Metal-Insulator Transition in One-dimensional Hubbard Superlattices

Thereza Paiva and Raimundo R. dos Santos
Instituto de Física, Universidade Federal Fluminense
Av. Litorânea s/n, 24210-340 Niterói RJ, Brazil
(March 24, 2022)

We study the Metal-Insulator transition in one-dimensional Hubbard superlattices (SL’s), modelled by a repeated pattern of repulsive (i.e., positive on-site coupling) and free sites. The evolution of the local moment and of the charge gap (calculated from Lanczos diagonalization of chains up to 18 sites), together with a strong coupling analysis, show that the electron density at which the system is insulating increases with the size of the free layer, relative to the repulsive one. In the insulating state, the mechanism of interaction between fermions separated by a free layer is the analog of superexchange, and the charge gap display universal features.

Considerable insight into the MIT problem should therefore be gained by seeking instances in which such displacement can occur.

Motivated by the oscillatory exchange coupling in magnetic metallic multilayers [10], we have recently studied the effects of electronic correlations in superlattices (SL’s), through a one-dimensional Hubbard-like model. In spite of its simplicity, a number of remarkable features were found, in marked contrast with the otherwise homogeneous system [11]: Local moment weight could be transferred from repulsive to free sites; SDW quasi-order was wiped out as a result of frustration; and strong SDW correlations (in a subset of sites) could set in above half-filling. Since the combination of strong correlations with SL structures can modify the magnetic properties in such non-trivial way, transport properties should, most likely, be also affected. With this in mind, here we investigate the MIT transition in this one-dimensional Hubbard superlattice model.

The model consists of a periodic arrangement of \( L_U \) sites (“layers”) in which the on-site coupling is repulsive, followed by \( L_0 \) free (i.e., \( U = 0 \)) sites, such that the Hamiltonian is written as

\[
\mathcal{H} = -t \sum_{i, \sigma} \left( c^\dagger_{i \sigma} c_{i+1 \sigma} + \text{H.c.} \right) + \sum_i U_i n_{i \uparrow} n_{i \downarrow}
\]

(1)

where, in standard notation, \( i \) runs over the sites of a one-dimensional lattice, \( c^\dagger_{i \sigma} (c_{i \sigma}) \) creates (annihilates) a fermion at site \( i \) in the spin state \( \sigma = \uparrow \) or \( \downarrow \), and \( n_i = n_{i \uparrow} + n_{i \downarrow} \), with \( n_{i \sigma} = c^\dagger_{i \sigma} c_{i \sigma} \). The on-site Coulomb repulsion is taken to be site-dependent: \( U_i = U > 0 \), for sites within the repulsive layers, and \( U_i = 0 \) otherwise; throughout this paper, numerical values of \( U \) will be given in units of \( t \). It is important to notice that the SL structure breaks particle-hole symmetry even on bipartite lattices, as it can be seen through a simple Hartree-Fock argument: The exchange splitting is zero on free sites and non-zero on the repulsive ones, thus giving rise
to a non-uniform shift in the symmetric one-body local density of states. Differently from the homogeneous system, particle-hole symmetry cannot be restored by a uniform shift in the chemical potential.

The MIT in this model is studied numerically in the canonical ensemble. In addition to the numbers of sites, \(N_s\), and electrons, \(N_e\), another important parameter is the number of periodic cells, \(N_c = N_s/N_b\), for a basis with \(N_b = L_U + L_0\) sites; in some cases, we were able to reach lattices with \(N_s = 18\) sites. The ground state \(\langle \psi_0 \rangle\) and energy of Eq. (1) are obtained with the aid of the Lanczos algorithm [12–14]: Starting with a trial state, the Hamiltonian is used to generate a second state, orthogonal to the first, so one ends up with a \(2 \times 2\) representation for the Hamiltonian [13]. The diagonalization is trivial, leading to an estimate for the ground state and energy, which are used as new inputs for the subsequent iteration. This process is repeated until numerical convergence for the ground state energy has been achieved. In order to improve extrapolations to the thermodynamic limit, boundary conditions were chosen such that the Fermi momentum was always one of the allowed \(k\)-values [15]. The influence of the results can be assessed by simultaneously fixing system size, occupation and SL configuration, and performing calculations for different boundary conditions: the ground state energy turned out to be quite insensitive to the condition imposed (at most of the order of 1%) and similarly for the local moment. When dealing with the charge gap (see below), the above mentioned choice has the additional advantage of providing a trend (with system size) free from oscillations [15].

