

MONTE-CARLO STUDY OF THE THREE-DIMENSIONAL CONSERVED-ORDER-PARAMETER ISING MODEL VIA FINITE-SIZE SCALING ANALYSIS

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Abstract. The critical properties of the three-dimensional simple-cubic Ising model (spin=1/2) with nearest-neighbor interactions were investigated by means of the Monte Carlo Wang-Landau, Metropolis, and heat-bath algorithms. We considered a variant of the aforementioned model wherein the magnetization is fixed at the zero value, conserved-order-parameter (COP) Ising model. The calculation was focused on the specific heat and Binder energy cumulant for lattices with linear size $L = 4-60$. The accumulated data was analyzed by finite-size scaling analysis; the thermal critical exponent γ_t and critical temperature K_c were estimated for all algorithms and the resulting values are compatible with those of the normal version. Also, the analysis revealed the necessity of corrections to interpret correctly the Monte Carlo data.

1. INTRODUCTION

The two-dimensional Ising model has received much attention in the equilibrium statistical physics as the prototype for phase transitions, since it was exactly solved on an infinite square lattice. It has also a wide-range of applications, as in liquid-vapor phase transition, physical chemistry and mixtures, etc. However, its three-dimensional counterpart has not yet been solved analytically but various attempts have been done (numerical methods, renormalization group, Monte Carlo, finite-size scaling) to shed light, mainly, on its critical behavior. The critical properties concern always an infinitely bulk system, since the phase transitions appear in such a system. In Monte Carlo (MC) simulations the criti-

cal behavior is extracted from the results obtained on a finite-size system by means of finite-size scaling (FSS). The finite size refers to the spatial size of the system.

One of the objects of finite-size scaling method is to find the critical exponents that, together with other universal parameters, characterize the universality class. Such a class consists of several systems with different interactions and lattice structure but displaying identical behavior in the neighborhood of the respective critical point; as a result they have the same critical exponents. These exponents offer the most direct test of universality, thus their precise calculation is one of the main goals of statistical mechanics. However, in an experiment the exponents cannot be measured with infinite precision

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thus causing doubts about the universality class a specific system belongs.

The systematic study of finite lattices started from the seminal paper by Ferdinand and Fisher [1]. They studied the specific heat singularity of the two-dimensional spin-1/2 Ising model confirming that the thermal properties obey finite-size scaling. They also observed a shifting and rounding of the critical temperature as a result of the finite dimensions of the system, see Fisher [2], Barber [3], Privman [4], and Binder [5].

In the present work, we shall deal with the study of the critical properties of a variant of the three-dimensional Ising model using the MC method in conjunction with FSS. This is the one with constant magnetization, called *conserved-order-parameter* (COP) Ising model. The critical behavior of this version of Ising model has not yet been studied systematically, in contradistinction to the normal one (i.e., without any constraint) for which, in spite of the non-existence of an exact solution, investigations by various methods have fixed the first significant digits of the critical temperature T_c and exponents, thermal y_t , magnetic y_h , and leading irrelevant y_l . Landau [6] investigated the unconstrained three dimensional Ising model on simple cubic lattices ($L \leq 20$) with periodic boundary conditions and free edges, leading to $\nu = 0.64$, $\beta = 0.312$, $\gamma = 1.25$, using FSS. Ferrenberg and Landau [7], investigated a similar system on lattices with sizes $8 \leq L \leq 96$ focusing on $K_c = J/(k_B T_c)$ (J interaction constant) and the ν exponent; by examining the finite size behavior of these lattice systems, they concluded that $K_c = 0.2216595 \pm 0.0000026$, $\nu = 0.627 \pm 0.002$ using large size lattices ($24 \leq L \leq 96$), while using smaller ones, they included a correction term leading to $\nu = 0.6289 \pm 0.0008$. Blöte *et al.* [8] performed MC simulations on three Ising models (three dimensional) belonging to the same universality class; their data was obtained by cluster algorithms and analyzed by FSS leading to $K_c = 0.2216546 \pm 0.0000010$, $y_t = 1.587 \pm 0.002$, and $y_l = -0.82 \pm 0.06$. In a subsequent paper, Deng and Blöte [9] investigated several three dimensional Ising models by means of MC simulations and FSS; the data was simultaneously analyzed thus providing improved accuracy, leading to $y_t = 1.5868 \pm 0.0003$ and $y_l = -0.821 \pm 0.005$.

