Accurate computation of critical properties for the 2-D Ising model on periodic networks through finite size scaling analysis

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The aim of this article is to study in a rigorous way at the computational level the critical properties of 2D Ising Model. We have used the Metropolis algorithm for a square lattice with periodic boundary conditions in a ferromagnet without external field. We will also address the effect of an external magnetic field, and lattices with triangular and hexagonal symmetry.

I. INTRODUCTION

Simulations are carried out for the 2D Ising model over a square lattice of L×L nodes with periodic boundary conditions in a ferromagnet (with coupling constant J=1), ruled by the hamiltonian

$$\mathcal{H} = -J \sum_{<ij>} \sigma_i \sigma_j - h \sum_i \sigma_i$$

where $\sigma_i = \pm 1$ are the allowed spins of the $V = L^2$ particles.

Let us define $\epsilon = E/V$ (energy per site), u(internal energy), C(heat capacity), m(magnetization) and χ (susceptibility):

$$u = \frac{\sum_{\{\sigma_i\}} H(\{\sigma_i\}) e^{-\beta H(\{\sigma_i\})}}{V \sum_{\{\sigma_i\}} e^{-\beta H(\{\sigma_i\})}} \qquad m = \frac{\sum_i \sigma_i}{V}$$

$$C \equiv \frac{du}{dT} = \beta^2(<\epsilon^2> - <\epsilon>^2)$$

$$\chi \equiv \frac{d<m>}{dh} = \beta(<m^2> - <m>^2)$$

According to the exact solution given by Onsager, the mean magnetization for $V \to \infty$, and h=0, is

$$<m> = \begin{cases} (1-(\sinh(2\beta))^{-4})^{\frac{1}{8}}, & \beta \geq \beta_c \approx 0.440687 \\ 0 & \text{otherwise.} \end{cases}$$

This corresponds to a phase transition, thus telling us that in our simulations we will see that at high temperatures spins are random and uncorrelated, but as the temperature is lowered the interactions between them encourage nearby spins to point in the same direction, giving rise to correlations. Groups of adjacent spins which are correlated (tend to point in the same direction) are called clusters. As we approach β_c, the typical size ξ of these clusters, known as correlation length, diverges giving place to arbitrarily large areas in which the spins are pointing mostly up or mostly down [1].

II. METROPOLIS ALGORITHM

At each sweep ("time step") we pick the spins to be updated according to: first for those such that i+j is even and afterwards the rest [2]. Each spin is flipped according to the probability rule:

$$W(\{\sigma_i\}_{old} \to \{\sigma_i\}_{new}) = \begin{cases} 1 & E_{new} < E_{old} \\ e^{-\beta(E_{new}-E_{old})} & E_{new} \geq E_{old} \end{cases}$$

which guarantees that a stable equilibrium will be reached.

Fig. 1 displays the square lattice for L=32 on which we have implemented the Metropolis algorithm. We show as blue dots spin s=-1 and as red dots those with spin s=1.

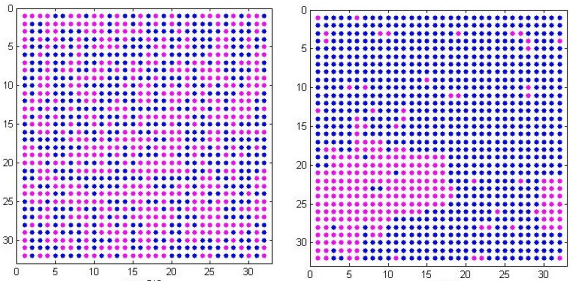

FIG. 1. On the left there is the initial state of the system where the spin of the particles is randomly generated. On the right we show (after a few sweeps) the state of a system for $\beta = 1$, for which we expect almost complete magnetization.

