Charge dynamics in the Mott insulating phase of the ionic Hubbard model

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I extend to charge and bond operators the transformation that maps the ionic Hubbard model at half filling onto an effective spin Hamiltonian. Using the transformed operators I calculate the amplitude of the charge density wave in different dimensions D. In 1D, the charge-charge correlations at large distance d decay as \( d^{-3} \ln^{-3/2} d \), in spite of the finite charge gap, due to remaining charge-spin coupling. Bond-bond correlations decay as \((-1)^d d^{-1} \ln^{-3/2} d\) as in the usual Hubbard model.

**I. INTRODUCTION**

The ionic Hubbard model (IHM) has been proposed in the 80’s for the description of the neutral-ionic transition in mixed-stack charge-transfer organic crystals.\(^1\)\(^2\) In the 90’s the interest on the model increased due to its potential application to ferroelectric perovskites.\(^3\)\(^9\) The model in any bipartite lattice can be written as:

\[
H = H_0 + H_t; \quad H_0 = \frac{\Delta}{2} \sum_{i \sigma} (-1)^i n_{i \sigma} + U \sum_i n_{i \uparrow} n_{i \downarrow},
\]

\[
H_t = -t \sum_{i \delta \sigma \delta' \sigma'} c_{i+\delta \sigma}^\dagger c_{i \delta \sigma'},
\]

where \(i + \delta\) denote the nearest neighbors of site \(i\), and odd \(i\) correspond to the sublattice with on-site energy \(-\Delta/2\).

At zero temperature, in the strong coupling limit \(t = 0\), the system is in the Mott insulating (MI) phase for \(U > \Delta\) (all sites are singly occupied), and in the bond insulating (BI) phase for \(U < \Delta\) (all sites with odd \(i\) doubly occupied). In one dimension (1D), for finite \(t\), field theory calculations pointed out the existence of a third intermediate phase, the spontaneous dimerized insulator (SDI) between the other two.\(^8\) For fixed \(\Delta\), as \(U\) increases, first a transition at \(U_c\) (involving mainly charge degrees of freedom) between the BI and the SDI takes place, and then for \(U_s > U_c\), the spin gap closes as in usual Kosterlitz-Thouless transitions. The physics has some similarities to that of the extended Hubbard model for small \(U\) and nearest-neighbor repulsion \(V\).\(^9\)\(^-11\)

The phase diagram of the 1D IHM has been calculated numerically using the method of jumps of Berry phases,\(^9\) which in this case coincides with the method of crossings of appropriately chosen excited states.\(^9\)\(^10\) The charge Berry phase is a measure of the polarization and therefore detects the ferroelectric charge transition,\(^4\)\(^-6\) while the spin Berry phase jumps at the point where the spin gap closes.\(^12\) For small \(t\), \(U_s - U_c \approx 0.6t\) was obtained for the width of the SDI phase.\(^9\)

Due to the fact that the spin gap is exponentially small for \(U\) smaller but near \(U_s\), direct numerical calculation of it or of appropriate correlation functions are unable to find a sharp transition at \(U_s\).\(^13\)\(^14\) The same difficulty happens in the Hubbard chain with correlated hopping.\(^15\)

where the existence and position of the transition is confirmed by field theory\(^16\)\(^17\) and exact\(^18\) results. In the IHM some controversy remains about the existence of \(U_s\) and the nature of the phase for \(U > U_c\) in the case of absence of a second transition. Wilkens and Martin\(^13\) suggested that the MI phase does not exist (the spin gap remains open for any finite \(U\)). This is in contradiction with the strong coupling expansion for \(t \ll U - \Delta\), which maps the IHM onto an effective spin Hamiltonian \(\tilde{H}\) with closed spin gap.\(^2\)\(^14\) Wilkens and Martin\(^13\) argued that since \(\tilde{H}\) has an additional symmetry with respect to \(H\) (translation to a nearest neighbor \(T_3\)), \(\tilde{H}\) seems to have lost part of the physics of \(H\), which might be essential.

