Phase diagram of the $t-t'-U$ chain at half filling

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We study the half filled Hubbard chain including next-nearest-neighbor hopping $t'$. The model has three phases: one insulating phase with dominant spin-density-wave correlations at large distances (SDWI), another phase with dominant spin-dimer correlations or dimerized insulator (DI), and a third one in which long distance correlations indicate singlet superconductivity (SS). The boundaries of the SDWI are accurately determined numerically through a crossing of excited energy levels equivalent to the jump in the spin Berry phase. The DI-SS boundary is studied using several indicators like correlation exponent $K_{\rho}$, Drude weight $D_{\rho}$, localization parameter $z_L$ and charge gap $\Delta_c$.

INTRODUCTION

Superconductivity in low dimensional systems has been a subject of interest in the last years. The physics of the negative-$U$ Hubbard model\textsuperscript{1} as well as that of the ladder\textsuperscript{2,3} suggest that the opening of a spin gap $\Delta_s$ is a key ingredient to superconductivity. In fact, a non zero $\Delta_s$ suggests the existence of bound pairs of electrons (like Cooper pairs), which if mobile can lead to a SS state. The indications of resonance valence bond superconducting states in effective low energy models for 2D cuprates, like the generalized $t-J$\textsuperscript{4,5} or the Hubbard model with correlated hopping\textsuperscript{6} are also consistent with this picture. Closely related with the latter system is the Hubbard model with an extra nearest-neighbor exchange $J'$\textsuperscript{7} for which also strong signals of superconductivity have been found.\textsuperscript{8,9}

The half-filled Hubbard model with additional next-nearest-neighbor hopping $t'$ in one dimension is appealing because, for weak $U$, one expects the existence of a metallic phase when $t'>0.5t$,\textsuperscript{10,11} and, from previous studies of the frustrated Heisenberg chain,\textsuperscript{12,13} one expects the opening of a spin gap for large $U$ and $t'/t>\sqrt{R_c}$ with $R_c=0.241167$.\textsuperscript{14} In addition, this model might be valid as an effective model for several one dimensional cuprates.\textsuperscript{14,15} The corresponding Hamiltonian is:

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

Using weak coupling renormalization group, Fabrizio obtained that a spin gap opens for $t'>0.5t$, and that for $\Delta_s \neq 0$ SS correlations dominate in the metallic phase while spin dimer correlations are the largest at long distances in the insulating phase.\textsuperscript{16} Later studies using density matrix renormalization group (DMRG) sketched an approximate phase diagram,\textsuperscript{16} confirmed the SS character in the metallic phase,\textsuperscript{17} and determined some points where approximately the charge transition SS-DI takes place.\textsuperscript{17,18}

In this work we present further evidence of the dominance of SS correlations in the metallic phase by calculating the correlation exponent $K_{\rho}$. We also obtain more information on the metal-insulator transition using numerical calculations of the Drude weight $D_{\rho}$, localization indicator $z_L$\textsuperscript{19,20,21} and charge gap $\Delta_c$. Furthermore, we determine the opening of the spin gap $\Delta_s$ using the crossing of singlet and triplet excitations.\textsuperscript{12,22} which is equivalent to the jump of the spin Berry phase.\textsuperscript{23} This method has been shown before to lead to very accurate results for this transition, even if the size $L$ of the systems considered is less than 13.\textsuperscript{5,22,24,25,26,27,28,29} As an example, the resulting opening of the spin gap for the Hubbard model with correlated hopping\textsuperscript{5,27} coincides with field theory results in the weak coupling limit,\textsuperscript{5,30} and with exact results when the number of doubly occupied sites is conserved.\textsuperscript{33} Moreover, this method allowed us to determine the complete boundary of the SDWI phase.

In Section II we present the results for the spin transition and briefly describe the method used. In Section III, we discuss our results for the correlation exponent $K_{\rho}$. In Section IV we explain briefly the meaning of the localization indicator $z_L$, present results for it, for the Drude weight $D_{\rho}$, and for the charge gap $\Delta_c$, and use this information to draw a tentative a phase diagram. Section V contains a summary and discussion.

