# First-order transition in the *XY* model on a fully frustrated simple cubic lattice

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We study the nature of the phase transition in the fully frustrated simple cubic lattice with the *XY* spin model. This system is the Villain's model generalized in three dimensions. The ground state is very particular with a 12-fold degeneracy. Previous studies have shown unusual critical properties. With the powerful Wang-Landau flat-histogram Monte Carlo method, we carry out in this work intensive simulations with very large lattice sizes. We show that the phase transition is clearly of first order, putting an end to the uncertainty which has lasted for more than 20 years.

## I. INTRODUCTION

One of the most fascinating tasks of statistical physics is the study of the phase transition in systems of interacting particles. Much progress has been made in this field since 50 years. Finite-size theory, renormalization-group analysis, numerical simulations, etc. have contributed to the advance of the knowledge on the phase transition. Exact methods have been devised to solve with mathematical elegance many problems in two dimensions. But as improvements are progressing, new and more complicated challenges also come in from new discoveries of materials and new applications. Renormalization group which has predicted with success critical behaviors of ferromagnets has many difficulties in dealing with frustrated systems. Numerical simulations which did not need huge memory and long calculations for simple systems require now new devices and new algorithms to improve convergence in systems with extremely long relaxation time or in systems whose microscopic states are difficult to access. One class of these systems is called "frustrated systems" introduced in the 1970s in the context of spin glasses. These frustrated systems are very unstable due to the competition between different kinds of interactions. However, they are periodically defined (no disorder) and therefore subject to exact treatments. This is the case of several models in two dimensions [1], but in three dimensions frustrated systems are far from being understood even on basic properties such as the order of the phase transition (first or second order, critical exponents, etc.). Let us recall the definition of a frustrated system. When a spin cannot fully satisfy energetically all the interactions with its neighbors, it is "frustrated." This occurs when the interactions are in competition with each other or when the lattice geometry does not allow them to satisfy all interaction bonds simultaneously. A well-known example is the stacked triangular antiferromagnet (STA) with interaction between nearest neighbors (NNs).

The frustration in spin systems causes many unusual properties such as large ground-state (GS) degeneracy, successive phase transitions with complicated nature, partially disordered phase, reentrance, and disorder lines. Frustrated systems still constitute at present a challenge for investigation methods. For recent reviews, the reader is referred to Ref. [2].

In this work, we are interested in the nature of the phase transition of the classical *XY* spin model in the fully frustrated simple cubic lattice (FFSCL) shown in Fig. 1. Although phase transition in strongly frustrated systems has been a subject of intensive investigations in the last 20 years, many aspects are still not understood at present. One of the most studied systems is the STA with Ising [3], *XY*, and Heisenberg [4,5] spins. The cases of *XY* (*N*=2) and Heisenberg (*N*=3) STAs have been intensively studied since 1987 [6–13], but only recently that the 20-year controversy comes to an end [14–23]. For details, see, for example, the review by Delamotte *et al.* [4].

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.
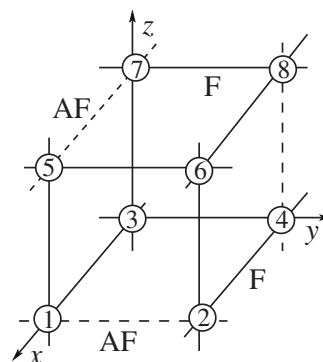


FIG. 1. Fully frustrated simple cubic lattice. Broken (solid) lines denote antiferromagnetic (ferromagnetic) bonds.