III. STATISTICAL ERROR ESTIMATION

The first problem we have to face is that there exists a correlation between the magnetization of two consecutive sweeps, which affects the needed number of samples N. The larger the correlation, the larger number of samples we need. The autocorrelation is computed by:

$$A(k) \equiv \frac{<m_i m_{i+k}> - <m_i><m_{i+k}>}{<m_i^2> - <m_i>^2}$$

which tends to $A(k) \propto e^{-k/\tau_{exp}}$. It should be noted that τ_{exp} is really difficult to evaluate because we have observed that the range of values of k where the approximation is valid depends on the size of the lattice. Therefore, the integrated autocorrelation time is discretized as [2]:

$$\tau_{int}(N) = \int_0^N dk A(k) \approx \frac{1}{2} + \sum_{k=1}^{N} A(k)$$

Here we have aproximated the integral with a trapezoidal discretization. The upper limit of the sum can be changed by T, cutting off the summation once $T > 6\tau_{int}(T)$.

Hence we have to take into account this correlation every time in our simulations: we wait $20\tau_{int}$ (arbitrary value) until the system stabilizes and consider we have an uncorrelated sample each $2\tau_{int}$ sweeps, which corresponds to a correlation of $e^{-2} \approx 0.135$ (small enough).

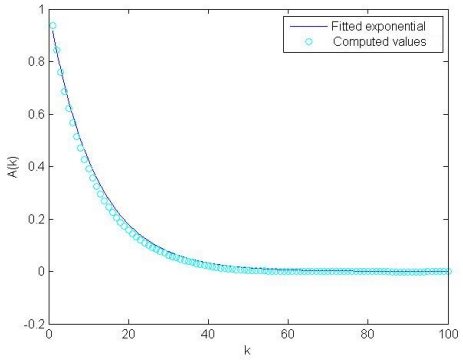

FIG. 2. Autocorrelation function for L=16 ($\tau_{exp} = 11.6596$)

With these preliminars, we are able to calculate the magnetization for some values of β and L. For each point of the plot shown in Fig. 3, we have computed the mean of 50 effective values, where each effective value is the mean of 2τ samples. Thus, values are uncorrelated and applying the central value theorem we know that the mean magnetization will tend to the real value.

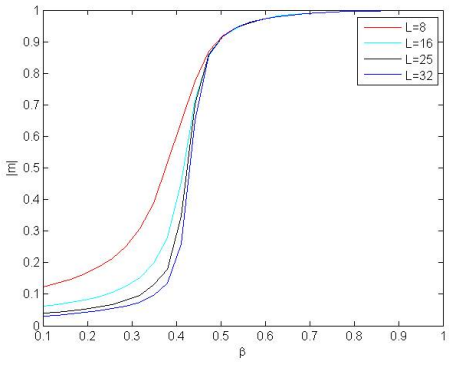

FIG. 3. Mean value of magnetization.

Here, we do observe a phase transition since the slope of magnetization becomes steeper when we go to larger systems, tending to Onsanger's solution. However, more sophisticated techniques are required in order to locate it accurately.

IV. REWEIGHTING TECHNIQUE

The partition function for a given temperature β_0 is $Z(\beta_0) = \sum_{\{s\}} e^{-\beta_0 H(\{s\})} = \sum_E \Omega(E) e^{-\beta_0 E}$ where $\Omega(E)$ denotes the number of states with the same energy E. Thus, $P_{\beta_0}(E) \propto \Omega(E) e^{-\beta_0 E}$. Hence, $P_\beta(E) \propto \Omega(E) e^{-\beta E} \propto P_{\beta_0}(E) e^{-(\beta-\beta_0)E}$.

Therefore, using this reweighting technique we can obtain the value of a given quantity, such as the energy or the specific heat, for all values of β by having only executed a massive simulation for a given β_0.

$$< f(E,M) >= \frac{\sum_{i=1}^{N} f(E_i, M_i) e^{-(\beta-\beta_0)E_i}}{\sum_{i=1}^{N} e^{-(\beta-\beta_0)E_i}}$$

