Numerical study of a superconductor-insulator transition in a half-filled Hubbard chain with distant transfers

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The ground state of a one-dimensional Hubbard model having the next-nearest neighbor hopping \((t')\) as well as the nearest-neighbor one \((t)\) is numerically investigated at half-filling. A quantum Monte Carlo result shows a slowly decaying pairing correlation for a sizeable interaction strength \((U \leq 2t)\), while the system is shown to become insulating for yet larger \(U > U_C \sim 3t\) from a direct evaluation of the charge gap with the density-matrix renormalization group method. The results are consistent with Fabrizio’s recent weak-coupling theory which suggests a transition from a superconductor into an insulator at a finite \(U\).

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For the past several years, the existence of a gap in the spin excitation has been suspected to be a key in the superconductivity in one-dimensional (1D) strongly correlated systems. This view has motivated intensive studies on ladder systems and systems with dimerized or frustrated spin-spin interactions. Some of these studies have revealed that the existence of a spin gap can indeed lead to a dominance of pairing correlations even in purely repulsive models. More recently, Fabrizio studied a 1D Hubbard model having the next-nearest neighbor (NNN) hoppings in addition to nearest-neighbor (NN) ones. Such a model may have some relevance to the 1D cuprates with large ratios of next-nearest neighbor (NNN) hoppings in addition to nearest-neighbor (NN) ones. Such a model may have some relevance to the 1D cuprates with large ratios of NNN to NN transfers, such as SrCuO\(_2\) having a zigzag structure or the recently discovered superconductor, Sr\(_{0.4}\)Ca\(_{13.6}\)Cu\(_{24}\)O\(_{41.8}\)\(_x\), where layers of 2-leg ladders alternate with layers of 1D chains with 90° Cu-O-Cu bond angles. Making use of a weak-coupling renormalization, Fabrizio has predicted the existence of a spin gap in a certain parameter regime and also a ‘superconductor-insulator transition’ (or more precisely a transition from a metal with dominating pairing correlation to an insulator since we are talking about 1D systems) at a certain Hubbard interaction \(U = U_C\) at half-filling. A transition from a superconductor directly into an insulator is intriguing, but it is beyond the scope of the weak-coupling theory to establish where (i.e., for which finite value of the interaction strength) the transition actually takes place.

The purpose of the present study is to look into the transition numerically, and to actually evaluate \(U_C\). Our strategy here is to employ two complementary approaches: the quantum Monte Carlo (QMC) method for small \(U\)’s and the density-matrix renormalization group (DMRG) for large \(U\)’s. Combination of the two has indeed enabled us to establish the existence of such a transition at \(U_C \sim 3t\).

The Hamiltonian under consideration is given, in standard notations, as

\[
\mathcal{H} = -t \sum_{i\sigma} (c_{i\sigma}^\dagger c_{i+1\sigma} + \text{h.c.}) - t' \sum_{i\sigma} (c_{i\sigma}^\dagger c_{i+2\sigma} + \text{h.c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow},
\]

(1)

where \(t\) and \(t'\) are NN and NNN hoppings, respectively, and \(U\) is the Hubbard repulsion. We focus our attention to half-filling, \(n = 1\), where the signs of \(t\) and \(t'\) are irrelevant due to an electron-hole symmetry. Here we shall take \(t > 0\) and \(t' < 0\).

Let us first recapitulate Fabrizio’s weak-coupling theory. If \(|t'/t|\) is small enough, the system can be mapped to the \(t' = 0\) case, because there is no essential difference in the vicinity of the Fermi level. For \(|t'| \geq t_c(n)\), on the other hand, the Fermi level intersects the one-electron band at four \(k\)-points (\(\pm k_F^1\) and \(\pm k_F^2\)), where \(t_c(n)\) is a function of the band filling (with \(t_c(1) = 0.5t\)). Namely, there are two right-moving and two left-moving branches in the terminology of the weak-coupling Tomonaga-Luttinger (TL) theory. When the Umklapp processes are absent, the situation is, as far as the weak-coupling picture is concerned, essentially identical to the two-leg Hubbard ladder, where a spin gap opens when the two Fermi velocities are not too different. Thus a spin gap also opens in the present model for a certain range of the ratio of the Fermi velocities, i.e., for \(|t'| > t'_c(n)\)(\(> t_c(n)\)). In the presence of a spin gap, the pairing correlation dominates for small enough \(U\) in the two-leg ladder when doped (i.e., at non-half-filling) and this is also the case with the present NNN model.

