Abstract

Since P. Anderson's proposal in 1973, the quantum spin liquid (QSL) has attracted much attention as an exotic quantum state of matter that does not show any symmetry breaking even at absolute zero temperature owing to strong quantum fluctuations. Further research related it to the topology and revealed the topological order and fractionalization into nonlocal quasiparticles. In 2006, A. Kitaev brought his honeycomb model with the QSL ground state to this field, now called the Kitaev model. This model is a two-dimensional spin-1/2 honeycomb model with bond-dependent anisotropic interactions. In the QSL state, the spin degree of freedom is fractionalized into itinerant Majorana fermions and localized static $\mathbb{Z}_2$ gauge fields, which comprise non-Abelian anyons under an external magnetic field. Although such anisotropic interactions appear to be difficult to realize in actual materials, in 2009, G. Jackeli and G. Khaliullin proposed that materials with edge-sharing octahedral lattice can generate them via the localized magnetic moments arising from spin-orbital entanglement. Following this mechanism, many candidate materials were proposed. Among them, a van der Waals material α-$RuCl_3$ has been intensively studied as a prime candidate. Notably, recent research revealed that it exhibits hallmarks of the Kitaev spin liquid as identified by several experimental techniques, such as Raman scattering, inelastic neutron scattering, and half-quantization of the thermal Hall conductivity. However, α-$RuCl_3$ shows a zigzag-type antiferromagnetic order at zero magnetic field, limiting further detailed studies and applications.

In this thesis, we propose the possibility of the Kitaev spin liquid at zero magnetic field by making van der Waals heterostructures of α-$RuCl_3$ and a ferromagnet CrX_3 (X=Cl and I). Using the *ab initio* calculations, we find that in the case of X=Cl the zigzag order is suppressed by the proximity effect of the ferromagnetic $CrCl_3$ layer, while the Kitaev interaction is still relevant in the α-$RuCl_3$ layer. Notably, the induced Ru moment is close to the value observed in the QSL of the bulk material under a magnetic field, signifying the realization of the QSL at zero magnetic field in the heterostructure. Furthermore, based on the *ab initio* results, we show that the effective pseudospin model retains dominant Kitaev-type anisotropic interactions in the α-$RuCl_3$ layer. In contrast, in the case of X=I, the system is on the verge of an insulator-metal transition by carrier doping through

interlayer hybridization. Our results indicate that van der Waals heterostructures provide a new platform for studying not only the magnetic but also the electronic properties of the Kitaev magnets.