Università degli studi di Trieste
Corso di laurea magistrale in Fisica della materia

Laboratorio di Fisica Computazionale

Unit IX
Ising model

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Programming language used:
Python

Contents

1 Ising model on a square lattice

The aim is to simulate the behaviour of an *interacting ensemble of atomic magnetic momenta* disposed on a 2D square lattice, in equilibrium with a thermal bath[1] and in absence of an external magnetic field. To do so, we need a model that describes:

- energy: how do these object interact? (i.e. what is the system hamiltonian?)
- evolution: what is the system dynamics? (i.e. how to generate the actual micro-states trajectory in the phase space?)

1.1 Energy model: Ising hamiltonian

For ease sake we will refer to atomic magnetic momenta as "spins". The simplest energy model of interacting spins on a lattice we can build is indeed *Ising model*. It comes from the most general Heisemberg model, but unlike that, it only consider the possibility for the single spins to be $s_i = \pm 1$, it just takes into account nearest neighbor interactions and allows a unique interaction constant between all the spins. Mathematically, this results into:

$$\mathcal{H} = -\frac{J}{2} \sum_{\langle i,j \rangle} s_i s_j \tag{1}$$

where, depending on the sign of J, two possibilities arise: if $J > 0$ the hamiltonian describes a system in which spin alignment is energetically favoured. Otherwise, if $J < 0$ the anti-alignment is preferred.

The reason why we are deepening this model is that, despite its triviality, it has gained a certain importance in Physics: the Ising model alongside with its generalization have been the starting point for many theoretical efforts in the description of interesting properties and phenomena in materials.
In particular, with the hamiltonian (1) we have at disposal a first rough model to depict (spontaneous) *ferromagnetism* ($J > 0$) and *anti-ferromagnetism* ($J < 0$) alongside the corresponding phase transition.

1.2 System dynamics

Once we fixed the hamiltonian, we must set the system dynamics that reproduces the temporal evolution process. Starting from a certain configuration, how we generate new micro-states?
Here is where the *Metropolis Monte Carlo* algorithm comes into play: we randomly choose a spin on the lattice, flip it, evaluate the corresponding energy change and - since we are dealing with a canonical ensemble - the new configuration is accepted or rejected comparing the factor $e^{-\beta \Delta E}$ with a random number in $[0, 1[$.

1.3 Boundary conditions

Moreover, since we cannot simulate an infinite system, we basically have two choices for what happens at the simulation cell edge. The first - known as *Open Boundary Condition* - is the more straightforward and take as nearest neighbors of an external spin the available ones on the finite simulation cell (in a 2D square lattice 3 NN for a spin on the sides and 2 NN for a spin on the corners). In the second - referred to as the *Periodic Boundary Condition* - a spin that lies on the edges, beside having as nearest neighbors the spins available on the cell as before, is connected with the spin sitting on the opposite side of the cell itself (so that on a 2D square lattice every spin has 4 NN, including the ones on the corners).
Throughout the entire unit we will use the PBC, but later we are going to analyze back further differences of the two conditions in more detail.

[1] We are thus in the context of the *canonical ensemble*, for which hold the same consideration done in Unit VII

1.4 Interesting physical quantities

The "instantaneous" physical quantities we will look at are[2] the *energy per spin* e and the *magnetization per spin* m:

$$e \equiv \frac{E}{N} = -\frac{J}{2N}\sum_{\langle i,j\rangle} s_i s_j \qquad\qquad m \equiv \frac{M}{N} = \frac{1}{N}\sum_{i}^{N} s_i \tag{2}$$

In this case m is also called *order parameter*. In fact, the Ising model brings with it the possibility for the system to undergo a second order phase transition: in the thermodynamic limit (large N), under a certain critical temperature T_C the spins spontaneously (i.e. without an external magnetic field!) align reaching the hamiltonian ground state with $E_0/N = -2J$. The magnetisation thus become a good parameter that allows to distinguish between the "disordered" phase above T_C where $|m| = 0$, and the "ordered" phase below T_C where $0 < |m| \leq 1$.