An important difference, however, appears at half-filling, where Umklapp processes emerge. In the two-leg ladder, in which the Umklapp process is a two-electron scattering process at half-filling, an infinitesimal \(U\) is enough to make the Umklapp process relevant in the renormalization, leading to an opening of a charge gap. In contrast, Umklapp processes are only higher-order at half-filling in the present NNN model, in which a four-electron scattering is involved.

The dominant pairing considered in Fabrizio’s weak-
coupling picture is
\[ c_{k_1^+c^* - k_2^+c^*} - c_{k_1^+c - k_2^+c} \],
(2)
which has the correlation function of the form \( \sim 1/r^{1/2K} \)
\((r: the real space distance). This pairing dominates over
a charge-density wave (or dimer wave in Fabrizio’s termin-
ology) whose correlation is \( \sim 1/r^{2K} \). If we assume that
the analysis may be extended to finite \( U \)'s, the renor-
malization equation has such a structure that \( K \geq 0.5 \) for
\( U \leq U_C \) (with \( K \rightarrow 1 \) for \( U \rightarrow +0 \)), where the pair-
ing correlation is the most slowly- decaying \( 1/r^{0.5} \) in the
weak-coupling limit as in doped two- and three-
leg Hubbard ladders). As \( U \) is increased the Um-
lapp process becomes relevant to make the system insu-
lating precisely when the two functional forms coincide
\( 1/r^{1/2K} = 1/r^{2K} \), i.e., at \( U = U_C \).

Now let us turn to our numerical analysis for finite \( U \)'s.
We take \( t' = -0.8t \) as a typical value of \( t' > t_c = 0.5t \).
We first present the QMC result of the pairing correlation
function in the ground state. We have adopted the pro-
jector Monte Carlo method, in which we implement the
stabilization procedure adopted by several authors.

We have taken projecting time \( \tau \) of up to \( \sim 60/t \) with
Trotter slices \( L \) of \( \tau/L \leq 0.2/\bar{U} \) to assure the con-
vergence of the correlation function. The details of the
calculation is similar to that for the two-leg Hubbard
ladder in ref. 5. We take 60 electrons on 60 sites with
\( t' = -0.78t \). For this set of parameters, the energy levels
of the two branches of the one-electron band structure
becomes very close to each other at the Fermi level. It
has been revealed for two-leg and three-leg Hubbard
ladders that such an alignment is desirable to mimic infinite
systems, and is indeed necessary in order to obtain corre-
lation functions consistent with the weak-coupling theory
at large distances. This applies to the present model as
well. As suggested in ref. 5, this may be an indication that
the offset between the discrete energy levels has to
be smaller than the spin gap in order to obtain results
consistent with the weak-coupling theory in finite size
systems.

For this parameter set the Fermi wave numbers satisfy
a relation \( k^1_F - k^2_F = \pi/2 \), so that the relevant pairing
correlation becomes NNN pairs in real space according to
eqn.2, since \( | \exp(i k^1_F \Delta x) - \exp(i k^2_F \Delta x) | \) takes its maxi-
mum at \( \Delta x = 2 \). Thus we study the pairing correlation,
\[ P(r) \equiv \langle \hat{O}^\dagger \hat{O} \rangle \]
\[ \hat{O} = (c^{+}_{i1} c^*_{i1+2} - c^{+}_{i4} c^*_{i4+2}) / \sqrt{2}. \]
(3)

Figure 1 shows the pairing correlation function for a pe-
riodic 60-site system with \( U = t \). The pairing correlation
is clearly enhanced over the non-interacting case, and a
slowly decaying component close to \( 1/r^{0.5} \) can be seen
at large distances. The behavior is similar to that for
two-leg and three-leg Hubbard ladders.

Figure 2 is a similar plot for a larger \( U = 2t \), about the
largest \( U \) for which the negative-sign problem in QMC is
overcome. In this case, the enhancement is smaller than
that for \( U = t \), which suggests that the exponent \( K \) is in-
deed a decreasing function of \( U \). However, the existence
of the enhancement itself implies that the charge gap is
still closed there, because otherwise the pairing correlation
would decay exponentially. The exponent at large
distances is seen to be close to unity, which indicates
a proximity to the superconductor-insulator transition,
so that \( U_C \) should lie somewhere above, but not too far
from, \( U = 2t \).

