論文の内容の要旨

論文題目
Modern Monte Carlo approaches to classical spin systems: Irreversible algorithm and massive parallelization applied to chiral magnets

(大規模モンテカルロシミュレーションによるカイラル磁性体の研究)

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This thesis considers modern Monte Carlo approaches and their applications to classical Heisenberg spin models of chiral magnets. Markov chain Monte Carlo method allows us to study any statistical models without any approximation in principle. Chiral magnets, in which spins build a collective textures, show complex ordering structures with large length scales. Such structures obstruct efficient Monte Carlo simulations and requires large-scale Monte Carlo simulations. In this thesis, we tackle phase transitions in chiral magnets by using an irreversible Monte Carlo algorithm, which breaks detailed balance, and massively parallelized Monte Carlo simulations implemented on GPUs.

The thesis is composed of three parts. In the first chapter of Part I, we introduce the concept of Markov chains and their fundamental properties. Any Markov chain has a unique stationary distribution and converges to it if the balance, the irreducibility, and the aperiodicity conditions are satisfied. These conditions are important in the sense that Markov chain Monte Carlo algorithms are guaranteed to give correct results. Time scales such as the relaxation time and the correlation time in Markov chains are also discussed. The correlation time is especially relevant in practical Monte Carlo simulations because it can be estimated in a relatively short time by the autocorrelation function. Slowing down of time scales in Markov chains and the dynamical critical exponent is discussed in connection with the efficiency of algorithms. Next, various Markov chain Monte Carlo algorithms are discussed focusing on their pros and cons. In the last section of the chapter, we introduce the concept of lift of Markov chains. It is a class of irreversible Markov chains, and may enhance decorrelation. In the last chapter, we discuss recently introduced event-chain Monte Carlo algorithm. The event-chain algorithm was originally developed in particle models. Recently, the algorithm is generalized to continuous spin systems. We applied the event-chain algorithm to classical Heisenberg spin models such as the three-dimensional ferromagnetic model, the antiferromagnetic model on the triangular lattice, and the three-dimensional spin glass model. We found that the algorithm reduces the

dynamical critical exponent of the ferromagnetic model. This is, to our knowledge, the first irreversible algorithm which realizes a reduction of the exponent in finite-dimensional models with finite-temperature phase transition. We also found that the algorithm is more efficient than a conventional algorithm in the antiferromagnetic model. However, unfortunately, in the spin glass model, the algorithm does not work well, and even worse than a conventional algorithm. We discuss the performance in connection with the discrete nature of the order parameter of the spin glass model.

In Part II, we discuss a classical Heisenberg spin model of a uni-axial chiral magnet in three dimensions. Because of the Dzyaloshinskii–Moriya (DM) interaction, the model has a helical structure in the low temperature region without magnetic fields, and a non-trivial spin structure, called the chiral soliton lattice, in the presence of a magnetic field perpendicular to the helical axis. In the first chapter, we overview a theory of a one-dimensional continuum model at zero temperature. The continuum model shows a phase transition at a finite field between the chiral soliton lattice and the paramagnetic phases. We also briefly review results of some experimental works using $Cr_{1/3}NbS_2$ on its phase diagram. Many experiments show qualitatively the same phase diagram. Moreover, some experiments report a change of some physical quantities, the magnetoresistance and the ac susceptibility, depending on the magnetic field. In the next chapter, we detail the simulation method used in the actual Monte Carlo simulations. We use the event-chain algorithm to make the correlation time short. Indeed, the autocorrelation function in the event-chain algorithm decays much faster than that in a conventional algorithm. With the event-chain algorithm, we performed large-scale Monte Carlo simulations of the system with more than 10^6 spins. Using finite-size scaling analyses, we show that the system without any magnetic field undergoes a continuous phase transition with the critical exponents of the three-dimensional XY universality class. A phase transition in the system changes depending on the magnetic field. When the magnetic field is weak, a phase transition similar to that in the zero magnetic field case occurs. On the other hand, when the magnetic field is slightly larger, a completely different phase transition occurs with strong divergences in the specific heat and the uniform magnetic susceptibility. This strongly implies that at least one critical point exists in the phase diagram. The critical exponent of the phase transition of the system with the weak magnetic field is also analyzed by a finite-size scaling form, and it again belongs to the three-dimensional XY class. In the end of the chapter, we discuss the order of the phase transition with larger magnetic field and the phase diagram.

In Part III, melting transition of skyrmions which emerge in a two-dimensional chiral magnet is studied. Skyrmions are topological excitations with local energies, and stable particle-like objects. They are also thermodynamically stable in chiral magnets because of the bi-axial DM interaction. In the first chapter of the part, we review phase diagram of chiral magnets obtained by experiments. We discuss a difference between three-dimensional bulk materials and (quasi-)two-dimensional thin films. After that, we review the famous Kosterlitz–Thouless–Halperin–Nelson–Young (KTHNY) theory of two-dimensional melting of particles with/without a periodic substrate. In the next chapter, details of our Monte Carlo simulations are presented. Due to a large free-energy barrier to create/destroy one skyrmion, conventional Monte Carlo algorithms cannot equilibrate the system for a very long time. We thus fix the number of skyrmions that is estimated to be the thermodynamic dominant value to avoid the difficulty. The system is simulated with massive parallelization using GPUs. In the last chapter, we present our Monte Carlo results and discuss the phase diagram. With an interpretation of skyrmions as point particles, we compute the correlation functions of the orientational and the positional orders. In the low temperature region, the positional correlation decays algebraically with a long-range correlation in the orientational order. This means that skyrmions form a typical two-dimensional solid rather than a crystal, which has long-range positional and correlation orders. With increasing temperature, the skyrmion solid state melts into a liquid phase in one step. This is consistent with the KTHNY theory of melting transition of particles in a weak incommensurate periodic substrate.