THE SPIN TRANSITION

This transition can be determined by a topological transition (a jump in the spin Berry phase), which is equivalent to a suitable crossing of excited energy lev-
els. The basic idea of this crossing is that, in confor-
mal invariant systems (corresponding to fixed points in 
weak coupling theory plus renormalization group), the lowest excitation energy determines the dom-
inant correlations at large distances. In gauge invariant form, it can be numerically 
calculated as:
\[ \gamma_s = -\lim_{N \to \infty} \text{Im} \left[ \ln \Pi_{i=0}^{N-2} \langle g(\Phi_i, -\Phi_i)g(\Phi_{i+1}, -\Phi_{i+1}) \rangle \langle g(\Phi_{N-1}, -\Phi_{N-1})g(2\pi) \rangle \right]. \] (2)
where \( \langle g(\Phi_i, -\Phi_i) \rangle \) is the ground state of \( \hat{H}(\Phi_i, -\Phi_i) \), and \( \langle g(2\pi) \rangle = \exp\left[ \frac{2\pi i}{U} \sum_j J(n_j - n_{j+1}) \right] g(0, 0) \). The Hamiltonian \( \hat{H} \) differs from \( H \) in that the hopping term has the form \( -t \sum_{\sigma} \bar{c}_{i+1, \sigma} c_{i\sigma} e^{i\phi_{\sigma}/L} + \text{H.c.} \).

The Berry phase \( \gamma_s \) can take only two values: 0 or \( \pi \) (modulo \( 2\pi \)). The jump between these values is related to the change in the difference between electric polarization from spin up and down by \( \Delta \gamma_s = (2\pi/e) \Delta(P_1 - P_1) \).

The position of the jump of \( \gamma_s \) coincides with the singlet-triplet crossing of the energy levels: the crossing of a singlet even under inversion with an odd triplet, with \( K = 0 \). The boundary conditions are periodic (antiperiodic) for system lengths \( L = 4n \) \((4n + 2)\), with \( n \) integer (they are opposite to the so called closed shell ones).

The same crossing is the one which determines the opening of the spin gap (the Kosterlitz-Thouless transition in the spin sector) according to conformal field theory, after bosonizing the problem and using renormalization group. This theory predicts a \( 1/L^2 \) scaling of the transition point.

We have calculated the transition for \( L = 8, 12 \) and \( 16 \). The restriction to \( L \) values multiple of four is due to the fact that other system sizes lead to frustration of the spin-density waves (or classical antiferromagnetic ordering) expected for large \( U \). In particular, for \( t = 0 \) the even and odd sites are decoupled and, to avoid frustration of the AF classical order in each subsystem, \( L/2 \) should be even. We have fitted the resulting three points with a straight line \( a + b/L^2 \) in \( 1/L^2 \). The transition point in the thermodynamic limit is determined by \( a \) and its error gives an indication of the fit quality.

In Fig. 4 we show the results for the spin transition for \( U \leq 10 \) (we have chosen \( t = 1 \) as the unit of energy). For \( t' < 0.5 \) we obtain that the transition takes place at \( U = 0 \) for all \( L \). For positives values of \( U \), \( \gamma_s = \pi \) and \( \Delta_c = 0 \), while for negative \( U \), \( \gamma_s = 0 \) and \( \Delta_c \neq 0 \), as in the ordinary Hubbard model. At the point \( U = 0 \), \( t' = 0.5 \), the spin transition line deviates \( 90^\circ \), and for positive \( U \) its shape is like a nose, with a maximum value of \( t' = 0.564 \pm 0.001 \) taking place near \( U = 4.5 \). The errors of the points shown in Fig. 4 are less than 0.003.

