Metallic interface at the boundary between band and Mott insulators

S. S. Kancharla[1] and E. Dagotto[1,2]
[1]*Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA*
[2]*Department of Physics and Astronomy, University of Tennessee, Knoxville, Tennessee 37996, USA*
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Motivated by experiments on atomically smooth layers of $LaTiO_3$, a Mott insulator, sandwiched between layers of $SrTiO_3$, a band insulator, a simple model for such heterostructures is studied using quasi-one-dimensional lattices and the Lanczos method. Taking both the local and long-range Coulomb interactions into account, and computing the layer dependent local density of states, a metallic state was found at the interface whose extent strongly depends on the dielectric constant of the material. We also observed that the antiferromagnetic correlations in the bulk Mott phase persist into the metallic region. Our conclusions are in excellent agreement with recently reported results for this model in the opposite limit of infinite dimensions, thus providing an alternative tool to study electronic reconstruction effects in heterostructures.

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I. INTRODUCTION

The physics of nanostructures comprising atomically smooth layers of correlated electron materials with abrupt interfaces is a rapidly growing field spurred by experimental advances. Apart from the technological promise of new devices, these systems are of fundamental interest for the novel phases that could occur at the interfaces of bulk systems. Correlated electron systems in the bulk are characterized by strong interactions and often exhibit a variety of competing states in close proximity within their phase diagrams. Fabricating dissimilar layers of these materials it has become possible to achieve the enhancement of properties compared to the bulk, such as the polarization increase observed in superlattices made up of ferroelectric $BaTiO_3$ interspersed with paraelectric $CaTiO_3/SrTiO_3$, as compared to pure $BaTiO_3$ with identical volume.[1] In other experiments, coexistence of ferromagnetism and singlet superconductivity has been observed in artificially fabricated superconductor (S)–ferromagnet (F) structures,[2,3] as well as the transfer of charge from a ferromagnet to a superconductor.[4]

In this work, we shall be concerned with the reorganization of charge and the interfacial state located at the boundary between a Mott insulator (MI) and a band insulator (BI), in the context of the experiments performed by Ohtomo *et al.*[5] These experiments involve the fabrication of a system with an arbitrary number of layers n of $LaTiO_3$, a MI, sandwiched in between m layers of $SrTiO_3$, a BI, on either side. The transport properties of this heterostructure (HS) revealed metallic behavior at the interface between the two types of insulators. Pioneering theoretical studies of this system by Okamoto and Millis[6,7] used the Hartree approximation to treat the long-range Coulomb interaction and a dynamical mean-field theory (DMFT) to treat the local Coulomb repulsion. DMFT incorporates dynamical correlations exactly in the limit of infinite coordination and reduces the problem of each infinite layer to that of a single site coupled to a self-consistent bath. Consequently, the entire problem is mapped onto a one-dimensional chain of independent impurity problems, coupled to each other via a self-consistency condition incorporating the hopping between layers, and a Hartree mean field for the long-range Coulomb interaction.

In this paper, we employ an alternative approach by considering a simplified one-band model for a finite heterostructure using a quasi-one-dimensional geometry. This limit of one dimension is the complete opposite to that of infinite dimensions that has been pursued in previous literature for this model.[6] Our main goal is to verify the conclusions of previous investigations, and to provide alternatives to DMFT for the study of HS systems involving correlated electrons. We treat the local and nonlocal Coulomb interactions exactly using the Lanczos method. Since the lattice parameters for $SrTiO_3$ and $LaTiO_3$ differ by only $\sim$1.5% we neglect effects of strain at the interface and, as in earlier work,[6,7] we focus on the relevant electronic degrees of freedom within the Ti band to define the Hamiltonian. We obtain the charge profile through the HS, along with the position dependent local density of states (DOS), and find a very good agreement with previous results.[6] In general, we observe that the strongest variation of the density moving from a MI to a metallic region, and then onward to a BI, occurs over a span of three to four unit cells. Furthermore, the antiferromagnetic (AF) correlations in the bulk Mott phase persist in the metallic interface. Similar results for the charge profile are found by extending our system to a two-leg ladder.