As for the temporal averages of these two quantities, we know that they are converted into ensemble averages $\langle e\rangle$ and $\langle m\rangle$ in the statistical mechanics framework and can be numerically evaluated through the Metropolis technique. The investigation of the temperature dependence of the average energy and magnetization per spin will allow us to study the phenomenon of phase transition, at least from a qualitative point of view.

The last two quantities of interest in this unit are the *linear response functions* $c \equiv C/N$ and $\chi \equiv X/N$, related to the intrinsic stochastic fluctuations at the equilibrium of the canonical ensemble:

$$c \equiv \frac{C}{N} = \frac{1}{N}\frac{\partial\langle E\rangle}{\partial T} = \frac{1}{Nk_BT^2}\left(\langle E^2\rangle - \langle E\rangle^2\right) \tag{3}$$

$$\chi \equiv \frac{X}{N} = \lim_{H\to 0}\frac{1}{N}\frac{\partial\langle M\rangle}{\partial H} = \frac{1}{Nk_BT}\left(\langle E^2\rangle|_{H=0} - \langle E\rangle|^2_{H=0}\right) \tag{4}$$

The emergence of the second order phase transition is even more evident for c and χ since a rapid change in $\langle e\rangle$ and $\langle m\rangle$ implies a singularity in the response functions. Indeed, when larger and larger fluctuations of determined physical quantities (such as E or M) appears while changing external parameter (such as T), this typically signals that a phase transition is approaching.

[2]Provided that we will work with 2D square lattice with linear size L, the total number of sites is $N = LxL$

2 Numerical results

In our computational experiment[3], the lattice spins dynamics is implemented by the Metropolis algorithm and, as we learnt back in unit VII, this means the whole stochastic process is affected by correlation. To achieve a fair level of statistical independence among two following configurations, the numerical estimation of E and M is implemented by updating their values just after a certain number of trial moves has been carried out on randomly chosen spins. We fixed this specific number as N so that, on average, all the lattice sites are in principle tested in the meanwhile.

2.1 Study of equilibration time

By definition, the considered system is described in the context of the canonical ensemble, so a question that arises quite spontaneously is: since we start from a random configuration, how many Monte Carlo steps are needed for the system to reach the thermal equilibrium?

A relatively simple way to proceed is plotting the *instantaneous* energy and magnetization per site and then manually checking at which point the trend stabilizes: this trick can be repeated for different values of temperature at a time. However, the larger and larger energy fluctuations that characterize the system as T grows make this estimation not trivial. One direct consequence is that the values one finds might depend, on some extent, on the personal criterion employed. Anyway, since we are interested in a qualitative estimation, this issue will not prevent us from drawing a conclusion on the global trend.

In Fig 2.1 are reported the collected data for three different lattice sizes[4]. What strikes most is the sharp increase around a value of T compatible with the expected T_C for such a system[5]. This could be interpreted as the first sign of the critical behaviour of the Ising spin lattice model: as T_C is approached, the spin lattice exhibit correlations on wider an wider scales. Therefore the time needed to get two following independent configuration dramatically increases, as well as the number of MC steps necessary to obtain numerically thermal equilibrium.

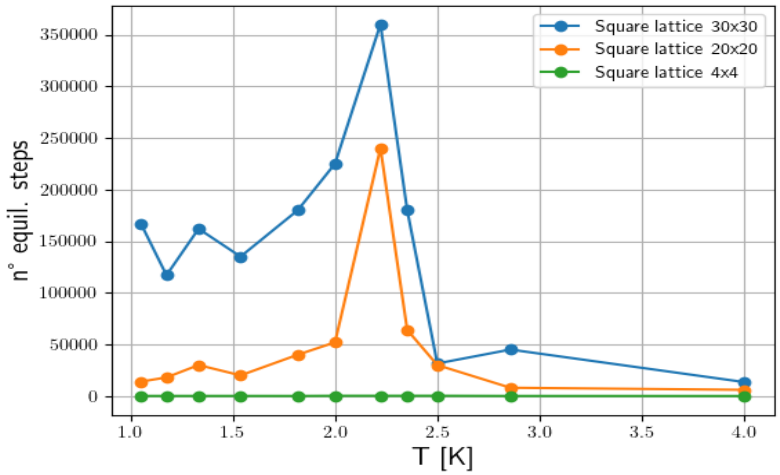


Fig 2.1 Number of MC equilibration steps as function of T.

