Abstract

The *quantum spin liquid* (QSL) is an exotic quantum state of matter, which does not show any long-range ordering down to the lowest temperature (T). This state has evaded full understanding for nearly half a century despite the intensive research. However, the recently-introduced Kitaev model brought a significant breakthrough in understanding of QSLs. The model provides an exact QSL ground state, with an explicit form of fractionalization of the spin degree of freedom into itinerant Majorana fermions and $\mathbb{Z}_2$ fluxes. One of the advances driven by this breakthrough was the discovery of an unconventional finite-T phase transition from paramagnet to the QSL on a three-dimensional (3D) hyperhoneycomb lattice. The finding brings up fundamental questions on universality and diversity of the phase transitions to QSLs. Meanwhile, in a two-dimensional (2D) case, a peculiar finite-T transition was reported for a *chiral spin liquid* (CSL), a QSL with broken time-reversal symmetry. This naturally poses a question for the phase transitions in 3D CSLs. These are, however, theoretical challenges since numerical methods used thus far are insufficient due to severe limitation in the system sizes. Another important advance has been made for materials exploration of the Kitaev-type QSL. Although most of the candidates exhibit magnetic long-range ordering at low T due to non-Kitaev interactions, it was found that an external magnetic field may induce a QSL by suppressing the long-range orders; in particular, in α-RuCl$_3$, a Majorana topological state was recently evinced by the half-quantized thermal Hall conductivity. Theoretically, the effects of non-Kitaev interactions and a magnetic field are not fully understood, since they break the exact solvability of the Kitaev model and most of the previous studies have been limited to numerical calculations for small-size clusters.

In this thesis, we develop two numerical techniques to solve these problems. One is a technique for the pure Kitaev models, which reduces the computational cost drastically. We apply this technique to study the finite-T transitions in the 3D Kitaev models defined on the hyperoctagon and hypernonagon lattices. The other is a technique applicable to the models including non-Kitaev interactions and a magnetic field, which alleviates the negative sign problem. We test this technique for the 2D Kitaev model in a magnetic field.

In the numerical technique for the pure Kitaev models, we adopt a sophisticated update method based on the kernel polynomial expansion of Green's functions in the quantum Monte Carlo (QMC) method on the basis of a Majorana fermion representation. It enables us to perform large-scale simulations with the computational cost of $\mathcal{O}(N^2)$, whereas the conventional method costs $\mathcal{O}(N^4)$, where N is the number of quantum spins in the system. Using this technique, we can reach up to $N \sim 2600$, which is a

big advance compared to $N \sim 900$ in the previous studies.

By applying this technique to the Kitaev model on the 3D hyperoctagon lattice, we find a finite-T transition of the same nature as for the hyperhoneycomb case. From careful analyses of the finite-size effects, we find that the critical temperature is lower than that in the hyperhoneycomb case. Considering that the gap for $\mathbb{Z}_2$ flux excitations is smaller than that in the hyperhoneycomb case, our result supports that the critical temperature of this topological transition is set by the loop tension of the excited $\mathbb{Z}_2$ fluxes.

We also apply the method to the 3D hypernonagon lattice, on which the odd-length cycles allow a phase transition to a CSL. We find that the system exhibits a first-order transition from paramagnet to the CSL. At this transition, in addition to time-reversal symmetry, the lattice symmetry is broken by nonuniform spatial alignment of the $\mathbb{Z}_2$ fluxes, which has a different pattern from those found in the previous studies. Furthermore, our results indicate that the phase transition accompanies the topological change caused by proliferation of excited loops similar to other 3D cases. By variational calculations, we explore the ground-state phase diagram and find five distinct CSL phases, all of which possess nonuniform orderings of the $\mathbb{Z}_2$ fluxes.

Next, we develop a QMC technique applicable to the Kitaev models with non-Kitaev interactions and in a magnetic field. Our technique relies on the Hubbard-Stratonovich transformation to handle the interactions and the Popov-Fedotov transformation from quantum spins to complex fermions. The conventional QMC simulation based on these transformations is known to lead to severe negative sign problems. In order to alleviate this difficulty, we introduce the so-called asymptotic Lefschetz thimbles in the QMC simulation (ALT-QMC), in which the integration domain for the Hubbard-Stratonovich fields is shifted to appropriate manifolds in the complex space.

We test the ALT-QMC technique for the Kitaev model in a magnetic field. For a small cluster, by visualizing the asymptotic Lefschetz thimbles with the saddle points and zeros of the fermion determinant, and following the time evolutions of the QMC samples explicitly, we clarify how the ALT-QMC technique alleviates the negative sign problem. We extend this technique to larger clusters and demonstrate the potential of studying lower-T regions in a magnetic field compared to the conventional method.

To summarize, in this thesis, we developed numerical methods to study the finite-T properties of the Kitaev models and its extensions. First, we improved the QMC technique on the basis of the Majorana fermion representation by introducing a sophisticated update technique. We applied this method to the Kitaev models on the 3D hyperoctagon and hypernonagon lattices and revealed the nature of finite-T transitions from paramagnet to the QSL and CSL. Our results will stimulate further exploration of exotic finite-T transitions in other 3D Kitaev models. Next, we developed a QMC technique on the basis of the complex fermion representation by introducing the asymptotic Lefschetz thimbles. By testing the method for the 2D Kitaev model in a magnetic field, we demonstrated that it alleviates the negative sign problem. Our results open the possibility of exploration of the effects of non-Kitaev interactions and magnetic field.