“Superconductor”-insulator transitions in a Hubbard chain with nearest-neighbor and bond-charge interactions

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We consider a half-filled generalized Hubbard chain with electron-hole symmetric correlated hopping and on-site and nearest-neighbor repulsions $U$ and $V$ respectively. In addition to the insulating charge- and spin-density wave phases for large $V$ and $U$ respectively, we identify a phase with dominant superconducting correlations at large distances for small $U$ and $V$. Using two Berry phases (one associated to the charge and the other to the spin degrees of freedom) as discrete order parameters, we construct a phase diagram for the three thermodynamic phases.

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After the discovery of high-$T_c$ systems, there has been an increase in the interest on purely electronic models exhibiting superconductivity, particularly those with correlated hopping\cite{1,5}. A hopping dependent on the occupation of the two sites involved is to be expected in nature, and together with the on-site ($U$) and nearest-neighbor ($V$) repulsions, have been discussed already by Hubbard in 1963\cite{10,11}. The resulting extended model (and a related one\cite{12}) has been studied by several groups\cite{13,14,15}, with particular emphasis in phase transitions like the Mott metal-insulator one. At half-filling and when the hopping term which changes the double occupancy $t_{AB} = 0$, Strack and Vollhardt obtained two regions of parameters for which the exact ground state in arbitrary dimension is a charge-density wave (CDW) or a spin-density wave (SDW) with maximum order parameter\cite{13}. These regions were later extended\cite{15,6} and a phase diagram constructed\cite{16}.

In one dimension (1D) the result is represented by the dashed line in Fig. 1 (b),(c). However, the nature of the third thermodynamic phase present in the diagram has not been clearly elucidated, no exact result exist for the third thermodynamic phase present in the diagram\cite{17,18}. However, the nature of a thermodynamic phase other than the CDW or SDW ones, therefore, each thermodynamic phase is determined by the correlation functions (charge-charge, spin-spin or pair-pair) with the lowest decay at large distances. Calculation of the correlation exponents and other arguments allow to identify the thermodynamic phase as a Tomonaga-Luttinger liquid in which the superconducting pair-pair correlations are the greatest at large distances.

The Hamiltonian for a ring of $L$ sites with electron creation operators satisfying arbitrary boundary conditions for both spins $c_{j+1,\sigma}^{\dagger} = e^{i\Phi_{j+1}\sigma}c_{j\sigma}^{\dagger}$ can be written in terms of the operators $c_{j\sigma}^{\dagger} = e^{-ij\Phi_{j}}/Lc_{j\sigma}^{\dagger}$ satisfying $c_{j+L\sigma}^{\dagger} = c_{j\sigma}^{\dagger}$ as:

$$H(\Phi_{1}, \Phi_{L}) = \sum_{j\sigma}( -\frac{1}{2}\tilde{w}(\Phi_{j}) c_{j+1\sigma}^{\dagger}c_{j\sigma}(t_{AA}(1-n_{i,\bar{\sigma}})(1-n_{i+1,\bar{\sigma}})$$

$$+t_{AB}[n_{i,\bar{\sigma}}(1-n_{i+1,\bar{\sigma}})+n_{i+1,\bar{\sigma}}(1-n_{i,\bar{\sigma}})]$$

$$+t_{BB}n_{i,\bar{\sigma}}n_{i+1,\bar{\sigma}} + h.c.)$$

$$+U \sum_{j} n_{j\uparrow}n_{j\downarrow} + V \sum_{j\sigma\sigma'} n_{j+1\sigma}n_{j\sigma'} (1)$$

In 2D, this Hamiltonian has been derived as an effective one-band model for cuprate superconductors\cite{25}. We restrict the parameters to $t_{AA} = t_{BB} = 1$, $0 < t_{AB} \leq 1$, interpolating between the usual extended Hubbard model $t_{AB} = 1$\cite{18}, and the case $t_{AB} = 0$, for which
some exact results are known \[ \text{[1]} \text{[2]} \text{[3]} \text{[4]}, \] particularly the boundaries of the CDW and SDW phases \[ \text{[5]} \text{[6]} \], and the exact ground state for \( V = 0 \) \[ \text{[4]} \]. Unfortunately this state is rather pathological, highly degenerate, and at half-filling it is insulating even for small \( U \), in spite of the absence of a charge gap for \( U < 4 \), for geometrical reasons \[ \text{[7]} \text{[8]} \]. Thus, it is necessary to include the effect of \( t_{AB} \) to draw general conclusions on the nature of the Mott or superconductor-insulator transition.

