Abstract

The quantum spin liquid (QSL) is an exotic quantum state in insulating magnets, in which long-range magnetic ordering is suppressed by strong quantum fluctuations even in the ground state. Despite the intensive researches for nearly half century, the identification of QSLs remains elusive so far. The main difficulty lies in the fact that the QSLs are not characterized by any conventional order parameter within the Landau-Ginzburg-Wilson theory. In the last decade, however, a breakthrough was brought by the seminal Kitaev model. The simple $S = 1/2$ model provides an exact QSL ground state even in two dimensions. Furthermore, the Kitaev model and its extensions have relevance to real materials with both strong electron correlation and spin-orbit coupling. The breakthrough has stimulated extensive search for the Kitaev QSLs from both experimental and theoretical points of view.

Although the Kitaev model is soluble in the ground state, no exact solution is available at finite temperature (T). Finite-T properties are important for the understanding of existing and forthcoming experiments and also the identification of QSLs in real materials. Recently, there has been substantial progress in the numerical study of finite-T properties of the Kitaev model. One of the remarkable findings is an exotic finite-T phase transition between QSL and paramagnet reported for an extension of the Kitaev model defined on a three-dimensional hyperhoneycomb lattice. This phase transition is not accompanied by any symmetry breaking, and can be explained by topological excitations specific to three-dimensional systems, namely, proliferation of loops composed of the emergent gauge fluxes. Although the Kitaev model can be extended to any tri-coordinate lattices, such an exotic phase transition has not been studied for other lattices thus far. It is interesting to investigate the thermodynamic properties of other three-dimensional Kitaev models for clarifying the universal aspects of the unconventional phase transition and exploring further exotic transitions.

In this thesis, we study finite-T behavior of the Kitaev model on another three-dimensional lattice, the hyperoctagon lattice, by using unbiased numerical simulations. In order to simulate sufficiently large systems beyond the previous study for the hyperhoneycomb case, we adopt a sophisticated update method based on the kernel polynomial expansion of Green functions in the quantum Monte Carlo

technique on the basis of a Majorana fermion representation. It enables us to perform the massively parallel simulation with the computational cost of $\mathcal{O}(N^2)$, whereas the conventional algorithm costs $\mathcal{O}(N^4)$, where N is the number of spins. Using this technique, we can reach up to $N = 2048$, much larger system sizes than the previous studies.

We find that the hyperoctagon model also shows a phase transition at finite T between the high-T paramagnet and the low-T QSL phase, similar to the hyperhoneycomb case. We discuss the nature of the phase transition from the unbiased numerical data for the specific heat, entropy, thermal average and fluctuations of the static gauge fluxes, and Wilson loop. We compare the results with those for the hyperhoneycomb case. We obtain the presice estimate of the critical temperature from the system-size extrapolations for two types of clusters with different boundary conditions. We find that the critical temperature is considerably lower than that in the hyperhoneycomb case, which is explained by the smaller flux gap in the hyperoctagon case. We also show that the low-T state below the critical temperature is likely consistent with the ground state deduced by a variational argument in the previous study. Finally, we discuss the phase transition in the anisotropic limit of the Kitaev exchange couplings, the so-called toric-code limit.