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

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Abstract. 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 super-antiferromagnetic (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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1 Introduction

The Ising square lattice with nearest-neighbor coupling (nn) is an exactly soluble model 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 [1–7]. 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 [3–5] 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:

$$\mathcal{H} = J_{nn} \sum_{<i,j>} S_i S_j + J_{nnn} \sum_{(i,j)} S_i S_j \qquad (1)$$

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 [1–7] develops at low temperatures superantiferromagnetic order for $R > 0.5$. Note that there is no loss of generality in considering only $J_{nn} > 0$ since the critical behavior associated with the SAF ordering is the same if $J_{nn} \to -J_{nn}$.

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 [1–7]. 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. [8–10] 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 [8–10]. It appears that this scenario has been further supported by the study of Buzano and Pretti [11]. These authors studied the same model with an additional 4-body coupling using again the CVM and concluded that a first-order behavior is expected for a very large part of the parameter space reproducing also the results of [8–10]. However, they also considered the limiting case ($J_{nn} = 0$), where the exact solution of Baxter model [12] applies, observing again a large part of the parameter space in which the CVM predicts first-order behavior. Thus, the CVM

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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 [13]. Notwithstanding that, a recent Monte Carlo simulation [14] 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. In the light of the above controversial situation, it is of interest to follow 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 ($R = 1$) using a new efficient entropic sampling technique, presented in the next section. In Section 3 we present our numerical data and a finite-size analysis, yielding accurate estimates for the critical exponents. Our conclusions are summarized in Section 4.

2 The CRMES Wang-Landau entropic sampling scheme

Flat histogram methods [15–19] 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. The random walk of this entropic simulation takes place only in the appropriately restricted energy space [18] and the method may be efficiently combined with the N-fold way [16,19]. The approximation of canonical averages, in a temperature range of interest, is as follows:

$$\langle Q\rangle = \frac{\sum_E \langle Q\rangle_E G(E) e^{-\beta E}}{\sum_E G(E) e^{-\beta E}} \cong \frac{\sum_{E\in(E_1,E_2)} \langle Q\rangle_{E,WL} \widetilde{G}(E) e^{-\beta E}}{\sum_{E\in(E_1,E_2)} \widetilde{G}(E) e^{-\beta E}}. \quad (2)$$

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

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

The approximate density of states used in equation (2) is obtained from the DOS determined in the last WL-iteration ($\widetilde{G}(E) = G_{WL}(E)$). 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 [19]. 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 [18,19]. The rest of the details and the N-fold implementation can be found in [15–19].

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). Alternatively the energy density function may be used in a simpler way to restrict the energy space [19]. The finite-size extensions of the critical energy subspaces ($\Delta\widetilde{E}$) obey the following law [18,19], from which α/ν may be estimated:

$$\Psi \equiv \frac{\left(\Delta\widetilde{E}\right)^2}{L^d} \approx L^{\frac{\alpha}{\nu}}. \quad (4)$$

Furthermore, following a similar procedure we may also estimate the critical exponent γ/ν, as already shown in [19]. Again, let $\widetilde{M}$ be the value maximizing the order parameter density at some pseudocritical temperature, for instance at the susceptibility pseudocritical temperature. For a diverging specific heat (susceptibility) the pseudocritical temperature T_L^* is the temperature corresponding to the maximum of the specific heat (susceptibility). For the cumulant finite-size anomaly the pseudocritical temperature corresponds to the minimum of the cumulant. The end-points ($\widetilde{M}_\pm$) of the magnetic critical subspaces (CrMMS) are located by the condition:

$$\widetilde{M}_\pm : \frac{P_{\widetilde{M}_\pm}(T_L^*)}{P_{\widetilde{M}}(T_L^*)} \le r \quad (5)$$

and the corresponding finite-size extensions of critical magnetic subspaces obey close to a critical point, the "susceptibility" scaling law [19]:

$$\Xi \equiv \frac{\left(\Delta\widetilde{M}\right)^2}{L^d} \approx L^{\frac{\gamma}{\nu}}. \quad (6)$$

3 Numerical evidence. Finite - size scaling analysis

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 [3]. We have used this rms order parameter and also, as an alternative, the sum of the absolute values of the four sublattice magnetizations. 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 very good agreement with the corresponding estimates obtained via our entropic scheme.

Next, we search 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 $R = 1$, we did not observe such double peaks. In contrast when we used our algorithm to generate the corresponding DOS of the triangular (SAF) model considered by Rasteli et al. [14], 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 [20,21]. 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. [8–10]. 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 [14] indicating a first-order transition, while for the present square model a behavior characteristic of a second order critical point was observed [20]. It appears that the first-order prediction of the CVM is false at least for the case $R = 1$.

