Theoretical Study of Novel Magnetism and Electronic States in Spin-Charge-Orbital Coupled Systems

その他のタイトル	スピン・電荷・軌道結合系における新奇な磁性と電子状態の理論的研究
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論 文 の 内 容 の 要 旨

論文題目　Theoretical Study of Novel Magnetism and Electronic States in Spin-Charge-Orbital Coupled Systems
（スピン・電荷・軌道結合系における新奇な磁性と電子状態の理論的研究）

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Interplay between spin and charge degrees of freedom in electrons has drawn considerable interest as one of the major topics in condensed matter physics. It has long been studied in a wide range of viewpoints, from a fundamental mechanism of magnetic ordering to application to electronic devices. On the other hand, the orbital and lattice degrees of freedom have also been extensively studied as it gives rise to fascinating phenomena, such as a colossal magnetoresistive effect, multiferroics, and a new type of Mott insulator stabilized by the spin-orbit coupling. Such interplay between multiple degrees of freedom in electrons has brought new concepts: exotic magnetic orders, anomalous transport phenomena, and colossal responses to external fields. These new concepts will be useful for designing and engineering exotic orders, which are important for applications. However, the microscopic understanding has not been fully obtained because it is difficult to deal with many ingredients in the problems, such as competition and cooperation between electron degrees of freedom, quantum and thermal fluctuations, and geometrical lattice structures. In order to explore further new concepts and provide deeper understanding of their microscopic origins, it is necessary to construct simple models describing the essential aspects of each phenomenon and carry out systematic and comprehensive analyses of the models.

The objective of the present thesis is to theoretically investigate new types of magnetic ordering brought by the interplay between multiple degrees of freedom in itinerant electron systems. We aim to clarify their origins from the microscopic viewpoints and their effects on electronic structure, transport properties, and magnetoelectric effects. For these purposes, we study the essential and universal aspects of such peculiar magnetism and electronic properties in several fundamental models for itinerant electrons, such as the multi-orbital Hubbard model, periodic Anderson model, Kondo lattice model, and their

extensions. We examined physical properties in the ground state as well as at finite temperatures of the models by using analytical and numerical methods in a complementary way, such as perturbation theory, variational calculation, mean-field approximation, and Monte Carlo simulation. We mainly discussed three exotic magnetic orders: toroidal order in spin-charge-orbital coupled systems, partial disorder in the systems with the hybridization between itinerant and localized electrons, and multiple-Q orders with noncollinear and noncoplanar spin textures in spin-charge coupled systems.

First, we investigated the emergence of a toroidal ordered state in metals and its influence on the electronic and transport properties. The toroidal order, which is an alignment of toroidal moments defined by a vector product of magnetization and electric polarization, has recently attracted interest in multiferroic insulating materials. We showed that such an exotic order is realized even in metallic systems on lattice structures where the spatial-inversion symmetry (parity) is preserved globally but broken intrinsically at each magnetic site. Considering an effective Hubbard-type model with a site-dependent antisymmetric spin-orbit coupling on a stacked honeycomb lattice, we clarified that a ferroic ordering of microscopic toroidal moments modulates the band dispersions with shifting the band bottom. We also found that the toroidal magnetic order shows the highly anisotropic Hall effect and two different types of magnetoelectric effects. These anomalous transport properties suggest that the toroidal magnetic order induces an intrinsic Hall response even without an external magnetic field. Furthermore, we showed that the spontaneous toroidal magnetic order is indeed stabilized in the effective model by the mean-field calculations. We also clarified the temperature dependence of the anomalous magnetoelectric responses. We discuss our results for a candidate material and how the toroidal order in metals is detected and controlled experimentally.

We further investigated the effect of the local parity breaking, with heavy-fermion systems in mind. We here examined the simplest case with local parity breaking: a quasi-one-dimensional system composed of zig-zag chains. We focused on an antiferromagnetic order, which is considered as an odd-parity multipole order composed of toroidal and quadrupole components. Starting from the periodic Anderson model with the antisymmetric spin-orbit coupling between itinerant and localized electrons, we derived a low-energy effective model with the antisymmetric exchange coupling between itinerant electrons and localized spins. We found that the effective antisymmetric exchange coupling favors the staggered antiferromagnetic order on zig-zag chains. We showed that such antiferromagnetic order exhibits the band deformation and magnetoelectric effect due to the active toroidal component. Moreover, we clarified that the antiferromagnetic order is realized at and near half filling in the ground state by variational calculations and at finite temperatures by Monte Carlo simulation. These results suggest that the odd-parity multipole order will be widely observed in heavy-fermion systems without local inversion symmetry.