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## II. MODEL AND WANG-LANDAU ALGORITHM

We consider the FFSCL shown in Fig. 1. The spins are the classical *XY* model of magnitude $S=1$. The Hamiltonian is given by

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

where $\mathbf{S}_i$ is the *XY* spin at the lattice site $i$ and $\Sigma_{(i,j)}$ is made over the NN spin pairs $\mathbf{S}_i$ and $\mathbf{S}_j$ with interaction $J_{ij}$. Hereafter we suppose that $J_{ij}=-J$ ($J>0$) for antiferromagnetic (AF) bonds indicated by broken lines in Fig. 1, and $J_{ij}=J$ for ferromagnetic (F) bonds. This model is a generalization in three dimensions of the two-dimensional (2D) Villain's model [24] which has been extensively studied [25–27]: every face of the cube is frustrated because we know that a plaquette is frustrated when there are an odd number of AF bonds on its contour [2,24]. To describe the model, let us look first at the *xy* plane (Fig. 1). There, all interactions are F, except one AF line out of every two in the *y* direction. The same is for the *yz* (*zx*) plane: one AF line out of every two in the *z* (*x*) direction. Note that there is no intersection between AF lines. Each plane is thus a 2D Villain's model. Let us define by formulas the interactions of this model. At the lattice site defined by three integers $(l,m,n)$ in the Cartesian coordinates, there are three interaction bonds with the NNs in increasing *x*, *y*, and *z* directions. The *x*, *y*, and *z* bonds are given by

$$J_x(l,m,n) = (-1)^{\mathrm{mod}(m,2)\mathrm{mod}(n,2)},$$

$$J_y(l,m,n) = (-1)^{\mathrm{mod}(n+1,2)\mathrm{mod}(l,2)},$$

$$J_z(l,m,n) = (-1)^{\mathrm{mod}(l+1,2)\mathrm{mod}(m,2)}.$$

These formulas are written using the convention that at the coordinate origin, one has $l=m=n=0$ (see Fig. 1).

Let us recall some results on the present model. For the classical *XY* model on the FFSCL, the GS is 12-fold degenerate with noncollinear spin configurations [28]. For convenience, let us define the local field acting on the spin $\mathbf{S}_i$ from its neighbors as $\mathbf{h}_i=\Sigma_j J_{ij}\mathbf{S}_j$. The GS can be calculated by noticing that the local field is the same at every site and is equal to $|\mathbf{h}|=2\sqrt{3}$, so that [28]

$$\mathbf{h}_5 = 2(\mathbf{S}_2 + \mathbf{S}_3 + \mathbf{S}_4), \tag{2}$$

$$\mathbf{h}_6 = 2(\mathbf{S}_1 + \mathbf{S}_3 - \mathbf{S}_4), \tag{3}$$

$$\mathbf{h}_7 = 2(\mathbf{S}_1 - \mathbf{S}_2 + \mathbf{S}_4), \tag{4}$$

$$\mathbf{h}_8 = 2(\mathbf{S}_1 + \mathbf{S}_2 - \mathbf{S}_3), \tag{5}$$

where the factor of 2 results from the symmetric neighbors lying outside the cube and $J_{ij}= \pm 1$ depending on the bond that has been used. Putting into square these equalities and using $\mathbf{h}^2=12$, $\mathbf{S}_i^2=1$ ($i=1,\ldots,8$), one has three independent relations which determine the relative orientation of every spin pair:
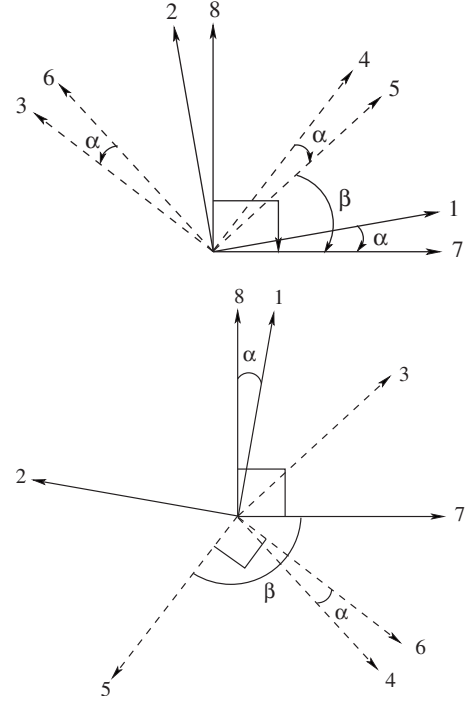


