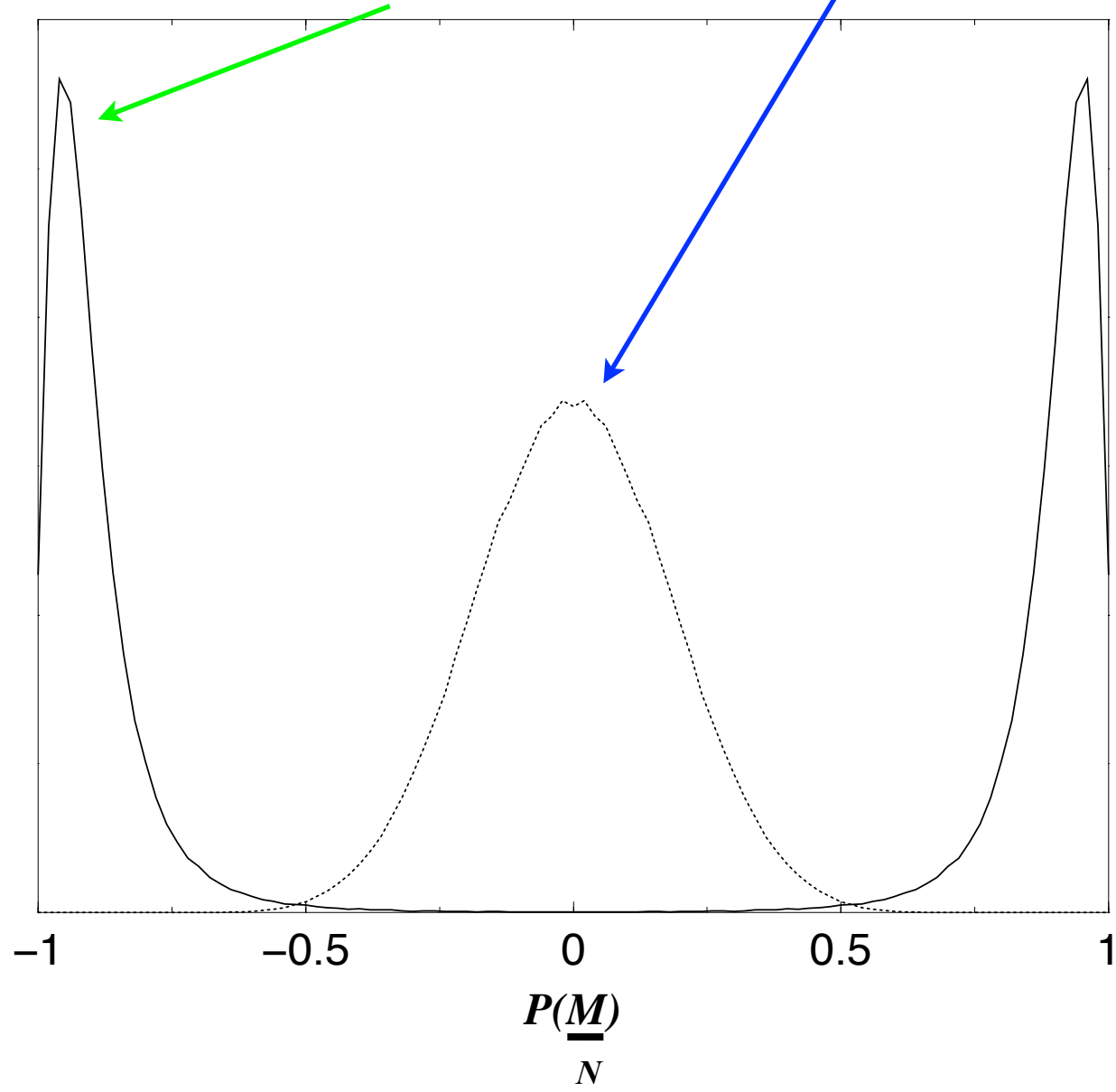


Fluctuations! do, as usual, temporal averages: $\langle M \rangle / N$, $\langle E \rangle / N$



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

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

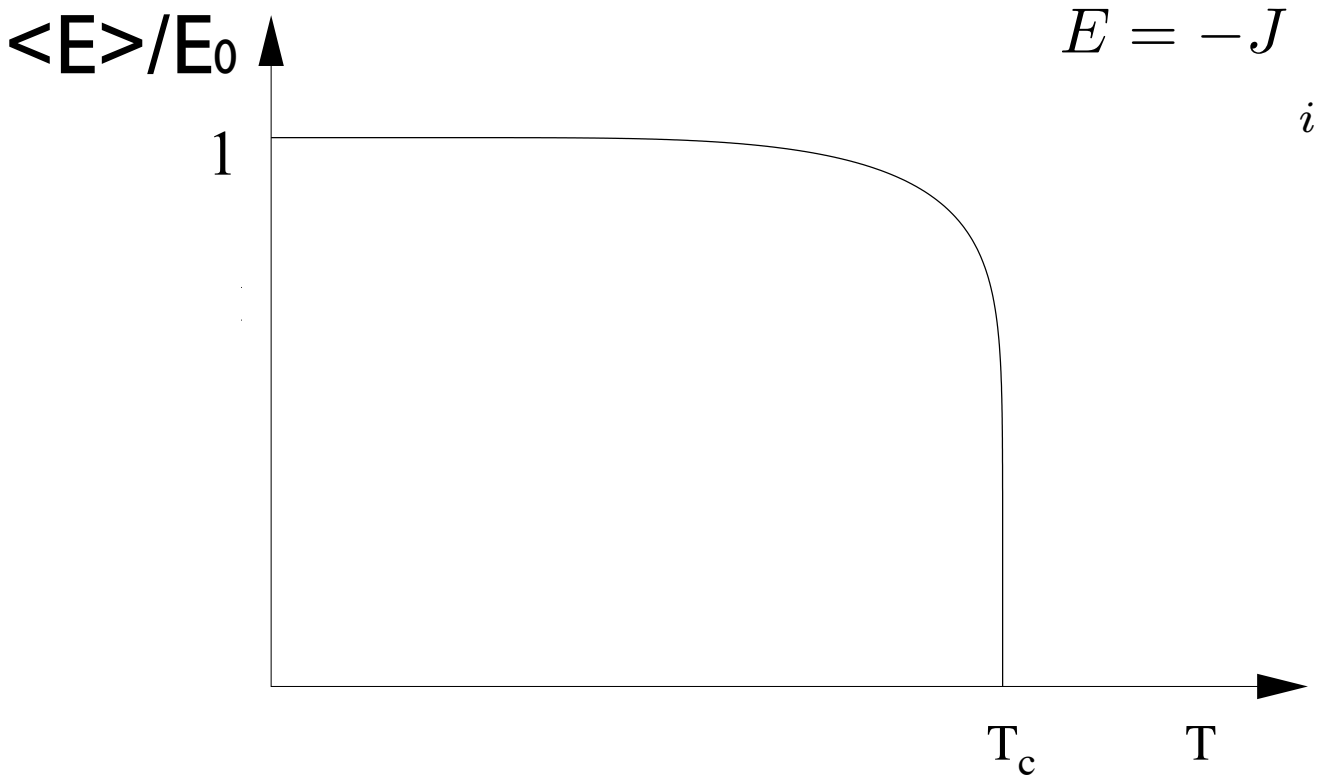


(data collected during time evolution, at equilibrium)

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...

