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MAGNETIC CRITICAL BEHAVIOR OF THE THREE-DIMENSIONAL ISING MODEL BY ENTROPIC SAMPLING IN DOMINANT ENERGY SUBSPACES

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Abstract. We apply a new entropic scheme to study the critical behavior of the three-dimensional (3D) Ising model on a cubic lattice. This method (CrMES entropic sampling scheme) has been recently shown to be an efficient and accurate alternative to the traditional Metropolis method. It utilizes a Wang-Landau (WL) random walk in an appropriately chosen dominant energy subspace. Via this process it generates, in one-run, good approximations for the density of energy states and the microcanonical estimators of the magnetic properties of the system by updating (E,M) histograms during the high-level WL iterations. Applying this procedure we present a convincing finite-size analysis of the magnetic critical behavior of the 3D Ising model and we estimate the relevant critical exponents. Finally, the far tail regime of the order-parameter probability distribution is discussed.

1. INTRODUCTION

In recent years there has been a growing interest in obtaining accurate estimates of critical parameters for the 3D Ising model. The Hamiltonian that describes the model is given by:

$$H = -J_{nn}\sum_{<ij>} S_i S_j, \qquad (1)$$

where the nearest-neighbor (J_{nn}) interactions are assumed to be positive (ferromagnetic). The system, as it is well-known, develops at low temperatures ferromagnetic order. Nevertheless, despite the intense effort made, the model has defied exact solution [1,2] and though it has been investigated extensively by various numerical methods, is still a matter of sophisticated numerical analysis [3-31]. The critical properties of the model, i.e., the critical temperature T_c, the thermal and magnetic scaling exponents y_t and y_h, and also the leading thermal irrelevant exponent y_i seem to be known with good accuracy [22,25]. However, the absence of exact results creates, at least in principle, a motive for disagreements [25,30]. For many years, reliable estimates for T_c and the critical exponents have been obtained by series expansion data, ε-expansion studies, Monte Carlo renormalization group studies and the coherent anomaly method [3-10,16-21,31].

Traditional Monte Carlo importance sampling and histogram techniques, have been used also to investigate the 3D Ising model [11-15,23-25], but only recently [25] such studies have provided accurate

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estimates of the critical exponents. There are two reasons for the modest accuracy obtained in these Monte Carlo simulations. Firstly, extended runs are necessary to reduce the systematic and statistical errors, which arise due to the finite number of samples taken. Secondly, corrections to scaling are much more important in three than in two dimensions. The leading irrelevant thermal exponent for the 3D Ising model has the value y_i =-0.821(5) [25] and this means that corrections decay relatively slowly. The two effects of finite sampling time and finite system size become intertwined and jeopardize the finite-size scaling analysis. The aim of this paper is to provide a convincing finite-size analysis of the magnetic critical behavior of the 3D Ising model and an accurate estimation of the the relevant critical exponents, via a new promising numerical procedure, based on a WL random walk [32,33] in an appropriately chosen dominant subspace [34]. This method has been recently put forward by the present authors and has been tested successfully on the 2D Ising model [35]. It implements the WL diffusion in order to accumulate appropriate energy-magnetization histograms. Since the WL process yields a flat histogram at any stage, the method mimics an entropic sampling scheme, as explained in the text. The present application is also one more reliability test of this method.

The layout of the paper is organized as follows. In the next section we outline the entropic technique implemented here to generate numerical estimates accurate in the critical region for all magnetic and thermal finite-size anomalies. In Section 3 we present a finite-size analysis of the magnetic properties, yielding accurate estimates for the critical exponents. In Section 4 we study the order-parameter distribution of the 3D Ising model and attempt to observe its asymptotic behavior in the far tail regime. Finally, our conclusions are summarized in Section 5.