2.2 Random vs ordered starting configuration

We mention by passing that we tried as well to study the dependence of the equilibration time on the specific initial configuration. In particularly, this was done by setting a "chessboard" starting pattern instead of a random one and let the algorithm run as always. We observed something different was going on, but the variability of the data was so high that, even with different runs, it was not possible to recognize a general trend out of them as before, making this qualitative study fairly inconclusive.

[3] By convention both J and k_B are set to 1.
[4] Although not appreciable with the chosen plot scale, the trend for the $4x4$ is similar to the others'.
[5] The theoretical value of T_C in the thermodynamic limit correspond to $T_C = 2.269K$.

2.3 Temperature dependence of some physical quantities

We now intend to check whether - and to what degree - the numerical implementation of this simple model reproduces some well-known experimental results. If it effectively did, we would have proven, at least qualitatively, this rough framework is indeed suitable to describe at a basic level the behaviour of a certain class of materials and the physical phenomena that rule them, such as the second order phase transition in elementary ferromagnetic systems. To do so, we study the temperature dependence of the physical quantities presented in §1.4 and look for evidences of a critical phenomenon and possibly identify when it occurs.

In Fig 2.2 are shown the collected data for different lattice sizes, for all of which the appropriate equilibration length has been chosen according to what done in §2.1. At the same time, the number of Monte Carlo steps has been fixed so that the overall collected points are 10^4, independently from the linear dimension L.

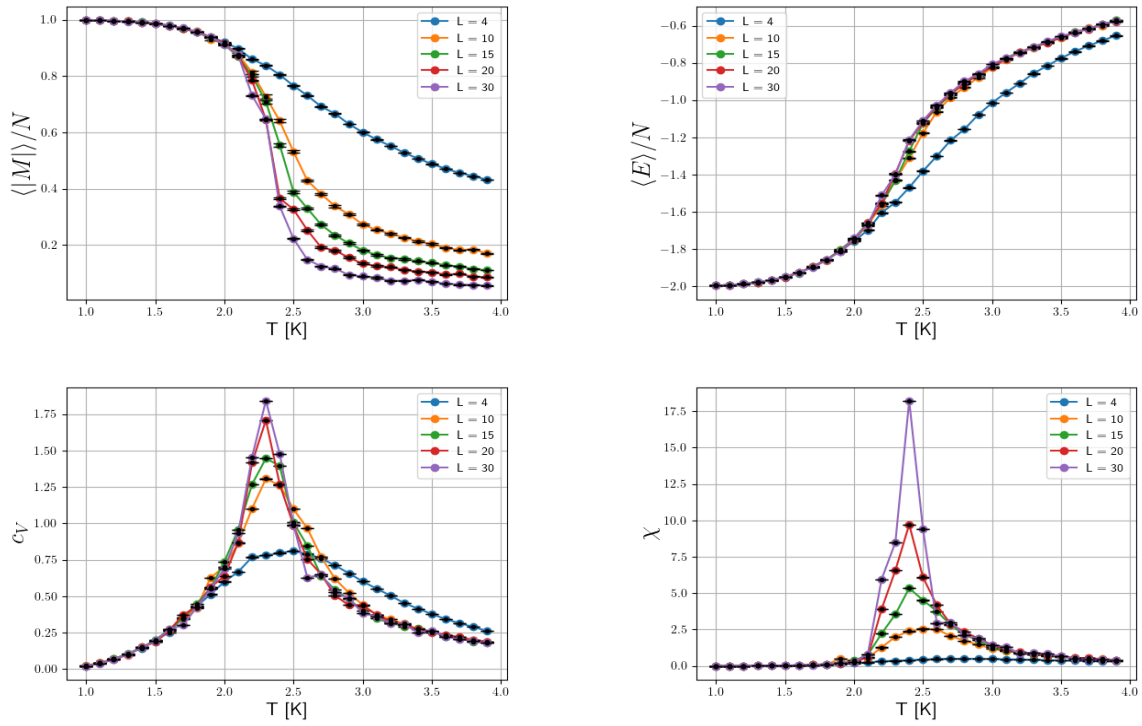


Fig. 2.2 Numerical simulation for the quantities a) $\langle |M| \rangle / N$, b) $\langle E \rangle / N$, c) c_V, d) χ.

