993SM - Laboratory of Computational Physics Unit X November 27, 2023

Maria Peressi
Università degli Studi di Trieste - Dipartimento di Fisica
Sede di Miramare (Strada Costiera 11, Trieste)
e-mail: peressi@units.it
tel.: +39 040 2240242

- more on Ising model

- Variational Monte Carlo

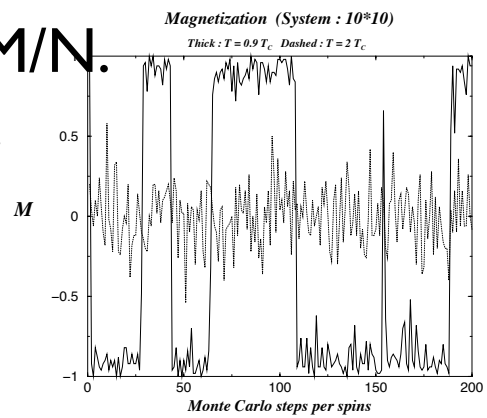
Exercise

(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

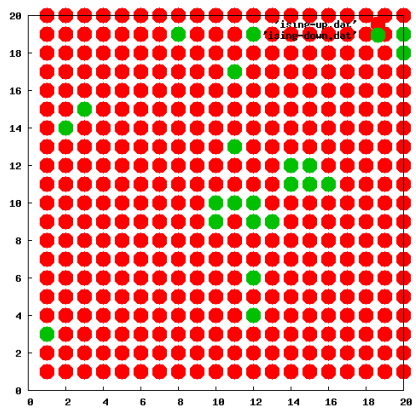
(a) Choose L=30, T=2, and initially spin=±1 randomly. ...

Plot a snapshot of the spin pattern: does the system appear ordered or disordered?

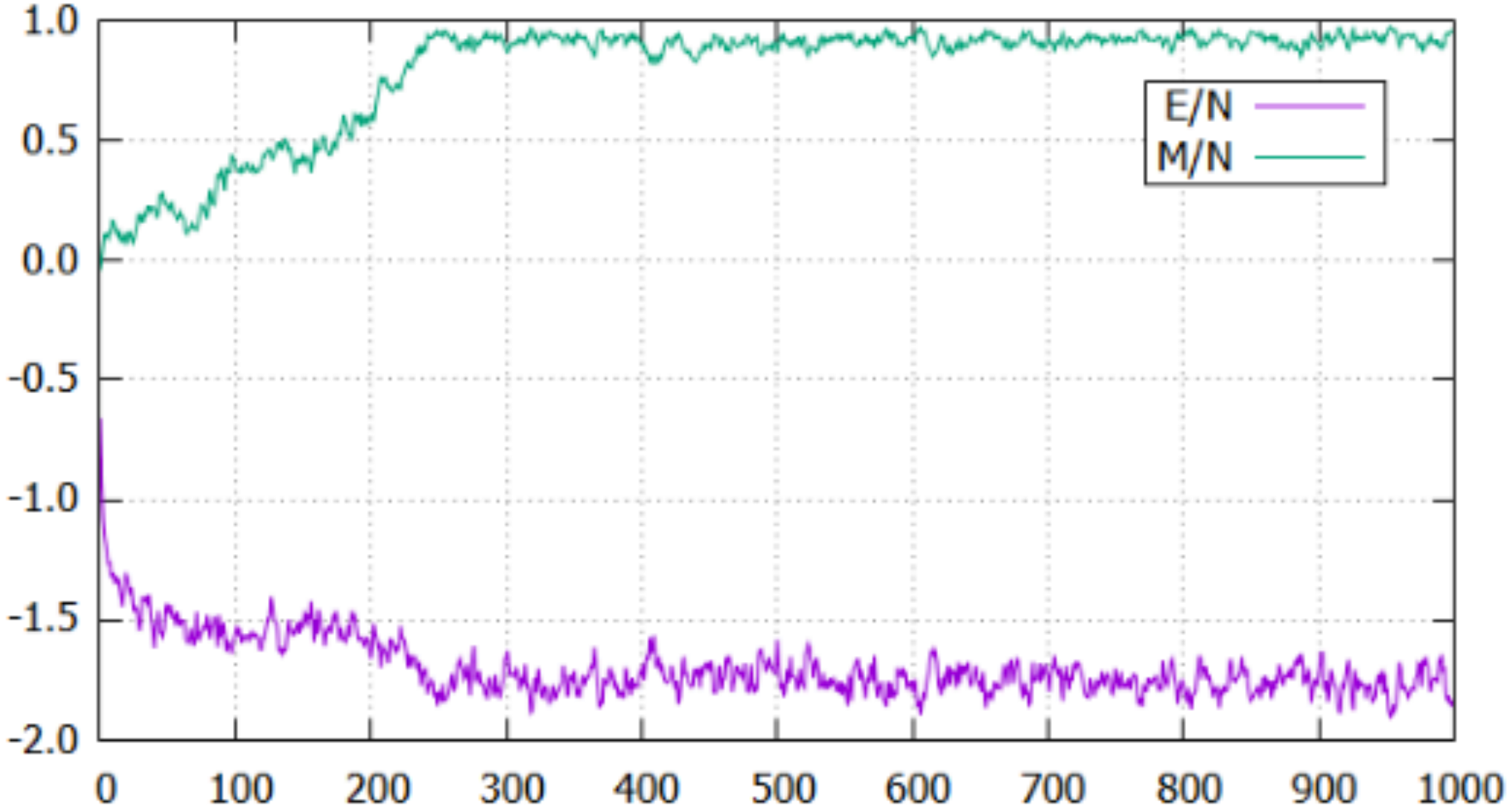
it should appear **ordered...**

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:



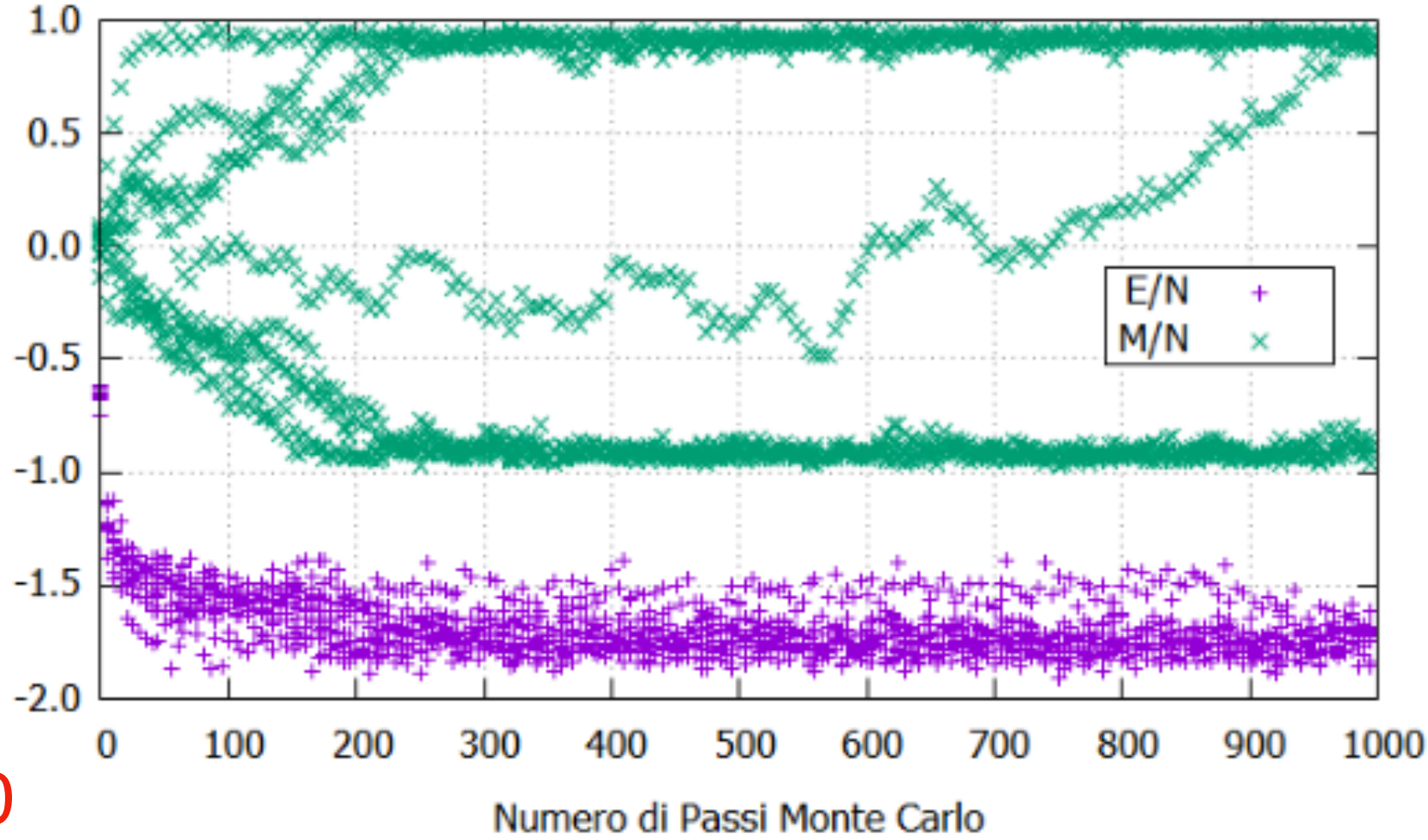
Some results that you should obtain…



L=30

(a) Energia media e magnetizzazione per spin al variare del tempo (ossia all'aumentare dei passi Monte Carlo svolti) per un sistema a temperatura $T = 2.0$.
Si noti che dopo circa 300 passi Monte Carlo il sistema sembra stabilizzarsi.