2. THE CRMES WANG-LANDAU ENTROPIC SAMPLING SCHEME

For many years traditional Monte Carlo sampling methods have been used almost exclusively in the study of critical phenomena [36-38]. However, in the last decade a considerable shift to entropic sampling methods or flat histogram methods is taking place [38]. This is particularly true in studies of critical behavior of complex systems, where the entropic schemes are expected to be much more efficient [38]. Recently, the present authors have presented a simple and efficient implementation of an entropic method [35]. This method is based on a systematic restriction of the energy space as we increase the lattice size and on the WL diffusion process. The random walk takes place only in the appropriately restricted energy space and this restriction produces an immense speed up of the WL process [34,35]. For the temperature range of interest, that is the range around a critical point, this scheme determines all finite-size anomalies using a one-run entropic strategy employing what we have called the ‘critical minimum energy subspace WL (CrMES-WL)-entropic sampling method’. We implement the high-levels (that is the levels where the detailed-balanced condition is quite well obeyed) of the WL random walk process to determine appropriate microcanonical estimators. The method is efficiently combined with the N-fold way [39,40] in order to improve statistical reliability but also to produce broad-histogram (BH) estimators [41,42] for an additional calculation of the density of states (DOS). The independent approximation of the density of states by the BH method provides a useful test, by which one can judge the effect of the DOS approximation on the magnetic properties calculated by the entropic scheme. In order to give a brief comprehensive description of the scheme let us start with the original statements of the CrMES restriction.

According to the CrMES method [34,35] the specific heat peaks are approximated by:

$$C_L^*\left(\tilde{E}_-,\tilde{E}_+\right) = N^{-1}\left(T_L^*\right)^{-2}\left\{\tilde{Z}^{-1}\sum_{\tilde{E}_-}^{\tilde{E}_+} E^2 \exp\left[\tilde{\Phi}(E)\right] - \left(\tilde{Z}^{-1}\sum_{\tilde{E}_-}^{\tilde{E}_+} E \exp\left[\tilde{\Phi}(E)\right]\right)^2\right\}, \tag{2}$$

$$\tilde{\Phi}(E) = \left[S(E) - \beta E\right] - \left[S(\tilde{E}) - \beta\tilde{E}\right], \quad \tilde{Z} = \sum_{\tilde{E}_-}^{\tilde{E}_+} \exp\left[\tilde{\Phi}(E)\right], \tag{3}$$

where the total energy range (E_{min},E_{max}) is restricted using the definitions:

$$\left(\tilde{E}_-,\tilde{E}_+\right),\ \tilde{E}_\pm = \tilde{E} \pm \Delta^\pm,\ \Delta^\pm \geq 0 \tag{4}$$

with respect to the value $\tilde{E}$ producing the maximum term in the partition function of the statistical model, for instance the Ising model, at some temperature of interest. To implement the above restriction we request a specified accuracy and we impose the condition:

$$\left|\frac{C_L^*(\Delta_\pm)}{C_L^*}-1\right|\le r \tag{5}$$

where r measures the relative error and it will be set equal to a small number (r = 10^{-6}), andC^*_L is the value of the maximum of the specific heat obtained by using the total energy range. With the help of a convenient definition [34,35], we can specify the minimum energy subspace satisfying the above condition and it has been numerically verified that the finite-size extensions (denoted by: $\Delta\tilde{E}\equiv\min(\tilde{E}_+-\tilde{E})$ close to a critical point obey the 'specific heat' scaling law [34]:

$$\Psi\equiv\frac{\left(\Delta\tilde{E}^*\right)^2}{L^d}\approx L^{\frac{\alpha}{\nu}}. \tag{6}$$

To locate the CrMES, we may follow the method described in Ref. [34], or an even simpler restriction based on the energy probability density [35]. Alternative definitions for the CrMES have been described in Ref. [35].

Let us now discuss the idea of producing accurate estimates for finite-size magnetic anomalies by using a simple method based on the WL random walk in an appropriately restricted energy subspace (E_1,E_2). We implement this scheme and at the same time we accumulate data for the two-parameter (E,M) histogram, where M is the uniform magnetization, any other convenient order-parameter, or in general some other property of the spin configurations of the system. The approximation of canonical averages, in a temperature range of interest, is as follows:

$$\left\langle M^n\right\rangle=\frac{\sum_E\left\langle M^n\right\rangle_E G(E)e^{-\beta E}}{\sum_E G(E)e^{-\beta E}}\cong\frac{\sum_{E\in(E_1,E_2)}\left\langle M^n\right\rangle_{E,WL}G_{WL}(E)e^{-\beta E}}{\sum_{E\in(E_1,E_2)}G_{WL}(E)e^{-\beta E}}. \tag{7}$$