Recently, a detailed study of different observables of the 1D IHM was made, using density-matrix renormalization group (DMRG), including a careful finite-size scaling analysis.\(^19\) The results indicate the present of two transitions and are consistent with the phase diagram found using topological transitions,\(^9\) although a smaller width of the SDI phase is suggested. Surprisingly, the authors find a power law decay of charge-charge correlation functions in the MI phase, in spite of a the presence of a charge gap \(\sim U - \Delta\).

Here I report calculations of charge expectations values, and in one dimension, the long distance behavior of charge-charge and bond-bond correlation functions using the mapping to a spin Hamiltonian, valid for \(t \ll U - \Delta\). This might seem surprising at first sight, since charge fluctuations are frozen in \(\tilde{H}\). However, the relevant information is contained in the transformed operators. This has some similarities with the case of the cuprates, in which Cu and O contributions to the photoemission spectra were successfully calculated using effective one-band models.\(^20\)\(^-23\) Also, while a \(t-J\) model is enough to explain the observed dispersion in photoemission measurements in Sr\(_2\)CuO\(_2\)Cl\(_2\), the mapping of the operators\(^24\)\(^25\) is crucial to explain the observed intensities.\(^25\)

The transformation on the operators is performed in Section II. Section III contains the results for expectation values of different quantities, and Section IV is a discussion.
II. THE CANONICAL TRANSFORMATION

In this Section, I use the canonical transformation plus projection onto the low-energy subspace that maps $H$ into a spin Hamiltonian $\tilde{H}$, to transform charge and bond operators in one direction ($\delta = \pm 1$)

$$n_i = n_i^\dagger + n_i, \quad b_i = \sum_{\delta \sigma} \delta(c_{i+\delta \sigma}^\dagger c_{i \sigma} + \text{H.c.}),$$

(2)

and discuss some symmetry properties. For our purposes, it is enough to work up to second order in $t/(U - \Delta)$. Thus

$$\tilde{H} = Pe^{-S}He^S P = P(H + [H,S] + \frac{1}{2}[[H,S],S] + \ldots) P,$$

(3)

where $P$ is the projector over the ground state subspace of $H_0$, in which $n_i \equiv 1$ for all $i$, and $S$ is chosen in such a way that linear terms in the hopping term $H_1$ are eliminated: $H_1 + [H_0,S] = 0$. Taking matrix elements of this equation between eigenstates of $H_0$, one obtains:

$$\langle n|S|m \rangle = \frac{\langle n|H_1|m \rangle}{E_m - E_n},$$

(4)

where $E_j$ is the energy of the eigenstate $|j\rangle$ of $H_0$. From Eqs. (3) and (4), proceeding in a similar way as done below, one obtains the known result:  

$$\tilde{H} = \frac{4t^2U}{(U^2 - \Delta^2)} \sum_{\langle ij \rangle} (S_i \cdot S_j - \frac{1}{4}).$$

(5)

The most important correction to $\tilde{H}$ in higher order is a next-nearest-neighbor exchange of order $t^4$, which does not affect the physics for $t \ll U - \Delta$. The effective Hamiltonian $\tilde{H}$ to all orders in $t$ is invariant under a nearest-neighbor translation $T_\delta$, while $H$ is not. This is simply a consequence of the fact that to all orders $\tilde{H}$ is a purely spin Hamiltonian, since the charge degrees of freedom are frozen ($n_i \equiv 1$ for all $i$). Then $\tilde{H}$ is invariant under the electron-hole transformation $T_{ch}: c_{i \sigma}^\dagger \rightarrow \sigma c_{i \sigma}$, which leaves invariant all spin operators. Since the original Hamiltonian $H$ is invariant under the product $T_\delta T_{ch}$, then $H$ should also be invariant under $T_\delta$. However other transformed operators, like $\tilde{n}_i$, below, are not invariant under $T_\delta$.