We also proposed a further interesting situation related to the local parity breaking, which is brought by strong electron correlations in spin-charge-orbital coupled systems. In such situation, a spontaneous electronic order accompanies generally a breaking of the global inversion symmetry, which gives rise to intriguing noncentrosymmetric physics, such as new types of band modulations and magnetoelectric effects, depending on its order parameter. Considering a minimal two-orbital model on a honeycomb lattice, we performed the complete analysis of the symmetry of possible spin, charge, and orbital orders and the mean-field analysis of their competition. We found that the system at 1/4 electron filling exhibits an interesting spin-orbital ordered state showing two different types of magnetoelectric effects. We also found a charge-ordered state with the antisymmetric spin splitting at different valleys in the band structure, and a paramagnetic insulating state showing the quantum spin Hall effect. These results reveal that the interplay between electron correlations, the spin-orbit coupling, and proper lattice structures with the local parity breaking leads to new fundamental physics in the spin-charge-orbital coupled systems. The resultant electronic structure and magnetoelectric responses by spontaneous electronic orders provide promising playgrounds in the local parity breaking.

Next, we investigated heavy-fermion physics on geometrically frustrated lattices. We focused on the possibility to have a peculiar partial disorder, i.e., coexistence of magnetic order and nonmagnetic sites. Such partial disorder was observed in several rare-earth compounds with frustrated lattice structures, but the detailed nature of the partial disorder was not clarified yet. To clarify the nature and mechanism of partial disorder, we studied partial disordered states in the periodic Anderson model on the triangular lattice. We found that, by the Hartree-Fock approximation, three-sublattice partial disordered states are stabilized in the ground state at and near commensurate fillings. Furthermore, we analyzed these states in detail by using the dynamical mean field theory. Comparing the results with those by the mean-field approximation, we elucidate the effect of electron correlations and quantum/thermal fluctuations. Our results provide deeper understanding of the frustration-induced phenomena in heavy-fermion systems.

Finally, we discussed noncollinear and noncoplanar magnetic orders characterized by multiple-Q wave vectors appearing in spin-charge coupled systems. While they have been found in itinerant electron systems on a wide range of lattice structures: square, triangular, simple cubic, and face-centered-cubic lattices, unified understanding of their stabilization mechanism has not been obtained. We here clarified a general mechanism of the multiple-Q instabilities in itinerant magnets, originating from a simple topology of the Fermi surface: (d-2)-dimensional connections of the Fermi surfaces in the extended Brillouin zone (d is the system dimension). This mechianism is distinct from the perfect nesting that corresponds to a (d-1)-dimensional connection, and the spin-orbit coupling, which is relevant in multiferroic materials and skyrmion crystals. The new universal mechanism was obtained by the detailed analysis of the fourth-order perturbation in term of the spin-charge coupling. Our study reveals "hidden" instabilities of the Fermi surfaces to noncollinear and noncoplanar magnetic orders. In addition, it is expected that the mechanism will be applicable to multi-orbital/sublattice systems, possibly leading to multiple-Q spin-orbital orders and multiple-Q superconducting states.

As a representative example of such multiple-Q states, we studied a triple-Q state with noncoplanar spin texture on the simple cubic lattice in detail. We showed that the triple-Q magnetic order induces the three-dimensional massless Dirac electrons on the cubic lattice, which leads to the emergence of a pair of Weyl electronic states in applied magnetic field. Furthermore, we demonstrated that the triple-Q magnetic order is indeed stabilized in the Kondo lattice model and the periodic Anderson model. We found that the system exhibits gapless surface states, which do not have ordinary closed Fermi surfaces but have the Fermi "arcs" connecting the bulk Dirac points. We also showed that the triple-Q ordered state turns into a topological insulator under appropriate perturbations. This result sheds new light on the topological aspect of the multiple-Q states.

We also systematically explored charge-ordered states on the cubic lattice in the periodic Anderson model with focusing on competition and cooperation between charge and magnetic orders. By examining the ground-state phase diagram, we found that the model exhibits three different charge-ordered states at 3/2 filling. Despite the absence of apparent geometrical frustration in the cubic lattice, one of the charge-ordered states shows a noncoplanar triple-Q magnetic order. The origin is likely to be the emergent geometrical frustration induced by charge order. This peculiar charge-ordered state is identified for the first time, to our knowledge.

The results in this thesis unveiled novel orders, which exhibit peculiar electronic structure, transport, and magnetoelectric effects, as a consequence of the interplay between spin, charge, orbital, and lattice degrees of freedom. The stabilization mechanism that we presented will give a guide to engineering such exotic orders and associated anomalous electronic properties in real compounds. Moreover, our present analysis will provide useful reference for understanding the physics in itinerant magnets, which has further potential for novel transport and magnetoelectric properties useful in applications in electronics and spintronics.