

Theoretical study on electronic properties at interfaces of strongly correlated electron systems

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Artificial heterostructures of strongly correlated electron systems, such as transition metal oxides, are currently one of the fascinating research topics in condensed matter physics. Recent progress in fabricating multi-layered structures has stimulated great interest in understanding the interface physics, leading to an extensive study of several classes of oxides heterostructures. As is well known, the transition metal oxides have a complex and rich phase diagram. Therefore, the interface between these materials is anticipated to display novel physical properties resulting from the competition of different ordered phases.

A prototypical example is the conducting interface between correlated insulators, such as the $\text{LaTiO}_3/\text{SrTiO}_3$ superlattice, where the mixed Ti valence dramatically changes the electronic properties around the interface layers. The $\text{LaMnO}_3/\text{SrMnO}_3$ heterostructure further evidences the presence of a variety of electronic and magnetic phases which are specific to the heterointerface. Moreover, the metal-insulator transition and anomalous transport properties are also reported in the $\text{LaVO}_3/\text{SrVO}_3$ superlattice, when the number of LaVO_3 or SrVO_3 layers is altered. These results imply the complex interplay of different electronic states near the interface, and pose the emergence of remarkable new phenomena.

In this thesis, we shed light on the interface physics of strongly correlated electron systems with particular focus on possible electronic/magnetic properties as well as correlation effects. Our main interest is put toward the interface-specific phases driven by the strong electron-electron interaction. To accomplish our goal, we explore heterostructures based on the Mott insulators employing two mean-field approximations: one is the Hartree-Fock (HF) approximation that provides a reasonable description for electronic and magnetic ordered phases, and the other is (inhomogeneous) dynamical mean-field theory (DMFT) that enables us to non-perturbatively deal with the electron correlation effects.

The conducting interface between correlated insulators has been observed in several types of the heterostructure. Taking an example of $\text{LaTiO}_3/\text{SrTiO}_3$, we first discuss possible electronic states at the interface of Mott insulator

(MI) and a band insulator by using the HF approximation. The obtained phase diagram displays various spin/charge orderings that appear only around the interface. For example, the antiferromagnetic (AF) ordering in the MI region can induce a canted AF state at the interface layer, which displays a first-order metamagnetic transition in external magnetic fields. It is pointed out that these behaviors are explained by the strong spin/charge coupling near the interface. This mechanism is further confirmed by both the obtained charge-ordered state at the interface, and its reentrant transition under the magnetic fields.

Recently another type of the metallic interface has been reported in heterostructures of topological band-insulators (TI), whose interface (edge) state is protected by the bulk topology. To clarify correlation effects on such topological edge mode, the proximity effects between the MI and the TI is investigated within the framework of DMFT. We elucidate that the edge state of the TI penetrates into the MI side, and forms a strongly renormalized mid-gap state inside the Mott-Hubbard gap. Intriguingly, this mid-gap state still keeps a signature of the helical energy spectrum, and is robustly stable in spite of the strong Coulomb repulsion.

In many cases, the electronic states near the interface are strongly influenced by changes in the superlattice periodicity. We next aim to explain such dependence in terms of correlation effects, focusing on the MI/metal superlattice structure, such as $\text{LaVO}_3/\text{SrVO}_3$. The DMFT result shows that an anisotropic Fermi liquid emerges in the ground state. Interestingly, the corresponding quasi-particle weight displays an even-odd oscillation depending on the number of metal layers, which accompanies a detectable change in the electrical resistivity. Moreover, our simple model succeeds in a reasonable explanation of some experimental findings in the $\text{LaVO}_3/\text{SrVO}_3$ superlattice, including the metal-insulator transition and the characteristic temperature-dependence of the resistivity.

In this thesis, we elucidate that the interplay of different electronic states leads to a variety of unusual interface phenomena. In order to achieve a comprehensive understanding, it would be also interesting to see other important aspects, such as the multi-orbital physics, the lattice relaxation and the effects of strain field. These are left as future problems.