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Physics of metal-corrrelated barrier with chemical modulation-metal heterostructure

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ABSTRACT

Barrier planes described by the Ionic Hubbard model sandwiched between metallic planes on both sides are studied using unrestricted Hartree Fock. For zero onsite correlation, the presence of the metallic interface generates an additional gap in the energy spectrum away from half filling, if the chemically modulated potential in the barrier planes exceed a critical value. There is an insulator–metal–insulator transition as we tune onsite correlation for fixed strength of chemical modulation. The metallic behaviour penetrates the barrier planes due to proximity effect. The variation of the gaps for varying numbers of intermediate planes is also determined.

1. Introduction

The physics of interface is an active research area for some time now [1–8]. The emergence of unexpected new properties has played a big hand in this. The interface of a band insulator and Mott insulator was shown to have metallic properties [2], which becomes superconducting on lowering the temperature [4,5]. Theoretically the subject has been studied using different methods like restricted Hartree Fock [2], two site DMFT [3], single site DMFT [7,8] and Lanczos [6].

In this article we have studied a metal-quasi 2D barrier-metal heterostructure. The barrier planes are described by the Ionic Hubbard Model, which describes a band insulator with onsite correlation. Thus the barrier planes describe a band insulator in the absence of onsite correlation U and a Mott insulator in the absence of chemical modulation for $U \geq U_c$, where U_c depends on the dimensionality of the system. The ionic Hubbard model has been widely studied by various groups using various techniques like single site DMFT [9,10], quantum monte carlo [11] and cluster DMFT [14] in 2D, DMRG in 1D [12] and two site DMFT in quasi 2D [13]. At half filling a single site DMFT solution which assumes a paramagnetic solution yields a metallic phase which separates the Mott insulator and band insulator phases [9,10]. A solution which incorporates long range anti-ferromagnetic ordering in quasi 2D, using two site DMFT, however shows that the system is insulating for all interaction strengths.

The Mott insulator-band insulator heterostructure has been studied using restricted Hartree Fock [2], inhomogeneous two site DMFT [3] and in quasi one dimensional lattices using Lanczos method [6]. The metal-Mott insulator-metal heterostructure has been studied in detail in the near past [7,8,15]. The role of disorder on the Mott planes sandwiched between two metallic planes has also been investigated by the present authors. [16].

Spatial variations in the planes and along the z direction play a crucial role in determining the correct ground state of a highly inhomogeneous systems like heterostructures. The DMFT method which have been quite successfully applied to Mott insulators, essentially reduces the problem to single site and incorporates the temporal quantum fluctuations at that site in an exact way at the cost of neglecting the spatial inhomogeneity. In the present problem, the in plane variation is totally ignored in a one site inhomogeneous DMFT (IDMFT) [17–20] approach. The two site IDMFT method though capable of capturing planar long range order like planar antiferromagnetism, is insufficient to capture the regime where the two orders start to cancel each other leading to short range ordering. With this in mind we have adopted the method of unrestricted Hartree Fock (UHF), which gives the solution in a self-consistent way while retaining the spatial inhomogeneity, an important requisite of the heterostructure problem. The UHF method did show some remarkable features in the spectrum and order parameters of the metal-correlated barrier-metal heterostructure problem because of inclusion of in plane correlation [15]. The Hartree Fock method has been used successfully to describe the ground state of the ionic Hubbard model even in 1D and was shown to be in excellent agreement with real space RG calculation [21]. In 2D t-t' Hubbard model, calculation at half filling using UHF were in good agreement with Monte Carlo calculations [23].

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1.1. Model and method

The Hamiltonian for the system is

$$\mathcal{H} = -\sum_{ij\alpha\sigma} t_{ij}^{\parallel} c_{i\alpha\sigma}^{\dagger} c_{j\alpha\sigma} - t\sum_{i\alpha\sigma}[c_{i\alpha\sigma}^{\dagger} c_{i\alpha+1\sigma} + h.c.] - \mu\sum_{i\alpha\sigma} c_{i\alpha\sigma}^{\dagger} c_{i\alpha\sigma} + \sum_{i\in B,\alpha} W_{\alpha}(n_{i\alpha\uparrow} + n_{i\alpha\downarrow}) + \sum_{i\alpha} U_{\alpha}\left(n_{i\alpha\uparrow} - \frac{1}{2}\right)\left(n_{i\alpha\downarrow} - \frac{1}{2}\right). \quad (1)$$

Here the label α indexes the planes, and the label i indexes sites of the two-dimensional square lattice in each plane. The operator $c_{i\alpha\sigma}^{\dagger}$ ($c_{i\alpha\sigma}$) creates (destroys) an electron of spin σ at site i on the plane α. We set the in-plane hopping $t^{\parallel}$ to be nearest neighbor only, and equal to t, the hopping between planes, so that the lattice structure is that of a simple cubic lattice. We take $W_{\alpha} = W$ for the B sites and $W_{\alpha} = 0$ for the A sites (W is therefore the disorder strength). We also take onsite electronic correlation $U_{\alpha} = U$ for the barrier planes, and zero for the metallic planes. The chemical potential μ is calculated by taking the average of the $N/2$ th and the $N/2 + 1$ th energy level. The plane index $\alpha = 1, m$ corresponds to the metallic layers. All the other α values in between correspond to the barrier planes. For the quasi 2D geometry taken by us total number of sites $N = m \times L^2$, where m is the total number of layers and L^2 is the number of sites in the planes.