M. Dirindin, 2021

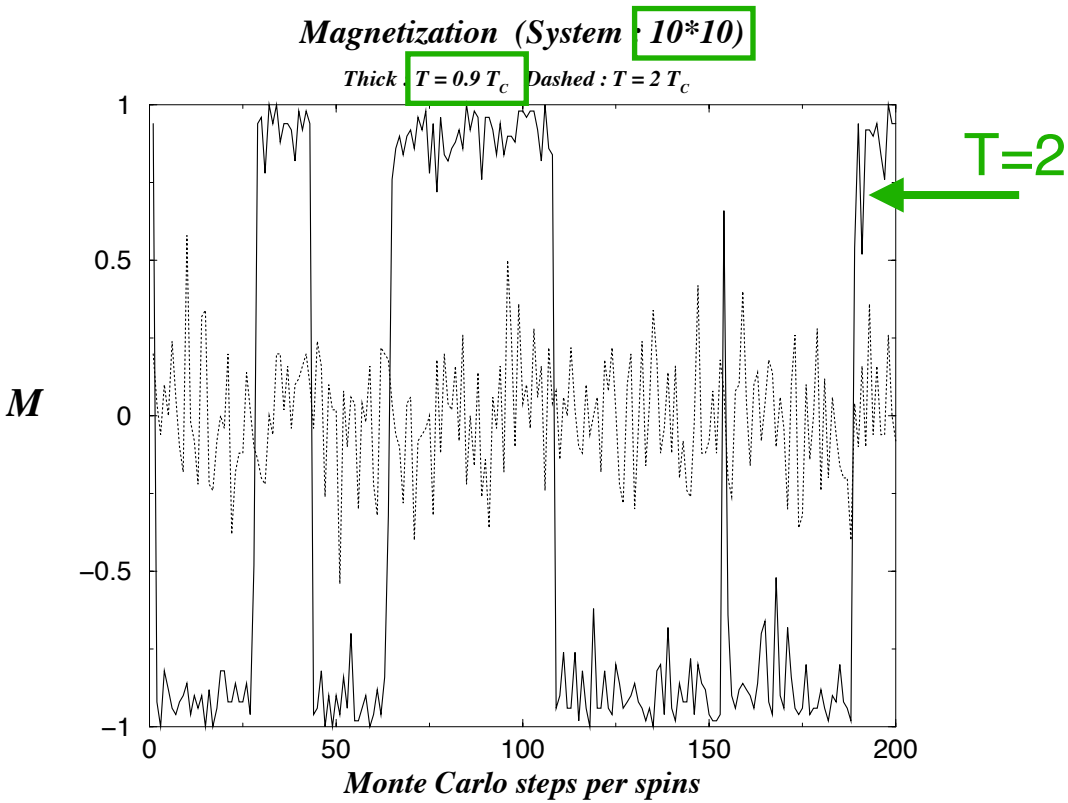


L=30

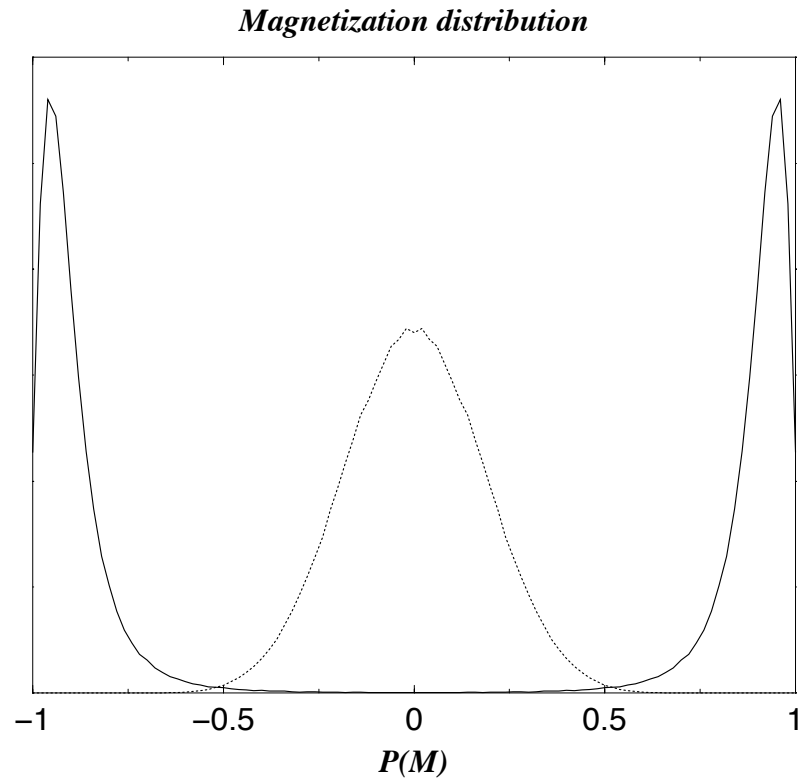
Figura 3: Energia e magnetizzazione per spin per 10 valori diversi di seed. Si noti come la maggior parte dei seed raggiunga l'equilibrio dopo circa 250 iterazioni, mentre un seed raggiunge l'equilibrio dopo appena 50 iterazioni ed un'altro lo raggiunge dopo 1000 passi Monte Carlo.

M. Dirindin, 2021

results for a smaller system:

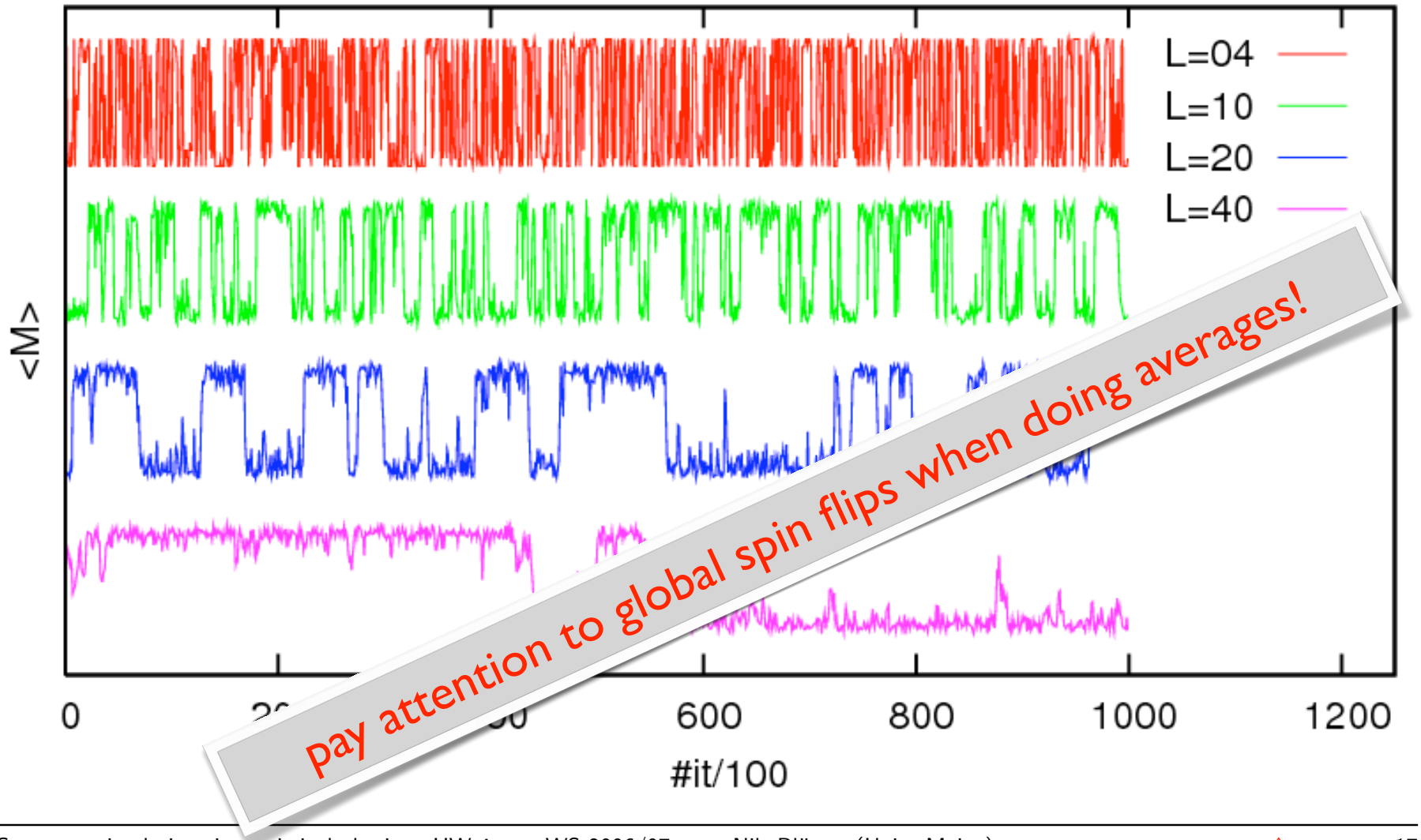


T=2



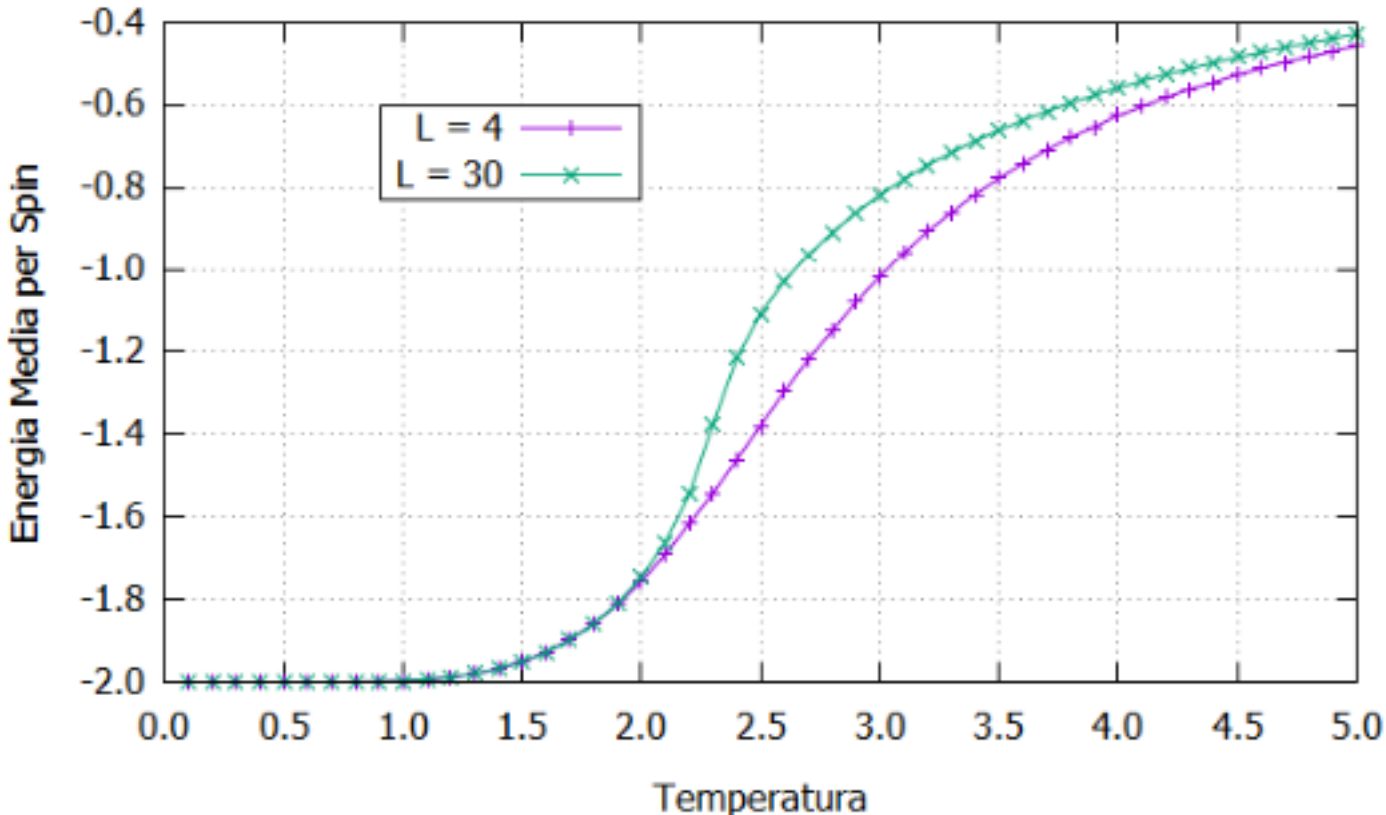
results for system of different size:

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



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



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)

(here K_{NN}=J)

D.P. Landau, PRB 13, 2997 (1976)

4x4

TABLE I. Comparison of Monte Carlo data and analytic values of the reduced internal energy per spin for an $N = 4$ square lattice with p.b.c.

kT/K_{nn}	$\langle U/U_0 \rangle_{anal}$	$\langle U/U_0 \rangle_A$ [a]	σ [b]	σ' [b]	$\langle U/U_0 \rangle_B$ [b]	σ [b]	σ' [b]
1.087	0.997 24	0.997 47	0.000 26	0.000 26	0.997 36	0.000 26	0.000 42
1.449	0.980 06	0.978 41	0.000 76	0.000 86	0.980 89	0.000 73	0.001 37
1.811	0.926 93	0.927 40	0.001 46	0.002 08	0.924 71	0.001 50	0.002 96
2.173	0.819 21	0.816 45	0.002 36	0.003 76	0.814 67	0.002 34	0.004 87
2.536	0.675 08	0.675 57	0.002 85	0.004 46	0.671 57	0.002 83	0.005 89
2.898	0.540 69	0.541 85	0.002 90	0.004 33	0.532 22	0.002 92	0.005 83
3.260	0.438 73	0.437 28	0.002 85	0.003 99	0.435 34	0.002 77	0.005 13
3.622	0.366 35	0.361 40	0.002 60	0.003 78	0.370 79	0.002 67	0.004 46

[a] Run A was made by going through the lattice in order. Run B was made by choosing the reference spin randomly.

[b] σ is the standard deviation of $\langle U/U_0 \rangle$ obtained assuming uncorrelated data. σ' is the standard deviation obtained using the coarse-grained technique described in the text. Values of the standard deviation which are too small to account for the discrepancy with the analytic values are underlined.

choice of the reference spin:

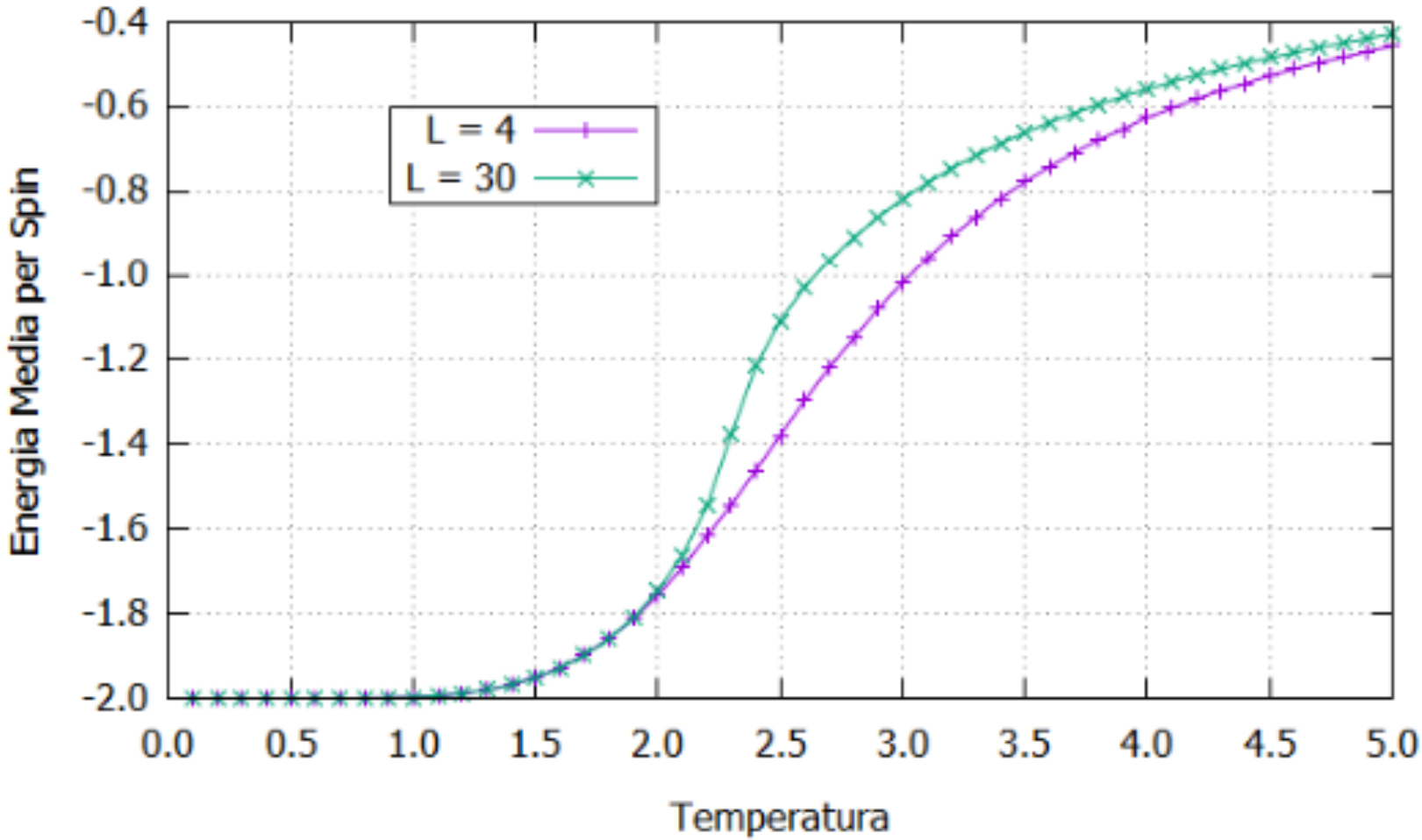
in order

randomly

Ising model: size problems

We cannot simulate an INFINITE system!

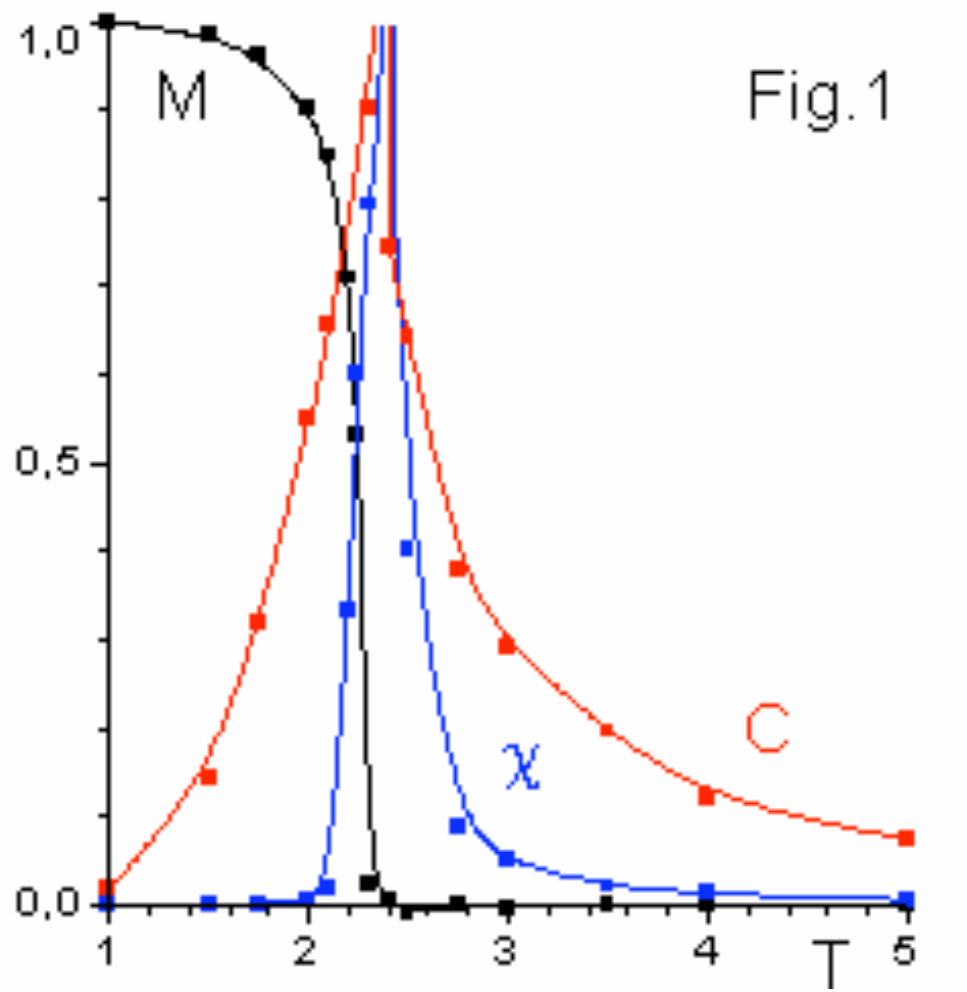
size effects with PBC on E(T):



