Critical point determination from probability distribution functions in the three dimensional Ising model

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In this work we propose a new numerical method to evaluate the critical point, the susceptibility critical exponent and the correlation length critical exponent of the three dimensional Ising model without external field using an algorithm that evaluates directly the derivative of the logarithm of the probability distribution function with respect to the magnetisation. Using standard finite-size scaling theory we found that correction-to-scaling effects are not present within this approach. Our results are in good agreement with previous reported values for the three dimensional Ising model.

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I. INTRODUCTION

The Ising model has a great importance in statistical mechanics since a great variety of techniques and methods, analytical and numerical, have been formulated first on this model. There are several numerical algorithms that can be used to study the critical behavior in spin systems, we can mention three types:

- Those that require adjusting a control parameter, like the standard Monte Carlo or the Wolff algorithms.
- Algorithms that not required to fine tune any parameter, examples of those kind are the Invasion Cluster Algorithm, algorithms based on Self Organisation or the Locally Cluster Algorithm.
- Algorithms that evaluate the Density of States in the microcanonical ensemble.

In this work we propose a new methodology based on the algorithm proposed by Sastre et al. for the evaluation of effective temperatures in out of equilibrium Ising-like systems. The algorithm is a canonical generalisation of the work proposed by H"uller and Pleimling for the evaluation of the density of states in the two and three dimensional Ising model. It is important to point out that variations of this algorithm have been successfully implemented in fluids with discrete potential interaction. The microcanonical version was used in to evaluate thermodynamic properties in the supercritical region and in for the evaluation of the Hight Temperature Expansion coefficients of the Helmholtz free energy. The canonical version was used for the evaluation of the critical temperature and the correlation length critical exponent in the Square-Well fluid with interaction range of 1.5 times the particle diameter.

Our aim in this work is to prove that a completely new methodology can be used to study critical phenomena on Ising-like systems. In particular we want to evaluate the critical temperature and the critical exponents for the correlation length, $\nu$, and the susceptibility, $\gamma$, in the three dimensional Ising model in an efficient way.

This article is organized as follows: in section II we explain the basic definitions for the Ising model and the algorithm used in this work, in section III we apply the method to evaluate the critical point and the critical exponents. We made our concluding remarks in the section IV.

II. PROBABILITY DISTRIBUTIONS FOR THE ISING MODEL

For a better understanding of the algorithm used in this work we will review first how the algorithm proposed by H"uller and Pleimling in the microcanonical ensemble works. The algorithm uses a variation of the transition variable method in order to evaluate the entropy as function of the energy and the magnetisation.

The hamiltonian for the Ising model on a three dimensional cubic lattice without external field and nearest neighbors interaction is

$$\frac{1}{k_B T} H = -\beta^{-1} \sum_{\langle i,j \rangle} \sigma_i \sigma_j,$$  (1)

where $\sigma_i = \pm 1$ is the spin in the $i$ th site, $\beta = k_B T/J$ is the control parameter and $J > 0$ is the coupling between first nearest neighbor spins. The notation $\langle i, j \rangle$ indicates that the summation runs over all nearest neighbors pairs on the lattice. If we consider a system with periodic boundary conditions and $N = L^3$ spins, the magnetisation, $M = \sum_i \sigma_i$, and the energy will be bounded. Moreover, when a spin is flipped in the system we observe that $\Delta M = \pm 2$ and $\Delta E/J = \pm 4 \eta$, $\eta = 0, \pm 1, \pm 2, \pm 3$.

In the standard microcanonical notation $\Omega(E_\mu, M_k)$ is the number of microstates that share the same magnetisation $M_k$ and energy $E_\mu$, for simplicity we will use $\Omega_{\mu,k}$ for this number. When the systems is in a given macrostate $\Omega_{\mu,k}$ and we flip a spin at random we can reach a new macrostate $\Omega_{\nu,1}$, with $E_\nu = E_\mu + 4 \eta J$ and
$M_k = M_l \pm 2$. The probability of reach $\Omega_{\nu,l}$ starting from $\Omega_{\mu,k}$ will be given by

$$P_{(\mu,k),(\nu,l)}^{(m)} = \frac{V_{(\nu,l),(\mu,k)}}{N\Omega_{\mu,k}}, \quad (2)$$

the superscript (m) denotes that we are working in the microcanonical ensemble and $V_{(\mu,k),(\nu,l)}$ indicates how many ways the system can reach $\Omega_{\nu,l}$ starting from $\Omega_{\mu,k}$, this quantity is purely geometric. We can also obtain the reverse probability with

$$P_{(\nu,l),(\mu,k)}^{(m)} = \frac{V_{(\mu,k),(\nu,l)}}{N\Omega_{\nu,l}}. \quad (3)$$