The first upper plot on the left depicts something we can observe in common magnets: at sufficiently low temperatures[6], the mean (absolute) magnetization per site is clearly different form zero (tends to 1 as $T \to 0$): by definition, the system exhibit a net magnetization. Its equilibrium configuration is strongly determined by the fact that exchange effects are sufficiently large to cause neighbouring atomic spins to spontaneously align and this gives rise to what is called "spontaneous magnetic order". On the other hand, since at higher temperatures $\langle m \rangle$ drops to zero, we can conclude that thermal fluctuations completely eliminate any alignment and so the system tends to be "magnetically disordered".

There is another feature that jumps out and that enrich our interpretation: if the transition from magnetic order to magnetic disorder appears to be rather flat for small values of L, as the lattice dimension increases it gets more and more sloping, keeping however smooth. We can imagine that for $N \to \infty$ the trend would reasonably look like the curve in Fig 2.3, as Onsager predicted in a seminal work where he managed to provide the analytical solution of this model.

[6] In what follows, we are going to to address from a quantitative point of view the question of what is meant by a "sufficient low" temperature

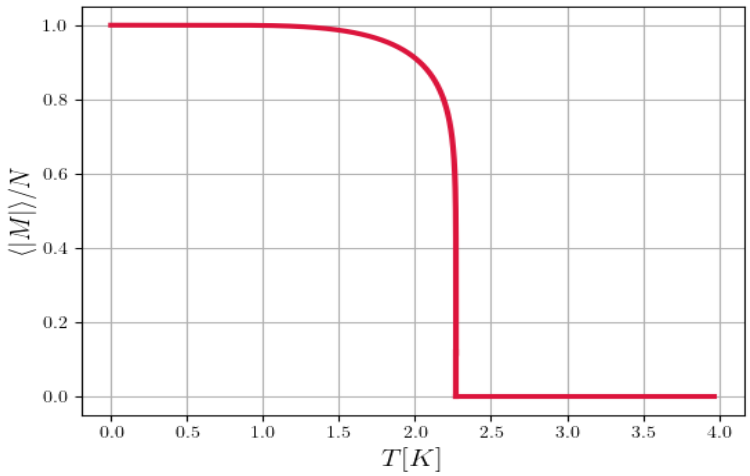


Fig 2.3 Asymptotic trend of $\langle m \rangle$ as function of T, from Onsager theoretical prediction (1944).

This peculiar characteristic can be interpreted as a typical sign of the emergence of a second order phase transition, where, in the thermodynamic limit, the magnetization - that we took indeed as "order parameter" - *continuously* increases from zero (disordered configuration) to finite values (ordered configuration) after a certain *critical temperature* is crossed when lowering T.

We take the opportunity to emphasize that, within the context of Statistical Mechanics, the formalism behind the introduction of the thermodynamic limit is rather subtle and still recently has been subject of discussion. It is a mathematical idealisation that serves as a guide to understand what happens in the real world, but does not actually describe it: a real system, indeed, usually have N and V very large, but not infinite! However, the existence of the phase transition and the presence of states with different symmetries (order-disorder), is owed to a large degree to the singularity of the thermodynamic limit. Thus, it is thanks to this prescription that our theoretical model can hope to describe - at least qualitatively - the critical behaviour of a macroscopic ensemble of particles.

