Flat energy-histogram simulation of the phase transition in an Ising fully frustrated lattice

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Abstract
We show in this paper the results of the phase transition of the so-called fully frustrated simple cubic lattice with the Ising spin model. We use here the Monte Carlo method with the flat energy-histogram Wang–Landau technique which is very powerful for detecting weak first-order phase transition. We show that the phase transition is clearly of first order, providing an answer to a question raised 25 years ago.

1. Introduction
Statistical physics provides powerful methods for studying the behavior of systems of interacting particles. In particular, different kinds of transition from one phase to another have been efficiently studied over the last 40 years by exact methods [1], renormalization group, high–low-temperature expansions [2], numerical simulations, etc. Experiments have verified most of these theoretical results. Among the most studied subjects is the effect of frustration in spin systems. Frustration is known to be the origin of spectacular properties such as large ground state (GS) degeneracy, successive phase transitions, partially disordered phases, re-entrance and disorder lines. Though these aspects have been found in exactly solved models [3], we believe that many of these features remain in complicated frustrated systems where exact solutions are not available. These general frustrated systems still constitute a challenge for theoretical physics [4].

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, for instance incompatible nearest-neighbor (NN) and next-nearest-neighbor (NNN) interactions, or when the lattice geometry does not allow a spin to satisfy all interaction bonds simultaneously, such as a triangular antiferromagnet. Apart from a few two-dimensional frustrated Ising systems where exact methods have been devised for mathematically elegant solutions [3, 5–7], most systems have recourse to numerical simulations and various approximations. One of the most studied systems is a stacked triangular antiferromagnet (STA) with interaction between NNs. This system with Ising [8], XY and Heisenberg spins [9, 10] has been intensively studied since 1987 [11–17], but it is only recently that the 20-year controversy has come to an end [18–27]. Note that numerical simulations now require new efficient algorithms to deal with frustrated systems [26, 27].

There is another fully frustrated system. Initially defined in two dimensions on a square lattice by Villain [28], this model has been generalized in three dimensions by Blankschtein et al [29] as shown in figure 1. A detailed description of the model will be presented in section 2. The nature of the phase transition in the classical XY [30] and Heisenberg [31] spin models has recently been investigated. It was shown that it is a first-order transition putting an end to a 25-year-long controversy [32, 33]. In this paper, we extend our study to the case of the Ising spin model.

In section 2 we describe the model and give some technical details of the Wang–Landau (WL) methods as applied in the present paper. Section 3 shows our results. Concluding remarks are given in section 4.
The Hamiltonian is given by
\[ \mathcal{H} = -\sum_{(i,j)} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j, \] (1)
where \( \mathbf{S}_i \) is the Ising spin of values \( \pm 1 \) at the lattice site \( i \), \( \sum_{(i,j)} \) is made over the NN spin pairs \( \mathbf{S}_i \) and \( \mathbf{S}_j \) with interaction \( J_{ij} \). We take \( J_{ij} = -J \) (\( J > 0 \)) for antiferromagnetic bonds indicated by discontinuous lines in figure 1, and \( J_{ij} = J \) for ferromagnetic bonds indicated by continuous lines. The two-dimensional (2D) Villain model has been intensively studied with the Ising model [28, 34, 35].

Let us recall some results for the present model. The GS degeneracy is infinite due to the fact that each face of the cube is frustrated, there is thus an infinite number of spins to arrange in an infinite crystal. Note that the ferromagnetic state is one of the GS spin configurations. In an early Monte Carlo (MC) study [38], it was shown that as the temperature \( T \) increases, the system selects the long-range ferromagnetic state at low \( T \) but goes to a partially disordered phase where two of the eight sublattices of the cube are disordered. The passage to this phase does not have the characteristics of a phase transition. The specific heat shows a ‘shoulder’ at \( T \approx 0.7 \) (in unit of \( J/k_B \)), far below the transition temperature for the whole system occurring at \( T \approx 1.345 \). Note that the nature of the low-\( T \) ordering of the present model has still not been elucidated. However, in 1987 we showed [5] in an exactly solved 2D model that a partial disorder can coexist with an order at equilibrium. Therefore, we believe that the early observation of two disordered sublattices in an ordered phase may have the same origin rooted in the frustration and in order selection by entropy [28, 34, 35]. The shoulder of the specific heat may turn out to be a true phase transition. This point has to be checked with careful MC simulations using very large lattice sizes. This is a formidable task, but it is not the purpose of this work. In the present work, we concentrate our attention on the nature of the overall phase transition occurring at a higher temperature. Using the Landau–Ginzburg–Wilson theory, Blankschtein et al [29] found a weak first-order transition. Our previous work in 1985, using a standard MC algorithm with short runs and small lattice sizes permitted by the computing capacity at that time [38], shows a second-order transition with unusual critical properties in contradiction to the prediction of Blankschtein et al. Subsequent MC works [36, 37] with sizes up to \( L = 30 \) have also shown a transition with a second-order aspect. In the light of new results on frustrated systems obtained not only with new efficient MC algorithms but also using today’s huge computer capacity [26, 27, 30, 31], we study this problem again in order to get a clear answer to that question.