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 $\left\langle M^n\right\rangle$ are determined from the $H_{WL}(E,M)$ histograms, which are obtained during the high-levels of the WL process:

$$\left\langle M^n\right\rangle_E\cong\left\langle M^n\right\rangle_{E,WL}\equiv\sum_M M^n\frac{H_{WL}(E,M)}{H_{WL}(E)},\quad H_{WL}(E)=\sum_M H_{WL}(E,M) \tag{8}$$

and the summation in the uniform magnetization (M) runs over all values generated in the restricted energy subspace (E_1,E_2). The accuracy of the magnetic properties obtained from the above averaging process depends on the WL levels used in the averaging. Using only the high-levels of the WL process, where the incomplete detailed balanced condition has not significant effect on the microcanonical estimators constructed from the cumulative histograms, yields smooth and excellent approximations as shown in Ref. [35]. 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 [32,34]. Details and the N-fold implementation can be found in Refs. [39,40].

Consider now, the probability density of the order-parameter at some temperature:

$$P_T(M)\cong\frac{\sum_{E\in(E_1,E_2)}\frac{H_{WL}(E,M)}{H_{WL}(E)}G_{WL}(E)e^{-\beta E}}{\sum_{E\in(E_1,E_2)}G_{WL}(E)e^{-\beta E}} \tag{9}$$

If $\tilde{M}$ is the value that maximizes (9), we locate the magnetic critical subspaces (CrMMS) by:

$$\tilde{M}_\pm:\ \frac{P_{T_{L,\chi}}\left(\tilde{M}_\pm\right)}{P_{T_{L,\chi}}\left(\tilde{M}\right)}\le r \tag{10}$$

and the corresponding finite-size extensions ($\Delta\tilde{M}$) of critical magnetic subspaces obey close to a critical point, the 'susceptibility' scaling law [22]:

$$\Xi\equiv\frac{\left(\Delta\tilde{M}\right)^2}{L^d}\approx L^{\frac{\gamma}{\nu}} \tag{11}$$

Eqs. (6) and (11) provide additional routes for estimating the involved critical exponents.

3. FINITE-SIZE SCALING ANALYSIS. MAGNETIC SRITICAL EXPONENTS

As mentioned in the introduction, the 3D Ising model has been investigated extensively by various numerical methods and from these studies the critical properties of the model are well known. Refined esti-

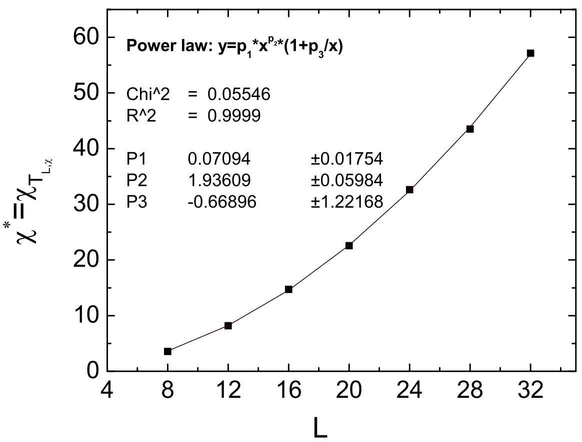

Fig. 1. Finite-size scaling behavior of the susceptibility peaks.

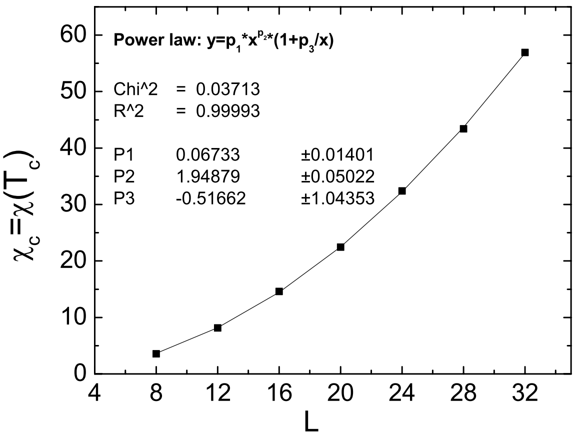

Fig. 2. Finite-size scaling behavior of the critical susceptibility.

mates are [22]: T_c = 4.51152..., $K_c = 1/T_c$ = 0.2216546±0.0000010 for the critical temperature, y_t=1.587±0.002 and y_h = 2.4808±0.0016 for the thermal and magnetic scaling exponents respectively. The correlation length exponent is given by (hyperscaling is assumed): $\nu=1/y_h$=0.630±0.001, the ratio $\gamma/\nu = 2y_h-d$ =1.9616±0.0032 and, finally, the exponent of the critical isotherm is given by: δ= 4.778±0.018.