FIG. 2. Two of the 12 ground-state configurations of the fully frustrated simple cubic lattice. The numbers indicate the spins at the sites defined in Fig. 1. The angle $\alpha$ is $\alpha=\arccos(\frac{1+\sqrt{2}}{\sqrt{6}})$. Upper: $\beta=\pi/4$; lower: $\beta=-3\pi/4$.

$$\mathbf{S}_2 \cdot \mathbf{S}_3 + \mathbf{S}_3 \cdot \mathbf{S}_4 + \mathbf{S}_2 \cdot \mathbf{S}_4 = 0, \tag{6}$$

$$-\mathbf{S}_1 \cdot \mathbf{S}_3 + \mathbf{S}_3 \cdot \mathbf{S}_4 + \mathbf{S}_1 \cdot \mathbf{S}_4 = 0, \tag{7}$$

$$\mathbf{S}_1 \cdot \mathbf{S}_2 + \mathbf{S}_2 \cdot \mathbf{S}_4 - \mathbf{S}_1 \cdot \mathbf{S}_4 = 0. \tag{8}$$

There are 12 solutions of these equations which can be described as follows [28,29]. Consider just one of them shown in the upper figure of Fig. 2: on a *yz* face, the spins (displayed by continued vectors) on a diagonal are perpendicular, i.e., $\mathbf{S}_1 \perp \mathbf{S}_2$, $\mathbf{S}_7 \perp \mathbf{S}_8$. In addition, the orthogonal dihedron $(\mathbf{S}_1,\mathbf{S}_2)$ makes an angle $\alpha=\arccos(\frac{1+\sqrt{2}}{\sqrt{6}})$ with the dihedron $(\mathbf{S}_7,\mathbf{S}_8)$. On the other *yz* face the spins (displayed by discontinued vectors in Fig. 2) are arranged in the same manner: $\mathbf{S}_5 \perp \mathbf{S}_6$, $\mathbf{S}_4 \perp \mathbf{S}_3$, and the dihedron $(\mathbf{S}_4,\mathbf{S}_3)$ makes an angle $\alpha$ with the dihedron $(\mathbf{S}_5,\mathbf{S}_6)$. Note that the dihedron $(\mathbf{S}_5,\mathbf{S}_6)$ makes a turn angle $\beta=\pi/4$ with respect to the dihedron $(\mathbf{S}_7,\mathbf{S}_8)$, and that the sum of the algebraic angles between spins on each face of the cube is zero.

There is another choice shown in the lower part of Fig. 2 where everything is the same as described above except $\beta=-3\pi/4$. One has therefore two configurations with the choice of the *yz* faces. If one applies the same rule for the spins on the *xy* faces and the *xz* faces, one obtains in all six configurations. Finally, together with their six mirror images, the total degeneracy is 12 [29].

The above description of the GS shows an unusual degeneracy which can help to understand the first-order transition shown below by relating this system to a Potts model where the GS degeneracy plays a determinant role in the nature of

phase transition. Note however that all simulations have been carried out with the initial Hamiltonian (1); no GS rigidity at finite temperature ($T$) has been imposed.

The first investigation of the nature of the phase transition of this model by the use of Metropolis Monte Carlo (MC) simulations has shown a second-order transition with unusual critical exponents [29]. However, the MC technique and computer capacity at that time did not allow one to conclude the matter with certainty. Recently, Wang and Landau [30] proposed a MC algorithm for classical statistical models which allowed one to study systems with difficultly accessed microscopic states. In particular, it permits one to detect with efficiency weak first-order transitions [22,23]. The algorithm uses a random walk in energy space in order to obtain an accurate estimate for the density of states (DOS) $g(E)$ 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 $g(E)^{-1}$.