Exercise

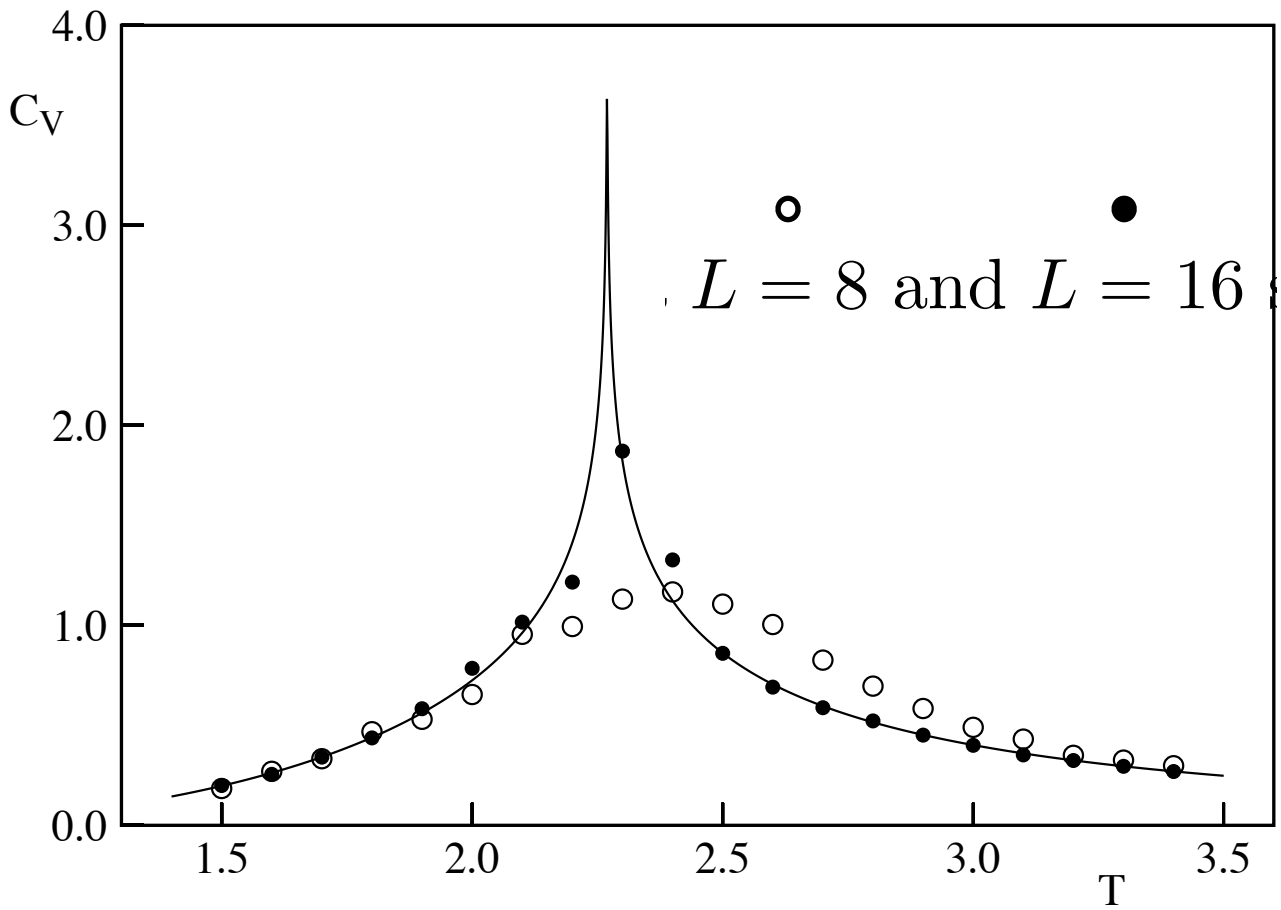
(a) Choose L=30, T=2, and initially spin=±1 randomly. ...

Calculate also c and χ.



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

We cannot simulate an INFINITE system!

INTERFACE EFFECTS: example of energy (units of J) for HALF UP/HALF DOWN configurations:

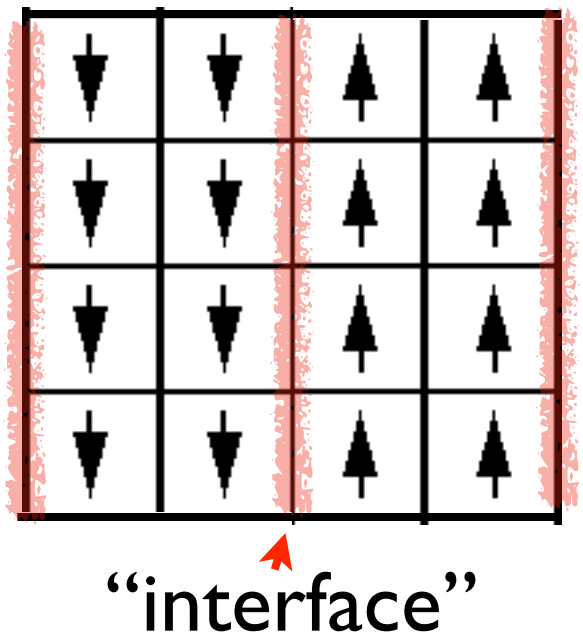
L=2	E= 0
L=4	E=-1
L=8	E=-1.5
L=16	E=-1.75
L=20	E=-1.8
L=32	E=-1.875

32 pairs, 4 of them with "wrong" intractions

=>

E = (-32 +8 +8) /16 = -1

2 x L x L. 2 x L



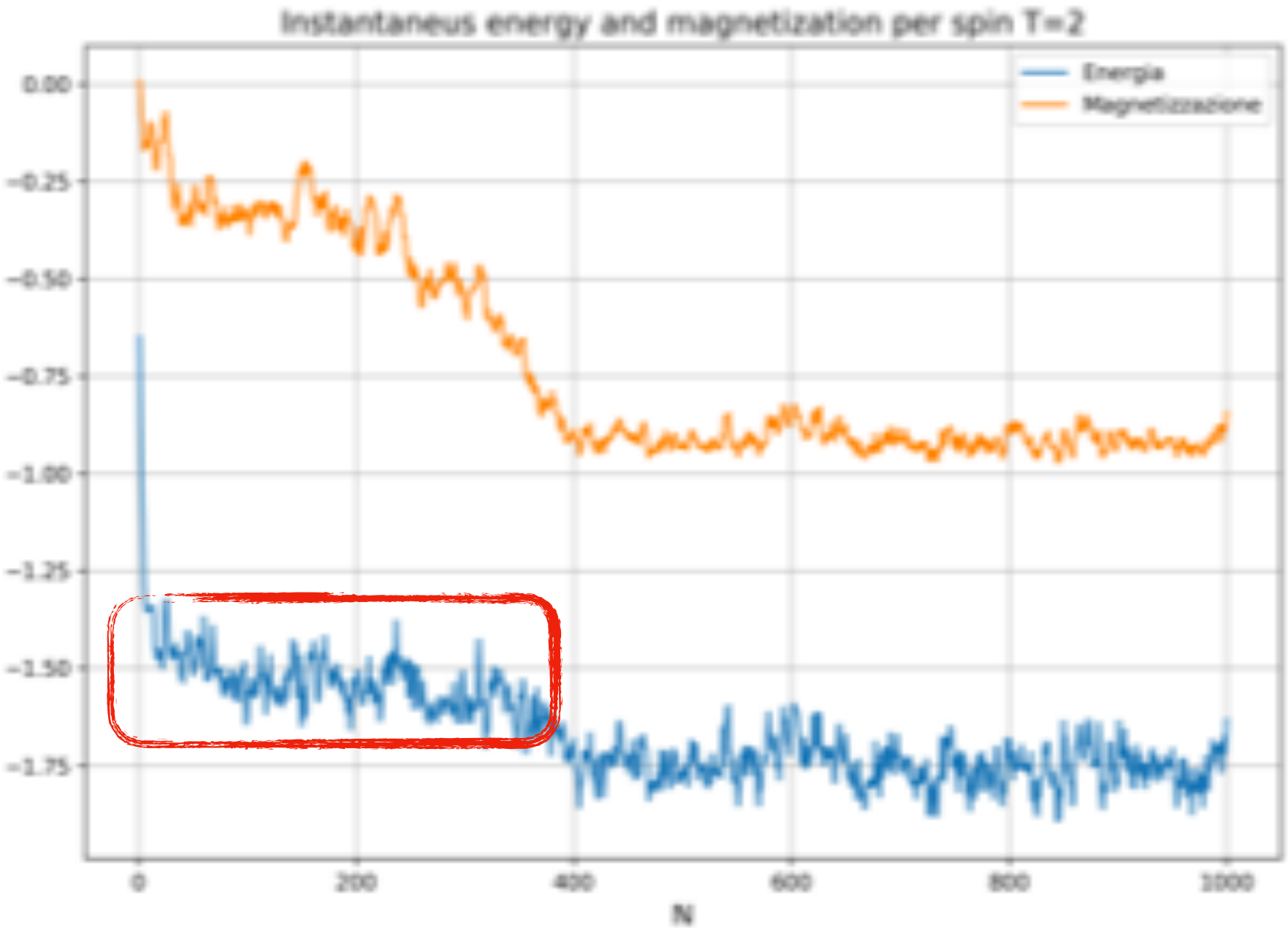
with PBC

"interface"

···· for an infinite system: E=-2

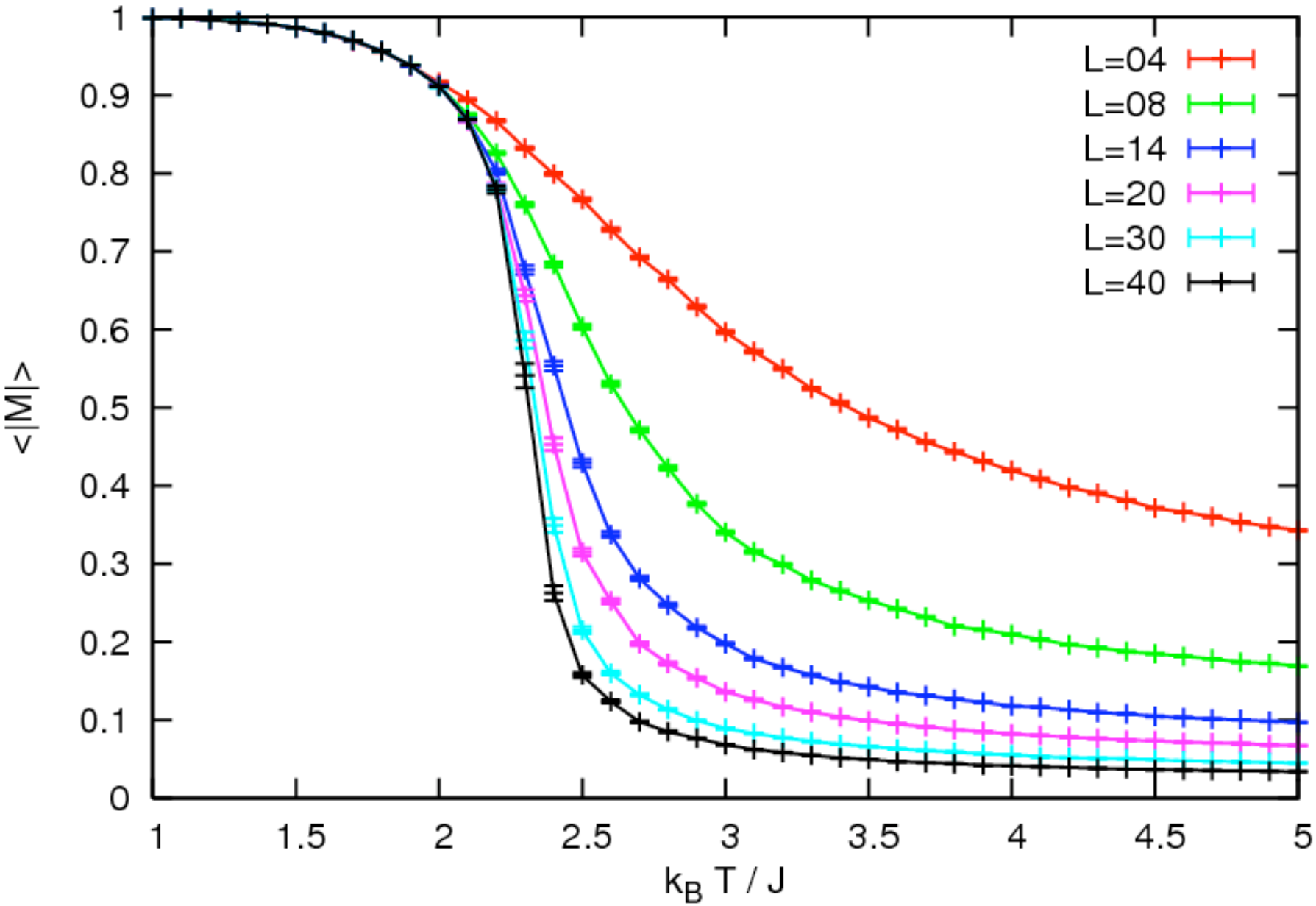
We have a ("interface") term proportional to 1/L

important monitoring E(t) and M(t) at the same time to identify possible metastable states

