Monte Carlo studies of the square Ising model with next-nearest-neighbor interactions

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We apply a new entropic scheme to study the critical behavior of the square-lattice Ising model with nearest- and next-nearest-neighbor antiferromagnetic interactions. Estimates of the present scheme are compared with those of the Metropolis algorithm. We consider interactions in the range where superantiferromagnetic (SAF) order appears at low temperatures. A recent prediction of a first-order transition along a certain range (0.5-1.2) of the interaction ratio $(R = J_{nnn}/J_{nn})$ is examined by generating accurate data for large lattices at a particular value of the ratio (R = 1). Our study does not support a first-order transition and a convincing finite-size scaling analysis of the model is presented, yielding accurate estimates for all critical exponents for R = 1. The magnetic exponents are found to obey "weak universality" in accordance with a previous conjecture.

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I. INTRODUCTION

Spin models with competing interactions are of great theoretical and experimental interest and have been for long time the subject of many investigations. Such interactions may give rise to complicated spatial orderings and produce complex and rich critical behavior [1]. The transitions between ordered and disordered phases may be continuous or of first order with a tricritical point between them, but no general classification exists, connecting the symmetry of spin structures and the range of interaction with the expected critical behavior. The Ising square lattice with nearest-neighbor coupling (nn) is an exactly soluble model [2] and almost all its properties are well known. With the addition of next-nearest-neighbor (nnn) interactions the problem is no longer exactly soluble and several approximate methods have been applied to attack this more general problem and to understand the effect of adding the nnn-coupling on the critical behavior of the system [3, 4, 5, 6, 7, 8, 9]. Of particular interest is the case of competing interactions, where the ground state is an arrangement with superantiferromagnetic (SAF) order in which ferromagnetic rows (columns) alternate with opposite oriented spins. The T=0 phase diagram is well known [5, 6, 7] and the SAF-order can be obtained in both cases of a ferromagnetic or an antiferromagnetic nn-coupling. The system, in zero-field, is governed by the Hamiltonian:

$$\mathcal{H} = J_{nn} \sum_{\langle i,j \rangle} S_i S_j + J_{nnn} \sum_{(i,j)} S_i S_j \tag{1}$$

where here both nearest-neighbor (J_{nn}) and next nearest-neighbor (J_{nnn}) interactions will be assumed to be positive (antiferromagnetic) and the system as is well known [3, 4, 5, 6, 7, 8, 9] develops at low temperatures superantiferromagnetic order for R > 0.5.

Several previous studies have suggested that the above system may possess "anomalous" exponents, and a non-universal critical behavior with exponents depending on the coupling ratio $R = J_{nnn}/J_{nn}$ has been the commonly accepted scenario for many years [3, 4, 5, 6, 7, 8, 9]. However, recently the interest on the subject has been renewed and some attempts to re-examine the behavior of this model have taken place. In several papers Lopez et.al [10, 11, 12] have used the cluster variation method (CVM) to study this model and have concluded that the system undergoes a first-order transition for a particular range of the coupling ratio (0.5-1.2). Thus, a different scenario predicting first order transitions between ordered and disordered phases, followed by continuous transitions outside the first-order region has been proposed [10, 11, 12]. It appears that this scenario has been further supported by the study of Buzano and Pretti [13]. These authors studied the same model with an additional 4-body coupling using again the CVM and concluded that according to this method a first-order behavior is expected for a very large part of the parameter space reproducing also the results of [10, 11, 12]. However, they also considered the limiting case ($J_{nn} = 0$), where the exact solution of Baxter model [14] applies, observing again a large part of the parameter space in which the

