論 文 の 内 容 の 要 旨

論文題目

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 enhance the transition temperatures and the order parameters of the magnets and superconductors. In this thesis, we elucidate the role of the electron correlation for such materials, and propose guiding principles to improve it.

To achieve these grand challenge, it is crucial to calculate different materials within a unified theoretical framework to clarify the general physics. Such a method should be able to substantially take the strong correlation effect into account and have a wide and flexible framework. For these reasons, we employ the dynamical mean-field theory 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. Therefore, one of our purposes is to understand this problem through a study on an itinerant ferromagnet $SrRuO_3$ (SRO) whose Curie temperature is 150-160K. SRO has a strong SOC about 140meV and strong electronic correlations because the bandwidth is comparable to the on-site interaction. For this material, it is known that the easy-axis (EA) is sensitive to the difference between the samples, and several kinds of the EA have been found in experiments. In particular, [110] and [001] have been reported as the EA for the thin films and single crystals, respectively. Other experiments found that the EA approaches from [001] to [110] with increasing temperature. One possible origin is the electron correlation because the effective interaction strength of SRO thin films is slightly larger than that of the single crystals due to the screening of the interactions and the strains originating from the substrate.

In order to study this 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 there adopt a pseudo-cubic lattice while SRO has an orthorhombic structure. We use this procedure to focus on the correlation effect apart from the crystal field one on the EA problem. Similarly, we use the orbital SO(3)-symmetric Slator-Kanamori interaction. Moreover, we study the sample dependence of the correlation by scaling the one-body terms by $\pm 4\%$. Note that the magnetic anisotropy arises only from the SOC term here.

We compare the free energy for [001] and [110] EAs within the DMFT. As a result, when the bandwidth is wider (narrower), [001] ([110]) tends to be the EA. Furthermore, there is an EA transition from [001] to [110] at 21K 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 21K. 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 is elucidated 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 40-50K, 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 Fermi liquid to bad metal behavior at 56K. We clarify that this crossover is the origin of the anomalies and confirm that such properties are reproduced by this crossover.

The thesis next studies $CeCo_5$ which is a potential candidate of hard magnets, and we here propose a guideline of design for better permanent magnets. To improve magnets, the rare-earth

elements are added to typical magnets Fe or Co. Cerium, classified as a light rare-earth, is a rather rich element and has potential of the valence fluctuation and volume collapse in the future. In the thesis, we discuss the valence change effect and propose the way to improve $CeCo_5$ performance.

As a first step, we employ the local density approximation and the constrained random phase approximation to derive an *ab initio* Hamiltonian including 42 bands consisting of *s*-, *d*- and *f*-orbitals of Ce and Co. In addition, we study the filling change effect of Ce *f*-orbital because this should have large impacts on the magnetic properties. We apply the DMFT to solve this model to take the local correlation into account. Thus, we found that the magnetization becomes maximum when the electron density of Ce *f*-orbital is 1.1. The performance (maximum energy production) as a permanent magnet is then 20% improved at most. Our results offer that one promising procedure is to increase the *f*-orbital filling for Ce.

In the last part of the thesis, we study the cuprate heterostructure. Such systems recently opened another way to realize the superconducting transition temperature T_c beyond bulk systems. While the heterostructure systems allows additional degrees of freedom, inhomogeneity, several distinctive phenomena have been found in comparison with the bulk. For example, a $La_2CuO_4/La_{2-x}Sr_xCuO_4$ heterostructure experiment reported that T_c is pinned at 40K for x=0.15-0.45, which is the highest T_c obtained in hole-doped La_2CuO_4, while T_c 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.

One previous theoretical study by Misawa et al. elucidated that there is a phase separation (PS) between antiferromagnetic (AF) insulator (x=0) and *d*-wave superconducting (dSC) state (x~0.19) in the bulk system. In addition, they showed that any layers with x=0-0.19 are not allowed in the heterostructure systems and the doping x in the PS region always moves to the PS boundary. As a result, the hole-doping 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 the T_c is pinned or not by finite temperature simulations.

To elucidate this point, we apply the 2×2-site DMFT to solve the single-band Hubbard model, which is the elementary one for the cuprate, and study a finite temperature phase diagram of the bulk system, including AF, dSC and PS between AF and paramagnetic metal. The results illustrate that the practical T_c should be maximized at the PS boundary (x~0.16), and agree with the experiment. This suggests the doping and T_c are pinned at the PS boundary. In practice, we simulated 5-layer heterostructures and directly confirmed that the hole-doping x always moves to the boundary if x at each layer is located at the inside of the PS region. Our results strongly

suggest that the anomalous T_c pinning in the heterostructure originates from the PS. Therefore, we suggest that it is crucial to consider the PS for realizations of higher T_c at the interfaces.