博士論文(要約)

論文題目 Theoretical Study of Spin-Charge Coupled Systems on Frustrated Lattices
（フラストレート格子上のスピン電荷結合系に関する理論研究）

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Coupling between localized spins and itinerant electrons have been one of the major topics in condensed matter physics. In the past few decades, studies on the coupling have revealed that the electronic structure of the itinerant electrons are strongly modified by the coupling giving rise to peculiar properties such as colossal magneto-resistance and metal-insulator transitions. On the other hand, the itinerant electrons mediate effective spin-spin interaction between the localized spins, inducing unusual magnetic properties such as spin grass behavior. Furthermore, stimulated by recent experimental studies on metallic magnetic oxides, the studies on the spin-charge coupled systems have expanded to wider class of materials. One of such systems are magnetic compounds on frustrated lattices, for example, pyrochlore oxides and stacked triangular magnetic compounds such as delafossites.

In the pyrochlore lattice, in the classical limit, the localized Ising spin model with local [111] anisotropy on the anisotropy axis (spin-ice model) exhibit macroscopic degeneracy in the ground state when the nearest-neighbor (NN) interaction is ferromagnetic. Due to the macroscopic degeneracy, the system remains paramagnetic to absolute zero temperature. Also, the system become supersensitive to external stimuli and perturbations, which often give qualitative changes to the thermodynamic phase diagram. A similar situation is realized in the triangular magnets when the NN interaction is antiferromagnetic, inducing various non-trivial behaviors such as Kosterlitz-Thouless (KT) type transitions, and partial disorder in the stacked triangular magnets.

An interesting question is, that when these spins are coupled to itinerant electrons, how does the peculiar spin textures induced by the geometrical frustration affects electronic states of the itinerant electrons and, as the consequence, the transport properties. Recent numerical studies on the electronic states of Falikov-Kimball model with strong local correlation between the localized particles have shown that the local correlation induced by geometrical frustration gives significant effect on the electronic structure, such as absence of Anderson localization. These fact indicates that the itinerant electrons coupled to localized spins are likely to show qualitatively different behavior compared to the completely random case. Indeed, recent experiments on the frustrated metallic magnets are known to show various peculiar conduction properties. The local correlation induced by geometrical frustration is expected to take key roles in these phenomena.

On the other hand, magnetic behavior in these systems are also of great interest. In the frustrated systems, perturbation such as further neighbor interactions are known to induce qualitative changes in the magnetic phase diagram. Hence, the effective further neighbor interactions as well as non-perturbative effects such as Slater mechanism induced by itinerant electrons can be a source for inducing non trivial magnetic behavior in these magnets.

To address these questions, we studied Ising-spin Kondo lattice models on frustrated lattices; pyrochlore, kagome, and triangular lattices. By using an unbiased Monte Carlo (MC) simulations which is free of any biased approximations, we numerically analyzed the thermodynamic properties of the Kondo lattice models. Combining this method with other approaches such as perturbation theories and mean-field type approaches, we theoretically investigate magnetic and electronic properties of these models. The major conclusions are as follows.

Stimulated by the recent studies on a chromium delafossite, we investigated the emergence and stability of collinear Ising-spin Kondo lattice models on a triangular lattice. By using the MC simulation with numerical diagonalization, along with a KT-like state, two-sublattice stripe order, and three-sublattice ferrimagnetic order, we confirmed that a three-sublattice partial disorder is stabilized at a finite temperature region with electron density around 2/3. In the previous studies on partial disorder, it have been shown to be fragile against thermal fluctuations, and our result presented here is the first example of partial disorder in two-dimensions. To further investigate the stabilization mechanism of the partial disorder, we calculated the electronic density of states (DOS) for itinerant electrons using mean-field type argument and MC simulation. From these results, we confirmed that the partial-disorder is stabilized by the so called Slater mechanism, which the magnetic super-structure gives rise to energy gap in the electronic DOS. We also conducted the MC simulation in a kagome lattice Kondo lattice model, and confirmed that the partial-disorder is also present in this model. These results implies that the stabilization of partially disordered states by itinerant electrons are widely observed in the two-dimensional frustrated lattices.

On the other hand, in the three-sublattice ferrimagnetic order at electron density above 2/3, we confirmed that the itinerant electrons in this phase exhibits a spin-polarized Dirac node at the Fermi level. By analyzing the low energy Hamiltonian for itinerant electrons, we confirmed that the Hamiltonian 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 view point of industrial application, the spin-polarized nature of carrier is expected to be useful as a spin-current generator, either by filtering out the electrons with opposite spins, or by a spin-transistor.

