

# Stacked Triangular XY Antiferromagnets: End of a Controversial Issue on the Phase Transition

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We show in this paper by using the Wang-Landau flat-histogram Monte Carlo method that the phase transition in the XY stacked triangular antiferromagnet is clearly of first-order, confirming results from latest Monte Carlo simulation and from a nonperturbative renormalization group, putting an end to a long-standing controversial issue.

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## I. INTRODUCTION

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 (GS) degeneracy, additional GS symmetries, successive phase transitions with complicated nature. Frustrated systems still challenge theoretical and experimental methods. For recent reviews, the reader is referred to Ref. 1.

Let us confine our discussion on the nature of the phase transition in strongly frustrated spin systems. Since the nature of the phase transition depends on the symmetry and the dimension of the system, we have to examine first its GS properties. Of course, the nature

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of the order parameter defined according to the system symmetry determines the properties of the phase transition. 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<sup>1</sup> to fully satisfy simultaneously the three AF bond interactions on each equilateral triangle. The GS configuration of both Heisenberg and XY models is the well-known 120-degree structure.

The phase transition in strongly frustrated spin systems is 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). The case of XY and Heisenberg spins on the STA has been intensively studied mostly since 1987. There are good recent reviews on the subject (see for example reviews by Delamotte et al<sup>2</sup>). Let us briefly recall here some main historical developments and actual situation. In the XY and Heisenberg cases, different materials give different experimental results. The anomalous dimension is found negative in many materials and in most numerical simulations, the scaling relations are violated and no universality in the exponents was found in early simulations. This situation is briefly described in the following. Kawamura<sup>3,4</sup> has conjectured by the two-loop RG analysis in  $d = 3$  the existence of a new universality class for frustrated magnets. Since then there have been many other perturbative calculations with contradictory results.<sup>5,6</sup> From 2000, there has been a number of papers by Tessier and coworkers<sup>7,8,9</sup> using a nonperturbative RG study of frustrated magnets for any dimension between two and four. They recovered all known perturbative results at one loop in two and four dimensions as well as for  $N \rightarrow \infty$ . They determined  $N_c(d)$  for all  $d$  and found  $N_c(d = 3) = 5.1$  below which the transition is of first order. However, they found the existence of a whole region in the flow diagram in which the flow is slow. As a consequence, for  $N = 2, 3$ , they found pseudo-critical exponents in good agreement with some experimental data. This allowed them to account for the nonuniversal scaling observed in XY and Heisenberg frustrated magnets. The only problem in this nonperturbative technique is that the Hamiltonian is truncated at the beginning. Giving this fact, we have to be careful about its conclusion. As will be seen in this paper, the nonperturbative results are so far well

confirmed. Early MC results on XY STA have been reviewed by Loison.<sup>10</sup> Until 2003, all numerical simulations found ambiguous results for this model and never a clear first-order transition. A numerical breakthrough has been realized with the results of Itakura<sup>11</sup> who used an improved MC renormalization-group scheme to numerically investigate the renormalization group flow of the Heisenberg and XY STA and its effective Hamiltonian which is used in the field-theoretical studies. He found that the XY STA exhibits clear first-order behavior and there are no chiral fixed points of renormalization-group flow for  $N=2$  and 3 cases. In 2004, Peles et al<sup>12</sup> have used a continuous model to study the XY STA by MC simulation. They found evidence of a first-order transition. In 2006, Kanki et al<sup>13</sup>, using a microcanonical MC method, have found a first-order signature of the XY STA. While these recent simulations have demonstrated evidence of first-order transition for the XY STA in agreement with the nonperturbative RG analysis, all of them suffer one or two uncertain aspects: the work of Itakura has used a truncated Hamiltonian, the work of Peles et al has used standard MC methods and the work of Kanki et al used a traditional microcanonical MC technique. At present, we have a very high-performance technique at hand for weak first-order transitions. This is a very good opportunity to test it on the XY STA and to say a last word on the nature of the phase transition of this system by using the full Hamiltonian, confirming or rejecting the nonperturbative RG and recent MC results. That is the purpose of this work.

We study again here the XY STA with high-resolution MC technique which is very efficient specially for weak first-order transition.<sup>14</sup> Our aim is to try to put an end to the controversy which has been lasting for 20 years. We will recall some important numerical results in the next section.

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

## II. MONTE CARLO SIMULATION: WANG-LANDAU ALGORITHM

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

$$\mathcal{H} = J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J' \sum_{\langle i,k \rangle} \mathbf{S}_i \cdot \mathbf{S}_k \quad (1)$$

where  $\mathbf{S}_i$  is the XY spin at the lattice site  $i$ ,  $\sum_{\langle i,j \rangle}$  indicates the sum over the NN spin pairs  $\mathbf{S}_i$  and  $\mathbf{S}_j$  in a  $xy$  triangular plane, while  $\sum_{\langle i,k \rangle}$  indicates that of NN spin pairs between adjacent planes.  $J$  and  $J'$  are in-plane and inter-plane interactions, respectively. We shall suppose that  $J = 1$  (antiferromagnetic) and  $J' = -1$  (ferromagnetic) in the following.

