Phase transition in Heisenberg stacked triangular antiferromagnets: End of a controversy

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By using the Wang-Landau flat-histogram Monte Carlo (MC) method for very large lattice sizes never simulated before, we show that the phase transition in the frustrated Heisenberg stacked triangular antiferromagnet is of first order, contrary to results of earlier MC simulations using old-fashioned methods. Our result lends support to the conclusion of a nonperturbative renormalization group performed on an effective Hamiltonian. It puts an end to a 20-year-long controversial issue.

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I. INTRODUCTION

When a spin cannot fully satisfy energetically all the interactions with its neighbors, it is "frustrated." This situation occurs when the interactions are in competition with each other or when the lattice geometry does not allow one to satisfy all interaction bonds simultaneously as seen, for example, in the triangular lattice with an antiferromagnetic interaction between the nearest neighbors. The effects of the frustration in spin systems have been extensively investigated during the last 30 years. Frustrated spin systems are shown to have unusual properties such as large ground-state (g.s.) degeneracy, interesting g.s. symmetries, successive phase transitions with a complicated nature, and partially disordered phase, reentrance and disorder lines. Frustrated systems still constitute at present a challenge for theoretical, experimental, and simulational methods. For recent reviews, the reader is referred to Ref. [1].

The nature of the phase transition in strongly frustrated spin systems has been a subject of intensive investigations in the last 20 years. Theoretically, these systems are excellent testing grounds for theories and approximations. Many well-established methods such as renormalization group (RG), high- and low-temperature series expansions, etc., often failed to deal with these systems. Experimentally, data on different frustrated systems show a variety of possibilities: first-order or second-order transitions with unknown critical exponents, etc. (see reviews in Ref. [1]). One of the most studied systems is the stacked triangular antiferromagnet (STA): the antiferromagnetic (AF) interaction between nearest-neighbor (NN) spins on the triangular lattice causes a very strong frustration. It is impossible [1] to fully satisfy the three AF bond interactions on each equilateral triangle. The g.s. configuration of both Heisenberg and *XY* models is the well-known 120° structure. The cases of *XY* ($N=2$) and Heisenberg ($N=3$) spins on the STA have been intensively studied since 1987. For details, see, for example, the review by Delamotte *et al.* [2]. Let us briefly recall here some main historical developments. Kawamura [3,4] has conjectured by a two-loop RG analysis and Monte Carlo (MC) simulations that the transition in *XY* and Heisenberg models belong each to a new universality class in dimension $d=3$. Since then, there have been many other calculations and simulations with contradictory results. For example, Azaria *et al.* [5] suggested from a nonlinear σ model that if the transition is not of first order or mean-field tricritical, then it should be O(4) universality. Numerical simulations [6–8], however, did not confirm these conjectures. Antonenko *et al.* [9] went further in a four-loop RG calculation with a Borel resummation technique. They concluded that the transition is of first order. From 2000, Tissier and co-workers [10–12] have carried out a nonperturbative RG study of frustrated magnets for any dimension between two and four. They recovered all known perturbative one-loop results in two and four dimensions as well as for the infinite spin-component number $N\rightarrow\infty$. They determined $N_c(d)$ for all d and found $N_c(d=3)=5.1$ below which the transition is of first order in contradiction with the conjecture of the existence of a new chiral universality class by Kawamura [3,4]. They explained why theories and simulations have encountered so far many difficulties by the existence of a whole region in the flow diagram in which the flow is slow: the first-order character for $N=2,3$ is so weak that the transition has a second-order aspect with "pseudocritical" exponents. They calculated these pseudoexponents and found that they coincided with some experimental data. While this scenario is very coherent, we note that in this nonperturbative RG technique, the real Hamiltonian is truncated at the beginning and replaced by an effective one. However, as will be seen in this paper, the nonperturbative results are well confirmed.