In the current COP three dimensional Ising model, the magnetization is fixed to $M=0$ [10], which is one of the possible values for M . One of the main consequences of this choice is the restriction of the possible spin configurations in a MC simulation. The data was generated by extensive MC cal-

culations using the Metropolis, heat-bath [10], and Wang – Landau (WL) sampling methods, [11]. The advantage of the latter algorithm over the former two, is that the temperature is not specified *a priori*. The chosen temperature for the Metropolis and heat-bath is the critical one. The WL algorithm estimates in a single run the density of states (DOS) $g(E)$, performing a random walk with an acceptance ratio $P(E_i \rightarrow E_j) = \min\{1, [g(E_j)/g(E_i)]\}$, E_i and E_j are the energies before and after the transition, respectively, and aiming at sampling a flat histogram in energy, [11]. The WL algorithm overcomes the difficulties, such as critical slowing down and long relaxation times in systems with complex energy landscape. This algorithm has been applied to a wide range of systems, spanning from the Ising model [12, 13], Potts [14], to glassy systems [15], polymers [16], DNA [17], and the Baxter-Wu model [18]. As the construction of the respective DOS is gradual, to achieve convergence of $g(E)$ to its proper value rapidly it is scaled by a modification factor f , which changes from an initially large value (usually, $f = e$) iteratively to nearly unity in a finite number of iterations according to the prescription $f_{j+1} = \sqrt{f_j}$, j is the order of iteration; in the current investigation the WL algorithm performed 24 iterations.

In this analysis, the major goal is to estimate the critical temperature and exponents of this version of Ising model and deduce whether the current Ising model belongs to the same universality class as the normal one. This is achieved by studying the finite-size behavior of the specific heat and Binder energy cumulant $V_L = 1 - \langle E^4 \rangle / (3 \langle E^2 \rangle^2)$, henceforth called Binder cumulant. In the former case, we associate, for every value of L , a temperature $T_c(L)$, called ‘pseudocritical temperature’, with the maximum value C_L^* of the specific heat, while, for the latter we associate for the same value of L another ‘pseudocritical temperature’ $T_V(L)$ with the minimum value V_L^* of the Binder cumulant; the asterisk will be suppressed for simplicity. In each case, a sequence of “pseudocritical temperatures” is formed and these sequences converge to the critical temperature T_c of the infinite system, $L \rightarrow \infty$. The previous calculations were carried out through the WL process.

The layout of the paper is as follows. In the next section we discuss the Wang-Landau, the Metropolis, heat-bath algorithms, and the newly proposed CrMES method [13]. In section 3 we apply the FSS to the Ising model under consideration and we close with the conclusions and discussions in section 4.

2. THE SIMULATION METHOD

As stated above, the main goal is to study the thermal properties in the critical region of the three-dimensional ferromagnetic isotropic COP Ising model on a simple cubic lattice with linear size L and periodic boundary conditions. The lattice is considered to be free of defects, impurities, or any other imperfections, that can influence the value of the critical temperature and exponents. The Hamiltonian of the system, in the absence of any external field and under the restriction of fixed magnetization ($M = 0$) is,

$$H = -J \sum_{\langle ij \rangle} S_i S_j, \quad S_i = \pm 1, \quad i = 1, \dots, N;$$