Results for larger values of \( U \) are shown in Fig. 2. For \( t, t' \ll U \), to leading order in \( 1/U \) the model is equivalent to the Heisenberg chain including next-nearest-neighbor exchange:
\[ H = \sum_i \left( J S_i \cdot S_{i+1} + J' S_i \cdot S_{i+2} \right) \] (3)
with \( J = 4t^2/U \), \( J' = 4t'^2/U \). Previous studies of this model using the method of crossings of excitation levels plus a detailed knowledge of the size dependence have established the critical value \( R_c = (J'/J)_c \approx 0.241167 \) at the transition. Then, for \( U \to \infty \), \( \Delta_c \) should open at \( t'_c = \sqrt{R_c} \). Our results are consistent with this fact. A fit of our transition points at \( U = 15, 20, 30, \) and 50 with
the parabola $t'_e - \sqrt{R_e} = a + b/U + c/U^2$ gives $c = 3.6$ and $a = b = 0$ within our numerical error for $t'_e$ (less than $5 \times 10^{-4}$). The fact that $b = 0$ is also consistent with the strong coupling expansion: $b$ is proportional to the first correction to Eq. (9), which is of order $t^2t'/U^2$. However, the electron-hole transformation $c_{\sigma} \rightarrow c_{\sigma}$ changes the sign of both hoppings but should leave invariant the spin gap at half filling. Then, all the corrections to $H$ of order $1/U^2n$ with $n$ integer should either vanish or be irrelevant for the spin gap since they change sign under electron-hole symmetry.

**CORRELATION EXPONENT IN THE METALLIC PHASE**

In the metallic phase, the analysis based on bosonization and renormalization group [10] shows that there is only one gapless charge model and the spin modes are gapped ($\Delta_s \neq 0$). This analysis is valid at weak coupling and requires that $t' > 0.5$. In this case, there are four Fermi points at wave vectors $\pm k_{F1}$ and $\pm k_{F2}$. The decay of the different correlation functions at large distances is determined by the correlation exponent $K_\rho$. Depending on the value of this exponent, the slowest asymptotic decay corresponds either to spin dimer-dimer correlation functions or to superconducting ones. At half filling the former have the following decay:

$$\chi_{DW}(x) = \langle O_{DW}(x)O_{DW}(0) \rangle \sim \frac{\cos[2(k_{F2} - k_{F1})x]}{x^{2K_\rho}},$$

where $O_{DW}(x) = S^+(x)S^-(x + a) + S^+(x + a)S^-(x)$. (5)

For the dominant superconducting correlations one has

$$\chi_{SC}(x) = \langle \Delta(x)\Delta^\dagger(0) \rangle \sim \frac{1}{x^{1/2K_\rho}},$$

where

$$\Delta(x) = \sum_{p=\pm} \psi_{p_{k_{F1}\uparrow}}(x) : \psi_{-p_{k_{F1}\downarrow}}(x)$$

$$- \psi_{p_{k_{F2}\uparrow}}(x) : \psi_{-p_{k_{F2}\downarrow}}(x).$$

An analysis similar to that of Schulz [11] extended to this case with 4 Fermi points leads to the following relations involving the correlation exponent $K_\rho$:

$$\pi v_\rho = \frac{1}{\kappa n^2}, D_c = \frac{2v_\rho K_{\rho^2}}{\pi}.$$  

Here, the subscript 1 or 2 in $K_\rho$ is due to the fact that, in finite systems, when $K_\rho$ is calculated using these expressions the results differ. In the above equation $v_\rho$ is the charge velocity, $\kappa$ is the compressibility and $D_c$ is the Drude weight. In finite systems these quantities can be calculated as:

$$E(K = 2\pi/L) - E(K = 0) = \frac{2\pi}{L}v_\rho.$$  

$$\frac{1}{\kappa n^2} = L E(N + 2) + E(N - 2) - 2E(N).$$  

$$D_c = \frac{L}{2} \frac{\partial^2 E_0(L, \Phi)}{\partial \Phi^2} |_{\Phi = \Phi_0},$$

where $E(K)$ is the energy of the lowest singlet with total wave vector $K$, $E(L, N)$ is the ground state energy for length $L$ and $N$ particles, and $E_0(L, \Phi)$ is $E(L, \Phi)$ in the presence of a flux $\Phi h/(2\pi)$ threading the ring. Unless otherwise stated, the boundary conditions correspond to the “closed shell” ones (those which lead to the minimum energy): $\Phi = 0$ ($\pi$) for $N = 2n$ with $N$ odd (even).