1.2. Calculated quantities

We have calculated the energy spectrum, charge and spin profile, and the optical conductivity. The charge at site i is given by $C_i = n_{i,\uparrow} + n_{i,\downarrow}$. The spin at a particular site is given by $S_i = |(n_{i,\uparrow} - n_{i,\downarrow})|$. The low frequency optical conductivity is calculated using the Kubo formula. In this paper, $\sigma_{zz}(\omega)$ is calculated in units of $\pi e^2/\hbar a_0$. For details of the calculation procedure see previous works [24,22]. We have performed finite size scaling of each of our transport results. The value of $\sigma_{zz}(\omega)$ is calculated for multiples of a small $\omega = \omega_r$, where ω_r is twice the lowest ω that we can access for a particular system size.

1.3. Analysis of our results

In Fig. 1, W positive/negative corresponds to repulsive/attractive potential in the barrier planes. Let us look at a few known limits first to understand the results obtained in Fig. 1. In the absence of the metallic planes, there is only one gap which opens at half filling. This gap is identical to W. For such a system, in the absence of U any non-zero W leads to a homogeneous charge density wave (CDW) profile throughout the system. On the other hand, in the absence of any charge modulation, the onsite Coulomb repulsion U opens a gap at half filling above a certain critical U_c. This gapped phase has homogeneous spin density wave extending throughout the system. Thus without the metallic planes the system is a CDW insulator without U and a SDW insulator without W for $U > U_c$.

In the presence of metallic planes, for $W=0$ on the boundary planes, we [15] find that, above U_c, the system is an antiferromagnetic insulator, while below this value the system is gapless with no spin density wave order but still with considerable charge inhomogeneity due to charge reconstruction along the z direction. The energy spectrum is found to have multiple gaps as the correlation strength is increased.

What happens in the other limit of $U=0$ but finite W in the presence of metallic planes? This has been answered in Fig. 1. As we increase W there is a gap at half filling due to CDW ordering in the system. The value of this gap is suppressed from the bare value due to the presence of the metallic planes which introduces midgap states (Fig. 1a). This also makes the CDW ordering highly inhomogeneous along the z direction. On further increasing W, beyond a certain critical value a second gap opens in the spectrum, this time away from half filling (Fig. 1b).

For general m, the filling at which the second gap opens up is given by 0.5 + sign(W) × (1/m). Above this value W_g, The CDW induced in the barrier planes becomes very strong compared to the CDW in the metallic planes. A CDW pattern arises in the metallic planes also due to proximity effect and a new band emerges. For positive/negative W the second gap opens at $W=4/-4$. The states below this new band gap now correspond to the induced B sites on the metallic planes and the states above the gap correspond to actual B sites from the barrier planes. In Fig. 1c we plot the two gaps with respect to variation in number of barrier layers. We find that both gap though varying differently attains a fixed value at around $m=11$. The CDW ordering in the barrier planes becomes more and more robust as we increase m which in turn strengthens the induced CDW ordering in the metallic planes. As such the energy difference between the A sites and the induced B sites increases with m which enhances the gap at half filling. As the CDW ordering in the barrier planes and the induced CDW ordering in the metallic planes both becomes stronger with increasing m, the relative difference between the induced B sites in the metallic planes and the actual B sites in the barrier planes is reduced with increasing m and a saturation is reached at around $m=11$. Because of this, the gap away from half filling decreases with m and reaches a fixed value near $m=11$.

These results which are essentially *exact* show that the system very interestingly shows insulating behaviour away from half filling for a value of site potential greater than a critical value, on the introduction of metallic interfaces on either side. This has tremendous practical application as one can tune the system from metal to insulator by taking the system at away from half filling and right at the value where there is a gap. If the site potential strength is varied the value of this gap away from half filling can be changed and the system can become a metal also.

In Fig. 2a, we show the modulation of the gap at half filling for $W=1$ as we increase U. The band gap is suppressed by U down to zero, after which there is a large gapless region. The low U region corresponds to a CDW phase, where U has started to compete with the chemical modulation with the latter being dominant. The large gapless region corresponds to a highly inhomogeneous phase, with no spin order till $U=6$ and with gradually diminishing but nonzero charge order. Above $U=6$, spin order starts to pick up gradually, though there is still a remnant weak charge order also.

Fig. 2b shows the variation of the two gaps in the energy spectrum for $U=7$, for both spins with variation in W. In the absence of W, the opening up of two gaps in the energy spectrum was first shown by us in a previous work [15]. For positive values of W, till $W=1$, both the gaps for both spins fall monotonically with increasing W. There is small spin asymmetry which is a signature of spontaneous symmetry breaking of the up and down spin sectors for such a system.

While for positive W the B sites are avoided by the electrons, the repulsion of the electrons to the metallic planes takes place uniformly for both up and down spins because there is very small charge modulation in the metallic planes and since there is U on all the barrier plane sites, they would all like to push electrons away to the metallic planes, without paying the cost of U.

Fig. 2c shows the plots of energy for both spin species and the total energy as we modulate W for $U=7$. The total energy increases monotonically with increasing W. The energy for the two spin species are different for the entire parameter range where there is both charge and spin order. This can be explained in a simple way in terms of average charge and spin order in different planes. In the presence of both charge and spin order the effective site