Due to the periodic boundary conditions used, the many-body eigenstates of \( H \) for any fluxes \( \Phi_\sigma \), can be classified according to their total wave vector \( K \) with \( KL/2\pi \) integer (instead, the wave vectors \( K \) in the representation of \( c_\sigma \) are shifted and cover all real values as the \( \Phi_\sigma \) are varied \[ \text{[1]} \text{[2]} \text{[3]} \text{[24]}. \] If an eigenstate \( |e_K(\Phi_\uparrow, \Phi_\downarrow)\rangle \) of \( H(\Phi_\uparrow, \Phi_\downarrow) \) with a given \( K \) does not have an accidental degeneracy with another eigenstate with the same \( K \) in the interval \( 0 \leq \Phi_\uparrow = \Phi_\downarrow = \Phi \leq 2\pi \), then this state can be followed adiabatically as \( \Phi \) is varied, and a many-body generalization of Zak’s Berry phase \[ \text{[19]} \] can be defined for it \[ \text{[24]} \]. For the explicit calculation, it is more convenient to use the numerically gauge invariant expression \[ \text{[24]} \text{[24]}, \] discretizing the interval \( 0 < \Phi < 2\pi \) into \( N \) points \( \Phi_i = 2\pi i/N : \)

\[
\gamma_c(e_K) = \lim_{N \to \infty} \frac{\text{Im}[\text{ln}(\Pi_{i=0}^{N-2}\langle e_K(\Phi_i, \Phi_i) | e_K(\Phi_{i+1}, \Phi_{i+1}) \rangle \langle e_K(\Phi_{N-1}, \Phi_{N-1}) | e_K(2\pi) \rangle)]}{\langle e_K(\Phi_{N-1}, \Phi_{N-1}) | e_K(2\pi) \rangle}, \tag{2}
\]

where \( |e_K(2\pi)\rangle \) represents \( |e_K(2\pi, 2\pi)\rangle \) obtained directly from \( |e_K(0, 0)\rangle \) \[ \text{[24]} \],

\[
|e_K(2\pi)\rangle = \exp[i \frac{2\pi}{L} \sum_{j\sigma \rho} j^\dagger_{j\rho} c_{j\sigma} |e_K(0, 0)\rangle]. \tag{3}
\]

In practice \( N = 10 \) points are more than enough to define if \( \gamma_c(e_K) \) is 0 or \( \pm \pi \) with six digits accuracy. In few cases in which this was not the case, we increased \( N \) until the same level of accuracy was obtained. Note that in contrast to previous cases \[ \text{[21]} \text{[24]}, |e_K(\Phi, \Phi)\rangle \) is not necessarily the ground state. In particular, for most of the parameters inside the S phase, there is a crossing of the energy levels between \( K = 0 \) and \( K = \pi \). As a consequence, the ground-state energy \( E_\sigma(\Phi, \Phi) \) has local minima around \( \Phi = 0 \) and \( \Phi = \pi \) (see Fig. 2) and its form is suggestive of anomalous flux quantization (AFQ), \( \text{i.e. } E_\uparrow(\pi) = E_\uparrow(0) \) in the thermodynamic limit, as expected if superconducting correlations dominate at large distances \[ \text{[4]} \text{[4]} \text{[4]} \text{[4]}. \]

In analogy to the fact that from the ground-state energy \( E_\sigma(\Phi_\uparrow, \Phi_\downarrow) \) one can calculate a charge stiffness (Drude weight) and a spin stiffness as \[ \begin{align*}
D_c &= (L/2)^2 \partial^2 E_\sigma(\Phi, \Phi) / \partial \Phi^2, \quad D_s &= (L/2)^2 \partial^2 E_\sigma(\Phi, -\Phi) / \partial \Phi^2, \quad \text{for } \Phi = 0, \end{align*} \]
for which \( \Phi_\uparrow + \Phi_\downarrow = \pi \), we define the spin Berry phase as that captured varying \( \Phi_\uparrow \) from 0 to \( 2\pi \), keeping \( \Phi_\downarrow = -\Phi_\uparrow \) in the cycle:

\[
\gamma_s(e_K) = -\lim_{N \to \infty} \frac{\{\text{Im}[\text{ln}(\Pi_{i=0}^{N-2}\langle e_K(\Phi_i, -\Phi_i) | e_K(\Phi_{i+1}, -\Phi_{i+1}) \rangle \langle e_K(\Phi_{N-1}, -\Phi_{N-1}) | e_K(2\pi) \rangle)] \times \langle e_K(\Phi_{N-1}, -\Phi_{N-1}) | e_K(2\pi) \rangle \}). \tag{4}
\]