Let us recall some results on the *XY* case. Early MC results on the *XY* STA have been reviewed by Loison [13]. Until 2003, all numerical simulations found a second-order transition with exponents. A numerical breakthrough has been realized with the results of Itakura [14] who used an improved MC RG scheme to investigate the RG flow of the effective Hamiltonian used in field-theoretical studies for the *XY* STA. He found that the *XY* STA exhibits a clear first-order behavior and there are no chiral fixed points of RG flow for $N=2$. In 2004, Peles *et al.* [15] used a continuous model to study the *XY* STA by MC simulations. They found evidence of a first-order transition. In 2006, Kanki *et al.* [16],

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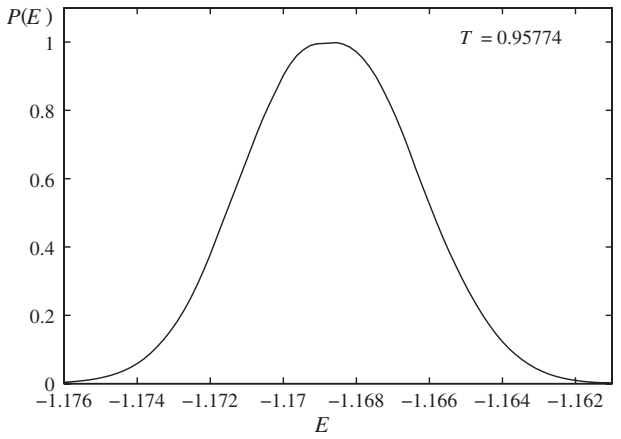

FIG. 1. Energy histogram for $N=96$ at T_c indicated in the figure.

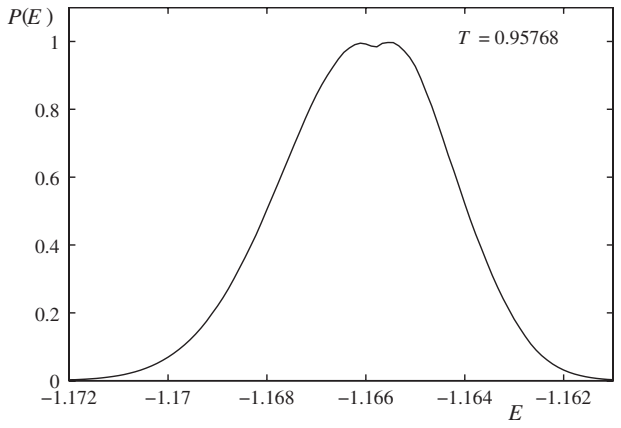

FIG. 2. Energy histogram for $N=120$ at T_c indicated in the figure.

using a microcanonical MC method, found a first-order signature of the *XY* STA. Bekhechi *et al.* [17] used in 2006 a new MC technique called "short-time dynamics" to show that the critical exponents β and ν of the model are nonuniversal with respect to a parameter which does not change the system symmetry. This is inconsistent with a second-order transition. Therefore they concluded, by exclusion, that the transition in the *XY* STA should be weakly of first order.

While these recent simulations have demonstrated evidence of first-order transition for the *XY* STA in agreement with the nonperturbative RG analysis, they might suffer one or two uncertain aspects: the work of Itakura [14] used a truncated Hamiltonian, the work of Peles *et al.* [15] used standard MC methods with a risk of critical slowing down, the work of Kanki *et al.* [16] used a traditional microcanonical MC technique with a uncertainty on a sufficient covering of microscopic states, and the work of Bekhechi *et al.* [17], although being able to get rid of the critical slowing down, gives only indirect evidence of the first-order character. Using a very-high-performance technique for weak first-order transitions, the so-called Wang-Landau flat-histogram method [18], we have recently carried out simulations on the *XY* STA. We have found clearly a first-order transition in that system, confirming results of other authors and putting an end to the controversy that which has lasted for 20 years [19].

For the Heisenberg case, Itakura [14] found, as in the *XY* case mentioned above, the absence of chiral fixed points of RG flow. However, he could not find numerical evidence of the first-order transition. He predicted that if the transition is of first order for the Heisenberg spins, it should occur at much larger lattice sizes, which he was not able to perform at that time. Indirect evidence of the first-order character of the Heisenberg case has been recently given by Zelli *et al.* [20] using the short-time dynamics MC simulation: they found, as for the *XY* case [17] discussed above, a nonuniversal behavior of the critical exponents, which is inconsistent with a second-order transition. Encouraged by the high performance of the Wang-Landau method, we decided to study the Heisenberg case in this work using the full Hamiltonian with very large lattice sizes. As shown below, we find indeed a first-order transition in this case.