Now, since numerical simulations force us to work with finite samples, they must rely on "finite size scaling" theory for reliable data extrapolation and analysis. This mechanism, along with the choice of periodic boundary conditions, allows to describe the build-up of bulk properties when a small system is increased in size: this is the ultimate reason why we performed simulations on latices of increasing L.
Table 2.1 report an estimate of the critical temperature as a fitting parameter of the absolute mean magnetization data. The interpolating curve we thought could describe the best the obtained points is the sigmoid and the parameter of interest is the one corresponding to the inflection point, x_0:

$$f(x) = \frac{L}{1 + e^{-k(x - x_0)}} + c \tag{5}$$

Although the asymptotic Onsager solution looks different, for the considered values of L in this temperature range this $f(x)$ seems indeed a satisfying approximation.

lattice size L	estimated $T_C[K]$
4	2.68 ± 0.1
10	2.46 ± 0.1
15	2.40 ± 0.1
20	2.37 ± 0.2
30	2.33 ± 0.2

Tab 2.1 Numerical estimation of T_C from the plots.

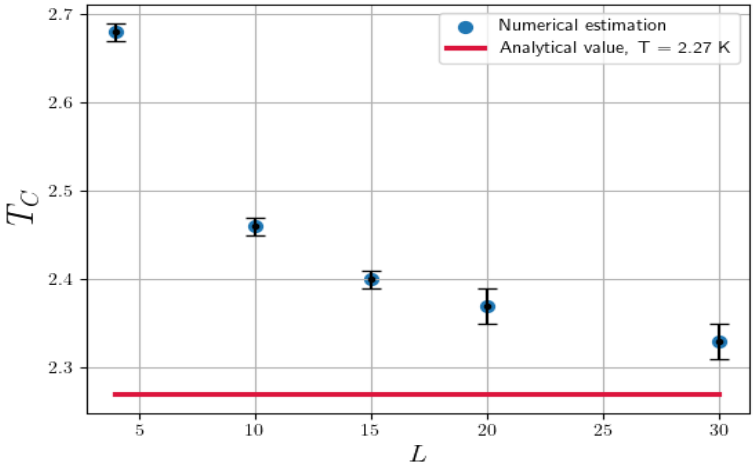


Fig 2.4 Numerical T_C vs linear lattice size L.

As fig. 2.4 shows, the so estimated value of the critical temperature decreases as the lattice size grows, apparently approaching the theoretical prediction of $T_C = 2.27K$.

Other interesting information can be inferred looking at the *specific heat* and *magnetic susceptibility*. As L is increased, the corresponding curves exhibit sharper and sharper peaks near the estimated T_C. This behaviour is typical of strongly correlated systems, where critical fluctuations - that c_V and χ describe by definition - develop with increasing system size around a threshold temperature. In the thermodynamic limit the Curie temperature is indeed a critical point for the magnetic system: the magnetic susceptibility is theoretically infinite and, although there is no net magnetization, spin correlations fluctuate at all length scales. The same goes for energy fluctuations and specific heat: as T is increased energy fluctuations make favorable for the system to reach a stable state that is far away from the hamiltonian ground sate with $E_0/(JN) = -2$.

In fig. 2.5 are reported the specific heat curves whose points, instead of passing through the energy variance, have been obtained by performing the numerical derivative on the $\langle e \rangle$ dataset. As can be noticed, the general appearance is similar to the one in fig. 2.2.c, but since this method is rather sensible to the mean energy fluctuations that are particularly stronger around T_C, the peak shapes are less defined. As a consequence, under equal conditions on the temperature spacing sampling, the variance method is to be preferred.

To conclude this second part of the analysis, the presence of fluctuations on pretty all ranges is then a net marker for a second order (or continuous) phase transition and can thus help us to identify and better understand critical phenomena such as the spontaneous magnetization.

All the aforementioned characteristics have an elegant and deeper description in the context of *spontaneous symmetry breaking* theory, where the symmetries that rule the hamiltonian are compared to the ones of the system states and where a difference between the two can be attributed to physical phase transitions of the considered system. This innovative approach, however, goes well beyond the original goal of this report and we just mention it so that can be used as an inspiration for a more comprehensive study of the subject.