II. MODEL HAMILTONIAN

Consider a HS with n layers of $LaTiO_3$ sandwiched in between m layers of $SrTiO_3$. A one-dimensional analog of this system is shown in Fig. 1(a). La and Sr carry a bare valence of +3 and +2 within $LaTiO_3$ and $SrTiO_3$, respectively. The condition of charge neutrality requires that substitution of Sr by La in n layers adds n electrons per unit area of each layer to the system. The essential dynamics is then governed by the interplay of the electrons hopping on the Ti sites, with their mutual long-range repulsion, and the attractive potential produced by the surplus positive charge of the La ions.

The Hamiltonian for this $(n+2m)$-sized HS in one dimension can then be written as

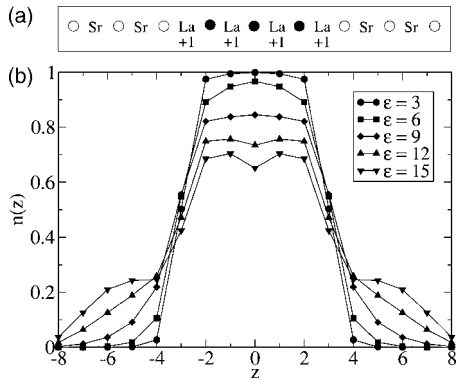

FIG. 1. (a) Circles denote Ti sites surrounded by La in the central Mott region and Sr in the band insulator. (b) Charge density across the 16-site heterostructure for $U=20t$ and ϵ varying from 3 to 15.

$$H = H_t + H_U + H_{coul}, \tag{1}$$

where

$$H_t + H_U = -t \sum_{\langle ij\rangle\sigma ij=1}^{n+2m} (d_{i\sigma}^{\dagger} d_{j\sigma} + \text{H.c.}) + U \sum_{i=1}^{n+2m} n_{i\uparrow} n_{i\downarrow}, \tag{2}$$

$$H_{coul} = \frac{1}{2} \sum_{i\neq jij=1}^{n+2m} \frac{e^2 n_i n_j}{\epsilon |\vec{R}_i - \vec{R}_j|} - \sum_{i=1}^{n+2m} \sum_{j=m+1}^{m+n} \frac{e^2 n_i}{\epsilon |\vec{R}_i - \vec{R}'_j|}. \tag{3}$$

Here H_t and H_U represent the nearest-neighbor hopping and onsite Coulomb repulsion through the HS on the Ti sites. Note that U is present on all the sites of the HS and not just in the MI region. The first term in H_{coul} denotes the long-range Coulomb repulsion between the electrons, with ϵ being the dielectric constant of the host lattice. The second term represents the long-range attractive potential between electrons on the Ti sites and the La ions located at $\vec{R}'_j = \vec{R}_j + 1/2a$, with a being the lattice constant. The dielectric constant ϵ is a strong function of temperature and frequency and also there is considerable uncertainty in the literature on the values of U for the system. Hence we investigate the properties of the above Hamiltonian over a range of parameters, $8t < U < 20t$ and $3 < \epsilon < 15$ at $T=0$, using the Lanczos technique[8] with open boundary conditions. We set $t = 0.3$ eV and $a = 4$ Å for simplicity.

III. RESULTS

First, we present in Fig. 1(b) results for the charge profile through a 16-layer (i.e., 16-site) HS with $U=20t$, as a function of the dielectric constant ϵ. The structure is made up of six La ions in the center and corresponds to a net free charge of six electrons. We shift the coordinate axis such that the center of the HS is $z=0$. For $\epsilon=3$, the charge density at the center is very close to 1 but it rapidly drops over four sites to a very small number, where the system approaches a BI. The intermediate region where the density lies between 1 and 0 is expected to be metallic. The strongest variation of the density moving from a MI to a BI via a metallic region occurs over three to four unit cells. Increasing ϵ reduces the confinement of electrons in the central region within the MI and increases the width of the crossover metallic region.