The paper is organized as follows. Section II is devoted to the description of the model and the technical details of the Wang-Landau (WL) methods as applied in the present paper. Section III shows our results. Concluding remarks are given in Sec. IV.

II. MONTE CARLO SIMULATION: WANG-LANDAU ALGORITHM

We consider the stacking of triangular lattices in the z direction. The spins are the classical Heisenberg model of magnitude $S=1$. The Hamiltonian is given by

$$\mathcal{H} = J\sum_{(i,j)} \mathbf{S}_i \cdot \mathbf{S}_j, \tag{1}$$

where S_i is the Heisenberg spin at the lattice site i and $\Sigma_{(i,j)}$ indicates the sum over the NN spin pairs S_i and S_j both in the xy planes and in adjacent planes in the z direction. For simplicity, we suppose the same antiferromagnetic interaction J $(J>0)$ for both in-plane NN pairs and interplane NN ones.

Recently, Wang and Landau [18] proposed a Monte Carlo algorithm for classical statistical models. The algorithm uses a random walk in energy space in order to obtained an accurate estimate for the density of states, $g(E)$, which is defined as the number of spin configurations for any given E. This method is based on the fact that a flat energy histogram $H(E)$ is produced if the probability for the transition to a state of energy E is proportional to $g(E)^{-1}$. At the beginning of the simulation, the density of states (DOS) is set equal to 1 for all possible energies, $g(E)=1$. We begin a random walk in energy space (E) by choosing a site randomly and flipping its spin with a probability proportional to the inverse of the momentary density of states. In general, if E and E' are the energies before and after a spin is flipped, the transition probability from E to E' is

$$p(E \to E') = \min[g(E)/g(E'),1]. \tag{2}$$

Each time an energy level E is visited, the DOS is modified by a modification factor $f>0$ whether the spin flipped or not—i.e., $g(E) \to g(E)f$. At the beginning of the random walk, the modification factor f can be as large as e^1

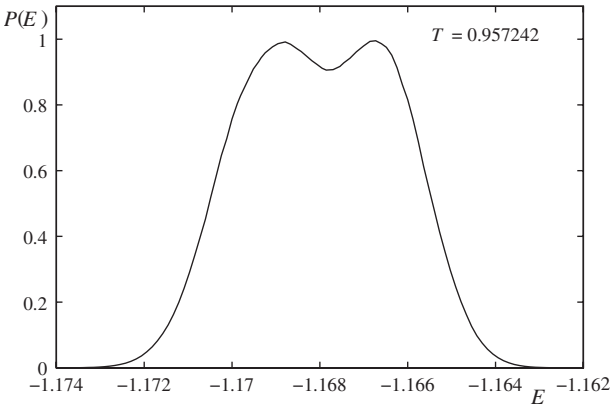

FIG. 3. Energy histogram for $N=150$ at T_c indicated in the figure.

$\simeq 2.718\,281\,8$. A histogram $H(E)$ records how often a state of energy E is visited. Each time the energy histogram satisfies a certain "flatness" criterion, f is reduced according to $f \to \sqrt{f}$ and $H(E)$ is reset to zero for all energies. The reduction process of the modification factor f is repeated several times until a final value f_{final} which close enough to 1. The histogram is considered as flat if

$$H(E) \geqslant x\,\% \times \langle H(E) \rangle \tag{3}$$

for all energies, where $x\%$ is chosen between 70% and 95% and $\langle H(E) \rangle$ is the average histogram.

The thermodynamic quantities [18,21] can be evaluated by $\langle E^n \rangle = \frac{1}{Z} \Sigma_E E^n g(E) \exp(-E/k_B T)$, $C_v = \frac{\langle E^2 \rangle - \langle E \rangle^2}{k_B T^2}$, $\langle M^n \rangle = \frac{1}{Z} \Sigma_E M^n g(E) \exp(-E/k_B T)$, and $\chi = \frac{\langle M^2 \rangle - \langle M \rangle^2}{k_B T}$, where Z is the partition function defined by $Z = \Sigma_E g(E) \exp(-E/k_B T)$. The canonical distribution at any temperature can be calculated simply by $P(E,T) = \frac{1}{Z} g(E) \exp(-E/k_B T)$.