$$M = \sum_{i=1}^N S_i = 0, \quad (1)$$

where $J > 0$ is the interaction constant and $N = L^3$, the number of lattice sites. The summation extends over all nearest-neighbor pairs on the lattice. In studying critical phenomena, it is usual to deal with the dimensionless parameter $K = J/(k_B T)$ (inverse temperature, k_B is Boltzmann constant) instead of the temperature T itself. The Metropolis, heat-bath and WL algorithms were implemented on lattices with $4 \leq L \leq 60$ and the density of states (DOS) was stored as a function of the energy. The single spin-flip algorithm was adapted to the non-local spin exchange version, to keep the constraint $M = 0$; this version is also more effective than the Kawasaki algorithm. To carry out this calculation, the system was divided into two groups, one with spin-up lattice sites (positive group) and one with spin-down lattice sites (negative group); each MC movement consists of a two-spin flip, in that, one spin, chosen at random from the positive group and similarly one from the negative, are exchanged.

For the Metropolis and heat-bath algorithms, the states were chosen randomly with transition probability $P(S \rightarrow S') = \min\{1, \exp[-\beta \Delta E]\}$ and $P(S \rightarrow S') = [1 + \exp[-\beta \Delta E]]^{-1}$, respectively; $\Delta E = E[S'] - E[S]$ is the energy change.

After the calculation of the density of states $g(E)$, one can evaluate useful thermodynamic quantities, because of the Boltzmann relation $S(E, V, N) = k_B \log g(E, V, N)$. However, before proceeding to this end, we outline a new method for speeding up the numerical calculations, called 'Critical Minimum Energy Subspace' (CrMES) technique, [13,18]. We consider, initially, the specific heat per site for a lattice of linear size L at temperature T ,

$$c_L(T) = L^{-d} T^{-2} \left\{ Z^{-1} \sum_{E_{\min}}^{E_{\max}} E^2 \exp[S(E) - \beta E] - \left(Z^{-1} \sum_{E_{\min}}^{E_{\max}} E \exp[S(E) - \beta E] \right)^2 \right\}, \quad (2)$$

where the Boltzmann constant was set $k_B = 1$, thus $\beta = 1/T$, d is the spatial dimension ($d=3$) and Z the 'partition function' of the system,

$$Z = \sum_{E_{\min}}^{E_{\max}} \exp[S(E) - \beta E]. \quad (3)$$

As we are interested in the behavior of $c_L(T)$ in the critical region, there is no need to calculate it for the whole range of energies $[E_{\min}, E_{\max}]$, but for a much smaller subinterval. To be specific, let's suppose we are interested in obtaining an accurate approximation of c_L at the pseudocritical temperature $T_c(L)$. We can easily determine a value \tilde{E} of energy corresponding to the maximum value of the term $\exp[S(E) - \beta E]$ of the partition function. Thus the CrMES technique proposes the estimation of DOS in a subrange $[\tilde{E}_-, \tilde{E}_+]$ with $\tilde{E}_{\pm} = \tilde{E} \pm \Delta^{\pm}$, $\Delta^{\pm} > 0$. The errors involved in this approximate computation for the summation are much smaller than the ones resulting from the approximate computation of $S(E)$ by the WL algorithm. The relative error in computing the specific heat from (2), using the restricted subinterval $[\tilde{E}_-, \tilde{E}_+]$ with respect to the total energy range $[E_{\min}, E_{\max}]$, is taken to be smaller than a predefined value r . That is, $|\left[c_L(\tilde{E}_-, \tilde{E}_+) / c_L(E_{\min}, E_{\max}) \right] - 1| \leq r$ and r is chosen to be $r = 1 \cdot 10^{-6}$, much smaller than the corresponding error in determining the DOS, for more see [13].

3. FINITE-SIZE SCALING ANALYSIS

The FSS is based on the assumption that the free energy of a system in the absence of an external magnetic field scales as,

$$F(L, t) = L^{-\psi} F_0(tL^{\theta}), \quad (4)$$

where $\psi = (2-\alpha)/\nu$, $t = |(T - T_c)/T_c|$; α, ν , are the specific heat and correlation length critical exponents, respectively. The scaling of the correlation length, $\xi = \xi_0 t^{-\nu}$ suggests that $\theta = \nu^{-1}$. The scaling function $F_0(x)$ is universal.