2.4 Periodic Boundary Conditions vs Open Boundary Conditions

We come back to the question on how different periodic conditions can afflict the simulation.
While the results discussed in §2.3 have been obtained with *periodic* boundary conditions in order to properly implement the thermodynamic limit, we repeat the runs using this time *open* boundary conditions and will study potential deviations. The modified part of the code concern the energy calculation: this naturally lead to different values of expected mean energy, as can be easily noticed looking at the

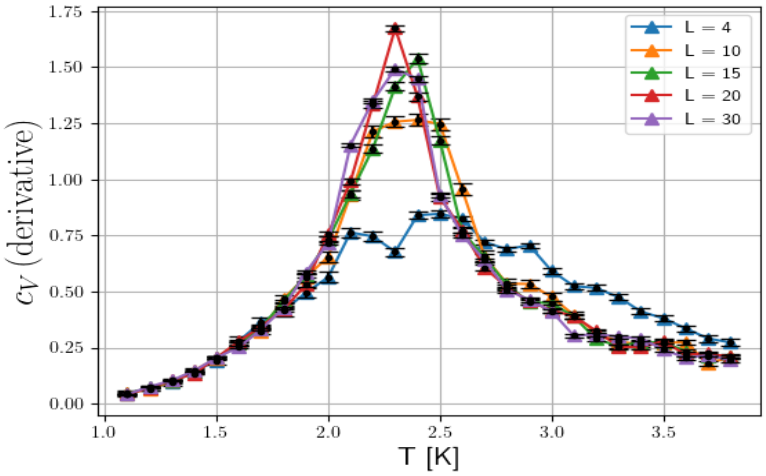


Fig 2.5 Specific heat from "direct" calculus, for various L.

ground state energy:

$$\begin{cases} e_0 = \frac{-\frac{1}{2}(4*N)}{N} = -2 & \text{with Periodic BC} \\ e_0 = \frac{-\frac{1}{2}\left(2*4+3*4(L-2)+4*(L-2)^2\right)}{N} = \frac{-2(L-1)}{L} & \text{with Open BC} \end{cases} \tag{6}$$

It is just for large L that the different surface terms in the OBC framework become negligible compared to the bulk interaction contribution and the two values asymptotically converges. This mathematical prediction is promptly confirmed by the simulations.

Indeed, this intrinsic energy disparity directly affect the system critical behaviour, as can be seen in fig. 2.6. The plots are the analogous of the ones in fig. 2.2, but with an evident difference: the asymptotic value of T_C - the same as before - is now approached in the opposite direction, from below. Now, the fact that the two dynamical models share the same asymptotic critical temperatures is due to the equivalence between the Open and the Periodic prescriptions for the edges behaviour in the thermodynamic limit. On the other hand, the fact this value is reached from below with increasing L might be traced back to a *topological* difference. Remember that now the spins on the boundary do not interact with the ones on the opposite side: if we start from a (partially) ordered configuration at low temperature and increase T, in such a closed system with finite size it is easier to trigger those critical fluctuation that, correlating the system on all posible lenght scale, bring the lattice to a completely disordered configuration. Taking larger and larger lengths L the effect of the borders becomes less important and the system witness a phase transition whose threshold value gets closer and closer to the ideal one.

Retracing what has been done in §2.3, with a series of interpolations on the absolute mean magnetization curves, we obtain a numerical estimation of the critical temperature for different lattice sizes. The results are reported in tab. 2.2.

lattice size L	estimated $T_C[K]$
4	1.86 ± 0.2
10	2.08 ± 0.1
15	2.12 ± 0.1
20	2.15 ± 0.1
30	2.21 ± 0.2

Tab 2.2 Numerical estimation of T_C from the plots: Open BC.