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CVM predicts first-order behavior. Thus, the CVM fails to predict the true second order critical behavior for the Baxter model and, this is of course, an obvious reason for suspecting the CVM. It is quite possible that the CVM, in any finite-order approximation, could produce misleading "mean-field" behavior not unlikely with other variational methods [15]. Yet, the relevant questions are very important for a better understanding of the critical behavior of systems with competing interactions. Notwithstanding that, a recent Monte Carlo simulation [16] of a quite "similar model" has provided strong evidence of first order behavior. This last model includes nn- and nnn-antiferromagnetic couplings but now the model is defined on the triangular lattice. Having to deal with the same hamiltonian and a similar ground state arrangement (SAF-arrangement) one should naively expect the same critical behavior for the two models, assuming a simple universality in which the underlying lattice is immaterial in 2D. In the light of the above controversial and at the moment unsettled situation, it is of interest to follow again the traditional finite-size scaling analysis to re-examine the above prediction. As a first attempt, we study here the square model for a particular value of the coupling ratio, R=1, included in the above range, and using a new complementary and efficient numerical method we generate accurate finite-size data for quite large lattices. The rest of the paper is organized as follows. In the next section we outline the entropic sampling technique implemented here to generate numerical estimates accurate in the critical region for the case R=1. In section 3 we explain why our numerical data are not supporting a first-order transition and then we present a finite-size analysis, yielding accurate estimates for the critical exponents. These are compared with estimates existing in literature and an old conjecture of K. Binder and D. P. Landau [5] assuming "weak universality" is reinforced. Our conclusions are summarized in section 4.

II. THE CRMES WANG-LANDAU ENTROPIC SAMPLING SCHEME

Traditional Monte Carlo sampling methods have been used for many years in the study of critical phenomena [17] and the first Monte Carlo approaches to the present model were indeed carried out by the Metropolis method [4, 5, 6]. On the other hand, general flat histogram methods [17, 18, 19, 20] are alternatives to importance sampling and are expected to be much more efficient for studying a complex system. A simple and efficient entropic implementation of the Wang-Landau(WL) method has been presented recently by the present authors. This method is based on a systematic restriction of the energy space as we increase the lattice size. The random walk of this entropic simulation takes place only in the appropriately restricted energy space and this restriction produces an immense speed up of all popular algorithms calculating the density of energy states (DOS) of a statistical system [21, 22]. For the temperature range of interest, that is the range around a critical point, this scheme determines all finite-size anomalies using an one-run entropic strategy employing what we have called the "critical minimum energy subspace Wang-Landau (CrMES WL)-entropic sampling method". In this approach all (thermal and magnetic) properties are obtained by using the high-levels (that is the levels where the detailed-balanced condition is quite well obeyed) of the Wang-Landau random walk process to determine appropriate microcanonical estimators. The method is efficiently combined with the N-fold way [19] in order to improve statistical reliability but also to produce broad-histogram (BH) estimators for an additional calculation of the density of states (DOS).

The approximation of canonical averages, in a temperature range of interest, is as follows:

$$\langle Q \rangle = \frac{\sum_{E} \langle Q \rangle_{E} G(E) e^{-\beta E}}{\sum_{E} G(E) e^{-\beta E}} \cong \frac{\sum_{E \in (E_{1}, E_{2})} \langle Q \rangle_{E, WL} \widetilde{G}(E) e^{-\beta E}}{\sum_{E \in (E_{1}, E_{2})} \widetilde{G}(E) e^{-\beta E}}$$
(2)

The restricted energy subspace (E_1, E_2) is carefully chosen to cover the temperature range of interest without introducing observable errors. The microcanonical averages $\langle Q \rangle_E$ are determined from the $H_{WL}(E,Q)$ -histograms, which are obtained during the high-levels of the WL-process:

$$\langle Q \rangle_E \cong \langle Q \rangle_{E,WL} \equiv \sum_Q Q \frac{H_{WL}(E,Q)}{H_{WL}(E)}, \ H_{WL}(E) = \sum_Q H_{WL}(E,Q)$$
 (3)

