博士論文 (要約)

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)

速水　賢

The interplay between spin, charge, and orbital degrees of freedom in electrons in solids brings about rich physics. It has long been studied in a wide range of viewpoints, from a fundamental mechanism of electronic ordering to application to electronic devices. From such studies, many new concepts have been brought about, such as exotic magnetic orders, anomalous transport phenomena, and colossal responses to external fields.

The objective of this thesis is to theoretically investigate new types of magnetism and electronic states 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 structures, 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, dynamical mean-field theory, and Monte Carlo simulation. We mainly discussed novel magnetic and electronic orders in three systems: spin-charge-orbital coupled systems with the antisymmetric spin-orbit coupling, heavy-fermion systems on geometrically-frustrated lattices, and 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 found that the toroidal ordered state exhibits the highly anisotropic Hall effect and two different types of magnetoelectric effects. From these results, we proposed that the toroidal magnetic order induces an intrinsic Hall response even without an external magnetic field. Furthermore, we showed that, by mean-field calculations, the spontaneous toroidal magnetic order is indeed stabilized in an effective model for a heavy-fermion compound, UNi_4B.

We further investigated the effect of the local parity breaking, with heavy-fermion systems in mind. We here examined a prototype: 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 Kondo-type low-energy effective model with the antisymmetric exchange coupling between itinerant electrons and localized spins. We showed that the model indeed exhibits the multipole order at and near half filling in the ground state by variational calculations and simulated annealing, and also 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. Specifically, we considered a spontaneous electronic order with breaking the global inversion symmetry, which gives rise to intriguing noncentrosymmetric physics. Considering a minimal two-orbital Hubbard 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 composite ordered state showing two different types of magnetoelectric effects. We also found several insulating phases, such as 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. We have also examined an extension to a three-orbital model, bearing the relation to MX_2 in mind. 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.

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. We found that, by the Hartree-Fock approximation for the periodic Anderson model on the triangular lattice, three-sublattice partial disordered states are stabilized in the ground state at and near commensurate fillings. We also examined the effect of the spin anisotropy, external magnetic field, and carrier doping on the partially disordered states. Furthermore, we further analyzed the effect of quantum fluctuations on these states by using the dynamical mean-field theory. 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 system. While they have even 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). The results reveal "hidden" instabilities of the Fermi surfaces to noncollinear and noncoplanar magnetic orders. In addition, it is expected that the new universal 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 states 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 state in applied magnetic field, a topological insulator under appropriate perturbations, and peculiar surface states with Fermi "arcs" connecting the bulk Dirac points. Furthermore, we demonstrated that the triple-Q magnetic order is indeed stabilized in the Kondo lattice model and the periodic Anderson model. The results shed 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 of the physics in itinerant magnets, which has further potential for novel transport and magnetoelectric properties useful in applications in electronic and spintronics.