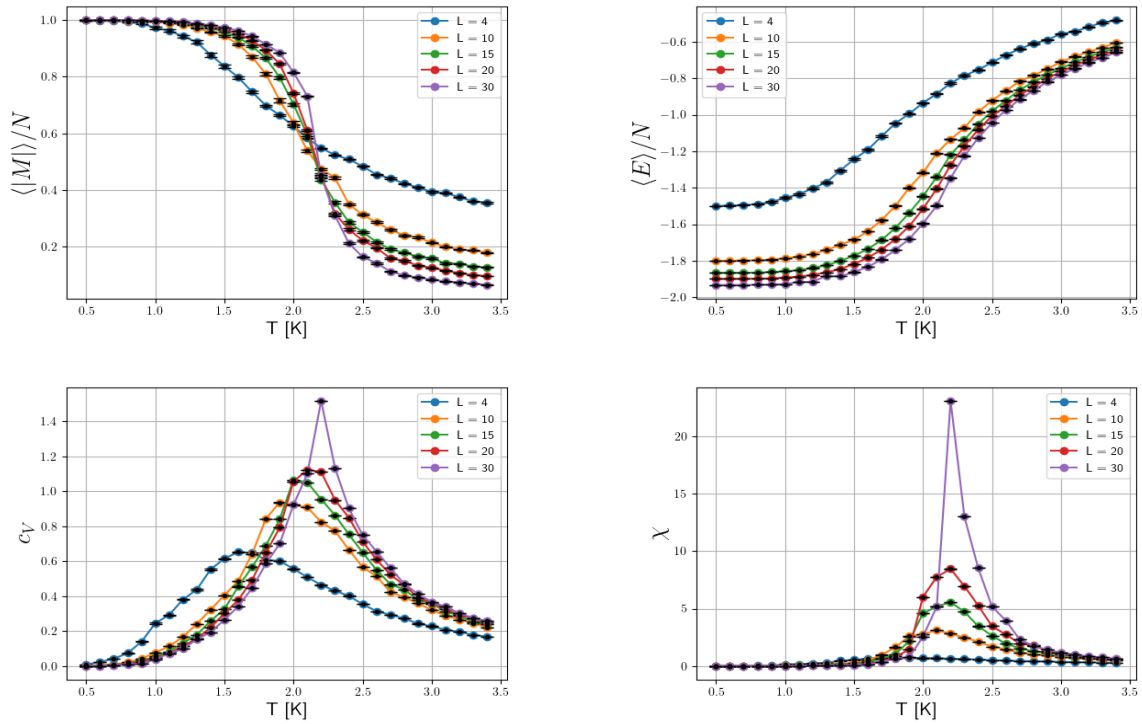


Fig. 2.6 Open BC: numerical simulation for the quantities a) $\langle|M|\rangle/N$, b) $\langle E\rangle/N$, c) c_V, d) χ.

In fig 2.7 are graphically shown the so obtained data: the increasing trend towards the theoretical value, the exact opposite of what obtained with the PBC, is well evident.