Ising model: fluctuations

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

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

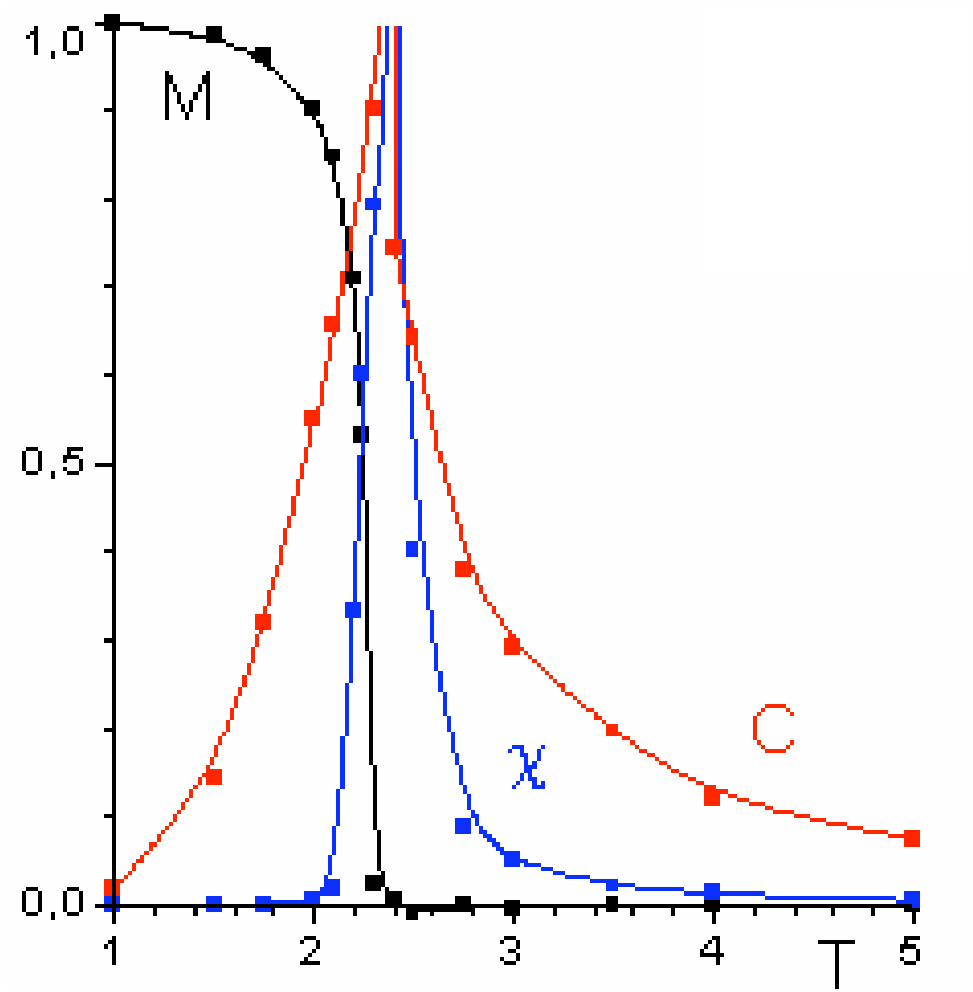
but also: $\chi = \lim\limits_{H \to 0} \dfrac{\partial \langle M \rangle}{\partial H}$, $\chi = \dfrac{1}{kT}\left(\langle M^2 \rangle - \langle M \rangle^2\right)$

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

```
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
```

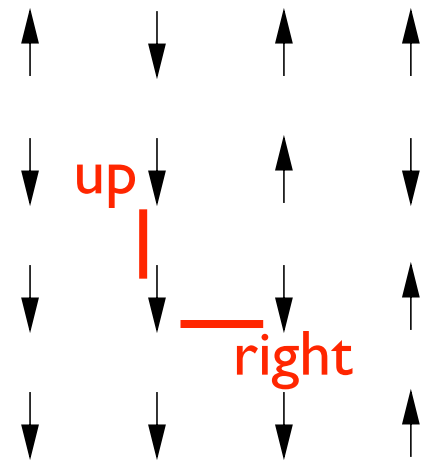
$$m = \frac{M}{N} = \frac{1}{N} \sum_{i=1}^{N} s_i$$

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

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

Ising model: energy

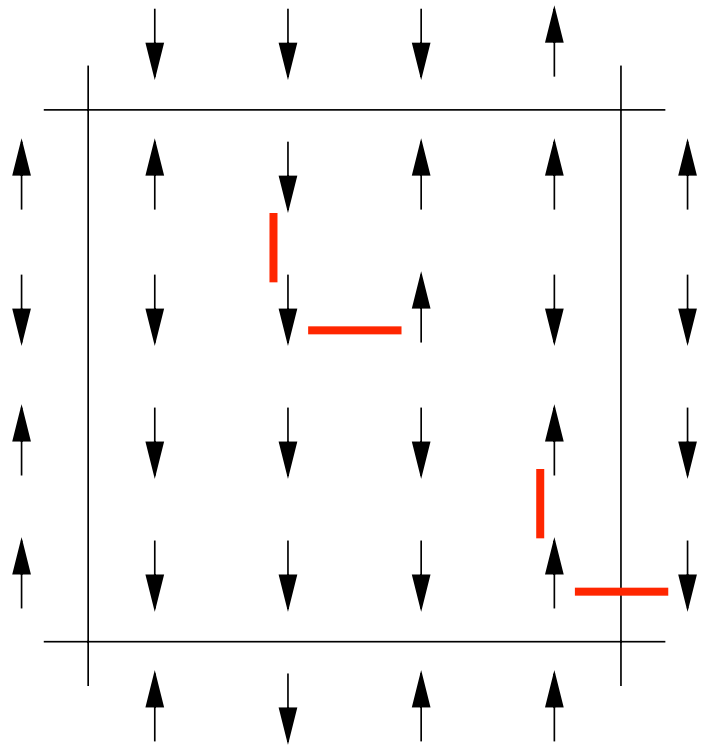
$$E = -J \sum_{i,j=\mathrm{nn}(i)}^{N} s_i s_j$$