We assess whether the system is metallic or insulating by calculating the local moment and the charge gap, as we now discuss in turn. The local moment at site \(i\) is defined as

\[
\langle S_i^2 \rangle = \frac{3}{4} \langle m_i^2 \rangle,
\]

where \(m_i = n_{i\uparrow} - n_{i\downarrow}\); ensemble averages should be understood as ground state averages, \(\langle \ldots \rangle \equiv \langle \psi_0 | \ldots | \psi_0 \rangle\). Being a measure of both magnetism and degree of itinerancy of the system, the local moment is useful in the investigation of the metallic or insulating character of the ground state. Indeed, in the case of a homogeneous lattice, for a finite value of the on-site repulsion \(U\), the local moment is sharply peaked at half-filling; in the completely localized limit, \(U = \infty\), \(\langle S_i^2 \rangle = 3/4\). Above half filling, \(\langle S_i^2 \rangle\) decreases due to an increase in the double occupancy of the states. Unlike the magnetization (or even the sublattice magnetization), \(\langle m_i \rangle\), which vanishes identically on a finite system due to the lack of spontaneous symmetry breaking, the local moment is always non-zero on a homogeneous lattice, except for \(\rho = 0\) and 2.

For a SL the site-dependent Coulomb repulsion leads to a non-uniform distribution of local moments throughout the lattice [15]. Figure 1 shows typical plots of the density dependence of the local moment at a repulsive site, for lattices with \(N_s = 12\). As the SL configuration is changed, the maximum value of \(\langle S_i^2 \rangle\) still approaches \(3/4\) as \(U\) is increased; its position is displaced to higher fillings, without showing any \(U\)-dependence. By analogy with the homogeneous case, one is led to identify this peak position with the density, \(\rho_I\), at which the system becomes an insulator; Fig. 1 then shows that \(\rho_I\) increases continuously with \(L_0\), for fixed \(L_U\). To see how this comes about, we should ask ourselves how can the SL be filled up with electrons in a way to obtain maximum hopping hindering and largest moment on the repulsive sites. In strong coupling this is equivalent to pin the electrons, and is achieved by placing two on each of the free sites (thus rendering them magnetically inert) and one on each of the repulsive sites (maximum polarization); this leads to

\[
\rho_I = \frac{2L_0 + L_U}{L_0 + L_U}.
\]

The maxima position of Fig. 1 are given exactly by Eq. (3), with \(U = 1\), and \(L_0 = 1, 2, 3, \text{and } 5\). Configurations with \(U > 1\) follow the same pattern, and reflect the fact that the layer thicknesses come into the definition of \(\rho_I\) only through the ratio \(L_U/L_0\). Also, note that in the limit of a uniform lattice, \(L_0 \rightarrow 0\), one has \(\rho_I \rightarrow 1\), thus recovering the insulating behavior exactly at half filling.

![Fig. 1. Local moment at a repulsive site versus \(\rho\) for 12 site chains with \(L_U = 1\) and \(L_0 = 1\) (a), 2 (b), 3 (c), and 5 (d). Squares and dotted lines respectively represent data for \(U = 0\) and \(\infty\) for the homogeneous system; triangles and circles respectively represent data for superlattices with \(U = 3\) and 12.](image)

The above discussion allows us to perform a strong coupling perturbation theory analysis [15]. Let us start with the dimerized SL configuration; the relevant Hilbert subspace is the one with repulsive and free sites being respectively singly and doubly occupied. The first non-trivial
contribution from the hopping term comes in fourth order, and gives rise to an effective Heisenberg Hamiltonian

$$\mathcal{H}_{\text{eff}} = J_2 \sum_{[k,\ell]} \mathbf{S}_k \cdot \mathbf{S}_\ell,$$

(4)

where $J_2 = 8t^4/|U|^3$, and $k, \ell$ are repulsive sites (i.e., next-nearest neighbors on the original dimerized lattice); trivial constants have been dropped from Eq. (4). Thus, the (magnetically inert) free sites intermediate the Heisenberg exchange interaction between moments on the repulsive sites; the analogy with the usual superexchange mechanism involving non-magnetic atoms arises here quite naturally. These arguments can be straightforwardly generalized to other configurations, with suitable changes: (i) within a repulsive layer ($L_U > 1$), spins interact via the usual second order Heisenberg exchange coupling $J_1 = 4t^2/|U|$; (ii) the first non-trivial coupling across a free layer of thickness $L_0$ only appears in $2(L_0 + 1)$-th order, and the exchange coupling becomes $\sim t^2(L_0+1)/|U|^{2L_0+1}$. The ensuing Heisenberg model is again defined only on the repulsive sites, with non-uniform, but periodic, exchange couplings. Away from strong coupling, numerical data are consistent with this picture [11].