For weak first-order transitions, MC simulations with the standard Metropolis algorithm can hardly give results with good precision even with the use of large sizes and long runs. This is because the algorithm does not allow us, among other difficulties, to easily sample rare microscopic states. Wang and Landau [39] have recently proposed an MC algorithm which allows the study of classical statistical models with difficult to access microscopic states. In particular, it permits the efficient detection of weak first-order transitions [26, 27, 30]. The algorithm uses a random walk in the energy space in order to obtain 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 of a 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 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 DOS. In general, if \( E \) and \( E' \) are the energies before and after a spin is flipped, the transition probability from \( E \) to \( E' \) is
\[ p(E \rightarrow E') = \min[g(E)/g(E'), 1]. \] (2)
Of course, to enhance the possibility of accessing rare states, some tricks have been devised. Each time an energy level \( E \) is visited, the DOS is modified by a modification factor \( f > 0 \) whether the spin is 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 \( e^1 \approx 2.7182818 \). 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 the final value \( f_{\text{final}} \) is close enough to one (see the detailed discussion given in [39]). The histogram is considered as flat if
\[ H(E) \geq x\% \langle H(E) \rangle \] (3)
for all energies, where $x\%$ is chosen between 70% and 95% and $\langle E \rangle$ is the average histogram. The WL method has been successfully applied to spin models in our recent papers [26, 27, 30]. We emphasize that for efficiency we consider here a multi subinterval energy scale within an energy range of interest [41, 42] $(E_{\text{min}}, E_{\text{max}})$ which does not include all possible energies of the system but only all energies in the region which will be used in applications. We divide this energy range into $R$ subintervals, the minimum energy of the $i$th subinterval is $E_{\text{min}}^i$ ($i = 1, 2, \ldots, R$), and the maximum is $E_{\text{max}}^i = E_{\text{min}}^i + 2\Delta E$, 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 subinterval $(E_{\text{min}}^i, E_{\text{max}}^i)$ with a flatness criterion $x\% = 95\%$. Note that we reject a 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 $(E_{\text{min}} + \Delta E, E_{\text{max}} - \Delta E)$.

The thermodynamic quantities [39, 40] can be evaluated by

$$\langle E^n \rangle = \frac{1}{Z} \sum_E E^n g(E) \exp(-E/k_B T),$$

$$C_v = \frac{\langle E^2 \rangle - \langle E \rangle^2}{k_B T^2},$$

where $Z$ is the partition function defined by $Z = \sum_E g(E) \exp(-E/k_B T)$. The canonical distribution at a temperature $T$ can be calculated simply by $P(E, T) = \frac{1}{Z} g(E) \exp(-E/k_B T)$.

The simulations have been carried out on a rack of several hundreds of 64-bit CPUs. For a given size $L$, the calculation takes, depending on $L$, from a few weeks to several months to have the required histogram flatness.

3. Results

We have started the simulations from the system linear size $L = 60$ (the system size is $L^3$). But only from $L = 90$ does a sign of first-order transition appear. Therefore, we use extremely large sizes up to 180. Periodic boundary conditions are used in the three directions. $J = 1$ is taken as the unit of energy in the following.

We show in figure 2 the energy per spin and the specific heat, for $L = 180$, using the flat histogram obtained with the WL method. Several remarks are in order.