Following Blöte *et al.* [8], the specific heat per lattice site, close to the critical point scales as,

$$c_L(T) = \rho_0 + L^{2y_i-d} [q_0 + q_1(K - K_c)L^{y_i}] + rL^{2y_i-d+y_i} + s_0L^{y_i-d}, \quad (5)$$

where leading analytic and singular terms were taken into account. By fixing the value of the irrelevant exponent at $y_i = -0.83$ and critical temperature $K_c = 0.2216547$, they estimated the value of the thermal critical exponent y_t using the five additional parameters $(\rho_0, q_0, q_1, r, s_0)$, $y_t = 1.60(2)$, but the errors for these parameters were large. In attempting to fit our results for the specific heat to the expansion (5), we found out that by omitting some terms in this expression, the errors are suppressed and the convergence is speeded up; therefore, we consider the expansion

$$c_L(T) = \rho_0 + q_0L^{2y_i-d} + rL^{2y_i-d+y_i}. \quad (6)$$

In Eq. (6) and all expressions hereafter, the leading irrelevant exponent y_i was fixed, $y_i = -0.821(5)$ [9], the only quantity kept constant everywhere, otherwise the accuracy of the fitting parameters will be very limited or, even, unaccepted. As a test, y_i was considered a free parameter, then the resulting uncertainties, in any fitting procedure, for this and the other parameters were, at least, as big as their absolute values. To facilitate further the calculations and make the results more reliable concerning the statistical errors, the lattices were divided into groups, $L = 4-60, 6-60, 8-60, \dots, 26-60$.

We started the fitting procedure, by attempting to fit to (6) the maximum values of the specific heat c_L at the pseudocritical temperature $T_c(L)$, resulting from the WL method. A usual way of performing the fitting process, e.g. in (6), was to choose the constant term ρ_0 in a somewhat arbitrary way such that this choice suits the scaling process concerning the results. In the current case, we followed a different route for this choice which is based on already known information about the critical exponents. This choice ensures stable fitting forms and small uncertainties in the results. Thus, we performed, firstly, preliminary fittings of the MC data to obtain estimates, for every lattice-group, for the constant term ρ_0 so that y_t is about 1.58. This rough estimation for y_t is implied, on the one hand, by the so far published results and, on the other hand, by the current partial results from the lattice-groups consisting of large lattices. This procedure was also carried out by all fitting attempts to follow, choosing, in each case, the proper parameter.

For the specific heat at the pseudocritical temperature, the respective values for ρ_0 in each lattice-

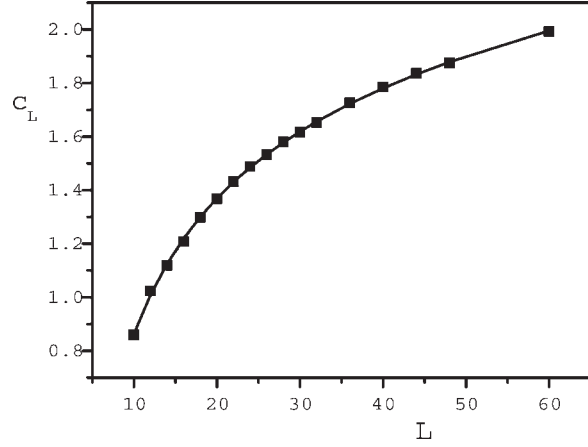


Fig. 1. The specific heat maxima according to the scaling expression (6) vs. L for the estimation of the thermal critical exponent y_t , for either temperature, through (7) and (9).

Table 1. Successive fittings for the maximum values of the specific heat at $T_c(L)$ (for the WL technique) by means of (6) for estimating the constant ρ_0 .