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

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

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

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
   .....
   .....
```

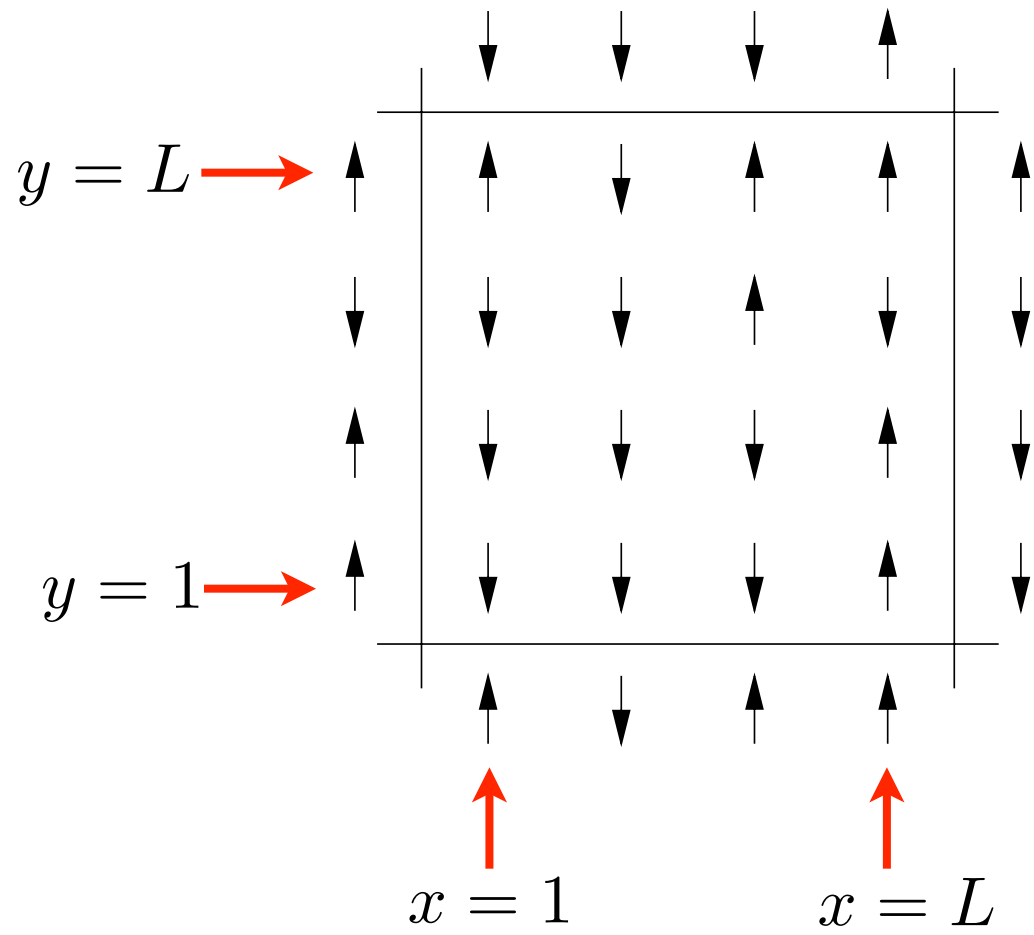
energy variation for `spin(x,y)` flip

`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

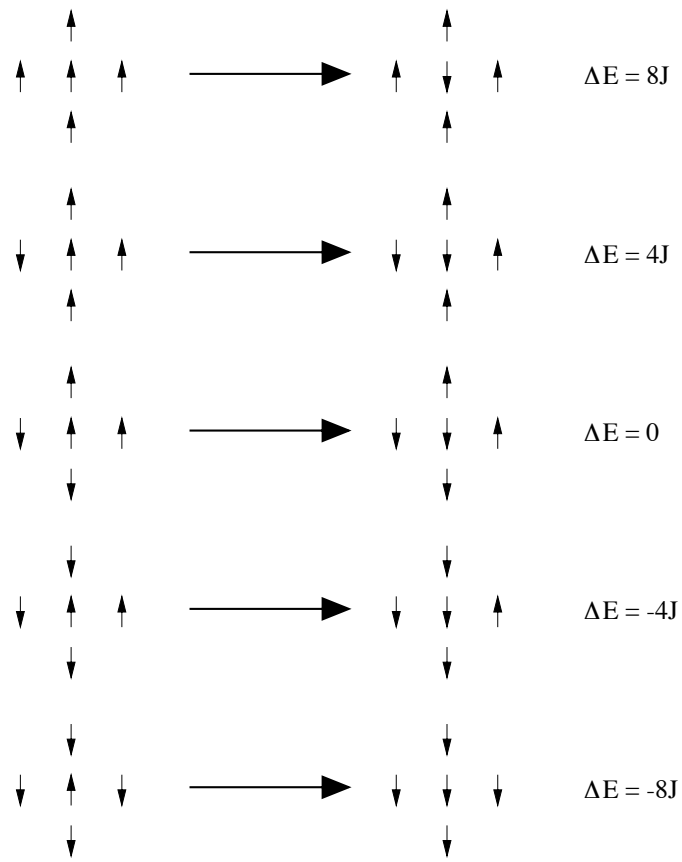
```
function DeltaE(x,y) result (DeltaE_result)
  !  periodic boundary conditions
.....
 if (x == 1) then
    left = spin(L,y)
    right = spin(2,y)
 else if (x == L) then
    left = spin(L-1,y)
    right = spin(1,y)
 else
    left = spin(x-1,y)
    right = spin(x+1,y)
 end if
 if (y == 1) then
    up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