In this work, we consider a energy range of interest [22,23] $(E_{\min}, E_{\max})$. We divide this energy range to R subintervals, and the minimum energy of each subinterval is $E^i_{\min}$ for $i = 1, 2, \ldots, R$, and maximum of the subinterval i is $E^i_{\max} = E^{i+1}_{\min} + 2\Delta E$, where ΔE can be chosen large enough for a smooth boundary between two subintervals. The Wang-Landau algorithm is used to calculate the relative DOS of each subinterval $(E^i_{\min}, E^i_{\max})$ with the modification factor $f_{\text{final}} = \exp(10^{-9})$ and flatness criterion $x\% = 95\%$. We reject the suggested spin flip and do not update $g(E)$ and the energy histogram $H(E)$ of the current energy level E if the spin-flip trial would result in an energy outside the energy segment. The DOS of the whole range is obtained by joining the DOS of each subinterval $(E^i_{\min} + \Delta E, E^i_{\max} - \Delta E)$.

III. RESULTS

We used a system size of $N \times N \times N$ where $N = 72$, 84, 90, 96, 108, 120, and 150. Periodic boundary conditions are used in the three directions. $J = 1$ is taken as the unit of energy in the following.

The energy histograms for three representative sizes $N = 96$, $N = 120$, and $N = 150$ shown in Figs. 1–3, respectively. As seen, for $N = 96$, the peak is very broad, a signature of the beginning of a double-maximum structure. The double peak begins really at $N = 120$. We note that the distance between the two peaks—i.e., the latent heat—increases with increasing size and reaches 0.0025 for $N = 150$. This is to be compared with the value $\simeq 0.009$ for $N = 120$ in the XY case [14–16,19]. Such a small value of the latent heat in the Heisenberg case explains why the first-order character was so difficult to observe. For increasing sizes, the minimum between the peaks will be deepened to separate completely the two peaks. Note that the double-peak structure is a sufficient condition, not a necessary condition, for a first-order transition. We give here the values of T_c for a few sizes: $T_c = 0.957\,74$, $0.957\,68$, and $0.957\,242$ for $N = 96$, 120, and 150, respectively.

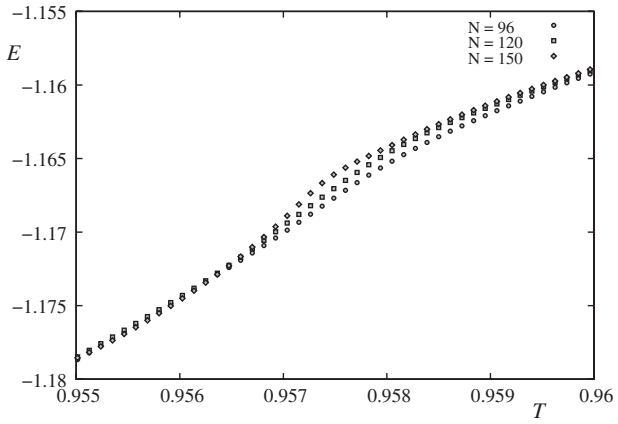

FIG. 4. Energy versus T for $N = 96, 120, 150$.

To explain why standard MC methods without histogram monitoring (see, for example, Ref. [3]) fail to see the first-order character, let us show in Fig. 4 the energy vs T obtained by averaging over states obtained by the WL method for $N = 96$, 120, and 150. We see here that while the energy histograms show already a signature of double-peak structure at these large sizes, the average energy calculated by using these WL histograms does not show a discontinuity: the averaging over all states erases away the bimodal distribution seen in the energy histogram at the transition temperature. Therefore, care should be taken to avoid such problems due to averaging in MC simulations when studying weak first-order transitions.