L	ρ_0
10-60	0.3770
12-60	0.3176
14-60	0.6090
16-60	0.7000
18-60	0.5823
20-60	0.5802
22-60	0.5130
24-60	0.5710

group appear on Table 1; the resulting mean value is $\bar{\rho}_0 = 0.53126 \pm 0.04449$, (Fig.1), thus (6) takes the form,

$$c_L(T) = 0.53126 + q_0L^{2y_i-d} + rL^{2y_i-d+y_i}. \quad (7)$$

Considering, now, the latter expression, we calculated, for every lattice-group, the values for (y_t, q_0, r) , see Table 2. Combining these estimates, we get the mean values,

Table 2. Successive fittings for the WL specific heat maximum values at $T_c(L)$ by means of the scaling expression (7).

L	q_0	y_t	r
10-60	0.83036(0.02214)	1.59194(0.00323)	-4.06023(0.13960)
12-60	0.81617(0.02882)	1.59394(0.00415)	-3.96191(0.18926)
14-60	0.88850(0.02212)	1.58422(0.00287)	-4.48261(0.15305)
16-60	0.91242(0.02737)	1.58122(0.00340)	-4.66116(0.19651)
18-60	0.88127(0.03168)	1.58509(0.00394)	-4.42327(0.23229)
20-60	0.88077(0.04178)	1.58516(0.00519)	-4.41936(0.31406)
22-60	0.86282(0.05360)	1.58740(0.00669)	-4.27742(0.41029)
24-60	0.87826(0.07137)	1.58549(0.00865)	-4.40179(0.56017)

$$\begin{aligned}\bar{y}_t &= 1.58681 \pm 0.00419, \\ \bar{q}_0 &= 0.86882 \pm 0.03154, \\ \bar{r} &= -4.33597 \pm 0.22852.\end{aligned}\quad (8)$$

Comparing the estimate for the thermal exponent y_t in (8) with that in Ref. [9], ($y_t=1.5868\pm 0.0003$), one observes excellent agreement, while with Malakis *et al.* [13] ($y_t = 1.5878(31)$) the agreement is good enough. The difference with Refs. [9] and [13], is in the respective errors and amplitudes, since the current model is not identical with these ones. Encouraged by this result, we extended the study to the MC specific heat values for the considered as exact value of the critical temperature $T_c = 4.5115217$ ($K_c = 0.2216547$) following the same procedure, as previously, for the calculation of the mean value \bar{p}_0 . In this case $\bar{p}_0 = -2.04584 \pm 0.06031$, thus, the scaling expression (6) is now rewritten as,

$$c_L(T) = -2.04584 + q_0 L^{2y_t-d} + r L^{2y_t-d+y_t}. \quad (9)$$

Fitting, now, the maximum values for the specific heat at T_c to (9), we estimate the parameters (y_t, q_0, r), for every lattice-group as it was done for the pseudocritical temperature; these values lead to the respective mean values,

$$\begin{aligned}\bar{y}_t &= 1.58691 \pm 0.00153, \\ \bar{q}_0 &= 1.53034 \pm 0.02251, \\ \bar{r} &= 0.63385 \pm 0.09607.\end{aligned}\quad (10)$$

Comparing the values for \bar{y}_t , (8) and (10), we observe that they are compatible and by combining them (since they result from the same MC process, the WL algorithm), we get,

$$\bar{y}_t = 1.58686 \pm 0.00007. \quad (11)$$

and $\bar{v} = 1/\bar{y}_t = 0.63018 \pm 0.00003$. The final value for \bar{y}_t in (11) is compatible with that in Ref. [9] ($y_t = 1.5868 \pm 0.0003$) improving the significant digits.