and the summations run over all values generated in the restricted energy subspace (E_1, E_2) . Finally, the approximate density of states used in (2) is obtained from the DOS generated after the last WL-iteration $(\tilde{G}(E) = G_{WL}(E))$ or from the broad-histogram (BH) approximation $(\tilde{G}(E) = G_{BH}(E))$. This last approximation may be easily calculated from appropriate microcanonical averages corresponding also to the high-levels of the WL-process, since in the N-fold implementation of the WL-process the necessary histograms for the application of the broad-histogram method [20] are also known. As mentioned above, the updating of appropriate histograms (Q may be any power of the order parameter or some other quantity) is carried out only in the high-levels of the WL-process. In these stages, the incomplete detailed-balance condition has not significant effect on the microcanonical estimators constructed from

the cumulative histograms as shown in [22]. Thus we have used only the WL-iterations: j=12-24 for lattices up to L=100 and the WL-iterations: j=16-26 for larger lattices. The initial modification factor of the WL-process is taken to be $f_1=e=2.718...$ and, as usual, we follow the rule $f_{j+1}=\sqrt{f_j}$ and a 5% flatness criterion [21, 22]. The rest of the details and the N-fold implementation can be found in [17, 18, 19, 20, 21, 22].

In the present implementation of the CrMES method we restrict the total energy range (E_{min}, E_{max}) to the minimum energy-subspace producing an accurate estimation for all finite-size anomalies. This restriction may be defined by requesting a specified accuracy on a diverging specific heat (or on a diverging susceptibility) as shown in [22]. Alternatively, the energy density function may be used in a simpler way to restrict the energy space. Thus, if \tilde{E} is the value maximizing the probability density, at some pseudocritical temperature (T_L^*) , the end-points (\tilde{E}_{\pm}) of the energy critical subspaces (CrMES) may be located by the condition:

$$\widetilde{E}_{\pm}: \frac{P_{\widetilde{E}_{\pm}}(T_L^*)}{P_{\widetilde{E}}(T_L^*)} \le r \tag{4}$$

where r is chosen to be a small number, independent of the lattice size. Both $r = 10^{-4}$ and $r = 10^{-6}$ have been used in the present study to estimate the relevant extensions of critical subspaces as discussed bellow. The resulting finite-size extensions of critical energy subspaces, denoted by $(\Delta \widetilde{E})$, obey the "specific-heat" scaling law [21]:

$$\Psi \equiv \frac{(\Delta \widetilde{E})^2}{L^d} \approx L^{\frac{\alpha}{\nu}} \tag{5}$$

Since the extensions of these energy subspaces satisfy very well the above scaling law, relation (5) is a new route for estimating the critical exponent α/ν [21, 22]. Furthermore, following a similar procedure we may also estimate the critical exponent γ/ν , as already shown in [22]. Again, let \widetilde{M} be the value maximizing the order parameter density at some pseudocritical temperature, for instance at the susceptibility pseudocritical temperature. The end-points (\widetilde{M}_{\pm}) of the magnetic critical subspaces (CrMMS) are located by the condition:

$$\widetilde{M}_{\pm}: \frac{P_{\widetilde{M}_{\pm}}(T_L^*)}{P_{\widetilde{M}}(T_L^*)} \le r \tag{6}$$

and the corresponding finite-size extensions of critical magnetic subspaces obey close to a critical point, the "susceptibility" scaling law [22]:

$$\Xi \equiv \frac{(\Delta \widetilde{M})^2}{L^d} \approx L^{\frac{\gamma}{\nu}} \tag{7}$$

Equations (equations (5) and (7)) provide additional routes for estimating the involved critical exponents.

