Abstract

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 such as skyrmion. Such a topologically-nontrivial spin texture may lead to an emergent electromagnetic field for itinerant electrons, which may result in unconventional transport phenomena, such as the topological Hall effect.

Among several different mechanisms for such topologically-nontrivial spin textures, multiple-spin interactions are intriguing because they can induce swirling spin textures in atomic scale, which lead to huge emergent electromagnetic fields. Interestingly, the multiple-spin interactions are naturally generated by spin-charge coupling as effective spin interactions mediated by itinerant electrons. Recently, the previous theoretical studies on itinerant magnets revealed that the four-spin interactions can induce noncollinear or noncoplanar spin orderings under special conditions where the ordering vectors have particular commensurate values. Although these results suggest the further possibility of more interesting magnetic and electronic phenomena in generic cases, it has not been fully investigated thus far mainly due to the following two reasons. One is that simple helical states have been believed to realize by the pairwise Ruderman-Kittel-Kasuya-Yosida (RKKY) interactions, except for the special conditions mentioned above. The other reason is that huge computational costs are required for the numerical analysis to treat the interplay between spin and charge degrees of freedom seriously for generic cases.

In this thesis, we explore the further 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 numerical difficulty mentioned above, we adopt a recently-developed numerical technique with its modification. This algorithm is based on the kernel polynomial method (KPM) for itinerant electrons and the Langevin dynamics (LD) for localized spins, which we call the KPM-LD method. We have performed the KPM-LD simulation by parallel processing on General-Purpose computing on Graphics Processing Units (GPGPU) up to the system size with 10^4-10^5 sites.

We discover two novel ground states in the Kondo lattice model at generic elec-

tron fillings in the weak spin-charge coupling region. One is the noncoplanar vortex crystal (VC) characterized by two ordering vectors that is stabilized in the weak limit of the spin-charge coupling. The VC has a spin density wave along one of the ordering vectors and a stripe of spin scalar chirality, a triple product of neighboring spins, along the other ordering vector. We find that the effective four-spin interactions play an important role in stabilizing the VC, and the mechanism is valid for generic electron fillings on generic lattices. In the VC, we show that alternative persistent current flows inside the bulk due to the emergent magnetic field associated with the stripes of spin scalar chirality.

The other novel state is the skyrmion crystal (SkX) with an unusually high topological number of two on a triangular lattice at zero magnetic field. This state appears for the slightly stronger spin-charge coupling than that for the VC. It is worth noting that it does not require either the DM interactions or external magnetic fields unlike the conventional SkXs. Furthermore, this state is the first example of a stable high-topological-number skyrmion. We also find that an external magnetic field induces successive transitions of topological numbers: from two to one, and to zero. Furthermore, we show the controllability of the period of SkXs by the electron filling and band dispersion.

We also study nonequilibrium phenomena in itinerant magnets, with focusing on the formation of magnetic domains in the Kondo lattice model. We clarify that the directional preference of magnetic domain walls (DWs) is predominantly determined by the electronic structure of itinerant electrons through the wave-number dependence around the peaks in the bare susceptibility.

Our results totally renew the phase diagram of the Kondo lattice model with classical localized spins in the weak coupling regime. This opens the great possibility for exotic electronic textures in itinerant magnets. The stabilization mechanisms emergent from the spin-charge coupling shown in our results may provide a deep insight of the exotic magnetic ordering observed in real materials. Our analysis on DWs provides a fundamental mechanism of the directional preference of magnetic domain walls in itinerant magnets which may be helpful for application to magnetic devices.