$1 \leq x \leq L$

$1 \leq y \leq L$

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?

```
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

(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?

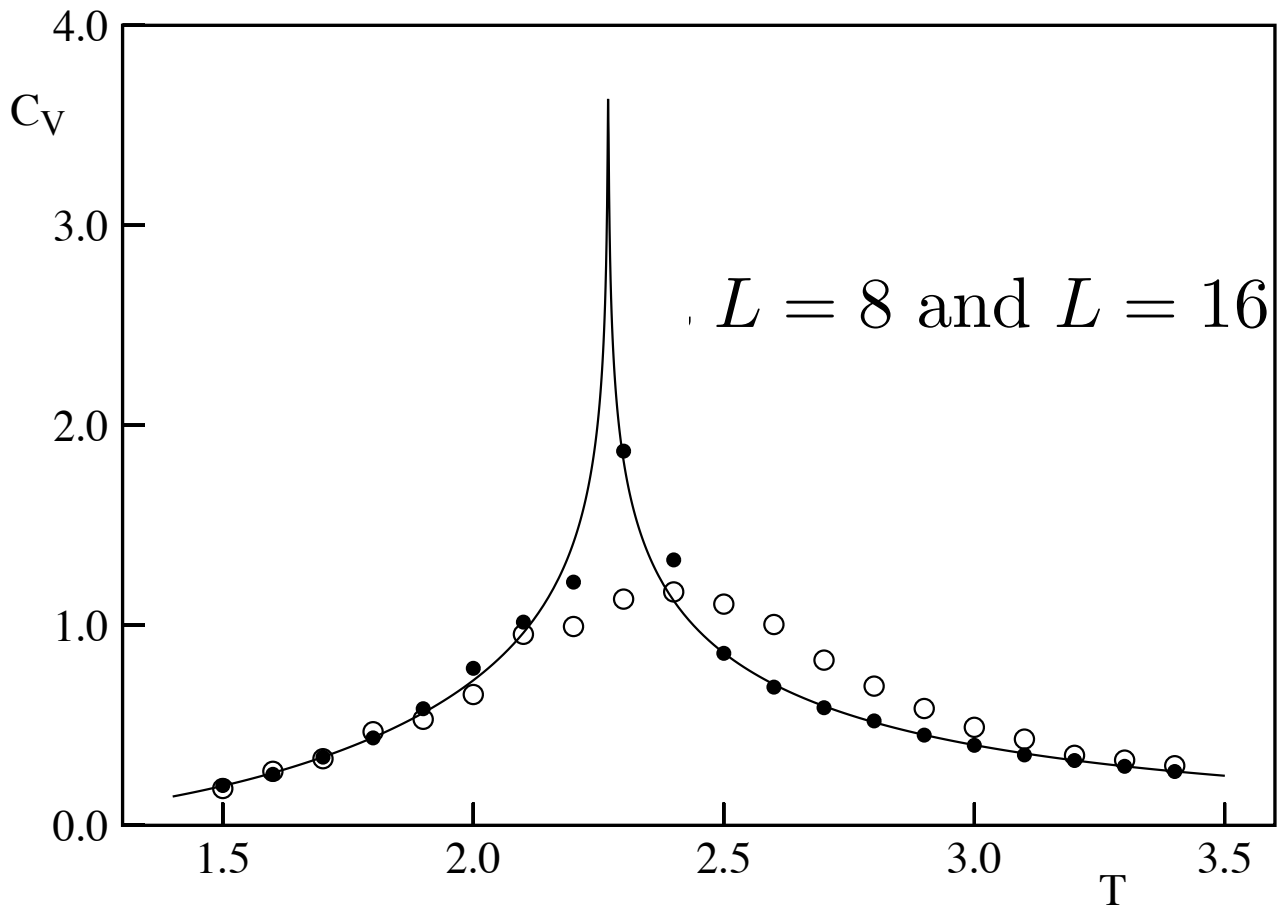
- necessary to give the ERROR ESTIMATE corresponding to the measured physical quantity !!!
- (see Tab. I of D.P. Landau, PRB 13, 2997 (1976), "Finite size behavior of the Ising square lattice")
- do also BLOCKING (called "coarse grained technique" in that paper)