III. NUMERICAL EVIDENCE. FINITE - SIZE SCALING ANALYSIS.

Let us first present an illustrative graph showing that the above-described entropic scheme yields accurate data for the application of finite-size scaling. We have used two different definitions for the order parameter. With the help of four sublattices of the SAF-ordering one may define a two-component order parameter and finally use its root-mean-square (rms) as done in [5].

$$M_{SAF}^{(1)} = \{M_1 + M_2 - (M_3 + M_4)\} / 4, \quad M_{SAF}^{(2)} = \{M_1 + M_4 - (M_2 + M_3)\} / 4$$

$$M_{SAF}^{(rms)} = \sqrt{\left(M_{SAF}^{(1)}\right)^2 + \left(M_{SAF}^{(2)}\right)^2}$$
(8)

We have used this rms order parameter and also, as an alternative, the sum of the absolute values of the four sublattice magnetizations ($M_{SAF} = \sum_{i=1}^{4} |M_i|/4$). The resulting behavior is very similar and the finite size extensions of the resulting CrMMS completely coincide supporting the identity of the two representations for the present system. Therefore, for large lattices only the second order parameter was used. For a particular temperature, T = 2.082, close to the critical temperature, we have calculated using long runs of the Metropolis algorithm several thermodynamic properties of the system for R = 1 and we have found good agreement with the corresponding estimates obtained via the entropic scheme described in the previous section. Figure 1 provides a comparison test between the Metropolis algorithm and entropic scheme. Let us consider the estimates of the Metropolis simulation for the susceptibility at the

above mentioned temperature as being the exact values. Then figure 1 presents the variation of the "relative errors" of the entropic scheme with lattice size and compare these with the statistical errors of the Metropolis simulation. From this figure it can be seen that the CrMES-WL entropic scheme provides estimates in the expected range. We conclude that similar accuracy should be expected for the temperature-range covered by the restricted energy subspaces.

Next, we search (using the approximate DOS: G(E)) for a double peak in the energy probability density which should be expected if the system undergoes a first-order transition as predicted by CVM. For R=1, using small temperature steps close to the specific heat pseudocritical temperatures, we did not observe such double peaks. In contrast when we used our algorithm to generate the appropriate DOS of the triangular (SAF) model considered by Rasteli et. al [16], the presence of the energy double-peaks reported by these authors was very clear. The finite-size behavior of the fourth-order cumulant (of the order parameter) is indicative for the order of the transition [23, 24]. We used this test in order to observe the behavior for the square lattice model and to examine the prediction for a first-order transition reported by Lopez et al. [10, 11, 12]. Comparing by this test the two models we had the opportunity to observe that the difference in the cumulant-behavior between them was again profound. For the triangular model the behavior was in very good agreement with that reported in [16] indicating a first-order transition, while for the present square model a behavior characteristic of a second order critical point was observed [23]. It appears that the first-order prediction of the CVM is false at least for the case R=1. The tricritical point, if it exists, could be in a lower temperature and the upper bound (1.2) given by Lopez et al. [10, 11, 12] could be an overestimation of the CVM.

Figure 2 presents the order-parameter cumulant behavior of the square lattice model for several lattice sizes close to the critical temperature. From this graph and by using the crossing method [23] we have estimated the critical temperature. Taking the average of all the crossing temperatures included in figure 2 we find: $T_c = 2.0823(17)$. Including in this averaging the smaller sizes L = 30 - 60 the estimate is: $T_c = 2.0821(13)$. Thus, $T_c = 2.0823(17)$ seems quite safe and it is also in good agreement with the estimates obtained by fitting the specific heat, susceptibility and energy-cumulant pseudocritical temperatures to a power law behavior with a correction term:

$$T_L = T_c + \alpha L^{-\lambda} \left(1 + \frac{b}{L} \right) \tag{9}$$

The above-mentioned fits, not shown for brevity, yielded respectively: $(T_c = 2.0825(5), \lambda = 1.20(4)), (T_c = 2.0828(8), \lambda = 1.197(50))$ and $(T_c = 2.0818(8), \lambda = 1.158(60))$