Now, we turn our attention to the MC results for the specific heat at the critical temperature T_c for the Metropolis and heat-bath algorithms, using the same scaling function (6). Following, as previously, the preliminary procedure, we estimate the mean value of the constant term p_0 , that is, $\bar{p}_0 = -1.58468 \pm 0.02896$ for the former and $\bar{p}_0 = -1.53581 \pm 0.02990$ for the latter algorithm, resulting from the entries on Table 3. Inserting the former value into (6), we estimate the parameters (y_t, q_0, r) for the Metropolis algorithm, see Table 4; from which we got the mean values,

$$\begin{aligned}\bar{y}_t &= 1.58685 \pm 0.00094, \\ \bar{q}_0 &= 1.29227 \pm 0.01090, \\ \bar{r} &= 0.18545 \pm 0.03806.\end{aligned}\quad (12)$$

Afterwards, inserting the latter mean value for p_0 into (6), we estimate the parameters (y_t, q_0, r) for the heat-bath algorithm, see Table 5, from which we got the mean values,

$$\begin{aligned}\bar{y}_t &= 1.58686 \pm 0.00098, \\ \bar{q}_0 &= 1.26758 \pm 0.01116, \\ \bar{r} &= 0.13958 \pm 0.03859.\end{aligned}\quad (13)$$

Comparing the estimates (11), (12), and (13) for y_t we observe that they are compatible, in that, their first four significant digits are identical, although the

Table 3. Successive fittings for the maximum values of the specific heat at T_c , for the Metropolis and heat-bath algorithms, by means of (6), for estimating the constant p_0 , in either case.

L	$p_0(\text{Metropolis})$	$p_0(\text{heat-bath})$
04-60	-1.66180	-1.61840
06-60	-1.59260	-1.53900
08-60	-1.55700	-1.50340
10-60	-1.52733	-1.48245

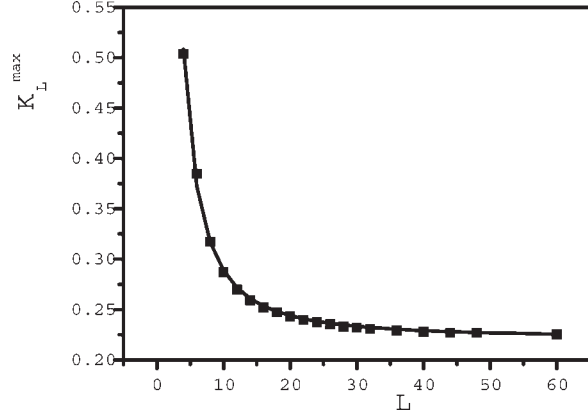


Fig. 2. The specific heat inverse pseudocritical temperature K_L^{\max} vs. L , from the scaling form (16). K_L^{\max} tends to the respective critical value K_c as $L \rightarrow \infty$, that coincides with the constant term in (16). An identical behavior is exhibited by the inverse pseudocritical temperature K_L^{\min} of the cumulant.

Table 4. Successive fittings for the maximum values at T_c of the Metropolis specific heat, by means of the scaling expression (6), to estimate (q_0, y_t, r) .

L	q_0	y_t	r
04-60	1.26305(0.00949)	1.58938(0.00088)	0.28562(0.02484)
06-60	1.28961(0.00823)	1.58705(0.00072)	0.19782(0.02499)
08-60	1.30282(0.00997)	1.58593(0.00084)	0.15001(0.03349)
10-60	1.31358(0.01284)	1.58505(0.00105)	0.10836(0.04665)

former is more accurate and we adopt it as the proper value for y_t .

Now, we carry on the calculations by applying the FSS to the pseudocritical temperatures resulting from the maximum values of the heat capacity for the various lattices, in order to find an estimate for the three-dimensional critical temperature of the COP Ising model, since we can pursue this calculation as far as $y_t = 1/\nu$ has been determined. The sequence of the specific-heat pseudocritical temperature tends to T_c as $L \rightarrow \infty$ and scales as [7],

$$T_c(L) = T_c + a_1 L^{-1/\nu} \quad (14)$$

for large lattices. If smaller lattices are included then correction terms are necessary, approximated by a single term with the suitable exponent w (more correction terms can also be included, but then the estimation becomes more complicated); in this