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!

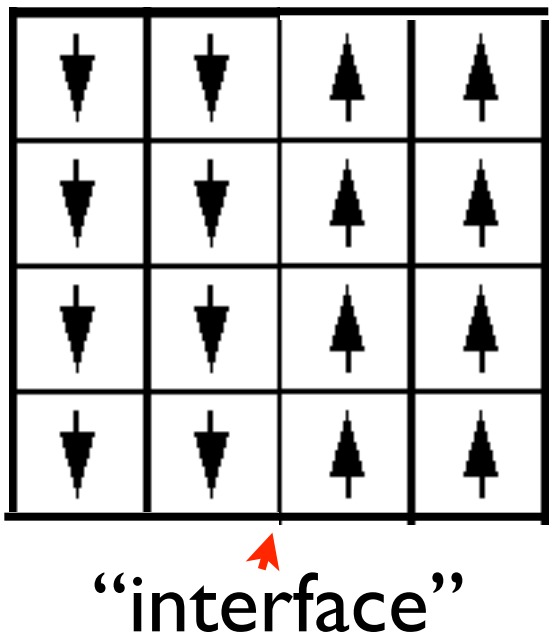


The temperature dependence of the specific heat C (per spin) of the Ising model

Ising model: size problems

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

Ising model: alternative dynamics

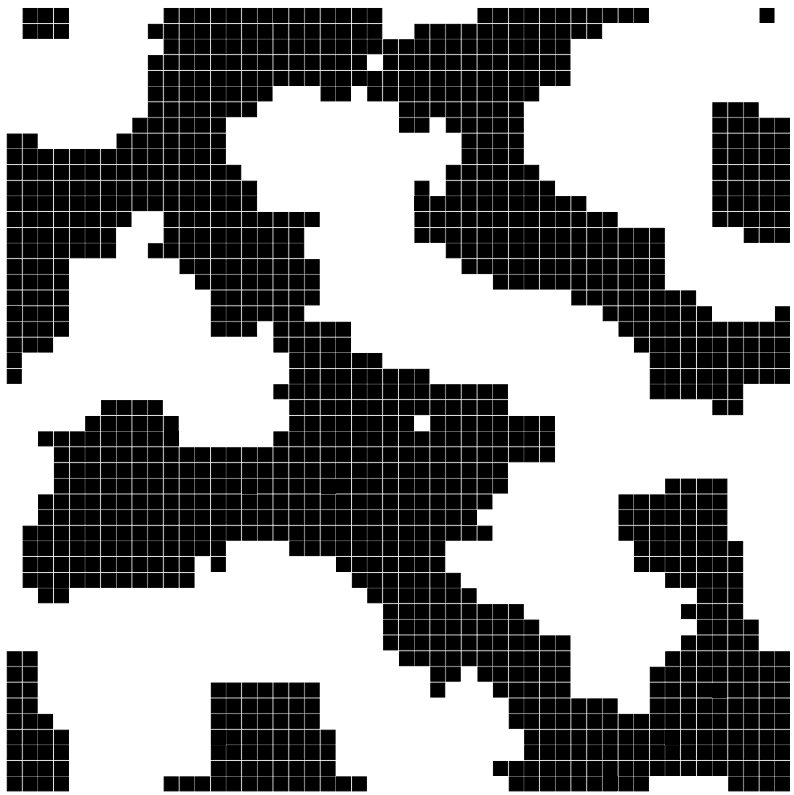
- in the SPIN FLIP dynamics the order parameter is not conserved (M changes during evolution)