Let us now try to estimate the magnetic critical exponent γ/ν . We employ the commonly used route of fitting the values of the susceptibility peaks and/or its values at the critical temperature ($T_c=2.0823$) to observe the scaling exponent. Figure 3 presents three scaling fitting attempts assuming a simple power law. The peaks of the susceptibility yield an estimate of the order 1.79, while the susceptibility values at the estimated critical temperature provide an estimate of the order 1.71. The exponent appears to acquire a value in this wide range ($\gamma/\nu=1.71-1.79$) if we vary the lattice sizes fitted and/or if we add corrections terms to the simple power law. Note that the estimated in [5] range is 1.71 ± 0.15 . The middle solid line in figure 3 shows that the average of the susceptibility in the two temperatures (T_c and $T_L^*(\chi)$) gives an estimate very close to the 2D-Ising value ($\gamma/\nu=1.75$). These observations seem to favor the original view of [5] that the system may obey a kind of "weak universality" [25]. According to this hypothesis the reduced exponent γ/ν will have the 2D-Ising value independent of R. To further check this conjecture let us analyze the scaling behavior of the finite-size extensions ($\Delta \widetilde{M}$) in equation (7). Figure 4 shows the behavior of these scaled extensions in the two temperatures T_c and $T_L^*(\chi)$) together with the behavior of their average. Fitting the numerical data to a law of the form:

$$y = \alpha L^w (1 + \frac{b}{L}) \tag{10}$$

we obtain very good fits and the estimates of γ/ν are for the three curves in the range $w=1.75\pm0.01$. Thus, the scenario of weak universality of $\gamma/\nu=1.75$ is greatly reinforced.

Frequently, the scaling of the specific heat is a difficult task but for the present model we have discovered that the scaling behavior of the average of our estimates in the two temperatures $(T_c \text{ and } T_L^*(C))$ is quite stable as one varies the lattice size. Figure 5 shows details of the fit for the "averaged" specific heat values and figures 6 and 7 show the analysis of the scaled extensions $(\Psi(\Delta \widetilde{E}))$ appearing in equation (5). Comparing the last two fits we find a unique case of stability and we confidently estimate:

$$\frac{\alpha}{\nu} = 0.412 \pm 0.005 \tag{11}$$

The above findings (estimate (11) and the weak universality $\gamma/\nu = 1.75$) may now be used to determine a consistent scheme for all critical exponents. Assuming hyperscaling, the correlation length exponent is estimated as

 $\nu=0.8292(24)$ and this value is consistent $(\frac{1}{\nu}=\lambda)$ with the estimates of the shift exponent found from the pseudocritical temperatures. The exponent β/ν should therefore be 0.125. A power law fit of our estimates of the order parameter at the critical temperature are in a good agreement with this value. The proposed set of exponents satisfies all scaling laws for a second order transition as can be easily verified.

IV. CONCLUDING REMARKS

In this paper we have considered the square-lattice Ising model with nearest- and next-nearest-neighbor antiferromagnetic interactions and found that the prediction of the cluster variation method of a first-order transition is not supported by the finite size behavior of the system (R=1). The original scenario [3, 4, 5, 6, 7, 8, 9] of a non-universal critical behavior with exponents depending on the coupling ratio has been strongly reinforced by our numerical study and "weak universality" [5, 25] seems to be well obeyed. The idea of using scaled extensions of dominant critical subspaces to estimate the thermal exponent α/ν and the magnetic exponent γ/ν seems to supply a quite accurate route for exponent estimation. In the present case the accurate estimation by this route of the thermal exponent is almost unique. Furthermore, the successful application of the scaling law (7) has been a helpful guidance in observing the "weak universality" of the magnetic critical exponents. The entropic sampling scheme applied in this study provides a better evaluation of the tail behavior of the critical distributions and this seems to be of importance for the accurate estimation of the finite-size extensions of the dominant subspaces used for the exponent estimation.

