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Large-scale calculation of ferromagnetic spin systems on the pyrochlore lattice

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ABSTRACT

We perform the high-performance computation of the ferromagnetic Ising model on the pyrochlore lattice. We determine the critical temperature accurately based on the finite-size scaling of the Binder ratio. Comparing with the data on the simple cubic lattice, we argue the universal finite-size scaling. We also calculate the classical XY model and the classical Heisenberg model on the pyrochlore lattice.

1. Introduction

Universality and scaling are two important concepts in critical phenomena [1,2]. The critical phenomena associated with the second-order phase transitions are classified into a limited number of universality classes defined not by detailed material parameters, but the fundamental symmetries of a system, that is, the spatial dimension D, the number of components of order parameter n, etc.

In some problems, the lattice structure plays an important role. Recently, the pyrochlore lattice has received a lot of attention because of its relation to the spin ice [3–5]. The pyrochlore lattice is a three-dimensional network of corner-sharing tetrahedra, and the illustration of the pyrochlore lattice is shown in Fig. 1. Antiferromagnetic spin systems on the pyrochlore lattice have frustration. The dilution effects on frustration were also studied for spin ice materials on the pyrochlore lattice [6,7]. It is also interesting to study ferromagnetic spin systems on the pyrochlore lattice in connection with the universality.

It is well known that Monte Carlo simulation is a standard method to study statistical physics of many-body problems [8].

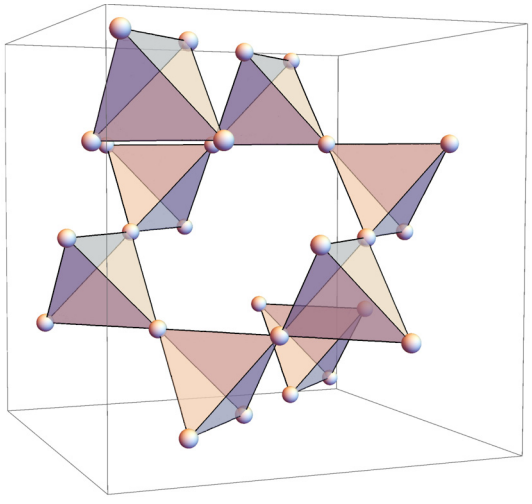

Fig. 1. (Color online.) The illustration of the pyrochlore lattice, which is a three-dimensional network of corner-sharing tetrahedra.

The single spin flip Metropolis method [9] is a robust algorithm for a wide range of subjects, but often suffers from the problem of slow dynamics; that is, it takes a long time for equilibration,

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for example, at temperatures near the critical temperature of the phase transition. To conquer the problem of slow dynamics, the cluster spin flip algorithms of Monte Carlo simulation have been proposed. The multi-cluster spin flip algorithm due to Swendsen and Wang (SW) [10] and the single-cluster spin flip algorithm due to Wolff [11] are typical examples.

For high-performance computing, the use of graphic processing unit (GPU) is a hot topic in computer science. The parallelization of cluster spin flip algorithm is not straightforward because the cluster labeling part of the cluster spin flip algorithm basically requires a sequential calculation, which is in contrast to the local calculation for the single spin flip algorithm. Komura and Okabe [12] proposed the GPU computing for the SW multi-cluster spin flip algorithm, where the ideas of Hawick et al. [13] and Kalentev et al. [14] were used in the cluster labeling part. Recently, Komura [15] proposed a refined version of the SW multi-cluster spin flip algorithm with a single GPU. Sample programs of the methods of Refs. [12] and [15] were published [16,17]. As applications, the large-scale Monte Carlo study of the two-dimensional XY model [18], and the phase transitions of the Ising model on the Penrose lattice (quasicrystal) [19] were studied.

In this paper, we perform the high-performance computation of the ferromagnetic Ising model on the pyrochlore lattice. We use the GPU algorithm by Komura [15] for the SW method. We determine the critical temperature accurately based on the finite-size scaling (FSS) [20] of the Binder ratio [21]. Comparing with the data on the simple cubic lattice, we argue the universal FSS [22,23]. We also calculate the classical XY model and the classical Heisenberg model on the pyrochlore lattice.

The remaining part of the paper is organized as follows: The model and the method are described in Sec. 2. The results are discussed in Sec. 3, while Sec. 4 is devoted to the concluding remark.

2. Model and simulation method

We deal with the classical spin models on the pyrochlore lattice. For the simulation, we use the 16-site cubic unit cell of the pyrochlore lattice [27], and the systems with $L \times L \times L$ unit cells with periodic boundary conditions are treated. We made simulations for the system sizes up to $L = 96$; the numbers of sites are $N\ (= 16L^3) = 14155776$.