- alternative: NN spin exchange (Kawasaki dyn.) (exchange two NN spins picked at random; M is conserved; this is equivalent to LATTICE GAS MODELS with fixed number of particles)

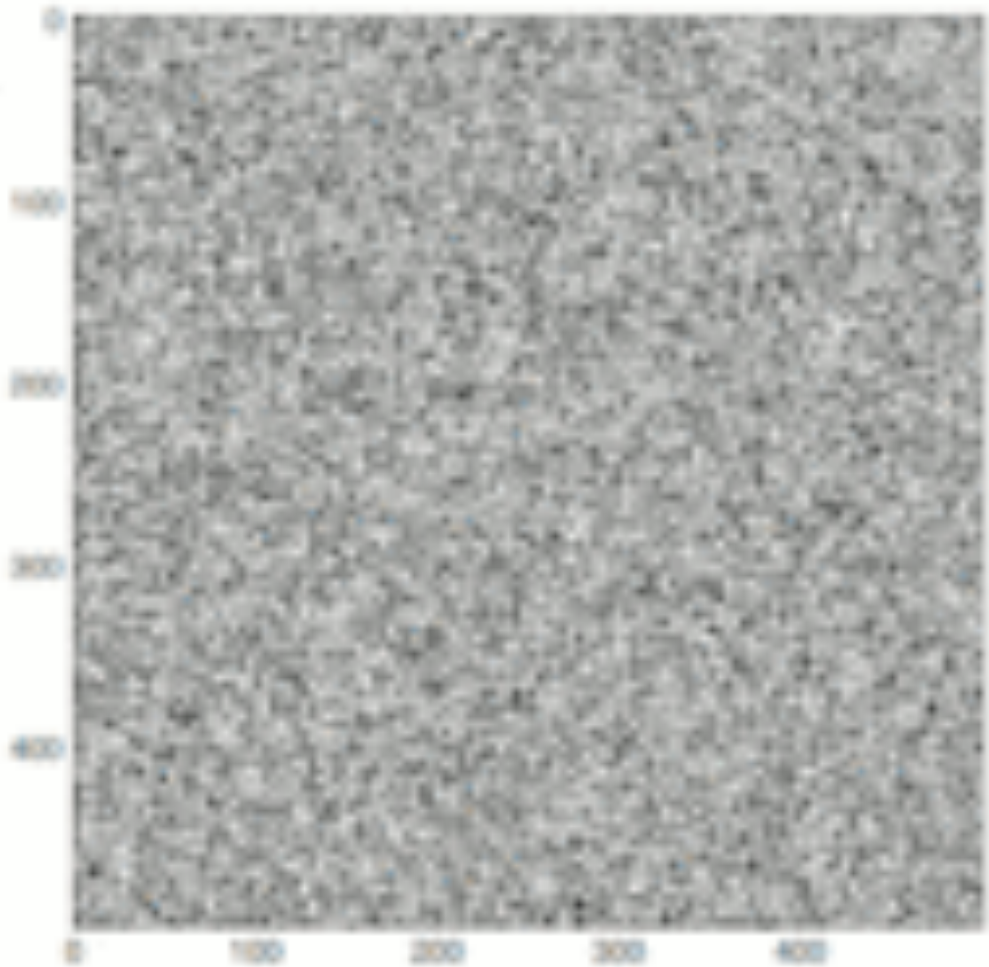
Ising model: Kawasaki dynamics

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

$$
\begin{aligned}
C &\sim |\Delta T|^{-\alpha} \\
\langle M \rangle &\sim |\Delta T|^{\beta} \quad \text{for } \Delta T < 0 \\
\chi &\sim |\Delta T|^{-\gamma} \\
\xi &\sim |\Delta T|^{-\nu}
\end{aligned}
$$

Program:

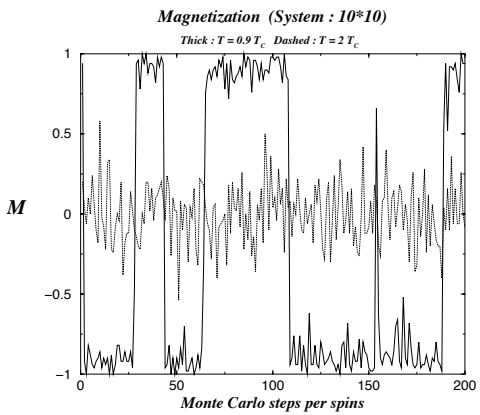
on