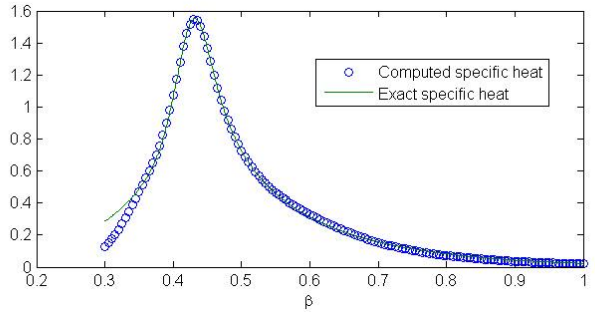

FIG. 4. Specific heat for L=16 obtained from a reweighting technique, which is compared with the exact solution computed with Mathematica by using the partition function for a finite lattice [3]. We have used a value $\beta_0 = 0.44$ and the simulation has been executed with 500,000 sweeps (as will be done always from now on).

V. FINITE SIZE SCALING

Let us define the dimensionless parameter t, called reduced temperature $t = 1 - \frac{\beta_c}{\beta}$. Near the phase transition it is known that the correlation length diverges as $\xi \sim |t|^{-\nu}$. The theory of renormalization group would be necessary to prove that this is an universal critical exponent independent of both the coupling constant J and the lattice we have chosen. There are, as well, other critical exponents which characterize the behaviour of C, m and χ near the critical temperature.

$$C \sim |t|^{\alpha} \quad m \sim |t|^{-\beta} \quad \chi \sim |t|^{\gamma}$$

A. First approach

In a system of finite size, the correlation length will not diverge and, thus, recalling that it represents the size of clusters, there is a neighbourhood of β_c where it will be simply L, thus having:

$$C \sim L^{\alpha/\nu} \quad m \sim L^{-\beta/\nu} \quad \chi \sim L^{\gamma/\nu}$$

Now, let's define the Binder parameters (introduced by Kurt Binder in 1981 [4])

$$U_{2p}(\beta) = 1 - \frac{< m^{2p} >}{3 < |m|^p >^2}, \quad p = 1, 2.$$

Since near $\beta = \beta_c$, $m \sim L^{-\beta/\nu}$, then $U_{2p} = 1 - \frac{C_p}{3}$, being C_p a constant which does not depend on L. Therefore, a first method to work out β_c is to observe the intersection point of either U_2 or U_4, as a function of β for different values of L.

We have chosen an initial value of β_0 using Fig. 3. Hence, we have calculated with Binder parameter method a new value for β_c^0. Then we have repeated this process taking as initial value β_c^0 obtaining thus β_c^1. And we have iterated until $\beta_c^n \approx \beta_c^{n+1}$.

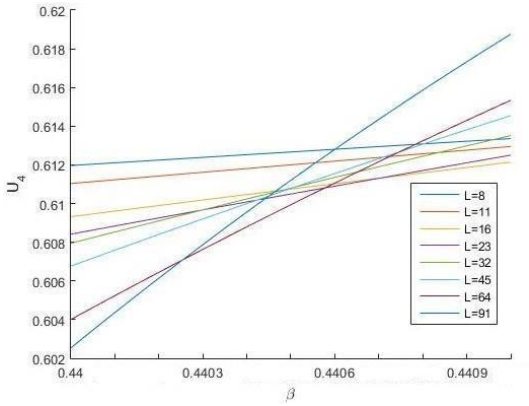

FIG. 5. Binder parameter U_4. The simulation has been done at $\beta_0 = 0.4405$, which corresponds to the last iteration. Notice that the horizontal scale has been magnified considerably.

B. Detailed computation of β_c

Fig. 5 shows that, although a considerable precision can be achieved, there is still some indeterminacy for β_c, and actually further improvements are possible without increasing the computational burden.