\[
|e_K(2\pi)\rangle = \exp[i \frac{2\pi}{L} \sum_{j\sigma \rho} j^\dagger_{j\rho} c_{j\sigma} |e_K(0, 0)\rangle], \tag{5}
\]

where \( \sigma = 1(-1) \) for spin up(down). While in general \( \gamma_c \) is a measure of the polarization in the system \( \text{[19]} \text{[21]} \text{[24]}, \) a change of \( \gamma_c \) in \( \pi \) corresponds to the change of polarization when one unit charge is displaced one lattice parameter, \( \gamma_s \) is a measure of the difference between the polarization of electrons with spin up and down.

At this point it is interesting to note the effect of the unitary transformation,

\[
c'_{j\uparrow} = c_{j\uparrow}, \quad c'_{j\downarrow} = (-1)^j c_{j\downarrow}, \tag{6}
\]

on \( H \). In the resulting Hamiltonian \( H' \), \( \Phi_\downarrow \) and \( U \) change sign, while the term in \( V \) transforms to an Ising interaction \( \tilde{V}' = V(n_{j\uparrow} - n_{j\downarrow})(n_{j+1\uparrow} - n_{j+1\downarrow}) \). Assuming in the following \( L \) even, and calling \( |e_K\rangle \) the state obtained from \( |e_K\rangle \) through the unitary transformation one has:

\[
\gamma_s(e'_K) = \pi + \gamma_c(e_K) \tag{7}
\]

The term \( \pi \) is due to the fact that the transformation interchanges the vacuum with the fully polarized ferromagnetic state \( |F\rangle \), for which \( \gamma_c(F) = \gamma_s(F) = \pi \). This can be easily seen from Eqs. (2)-(5), since all scalar products inside the logarithm are 1, except the last one, which is \(-1\).

We define the Berry phases of a thermodynamic phase, as the Berry phases of the corresponding ground state. For those cases in which two energy levels with different quantum numbers as functions of \( \Phi_\uparrow, \Phi_\downarrow \) cross in the ground state, we have chosen the state of lowest minimum of the energy \( E(\Phi_\uparrow, \Phi_\downarrow) \). In all cases we have found that this minimum corresponds to \( K = \Phi_\uparrow = \Phi_\downarrow = \pi \) for \( L \) multiple of four, and to \( K = \Phi_\uparrow = \Phi_\downarrow = 0 \text{ if } L/4 \text{ is a half integer. The chosen state has also the lowest energy averaged over the fluxes. The values of the Berry phases at the CDW and SDW thermodynamic phases are easy to determine using continuity arguments (\( \gamma_s, \gamma_c \) cannot jump unless there is a phase transition). In the limit of very large \( U \), for \( \Phi_\uparrow = \Phi_\downarrow = \Phi \), \( H \) is equivalent to a Heisenberg Hamiltonian with exchange constant \( J = 4t_{AB}^2/(U - V) \) independent of \( \Phi \). Then, all factors but the last in Eq. (2) are 1, the exponential in Eq. (3) introduces a factor -1, and \( \gamma_c(\text{SDW}) = \pi \). A Hartree-Fock wave function leads to the same result, in agreement with previous findings for a diatomic system \[ \text{[24]} \]. When \( \Phi_\uparrow = -\Phi_\downarrow \), the exchange terms in the large \( U \) limit depend on \( \Phi_\uparrow \). However we do not expect a transition if the Ising term (of the form of \( \hat{V}' \)) is increased.}
to the S phase near CDW state. These simple arguments cannot be extended
with spin up are displaced one lattice parameter to form a
tent with Eq. (7) and with the changes in polarization
and did not converge with the number of splittings
that

gamma = (0, 0). This result is consistent with Eq. (7) and with the changes in polarization
for both spins when in the Neel SDW state, all electrons
with spin up are displaced one lattice parameter to form a
CDW state. These simple arguments cannot be extended
to the S phase near \( U, V \sim 0 \). However for \( U = V = 0 \),
and \( 0 \neq t_{AB} \neq 1 \), the ground state is non-degenerate
for any fluxes \( \Phi_\uparrow, \Phi_\downarrow \), and therefore, it should be mapped
onto itself by the transformation Eq. (6). Then, Eq.
(7) implies that \( \gamma_s(S) = \pi + \gamma_c(S) \) (modulo \( \pi \)). Thus,
before actually computing the Berry phases one knows
that the \( \gamma \) are different for the three phases. We obtain
\( \gamma(S) = (0, \pi) \) numerically. In the non-interacting case
\( U = V = 0 \), \( t_{AB} = 1 \), \( \gamma \) ill defined due to a degeneracy
of the ground state for some values of \( \Phi_\uparrow, \Phi_\downarrow \) (correspond-
ing to a local maximum in the ground-state energy as a
function of flux) and the same value of \( K \). This is consistent
with previous numerical calculations, which found that \( \gamma_c \) in a metallic normal phase took arbitrary values
and did not converge with the number of splittings \( N \)