In our previous study [34] we have applied the CrMES-WL scheme to obtain the DOS for cubic Ising lattices with sizes L=4-32. From these data the specific heat peaks were determined and were subjected to finite-size analysis to yield accurate estimates of the thermal critical exponent in agreement with the above value. Furthermore, an accurate estimation of the thermal exponent has been also achieved recently by studying the fixed magnetization (M = 0) version of the model [43]. However, the methods calculating the one-parameter E-DOS provide only the thermal properties of statistical systems. In order to study the magnetic properties one has either to utilize traditional importance sampling or to employ a two-parameter (E,M) flat histogram method such as a two-dimensional WL random walk in the (E,M) space. This last method is expected to be very accurate for the estimation of magnetic properties but its implementation can be carried out only for relatively small systems [41]. The CrMES-WL entropic scheme presented in the previous section is an alternative which have been already applied successfully in a number of systems of quite large sizes. Here, this method is applied on the 3D Ising model in order to estimate only the ratio γ/ν, since the thermal ratio α/ν has been estimated in previous papers [34,43].

We shall use the finite-size analysis to estimate this exponent from the data of the critical susceptibility and the susceptibility values at its pseudocritical temperature. Furthermore, we shall also use the route via the scaled extensions of the dominant magnetic subspaces (Eq. (11)), to obtain an additional estimation of this exponent. In order to diminish the computational effort, the entropic scheme was applied only to sizes that are multiples of 4 (L = 8,12,16,20,24,28 and L = 32).

Fitting the values of the susceptibility peaks and its values at the critical temperature ($K_c = 1/T_c$ = 0.2216546±0.0000010) to a power law (including a correction) of the form:

$$y = aL^w\left(1+b/L\right) \qquad (12)$$

we present all the fitting parameters in Figs. 1 and 2. The estimates for the critical ratio are: γ/ν =1.936±0.060 and γ/ν = 1.949±0.050 respectively. The large error bounds of these estimates permit an agreement with the estimate from the literature given above, but this agreement is not very good. On the other hand, Fig. 3 shows the average scaling behavior of the finite-size scaled extensions of the CrMMS, as defined in Eq. (11) for the above two temperatures, that is the critical and the susceptibility's pseudocritical temperature. The estimate obtained now is γ/ν = 1.957±0.013, much

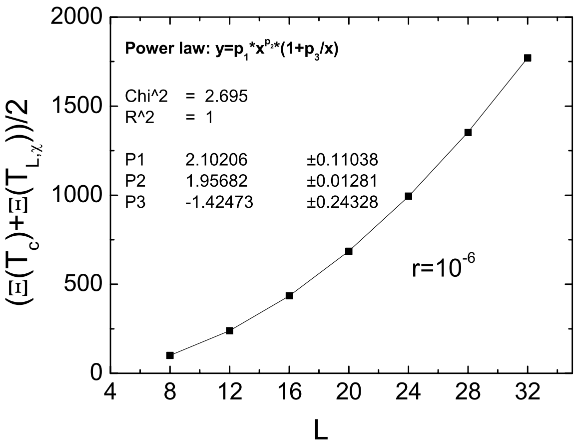

Fig. 3. Scaling behavior of dominant magnetic subspaces (CrMMS). The average of the two temperatures (critical and susceptibility's pseudocritical temperature) of the scaled extensions are fitted to the power law shown.