With some simple calculation we obtain that:

$$\frac{d<|m|^p>}{d\beta} = N(< e >< |m|^p > - < e|m|^p >)$$

$$\frac{dU_{2p}(\beta)}{d\beta} = \frac{N(<m^{2p}><e>+<m^{2p}e>-2\frac{<m^{2p}><|m|^p e>}{<|m|^p>})}{3<|m|^p>^2}$$

$$\frac{d\ln<|m|^p>}{d\beta} = N(\frac{<|m|^p e>}{<|m|^p>} - < e >)$$

Hence,

$$\frac{dU_{2p}}{d\beta} \sim L^{1/\nu}, \quad \frac{d<|m|>}{d\beta} \sim L^{(1-\beta)/\nu}, \quad \frac{d\ln<|m|^p>}{d\beta} \sim L^{1/\nu}$$

Thus, taking into account that $\{\frac{dU_{2p}}{d\beta}\}_{p=1,2} \propto L^{1/\nu}$ and $\{\frac{d\ln<|m|^p>}{d\beta}\}_{p=1,2} \propto L^{1/\nu}$, we can compute the parameter ν by fitting the logarithm of the maxima of the previous magnitudes as shown in Fig. 6:

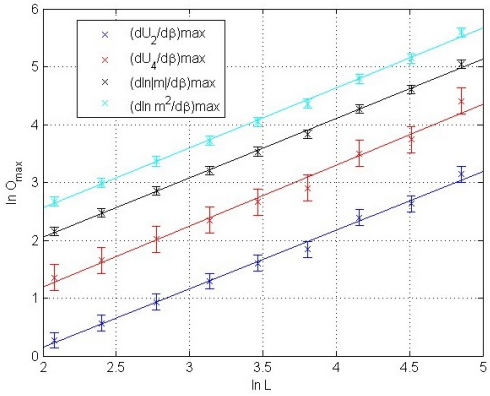

FIG. 6. Maxima of different magnitudes (see inset).

For each fitted line we can estimate a value of ν and then compute the mean and standard deviation. We obtain $\nu = 1.0037 \pm 0.029$, which compares very satisfactorily with a theoretical value of $\nu = 1$. (The error bars in the plot have been drawn considering a 95% confidence interval.)

Now, once ν is known, from the definition of the scaling variable $x = (\beta - \beta_c)L^{1/\nu}$, we can calculate the value of β_c with the location of the maxima of C, χ, $\{\frac{dU_{2p}}{d\beta}\}_{p=1,2}$, $\frac{d<|m|>}{d\beta}$, $\frac{d\ln<|m|^p>}{d\beta}\}_{p=1,2}$ by a simple fitting since: $\beta_{max_i}(L) = \beta_c + a_i L^{-1/\nu}$.

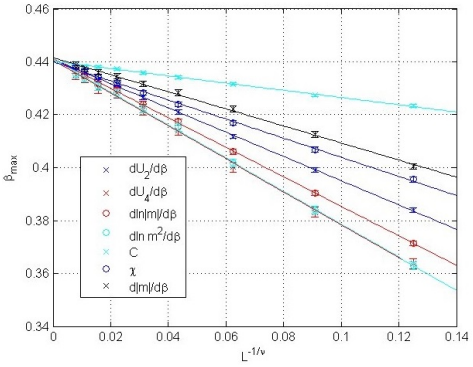

FIG. 7. Fitting of the location of the maxima of the observed quantities (see inset). The value of β_c is the intersection point of the plotted lines with the vertical axis.

Thus, we have finally obtained $\beta_c = 0.4407 \pm 0.0011$. The theoretical value of $\beta_c \approx 0.440687$ lays inside this interval, as expected.

VI. FURTHER RESULTS

A. External magnetic field

When considering a non-zero external magnetic field there is a spontaneous breakdown of the symmetry $\sigma \to -\sigma$ of the hamiltonian (since $H(\{\sigma_i\}) = H(\{-\sigma_i\})$ for $h = 0$ but not for $h \neq 0$), and, thus, there is no phase transition. This may be seen by noticing that there is no transition point where the slope of the magnetization diverges as $L \to \infty$.

