論 文 の 内 容 の 要 旨

論文題目: **Topological spin textures emergent from spin-charge coupling**
(スピン電荷結合が創発するトポロジカルなスピンテクスチャ)

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Topological aspects of the electronic states in solids have been one of the central issues in modern condensed matter physics. The research field was initiated by the discovery of the relation between the quantum Hall effect and a topological invariant called the first Chern number, which has continuously stimulated the growing vast area of the topological phases of matter. One of the recent examples is a topologically-nontrivial spin texture with noncollinear or noncoplanar spin configuration. Such a swirling spin texture leads to an emergent electromagnetic field for itinerant electrons, which may result in unconventional electronic states and transport phenomena, e.g., the Chern insulator, Dirac and Weyl semimetals, the spin Hall effect, and the topological Hall effect. The magnetic skyrmion is a typical example of such swirling spin textures, which has been attracting growing interest from not only fundamental physics but also potential applications to electronic devises.

Several different mechanisms have been proposed for such topologically-nontrivial spin textures, such as the spin-orbit coupling (Dzyaloshinskii–Moriya interaction) and the long-range dipolar interaction. Among them, the multiple-spin interactions are intriguing because they can induce swirling spin textures with rather small spatial sizes, which lead to larger emergent electromagnetic fields. Interestingly, the multiple-spin interactions are naturally generated by spin-charge coupling as effective spin interactions mediated by itinerant electrons. In most of the previous studies, however, such multiple-spin interactions have been neglected and effective spin-only models with minimal pairwise interactions called the Ruderman-Kittel-Kasuya-Yosida (RKKY) interactions, were studied. Nevertheless, the multiple-spin interactions often play an important role in the spin-charge coupled systems; for instance, the previous studies on a minimal Kondo lattice model revealed that the four-spin interactions can induce noncoplanar spin ordering under particular conditions. Although they point to the possibility of more interesting magnetic and electronic phenomena in itinerant magnets, such investigations have not been fully done thus far. The theoretical difficulty lies in the following two points. One is that the spin-charge coupled systems are more complicated than the spin-only models due to the additional charge degree of freedom. To discuss the keen competition between different magnetic states and the resultant electronic states, it is necessary to seriously treat the effect of spin-charge coupling without biased approximations. The other difficulty is that it is often desired to treat large system sizes in real space for considering spatially extended magnetic objects. Also, it is crucial to include spatial fluctuations. These are theoretical challenges, for which the conventional theories and numerical techniques are insufficient.

In this thesis, we explore the possibility of topologically-nontrivial spin textures and itinerant electronic states emergent from the interplay between spin and charge degrees of freedom. Specifically, we consider a minimal model for itinerant magnets, the Kondo lattice model with classical localized spins, and take into account both spin and charge degrees of freedom on an equal footing. To solve the difficulties mentioned above and go beyond the previous studies, we adopt a recently-developed numerical technique. This method is based on the kernel polynomial expansion (KPM) of the density of states for itinerant electrons and the Langevin dynamics (LD) for localized spins, which we call KPM-LD method. To further increase the efficiency, we modify the method by introducing the stochastic Landau-Lifshitz equation for the LD. We also developed a new optimization technique by introducing a local heating, which we call the simulated floating zone technique. We have performed the KPM-LD simulation by parallel processing on General-Purpose computing on Graphics Processing Units (GPGPU).

The first result shown in the thesis is the discovery of a new noncoplanar spin state as the generic ground state in a wide range of the electron filling in the weak spin-charge coupling regime. The spin pattern is characterized by two independent wave numbers, namely, a double-Q state. Interestingly, the noncoplanar spin structure comprises a vortex-antivortex crystal accompanied by the stripe of spin scalar chirality, the triple-product of neighboring three spins. Owing to an emergent magnetic field induced by the spin scalar chirality through the spin Berry phase mechanism, we find that a persistent electric current flows along the chiral stripes in an alternative direction. The results are found by the KPM-LD simulation for the Kondo lattice model on a square lattice, and later, confirmed by variational calculations based on the variational states that we construct from the numerical results. We also clarify the stabilization mechanism of the vortex crystals in the following two ways. Firstly, by a perturbation expansion in terms of the spin-charge coupling, we show that fourth-order terms (effective four-spin interactions) play an essential role in lowering the energy for the noncoplanar double-Q state compared to that for a single-Q helical state expected from the second-order RKKY interactions. Secondly, we explicitly evaluate the energy gain of the vortex crystals by considering the partial-gap formation of the Fermi surface. Our results indicate that single-Q helical states always have the instability toward the double-Q vortex crystals. The stabilization mechanism is generic irrespective of the electron filling and lattice structures. Indeed, we confirm that a similar vortex crystal is stabilized on a triangular lattice as well.

