Superconductivity from correlated hopping

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Abstract

We consider a chain described by a next-nearest-neighbor hopping combined with a nearest-neighbor spin flip. In two dimensions this three-body term arises from a mapping of the three-band Hubbard model for CuO$_2$ planes to a generalized $t - J$ model and for large O-O hopping favors resonance-valence-bond superconductivity of predominantly $d$-wave symmetry. Solving the ground state and low-energy excitations by analytical and numerical methods we find that the chain is a Luther-Emery liquid with correlation exponent $K_\rho = (2 - n)^2 / 2$, where $n$ is the particle density.

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Recently, there has been a considerable interest in obtaining the exact ground state of different strongly correlated systems, using a variety of techniques [1–9]. Although in some cases the model or the parameters are rather unrealistic, exact results are useful in clarifying the effect of different physical ingredients and as a test of approximations. Particularly interesting are those models in which the ground state is superconducting, or has dominant superconducting correlations in one dimension [4,8], because they display superconducting mechanisms which are different from the conventional electron-phonon one and might be relevant to the understanding of the high-$T_c$ systems.

Here we consider a one-dimensional (1D) system described by the Hamiltonian:

$$H_{t''} = t'' \sum_{i,\delta \neq \delta'} c_{i+\delta''}^\dagger c_{i+\delta'}^\dagger (\frac{1}{2} - 2 \mathbf{S}_i \cdot \mathbf{S}_{i+\delta}),$$

where in terms of ordinary fermion operators $c_{i,\sigma}^\dagger = \tilde{c}_{i,\sigma}^\dagger (1 - \tilde{c}_{i-\sigma}^\dagger \tilde{c}_{i-\sigma})$ (double occupancy at any site is forbidden), $\mathbf{S}_i$ is the spin operator at site $i$, and $i + \delta$ denote the nearest neighbors of site $i$. Eq. (1) can also be written in the form of a hopping of singlet pairs:

$$H_{t''} = 2t'' \sum_{i,\delta \neq \delta'} b_{i,\delta}^\dagger b_{i,\delta}^\dagger; \quad b_{i,\delta}^\dagger = \frac{1}{\sqrt{2}}(c_{i+\delta''}^\dagger c_{i+\delta'}^\dagger - c_{i+\delta'}^\dagger c_{i+\delta''}^\dagger)$$

In 2D, $H_{t''}$ was obtained as an important term in a systematic analytical derivation of a generalized $t - J$ model, starting from the extended three-band Hubbard model [10]. Also, a numerical study of a Cu$_4$O$_8$ cluster has shown that fitting of the energy levels using a generalized $t - J$ model improves considerably, and a correct ordering of the levels is obtained, if $H_{t''}$ is included [11]. If the direct O-O hopping $t_{pp}$ of the three-band model is large enough, $t''$ has opposite sign as the one which corresponds to a canonical transformation of the Hubbard model [11,12] and simultaneously the direct nearest-neighbor hopping $t'$ has the sign which agrees with the observed Fermi surface and other properties of hole-doped superconductors, and with the asymmetry in the magnetic properties between hole-doped and electron-doped cuprates [11,12,14].

A recent exact diagonalization of a $4 \times 4$ cluster shows that when $|t''/t| > 0.12$ with the sign of $t''$ corresponding to large $t_{pp}$, the system shows strong signals of $d$-wave superconductivity for realistic $J/t = 0.4$ and doping $x = 1 - n = 0.25$ [12]. The $d$-wave superconducting
susceptibility is strongly enhanced and the ground-state wave function has a significant overlap with a a simple short-range resonance-valence-bond state with superconducting off-diagonal long-range order (ODLRO) in the \( d \)-wave and \( s \)-wave channels (the former being the dominant). The fact that \( H_{t''} \) changes the physics dramatically is also evident in the symmetry of the ground state as a function of doping \([12]\). Another case of the three-band Hubbard model in wich \( H_{t''} \) is important is the limit \( t_{pp} << t_{pd} << \Delta \) where \( \Delta \) is the Cu-O charge transfer energy. In this case \( t'' \) becomes of the order of \( t \), as can be seen from a canonical transformation that eliminates double occupancy in the effective one-band Hubbard model \([13]\).

Unfortunately, although the saturation of the superconducting correlation functions in Ref. \([12]\) is an indication of ODLRO, a study of a small cluster cannot assure the presence of ODLRO in the thermodynamic limit. Instead, in 1D one can use powerful results obtained using conformal-field theory to relate the correlation exponents with thermodynamic quantities \([16]\), and then, the effect of \( H_{t''} \) on superconducting correlations can be determined unambiguously. As a first step, we drop the other terms of the generalized \( t - J \) model. This allows us to obtain analytical results and to isolate the effect of \( H_{t''} \).