By using the crossing method [20] for the order-parameter cumulant we have estimated the critical temperature. Taking the average of all the crossing temperatures of the curves corresponding to sizes $L = 70$–160 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's and susceptibility's pseudocritical temperatures to a power law behavior with a correction term: $T_L^* = T_c + \alpha L^{-\lambda}(1 + b/L)$. These fits, not shown for brevity, yield respectively: $T_c = 2.0825(5), \lambda = 1.20(4)$ and $T_c = 2.0828(8), \lambda = 1.197(50)$.

Let us now try to estimate the magnetic critical exponent γ/ν. We first fit the values of the susceptibility peaks and our estimates for the critical susceptibility ($T_c = 2.0823$) to a power law. Figure 1 presents three fitting attempts assuming a simple power law. The peaks of the susceptibility yield an estimate of the order of 1.79, while the critical susceptibilities yield an estimate of the order of 1.71. The exponent appears to acquire a value in this wide range ($\gamma/\nu = 1.71 - 1.79$) when we vary the lattice sizes fitted and/or when we add corrections terms to the simple power law. Note that the estimated

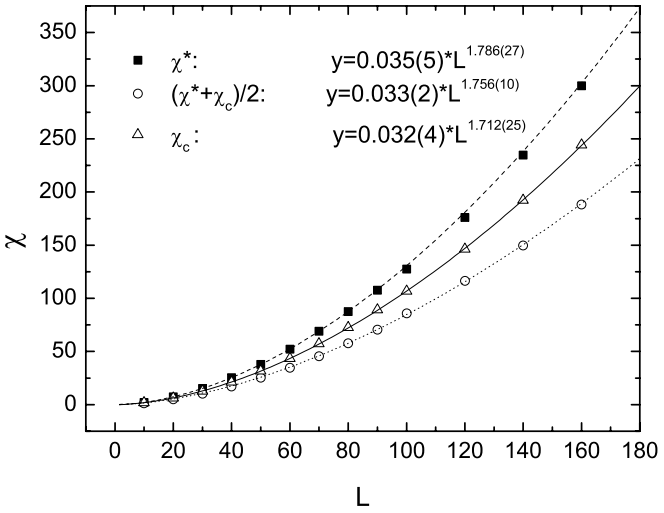

Fig. 1. Finite-size behavior of the susceptibility at the critical and its pseudocritical temperature. Fitting parameters to a simple power law are presented for the above estimates as well as for their average. Note, that only their average gives an exponent value very close to the 2D Ising value.

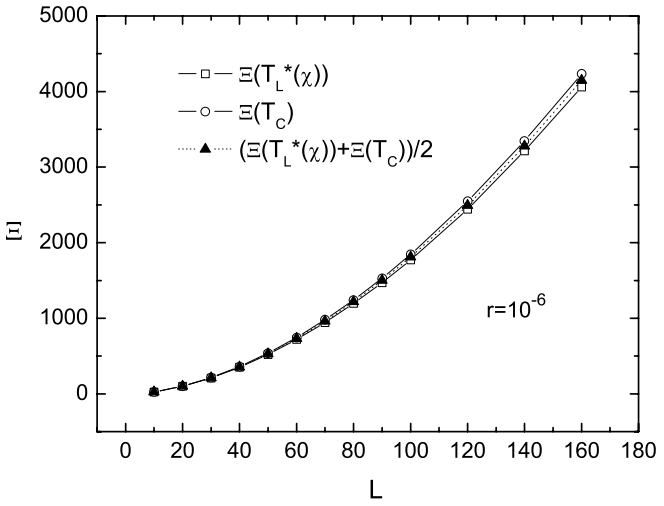

Fig. 2. Behavior of the scaled extensions $\Xi(\Delta\widetilde{M})$ at the critical and susceptibility's pseudocritical temperature. Their average is also shown. Fitting equation (6) to these data we have obtained very good estimates of the critical exponent γ/ν: 1.7545(27), 1.7536(45), 1.7541(28) respectively.

in [3] range is 1.71 ± 0.15. The middle solid line in Figure 1 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 [3] that the system may obey a kind of "weak universality". According to this hypothesis the "reduced" critical exponents, i.e. $\hat{\gamma} = \frac{\gamma}{\nu}$, $\hat{\beta} = \frac{\beta}{\nu}$, $\hat{\phi} = \frac{2-\alpha}{\nu}$ etc, are constant for systems obeying weak universality [22]. Thus, γ/ν will have the 2D-Ising value independent of R. Let us now analyze