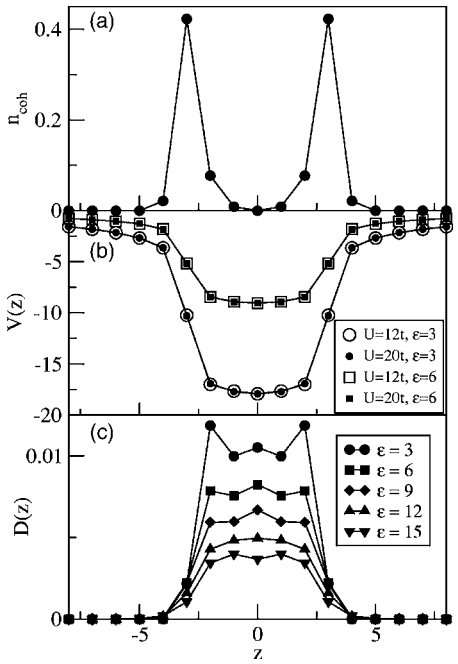

FIG. 2. (a) Coherent part of the total density, (b) effective single-particle potential, and (c) double occupancy across the heterostructure for $U=20t$ and ϵ varying from 3 to 15.

Since a metal is characterized by the presence of coherent quasiparticles, we calculate the coherent fraction[6] of the total density n_{coh} along the HS [Fig. 2(a)]. This quantity is defined as an integral over the spectral weight from $\omega=0$ up to the first point in the occupied band where the spectrum vanishes. We find that n_{coh} has a sharp peak in the crossover region reaching ~90% of the total density, decreasing to zero in the MI and BI regions. Both the results for the charge profile and n_{coh} are in excellent agreement with previous DMFT studies.[6] The density profile can be better understood by constructing an effective one-body potential $V(z)$ which is obtained by substituting the result of the density across the HS for a given U and ϵ into H_{coul} and setting H_{coul} equal to $\Sigma_z n_z V(z)$. Figure 2(b) shows $V(z)$ for $U=12t$, $20t$, and $\epsilon=3$, 6. It can be observed that the effective potential that confines the electrons to the MI region in the center is practically independent of U and only depends on ϵ. Increasing ϵ reduces the depth of the potential well and reduces the slope of the potential in the crossover metallic region.

In Fig. 2(c), we plot the double occupancy D along the HS for several dielectric constants, at a fixed value of $U=20t$. Note that D does not always follow the same behavior as the density through the HS. For $\epsilon=3$, where a clear MI phase prevails in the central region, D is suppressed at the center ($z=0$) relative to the maximum which occurs in the metallic state at the interface. Finally D goes to zero as the BI is approached. Increasing the dielectric constant the double occupancy shows no dip at the center relative to the crossover region and essentially follows the behavior of the density, implying that there is a wider metallic phase that now

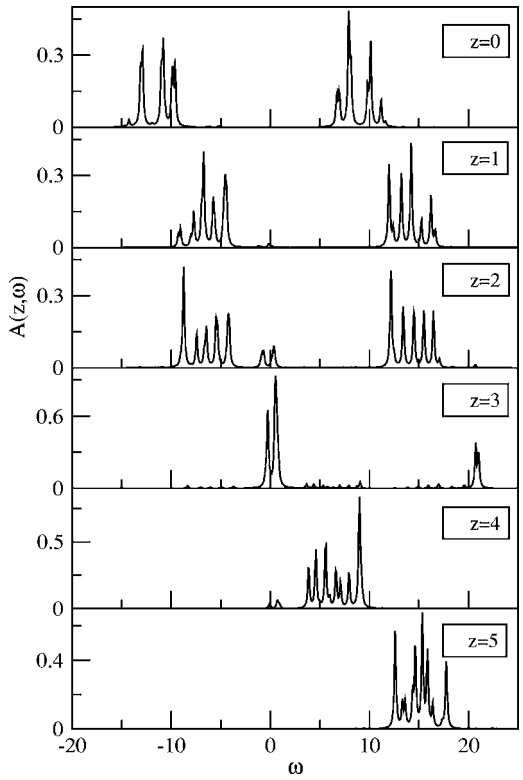

FIG. 3. Position dependent local density of states along the 16-site heterostructure for $U=20t$ and $\epsilon=3$.

evolves into a BI with no Mott phase in the center.