We summarize how this algorithm is applied here. At the beginning of the simulation, the 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 temporary 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

$$p(E \rightarrow E') = \min[g(E)/g(E'),1]. \tag{9}$$

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., $g(E) \rightarrow g(E)f$. At the beginning of the random walk, the modification factor $f$ can be as large as $e^1 \simeq 2.718\ 281\ 8$. A histogram $H(E)$ records the number of times 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 1. The histogram is considered as flat if

$$H(E) \geq x\% \langle H(E) \rangle \tag{10}$$

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

The thermodynamic quantities [30,31] can be evaluated by $\langle E^n \rangle = \frac{1}{Z}\Sigma_E E^n g(E)\exp(-E/k_B T)$, $C_v = (\langle E^2 \rangle - \langle E \rangle^2)/k_B T^2$, $\langle M^n \rangle = \frac{1}{Z}\Sigma_E M^n g(E)\exp(-E/k_B T)$, and $\chi = (\langle M^2 \rangle - \langle M \rangle^2)/k_B T$, 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 [32,33] $(E_{\min},E_{\max})$. We divide this energy range to $R$ subintervals, the minimum energy of each subinterval is $E_{\min}^i$ for $i=1,2,\ldots,R$, and the 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 WL algorithm is used to calculate the relative DOS of each
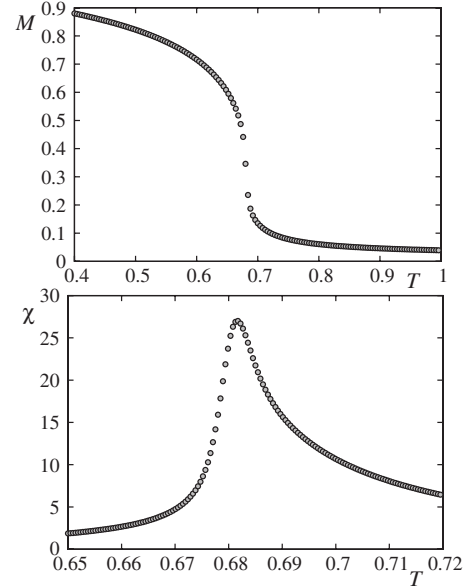


FIG. 3. Magnetization and susceptibility versus $T$ for $N=24$.

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 $N$ varies from 24 up to 48. We stop at $N=48$ because, as seen below, the transition at this size shows a definite answer to the problem studied here. Periodic boundary conditions are used in the three directions. $J=1$ is taken as the unit of energy in the following.

We show in Fig. 3 the magnetization and the susceptibility and in Fig. 4 the energy per spin and the specific heat, for $N=24$. All these quantities show a transition with a second-order aspect. However, we know that many systems show a first-order transition only at very large sizes. This is indeed the case. The energy histograms obtained by the WL technique for three representative sizes $N=24$, 36, and 48 are shown in Fig. 5. As seen, for $N=24$, the energy histogram, although unusually broad, shows a single peak indicating a continuous energy at the transition as observed before in Fig. 4. The double-peak histogram starts already at $N=36$ and the dip between the two maxima becomes deeper with increasing size, as observed at $N=48$. We note that the distance between the two peaks, i.e., the latent heat, increases with increasing size and reaches $\simeq 0.03$ for $N=48$. This is rather large compared with the value of $\simeq 0.009$ for $N=120$ in the $XY$ STA [17–19,22] and with 0.0025 for $N=150$ in the Heisenberg case [23]. We give here the values of $T_c$ for a few sizes: $T_c = 0.680\ 80 \pm 0.000\ 10$, $0.679\ 67 \pm 0.000\ 10$, and $0.679\ 19 \pm 0.000\ 10$ for $N=24$, 36, and 48, respectively.
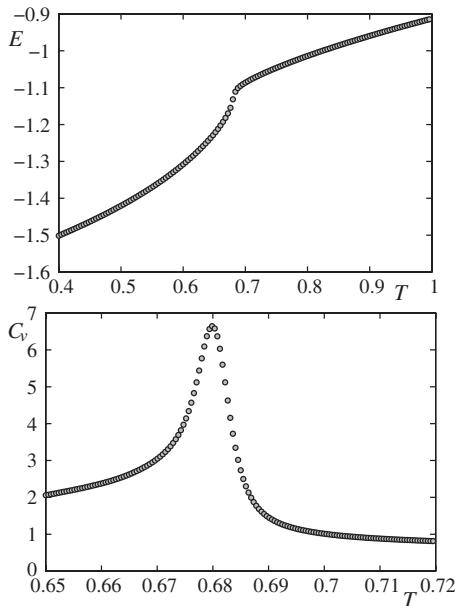
FIG. 4. Energy per spin and specific heat versus $T$ for $N=24$.