$/home/peressi/comp-phys/IX-ising/
[do: $cp /home/peressi/.../IX-ising/* .]

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

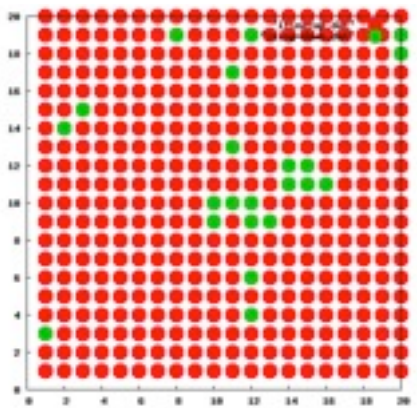
(a) Choose L=30, T=2, and initially spin=±1 randomly. ...

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). ..

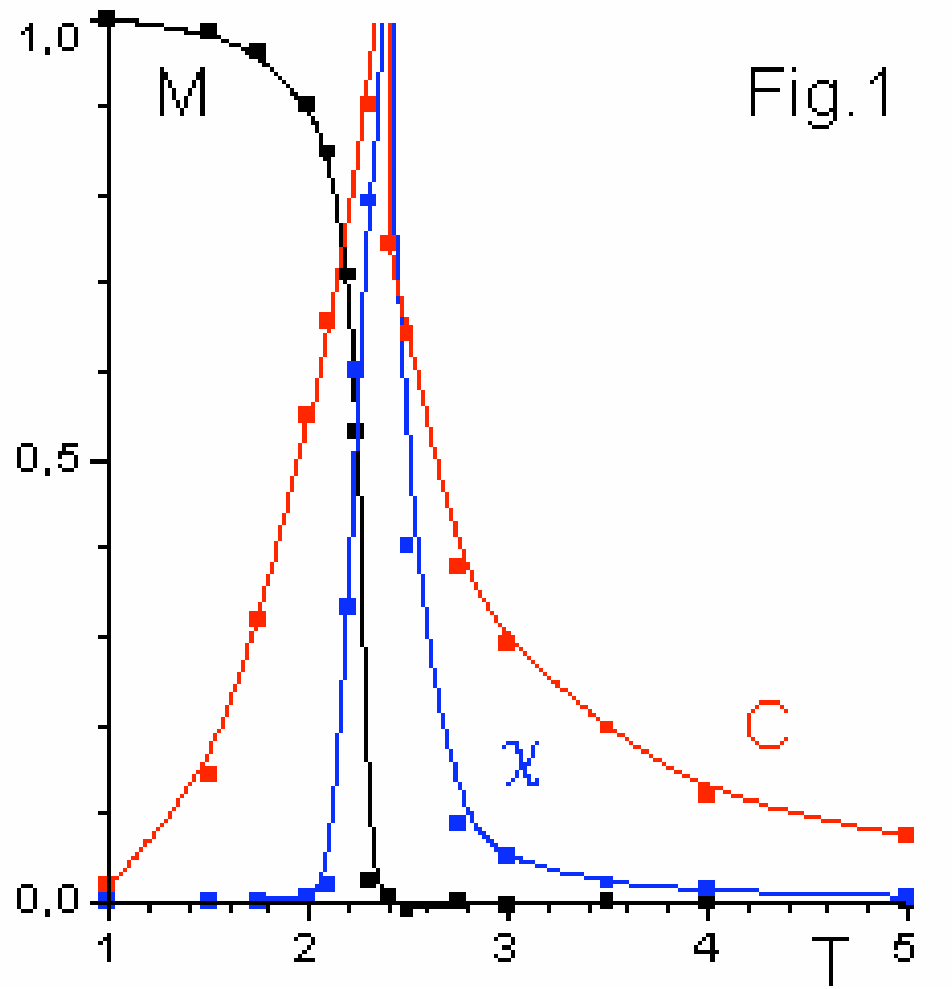
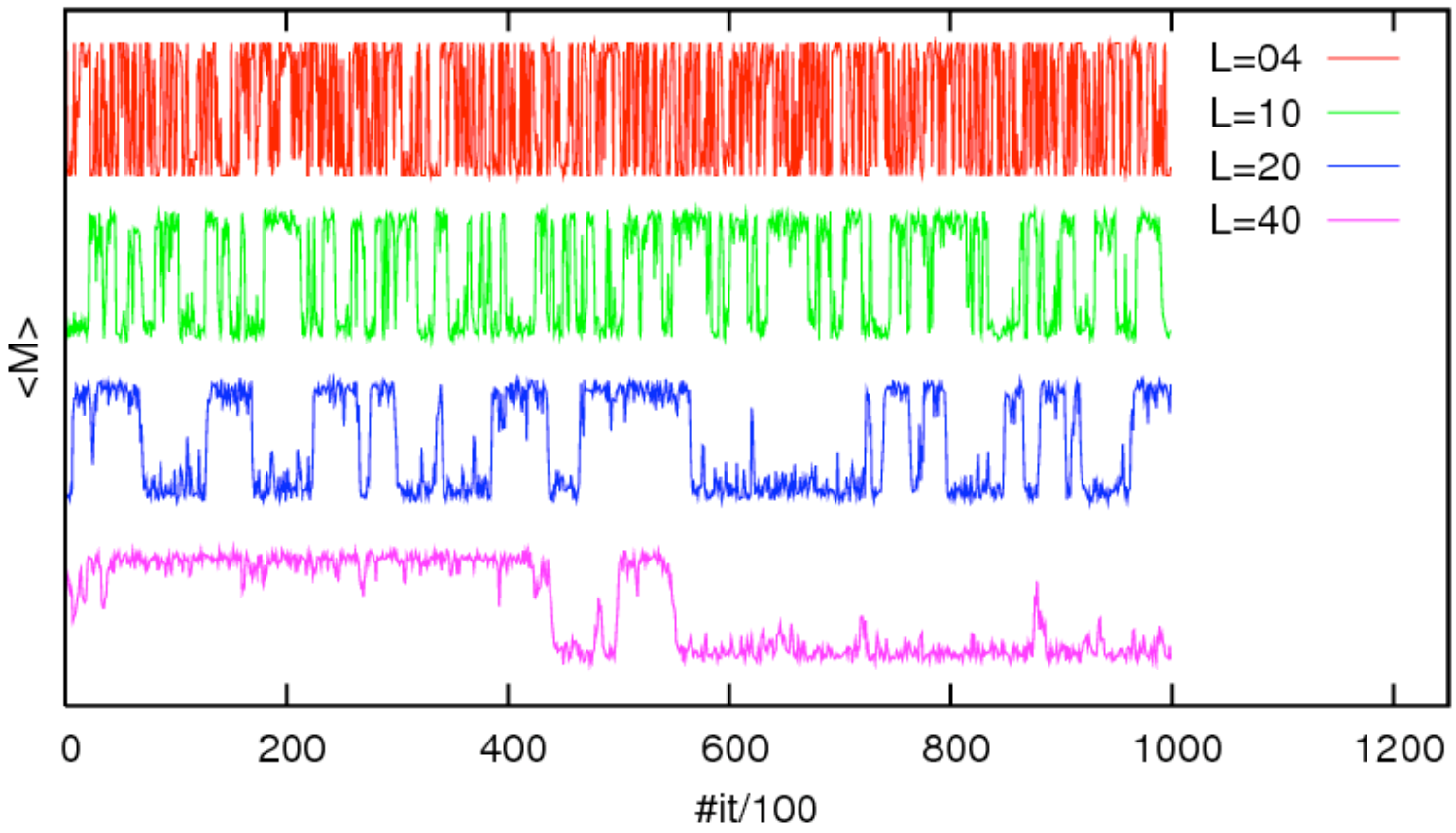


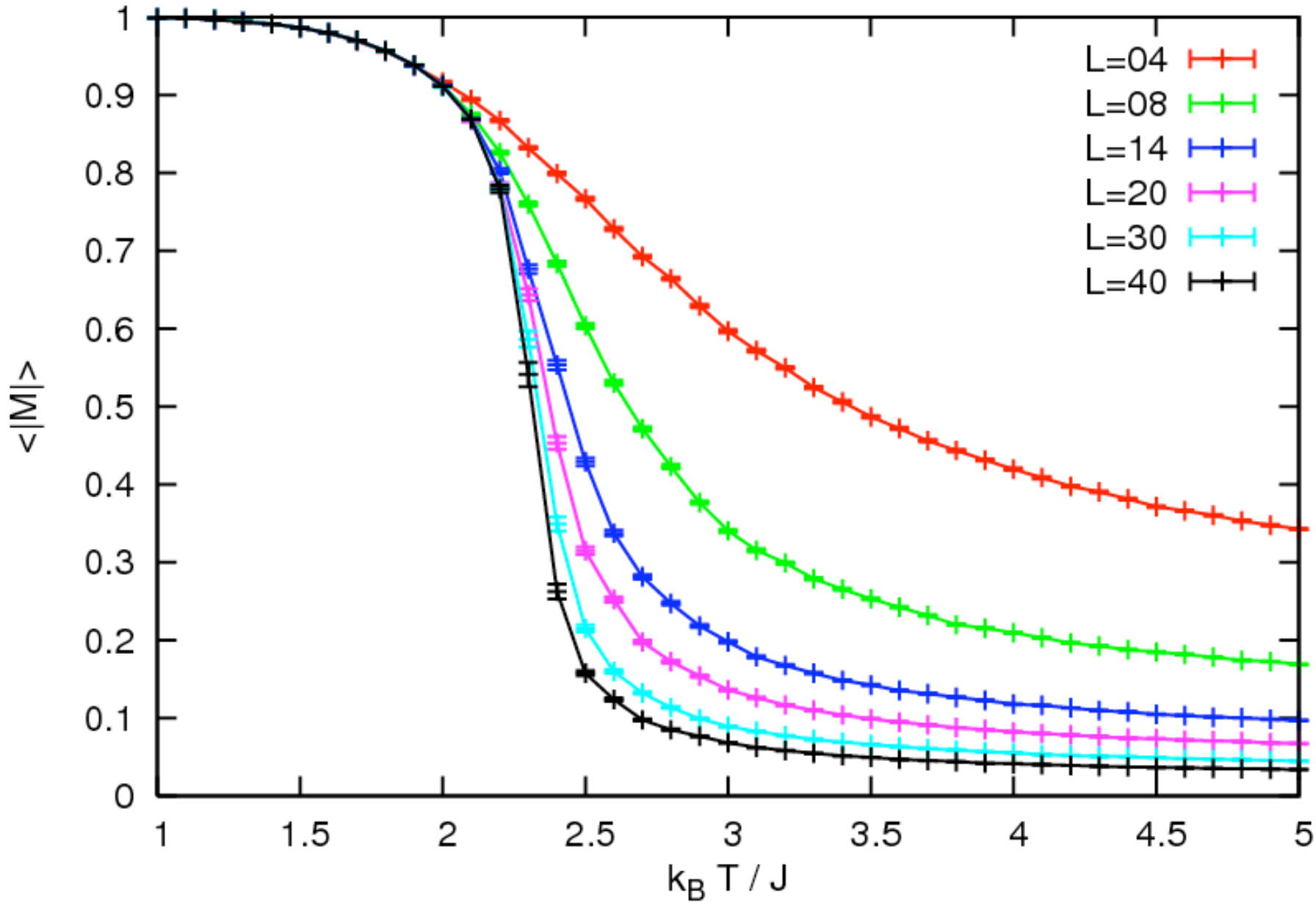
Fig. 1

Raw data: traces, covariance and autocorrelation time

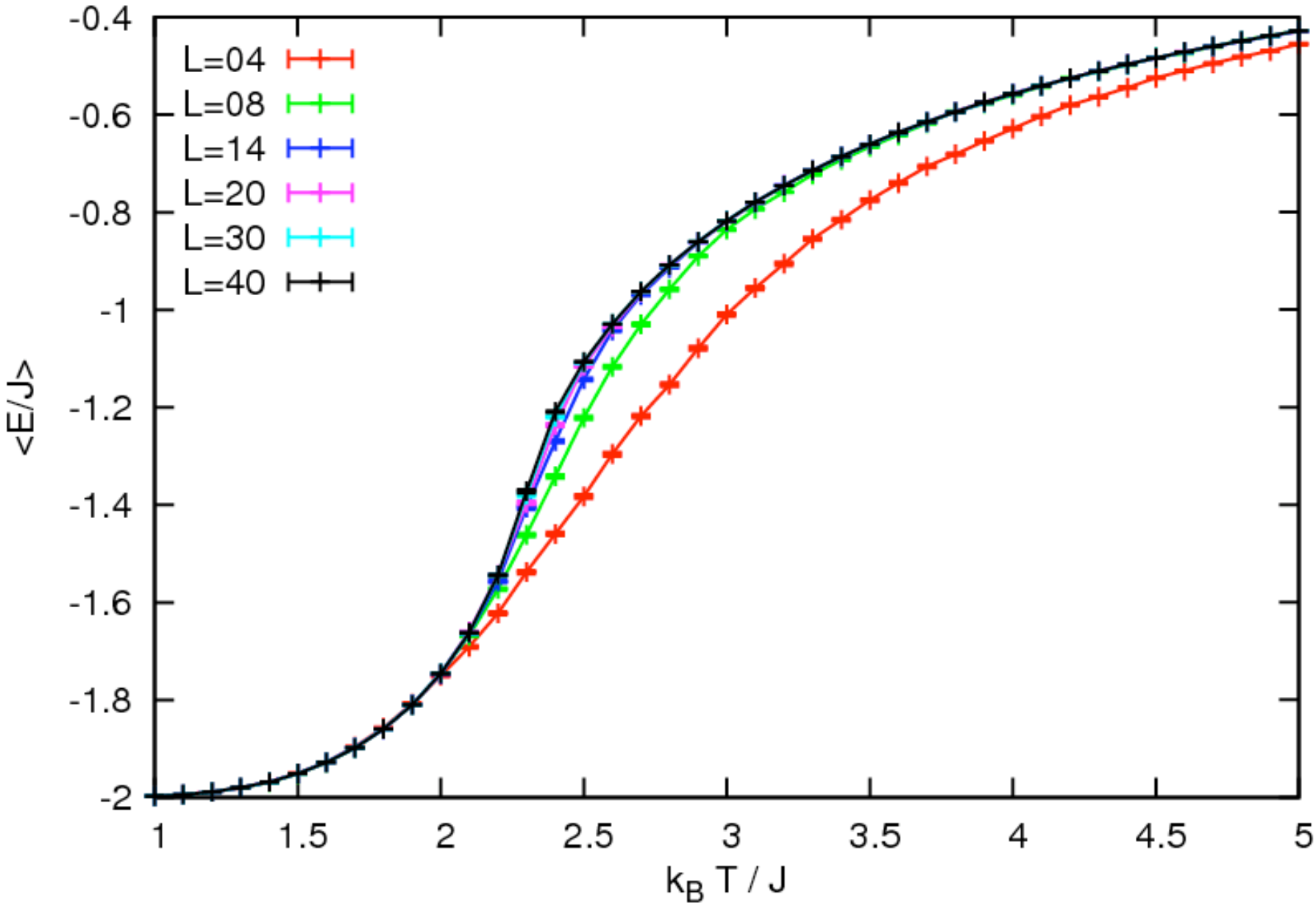