case, the scaling expression (14) takes the form [7],

$$T_c(L) = T_c + a_1 L^{-1/\nu} (1 + b_1 L^{-w}) \quad (15)$$

or, in terms of the inverse temperature $K = J/k_B T$,

$$K_c(L) = K_c + a L^{-1/\nu} (1 + b L^{-w}). \quad (16)$$

The exponent w is chosen as $w = -y_t$ [19], fixed as earlier, and y_t as in (11). To minimize the uncertainties and have stable fitting forms, we estimate, as in specific heat, for every lattice group, the value of the coefficient a such that the estimated value for K_c in each lattice group is 0.22; these preliminary calculations lead to the mean value $\bar{a} = 1.83943 \pm 0.02071$. Fitting the corresponding data to Eq. (16) (with the previous mean value for a , Fig. 2), we estimate K_c and b from the entries of Table 6 as,

Table 5. Successive fittings for the maximum values at T_c of the heatbath specific heat, by means of the scaling expression (6), to estimate (q_0, y_t, r) .

L	q_0	y_t	r
04-60	1.23664(0.01000)	1.58960(0.00095)	0.24522(0.02631)
06-60	1.26668(0.00820)	1.58691(0.00073)	0.14570(0.02498)
08-60	1.27974(0.01002)	1.58578(0.00086)	0.09830(0.03375)
10-60	1.28727(0.01337)	1.58514(0.00112)	0.06910(0.04856)

Table 6. Successive fittings for the specific heat inverse pseudocritical temperature $K_c(L)$ to the scaling expression (16), for the estimation of the inverse critical temperature K_c , and the amplitude b .

L	$K_c(L)$	b
08-60	0.22174(0.00002)	3.47238(0.00645)
10-60	0.22171(0.00002)	3.49938(0.00733)
12-60	0.22168(0.00001)	3.52411(0.00808)
14-60	0.22167(0.00001)	3.54705(0.00873)
16-60	0.22165(0.00001)	3.56854(0.00930)
18-60	0.22164(0.00001)	3.58881(0.00979)
20-60	0.22163(0.00001)	3.60798(0.01019)
22-60	0.22163(0.00001)	3.62610(0.01050)
24-60	0.22162(0.00001)	3.64315(0.01077)
26-60	0.22162(0.00001)	3.65911(0.01110)

$$\begin{aligned} \bar{K}_c &= 0.22166 \pm 0.00004, \\ \bar{b} &= 3.57366 \pm 0.06259. \end{aligned} \quad (17)$$

The value for K_c in (17) is compatible with that currently in use.

Binder, in order to facilitate the estimation of critical exponents, introduced a new quantity in the study of critical phenomena, that is, the cumulant V_L [20], which can be defined either for the magnetization [7,20] or energy [18,21]. Although V_L is not an experimentally measurable quantity, it was proved to be very important in critical phenomena, since it provides an independent route for calculating some of the critical exponents [7] and behaves differently in first- or second- order transitions. Far from the critical temperature and for small values of L , V_L exhibits a minimum (V_L^{\min}) at a temperature $T_{\min} \equiv T_v(L)$, which diminishes gradually on increasing L and, finally, V_L approaches the value (2/3) in the thermodynamic limit. The overall behavior of V_L is reflected

in Fig. 3 and was observed irrespective of the algorithm under consideration; the only observable variation is in the respective decay critical exponent s of the scaling relation,

$$V_L = a + bL^s(1 + qL^r), \quad (18)$$

where a correction term was added. For the WL algorithm $s = -2.49699 \pm 0.01092$, Metropolis $s = -2.50314 \pm 0.00528$ and heat-bath $s = -2.52254 \pm 0.00537$, while the constant term assumes the value $a = 0.66668 \pm 0.000005$ for all the algorithms, which is the expected value, since V_L tends to the limit (2/3) in the thermodynamic limit $L \rightarrow \infty$. The other coefficients (b, q, r) assume appropriate values, especially, r is negative to prevent divergence of the expression.