To gain physical insight into the 1D problem, let us consider a chain with only one vacant site (or hole). The action of the Hamiltonian Eq.(2) over a state in which the hole is localized at a given site, can be thought as a permutation of the hole with a nearest-neighbor singlet. Thus, to take maximum advantage of \( H_{t''} \), it is convenient that the spin configuration consists of a bond-ordering wave of non-overlapping singlets at each side of the hole (see Fig. 1). The subsequent motion of the hole does not alter the spin configuration, the problem becomes equivalent to a tight-binding model with next-nearest-neighbor hopping \( 2t'' \), and the resulting ground-state energy in the thermodynamic limit \(-4t''\) coincides with the lower bound of \( H_{t''} \) which can be obtained using Gerschgorin’s theorem \([17,9]\). This fact confirms that the spin configuration is the optimum one. When more than one hole is present in the system, in order to have all spins paired in singlets of nearest-neighbor particles, it is necessary that the distance between two successive holes is odd (the parity of this distance...
is conserved by $H_{t''}$. From the arguments given above, it seems clear that the ground state
is a combination of sequences of these singlets and holes (see Fig.1). Although we could not
prove analytically this statement for more than two holes, we have verified that the ground-
state energy of an open chain with 14 sites and any even number of particles is the same as
that of a spinless model (Eqs.(3) and (4)), obtained using the mapping sketched in Fig.1:
each singlet is replaced by a spinless fermion. For a chain of length $L$ and $N$ particles ($N$
even), the hopping, length and number of particles of the effective spinless fermion problem
are given by:

$$t = 2t''; \quad L' = L - N/2; \quad N' = N/2. \quad (3)$$

For example in Fig.1 $L = 14$, $N = 10$, and then $L' = 9$, $N' = 5$. In a chain with open
boundary conditions, the order of the singlets is conserved, and thus, the statistics of the
fermions in the equivalent problem does not play any role. We recall that the ground-state
energy of a spinless chain with open boundary conditions of length $L'$, $N'$ fermions and
hopping $t$ is (see for example Ref. [8]):

$$E = -|t| \left( \frac{\sin \pi \frac{2N'+1}{2L'+2}}{\sin \frac{\pi}{2L'+2}} - 1 \right). \quad (4)$$

Eqs.(3) and (4) describe the ground-state energy of $H_{t''}$ for a chain with open boundary
conditions. However, for the discussion below concerning the central charge and low-energy
excitations, it is more convenient to know the energy of $H_{t''}$ in a ring (periodic boundary
conditions). In this case, the mapping to the fermionic system can still be done: the fermionic
sign which arises under a cyclic permutation of the fermions can be absorbed taking periodic
(antiperiodic) boundary conditions if the number of fermions is odd (even). This corresponds
to an even number of particles not multiple of four (multiple of four) in the original system
described by $H_{t''}$. In both cases the energy can be written as:

$$E = -2|t| \frac{\sin \left( \pi \frac{N'/L'}{L'} \right)}{\sin \left( \pi / L' \right)} \quad (5)$$

Using Eq.(3), the ground-state energy per site $e = E/L$ of a ring of length $L$ and density
$n = N/L$ described by $H_{t''}$ is:
\[
e(n, L) = -4|t''| \frac{\sin\left(\frac{\pi n}{2-n}\right)}{L \sin\left(\frac{2\pi}{L(2-n)}\right)} \quad (6)
\]

We have also verified Eq. (6) for \( L = 14 \) and all \( n \) multiple of \( 1/7 \). From Eqs. (3) and (4) or Eq. (6) one obtains in the thermodynamic limit:

\[
e(n, \infty) = -\frac{2|t''|}{\pi} (2 - n) \sin\left(\frac{\pi n}{2-n}\right) \quad (7)
\]

The corresponding wave function can be obtained through the mapping procedure in a similar way as in Ref. [8].

To obtain the long-distance behavior of any correlation function, using results of conformal-field theory, one needs information about the low-energy excitations of the system \[16\]. It is easy to see that the low-energy triplet excitations on the ground state, act as barriers to the propagation of the holes. From arguments similar to those presented above for the one-hole case, one sees that the spin excitation of lowest energy is to change one singlet of nearest-neighbor particles into a triplet. For open boundary conditions in the equivalent fermionic problem, this is equivalent to changing a chain of length \( 2L' + 1 \) with \( 2N' + 1 \) particles into two equal chains of length \( L' \) with \( N' \) particles. Using Eqs. (3) and (4) we obtain that the value of the spin gap in the thermodynamic limit is:

\[
\Delta_s = |2t''|[1 + \cos\left(\frac{\pi n}{2-n}\right)] \quad (8)
\]

The gap is maximum for \( n = 0 \) and vanishes at \( n = 1 \).