(i) The energy at the largest size shows a ‘pseudo’ discontinuity at the transition temperature $T_c \simeq 1.34814$. We will see below that this discontinuity is confirmed by the double-peak canonical distribution at this temperature.

(ii) The specific heat shows a very strong size dependence. It should be noted that the specific heat is calculated from the fluctuation of the energy of the system at a given $T$ (see equation (5)), not by the derivative of $E$ with respect to $T$. Therefore, when the energy has a discontinuity at $T_c$ with two levels $E_1$ and $E_2$, the average energy is $E = (E_1 + E_2)/2$. It is the fluctuations of $E$ which give rise to $C_v$, and we will not see a delta-like function if $C_v$ is calculated by the energy derivative. This is the reason why in standard MC simulations with the Metropolis algorithm we do not see discontinuity in energy for weak first-order transition (what is sorted out of the simulation is an average energy). So, an energy histogram is needed if we want to see a weak first-order transition.

The energy histogram can be realized directly in the old fashioned manner by measuring the system energy at a given $T$ [43]. However, when the relaxation between rare states is very slow, we need the temperature-independent WL flat histogram technique as described above. We show the WL result in figure 3. As seen, for $L = 120$, the canonical distribution begins to show a sign of the double-peak structure. The dip between the two maxima becomes deeper with increasing size. Note that a ‘true’ discontinuity happens only when the dip comes down to $P(E) = 0$. This requires sizes much larger than $L = 180$. But for our present purpose, we need not study sizes larger than $L = 180$.

We note that the distance between the two peaks, i.e. the latent heat, increases with increasing size and reaches $\simeq 0.005$
for \( L = 180 \). This is very small compared to the value \( \simeq 0.03 \) for the XY case at \( L = 48 \), and to \( \simeq 0.0085 \) for the Heisenberg case at \( L = 90 \). The smallness of the latent heat in the present Ising case explains why one needs to go to an extremely large lattice size to detect the first-order transition.

We show in figure 4 the maximum of \( C_V \) versus \( L \) in a \( \ln-\ln \) scale; we find a straight line by a least-mean-square fit with a slope equal to \( \phi = 2.794 \pm 0.198 \). This means that \( C_V^{\text{max}} = A L^\phi \) where \( A \) is a constant and \( \phi \) is very close to the system dimension \( d = 3 \). The fact that \( C_V^{\text{max}} \) is proportional to the system volume is consistent with a first-order transition. For figure 4, we added error bars which come from independent random walks in the energy space performed for each size. The error given to the value of \( \phi \) was from the least-mean-square fit using these data points. In the WL method, the errors come from two essential factors: (i) the modification factor \( f \) which should be as close to 1 as possible at the final step (we took \( f = \exp(-8) = 1.00000001 \)), (ii) the flatness criterion \( x \) to stop the simulation (we took \( x > 95\% \)). The errors induced by such imperfect flatness are so small that the shapes of the curves in figure 3 do not change. The reader is referred to the original paper by Wang and Landau for details [39].

The weak first-order transition found here is thus in agreement with the Landau–Ginzburg–Wilson theory [29]. This is rather surprising because in other frustrated systems such as the STA mentioned in section 1, the renormalization group with low-order developments in \( \epsilon \) did not work properly.

### 4. Concluding remarks

We have shown in this paper the results obtained with the WL flat energy-histogram technique for the phase transition in an Ising fully frustrated simple cubic lattice. We found that the transition is clearly of first order. Note that the first-order character is so weak that it has been observed only at extremely large lattice sizes. This finding shows that early studies using the standard MC algorithm with short runs and much smaller sizes [38, 36, 37] are not correct. Our result confirms the prediction of the Landau–Ginzburg–Wilson analysis [29] putting an end to an uncertainty which has lasted for 25 years.

Together with our recent results [30, 31], we conclude that a fully frustrated simple cubic lattice undergoes a first-order transition for Ising, \( XY \) and Heisenberg spin models.

This study shows that one has to be very careful in studying complex systems by MC simulations: in some cases such as the one studied here, sizes as large as 80\(^3\) are still not sufficient to obtain a correct conclusion. Recent large-scale MC simulations using special purpose algorithms such as the WL technique have allowed us to settle several long-standing controversial questions [26, 27, 30, 31].

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