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Phase transitions on trimer lattices of magnetic dipoles

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Abstract: The heat capacity in a trimerized triangular lattice was studied using the GPU-optimized Metropolis algorithm. The presence of phase transitions is discovered, the reasons for their disappearance at certain lattice parameters are explained, and frustration estimates are made for systems with different lattice parameters.

Keywords: spin ice, phase transition, Monte Carlo methods

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Материалы конференции
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Фазовые переходы на тример решетках магнитных диполей

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Аннотация. При помощи GPU оптимизированного алгоритма Метрополиса исследованы теплоемкость в тримеризованной треугольной решетке. Обнаружено наличие фазовых переходов, объяснены причины их исчезновения при определённых параметрах решетки, сделаны оценки фрустрации систем с различными параметрами решетки.

Ключевые слова: спиновый лёд, фазовый переход, методы Монте-Карло

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Introduction

Artificial spin ices are nanomagnetic systems consisting of monodomain Ising-type nanomagnets that are lithographically defined onto two- and three-dimensional lattices [1, 2]. A distinctive feature of spin ice is a special lattice geometry, which makes any state of the system of magnetic moments energetically tense, and the artificial spin ice has non-zero entropy even at absolute zero [3]. Because of this property, such system can form phases, unusual for ordinary magnetic substances. However, studies in this area are facing computational problems, such as slow dynamics at low temperatures and exponential growth of computational time. For example, for the long-range action model, the complete enumeration algorithm cannot compute systems larger than $N = 40$ particles. Therefore, the probabilistic Monte Carlo methods, although affected by the problem of critical slowing down, are still among the most important for the study of spin ices.

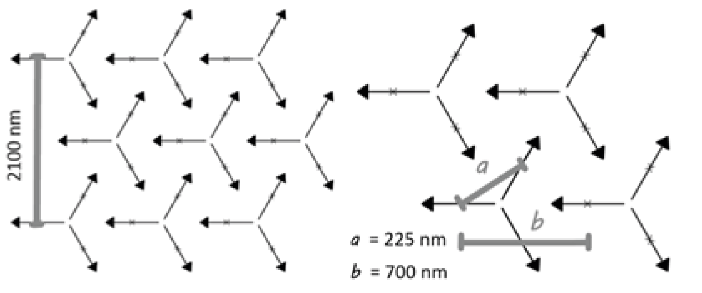

Fig 1. Trimerized triangular lattice with lattice parameters *a* and *b*

Trimerized triangular spin ice consists of repeating triplets (trimers) of particles arranged relative to each other at an angle of 60 degrees (Fig. 1) [4].

In this paper, we investigate the heat capacity [5] of a trimerized triangular point dipole spin ice, modeled by GPU-accelerated parallel Metropolis algorithm. The dependence of the heat capacity maximum on the lattice parameter *b*, as well as on the number of particles was investigated.

Model and computational methods

Energy of dipole-dipole interaction calculated by 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 *i*, *j* are the numbers of the interacting dipoles, *r* is the vector between the centers of the magnetic moments of the interacting dipoles, *m* is the value of the magnetic moment vector.

To study the properties of the system, we used the GPU-accelerated parallel Metropolis algorithm. The essence of the algorithm was to simultaneously independently simulate many systems at different temperatures. The calculations were performed on the NVIDIA A100 GPU, which allows to simultaneously simulate the system at 6912 temperatures. The probability of adopting a new configuration was calculated by the formula:

$$P\left(E_i \to E_j\right) = \min\left(\exp\left[\frac{\Delta E_{ij}}{k_B T}\right], 1\right). \quad (2)$$

After the new configuration is accepted, thermodynamics averages are recalculated. In this case we recalculate an average energy:

$$\left\langle E \right\rangle = \frac{\sum_i^N E_i}{N}. \quad (3)$$

Next, we can obtain the heat capacity by the formula:

$$C = \frac{\left\langle E^2 \right\rangle - \left\langle E \right\rangle^2}{NT^2}. \quad (4)$$

Therefore, the value of the heat capacity is calculated per particle and there is no direct dependence of the heat capacity on the number of particles.