The Binder cumulant pseudocritical temperatures scale according to the expression (16); by performing preliminary fitting, as earlier, we found that,

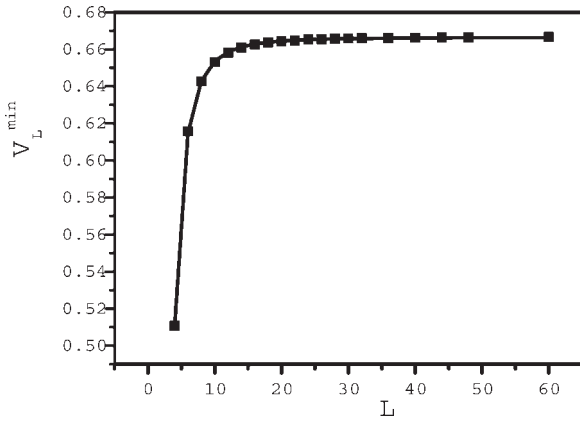


Fig. 3. Variation of the cumulant minimum with L . The early asymptotic behavior of V_L^{\min} towards its value ($2/3$) is obvious.

$\bar{a} = 2.19786 \pm 0.18271$. By fitting the MC values for T_L^{\min} to (16), as in respective case for the specific heat, the resulting mean values are,

$$\begin{aligned} \bar{K}_c &= 0.22169 \pm 0.00023, \\ \bar{b} &= -5.44779 \pm 0.59702. \end{aligned} \quad (19)$$

Comparing the values for K_c in (17) and (19), we observe that they are compatible, although the former is more accurate and is closer to the one in Refs. [7,8].

4. CONCLUSIONS AND DISCUSSIONS

The Wang-Landau, Metropolis and heat-bath algorithms were applied to the three-dimensional Ising model with constant order parameter. We analyzed the MC data for the specific heat and Binder energy cumulant by means of FSS to estimate the critical temperature and thermal critical exponent y_t ; the leading irrelevant exponent was fixed for all scaling attempts, since if it were variable, the induced errors would be large. The resulting values for y_t and K_c , confirm that the system belongs to the three-dimensional Ising universality class, since these values are consistent to the respective ones for the normal version of the model. The current analysis yields accurate estimations for the thermal exponent and critical temperature, as well.

The estimates (8,10,12,13) for y_t found directly from the MC calculations, can be utilized in two

ways: to determine rough bounds for y_t and draw conclusions concerning the significant digits of y_t .

As noted earlier, our main estimate $y_t = 1.58686 \pm 0.00007$ is in excellent agreement with the one of Deng and Blöte [9], ($y_t = 1.5868(3)$), (as well as the results in (12), (13)), while with Blöte *et al.* [8], ($y_t = 1.587(2)$), and Malakis *et al.* [13], ($y_t = 1.5878(31)$), the agreement is good. Also, our estimate is consistent with the one in Ferrenberg and Landau [7] ($y_t = 1.590 \pm 0.002$), Blöte *et al.* [22] ($y_t = 1.585(3)$). However, it is in disagreement with Landau [23] ($y_t = 1.590(2)$) and Baillie *et al.* [24] ($y_t = 1.602(5)$).

Comparing our estimate for the inverse critical temperature $K_c = 0.22166 \pm 0.00004$ with other ones, we find that the agreement is good with the results of Ferrenberg and Landau [7] (0.2216595 ± 0.0000026), Blöte *et al.* [8] (0.2216546 ± 0.0000010), Deng and Blöte [9] ($0.22165455 \pm 0.00000003$), Landau [23] (0.2216576 ± 0.0000022), Ito and Suzuki [25] (0.221657 ± 0.000003). However, it is in disagreement with Baillie *et al.* [24] (0.221652 ± 0.000003), Liu and Fisher [26] (0.22162 ± 0.00006) and Blöte and Kamieniarz [27] (0.221648 ± 0.000004).

These results ensure the correctness and reliability of the CrMES scheme, which can be used safely for the estimation of critical exponents.

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