The charge excitations, and in particular the charge velocity \( v_c \) can also be calculated using the equivalent model of spinless fermions. It should be taken into account that distances and therefore also momentum are changed in the mapping procedure. While the minimum excitation energy \( E_{\text{min}} \) of \( H_{t''} \) in a ring corresponds to \( q = 2\pi/L \), the corresponding momentum for the same energy in the equivalent spinless ring is \( q' = 2\pi/L' \). Calling \( v'_c \) the charge velocity of the spinless ring, we can write [18]:

\[
v_c = \frac{E_{\text{min}} - E}{2\pi/L} = \frac{L}{L'} \frac{E_{\text{min}} - E}{2\pi/L'} = \frac{L}{L'} v'_c \quad (9)
\]
In the thermodynamic limit \( v'_c = 2t \sin(\pi N'/L') \), and using Eqs.(3) and (9) one obtains:

\[
v_c = \frac{8|t''|}{2-n} \sin\left(\frac{\pi n}{2-n}\right)
\]

(10)

Expanding the denominator of Eq.(6) up to third order in the argument and using Eqs.(7) and (10), one can see that for \( L \to \infty \):

\[
e(n, L) = e(n, \infty) - c \frac{\pi v_c}{6L^2}
\]

(11)

where the number \( c = 1 \) is called the central charge [16,19]. This scaling law characterizes a Luther-Emery liquid [20]. In this liquid, the correlation functions are characterized by a single exponent \( K_\rho \). The superconducting pair-pair correlation functions depend on the distance \( d \) between pairs as \( d^{-1/K_\rho} \) for \( d \gg 1 \) and are the dominant correlation functions at large distances if \( K_\rho > 1 \) [16,21,18]. In this case a small coupling between different chains gives rise to superconductivity. \( K_\rho \) can be calculated in terms of the charge velocity and the compressibility \( \kappa \) [16,18]. Using Eq.(7) on obtains:

\[
\frac{1}{\kappa n^2} = \frac{\pi v_c}{2K_\rho} = \frac{\partial^2 e}{\partial n^2} = \frac{8\pi|t''|}{(2-n)^3} \sin\left(\frac{\pi n}{2-n}\right),
\]

(12)

and using Eq.(10), a very simple expression for the correlation exponent results:

\[
K_\rho = \frac{(2-n)^2}{2}
\]

(13)

This exact result allows to test numerical methods and approximations. As an example, we have calculated \( K_\rho \) in a ring of 14 sites from the expression \( K_\rho = \pi(\kappa n^2 D_c/2)^{1/2} \), obtaining \( \kappa \) and the Drude weight \( D_c \) numerically as in Ref. [18]. The comparison with Eq.(13) is shown in Fig.2. One can see that the agreement is very good except for a small deviation at the extreme densities. This deviation is mainly due to the discretization of the expression of the second derivative which enters the compressibility.

The system has dominant superconducting correlations for \( 0 < n < 2 - \sqrt{2} \). Inspection of Eq.(12) shows that there is no phase separation in the system for any density. This is in contrast to the \( t-J \) and other models proposed to the cuprates in which superconductivity
takes place near a region of phase separation \[21\]. In the dilute limit \(n \to 0\), \(K_{\rho} \to 2\), as in the negative \(U\) Hubbard model for large \(|U|\): the physics is like that of hard-core bosons which undergo Bose condensation. The same type of physics is expected in 2D in the dilute limit. We have confirmed this by numerical calculations in a 4\(\times\)4 cluster and comparison with a BCS-like wave function. Instead, for \(n \to 1\), \(K_{\rho} \to 1/2\), as in the case of spinless fermions. Addition of an attractive term like the superexchange \(J\) of the \(t-J\) model should extend the range of densities for which \(K_{\rho} > 1\) to larger values of \(n\). One also expects that addition of \(J\) should close the spin gap for \(n \sim 1\). The effect of the interplay of \(H_{\sigma}\) with the terms present in the \(t-J\) model in 1D has been studied quite recently by numerical methods \[22,23\]. The main result is that the regions of superconductivity and phase separation for \(n \sim 1\) shift to higher (lower) values of \(J/t\) if a small \(t''\) is added with the same (opposite) sign as the one which corresponds to a canonical transformation of the Hubbard model. Thus, as in 2D, the sign of \(t''\) favored for large \(t_{pp}\) in the mapping from the three-band Hubbard model \[10,12\] is more convenient for superconductivity for realistic doping.

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**FIGURE CAPTIONS**

Fig. 1: (a) Schematic representation of a typical state with definite occupation at each site among those which compose the ground state of the system. (b) state obtained from (a) replacing each singlet pair by a spinless fermion. Open circles denote vacant sites, closed circles joined by a full line represent a singlet $b^\dagger_{i\delta}$ (Eq. (2)), and up arrows represent spinless fermions.

Fig. 2: Correlation exponent $K_\rho$ obtained numerically in a ring of 14 sites (solid squares) in comparison with the exact result (solid line).
Fig. 1
Fig. 2