Density-matrix renormalization group study of quantum spin systems with Kitaev-type anisotropic interaction

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The proposal of the Kitaev model and its candidate material Na_2IrO_3 have introduced new playground of quantum spin systems. In this thesis, we theoretically study the effect of the Kitaev-type anisotropic interaction on quantum spin systems by using the unbiased numerical method, density-matirx renormalization group (DMRG) method. Especially, we focus on Na_2IrO_3 with the honeycomb lattice and $Ba_3IrTi_2O_9$ with the triangular lattice. The spin exchange interaction of these materials is dominated by the Kitaev interaction. We make clear the effect of the Kitaev interaction on quantum spin systems that is expected to lead to non-trivial phases.

We investigate the extended Kitaev-Heisenberg (KH) model as an effective spin model for Na_2IrO_3 that takes into account the Ir-Ir direct electron hoppings and trigonal distortion present in Na_2IrO_3. The KH model is too simple to explain zigzag antiferromagnetic (AFM) order that is observed in experiments. We find that the extended KH model naturally explains the zigzag AFM order. In order to obtain the zigzag AFM order, off-diagonal spin exchange interaction due to the trigonal distortion plays an important role. Other than the zigzag AFM phase, we also find the 120° AFM, FM, and two kinds of incommensurate phases next to the spin-liquid phase.

We further investigate the KH model on the triangular lattice that is expected to describe the physics of $Ba_3IrTi_2O_9$. By performing DMRG, we find the 120° AFM phase, Z_2-vortex crystal phase, dual Z_2-vortex crystal phase, nematic phase, Z_6 FM phase, and its dual phase, which is consistent with previous studies. The ground-state phase diagrams of these models on the honeycomb and triangular lattices are completely different.

In addition, we examine the entanglement entropy and entanglement spectrum of these models. Although the two quantities do not necessarily change at phase boundaries in general, the KH model on the triangular lattice shows the change at the boundaries. In contrast to the triangular lattice, the change of the distribution of the entanglement entropy and

entanglement spectrum of the extended KH model on the honeycomb lattice is obscure. However, we find that phase transitions between the Kitaev spin-liquid state and magnetically ordered states are well characterized by the entanglement spectrum due to its degenerate structure related to the exact-solvability of the Kitaev model.

The results obtained in this thesis show that the effect of the Kitaev interaction emerges in various non-trivial phases in quantum spin systems. This implies that our study on the Kitaev physics opens up a new field in quantum spin systems. Furthermore, our study contributes to the understanding of the physics of the materials with strong spin-orbit interaction, since the quantum spin systems with the Kitaev anisotropic interaction are expected to be relevant to iridate-oxide materials such as Na_2IrO_3 and $Ba_3IrTi_2O_9$.