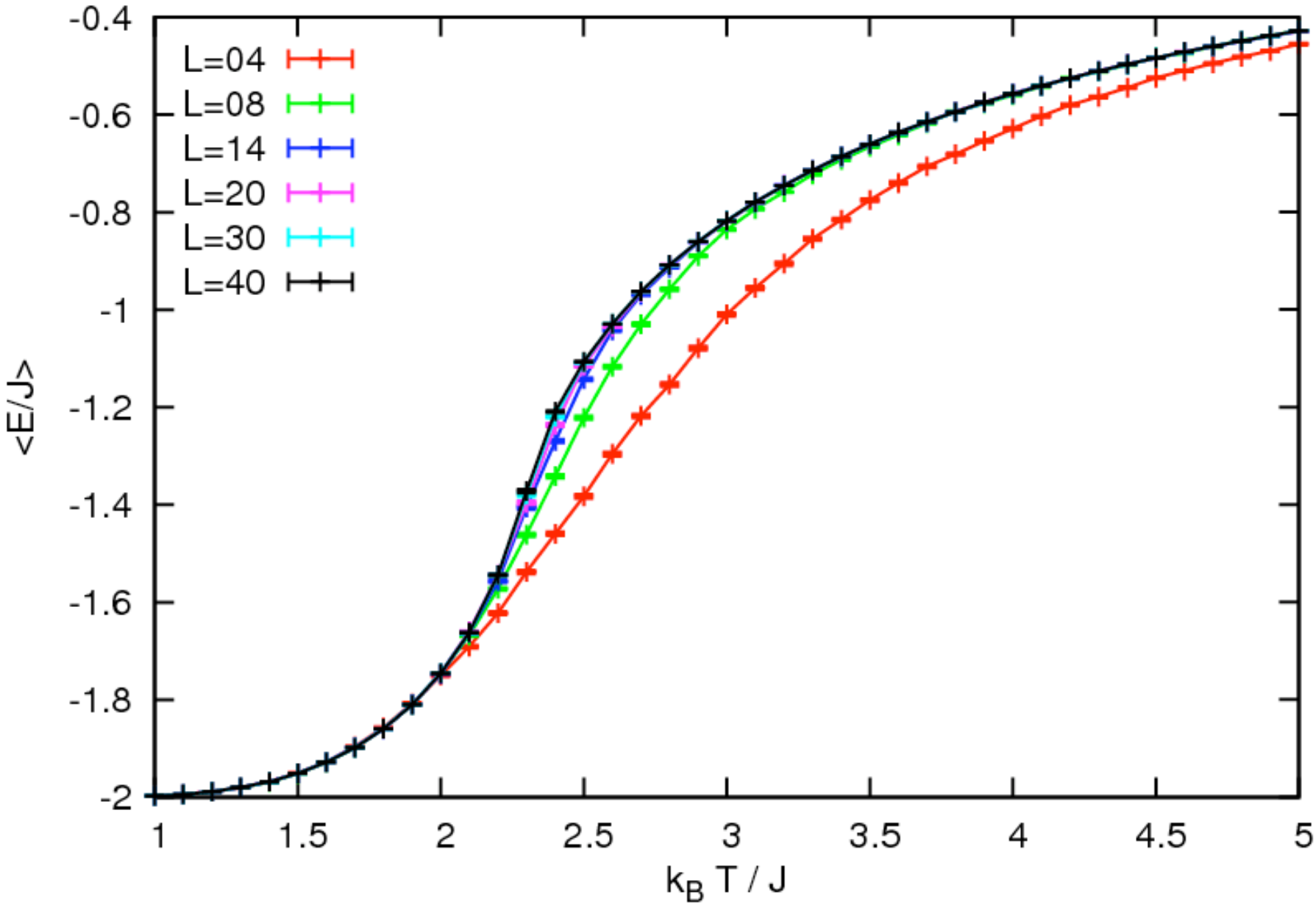


more on size effects…

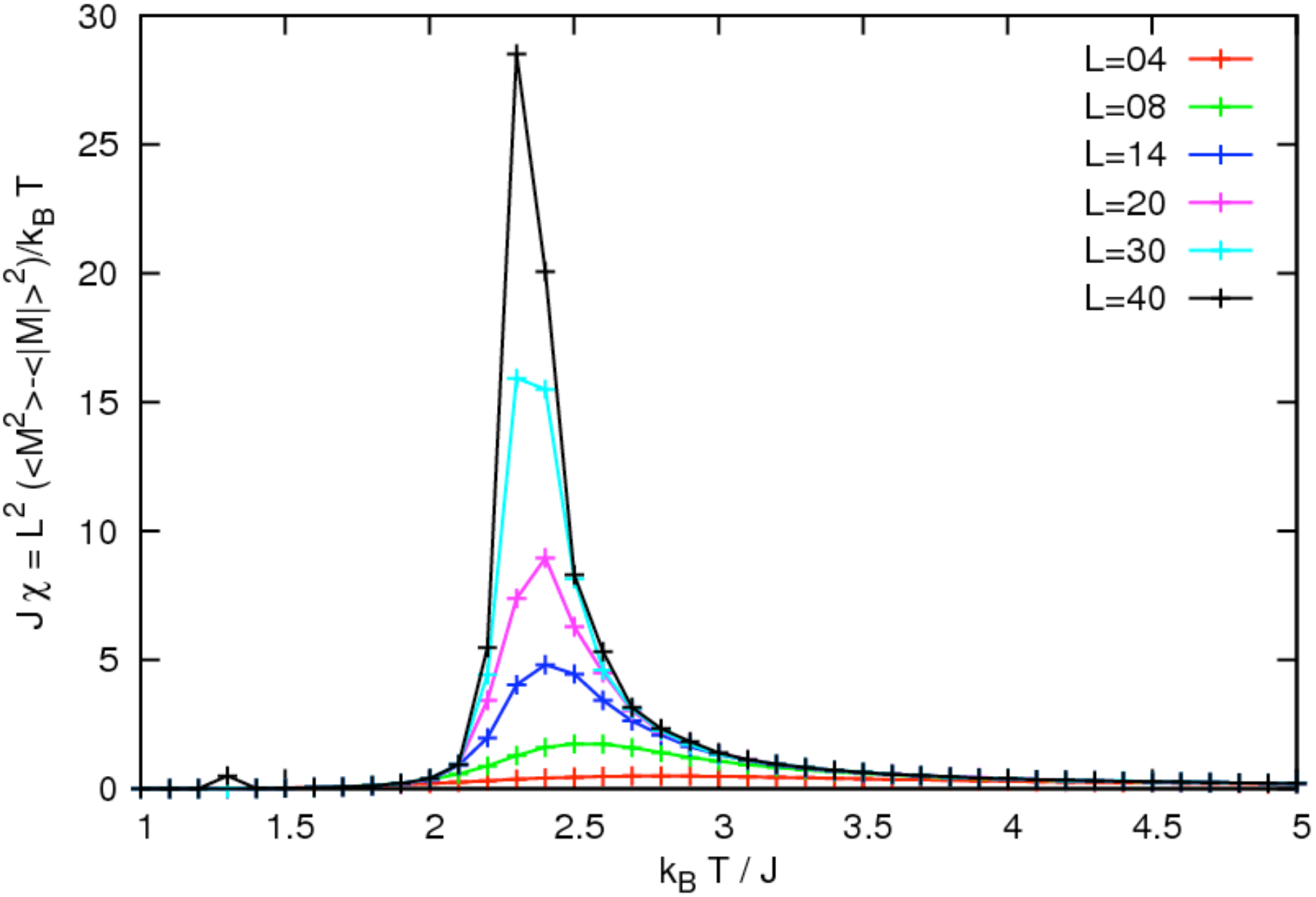
Magnetization (10^5 sweeps)



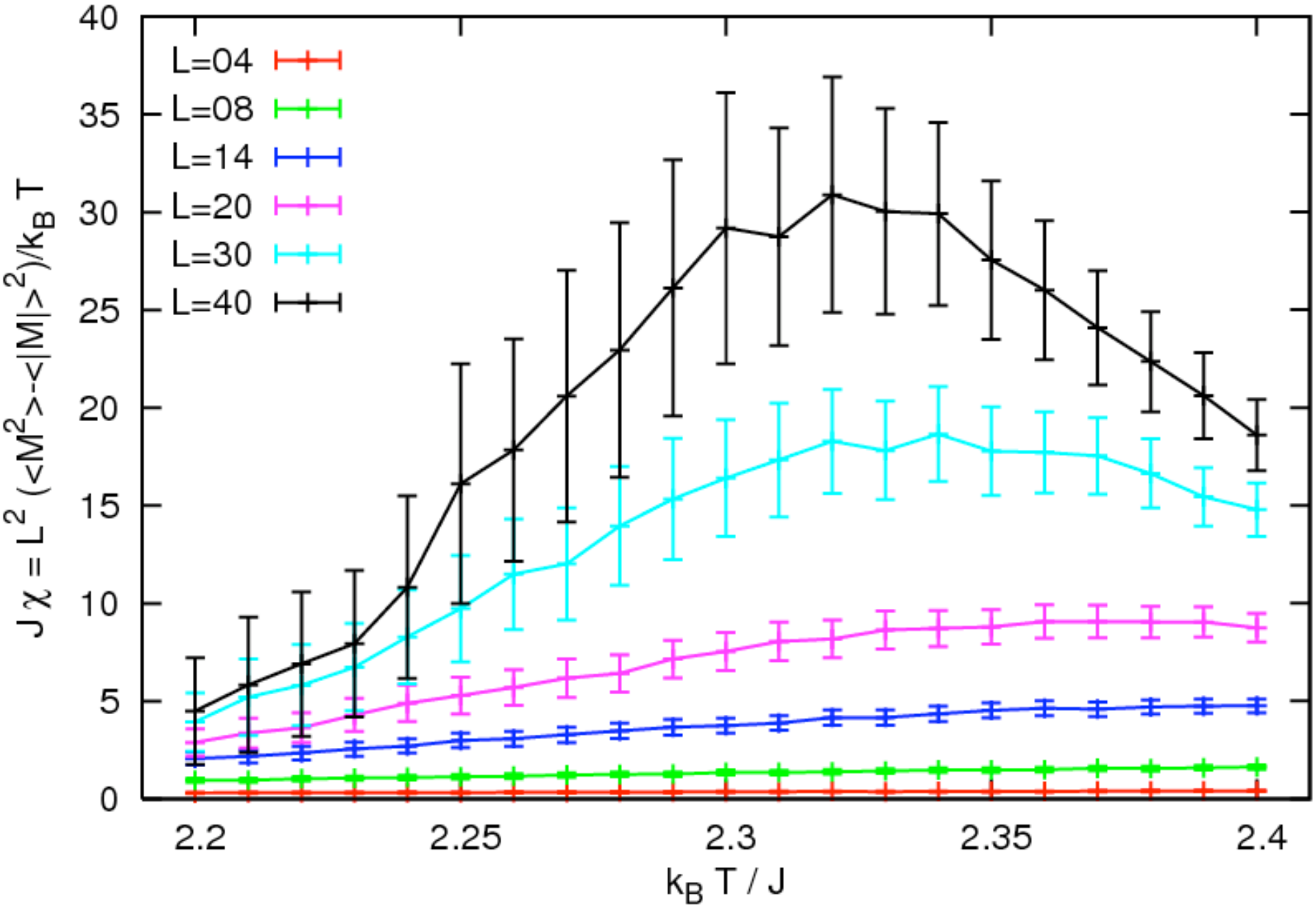
Energy (10^5 sweeps)