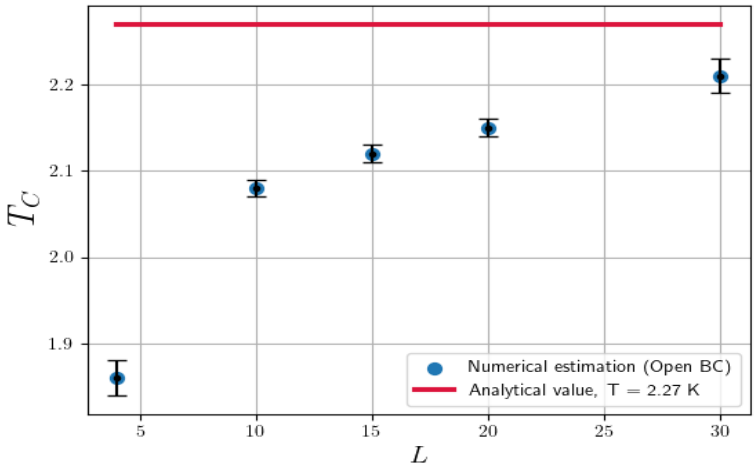
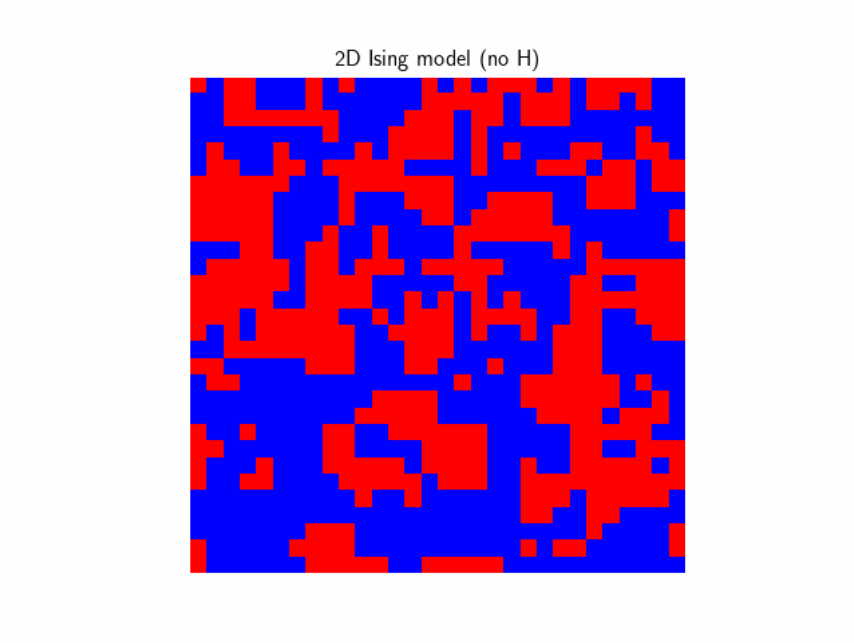


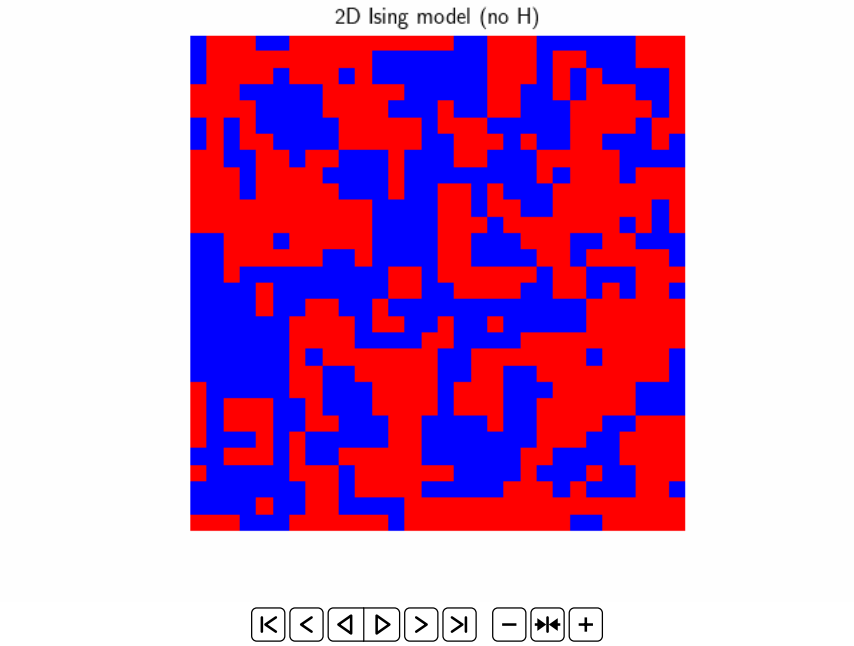
Fig 2.7 Numerical T_C vs linear lattice size L: Open BC.

2.5 Visualizing the evolving configurations (optional)

We conclude with a couple of animation that allow us to visualize the spin lattice variation during the evolution within the Metropolis algorithm. For curiosity sake we printed out the animation for two different starting configuration: One begins with the spin randomly chosen, while the second with an ordered "chessboard" configuration. Spin up $s_i = +1$ and spin down $s_i = -1$ are respectively mapped into red and blue pixels.



Random starting configuration, $L = 30$, $n_{MC} = 2 * 10^5$



Chessboard-like starting configuration, $L = 30$, $n_{MC} = 2 * 10^5$