FIG. 5. Energy histogram for several sizes $N=24$, 36, and 48 at $T_c$ indicated on the figure.

Note that the double-peak structure is a sufficient condition, not a necessary condition in old-fashion MC simulations (i.e., not the WL method), for a first-order transition. This is because in old-fashion MC simulations performed at a given $T$, we often encounter the situation where, at the transition, the system is spatially composed of two (or more) parts: the ordered phase with energy $E_1$ and the disordered phase with energy $E_2$. Since in old-fashion MC simulations we make histogram from the total system energy, i.e., $E_1+E_2$, the histogram will record the "average" energy $E_1+E_2$; therefore, the double-peak structure will not be seen. Such a coexistence at any time of the ordered and disordered phases in some first-order transitions makes it impossible in old-fashion MC simulations to detect two peaks. In our present WL flat-histogram method, the double-peak structure is obtained from the DOS histogram which gets rid of the problem of spatial coexistence of the two phases discussed above. Therefore, the double-peak structure is a necessary condition for a first-order transition as it should be.

Let us say a few words on the correlation length. It is known that the correlation length is finite at the transition point in a first-order transition. For very strong first-order transitions, this correlation length is short, so that the first-order character is detected in simulations already at small lattice sizes. For weak first-order transitions, the correlation length is very long. To detect it one should study very large lattice sizes as in the present paper. Direct calculation of the correlation length is not numerically easy. Fortunately, one has other means such as the WL method to detect more easily weak first-order transitions.

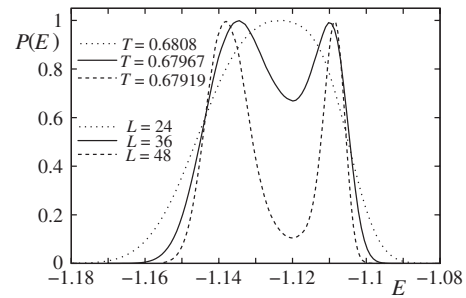To close this section, let us emphasize two points: (i) First, the first-order transition observed here may come from the fact that the GS of the present *XY* FFSCL model has a 12-fold degeneracy which is reminiscent of the 12-state Potts model. In three dimensions, the latter model has a first-order transition. Note however that this conclusion is not always obvious because the continuous degrees of the order parameter mask in many cases the symmetry argument based on discrete models [27]. (ii) Second, some other *XY* frustrated systems such as the fcc [34], hcp [35], and helimagnetic [36] antiferromagnets show also a first-order transition in MC simulations. Although the nonperturbative renormalization group has been extensively used for the STA case [4] due to its long-lasting controversy, we believe that the other cases are worth to study in order to verify that the validity of that theory is not limited to the STA but is universal for frustrated systems of vector spins.

## IV. CONCLUDING REMARKS

Using the powerful WL flat-histogram technique, we have studied the phase transition in the *XY* fully frustrated simple cubic lattice. The technique is very efficient because it helps to overcome extremely long transition time between energy valleys in systems with a first-order phase transition. We found that the transition is clearly of first order at large lattice sizes in contradiction to early studies using standard MC algorithm and much smaller sizes [29]. The result presented here will serve as a testing ground for theoretical methods such as the renormalization group which still has much difficulty in dealing with frustrated systems [4].

## ACKNOWLEDGMENTS

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