The transformed charge operator is:

$$\tilde{n}_i = Pe^{-S}n_ie^S P \cong P(n_i + [n_i,S] + \frac{1}{2}[[n_i,S],S]) P = 1 + P(SS - Sn_iS)P.$$

(6)

In the second equality I used the fact that $S$ applied to any state of the ground state manifold of $H_0$, gives an excited state. The only terms of $-PSn_iSP$ which do not cancel with $PSSP$ are those in which $n_i = 0$ or $n_i = 2$ after the first application of $S$. Using Eq. (4):

$$\tilde{n}_i = 1 + \sum_{\delta \sigma \sigma'} P[\frac{t}{U - (-1)^\delta \Delta} c_{i \sigma}^\dagger c_{i+\delta \sigma} c_{i+\delta \sigma'} c_{i \sigma'} + \frac{t}{U + (-1)^\delta \Delta} c_{i+\delta \sigma} c_{i \sigma} c_{i \sigma'} c_{i+\delta \sigma'}] P.$$

(7)

The first (negative) term correspond to charge $n_i = 0$ in the intermediate state and the excitation energy is $E_n - E_m = U + (-1)^{i+\delta} \Delta/2 - (-1)^i \Delta/2 = U - (-1)^i \Delta$. The sums over spins can be transformed as follows:

$$\sum_{\sigma \sigma'} Pc_{j \sigma}^\dagger c_{i \sigma} c_{i \sigma'} c_{j \sigma'} P = \sum_{\sigma \sigma'} Pc_{j \sigma}^\dagger c_{j \sigma'} (\delta_{\sigma \sigma'} - c_{i \sigma}^\dagger c_{i \sigma} P = \sum_{\sigma} Pn_{j \sigma}(1 - n_{i \sigma})P = S_j^+ S_i^- - S_j^- S_i^+ = \frac{1}{2} - 2S \cdot S_j.$$

(8)

And replacing this in Eq. (7):

$$\tilde{n}_i = 1 - (-1)^i \frac{2U \Delta t^2}{(U^2 - \Delta^2)^2} \sum_\delta (1 - 4S_i \cdot S_{i+\delta}).$$

(9)

This equation relates a charge operator with a purely spin operator. Although this might seem surprising at first sight, it is clear that in the strong coupling limit, virtual charge fluctuations are inhibited only for a ferromagnetic alignment of the spins. This shows that for finite $U$, some charge degrees of freedom remain coupled with spin, in contrast to the usual Hubbard model ($\Delta = 0$).

Using Eq. (2), to leading order in $t$, the transformed bond operator is:

$$\tilde{b}_i = Pe^{-S}b_ie^S P \cong P[b_i,S] P = \sum_{\delta \sigma \sigma'} \delta P[\frac{t}{U + (-1)^\delta \Delta} c_{i+\delta \sigma} c_{i \sigma} c_{i \sigma'}^\dagger c_{i+\delta \sigma'}^\dagger + \frac{t}{U - (-1)^\delta \Delta} c_{i \sigma}^\dagger c_{i+\delta \sigma} c_{i+\delta \sigma'} c_{i \sigma'} + \text{H.c.}] P.$$

(10)

The first term correspond to acting first with $S$ creating an excitation with a doubly occupied site at $i$, and an empty site at $i + \delta$, and then with $b_i$, restoring occupation 1 at each site. Using Eq. (8), I obtain:

$$\tilde{b}_i = \frac{-8tU}{U^2 - \Delta^2} \sum_\delta \delta S_i \cdot S_{i+\delta}.$$

The second member is a local measure of the asymmetry between the spin “bonds” involving site $i$ in the direction of $\delta$. Here there is no essential difference with the result for the ordinary Hubbard model.
III. OBSERVABLES AND CORRELATION FUNCTIONS

For $t \ll U - \Delta$, using Eq. (9) the amplitude of the charge density wave is given by:

$$A = \langle n_i - n_{i+\delta} \rangle_H = \langle \tilde{n}_i - \tilde{n}_{i+\delta} \rangle_H$$

$$= 2a \sum_\delta (1 - 4 \langle S_i \cdot S_{i+\delta} \rangle_H),$$

(11)

where the subscript in the expectation values indicates the Hamiltonian with which they are calculated and

$$a = \frac{2U\Delta t^2}{(U^2 - \Delta^2)^2}.$$  

(12)

In 1D, from the Bethe ansatz solution $1/4 - \langle S_i \cdot S_{i+\delta} \rangle_H = \ln 2 \approx 0.69$. This gives $A \approx 11.09a$. This result has also been obtained using Hellman-Feynman theorem and is in very good agreement with DMRG results.\cite{Note1}

For the square lattice $\langle S_i \cdot S_{i+\delta} \rangle_H \approx -0.3347$, and then $A \approx 18.74a$. In three dimensions, spin waves is a good approximation and gives $\langle S_i \cdot S_{i+\delta} \rangle_H \approx -0.3028$ which leads to $A \approx 26.9a$.