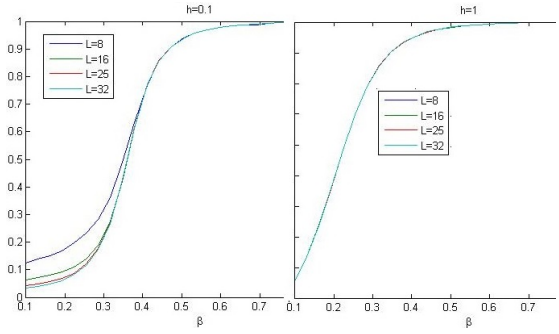

FIG. 8. Mean magnetization for h=0.1 (left) and h=1 (right).

But the clearest proof is the fact that we observe no interesection point in the following graphic:

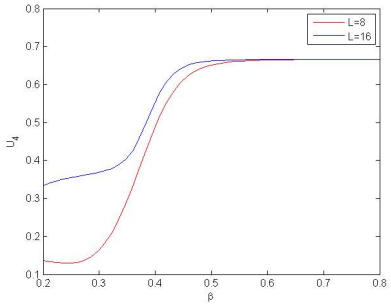

FIG. 9. Binder parameter U_4 for h=0.1 with L=8 and L=16.

B. Other planar lattices

Finally, we have repeated the simulation explained throughout this article for a triangular and an hexagonal lattice in order to verify that transition points are placed respectively at $\beta_c^T = \frac{ln(\sqrt{3})}{2} \approx 0.274653$ and at $\beta_c^H = \frac{ln(2+\sqrt{3})}{2} \approx 0.658479$ and that the value of the critical coefficient is $\nu = 1$ [5].

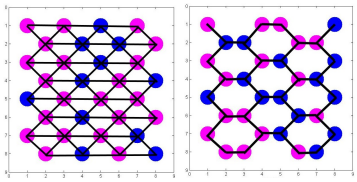

FIG. 10. Triangular(left) and hexagonal(right) lattices (L=8).

We obtain $\nu^T = 1.033 \pm 0.079$, $\nu^H = 1.084 \pm 0.119$, $\beta_c^T = 0.2744 \pm 0.00091$ and $\beta_c^H = 0.6599 \pm 0.0023$. Again, all theoretical values fall within the computed intervals.

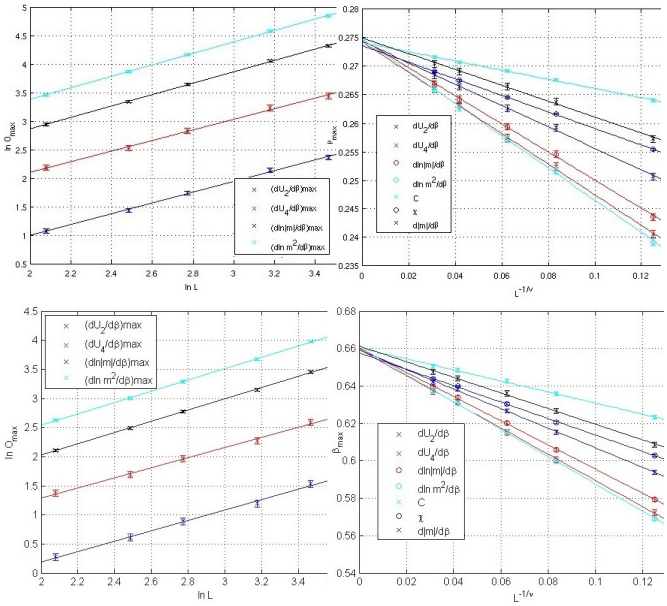

FIG. 11. Results obtained for ν (left), β_c (right) and for both triangular lattice (above) and hexagonal lattice (below).

VII. CONCLUSIONS

We have studied the critical behaviour of the 2D Ising model in different cases (with or without external magnetic field and in a square, triangular and hexagonal lattices). Moreover, we have been able to use some techniques based on the local behaviour of some functions characterized by their critical exponents so as to find out whether there is or not critical temperature and to work out its precise value. The calculus of β_c for square lattice has been obtained with a precision of 99.997%, with a computational cost of around 10 hours on an Intel(R) Core(TM) i7-2600 CPU @ 3.40GHz processor.

VIII. ACKNOWLEDGMENTS

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