# Abstract

Coupling between localized spins and itinerant electrons has been one of the major topics in condensed matter physics. In a spin-charge coupled system, the coupling between the localized moments and itinerant electrons often drives the magnetic and peculiar transport phenomena in these systems. When the electrons are coupled to localized moments on a frustrated lattice, the interplay between the spin-charge coupling and geometrical frustration is likely to induce novel magnetic and transport phenomena. Related to experimental studies on the metallic magnets with pyrochlore and triangular lattice structures, these effects have recently gained much interest in the field of strongly correlated electrons and statistical physics.

In this thesis, stimulated by these experiments, we theoretically investigate such possibility in Ising-spin Kondo lattice models. We studied the Kondo lattice models with localized Ising spins on frustrated lattices: triangular, kagome, and pyrochlore lattices. We analyzed thermodynamic properties of the models mainly by an unbiased Monte Carlo simulation which is free of any biased approximations. Combining this method with other approaches such as perturbation theories and mean-field approximations, we theoretically investigated electronic and magnetic properties of these models. The major results are as follows.

In the case of the triangular lattice, we investigated the emergence and stability of a peculiar magnetic state called partial disorder. We found that along with two-sublattice stripe order, three-sublattice ferrimagnetic order, and Kosterlitz-Thouless like state, a three-sublattice partial disorder is stabilized at a finite temperature region with electron density around 1/3 (two electrons per three sites). To the best of our knowledge, this is the first example of partial disorder in two dimensions. By calculating the electronic density of states for itinerant electrons using a mean-field type argument and Monte Carlo simulation, we concluded that the partial disorder is stabilized by the Slater mechanism, in which the magnetic super-structure gives rise to an energy gap in the electronic density of states. In addition, similar partially disordered state is also discovered in a kagome lattice model. These results imply that the stabilization of partially disordered states by itinerant electrons

is widely observed in the two-dimensional frustrated itinerant systems.

On the other hand, we discovered that the electronic structure exhibits a spin-polarized Dirac node at the Fermi level in the three-sublattice ferrimagnetically ordered phase found at electron density above 1/3 on the triangular lattice. By analyzing the low-energy effective Hamiltonian for itinerant electrons, we showed that it is essentially the same with that of graphene. This indicates that the peculiar electronic properties observed in graphene can be realized in magnetic oxides. Furthermore, from the viewpoint of industrial applications, the spin-polarized nature of Dirac electrons is expected to be useful for spintronics, e.g., as a spin-current generator or spin-transistor.

In the kagome lattice variant of the Ising-spin Kondo lattice model, we found that a peculiar ferrimagnetic state appears in a finite temperature region. In this state, all the triangles on the kagome lattice satisfy the two-up one-down local constraint, inducing a magnetic moment 1/3 of the fully saturated value. However, due to the geometrical structure of the lattice, the local constraint is insufficient for the spins to form a long-range order, leaving the system disordered. We call this phase a loop-liquid state, as it can be viewed as a collection of the up-spin loops with isolated down-spin sites. By the Monte Carlo simulation, we show that this model shows a rich phase diagram with various magnetic phases: ferromagnetic, partially ferromagnetic, $q = 0$ ferrimagnetic and $\sqrt{3} \times \sqrt{3}$ ferrimagnetic phases in addition to the loop-liquid state. We also show that, in the loop-liquid state, the optical conductivity shows a resonant peak corresponding to the formation of the loops.

We also considered a kagome model, in which the Ising spins are not collinear but aligned along the local noncoplanar axis, corresponding to an isolated $\langle 111 \rangle$ kagome plane of the pyrochlore spin-ice model. To investigate how the electronic state of itinerant electrons is affected by the local correlation in the localized spins, we first investigated the evolution of electronic state with respect to the magnetic moment perpendicular to the kagome plane by taking simple average over different spin configurations. As a consequence, we found that in the kagome-ice state, in which all the upward (downward) triangles retain two-in one-out (one-in two-out) spin configurations, an energy gap appears in the electronic density of states at the Fermi level for electron density 2/3. This is a peculiar insulating state without a magnetic long-range order. In this phase, associated with the energy gap formation, the Hall conductivity is quantized at a nonzero value. In addition, by using the Monte Carlo simulation, we confirmed that such a quantum anomalous Hall insulator is realized in applied magnetic field perpendicular to the plane.

In the last, we considered a pyrochlore model in which itinerant electrons are coupled with the spin-ice type Ising spins. We investigated the magnetic behavior of the Kondo lattice model in both the strong coupling limit and intermediate coupling case. The magnetic phase diagram in the weakto-intermediate coupling region of the spin-ice type Kondo lattice model is studied by using a Monte Carlo simulation using the polynomial expansion method. We mapped out the phase diagram for this model while varying electron density. As a result, we found a novel 32-sublattice magnetic phase with charge density wave along with other magnetic phases: ice-ferro, ice-($\pi$,0,0), and all-in/all-out ordered phases. By the analysis of the Ruderman-Kittel-Kasuya-Yosida interaction, we showed that the 32-sublattice order is driven by the effective third-neighbor interaction between the spins. An interesting feature of this phase is the controllability of charge density wave by magnetic field. By applying an external magnetic field along the $\langle 111 \rangle$ direction, we demonstrated that the system exhibits a transition to another 32-sublattice ordered phase, at which charge density wave pattern is switched to a different one.

On the other hand, in the strong coupling limit, we considered a spin-ice type double-exchange model with the NN antiferromagnetic superexchange interaction between the localized spins. By the polynomial expansion Monte Carlo method, we discovered that this model exhibits a peculiar phase with broken spatial inversion symmetry in an intermediate temperature region, in which the system remains magnetically disordered but four spins on each upward tetrahedron form an all-in/all-out type cluster. To address how this phase is realized, we developed a perturbation theory in the strong coupling limit which enabled us to construct an effective Ising-spin model. From the effective spin model, we revealed that the novel intermediate phase is stabilized by the emergent geometrical frustration induced by the second- and third-neighbor effective interactions. Also, from the analysis of the transport properties of the double-exchange model, we showed that this phase exhibits the spin Hall effect. The result is the first example of the spin Hall effect that takes place in the absence of the relativistic spin-orbit coupling.

The series of results indicate that, together with the geometrical structure of the lattices, effective long-range interactions induced by itinerant electrons give rise to qualitatively new magnetic behavior. In addition, the mechanism beyond simple exchange type interactions, such as the Slater mechanism, also plays a crucial role. Meanwhile, such novel magnetic states give rise to a number of peculiar properties in charge degrees of freedom, such as anomalous transport properties and charge density wave. The results we presented here will pave the way for further studies on the magnetic and electronic properties in the physics of frustrated spin-charge coupled systems. As the results shown here are numerically exact solutions, they will also provide reliable references for the studies on systems with quantum spins and other complex systems which are difficult to be treated in an unbiased manner.