Conference materials
UDC 538.91, 537.6
DOI: https://doi.org/10.18721/JPM.153.113

Application of hybrid multispin Monte Carlo method to artificial dipole ice on hexagonal and Cairo lattices

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Abstract: We apply the hybrid multispin Monte Carlo method to calculate the properties for artificial dipole ice on hexagonal and Cairo lattices. The method is based on combining a random selection of a set of spins (cluster) using the Monte Carlo with complete enumeration of all states of the selected cluster. The method works only for Ising models with a restricted radius of interaction. In addition, the method makes it possible to bring spin systems to the ground state at low temperatures.

Keywords: hybrid Monte-Carlo, dipolar antiferromagnets, spin ice, statistical thermodynamics

Funding: The results of studies related to the development of a theoretical model, samples and physical experiments were obtained within the framework of the state task of the Ministry of Education and Science of Russia (No. 0657-2020-0005). The results of research related to coding were obtained at the expense of the grant of the President of the Russian Federation for state support of the leading scientific schools of the Russian Federation (NSh-2559.2022.1.2). The results of research related to the development of algorithms were obtained within the framework of the state task of the Ministry of Education and Science of Russia (No. 075-00771-22-00).

Citation: Makarova K. V., Makarov A. G., Nefedev K. V. Application of hybrid multispin Monte Carlo method to artificial dipole ice on hexagonal and Cairo lattices. St. Petersburg State Polytechnical University Journal. Physics and Mathematics. 15 (3.1) (2022) 76–81. DOI: https://doi.org/10.18721/JPM.153.113

Материалы конференции
УДК 538.91, 537.6
DOI: https://doi.org/10.18721/JPM.153.113

Применение гибридного мультиспинового Монте-Карло метода для искусственного дипольного льда на гексагональной и Каирской решетках

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Аннотация. Для расчета характеристик искусственного дипольного льда на гексагональной и Каирской решетках мы применяем гибридный мультиспиновый Монте-Карло метод. Метод основан на сочетании случайного выбора набора спинов (кластера) методом Монте-Карло с полным перебором всех состояний выделенного кластера. Метод работает только для моделей Изинга с ограниченным радиусом взаимодействия. Кроме того, метод позволяет привести спиновые системы к основному состоянию при низкой температуре.

Ключевые слова: гибридный Монте-Карло метод, дипольные антиферромагнетики, спиновой лед, статистическая термодинамика

Финансирование: Результаты исследований, связанных с разработкой теоретической модели, образцов и физических экспериментов, получены в рамках государственного задания Минобрнауки России (№ 0657-2020-0005). Результаты исследований, связанных с программированием, получены за счет гранта Президента Российской Федерации для государственной поддержки ведущих научных школ Российской Федерации (НШ-2559.2022.1.2). Результаты исследований, связанных с разработкой алгоритмов, получены в рамках государственного задания Минобрнауки России (№ 075-00771-22-00).

Ссылка при цитировании: Макарова К.В., Макаров А.Г., Нефедев К.В. Применение гибридного мультиспинового Монте-Карло метода для искусственного дипольного льда на гексагональной и Каирской решетках // Научно-технические ведомости СПбГПУ. Физико-математические науки. 2022. Т. 15. № 3.1. С. 76–81. DOI: https://doi.org/10.18721/ JPM.153.113

Introduction

To calculate the properties of a system of interacting magnetic moments (spins) at a given temperature in thermodynamic equilibrium, it is necessary to determine the partition function, i.e., it is necessary to obtain information about all possible states (configurations). However, in practice, exact calculation of the partition function is possible only in very rare cases. Finding the properties of a full set of events is an important computational problem. Attempts are currently underway to solve this fundamental problem using Monte Carlo algorithms, a combination of Monte Carlo methods and machine learning.

One such method is the Metropolis–Hastings algorithm, which was proposed in 1953 [1]. The Metropolis–Hastings algorithm is one of the most important algorithms that have been developed in the last century [2]. This approach remains to this day one of the most popular not only in statistical mechanics, but also in an extremely wide field of diverse sciences.

