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Method for density-of-states calculation of dipole spin lattices

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Abstract: The solution to the problem of finding the probability density of all possible states (configurations) in dipole lattices, which also allows obtaining information about the degree of frustration in the system, is considered in the article. As an example, the Cairo lattice of 40 particles (dipoles) was used - a two-dimensional system of artificial spin ice, combining the geometry of square and Kagome lattices. Our method was created by combining the approximate polynomial algorithms of the MC-walk and the Greedy algorithm. We used the Greedy algorithm to obtain the energy data points for each possible spin excess, then partition the space into an equal number of intervals, and MC-walk to accumulate the data points. It was shown that the use of intervals makes it possible to ensure good performance of the method on the most degenerate energy regions but has a problem in finding data points on the least degenerate regions. The distribution of the density of states is constructed.

Keywords: density of states, Cairo lattice, algorithm development, ground state

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Метод расчета плотности состояний для дипольных решеток

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Аннотация. В статье рассматривается решение проблемы нахождения плотности вероятности всех возможных состояний (конфигураций) в дипольных решетках, также позволяющий получить информацию о степени фрустраций в системе. В качестве примера была использована Каирская решетка – двумерной системе искусственного спинового льда, совмещающей геометрии квадратной и кагоме систем из 40 частиц (диполей). Наш метод создан путем комбинирования приближенных полиномиальных алгоритмов МК-блуждания и Жадного алгоритма. Мы используем Жадный алгоритм для получения энергетических границ для каждого возможного спинового избытка, для последующего разбиения пространства на равное число интервалов, и МК-блуждания для накопления точек данных. Показано, что использование интервалов позволяет обеспечить хорошую работу метода на наиболее вырожденных энергетических участках, но имеет проблему в поиске точек данных на наименее вырожденных участках. Построено распределение плотности состояний.

Ключевые слова: плотность состояний, Каирская решетка, разработка алгоритма, основное состояние

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Introduction

Artificial spin ice is a nanomagnetic multiferroic artificial material consisting of nanoparticles of elongated shape. The magnetic moment of a particle consists of many spins, therefore it is called a superspin or macrospin. The behavior of magnetic moment of nanoparticles makes it possible to use the Ising model, since there are only two possible mutually exclusive orientations for it, 'up' or 'down'. Initially, artificial spin ice was understood as a two-dimensional artificial equivalent of spin ice on a pyrochlore lattice. Research on artificial spin ice is of major importance. Thermodynamic properties of systems are investigated. Theoretical work is usually aimed at confirming experimental observations. However, the most fundamental issue is developing algorithms that could allow calculating a complete group of events based on a sample from the state space. Currently, there are no theories and, consequently, technical, software capabilities for accurate calculation of the statistical sum of a large number (>40) of interacting particles of a fully connected model. Therefore, interest in the topic of artificial spin systems is constantly growing.

The method we used for calculating the density of states is independent of geometry and is suitable for studying any dipole lattices.

As an example, the Cairo lattice was used, which is a two-dimensional system of artificial spin ice that combines the geometry of the square and kagome systems [1].

Model and Computational Methods

A system of 40 dipoles was observed, since its dimension is large enough for the obtained data to have statistical value, and at the same time, it is still possible to calculate the exact values by exhaustive search, which is used for comparison.

The greedy algorithm made it possible to 'descend' to low-energy configurations in a relatively small number of operations, but rarely allows to find the ground state or configurations that are energetically close to it [2]. The algorithm can be reversed to find the highest energy in the system.

In the study, we applied this algorithm sequentially for various parameters of the spin excess M to obtain the graph for $E(M)$, which is the basis of the future three-dimensional graph of the density of states. For each M, there are two points that the boundary passes through: $E_{\max}$ and $E_{\min}$ (except $M = N$, where the lines converge). These are the maximum and minimum energies found for a fixed spin excess M respectively.

A random Monte Carlo walk over the system's energy spectrum was used to accumulate a statistically significant number of possible energy values [3]. The algorithm is simple: we generated a random spin configuration, calculated the system's total energy and saved the result. The operation was performed for each of the M possible using the MC averaging steps. The energy of the dipole-dipole interaction of a system of dipoles on the Cairo lattice is calculated using the formula:

$$E_{ij} = \frac{(\vec{m}_i \vec{m}_j)}{\left|\vec{r}_{ij}\right|^3} - 3\frac{(\vec{m}_i \vec{r}_{ij})(\vec{m}_j \vec{r}_{ij})}{\left|\vec{r}_{ij}\right|^5}, \quad (1)$$

where $\vec{m}_i$ is the value of the magnetic moment vector; $\left|\vec{r}_{ij}\right|$ is the vector between the centers of the magnetic moments of the interacting dipoles.

Due to energy degeneracies (states in which several configurations can correspond to the same energy value) some energies are much more common than others, serving to generate the function $g(E)$ corresponding to the upper part of the general three-dimensional density of states.

The step was calculated for dividing the energy space into intervals for each spin excess M using the formula:

$$step = \frac{E_{\max} - E_{\min}}{num}, \quad (2)$$

where *num* is the number of intervals.

Then, for each interval, the degeneracy multiplicity g (describing how many of the previously generated energies are included in each interval) was calculated.

The area under the graph S is equal to the binomial coefficient calculated using formula (3):

$$S = \frac{N!}{M!(N-r)!}. \quad (3)$$

For each spin excess, we multiplied $g(E_i)$ so that the area under the graph is equal to the corresponding binomial coefficient.