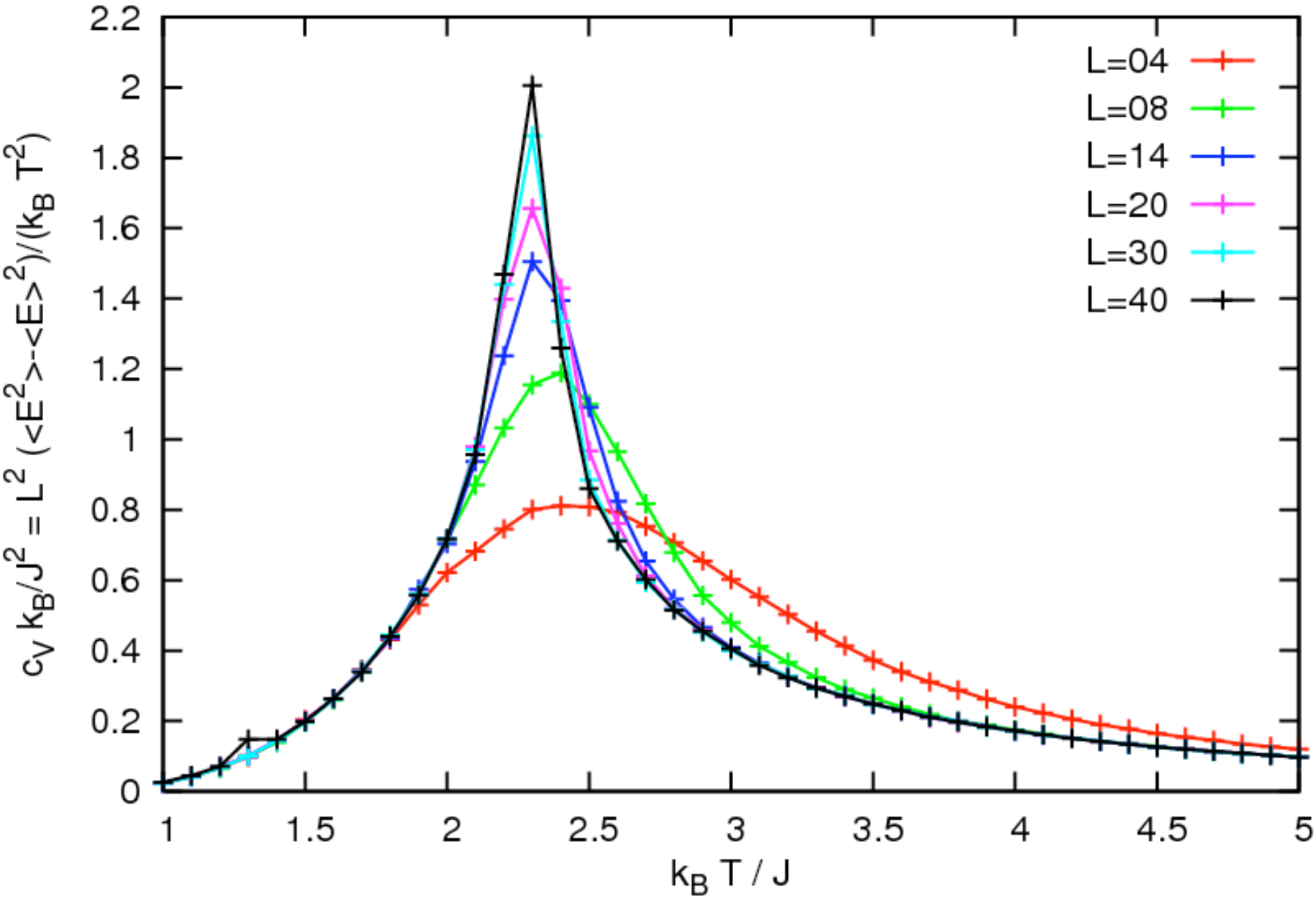
Magnetic susceptibility (10^5 sweeps)



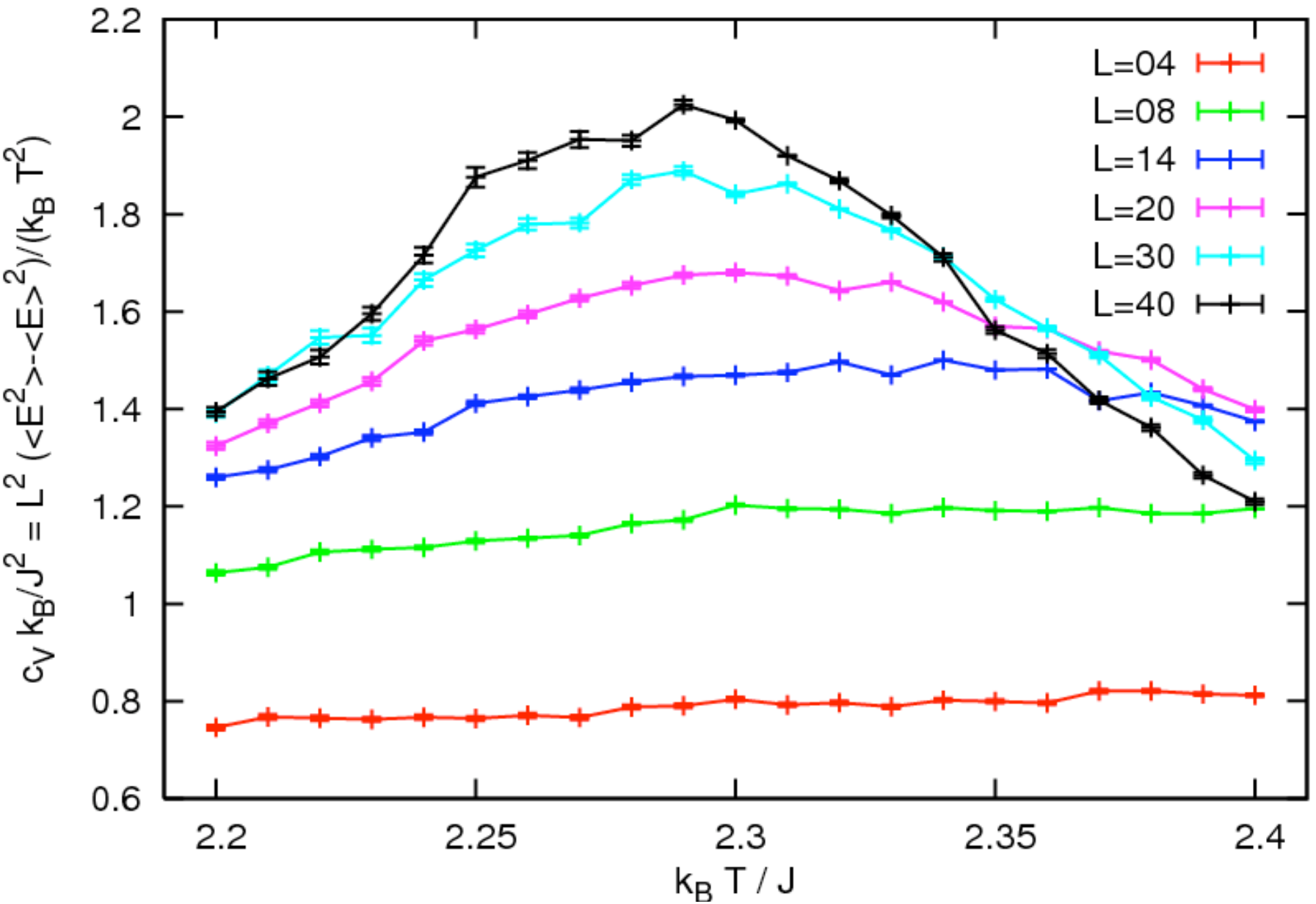
Magnetic susceptibility near T_c (10^6 sweeps)



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 . 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 T_c 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 fit,

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

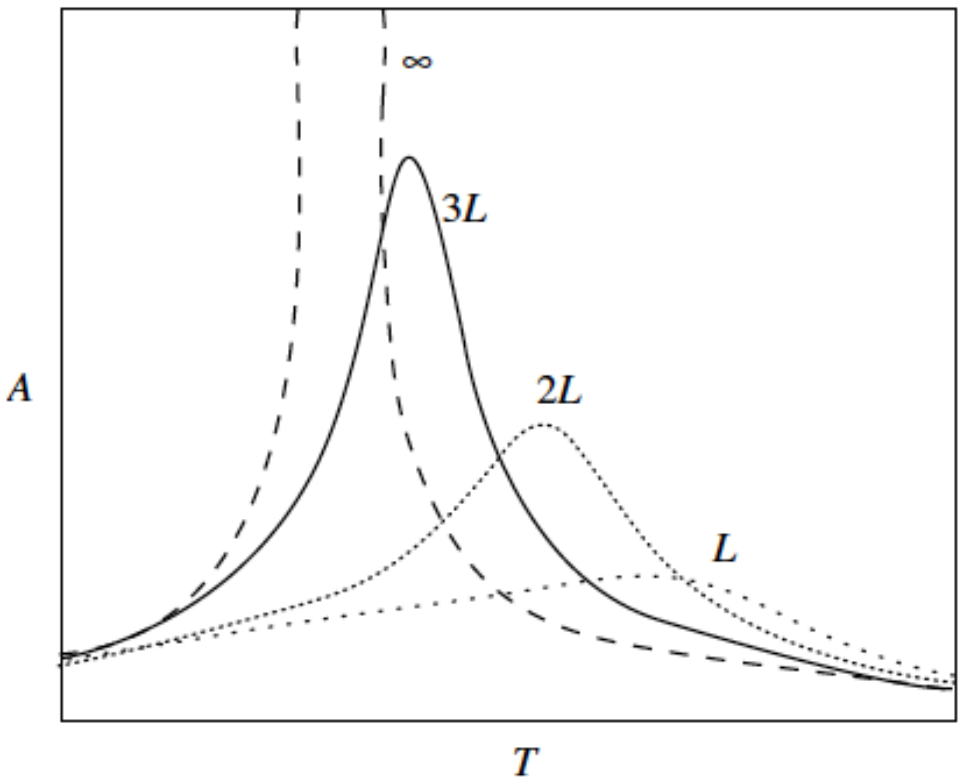


FIG. 1. Typical behaviour of a physical quantity A vs temperature close to the critical point for various system sizes. Figure taken from Thiissen[8].