Results and discussion

Graphs of the heat capacity per particle as a function of temperature were plotted for 1200 particles with different lattice parameters b (Fig. 1,*a*). Fig. 2, b shows some of them. It is easy to see that the graph for b = 560 shows a sharp increase in the region of a certain critical temperature. The heat capacity at b = 600 exhibits somewhat different behavior. There is no sharp increase at a certain critical temperature.

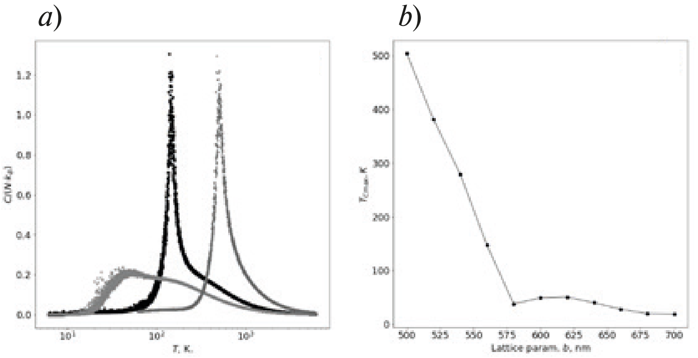

Fig 2. Heat capacity for b = 600, 560, 500 respectively (from left to right) (*a*); dependence of the maximum heat capacity on the lattice parameter (*b*).

Fig. 2, b shows the dependence of the maximum heat capacity on the lattice parameter b.

The flatness of the graph can be explained by the strong frustration of the systems having the parameter $b \approx 580$. For the initial study of frustrations in the system, we investigated low energy states (Fig. 3). The low energy states of closed vortexes and frustrated states of trimers having only two states are typical for parameter $b \leq 560$. The frustrated vortexes and low energy states of trimers for the parameter $b \geq 600$ are characteristic, and they have six possible states each.

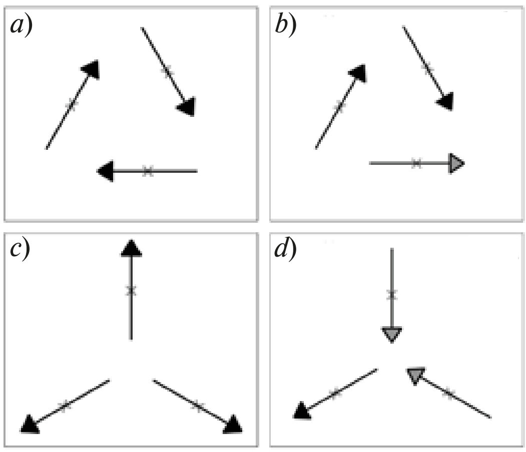

Fig. 3. Typical vortex configuration for low energy configuration for $b \leq 560$ and $b \geq 600$ (*a*, *b*) respectively; typical trimer configuration for $b \leq 560$ and $b \geq 600$ respectively (*c*, *d*).

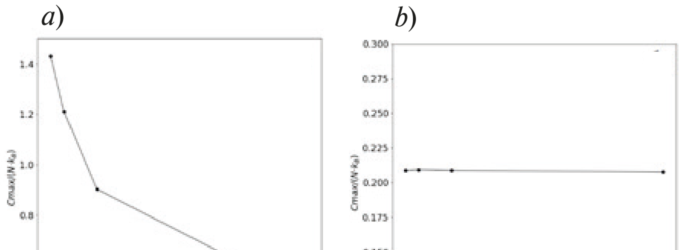

Fig. 4. The presence of a phase transition at b = 560 (*a*); absence at b = 600 (*b*).

Fig. 4 shows the dependence of the height of the heat capacity peak on the number of particles in the system. An increase in peak height indicates a phase transition. Systems with lattice parameters $b \leq 560$ exhibit a phase transition and systems with do not.

Systems with lattice parameters $560 < b < 600$ is extrimely frustrated and have very complex energy relief and cannot be investigate with the Metropolis method. We are planing to use Wang-Landay and parallel tempering methods in the future to overcome critical slowdown.

Conclusion

Phase transitions in trimerized triangular lattice were investigated, the causes of disappearance are explained, and estimates of the frustration of systems with different lattice parameters are made.

Additional studies are required by methods capable of overcoming the critical slowing down to determine the specific value of the lattice parameter and to investigate the nature of the disappearance of the phase transition.

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