As any spin flip can be reversed, the relation $V_{(\mu,k),(\nu,l)} = V_{(\nu,l),(\mu,k)}$ must be satisfied. For example, from the base state with $E_{\mu} = -3NJ$ and $M_k = N$ we can reach the state with $E_{\nu} = -3J(N-4)$ and $M_l = N-2$ in $N$ ways, then $V_{(\mu,k),(\nu,l)} = N$ and, as $\Omega_{\mu,k} = 1$, $P_{(\mu,k),(\nu,l)}^{(m)} = 1$. In the reverse process we have $\Omega_{\nu,l} = N$ then $P_{(\nu,l),(\mu,k)}^{(m)} = 1/N$. Combining equations (2) and (3) we obtain the important microcanonical relation

$$\frac{P_{(\mu,k),(\nu,l)}^{(m)}}{P_{(\nu,l),(\mu,k)}^{(m)}} = \frac{\Omega_{\nu,l}}{\Omega_{\mu,k}}. \quad (4)$$

The last equation can be used to evaluate the microcanonical derivatives

$$\frac{1}{T} = \frac{\partial S}{\partial E}, \quad (5)$$

and

$$-\frac{B}{T} = \frac{\partial S}{\partial M}, \quad (6)$$

where $B$ is the magnetic external field. The change on the entropy can be obtained using the following approximation

$$\Delta S = k_B \ln \left( \frac{P_{(\mu,k),(\nu,l)}^{(m)}}{P_{(\nu,l),(\mu,k)}^{(m)}} \right) \approx \Delta E \frac{1}{T} - \Delta M \frac{B}{T}. \quad (7)$$

In the simulation the probabilities can be estimated with the rate of attempts $T_{(\mu,k),(\nu,l)}$ to go from $\Omega_{\mu,k}$ to $\Omega_{\nu,l}$. The rate is given by the relation

$$T_{(\mu,k),(\nu,l)} = \frac{z_{(\mu,k),(\nu,l)}}{z_{(\mu,k)}}, \quad (8)$$

where $z_{(\mu,k)}$ is the number of times that the system spends in a macrostate $\Omega_{\mu,k}$, and $z_{(\mu,k),(\nu,l)}$ is the number of times that the system attempts to change from $\Omega_{\mu,k}$ to $\Omega_{\nu,l}$. In this method, once that we fix the ranges $[E_{\min}, E_{\max}]$ and $[M_{\min}, M_{\max}]$, where the simulation will be confined, the quantities $z_{(\mu,k),(\nu,l)}$ and $z_{(\mu,k)}$ can be estimated in the following way:

1. With $E_{\min} \leq E_{\nu} \leq E_{\max}$ and $M_{\min} \leq M_k \leq M_{\max}$ as initial state, a spin is chosen at random and $z_{(\mu,k)}$ is always incremented by 1.

2. We evaluate the new values $E_{\nu}$ and $M_k$ that the system would take if the chosen spin is flipped.

3. If $E_{\min} \leq E_{\nu} \leq E_{\max}$ and $M_{\min} \leq M_k \leq M_{\max}$ the quantity $z_{(\mu,k),(\nu,l)}$ is incremented by 1.

4. The spin flip attempt is accepted with probability $\min \{1, \frac{z_{(\mu,k),(\nu,l)}}{z_{(\mu,k)}}, \frac{z_{(\mu,k)}}{z_{(\nu,l)}}, \frac{z_{(\nu,l)}}{z_{(\mu,k)}} \}$. This condition assures that all macrostates are visited with equal probability, independently of their degeneracy.

The values $z_{(\mu,k),(\nu,l)}$ and $z_{(\mu,k)}$ can be initialized with any positive integer, a safe option is 1, and after a large number of spin flip attempts we will observe that $T_{(\mu,k),(\nu,l)} \rightarrow P_{(\mu,k),(\nu,l)}$.

Müller an Pleimling used this method for the determination of the microcanonically defined spontaneous magnetisation and the order parameter critical exponent for the Ising model in two and three dimensions. This algorithm is highly efficient for evaluate the ratios $\Omega_{\nu,l}/\Omega_{\mu,k}$ since it gives the freedom of restricting the calculations to a chosen range in the energy and magnetisation. Additional details of the method can be found in the original work [7].