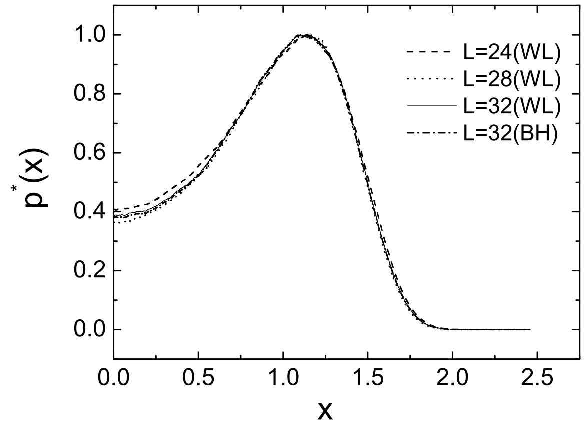

Fig. 4. Illustration of the universal scaling density function for various lattice sizes (see Eq. (13)).

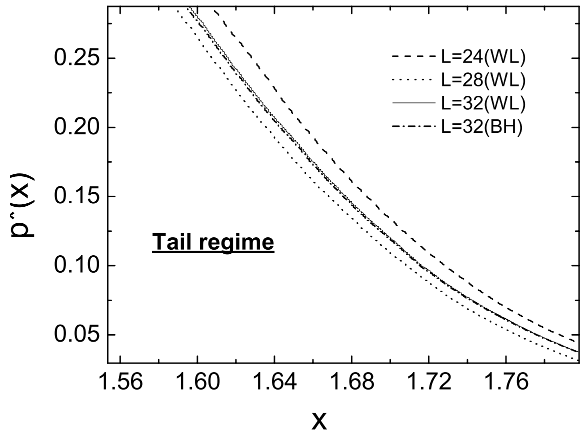

Fig. 5. The tail regime of the universal distribution illustrated in Fig. 4. The observed differences are discussed in the text.

closer to the best available estimate (see above γ/ν= 1.9616±0.0032), and all the errors of the fit-parameters are considerably smaller from the previous two fits obtained by the traditional method. Since, this property seems to be a common feature in all our studies [34,35,44], we shall speculate that the CrMES and CrMMS routes are superior to the traditional methods for the application of finite-size analysis.

4. ANALYSIS OF THE UNIVERSAL ORDER-PARAMETER DISTRIBUTION IN THE TAIL REGIME

Let us rescale the order-parameter density as usually [45]:

$$p^*(x)dx \cong p(m)dm,$$
$$x = m / \sqrt{\langle m^2 \rangle},\ m = M / N. \qquad (13)$$

Fig. 4 shows this universal distribution for the 3D Ising model for the lattice sizes L = 24,28 and L = 32, as obtained using our scheme described in Section 2. Also Fig. 5 shows for the same lattices the far tail regime of the corresponding distributions. It is evident from this graph that complete coincidence is not achieved at these sizes and this implies possible persistence of correction terms or statistical errors. Note however that, the small difference between the two approximations (WL and BH) shown for the lattice L = 32 reflects the magnitude of the statistical errors, coming only from the DOS approximation. To have a more complete picture of statistical errors different and longer runs should be compared. To analyze the tail behavior of these distributions we note that, the following conjecture has been put forward in the literature for the far tail regime (x>>1):

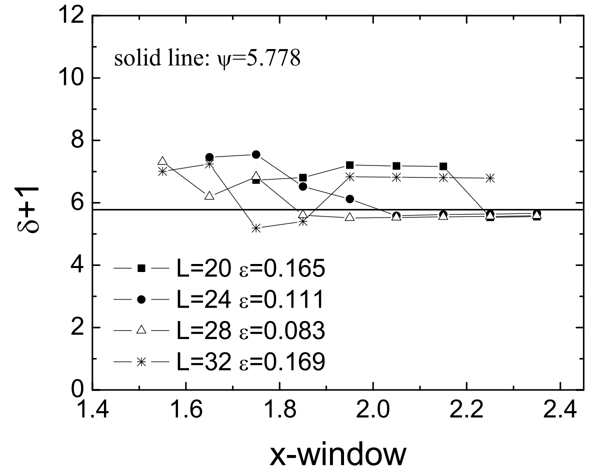

Fig. 6. An attempt to observe the value of the critical exponent δ+1 by fitting our data to Eq. (14). Note that, in these fits we have used *x*-windows corresponding to 100 magnetization values and we have suppressed the prefactor term by setting ψ= 1. The solid line shows the literature's estimate of δ+1.