The charge-charge correlation function is given by:

$$C_d = \langle n_i n_{i+d} \rangle_H - \langle n_i \rangle_H \langle n_{i+d} \rangle_H.$$  

(13)

To leading order, I can approximate $\langle n_i n_{i+d} \rangle_H \approx \langle \tilde{n}_i \tilde{n}_{i+d} \rangle_H$. The neglected term (see Eq. (6) ) $\langle P e^{-S_i} e^{S_{i+d}} \rangle_H$ involves charge fluctuations across the energy gap and therefore should lead to an exponentially decaying contribution, as in the usual Hubbard model. Using Eq. (9) in the form $\tilde{n}_i = 1 - (-1)^i 4aS_i \cdot S_{i+\delta} - z(-1)^ia + O(t^4)$, where $z$ is the number of nearest neighbors, and dropping the subscript $H$, one obtains to leading order in $t$:

$$C_d = 16a^2(-1)^d \sum_{\delta'} \left[ \langle S_i \cdot S_{i+\delta} \rangle \langle S_{i+d} \cdot S_{i+d+\delta} \rangle \right]$$

$$- \langle S_i \cdot S_{i+\delta} \rangle \langle S_{i+d} \cdot S_{i+d+\delta} \rangle.$$  

(14)

Note that the terms $O(t^4)$ in $\tilde{n}_i$ cancel exactly in Eq. (13). Thus, it is enough to include terms up to order $t^2$ in $\tilde{n}_i$ to obtain the result up to order $t^4$ in $C_d$. Using symmetry, I can write:

$$\langle S_i \cdot S_{i+\delta} \rangle \langle S_{i+d} \cdot S_{i+d+\delta} \rangle = 3\langle S_i^z S_{i+d}^z \rangle \langle S_{i+\delta}^z S_{i+d+\delta}^z \rangle$$

$$+ 6\langle S_i^z S_{i+d}^z S_{i+\delta}^z S_{i+d+\delta}^z \rangle,$$

(15)

and similarly for the other term inside square brackets of Eq. (14).

In 1D, the leading power-law decay can be determined using bosonization expressions for the XXZ model and correlation functions of the gaussian model.\cite{Note2} However, at the isotropic point, there are important logarithmic corrections. They can be calculated using expressions derived by Giamarchi and Schulz.\cite{Note3} Using $S_i^z \approx \cos(\pi l + \sqrt{2}\varphi(x))$ for the slowest decaying part of $S_i^z$,

the operator product expansion $S_i^z S_{i+\delta}^z \approx \cos(2\sqrt{2}\varphi(x))$, and

the results of section III B of Ref. 30, I obtain:

$$\langle S_0^z S_{d}^z S_{d+\delta}^z \rangle \approx d^{-4} \ln^{-2} d.$$  

(16)

Using symmetry again:

$$\langle S_0^z S_{d}^z S_{d+\delta}^z \rangle = \frac{1}{8} \sum_{\delta'} \langle S_\delta^z S_{-\delta}^z + S_0^z S_{\delta}^z \rangle \langle S_{d+\delta}^z S_{d-\delta}^+ + S_d^z S_{d+\delta}^+ \rangle$$

$$- \langle S_0^z S_{d}^z S_{d+\delta}^z \rangle.$$  

(17)

The first term in this equation turns out to be the dominant one, and therefore I explain it in more detail. Performing a Jordan-Wigner transformation from spin operators to fermions with annihilation operators $a_j$, going to the continuum limit using $a_j = i\partial L(x) + (-i)^j R(x)$, with $x = ja$, and then bosonizing one gets:

$$\sum_{\delta} \langle (a_j a_{j+\delta} + \text{H.c.}) \rangle$$

$$\rightarrow \sum_{\delta} \langle \delta^4 L(x) R(x + a\delta) + (-i)^4 R^4(x) R(x + a\delta) + (-1)^4 (-i)^4 R^4(x) R(x + a\delta) + (-1)^4 (-i)^4 R^4(x) \rangle$$

$$\rightarrow 2i[\partial L \partial R - R^4 \partial R^4 - (-1)^4 \partial L \partial R + (-1)^4 \partial R \partial R^4]$$

$$= 2i[2L \partial L - 2R \partial R + (-1)^4 \partial \partial R^4] + \text{c.c.}$$

$$\sim 2 \cos(\sqrt{2}\varphi(x))$$

(18)

where $c$ is a nonuniversal constant of the order of one.