The above equations lead to two independent ways of calculating $K_\rho$. A third possibility uses the geometric mean $\overline{K_{\rho}} = \sqrt{K_{\rho 1}K_{\rho 2}}$. In $K_{\rho 3}$ the charge velocity does...
not enter, and usually it leads to a more accurate result. The consistency of the three results in the thermodynamic limit is a test on the validity of the Luttinger liquid description, with gapless charge excitations. In fact, when the $K_{Dc}$ extrapolated to the thermodynamic limit start to deviate from each other one has a strong indication of a metal-insulator transition. For example, in the model with correlated hopping, the point where the $K_{Dc}$ start to deviate agrees with the jump in the charge Berry phase which corresponds to this transition.

In Fig. 3 we show the evolution of $K_{Dc}$ as $U$ increases, for $t' = 2.5$. Clearly, for $U = 10$ the extrapolated $K_{Dc}$ are inconsistent and the system is in the insulating phase. The metal-insulator transition seems to be near $U/t = 6$, where $K_{Dc} \sim 1/2$. For lower values of $U$, $K_{Dc}$ increases, which indicates that superconducting correlations are the dominant ones inside the metallic phase. This is in agreement with previous results.

![FIG. 4: Localization indicator $z_{Lc}$ and Drude weight $D_{c}$ as a function of $U/t$ for several system sizes $L$ and $t' = 2.5$.](image)

![FIG. 5: Same as Fig. 4 for $t' = 5$.](image)

THE CHARGE TRANSITION

In absence of disorder, the Drude weight $D_{c}$ defined in the previous section is an indicator of the metal-insulator transition. In particular, in the thermodynamic limit it should go to zero in the insulating phase. In recent years, Resta proposed to use as an alternative a localization indicator $z_{Lc}$. However, a simple symmetry argument shows that this expression gives an incorrect result for periodic systems with non integer number of particles per unit cell $n$. One of us and Ortiz have generalized this concept for correlated systems with rational $n$. Following a corresponding generalization for the charge Berry phase, in the present case, with $n = 1$ one has

$$z_{Lc} = |\langle g|e^{i\sum_{j}j_{\mu}n_{\mu}|g\rangle|\text{.}$$

and $z_{Lc} \to 0$ (1) for a metal (insulator) in the thermodynamic limit. Note that the operator entering Eq. (12) is a displacement operator in momentum space. Then, for an extended system with a well defined Fermi surface this operator shifts the Fermi surface and the scalar product vanishes ($z_{Lc} = 0$). Instead, for an uncorrelated band insulator the operator reproduces the same state and $z_{Lc} = 1$. Other cases with either disorder or correlations were also discussed before. One advantage of $z_{Lc}$ over $D_{c}$ is that it can be calculated with DMRG, although we are not considering this here.

In Fig. 4 we show the results for $D_{c}$ and $z_{Lc}$ as a function of $U$, for $t' = 2.5$ and $L = 8,12$. Both quantities vary smoothly with $U$. While the results point towards an insulating behavior for $U > 4t' = 10$ (in particular $z_{Lc} > 0.5$ and increases with system size) and a metallic behavior for small $U$ ($z_{Lc} \to 0$), it is not possible to determine accurately the critical value of $U$ for which the transition takes place. For large system sizes there is a level crossing in the ground state, and while for one of the states $z_{Lc}$ increases with $L$, for the other one $z_{Lc}$ decreases with size. This suggests to associate the crossing point with the metal-insulator transition, which gives $U_{c} = 1.75t'$. As showed in Fig. 5 when $t'$ is increased to $t' = 5$ the values of $D_{c}$ increase and those of $z_{Lc}$ decrease, suggesting an enlargement of the metallic region. However, from the dependence on $L$ of the corresponding quantities no safe conclusions can be drawn about the critical value of $U$ at which the transition takes place. For the same ratio $t' = 5$ we have also calculated numerically the charge gap, including DMRG results up to 20 sites, using the expression:

$$\Delta_{c} = E(L, N + 1) + E(L, N - 1) - 2E(L, N).$$
FIG. 6: Charge gap as a function of $1/L$ for $t' = 5$ and different values of $U$. From bottom to top: 2, 6, 8.5, 9, 10, and 20.

The results are shown in Fig. ?? together with a linear extrapolation to the thermodynamic limit. Although a straight line in $1/L$ fits well the results for all values of $U$, the extrapolated $\Delta_c$ becomes negative for $U \leq 6$, indicating again that finite size effects are important (since $\Delta_c$ should be either zero or positive). Nevertheless, for $U > 10$ it seems clear that the gap is open.

Unfortunately, the charge Berry phase does not jump at the metal-insulator transition, in contrast to the case of the Hubbard model with correlated hopping.[7, 27] The study of this transition using $K_{\rho i}, D_c, z_L$, and $\Delta_c$ as explained above is not enough to lead to a well defined phase boundary. With this information we can draw a tentative phase diagram, presented in Fig. 7 with large error bars for the metal-insulator DI-SS boundary. We also include some points obtained by other authors using larger systems.[17, 18] The boundary of the SDWI determined in section II is also plotted.

SUMMARY AND DISCUSSION

We have studied the phase diagram of the $t - t' - U$ model at half filling, using different quantities calculated mainly by numerical diagonalization of finite rings. Unfortunately, this model has large finite size effects in the regime in which there are four Fermi points in the non interacting case ($t' > 0.5t$). This can be checked by calculating correlation functions or other quantities as a function of size $L$ in the non interacting limit, either for a ring or with open boundary conditions. Kuroki et al. argue that one should choose system sizes for which the level structure of the different bands in the non interacting case is similar.[17]

The above mentioned difficulties prevented us to obtain quantitatively valid results for the metal-insulator transition. Nevertheless, our calculations of $K_{\rho}$ confirm the dominance of superconducting correlations in the metallic phase found earlier by analytical[10] and numerical[17] methods. Our tentative phase diagram also agrees with previous studies.[17, 18] For the spin transition, on the contrary, our results show the $1/L^2$ scaling expected from conformal field theory[12, 22] and, therefore, are reliable. Moreover, they converge with high precision to the known result in the strong coupling limit up to terms of order $1/U^2$. The jump of the spin Berry phase and the equivalent level crossing method have been successful in determining the opening of the spin gap in different SU(2) invariant models.[7, 22, 26, 27, 28, 29] and its validity has been confirmed by other analytical and numerical methods.[7, 27] In the present case, we became aware of recent DMRG results for this transition based on extrapolations of the dimer order parameter.[35] These results are very similar to ours except for a shift to larger $t'$ by about $\sim 0.7t$ for $U \sim 5t$. We believe that this might be due to difficulties in detecting an exponentially small dimerization order parameter or gap using DMRG.

An interesting question is what is the origin of the superconducting correlations in this system, where the only interaction is repulsive. An intuitive picture can be built starting from the strong-coupling limit $U \to \infty$, where the model is described by the spin Hamiltonian Eq. 3, whose properties are well known.[12] In the dimerized phase, at the Majumdar-Ghosh point $J' = 0.5J$ the ground state consists of nearest-neighbor spin singlets. These electron pairs are static and the system is insulating. However, when $U$ is reduced these pairs can overlap and become mobile, behaving similarly to bosons with short range repulsion, for which dominance of singlet superconducting correlations at large distance can be expected.
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