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Interface phenomena in correlated electron systems

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Abstract

We present theoretical studies of heterostructures comprised of a Mott insulator and a band insulator. A model calculation based on the Hartree–Fock approximation on $LaTiO_3/SrTiO_3$-type heterostructure is performed. It is found that spin and orbital ordering patterns in thin heterostructures differ from those in bulk $LaTiO_3$, and that $LaTiO_3/SrTiO_3$ interface region, about three unit cell wide, is always metallic. We further discuss strong correlation effects on the physical properties using dynamical-mean-field theory. It is shown that metallic behavior is supported by heavy quasiparticle bands centered at the interfaces.

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Keywords: Strongly correlated electron systems; Surface properties; Heterostructure

"Correlated electron compounds" are materials in which strong electron–electron and electron–lattice interactions produce new electronic phases, including interaction-induced ("Mott") insulators, many forms of spin, charge and orbital ordering, and high-temperature superconductivity [1,2]. Understanding their surface and interface properties is an important open scientific question and is necessary for the analysis of nanostructures and possible devices involving correlated electron materials. Many effects, including surface reconstruction [3], strain [4], and charge redistribution [5], may contribute to the physical properties. Thus it is preferable to study each effect separately first, and study the interrelation among them later. Recently, Ohtomo et al. [6] fabricated atomically controlled heterostructures of $LaTiO_3$ (a Mott insulator with d^1 configuration) and $SrTiO_3$ (a band insulator with d^0). In this system, the lattice distortion is minimized because of the similar lattice constants between the two materials, thus providing an ideal model system for studying the charge redistribution. Ref. [6] measured the distribution of charge originating from Ti d-shell in $LaTiO_3$ (leakage of electron to $SrTiO_3$ region is

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broad, about three unit cells wide) and transport properties. Surprisingly, the heterostructures are always metallic.

This paper reviews our recent progress in studying the physical properties of correlated heterostructures with the geometry reported in Ref. [6], and presents new results going beyond the Hartree–Fock(HF) approximation used in our previous work. We consider the heterostructure comprised of perovskite ABO_3-type materials reported in Ref. [6], in which finite number (n) of Mott-insulating $LaTiO_3$-layers are sandwiched between two semi-infinite number of band-insulating $SrTiO_3$ layers. (see the inset of Fig. 1) We take the d-electrons to hop between correlated B-sites according to a nearest-neighbor hopping and to feel a potential defined by (i) the Coulomb force arising from the extra charge on the La relative to Sr on A-sites (ii) the Coulomb force arising from the electrons on other B-sites and (iii) on-site "Hubbard U" interactions with the other d-electrons on the same site. For the d-electron, we assume a three-fold degenerate t_{2g}-band, termed t_{2g}-orbital model (for details, see Refs. [7,8]). We also present preliminary beyond HF results for the one-band Hubbard model.

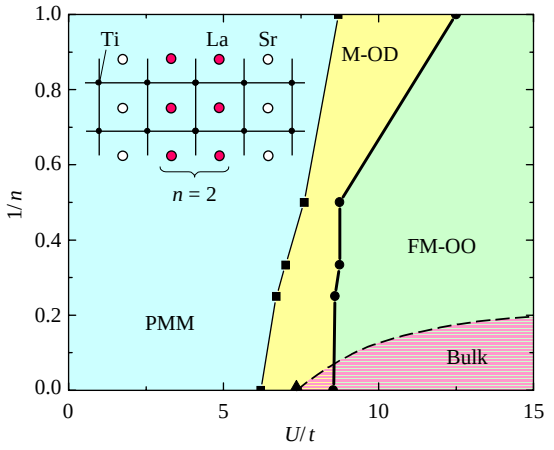

Fig. 1. Phase diagram as a function of inverse of layer number n and on-site Coulomb interaction U/t. Result for the t_{2g}-orbital model with $U'/U = \frac{7}{9}$, $J/U = \frac{1}{9}$ and $\varepsilon = 15U'(J)$ is an interorbital Coulomb (exchange) interaction, and ε is a dielectric constant. t is a transfer intensity. Inset: schematic view of the heterostructure projected on to the [0 1 1] plane.

Let us start with HF analysis. The crucial technical issue is the self-consistent screening of the long-range Coulomb interaction; in most cases, the highest-energy electron is very weakly bound. Thus, many iterations are required to obtain well-converged solution. The calculated ground state phase diagram for t_{2g}-orbital model is summarized in Fig. 1. PMM: paramagnetic metallic state, M-OD: two-dimensional magnetically ordered state with orbital disorder, FM-OO: ferromagnetic state with two-dimensional orbital order. Bulk-like spin and orbital orders are expected in large U and large n region denoted by Bulk. Thin heterostructures are seen to have different spin and orbital orderings from those observed in bulk. This is found to be due to charge leakage into the Sr-rich region, leading to a $\sim$3 unit cell wide edge region, which supports metallic behavior.

We further investigate the strong correlation effect beyond HF for single-band model applying the dynamical-mean-field theory (DMFT) approximation, as adapted for layer geometries by Ref. [9]. Here, the electron self-energy is assumed to be layer diagonal and to be independent of momentum parallel to the layers. The impurity model is solved in the two-site approximation [10], and charge distribution and parameters defining the impurity models are self-consistently determined. The long-range part of Coulomb interaction is treated at the Hartree level.

The characteristic feature of the HF results, that the charge decay length is about three unit cells wide, remains unchanged in DMFT. A more striking feature is the appearance of Hubbard bands and a heavy quasiparticle band. Fig. 2 shows charge densities coming from lower Hubbard band and coherent quasiparticle band near $\omega = 0$ in paramagnetic phase. (Position of layer is specified by z.) There is no electron deep in the Sr-rich region ($|z| \gg 5$). In the La-rich region ($z \sim 0$), the charge density is almost one and almost all the spectral weight is in the lower Hubbard band, indicating the insulating character. Around the interface region $z \sim \pm 5$, the charge density is dominated by a quasiparticle band near the Fermi level. These observations confirm the qualitative picture emerging from the Hartree–Fock calculations [7,8], of a near interface metallic band.

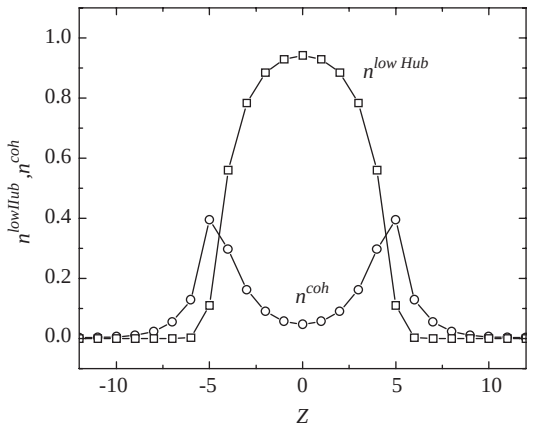

Fig. 2. Charge densities coming from lower Hubbard band $n^{\text{low Hub}}$ and coherent quasiparticle band n^{coh}. Single band model with $U/t = 16$, $\varepsilon = 15$ and $n = 10$. $+1$ charges corresponding to La-ions reside at $z = \pm 0.5, \pm 1.5, \ldots, \pm 4.5$.

Summarizing, we have theoretically studied the properties of correlated heterostructure. Via Hartree–Fock analysis and the dynamical-mean-field theory approximation, we found that the thin heterostructures show different spin and orbital orderings from those in the bulk. The edge region, where the charge density drops from ~ 1 to ~ 0, is about three unit cell wide and supports a heavy quasiparticle band and metallic conduction in the heterostructure.

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