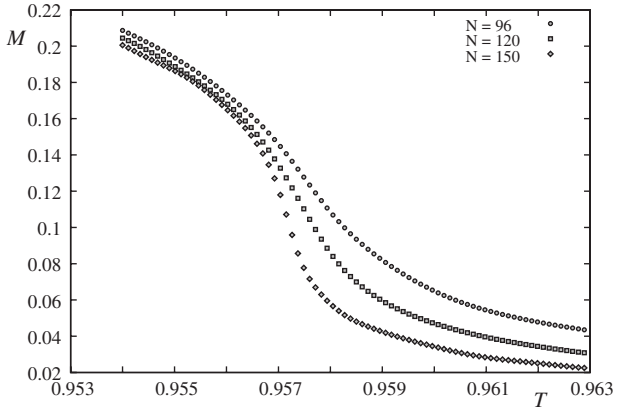

FIG. 5. Magnetization versus T for $N = 96, 120, 150$.

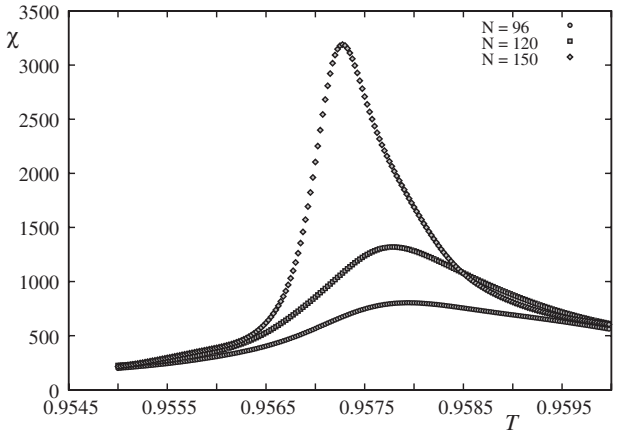

FIG. 6. Susceptibility versus T for $N=96,120,150$.

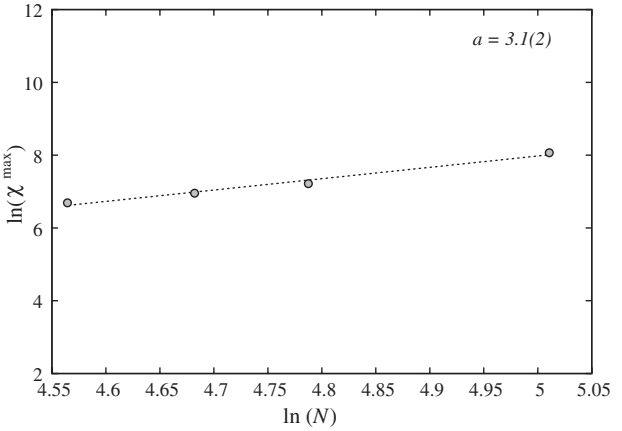

FIG. 7. Maximum of susceptibility versus $N=96$, 108, 120, and 150 on a ln-ln scale. The slope is 3.1. See text for comments.

Figures 5 and 6 show the magnetization and the susceptibility for three sizes $N=96$, 120, and 150. Again, here, one does not see with one's eye the discontinuity of the magnetization at the transition even for $N=150$. The averaging procedure erases, as for the energy, the detailed structure at the transition.

At this stage it is interesting to make another check of the first-order character: in a first-order transition, the maximum of the susceptibility should scale with the system volume—namely, N^d where d is the system dimension [24]. We plot in Fig. 7, χ^{max} versus N on a ln-ln scale. The slope of the straight line is ~ 3.1, which is nothing but d within errors. This is a very strong signature of a first-order transition.

IV. CONCLUDING REMARKS

We have studied in this paper the phase transition in the Heisenberg STA by using the flat-histogram technique invented by Wang and Landau. The method is very efficient because it helps to overcome the extremely long transition time between energy valleys in systems with a first-order phase transition. We found that the transition becomes clearly of first order only at a very large lattice size, confirming the result of a nonperturbative RG calculations using an effective average Hamiltonian [2] and that using a short-time MC simulation [20]. The present work hence puts definitely an end to the long-standing controversial subject on the nature of the phase transition in the Heisenberg STA. To conclude, let us emphasize that for complicated systems like this one, methods well established for simple systems such as ferromagnets may encounter difficulties in dealing with the nature of the phase transition. Such difficulties can be solved only with high-performance MC simulations as the one used here and a detailed analysis of the flow behavior as suggested by a nonperturbative RG calculation.

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