Indeed, the Metropolis algorithm has fundamental importance, but the one-spin approach is unfortunately insufficient at low temperatures. This phenomenon is called the 'critical slowing down' [3, 4].

Therefore, efforts are made to develop new approaches. For example, Melko et al. introduced loop flips into the Metropolis algorithm, performing simulations of a spin-ice model at low temperatures [3, 5]. There are combinations of the conventional Metropolis method with single spin rotations and replica exchange method [6, 7], and with the over-relaxation method, with the replica-exchange method [8]. There are Monte Carlo simulations combined with finite-size scaling [9].

In this paper, we applied the hybrid Monte Carlo method of our own design [10, 11], in which, instead of a single spin-flip, we use a complete enumeration of 2^{N_c} states of N_c spins (moments) within a small cluster that interact with a configuration of 'frozen boundary' of N_b spins or moments. The basic idea of our approach is to search for the thermodynamic equilibrium of subsystems of relatively small size at finite temperature at almost adiabatic process. Naturally, equilibrium is achieved significantly faster in small subsystems than in the entire system. If all subsystems with the same local Hamiltonian are physically and statistically equivalent, the statistical thermodynamic characteristics of one subsystem (replica) can be calculated only once to be used to calculate the thermodynamic averages.

Hexagonal Dipolar Spin Ice, Nearest Neighbors Model

'Artificial spin ice' (ASI) is not just an artificial analog of natural spin ice, which is to say, geometrically frustrated magnetic pyrochlores that imitate the ordering of the spins of water protons, but a convenient framework for developing and testing theoretical models of many interacting bodies and new statistical methods, as well as verifying their accuracy.

We use Ising-like point dipoles located on the edges of a two-dimensional hexagonal lattice with periodic boundary conditions. The magnetic moment of the dipole i is defined as $\vec{m}_i$ and is directed along the edges (see [10, 11] for details). An example of a dipole hexagonal lattice is shown in Fig. 1, *a*.

For the operation of the hybrid Monte Carlo method, we limited the radius of the dipole-dipole interaction to three coordination spheres according to the results [12]. To calculate the energy, it is necessary to determine the neighbors for each dipole. Each cluster dipole has 14 nearest neighbors (see Fig. 1, *b*). Since the boundary conditions are periodic, all elements in the system have the same number of neighbors.

For the method to work correctly, it is necessary to determine the clusters and boundaries of each hexagon. A hexagon is taken as a cluster, and the nearest neighbors of the hexagon dipoles are the boundary that interacts with the cluster and separates it from all other dipoles. The cluster is shown by red arrows in Fig. 1, *a* and consists of six dipoles. The cluster boundary is shown by blue arrows and consists of 24 nearest neighboring dipoles. In total, the cluster and the boundary block contain 30 dipoles, whose states can be easily enumerated by complete enumeration. This block will be subsequently used for sampling.

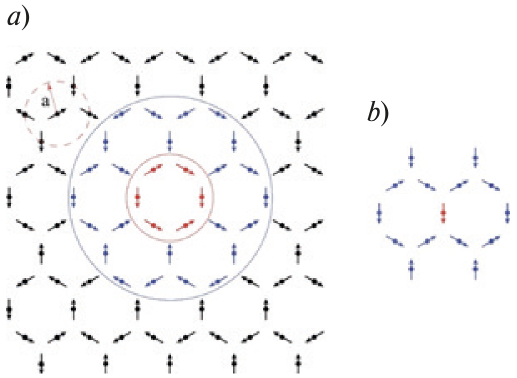

Fig. 1. Example of hexagonal lattice with Ising-like point dipoles (spins): cluster spins are marked in red (small circle) and border spins in blue color (large circle), which are used as subsystems in the hybrid Monte Carlo method (*a*); cluster spin and interacting dipole-dipole neighbors up to the third coordination sphere (*b*)

