博士論文 (要約)

Numerical studies by dynamical mean-field theory
on magnetism and superconductivity
in strongly correlated electron systems

(動的平均場理論を用いた強相関電子系における
磁性と超伝導の数値的研究)

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Various phenomena appear in strongly correlated electron systems. Among them, extensive effort has been devoted to the magnetism and high-T_c superconductivity for decades but there are still many unsolved problems. In particular, it is important for the progress both in fundamental physics and industry applications to elucidate how we are able to control their properties such as the transition temperatures of the magnets and superconductors. In this thesis, we elucidate the role of the electron correlation for such materials, and give understandings of unsolved problems.

To attack this challenge, we need a method which is able to sufficiently take the strong correlation effect into account and has a flexible framework to describe magnetic ordered and superconducting states. For this reason, we employ the dynamical mean-field theory (DMFT) or its extensions to multi-site and multi-orbital cases, which are able to include the local or short-range correlation exactly to describe the magnetism and high-T_c superconductivity.

The first target of this thesis is the ferromagnetism. The performance of magnets is determined by the magnitude of the magnetization, Curie temperature and magnetic anisotropy. Especially, while the magnetic anisotropy originating from the spin-orbit coupling (SOC) is a crucial factor, the effect of the electron correlations on it is still unclear. One of our purposes is to understand this problem through a study on an itinerant ferromagnet $SrRuO_3$ (SRO) whose Curie temperature is 137-165 K. SRO has a strong SOC and electronic correlations because the bandwidth is comparable to the on-site Coulomb interaction. Although SRO has the magnetic anisotropy, its easy axis (EA) is sensitive to the condition of the sample preparations. Several kinds of the EA, mainly [110] and [001] directions ([100], [010] and [001] are parallel to three nearest-neighbor Ru-Ru bonding directions), have been reported for the thin films and single crystals, respectively. Other experiments found that the EA changes from [001] to [101] with increasing temperature. We here propose the

electron correlation effect as a key to understand this controversial EA issue. Thin film samples, e.g., on $SrTiO_3$ substrates are expected to have slightly larger correlations than that in single crystals due to a larger orthorhombic distortion, which reduces the bandwidth. We confirm this tendency by comparing experiments.

In order to study the EA problem, we employ the generalized gradient approximation and the density functional theory to derive a tight-binding Hamiltonian consisting of three t_{2g} orbitals of Ru site, including the SOC term. In addition, we adopt a pseudo-cubic lattice while SRO has an orthorhombic structure. We use this procedure to focus on the correlation effect apart from the contribution from the ligand field effect on the EA problem. Similarly, we use the SU(2)-symmetric Slator-Kanamori interaction. Moreover, we scale the one-body terms to study sample dependences in terms of the correlation strength. Note that the magnetic anisotropy arises from the SOC term here. We compare the free energy for [001] and [101] EAs within the DMFT. As a result, when the bandwidth is wider (narrower), [001] ([101]) tends to be the EA. Furthermore, we found an EA transition from [001] to [101] at 22 K for the intermediate bandwidth. These results are consistent with the experiments because thin film (single crystal) samples should have stronger (weaker) correlations and correspond to the narrower (wider) bandwidth case. The temperature dependence of the EA is also qualitatively explained by the EA transition at 22 K. From the above results, we conclude that the sensitivity of the SRO's EA originates from the electron correlation. This is a significant result because it reveals that we need to include the correlation effects for the reliable evaluations of the magnetic anisotropy.

We also challenge to understand other unsolved problems of SRO, which include anomalous dips or peaks of the magnetoresistance, $d\rho/dT$ and dM/dT at 25-50 K, where ρ and M are the dc resistivity and the magnetization, respectively. For these issues, we again apply the DMFT to find a crossover from weakly to strongly spin-

fluctuating metal at 56 K. The enhanced spin fluctuation is induced and accompanied by each anomaly and its temperature dependence is consistent with the experiments. Our results support that the high-temperature region above the crossover temperature induces a bad-metallic behavior associated with the enhanced spin fluctuations.

An explanation of the non-Fermi liquid behavior of the optical conductivity is also attempted. Experiments have reported the optical conductivity of SRO in the infrared region has an anomalous decay $O(1/\omega^{0.5})$ which is slower than $O(1/\omega^2)$ as predicted in the Fermi liquid. We found that the density of states may play a significant role to demonstrate such an apparent decay and the realistic value of the optical conductivity observed in experiments. In addition, other mysteries of the optical conductivity include a suppression at ω=0 and a peak structure at several tens meV. We also provide a possible explanation for these problems. The crossover induces an unusual temperature dependence of the scattering rate, and it reproduces the experiments.

In the last part of the thesis, we study the heterostructure constructed from the copper-oxide high-T_c superconductors. Such systems recently opened another way to realize the superconducting transition temperature $T_{d\mathrm{SC}}$ beyond bulk systems. At the same time, distinctive phenomena have been found. For example, a $La_2CuO_4/La_{2-x}Sr_xCuO_4$ heterostructure experiment reported that $T_{d\mathrm{SC}}$ is pinned at 40 K, although the hole concentration x in the metallic side is varied in the range x=0.15-0.47, where 40 K is the highest $T_{d\mathrm{SC}}$ obtained in hole-doped La_2CuO_4, while $T_{d\mathrm{SC}}$ has a dome-like dependence on x in the bulk $La_{2-x}Sr_xCuO_4$. It is the last purpose of this thesis to understand the mechanism of this anomalous pinning for the future superconductivity engineering at finite temperature. A previous theoretical study at zero temperature elucidated that there is a phase separation (PS) between antiferromagnetic (AF) insulator (x=0) and d-wave superconducting (dSC) state in the underdoped region of the bulk system. In addition, they showed that the hole

concentration in this PS region is not allowed at any layers in the heterostructure systems and the doping x in the PS region is always readjusted to the PS boundary. As a result, the hole-doping concentration x at the metallic interface next to the insulating layer is pinned at the PS boundary. However, they studied only at zero temperature and it is necessary to clarify whether $T_{d\mathrm{SC}}$ is indeed pinned or not by finite temperature simulations because the phase separation must disappear at some temperature with the competition with the superconducting critical temperature. To elucidate this point, we apply a cluster extension of the DMFT to solve the single-band Hubbard model, which is a simple standard model for the cuprates.

We study a finite temperature phase diagram of the bulk, including AF, dSC and PS between AF and paramagnetic metal. The phase diagram suggests that the phase separation should pin $T_{d\mathrm{SC}}$ even at optimal hole doping. Furthermore, we simulated 5-layer heterostructures with a small interlayer electronic transfer and directly confirmed that the hole-doping concentration x is always readjusted to the border of the PS if x at that layer estimated from its chemical potential is located inside the PS region in the bulk. Our results at finite temperature including the superconducting and PS critical temperatures substantiate the mechanism proposed earlier at zero temperature and verify that the anomalous $T_{d\mathrm{SC}}$ pinning in the heterostructure originates from the PS by showing the PS critical temperature exceeds $T_{d\mathrm{SC}}$.