[Thijssen, Computational Physics (Cambridge University Press)]

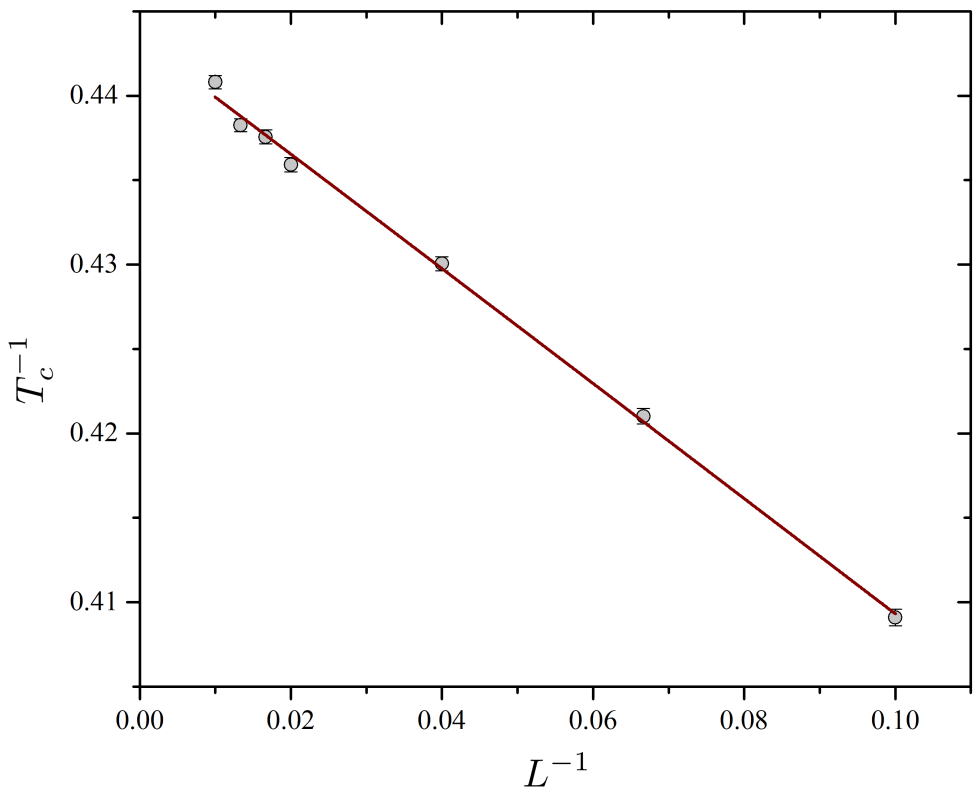


FIG. 9. (Color online) Inverse of the critical temperature T_c^{-1} vs inverse of lattice size L^{-1} for the 2D Ising model. The curve was fitted with a power law $T_c^{-1} = T_{c\infty}^{-1} - bL^{+1/\nu}$, and the critical exponent ν was determined.

$(L^{-1})^{-1/\nu}$

- 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:

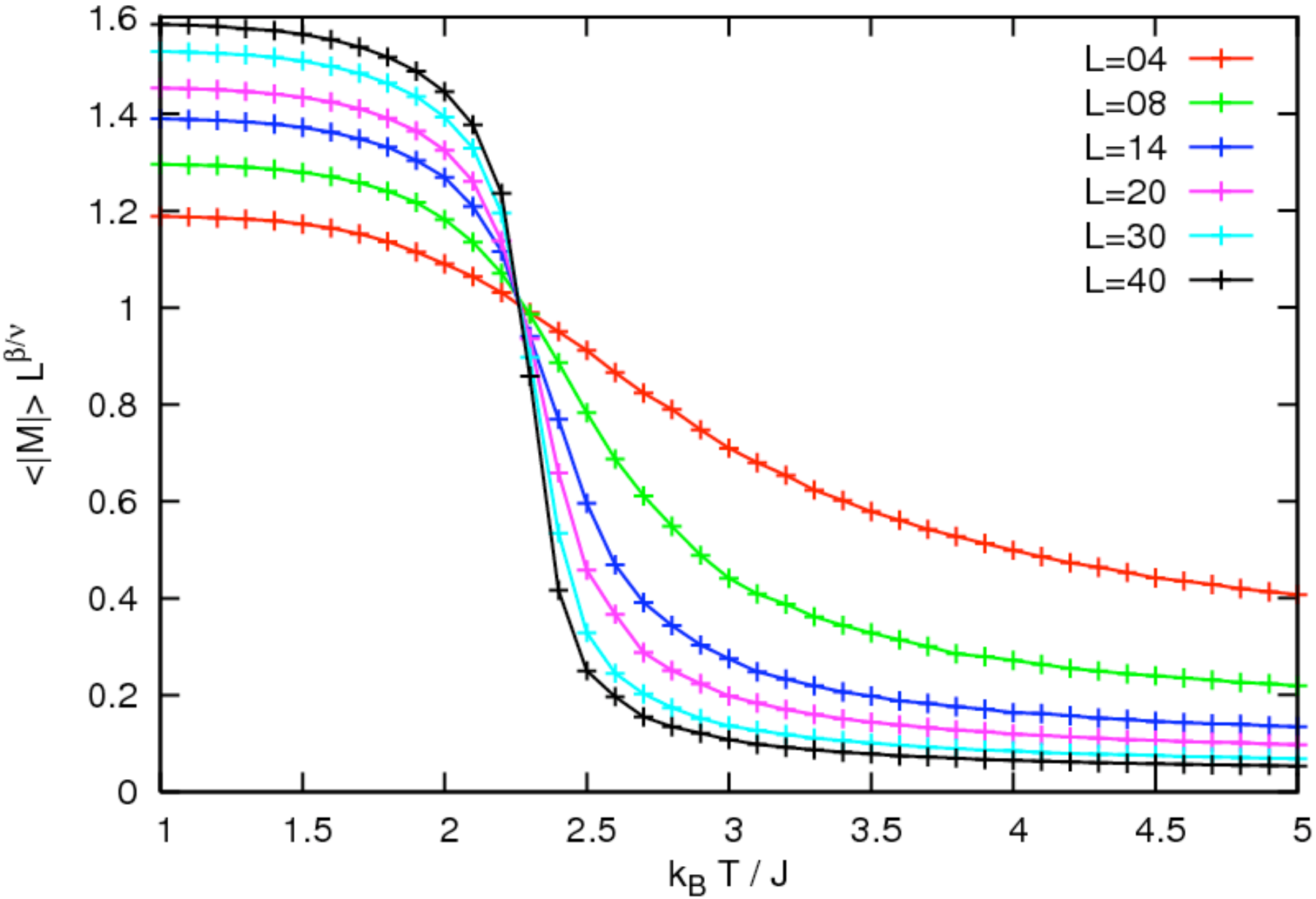
$$m(T) \sim (T_c - T)^{\beta} \to L^{-\beta/\nu} \tag{17.29}$$

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

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

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)

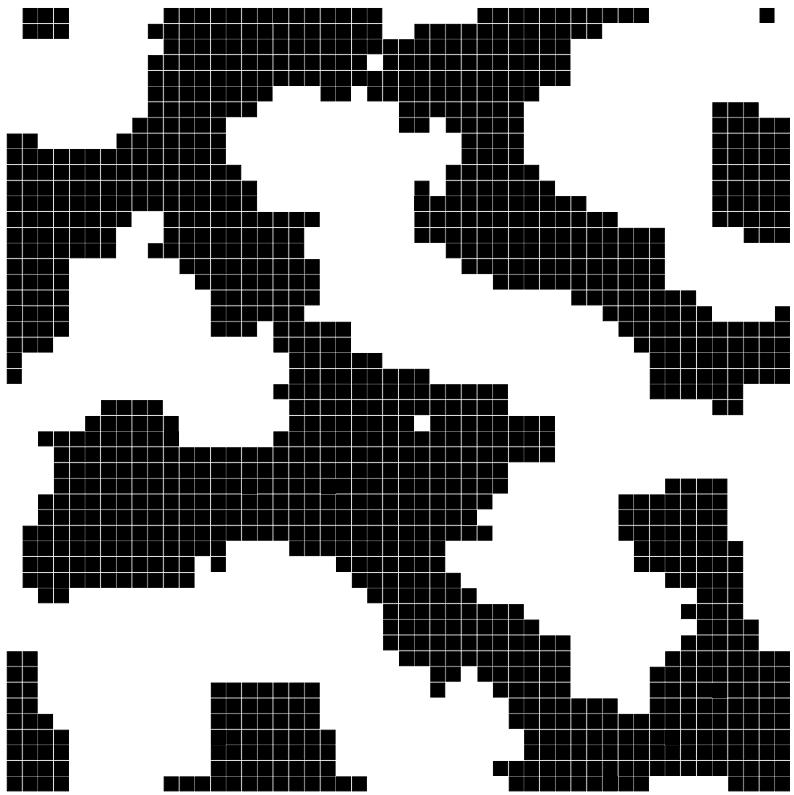
see e.g.: https://mattbierbaum.github.io/ising.js

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:

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

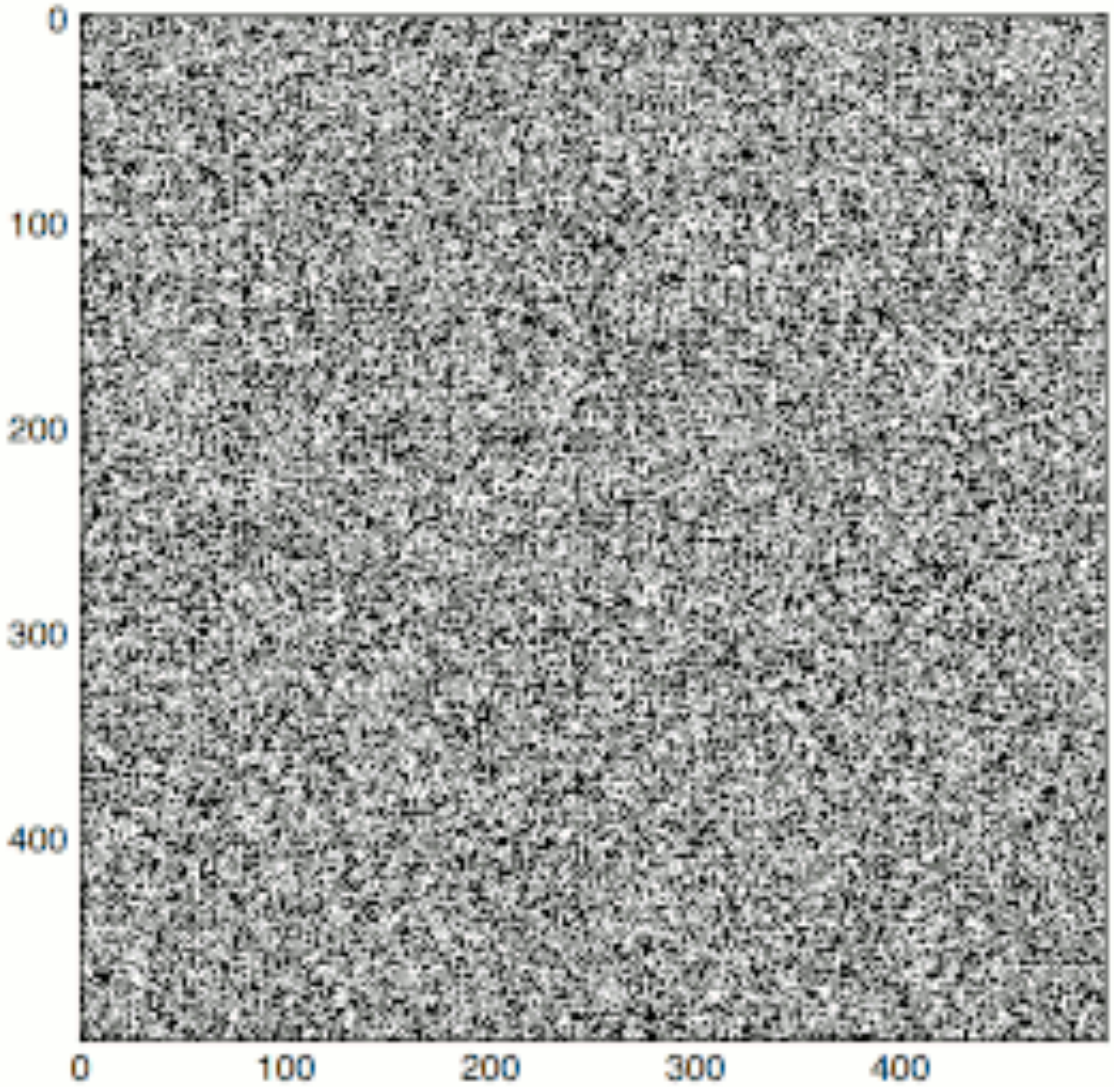
=> Trend to aggregation (diffusive behavior is limited to a transient)

- 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



500 x 500

parla di “inverse temperature beta” ???

T=?0, starting from random configuration

Ising model: other generalizations

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

Different behaviour according to the geometry and the kind of interactions.
Example: frustration in the triangular antiferromagnetic Ising model:

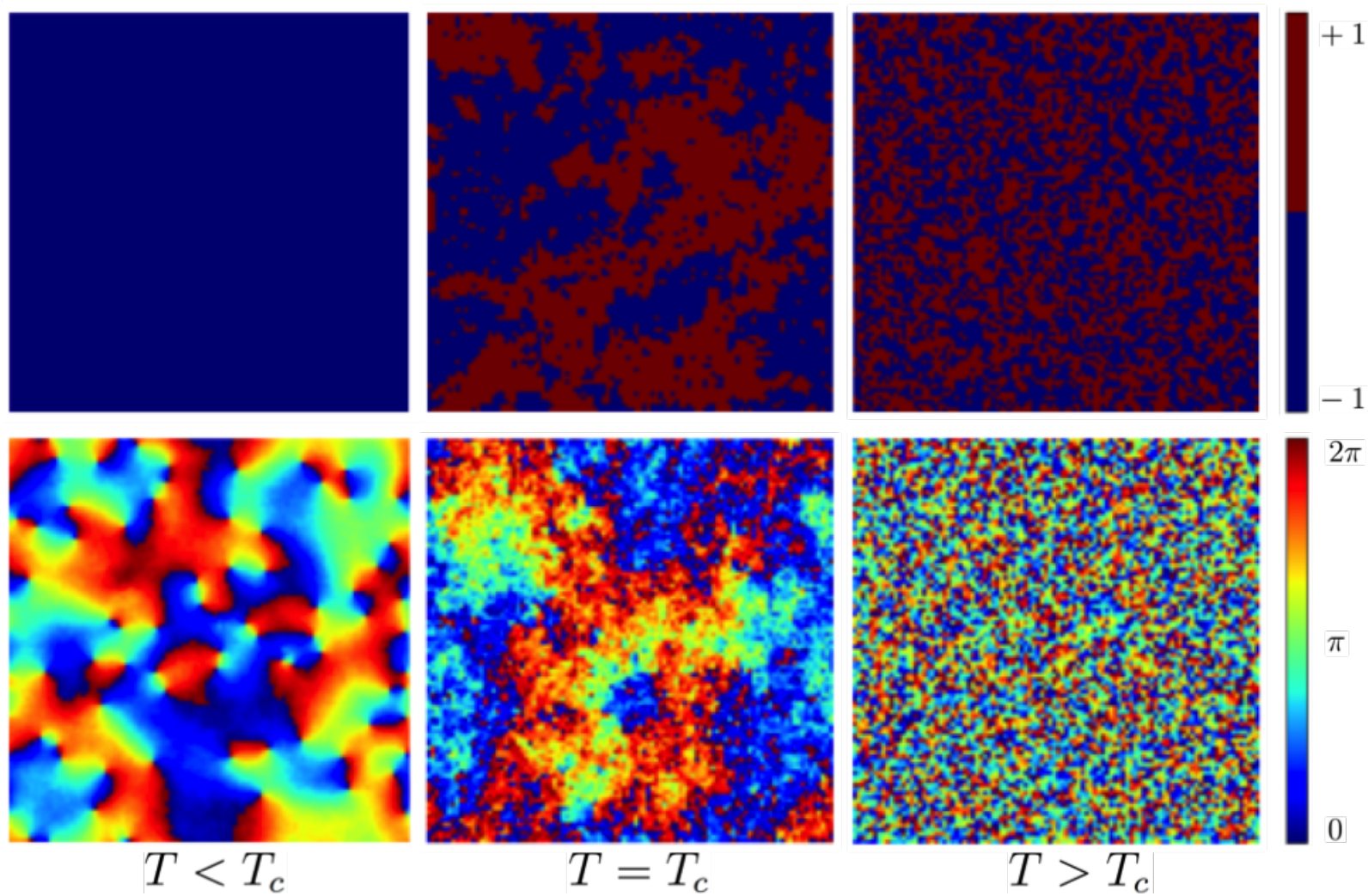
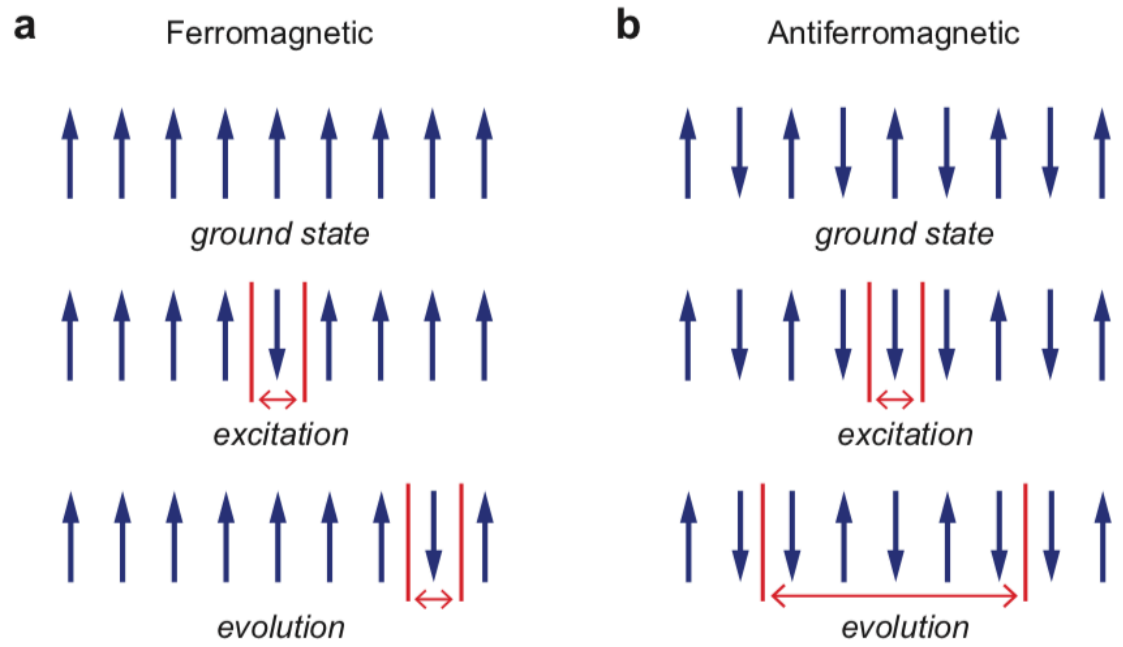


FIG. 15. (Color online) Behavior of the two dimensional Ising model (top) and XY model (bottom) at $T < T_c$, $T = T_c$ and $T > T_c$. For the Ising model, an $\uparrow$ spin ($s_i = 1$) is represented by red and a $\downarrow$ spin ($s_i = -1$) is represented by blue. For the XY model, because every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



a collective excitation of the spin structure in the lattice

With Spin exchange dynamics

Figure 1. (a) Magnon excitation and its evolution inside a ferromagnetic chain. In the ground state all the spins are in parallel alignment within each other. A magnon can be represented as a single reversed spin surrounded by two domain walls. It can propagate along the chain, but the domain walls will stay bounded to each other. (b) Same as (a) but for an antiferromagnetic chain, in the Ising limit. In the ground state, the spins are in antiparallel alignment. An excitation is achieved by creating two domain walls that separate two different AFM phases. Those two fractional excitations can independently propagate along the chain.