\[ \text{FIG. 1. Phase diagram in the } U, V \text{ plane for different values of } t_{AB}. \quad \text{Solid (empty) circles denote the points at which } \gamma_c \text{ (}\gamma_s\text{) jumps in } \pi. \quad \text{Dashed line corresponds to the exact result for } t_{AB} \to 0. \quad \text{Dashed-dotted line in (a) corresponds to } V = U/2. \]

The phase diagram for different values of \( t_{AB} \) is shown
in Fig. 1. Because of the unitary transformation Eq.
(6), the phase diagram is also that of \( H' \) interchanging
SDW and CDW phases. The results were obtained
calculating the boundaries for all chains of even length
\( L \leq 10 \) and extrapolating the results using the procedure following in Ref. [23]. For \( t_{AB} = 1 \), the S phase
is absent and the CDW-SDW boundary is very similar
to that found previously from the structure factors obtained
with Monte Carlo simulations [18]. However, this method
has an error \( \sim 0.05 \) in the critical value of \( V \).
There is in addition a systematic error due to the dis-
cretization of imaginary times which is difficult to estimate.
In our case, from the difference in the extrapolated values using up to 8 sites, or up to 10 sites, we estimate
the error to be one order of magnitude smaller. As long
as \( t_{AB} < 1 \), a superconducting phase appears, near the
CDW-SDW boundary for \( t_{AB} = 1 \), if \( U < 4 \), particularly
for small \( U \) and \( V \). This can be understood in part
by the fact that the energy of CDW and SDW states increase when \( t_{AB} \) decreases. This fact is particularly clear for large \( V \) or large \( U \) for which the ground-state energy per site is
\( E_{CDW} = U/2 - 2t^2_{AB}/(3V - U) \) and
\( E_{SDW} = V - 4t^2_{AB}/(U - V) \) respectively, and agrees roughly with the result of a generalized Hartree-Fock de-
coupling of the two- and three-body terms present in \( H \)
[17]. The exact results for \( t_{AB} = 0 \) [17], [18], show that for small \( t_{AB}, U \) and \( V \), it is energetically convenient
to destroy the CDW or SDW phase to take advantage of the kinetic energy terms in \( t_{AA} \) and \( t_{BB} \). However, the
fact that the S phase is more stable near the line in which
the CDW and SDW are degenerate is noticeable and un-
expected in these previous approaches. This is probably
related to the fact that the transition between the CDW
and SDW phases for \( t_{AB} = 1 \) is second order for \( U < U_c \)
and first-order for \( U > U_c \), where the position of the tricritical point \( U_c \sim 3 \pm 1 \) [18]. The S phase seems to
develop around the line of the second-order phase trans-
sition as long as \( t_{AB} < 1 \). Unfortunately, our method
can not determine the order of the transition and a more
precise value of \( U_c \) can not be given.

As \( t_{AB} \) decreases further, the region occupied by the S
phase increases and tends to the exact result for \( t_{AB} \to 0 \)
[16]. For small \( t_{AB} \) the finite-size effects become more im-
portant for the S-SDW phase boundary. For \( V = 0 \) and
\( t_{AB} = 0.1 \), the extrapolation using chains up to 10 sites
gives \( U_{S-SDW} = 3.901 \), while extrapolation including
\( L = 12 \) gives a value smaller by 0.016.
ably a finite-size effect. Thus, all calculations are con-

with the flux is calculated simultaneously with the Berry

addition, since the dependence of the ground-state energy

are the ground state for large distances for 0 < \( t_{AB} < t_{AA} = t_{BB} \)

and small \( U \) and \( V \). This thermodynamic phase, as well as the insulating CDW and SDW phases , which are the ground state for large \( V \) and large \( U \) respectively, are characterized by different quantized values of \( \gamma = (\gamma_c, \gamma_s) \), where \( \gamma_c, \gamma_s \) are Berry phases associated with charge and spin degrees of freedom respectively: \( \gamma(\text{S}) = (0, \pi) \), \( \gamma(\text{CDW}) = (0, 0) \), \( \gamma(\text{SDW}) = (\pi, \pi) \). The finite jumps in \( \gamma \) at the phase boundaries allowed us to define them sharply for each finite chain, and to obtain an accurate phase diagram through finite-size scaling. The use of topological quantum numbers to characterize the different thermodynamic phases should be useful in general for non-trivial highly correlated models, for which correlation functions in finite systems do not show sharp transitions and exact solutions in the thermodynamic limit are very rare.