The microcanonical algorithm counts all the attempts to change from a given macrostate to another, as long as the final macrostate is an allowed one, while the generalisation proposed in [6] adds an additional condition to the attempts count. The additional condition includes a "heat bath", then we will need to incorporate an extra factor in the ratio of probabilities

$$\frac{P_{(\mu,k),(\nu,l)}}{P_{(\nu,l),(\mu,k)}} = e^{-\frac{\Delta E}{k_B T}} e^{-\frac{\Delta M}{k_B T}} \quad (9)$$

here the absence of the superscript indicates that we are no longer in the microcanonical ensemble. Combining Equations (7) and (9) we get

$$\ln(P_{(\mu,k),(\nu,l)}) - \ln(P_{(\nu,l),(\mu,k)}) \approx -\Delta M \frac{B}{k_B T} \quad (10)$$

where we can drop the subscript $\mu$ and $\nu$, since the right hand side of the equation depends only on $\Delta M$. In the simulation the probabilities now can be estimated with the rate of attempts $T_{k,l}$ to go from a macrostate with magnetisation $M_k$ (level $k$) to a macrostate with magnetisation $M_l$ (level $l$). The quantity $T_{k,l}$ will be given now by the relation

$$T_{k,l} = \frac{z_{kl}}{z_k}. \quad (11)$$

where $z_{kl}$ is the number of times that the system attempts to change from level $k$ to level $l$ and $z_k$ is the number of times that the system spends in level $k$. For the estimation of the $z_{kl}$ and $z_k$ values, the detailed steps are now:
1. With $M_{\min} \leq M_k \leq M_{\max}$ as initial state, a spin is chosen at random and $z_k$ is always incremented by 1.

2. If the possible state $M_l$, that would be reached if the chosen spin is flipped, is allowed we evaluate $\Delta E$ between states $M_k$ and $M_l$, and the quantity $z_{kl}$ is incremented by 1 with probability $\min(1, e^{-\Delta E/k_B T})$.

3. The spin flip attempt is accepted with probability $\min(1, e^{-\Delta E/k_B T})$.

The values $z_{kl}$ and $z_k$ are initialized to 1 and after a large number of spin flip attempts we will observe that $T_{kl} \to P_{kl}$.

Now we obtain the derivative of $\ln P$, instead of the derivatives of $S$, with the following approach

$$\frac{\partial \ln P}{\partial M} \bigg|_k \approx \ln P_{kl} - \ln P_{lk} \approx \ln(T_{kl}/T_{lk}). \quad (12)$$

We will use the following function in our simulations

$$g(m) = L^{-d} \frac{\partial \ln P}{\partial m}, \quad (13)$$

where $m = M/L^d$, since it can be obtained directly from the transition rates with the approximation

$$g(m_k) \approx \frac{1}{2} \left[ \ln[(T_{k,k+1})/(T_{k+1,k})] - \ln[(T_{k,k-1})/(T_{k-1,k})] \right], \quad (14)$$

where $T_{k,k\pm1,k}$ are the transition rates from level $k$ to its adjacent levels and $T_{k\pm1,k}$ are the transition rates from the adjacent levels to level $k$.

We verified that this method is compatible with the ansatz proposed by Tsypin and Blöte for the three dimensional Ising model at the critical point

$$P(m) \sim \exp \left[ - \left( \frac{m}{m_0} \right)^2 - 1 \right] \left( a \left( \frac{m}{m_0} \right)^2 + c \right), \quad (15)$$

where $a$, $c$ and $m_0$ are size depending fitting parameters.

For $L = 12$ we performed three independent simulations at $\beta_c = 0.221654$, taken from Ref. [15], with different ranges in $m$. Our results are show in Figure 4 along with the curve given by Eq. (15), using $a = 0.268$, $c = 0.268$, $m = 0.3892$. Our simulations are in really good agreement with the ansatz, except at the extreme values of the curves, but this effect is also present in the results published by Tsypin and Blöthe.

**III. RESULTS**

![Graph of g as function of m for three different range simulations.](image)

**FIG. 1:** (Color online) Graph of $g$ as function of $m$ for three different range simulations. We observe that the restriction in range does not affects the computed value of $g$. The continuous line reproduces Eq. (15), with the parameters $a = 0.268$, $c = 0.859$ and $m_0 = 0.3892$ for $L = 12$. There is a really good agreement with our results, except in the extremes of the curves, as shown in the inset.

As we can see there is a change in the sign of the slope $\partial g/\partial m$ around $m = 0$ as function of $\beta$, then we can find $\beta_c(L)$ restricting our simulations around $m = 0$. We performed simulations restricting the intervals to $|m| \lesssim 0.1$ on several system sizes and temperature values in the three dimensional Ising model. The justification for this interval is that $g(m)$ is linear around $m = 0$ and the slope can be easily obtained from a linear fit to the simulation data. For every system size we evaluate the slope for several values of $\beta$, in Figure 5 we are illustrating how the evaluation of $\beta_c(L)$ is performed for the case $L = 12$. Here we used a linear fit to the curves of the slope as...
FIG. 2: (Color online) Symmetry breaking for the three dimensional Ising model with $L = 8$. For $\beta < \beta_c$ the curve cross the horizontal axis at $m = 0$ with a negative slope. For $\beta > \beta_c$ we have three crossings, at $m = 0$ and at $m = \pm m_{sta}$ and we observe that the slope at $m = 0$ is now positive.

function of $\beta$ in order to solve $\left( \frac{\partial g}{\partial m} \right)_{\beta = \beta_c} = 0$.