Recently, Wang and Landau<sup>14</sup> proposed a Monte Carlo algorithm for classical statistical models. The algorithm uses a random walk in energy space in order to obtain an accurate estimate for the density of states  $g(E)$ . 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 one for all energies,  $g(E) = 1$ . In general, if  $E$  and  $E'$  are the energies before and after a spin is flipped, the transition probability from  $E$  to  $E'$  is

$$p(E \rightarrow E') = \min [g(E)/g(E'), 1]. \quad (2)$$

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.  $g(E) \rightarrow g(E)f$ . In the beginning of the random walk the modification factor  $f$  can be as large as  $e^1 \simeq 2.7182818$ . 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  $f \rightarrow \sqrt{f}$  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  $f_{\text{final}}$  which is close enough to one. The histogram is considered as flat if

$$H(E) \geq x\% \cdot \langle H(E) \rangle \quad (3)$$

for all energies, where the flatness parameter  $0\% < x\% < 100\%$  controls the accuracy of the estimated  $g(E)$ , with increasing accuracy as  $x\%$  approaches unity.  $\langle H(E) \rangle$  is the average histogram.

Thermodynamic quantities<sup>14,15</sup> can be evaluated using the canonical distribution at any temperature  $T$  by  $P(E, T) = g(E) \exp(-E/k_B T)/Z$  where  $Z$  is the partition function defined by  $Z = \sum_E g(E) \exp(-E/k_B T)$ .

In this work, we consider a energy range of interest<sup>16,17</sup>  $(E_{\min}, E_{\max})$ . We divide this energy range to  $R$  subintervals, the minimum energy of each subinterval is  $E_{\min}^i$  for  $i = 1, 2, \dots, R$ , and maximum of the subinterval  $i$  is  $E_{\max}^i = E_{\min}^{i+1} + 2\Delta E$ , where  $\Delta E$  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  $(E_{\min}^i, E_{\max}^i)$  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  $(E_{\min}^i + \Delta E, E_{\max}^i - \Delta E)$ .

### III. RESULTS

We used the system size of  $N \times N \times N$  where  $N = 12, 18, 24, 30, 36, 48, 60, 72, 84, 90, 96, 108, 120$ . Periodic boundary conditions are used in the three directions.  $|J| = 1$  is taken as unit of energy in the following.

The energy histograms for two representative sizes  $N = 48$  and  $N = 120$  are shown in Figs. 1 and 2, respectively. As seen, for  $N = 48$ , the peak, though very large, does not show yet a double-maximum structure. Only from  $N = 90$  that the double-peak structure clearly appears. This 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:  $T_c = 1.458270, 1.457878, 1.457642, 1.457537$  for  $N = 48, 84, 96, 120$ , respectively. Note that this result is in excellent agreement with earlier MC simulations<sup>11,12,13</sup> using less sophisticated methods. 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. 3 the energy vs  $T$  obtained by averaging over states obtained by the WL method for  $N = 120$ . We see here that even at this big size, the average energy does not show a discontinuity as in a strong first-order transition: 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. We note that the distance between to peaks in Fig. 2, i. e. the latent heat, is  $\simeq 0.009$  in agreement with earlier works.<sup>11,12,13</sup>

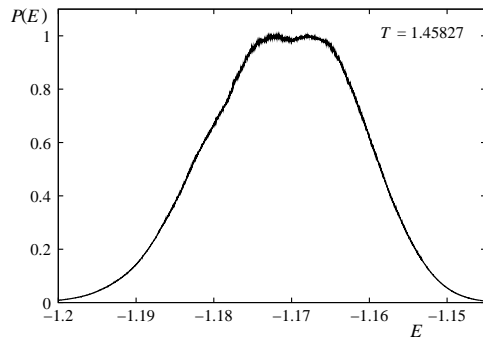


FIG. 1: Energy histograms for  $N = 48$  at  $T_c$  indicated on the figure.

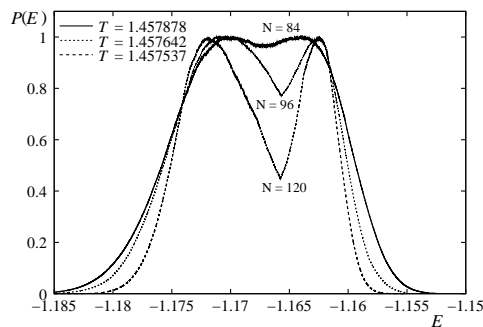


FIG. 2: Energy histograms for  $N = 84, 96, 120$  at  $T_c$  indicated on the figure.

#### IV. CONCLUDING REMARKS

We have studied in this paper the phase transition in the XY STA by using the flat histogram technique invented by Wang and Landau. The method is very efficient because it helps to overcome extremely long transition time between energy valleys in systems with a possible first-order phase transition. We found that the transition is clearly of first-order confirming therefore recent MC results using less efficient techniques. These results put

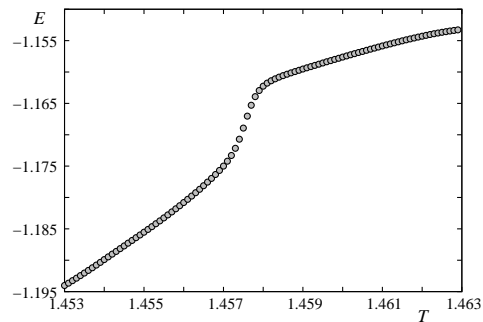


FIG. 3: Energy vs  $T$  for  $N = 120$ .

definitely an end to the 20-year long controversy and lend support to nonperturbative RG calculations using an effective average Hamiltonian.

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