In the kagome lattice variant of the Ising-spin Kondo lattice model, by using the same MC method used in triangular lattice, we confirmed that a peculiar ferrimagnetic state appears in the finite temperature region. We call this phase as loop liquid state. In the loop-liquid state, all the triangles in the kagome lattice satisfies two-up one-down local constraint, inducing magnetic moment 1/3 of the ferromagnetic order. 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. An interesting behavior of this phase is the critical region between the ferromagnetic state, which resides in the vicinity of this phase. From the symmetry consideration, the ferromagnetic order and loop-liquid state shares same properties; the mirror symmetry of spins along xy plane is broken due to the finite magnetic moments, but the translational symmetry and rotational symmetry of the lattice is preserved as the loop-liquid state shows no magnetic long-range order. As the consequence, the two phases are connected by a crossover across a partially ferromagnetic state which is an intermediate state between the loop-liquid state and ferromagnetic order. Another interesting behavior of this phase is observed in the conduction properties. By using the Kubo formula, we calculated optical conductivity in the loop-liquid state. The result shows a peak in the spectra at a frequency which roughly corresponds to the hopping. This is the sign of six-site loops which is present in the loop-liquid state, which can be an experimental signature for the loop-liquid state.

In the later half, we considered another class of Ising-spin systems, the ice-type models. In the ice-type models, different anisotropy axes are defined for each sublattices; the axes are defined along local [111] axis for the pyrochlore lattice, i.e., radially from the center of the tetrahedra that the spin belongs to. In these models, the spins become "frustrated" when the NN interaction is ferromagnetic, in contrast to the antiferromagnetic case for the collinear spin models.

In the study of ice-type models, we firstly considered a kagome-ice model, which corresponds to the isolated <111> kagome plane of the spin-ice model. To investigate how the electronic states of the itinerant electrons are affected by the local correlation in the localized spins, we first divided the spin configurations of the frustrated ground states into submanifolds by the magnetic moment perpendicular to the kagome plane. The evolution of electronic state with respect to the magnetic moment is investigated by taking simple average over different spin configurations in each manifold. As the consequence, we confirmed that in the kagome-ice state, which all the up-ward (down-ward) triangles retains two-in one-out (one-in two-out) spin configurations, the DOS for itinerant electrons forms energy gap at the Fermi level for electron density 2/3. This is a peculiar insulating state without a magnetic long-range order. In addition, by using the MC simulation, we confirmed that such insulating state is realized under ambient magnetic field perpendicular to the plane.

In the next, we considered the spin-ice model on a pyrochlore lattice to investigate how the magnetic behavior of the Kondo lattice model is affected by the spin-charge coupling by considering both the strong coupling limit and moderately coupled case. In the strongly coupled limit, we considered a spin-ice type double-exchange model with NN antiferromagnetic superexchange interaction between the localized spins. By the MC simulation using polynomial expansion method, we indicated that this model exhibits peculiar intermediate phase with broken spatial-inversion symmetry, which the four spins on the upward tetrahedra forms an all-in/all-out type clusters that are fluctuating thermally. To address how this phase is realized in this model, we developed a perturbation theory in the strong coupling limit which enabled us to construct an effective Ising-spin model. From the construction of the model and analysis using classical MC simulation, we confirmed that the novel intermediate phase is stabilized by the emergent geometrical frustration induced by the effective exchange interaction between the second and third NN localized spins. Also, from the analysis on the conduction properties of this model, we confirmed that this phase exhibit spin Hall effect. The result is a first example of spin Hall effect that takes place in the absence of spin-orbit coupling.

We also studied the magnetic phase diagram in the weak coupling region of the model by using the polynomial expansion MC method. By the MC simulation, we mapped out the phase diagram for this model with varying electron density. In the phase diagram, we confirmed a novel 32-sublattice magnetic phase with charge density wave (CDW) along with other magnetic phases: ice-ferro, ice-(π,0,0), and all-in/all-out order. By the analysis on the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction, we confirmed that the 32-sublattice order emerges in the region where NN interaction become less dominant due to the nodal structure of the RKKY interaction. Indeed, the magnetic configuration shows no favorable magnetic correlation in the tetrahedra. Instead, it shows antiferromagnetic correlation between the third neighbor spins along the chains. An interesting feature of this magnetic phase is the controllability of the CDW. By applying external magnetic field along <111> direction, we confirmed that there is another 32-sublattice order in the intermediate region which accompanies different type of CDW.

To summarize, by using the MC simulation, we studied the magnetic and electronic behavior of Ising-spin Kondo lattice models on frustrated lattices. We have shown that these models show varieties of novel magnetic states and associated exotic transport properties. In the triangular lattice model, we have shown first example of partially-disordered states in two-dimension and also presence of Dirac half-metal state. On the other hand, in the kagome lattice model, we show emergence of partial-disorder and loop-liquid state. In the ice-type variant of the kagome lattice model, we have shown that the local correlation gives rise to energy gap in the electronic DOS.

In the last, we investigated the phase diagram of spin-ice type model on a pyrochlore lattice, and shown that the model exhibits rich phase diagram. In the strong coupling limit, we have shown that an intermediate state with broken-spatial inversion symmetry. We also confirmed that the intermediate phase shows spin Hall effect in absence of spin-orbit coupling. On the other hand, in the weak coupling region, we indicated emergence of a novel 32-sublattice order which accompanies charge modulation.