I would like to remark that the bosonic fields $\varphi, \theta$ are not pure spin operators of the original Hamiltonian Eq. (1), because they come from operators already dressed by the transformation. The expression of the transformed original fermions for $\Delta = 0$ and any filling to lowest order in $t/U$ can be found in Refs. 24,25.

The first two terms of the last member of Eq. (18) lead also to contributions of order $1/d^4$ (without including logarithmic corrections). Using\cite{Note3}:

$$\langle \cos(\sqrt{2}\varphi(x)) \rangle \cos(\sqrt{2}\varphi(y)) \sim \frac{1}{|x - y|^{3/2}},$$

(19)

together with Eqs. (14) to (19), I finally obtain (except for some factor of the order of one):

$$C_d \approx 4\frac{U^2 \Delta t^4}{(U^2 - \Delta^2)^2} d^3 \ln^{-3/2} d.$$  

(20)

Note that factors $(-1)^d$ cancel, and then in spite of the even-odd oscillations in $\langle n_j \rangle$, these oscillations are absent in the charge-charge correlation functions.

Concerning the bond-bond correlation functions, using Eqs. (10), (19) and $\sum_\delta S_i \cdot S_{i+\delta} \sim \cos(\sqrt{2}\varphi(x))$, one obtains:
\[ \langle b_i b_{i+d} \rangle \approx 64 \frac{U^2 t^2}{(U^2 - \Delta^2)^2} (-1)^d d^{-1} \ln^{-3/2} d. \] (21)

These are much smaller than the spin-spin correlation functions, which behave like \( \langle S_i^x S_{i+d}^x \rangle \approx d^{-1/2} d \) at large distances, and have a larger prefactor.

**IV. DISCUSSION**

I have calculated several quantities of the ionic Hubbard model, using a mapping to a spin Hamiltonian valid for \( U > \Delta \) and \( t \ll U - \Delta \). In this limit the system is expected to be in the MI phase. This prediction is to be the case in 1D,8,9 and in fact the absence of a spin gap in the effective transformed Hamiltonian \( \tilde{H} \) is consistent with this.2,14 Also, the bond-bond correlation functions decay faster than the spin-spin ones at large distances, in contrast to what is expected in the SDI.

By construction, the symmetry of the observables is independent of the basis in which they are calculated, and this becomes clear after transformation of the operators. For example, the charge operator \( n_i \) is invariant under translation of one lattice parameter \( T \), while \( H \) is not. These symmetry properties are interchanged in the transformed operators \( \tilde{n}_i \) and \( \tilde{H} \), and the expectation value \( \langle \tilde{n}_i \rangle_H = \langle \tilde{n}_i \rangle_{\tilde{H}} \) is not invariant under \( T \). As a consequence, for any finite \( U \) there is a charge density wave. Its amplitude for \( t \ll U - \Delta \) is proportional to \( t^2 U/(U^2 - \Delta^2)^2 \) but with a coefficient larger than 20 which depends on dimension, and is near 53 in three dimensions.

The charge-charge correlation functions in 1D decay as \( d^{-3/2} \ln^{-3/2} d \) as a function of distance \( d \) for large \( d \) with a prefactor proportional to \( t^2 \Delta^2 \), in excellent agreement with recent DMRG calculations.9 This result for a finite charge gap, is in marked contrast to the general behavior found in 1D systems and is a consequence of the fact that coupling between charge and spin dynamics remains at low energies in the original basis (effective dressed charge and spin fields are separated at low energies). This fact is at variance with the low-energy spin-charge separation that takes place in translationally invariant models with quite general nearest-neighbor interactions17 (including the extended Hubbard model with nearest-neighbor repulsion \( V \) and the Hubbard model with correlated hopping10,16,17). An important difference is that in weak coupling the charge-spin interaction is a relevant operator in the IHM.14

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