The Hamiltonian of the classical spin models is given by

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \boldsymbol{s}_i \cdot \boldsymbol{s}_j, \tag{1}$$

where J is the coupling and $\boldsymbol{s}_i$ is an n-dimensional unit vector on the lattice site i; $n = 1$, 2, and 3 correspond to the Ising model, the classical XY model, and the classical Heisenberg model, respectively. The summation is taken over the nearest-neighbor pairs $\langle i, j \rangle$. We note that the coordination number of the pyrochlore lattice is six, which is the same as the simple cubic lattice.

We use the SW multi-cluster spin flip algorithm with a single GPU in the program of Refs. [15,17]. The embedded cluster idea of Wolff [11] is used for simulating the spin systems with continuous symmetry (XY model and Heisenberg model). Once we have the table which gives the nearest-neighbor sites for each site, we can use the CUDA program of Refs. [15,17]. The performance of the parallel computation with using the CUDA program was discussed in Refs. [15,17]. The system sizes we treat are $L = 32$ ($N = 524288$), $L = 48$ ($N = 1769472$), $L = 64$ ($N = 4194304$), and $L = 96$ ($N = 14155776$). We discarded the first 10,000 Monte Carlo Steps (MCSs) to avoid the effects of initial configurations, and the next 200,000 MCSs were used for measurement. We made five independent runs for each size; the average was taken over five runs, and the statistical errors were estimated.

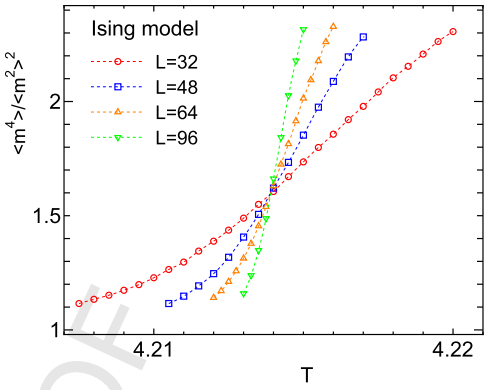

Fig. 2. (Color online.) The moment ratio of the Ising model on the pyrochlore lattice. The system sizes are $L = 32$ ($N = 524288$), $L = 48$ ($N = 1769472$), $L = 64$ ($N = 4194304$), and $L = 96$ ($N = 14155776$).

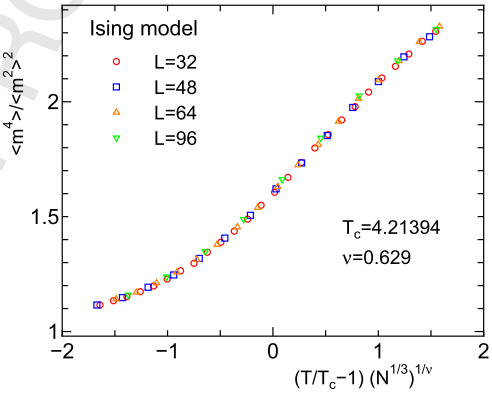

Fig. 3. (Color online.) The FSS plot of the moment ratio of the Ising model on the pyrochlore lattice. The system size N is $16L^3$. The choices of T_c and ν are given in the figure.

3. Results

3.1. Ising model

We start with the Ising model on the pyrochlore lattice. This model undergoes a second-order phase transition. To study the critical phenomena of second-order phase transition, it is convenient to calculate the moment ratio of the magnetization M [21]. In Fig. 2, we plot the temperature dependence of the moment ratio of the magnetization M;

$$U(T) = \frac{\langle M(T)^4 \rangle}{\langle M(T)^2 \rangle^2} = \frac{\langle m(T)^4 \rangle}{\langle m(T)^2 \rangle^2} \tag{2}$$

with $m = M/N$, which is essentially the Binder ratio [21] except for the normalization. The value of $U(T)$ becomes 1 for $T \to 0$, whereas it becomes 3 for $T \to \infty$. The system sizes are $L = 32$ ($N = 524288$), $L = 48$ ($N = 1769472$), $L = 64$ ($N = 4194304$), and $L = 96$ ($N = 14155776$). The temperature is measured in units of J; in other words, we take $J = 1$. The error bars are within the size of marks. We only show the data near the second-order phase transition. We see from Fig. 2 that the data with different L cross around $T = 4.214$, which yields the critical temperature T_c.

To get precise estimate of T_c, let us consider the FSS [20] of the moment ratio $U(T)$. The FSS of $U(T)$ is expected to take a form

$$U(t) = f_1\left(t\,(N^{1/3})^{1/\nu}\right), \tag{3}$$

where $t = (T - T_c)/T_c$, and ν is the critical exponent for the correlation length. We plot $U(T) = \langle m^4 \rangle / \langle m^2 \rangle^2$ as a function of $t(N^{1/3})^{1/\nu}$ in Fig. 3; all the data with different sizes are collapsed

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