FIG. 1. QMC result for the pairing correlation function,
\( P(r) \), plotted against the real space distance \( r \) in a
60-site half-filled Hubbard ladder with \( U = t \) and \( t' = -0.78t \).
The dashed line is the noninteracting result for the same sys-
tem size, while the straight dashed line represents \( \sim 1/r^{0.5} \).
The pairing correlation function takes negative values at dis-
tances \( r = 8, 16, 24 \), which are omitted in the plot.

FIG. 2. A plot similar to Fig.1 for \( U = 2t \) and \( t' = -0.78t \).
The straight dashed line represents \( \sim 1/r \).
The regime with larger \( U \) is exactly where we can introduce the DMRG method. The calculation has been done for system sizes up to \( L = 28 \) sites with \( t' = -0.8t \) here with an open boundary condition. We have kept up to 120 states per block with truncation errors smaller than \( 10^{-4} \) and mostly around \( 10^{-5} \sim 10^{-6} \). The charge gap \( \Delta_C(N) \) and the spin gap \( \Delta_S(N) \) for a half-filled \( N \)-site system are calculated by

\[
\Delta_C(N) = \frac{[E(N/2 + 1, N/2 + 1) + E(N/2 - 1, N/2 - 1) - 2E(N/2, N/2)]}{2},
\]

\[
\Delta_S(N) = E(N/2 + 1, N/2 - 1) - E(N/2, N/2),
\]

respectively, where \( E(N_{\uparrow}, N_{\downarrow}) \) is the ground state energy for \( N_{\uparrow} \) up-spin and \( N_{\downarrow} \) down-spin electrons. We have checked that as far as these quantities and the parameter values adopted here are concerned, \( \sim 100 \) states per block suffice for the convergence.

Figure 3 displays the charge gap for various values of \( U \) as a function of \( 1/L \) (the inverse system size). The results for 8- and 10-site systems are also obtained from the exact diagonalization in order to check the DMRG result. The system-size dependence is least-squares fit to second-order polynomials in \( 1/L \). The extrapolation to \( L \to \infty \) shows that the charge gap closes at \( U_C \sim 3t \). Although the estimated \( U_C \) may contain some errors due to finite-size effects, this result is consistent with the above QMC result that the pairing correlation exists for \( U = 2t \), which serves as a lower boundary for the existence of a spin gap. Thus the complementary QMC and DMRG results can indeed be combined to indicate a superconductor-insulator transition somewhere around \( 2t < U < 3t \).

**FIG. 3.** DMRG evaluation of the charge gap \( \Delta_C \) at \( t' = -0.8t \) plotted against \( 1/L \) for various values of \( U \). Dashed curve is a least-squares fit with second order polynomials in \( 1/L \).

The existence of a metallic phase at half-filling having a spin gap and a dominating pairing correlation is rather surprising. One might be tempted to explain the origin of the spin gap and superconductivity by regarding the model as essentially the same as the ‘\( t'-J-J' \)' model, where electrons hop with excluded double occupancies and interact with NN and NNN antiferromagnetic exchanges. This view, however, cannot be valid, because we are sitting on the half-filled point, where the \( t-J-J' \) model is trivially insulating. In this sense the spin gap in the metallic phase of the present model may not be regarded as simply arising from a frustration in antiferromagnetic exchange interactions \((J, J')\), which is consistent with Fabrizio’s remark in ref. 10 on the inverse doping effects on the spin gap between the present model and the \( t-J-J' \) model.

Finally we evaluate the spin gap using DMRG. Although the spin gap is a key concept in our motivation mainly in the metallic phase, we present here the result for the insulating phase, which is of greater interest in the context of strongly correlated systems such as 1D cuprates. The study of the spin gap in the metallic phase will be presented elsewhere. We have evaluated the magnitude of the spin gap at \( U = 8t \) with the same value of \( t' \) as above. In fig., we plot \( \Delta_S \) as a function of \( 1/L \). The extrapolation to the thermodynamic limit suggests an existence of a spin gap as large as \( \sim 0.16t \sim 0.17t \).

**FIG. 4.** DMRG evaluation of the spin gap for \( U = 8t \) and \( t' = -0.8t \) plotted against \( 1/L \).

To summarize, a transition from a metallic state with a dominating pairing correlation into an insulating state has been shown to occur at an intermediate strength of the interaction of \( \sim O(t) \). Further studies for other values of \( t' \) and \( U \), and for the doped phase is under way.

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