Next, we investigate the possibility of skyrmion crystals, which are usually characterized by three wave numbers (triple-Q states), stabilized by the spin-charge coupling. For this purpose, we consider the Kondo lattice model on a triangular lattice, as the hexagonal lattice symmetry allows three independent wave numbers for ordering. Performing both the KPM-LD simulation and variational calculations for a slightly larger spin-charge coupling than that for the vortex crystals above, we discover skyrmion crystals with an unusually high topological number n_{sk}=2 as a new ground state of itinerant magnets in a wide range of the electron filling. This is, to our knowledge, the first example of thermodynamically-stable magnetic skyrmion crystals with the high n_{sk} at zero magnetic field. More interestingly, we show that the system exhibits unique successive transitions with changing n_{sk} from two to one, and to zero in applied magnetic field. These transitions are accompanied by the switching of itinerant electron textures, such as circular currents and spin-charge density waves. We also find that the skyrmion size can be controlled by the electron filling and band dispersion.

The two discoveries urge the reconsideration of the phase diagram of the Kondo lattice model with classical localized spins in the weak spin-charge coupling region. In the conventional RKKY theory, it was believed that the model exhibits a single-Q helical order whose wave number depends on the electron filling and band structure. Some previous studies revealed noncoplanar orderings may occur at particular fillings where the Fermi surface has a special connection by the ordering vectors. Our results, however, completely renew the phase diagram: in the weak-coupling limit, the single-Q helical order is replaced by a noncoplanar double-Q order with a vortex crystal not only at the particular fillings but also for generic filling. Furthermore, in the region with a slightly larger spin-charge coupling, the double-Q state turns into a triple-Q skyrmion crystal with a high topological number n_{sk}=2. We note that the skyrmion state is a generalization of the noncoplanar ordered states found in the previous studies. Thus, our new findings provide a new generic phase diagram of itinerant magnets with weak spin-charge coupling.

Besides the stable ground states, we also study the nonequilibrium states in itinerant magnets, with focusing on the formation of magnetic domains. We perform the large-scale KPM-LD simulation by a sudden quench from the high-temperature limit to zero temperature. From the comparative study for different lattice structures and different magnetic orders, we clarify a microscopic mechanism of the shape of magnetic domains in the spin-charge coupled systems. We find that the directional preference of magnetic domain walls is rationalized by the wave-number dependence of the bare susceptibility, which is a dimensionless measure of the effective pairwise RKKY interaction. We also discuss the width of magnetic domain walls from the viewpoint of the RKKY interaction as well as the electronic state. In the case of the domain walls for noncoplanar spin states, we demonstrate that the chiral edge electric current is induced along the domain walls according to the Berry curvature in the band structure.

We also develop a new optimization technique to efficiently obtain the thermal equilibrium state by avoiding the freezing in a multiple-domain state. In our method, the system is heated up locally, and the heated region is steadily shifted, similar to the floating zone method for growing a single crystal with less lattice defect and impurity in experiment. Hence, we call the method the simulated floating zone method. Applying the technique in the KPM-LD simulation, we demonstrate that the optimization is substantially accelerated and the freezing problems are avoided. We also clarify that the efficiency is maximized when the local heating temperature is tuned to be comparable to the characteristic energy scale of the ordered state. The algorithm is very generic and applicable to a wide range of systems in any spatial dimensions.

The outcomes of this thesis will bring about a great impact on many fields from fundamental studies on itinerant magnets to applications in electronics and spintronics. First of all, our findings of new vortex crystals and skyrmion crystals with peculiar itinerant electronic textures will provide useful reference for understanding and controlling magnetic and itinerant electronic properties of itinerant magnets. Especially, our discovery of skyrmion crystals with an unusual high n_{sk} possessing the flexibility in n_{sk}, helicity, and size may provide a new design principle of magnetic skyrmions. Moreover, these discoveries renew the phase diagram of the Kondo lattice model in which the helical state was believed to realize at generic electron filling. Our finding of the directional preference of the domain walls may provide a deeper insight into the domain wall formation observed in several itinerant magnets such as pyrocholore oxides. Last but not least, our proposal of the simulated floating zone method will be widely used in similar optimization problems.