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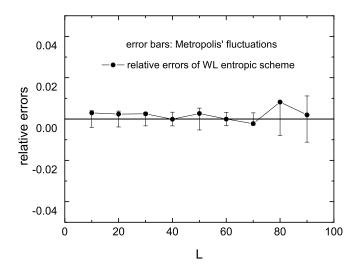


FIG. 1: Relative deviations of the CrMES entropic scheme used in this paper with respect to the Metropolis algorithm. The relative errors of the critical susceptibility are presented for L=10-90 and are compared to the statistical errors (indicated as error bars) of the corresponding Metropolis runs.

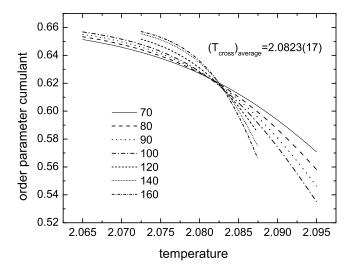


FIG. 2: Estimation of the critical temperature (R = 1). T_c is obtained as the average of the crossing points. The reduced fourth-order cumulant has been used.

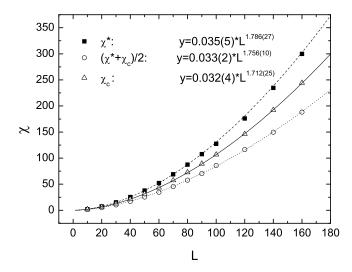


FIG. 3: Finite-size behavior of the susceptibility at the critical and its pseudocritical temperature. Fitting parameters to a simple power law are presented for the above estimates as well as for their average. Note, that only their average gives an exponent value very close to the 2D Ising value.

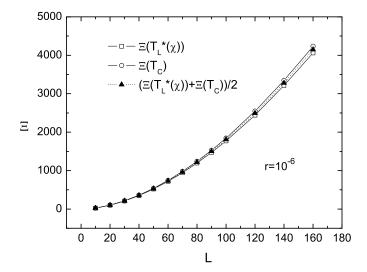


FIG. 4: Finite-size behavior of the scaled extensions $\Xi(\Delta M)$ at the critical and susceptibility's pseudocritical temperature. Their average is also shown. Fitting Eq. (10) to these data we have obtained very good estimates of the critical exponent γ/ν : 1.7545(27), 1.7536(45), 1.7541(28) respectively. These three estimates fall into a narrow range close to the 2D Ising value contrary to the wide range observed in figure 3.

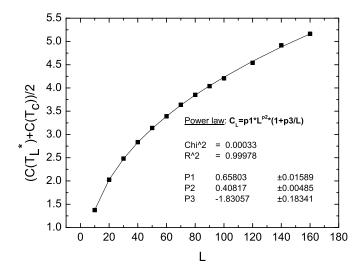


FIG. 5: Finite-size behavior of the specific heat's average at the critical and its pseudocritical temperature. Fitting parameters to the power law illustrated on the graph, are presented as well.

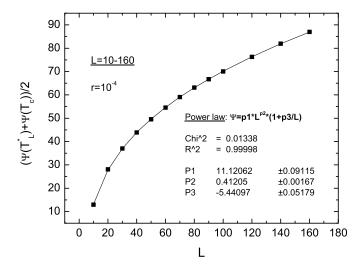


FIG. 6: Finite-size behavior of the average of scaled extensions $\Psi(\Delta \widetilde{E})$ (Eq. (5)) at the critical and and specific heat's pseudocritical temperature. Fitting parameters to the power law illustrated on the graph, are presented as well. The results are obtained through fitting all the available data

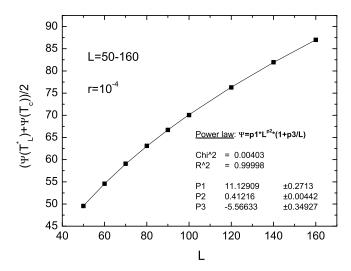


FIG. 7: Finite-size behavior of the average of scaled extensions $\Psi(\Delta \widetilde{E})$ at the critical and and specific heat's pseudocritical temperature. The results are obtained through fitting data from L=50 to 160 in order to check the stability of the fit.