The energy of the dipole-dipole interaction between dipoles is defined as

$$E = Da^3 \sum_{i<j} \left[\frac{(\vec{m}_i \vec{m}_j)}{\left|\vec{r}_{ij}\right|^3} - 3\frac{(\vec{m}_i \vec{r}_{ij})(\vec{m}_j \vec{r}_{ij})}{\left|\vec{r}_{ij}\right|^5} \right], \tag{1}$$

where $D = \mu_2/a3$ is the dipole coupling constant, $a = \sqrt{3}/2$ is the lattice parameter (Fig. 1, *a*) and $\vec{r}_{ij}$ is the radius vector between dipoles *i* and *j* with magnetic moments $\vec{m}_i$ and $\vec{m}_j$, respectively.

For systems with different numbers *N* of spins, we calculated the specific heat capacity $C(T)$ per spin depending on temperature

$$C(T) = \frac{1}{N} \frac{\langle E^2 \rangle - \langle E \rangle^2}{k_B T^2}, \tag{2}$$

where $\langle E \rangle$ is the average thermodynamic quantity, k_B is the Boltzmann coefficient, T is the temperature.

Hexagonal Dipolar Ice Thermodynamics and Ground State

Using our method, we obtained the specific heat (Fig. 2) for the hexagonal spin ice consisting of different numbers of spins; the data are presented in relative units.

The temperature behavior of the heat capacity has two peaks. An increase in one of the heat capacity peaks with an increase in the size of the system may indicate the presence of a phase transition. In addition, there is no low-temperature peak in the temperature behavior of heat capacity in the model of Ising-like point dipoles on a hexagonal lattice. The low temperature pick

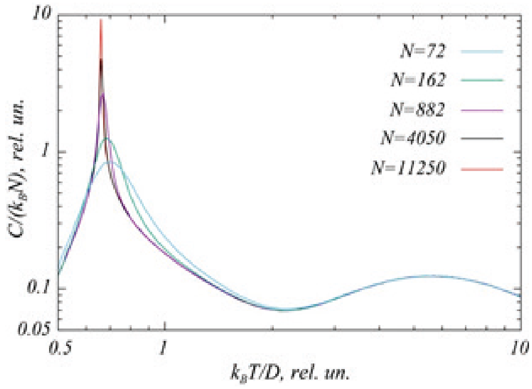

Fig. 2. Temperature behavior of specific heat for different numbers of spins on the hexagonal lattice, calculated by the hybrid Monte Carlo method

was discussed in [13, 14]. The presence of a peak is usually associated with a phase transition to a low-energy phase. The low-temperature transition to long-range order, which is discussed in [15], is absent in the nearest-environment model. Thus, the phase transition to an ordered phase in artificial macrospin ice materials is associated with the long-range nature of dipole interaction, which lifts the macroscopic degeneracy of the ground state.

Developing an algorithm to search for ground state is a fundamental problem. The multispin cluster Monte Carlo method allows to search for configurations of low-energy states. Fig. 2 from [16] shows an example of one of the ground state candidates for the hexagonal lattice of Ising-like dipoles obtained by our method.

Cairo Dipolar Ice, Nearest Neighbors Model

The Cairo lattice with periodic boundary conditions is shown in Fig 3, *a*. The lattice parameters were a = 472 nm, b = 344 nm, and c = 376 nm. The interaction radius and nearest neighbors of one of the dipoles of the cluster are shown in Fig. 3, *b*. To implement the hybrid multispin Monte Carlo method, five dipoles are taken as a cluster, and their nearest neighbors form a boundary (Fig. 3, *c*).

a) *b*) *c*)