Results and Discussion

The energy boundaries were calculated using a greedy algorithm. We generated 100,000 possible energy points for each spin excess M. NVIDIA CUDA parallel computing technology was used to speed up the implementation [4]. For each spin excess M, the energy space was divided into 1,000 intervals with an equal step. This approach made it possible to obtain a fairly correct (with respect to exhaustive search values) distribution of energies and multiplicity of degeneracies using a relatively small amount of data.

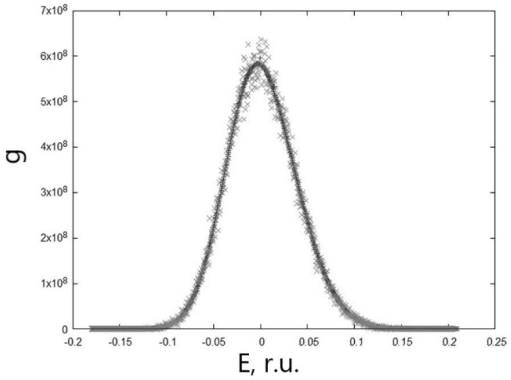

Fig. 1. Function $g(E)$ for spin excess $M = 0$ for exact solution (straight line) and approximate solution (dots).

Fig. 1 shows the $g(E)$ plot for the spin excess $M = 0$, on which the dark straight line is the distribution plot for the exact solution (also divided into intervals, otherwise we would obtain a different dimension), the brighter dots are the approximate data extracted using the algorithm. Evidently, the curves exhibit a similar shape along the entire length with a slight inaccuracy in the peak region, where the largest number of possible energies is located.

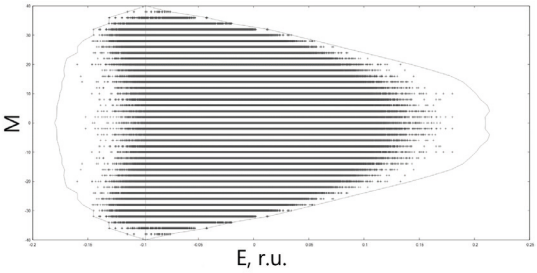

Fig. 2. $M(E)$ for all generated energy points found by the MC method and bounds found by the greedy algorithm.

However, it can be seen from Fig. 2 that the points generated by Monte Carlo do not occupy all the available space (that is also calculated by the approximate greedy algorithm). Because the multiplicities of degeneracy g for the energies located in the middle were much larger, the points along the edges were chosen much less often, or not chosen at all. Fig. 1 shows how strong the growth dynamics was in the middle, relative to the edges. This introduces an additional inaccuracy in the approximate method, requiring to search for solutions.

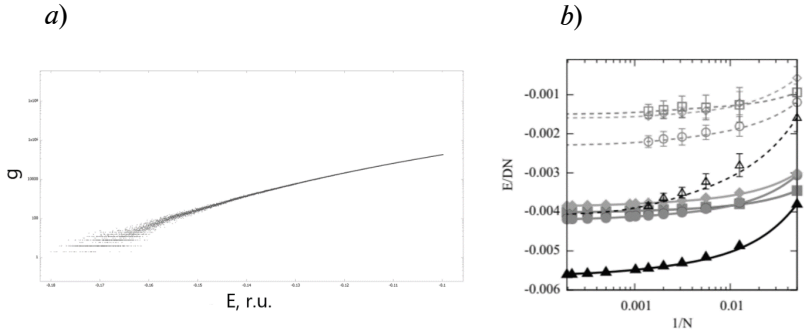

Fig. 3. Function $g(E)$ for the spin excess $M = 0$ (*a*); dependence of the ground state on the number of particles (*b*) [5].

We found from an exhaustive data search that the graph in the low-energy regions close to the ground state can be approximated by a straight line (Fig. 3, *a*) extended to a zone that is well calculated by the Monte Carlo method from the starting point (the ground state or a value close to it).

The first option is to improve the existing greedy algorithm to be able to search for lower energy points close to the ground state for each fixed spin excess M. However, improving of the greedy algorithm is a challenge in itself. A more promising option is to refine the existing method of the ground state energy calculation by scaling. Fig. 3, *b* shows a graph of the change in the minimum energy with a change in the size of the system for the Cairo lattice with different parameters [5].

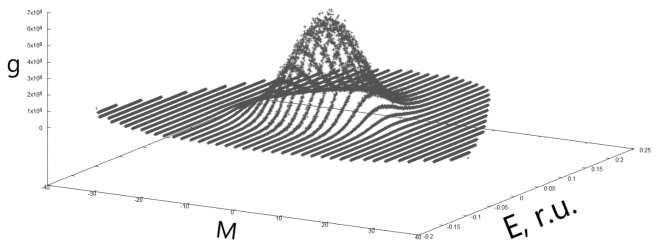

Fig. 4. Density of states (the axis x represents the energy E in arbitrary units; y the spin excess M; z the multiplicity of degeneracy g).

Finally, the binomial coefficients were calculated; the area under each $g(E)$ plot for each spin excess M has been proportionally increased to match the binomial coefficient.

The result is a density of states plot (Fig. 4). We will be able to calculate a fairly accurate DOS after improving the algorithm.

Conclusion

We used 2 approximate methods to construct a polynomial algorithm for finding the density of states for dipole lattices of artificial spin ice. We have found that our approach demonstrates good accuracy for a part of the system (in the center of the energy space) but does not perform well at the edges. We made suggestions about possible ways to solve the problem and improve the algorithm, based on previously obtained data.

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