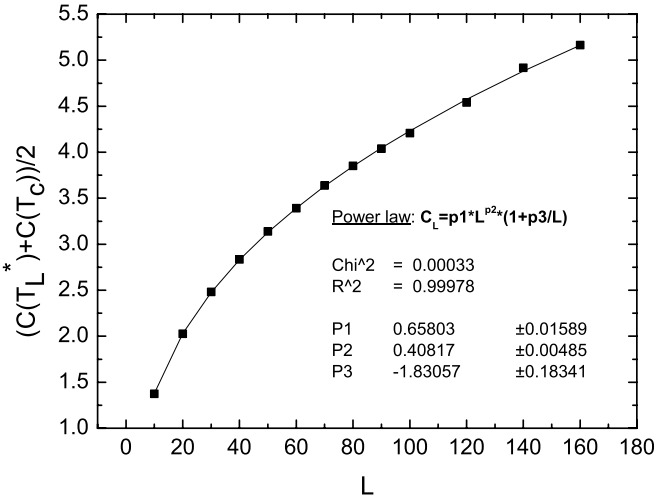

Fig. 3. Finite-size behavior of the specific heat's average at the critical and its pseudocritical temperature. Fitting parameters to the power law illustrated on the graph, are presented as well.

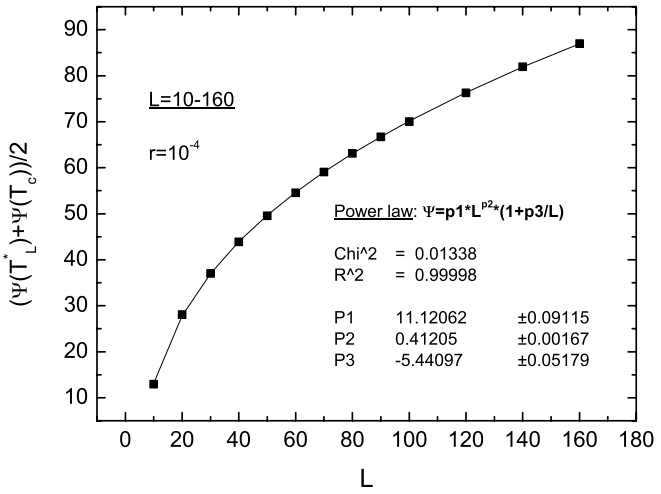

Fig. 4. Behavior of the average of scaled extensions $\Psi(\Delta\widetilde{E})$ at the critical and specific heat's pseudocritical temperature. Fitting parameters of the power law are given in the graph.

the scaling behavior of the finite-size extensions $(\Delta\widetilde{M})$ in equation (6). Figure 2 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: $y = \alpha L^w(1 + b/L)$ we obtain very good fits and the estimates of γ/ν, are for the three curves, in the range $w = 1.75 \pm 0.01$. Thus, the scenario of weak universality of $\gamma/\nu = 1.75$ is greatly reinforced.

Finally, consider the scaling of the specific heat. We have discovered that the behavior of the average of our estimates in the two temperatures (T_c and $T_L^*(C)$) is quite stable as one varies the lattice size. Figure 3 shows details of the fit for the "averaged" specific heat values and Figures 4, 5 show the analysis of the scaled extensions $(\Psi(\Delta\widetilde{E}))$ appearing in equation (4). Comparing the last

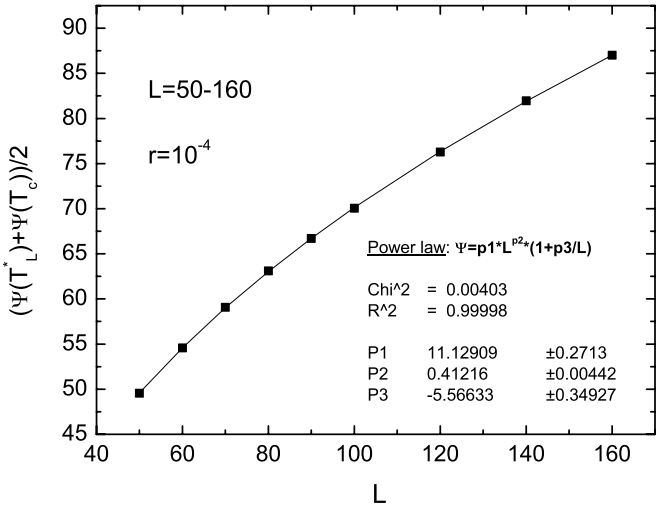

Fig. 5. Behavior of the average of scaled extensions $\Psi(\Delta\widetilde{E})$ at the critical and specific heat's pseudocritical temperature, for the range $L = 50$ to 160.

two fits we find a unique case of stability and we confidently estimate: $\alpha/\nu = 0.412 \pm 0.005$. Assuming hyperscaling ($\alpha = 2 - d\nu$), 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.

4 Concluding remarks

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 [1–7] of a non-universal critical behavior with exponents depending on the coupling ratio has been strongly reinforced by our numerical study and the conjecture of "weak universality" [3,22] seems to be well obeyed. Of course, an analogous study for a range of R-values would strengthen this last hypothesis. The idea of using scaled extensions of dominant critical subspaces to estimate the exponents α/ν and γ/ν seems to supply a quite accurate route for their estimation.

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