Previous numerical studies for finite \( t_{AB} \), well inside the S phase have shown the presence of mobile carriers [17], however the attempts to determine if the S phase is superconducting or not gave contradictory results [1]. On one hand, it has been established that for \( t_{AB} < 1 \), and small \( U \) and \( V \), the system behaves as a Tomonaga-Luttinger liquid with dominant superconducting correlations at large distances. On the other hand, no signs of AFQ were found for \( U = V = 0 \), and a generalized Hartree-Fock Bardeen-Cooper-Schrieffer (BCS) decoupling of the two- and three-body terms, shows that an ordinary singlet BCS superconducting solution is unstable. However, we find that this decoupling, for small \( U, V \), leads naturally to a \( p \)-wave triplet-pairing superconducting ground state. A similar BCS solution exists in 2D, which should be valid for small \( U, V \) and \( 1 - t_{AB} \). In addition, since the dependence of the ground-state energy with the flux is calculated simultaneously with the Berry phase \( \gamma_c \), we found that in most of the S phase there are signs of AFQ. An example is given in Fig. 2. The fact that no signals of AFQ are found for \( U = V = 0 \) is probably a finite-size effect. Thus, all calculations are consistent with the superconducting nature of the S phase.

Furthermore, for \( V = 0 \), the correlation exponent \( K_\rho > 1 \) for \( U < U_{\text{S-SDW}} \), while for \( U > U_{\text{S-SDW}} \) a gap opens in the charge sector \( \Phi \). Calculations of \( K_\rho \) for \( t_{AB} = 0.6 \) in rings of 8, 10 and 12 sites gave \( U_{\text{S-SDW}} = 2.05 \pm 0.05 \), in excellent agreement with the result 2.11 obtained with the Berry phases (see Fig. 1 (b)). The triplet nature of the S phase is supported by our numerical calculations of pair-pair correlation functions for \( L = 10 \) and the fact that for a singlet S phase one expects \( \gamma = (0, 0) \).

In summary, we have shown that in one dimension at half filling, the extended Hubbard model with correlated hopping \( H \) (Eq. (1)), and the model \( H' \) obtained from \( H \) through the unitary transformation Eq. (6), present a phase “S” with dominating superconducting correlations at large distances for \( 0 < t_{AB} < t_{AA} = t_{BB} \) and small \( U \) and \( V \). This thermodynamic phase, as well as the insulating CDW and SDW phases , which are the ground state for large \( V \) and large \( U \) respectively, are characterized by different quantized values of \( \gamma = (\gamma_c, \gamma_s) \), where \( \gamma_c, \gamma_s \) are Berry phases associated with charge and spin degrees of freedom respectively: \( \gamma(\text{S}) = (0, \pi) \), \( \gamma(\text{CDW}) = (0, 0) \), \( \gamma(\text{SDW}) = (\pi, \pi) \). The finite jumps in \( \gamma \) at the phase boundaries allowed us to define them sharply for each finite chain, and to obtain an accurate phase diagram through finite-size scaling. The use of topological quantum numbers to characterize the different thermodynamic phases should be useful in general for non-trivial highly correlated models, for which correlation functions in finite systems do not show sharp transitions and exact solutions in the thermodynamic limit are very rare.

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[26] For some parameters and values of $K$, there are accidental degeneracies at given values of $\Phi_\uparrow = \Phi_\downarrow$ (and $\Phi_\downarrow = -\Phi_\uparrow$) and precisely at these points $\gamma_c (\gamma_s)$ jumps in $\pi$.

[27] In terms of the $\hat{c}_{\uparrow\sigma}^\dagger$ operators, $|e_K(2\pi)\rangle$ is identical to $|e_K(0,0)\rangle$. Also for $\Phi = 0$, $\hat{c}_\uparrow^\dagger = \hat{c}_\downarrow^\dagger$. Then, writing $|e_K(2\pi)\rangle$ in terms of the $c_{\sigma\sigma}$ operators for $\Phi = 2\pi$ leads to Eq. (3).

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