Trace: magnetization for $T = 2.27 J/k_B \approx T_C$ (10^5 sweeps)



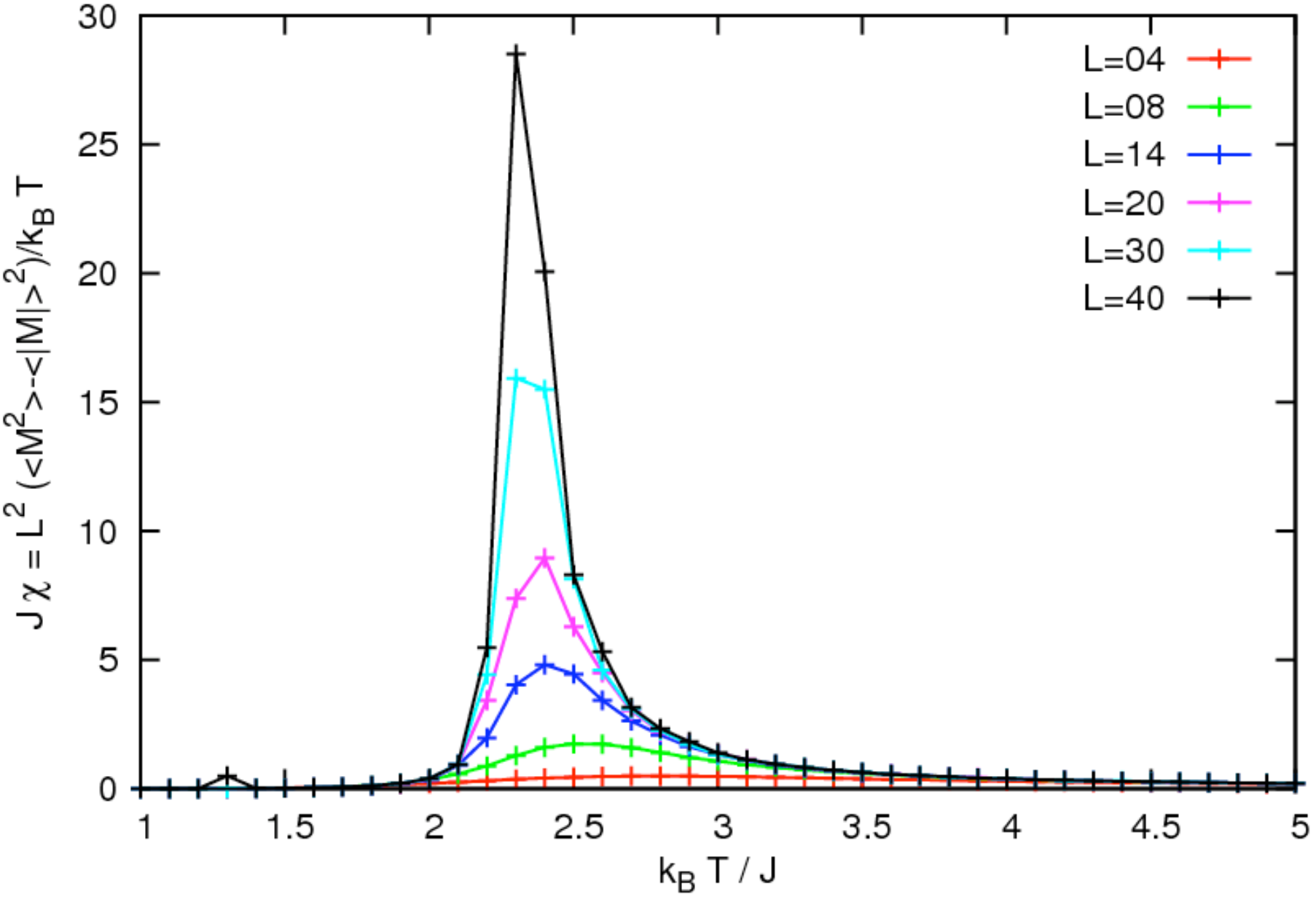
Magnetization (10^5 sweeps)



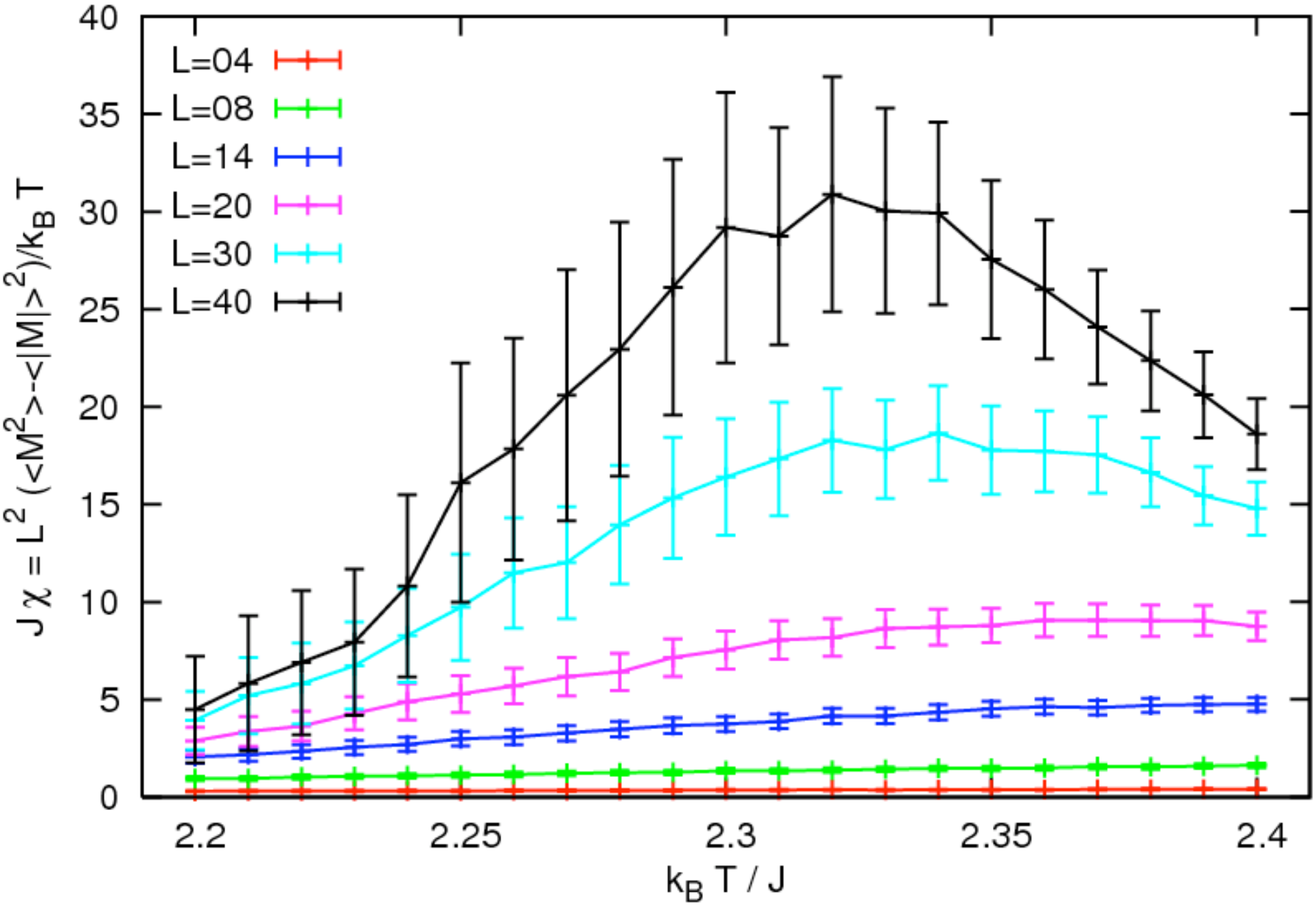
Energy (10^5 sweeps)



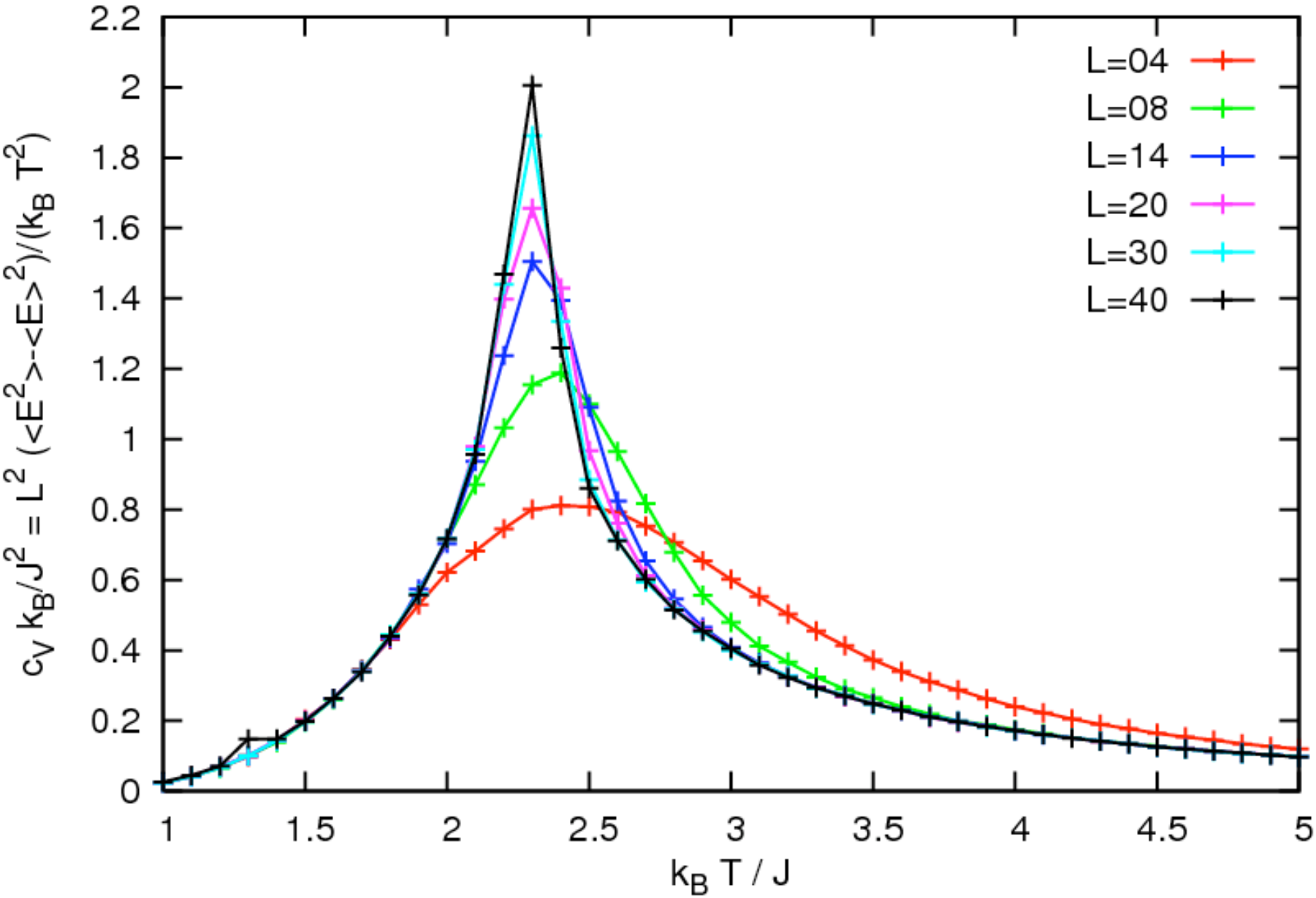
Magnetic susceptibility (10^5 sweeps)



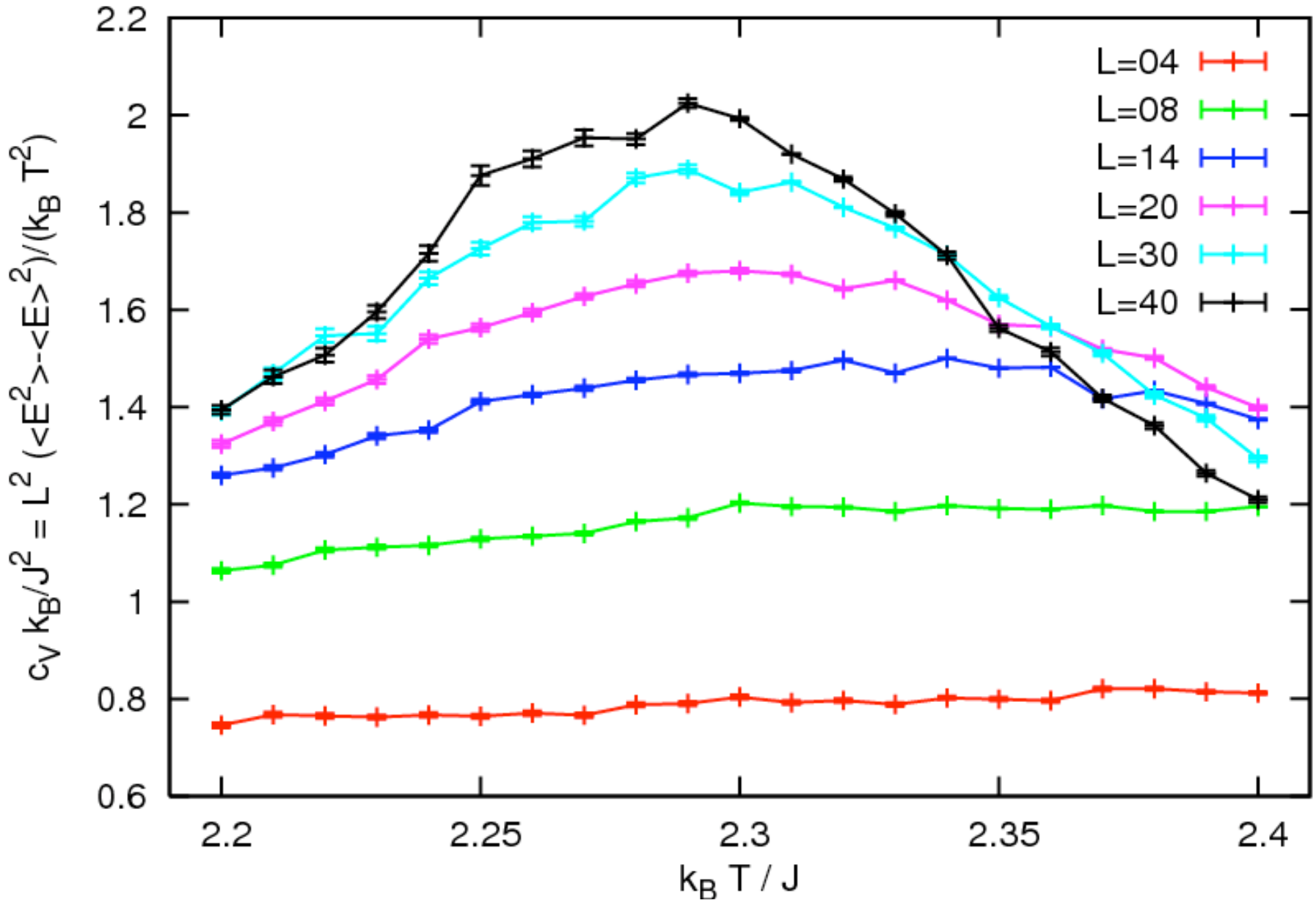
Magnetic susceptibility near T_c (10^6 sweeps)



Specific heat (10^5 sweeps)



Specific heat near T_c (10^6 sweeps)



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