In Fig. 3, we show the position dependent local DOS along the HS for $U=20t$ and $\epsilon=3$. At the center, $z=0$, we have a MI with density $n=0.999$ reflected by a Mott gap separating the lower and upper Hubbard bands. Moving to the adjacent site ($z=1$) the density is only slightly lower at $n=0.994$ but a low weight in-gap state appears at the chemical potential. This metallic phase extends up to site 4, beyond which the DOS reflects a BI with all the spectral weight above a finite gap approaching U. These results are in excellent agreement with those obtained earlier for this model using DMFT.[6]

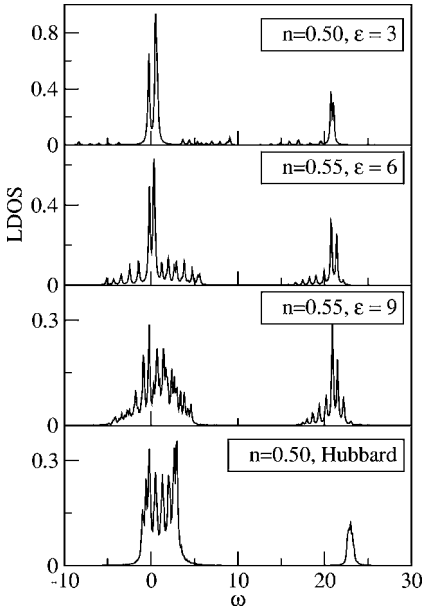

FIG. 4. Dependence of the local density of states on the dielectric constant for fixed density, $n\approx0.5$, $U=20t$. The lowest panel shows the same result for a uniform Hubbard model with periodic boundary conditions.

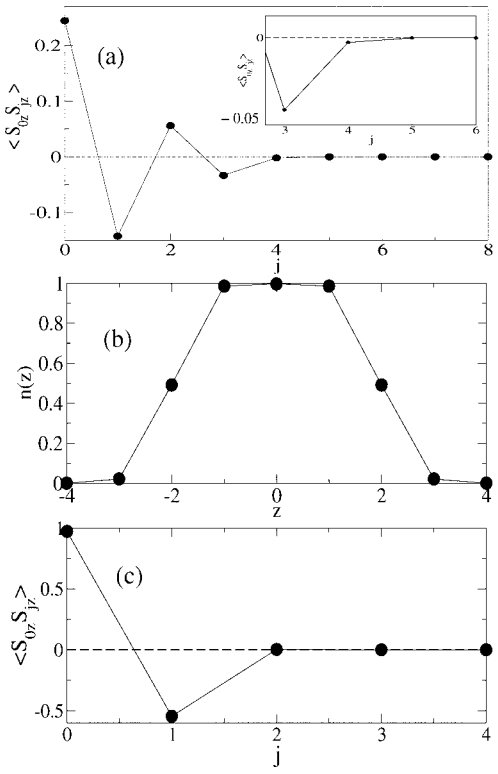

FIG. 5. (a) Spin-spin correlation function along the heterostructure. The inset shows the nonmagnetic outer layers. (b) Density profile in the two-leg ladder also shows a metallic interface. (c) Spin-spin correlation function for the two-leg ladder along the heterostructure for $U=20t$, $\epsilon=3$.

To clarify the nature of the metallic phase, in Fig. 4 we plot the local DOS for positions within the HS with comparable densities ($n\approx0.5$) but different ϵ, along with the spectral function for a quarter-filled uniform Hubbard chain of 16 sites under periodic boundary conditions. Both the partially occupied (lower Hubbard) and unoccupied (upper Hubbard) bands are significantly widened with the reduction of the dielectric constant and they develop long tails (although with low weight) as compared to the case with purely local interactions. For the lowest value $\epsilon=3$ most of the weight in the lower Hubbard band appears in a narrow feature arising from the onsite Coulomb repulsion, which is well separated from the tails arising from the long-range part of that interaction.