From here we can use the Finite size scaling ansatz for the critical temperature, given by the relation

$$\beta_c(L) \approx \beta_c + AL^{-1/\nu},$$

where $\beta_c$ is the critical control parameter for the infinite system, $A$ is a non universal parameter and $\nu$ is the critical exponent for the correlation length $[10]$. In principle Eq. (16) is valid for sufficiently large $L$ values. For small systems the last term changes to $L^{-1/\nu}(1 + BL^{-\omega})$, here the parameter $\omega$ is the scale correction exponent, whose reported value for the three dimensional Ising model is $\omega \approx 0.81$ $[17]$.

The simulations were carried out in systems with linear sizes $L = 8, 10, 12, 14, 16, 20$ and $24$, using $5N \times 10^6$ spin flip attempts and 120 independent runs for every set of parameters. With these values we obtain reliable data with less CPU time compared with standard canonical simulations, since most of the spin flips are discarded when the system falls outside of the restricted range. However, all attempts, successful or not, are used for the evaluation of the transition rates. We evaluated $T_c$ and $\nu$ performing a non-linear curve fitting to Eq. (16), in Figure 2 we show the evaluation of the critical point along with the $\nu$ critical exponent. We must emphasized that in our analysis the scale correction exponent is absent, which is a great advantage in numerical simulations that study critical phenomena. This feature is also observed in the evaluation of the critical temperature for the square-well fluid using an equivalent method $[10]$. We think that the absence of scale corrections are related to the fact that in this method we evaluate the critical point analyzing the behavior of the probability distribution of the order parameter around $M = 0$, while in most traditional methods the critical point is evaluated analyzing the behavior around the peaks of the probability distribution.

The results for the critical point is $\beta_c = 0.22165(65)$ and for the correlation length critical exponent we obtain $\nu = 0.6301(88)$, that are in good agreement with previous reported values, see Table I.

Once that we have the critical temperature we can proceed to evaluate the susceptibility critical exponent $\gamma$. We used the scaling ansatz for the probability distribution function at the critical point proposed in Ref. $[20]$

$$P(m, L) \approx \exp \left( -A_0 + A_2x^2 + A_4x^4 + \ldots \right),$$

(17)
FIG. 4: Evaluation of the critical temperature and the correlation length critical exponent for the three dimensional Ising model. The dashed line is a non-linear curve fit to Eq. (16). The results from the fit are $\beta_c = 0.22165$, $A = -0.2439$ and $1/\nu = 1.587$.

TABLE I: Critical parameters for the three dimensional Ising model obtained in this work and those from literature. The values between parenthesis indicate the uncertainty in the last digits.

| $\beta_c$ | $\nu$ | Source                  |
|----------|-------|-------------------------|
| 0.22165(65) | 0.6301(88) | This work               |
| 0.22165452(8) | 0.63020(12) | Butera and Comi [18]    |
| 0.221655(2)     | 0.6299(2)    | Deng and Blöte [19]      |
| 0.221654(2)     | 0.6308(4)    | Lundow and Campbell [17] |

where $x = mL^{\beta/\nu} << 1$ and $\beta$ is the order parameter critical exponent. As we are restricting our simulations to the range $|m| \leq 0.1$ we can use the next approximation

$$\frac{\partial \ln P}{\partial m} = 2A_2 mL^{2\beta/\nu} + O(x^3), \quad (18)$$

that we can combine with Eq. (18) to obtain the desired scaling relation

$$\frac{\partial g}{\partial m} \sim L^{-\gamma/\nu}. \quad (19)$$

For the three dimensional case we performed simulations at our estimated critical point $\beta_c = 0.22165$ and linear sizes $L = 8, 10, 12, 14, 16, 20$ and 24. In this case we used $N \times 10^7$ spin flip attempts and 120 independent runs for every $L$ value. The critical exponent $\gamma$ was obtained from a linear fit to Eq. (19) as shown in Figure 5. From this fit we obtain $\gamma/\nu = 1.973(10)$. From the fit we obtain the slope $\gamma/\nu = 1.973$. Again we observe that scaling correction exponents are absent.

IV. CONCLUSIONS

We have presented a new method for the evaluation of the critical temperature and the critical exponents for the correlation length $\nu$ and the susceptibility $\gamma$ on the three dimensional Ising model. Using the derivatives of the probability distribution function for the magnetisation and small system sizes we obtain reliable results that are in good agreement with the reported values. The method can be used in a restricted range on the magnetisation and this feature reduces the computational time in the simulations. One additional advantage of the method is that scale corrections are not present, at least in the three dimensional Ising model. In future works we will study if this advantage is present in other systems.
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