Further evidence in favor of the MIT being located at $\rho_I$ comes from the analysis of the charge gap, defined by

$$\Delta_c = E(N_c, N_e + 1) + E(N_c, N_e - 1) - 2E(N_c, N_e),$$

(5)

where, for a given SL configuration, $E(N_c, N_e)$ is the ground state energy for a chain with $N_e$ periodic cells and $N_c$ electrons. This gap is a measure of the charge excitation spectrum (i.e., the cost of adding extra particles): When extrapolated to the thermodynamic limit, a non-zero value indicates an insulating state, whereas a zero value corresponds to a metallic state. Before discussing our results, a comment is in order at this point. The Drude weight, which is proportional to the second derivative of the ground state energy with respect to the magnetic flux through the ring [17–19], is an elegant test of the metallic or insulating character of the system: It yields impressive results when Bethe-Ansatz data (corresponding to arbitrarily large lattices) are used [18]. For small systems, however, extrapolations with the charge gap appear to be more conclusive than those with the Drude weight [23,24].

Figure 2(a) shows charge gap data for the dimerized configuration, $L_U = L_0 = 1$. In this case $\rho_I = 3/2$, and extrapolation (through least-squares fits) of data towards $N_e \to \infty$ yields finite values for $\Delta_c$, for both $U = 6$ and 12, confirming the insulating character of this filling factor. By contrast, for $\rho = 5/3$, the data extrapolate to $\Delta_c \approx 0$, for both values of $U$, signaling a metallic state; for clarity, the only metallic case shown in Fig. 2(a) corresponds to $\rho = 5/3$, but this is a representative example for all $\rho \neq \rho_I$. For the configuration $L_U = 1$, $L_0 = 2$, $\rho_I$ is now 5/3, and Fig. 2(b) shows that the roles of fillings 5/3 and 3/2 have been reversed with respect to that of Fig. 2(a).

**FIG. 2.** Charge gap vs. the inverse number of cells for the SL configurations $L_U = L_0 = 1$ (a) and $L_U = 1$, $L_0 = 2$ (b), and densities $\rho = 3/2$ (empty symbols) and $\rho = 5/3$ (filled symbols). Circles and squares denote $U = 6$ and $U = 12$, respectively. The lines are least-squares fits to the data.

**FIG. 3.** Scaled extrapolated–charge-gap versus scaled on-site energy. Data for the configurations $(L_U, L_0)$ are represented as follows: (1,1) by squares; (1,2) by circles; (1,3) by up-triangles; and (2,2) by down-triangles. The full line is the Mott-Hubbard gap for the homogeneous system, calculated from the Lieb-Wu solution. The inset shows the intermediate coupling region.

Similarly to the homogeneous system, the gap increases with $U$. This similarity, however, goes beyond a simple qualitative trend: If both the extrapolated charge gap and the on-site coupling $U$ are scaled by $\rho_I$, strong coupling data for different $\rho_I$ fall on a universal function, as shown in Fig. 3. This function, in turn, reduces to the Mott-Hubbard gap for the homogeneous system ($\rho_I = 1$), known for any $U$ through the Bethe ansatz solution [3,22];
its asymptotic forms are $\Delta_c \sim (8\sqrt{tU}/\pi) \exp(-2\pi t/U)$, in weak coupling, and $\Delta_c \sim U$, in strong coupling. As $U$ decreases, the relative errors in extrapolating the gaps increase; nonetheless, the resulting fits to the scaled Lieb-Wu gap (shown as the inset of Fig. 3) are still satisfied within error bars.

In summary, within a simple model we have established that the superlattice structure induces a shift in the critical density at which the Mott-Hubbard transition occurs: It increases with the ratio between free and repulsive layer thicknesses. This comes about as a result of having to doubly (singly) occupy the free (repulsive) sites, in order to keep electronic motion to a minimum, i.e., to that resulting from quantum fluctuations. These insulating states have interesting properties: (i) fermions on free sites act as mediators of the magnetic exchange interaction between fermions on repulsive sites ('superexchange'); (ii) if properly scaled, the charge gap seems to follow a universal curve (reducing to that for the homogeneous system at half filling), for all superlattices. Experimental realizations of (effectively) one-dimensional systems undergoing Mott-Hubbard transitions are, by now, well established in organic compounds [23]. In Bechgaard salts, for instance, organic complexes are stacked along a given direction; their large anisotropy is responsible for the one-dimensional character of the system. Within closely related families of these compounds, some are insulators whereas others are metals, and an interesting possibility would be to stack layers of these different complexes, forming a one-dimensional superlattice, and investigate the evolution of the metal-insulator transitions with the superlattice structure; we hope the scenario proposed here stimulates experimental studies along these lines.

ACKNOWLEDGMENTS

The authors are grateful to M. A. Continentino, J. d’Albuquerque e Castro, G. Japaridze, and E. Müller-Hartmann for enlightening discussions and suggestions. Financial support from the Brazilian Agencies FINEP, CNPq and CAPES is also gratefully acknowledged. The authors are also grateful to Laboratório Nacional de Computação Científica (LNCC) for the use of their computational facilities.

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