Next, we present in Fig. 5(a) the spin-spin correlations, $\langle S_{0z}S_{jz}\rangle$, as a function of distance j from the central spin at 0. Clearly, AF order is favored in the central region with density close to 1, as is expected in a MI. As we move toward the outer layers of the HS, where the density is significantly reduced from 1 (beyond site 3), there is no alternation of sign in the spin-spin correlation function signifying a nonmagnetic state as we approach the BI. However, in the interven-

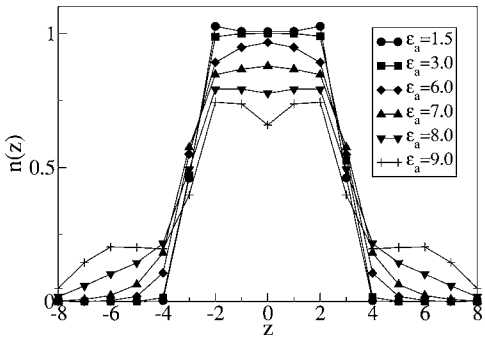

FIG. 6. Density profile through the HS as a function of ϵ_a for fixed $\epsilon_r=6$ and $U=20t$.

ing metallic interface we still have a clear signature of AF correlations as nearest-neighbor correlations (not shown) indicate. To check the robustness of our results we extend the system perpendicular to the interfacial direction by considering a two-leg ladder (a 2×9 system with each leg containing two Sr ions on either side of four La ions) with $U=20t$ and $\epsilon=3$. The density profile shown in Fig. 5(b) reveals a metallic region in between the MI and BI, as observed before for the one-dimensional (1D) case. In addition, from the spin-spin correlations along the ladder shown in Fig. 5(c) we find AF correlations in the central MI. Nearest-neighbor AF correlations persist in the metallic phase (not shown).[9]

Last, we consider a generalization of our model Hamiltonian where the dielectric constant that governs the attractive interaction of the ions, ϵ_a, differs from the dielectric constant ϵ_r for the electron-electron repulsion. In principle, there is no obvious reason why $\epsilon_a=\epsilon_r$. Our previous results simply followed Ref. 6 in these regards, but it is important to analyze the case $\epsilon_a \neq \epsilon_r$. The modified Coulomb term in the Hamiltonian then becomes

$$H_{coul}=\frac{1}{2}\sum_{i\neq j}^{n+2m}{}_{ij=1}\frac{e^2 n_i n_j}{\epsilon_r|\vec{R}_i-\vec{R}_j|}-\sum_{i=1}^{n+2m}\sum_{j=m+1}^{m+n}\frac{e^2 n_i}{\epsilon_a|\vec{R}_i-\vec{R}'_j|}. \quad (4)$$

The density profile through the HS for fixed $\epsilon_r=6$ and varying ϵ_a is shown in Fig. 6. For $\epsilon_a<\epsilon_r$ we see an increase in the density as we move away from the central Mott region, so that the density exceeds 1, and then drops across the metallic interface to approach zero in the BI region. When $\epsilon_a>\epsilon_r$ we see a suppression of density below 1 in the central MI and a metallic region which increases in width at the interface.

IV. SUMMARY AND CONCLUSIONS

To summarize, motivated by experiments on $LaTiO_3/SrTiO_3$ interfaces,[5] we have presented an exact diagonalization study of a simple one-band model for a correlated electron layered heterostructure in quasi-one-dimensional lattices, where a MI is sandwiched in between a BI. Considering exactly the long-range attractive Coulomb potential of the La ions and the repulsion between the electrons, we find that the interface supports a metallic state, in excellent agreement with previous studies of this model using DMFT and the Hartree techniques.[6,7]

The strongest variation of the density across the interface occurs over a region of three to four unit cells, whereas the actual width of the metallic region depends strongly on the dielectric constant of the material. The charge density depends only weakly on the local Coulomb interaction. Since the phenomena of interest occur over a very short spatial range at the interface, we believe that our results are valid even for HS much larger in the z direction than the sizes we considered here. We further check the robustness of our conclusions by extending the system to a ladder configuration, finding similar results for the charge profile. The central region with density close to 1 shows AF correlations characteristic of a MI which persist into the metallic phase.

The excellent agreement with DMFT does not imply that the self-energy for our system is relatively momentum independent, but that the observables such as charge density along the HS are unlikely to be strongly affected by momentum dependence of the self-energy. Cluster generalizations of DMFT such as cellular DMFT are likely to provide a better understanding of this issue. Important directions for future work using the method discussed here could involve realistic multiband models for other correlated electron phases including ferromagnetic and superconducting regimes. Also, the analysis of chain or ladder systems using density-matrix renormalization group or cluster generalizations of DMFT are possible, although the proper consideration of long-range Coulomb interactions are likely to pose a significant challenge to these methods.

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