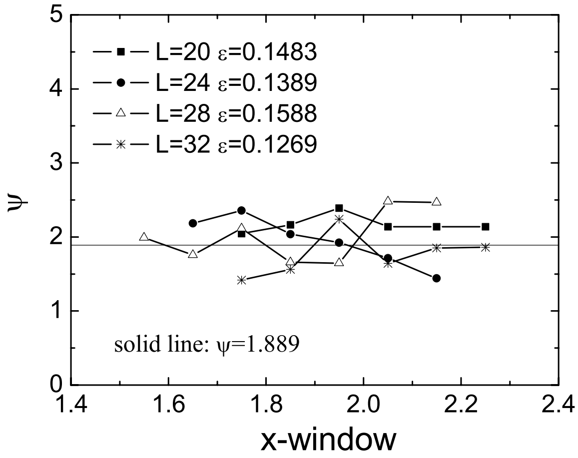

Fig. 7. A similar *x*-window fitting attempt by now treating the exponent y of Eq. (14) as a free parameter, assuming the validity of the conjecture ψ= (δ-1)/2. Note that, the averaged absolute errors shown are to be compared with those of Fig. 6.

$$p^*(x) \cong p_\infty x^\psi \exp\left(-a_\infty x^{\delta+1}\right),$$
$$\psi = \frac{\delta - 1}{2},\ x >> 1. \qquad (14)$$

For the 2D Ising model the study of [45-49] has provided some evidence for this conjecture and in particular for the prefactor and the relation of the exponent ψ to the critical exponent δ. For the 2D Ising model the exponent ψ should have the value ψ= 7. Smith and Bruce [45] have provided numerical support for this conjecture although this study was not completely conclusive since it only concerned relatively small lattices (*L*=32 and *L*=64) and the window in which the value was observed was quite narrow. However, our recent study of the 2D Ising model has considered large lattice sizes (*L*=80,100,120 and *L*=140) and has verified this conjecture in a very wide *x*-window [50].

Let us now attempt to observe the asymptotic behavior of the 3D universal distribution by using our data. First we attempt to fit our results in large *x*-windows corresponding to about 100 different magnetization values in the $x > 1$ regime by setting the prefactor exponent equal to one ($\psi = 1$). This means that we ignore the conjecture ψ=(δ-1)/2 and we attempt to estimate the exponent δ+1 of the power law in the exponential of Eq. (14). According to previous section this exponent should have the value δ+1 = 5.778±0.018. Fig. 6 shows the behavior of resulting estimates as well as the averaged over all *x*-windows relative absolute errors. The relative errors are defined by: $\varepsilon = \left\langle \left| w_i - w \right| / w \right\rangle$, where w = δ+1 = 5.778.

Finally, let us now accept the prefactor conjecture ψ=(δ-1)/2 and repeat the fitting attempts, by using the prefactor exponent (ψ) as a free parameter. Applying again the above described *x*-window fitting procedure we illustrate in Fig. 7 the behavior of the estimates for all the lattices used, together with the corresponding averaged absolute errors. Since these errors are of the same order with those in previous figure we cannot extract definite positive evidence for the prefactor conjecture from these absulute errors, but its validity seems to be supported from the comparison of the corresponding estimates shown in Figs. 6 and 7. We suspect that in order to clarify this situation we should have to study larger lattices, but also to use longer and refined simulations to avoid possible statistical errors.

5.CONCLUSIONS

The efficiency of our entropic method relays mainly on the restrictive CrMES technique developed recently by the present authors [34,35]. It is hoped that this new approach will increase our comprehension for the development of the critical behavior as the lattice size increases and will further facilitate the estimation of critical exponents via finite-size scaling. Furthermore, it is hoped that the presented one-run entropic scheme will provide a better alternative for the study of complex systems such as the RFIM [51] and systems with competing interactions [44]. 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 and this is in our opinion an additional important element of the scheme. In the case of a recent investigation of the SAF transition in the 2D Ising model with next-nearest neighbor interactions the very accurate estimation, by this route, of the thermal exponent and the observation of 'weak universality' for the magnetic exponents are very encouraging. The entropic sampling scheme offers 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. Finally, this is related to the reliability of the numerical data used here for the analysis of the asymptotic tail behavior of the universal critical distribution of the order-parameter.

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