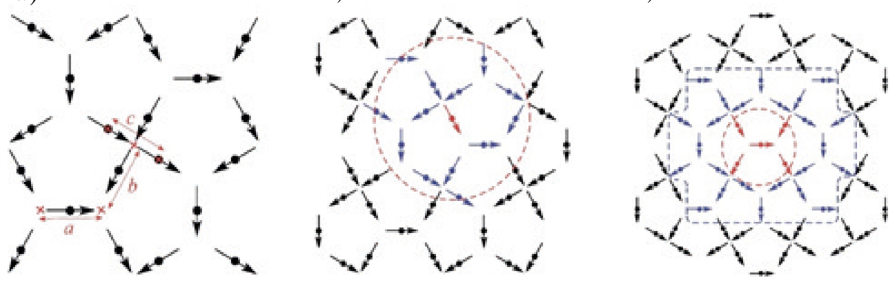

Fig. 3. Example of Cairo lattice with Ising-like point dipoles (spins): relevant parameters *a*, *b*, and *c* (*a*); the cluster spin and interacting dipole–dipole neighbors (*b*); cluster spins are marked in red (small circle) and border spins in blue (large rectangle), which are used as subsystems in the hybrid Monte Carlo method (*c*)

The energy of the dipole-dipole interaction in the Cairo lattice was calculated using Eq. (1).

Thermodynamics Cairo Dipolar Ice and Ground State

Calculating thermodynamic averages allowed calculating the temperature dependence of the specific heat capacity for the pentagonal Cairo lattice as a function of the given number of dipoles. The size of the cluster with the boundary had 29 dipoles. The lattice parameters were a = 472 nm, b = 344 nm, and c = 376 nm

As can be seen from Fig. 4, with an increase in the number of dipoles on Cairo lattice, there is no increase in the height of the heat capacity peak in models with a limited interaction radius.

The absence of size effects in the temperature behavior of the heat capacity is observed. The heat capacity peak height is the same for all studied systems with the number of particles $N = 80$, 500 and 980, in the nearest neighbors model.

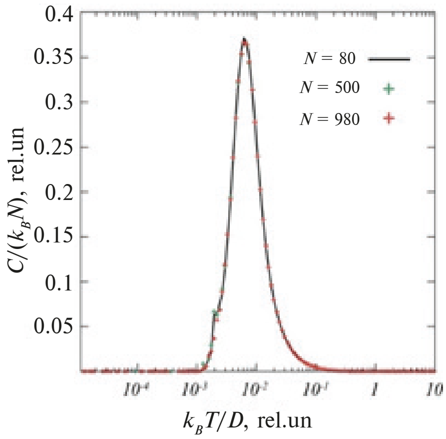

Fig. 4. Temperature behavior of specific heat of Cairo dipolar ice, calculated by hybrid Monte Carlo method

It should be noted that a model and, specifically, the interaction radius should be selected very carefully, since it is known that depending on the value of the interaction radius of Ising dipoles, the same model can lead to existence of several heat capacity peaks. For a limited interaction radius in the model of nearest neighbors, only one heat capacity peak is observed. Moreover, we calculated the ground state of the Cairo lattice of dipoles $N = 80$ dipoles (see [10], Fig. 8).

Conclusion

The hybrid multispin Monte Carlo method allows increasing the size of counting systems and to expand the amount of calculated statistical-thermodynamic parameters while preserving the accuracy and performance at the same level. Furthermore, the method allows to calculate the temperature dependence of thermodynamic quantities such as heat capacity and others, and in some cases solve the fundamental problem of searching for configurations of low-energy states or even ground states at $T \rightarrow 0$. It can be easily generalized to spin lattices of arbitrary dimensions, arbitrary Hamiltonian, arbitrary dilution, and external field.

Acknowledgments

The results of studies related to the development of a theoretical model, samples and physical experiments were obtained within the framework of the state task of the Ministry of Education and Science of Russia (No. 0657-2020-0005). The results of research related to coding were obtained at the expense of the grant of the President of the Russian Federation for state support of the leading scientific schools of the Russian Federation (NSh-2559.2022.1.2). The results of research related to the development of algorithms were obtained within the framework of the state task of the Ministry of Education and Science of Russia (No. 075-00771-22-00).

To perform the calculations, we used the computational resources provided by the Shared Facility Center “Data Center of FEB RAS” [17].

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Received 22.05.2022. Approved after reviewing 14.07.2022. Accepted 26.07.2022.