Real-space pairing in fermion systems

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A real-space tight-binding model of fermions involving the competition between an attraction V between the localized fermion pairs on different sites and an ordinary one-particle hopping t is introduced. The ground-state properties of its one-dimensional version are studied with use of numerically exact finite-chain calculations for up to $N=10$ sites. A transition of the essential singularity type between the band and the localized-pairs state is found for finite V/t.

The problem of pairing interactions in fermion systems has been very intensively investigated following the development of the Bardeen-Cooper-Schrieffer (BCS) theory of superconductivity.[1] The famous BCS reduced Hamiltonian describes the attractive interaction between the electronic pairs in momentum space. In this model the range of interaction is short, but the size of the Cooper pairs is large.[2] Thus, the BCS superconducting transition in three-dimensional isotropic compounds can be well described by a molecular-field—type Ginzburg-Landau or, equivalently, by the original BCS solution. An additional assumption requires that the pairing interaction be weak compared with the kinetic energy t. It has been recognized very early that superconductivity may appear even if some of these restrictions are relaxed. For instance, the pairing correlations in nuclear matter correspond to the vanishing-kinetic-energy situation.[3] Let us mention that such zero-kinetic-energy models can be solved exactly.[4] In numerous condensed-matter problems, especially in reduced dimensionalities, serious complications arise in the reciprocal space and one would rather prefer to formulate the Hamiltonian using localized atomiclike orbitals.

Such real-space formulations were used to treat the superconductivity in narrow d bands,[5] properties of amorphous materials,[6] bipolaron transitions,[7] and other problems.[8] These and related treatments[9,10] usually represent the real-space pairing by the negative-U Hubbard model. The considerations on U values entering the $U>0$ Hubbard models are already quite intricate,[11] and even less can be said about negative values of U. In one dimension (1D) the $U<0$ ground-state wave function can be obtained exactly,[12] but it is too complicated to decide whether it could lead to the superconductivity. Furthermore, for $t=0$ any Hubbard-type model becomes classical, rendering eventual applications to superconductivity questionable. Very recently Nozières *et al.*[13] have analyzed the transition between the weak (BCS-type) and strong (negative-U) coupling superconductivity and elaborated on the nonapplicability of the Hubbard model for $|U|\gg t$.

Here, we wish to propose a new model to describe the pairing transition with the features that it is defined in real space, is short ranged, and remains quantum mechanical for both weak and strong couplings. In contrast with the BCS model, the radius of pairs is zero (like diatomic molecules). In order to get a feeling for the properties of it, we investigate it numerically in 1D to extract the properties of its ground state and its low-lying excitations.

The Hamiltonian of this model is

$$H=\sum_{\substack{\langle ij\rangle \\ \sigma=\uparrow,\downarrow}} t_{ij}c_{i\sigma}^{\dagger}c_{j\sigma}-\sum_{\langle ij\rangle} V_{ij}(c_{i\uparrow}^{\dagger}c_{i\downarrow}^{\dagger}c_{j\downarrow}c_{j\uparrow}+c_{j\uparrow}^{\dagger}c_{j\downarrow}^{\dagger}c_{i\downarrow}c_{i\uparrow}) ,$$

$$\text{with } V_{ij}>0 , \quad (1)$$

where $c_{i\sigma}^{\dagger}$ creates a fermion with spin σ on site i and t_{ij} is the hopping integral between the sites i and j and is spin-independent. The interaction V_{ij} describes the hopping of pairs with opposite spins on the same site. This type of interaction has been considered by Kulik and Pedan[14] in their study of superconductivity in systems with structural disorder. V_{ij} favors the formation of pairs but also encourages their mobility.[15] It is in this respect that (1) differs from the aforementioned negative-U Hubbard model.

Let us now show how this model provides a mechanism for pair formation. First for $V_{ij}=0$, the fermions with different spin are uncoupled and thus uncorrelated, and, we have a system of two sets of free fermions whose properties are exactly known. In the opposite limit $t_{ij}=0$, H favors pair formation, as then each term in the sum in Eq. (1) acting on a singly occupied site vanishes. This system of paired fermions can be described by introducing $S=\frac{1}{2}$ pseudospins $\mathbf{T}_i$, with $T_i^{+}=c_{i\uparrow}^{\dagger}c_{i\downarrow}^{\dagger}$ and

$$T_i^z=\tfrac{1}{2}(n_{i\uparrow}+n_{i\downarrow}-1) .$$

$T_i^z=-\frac{1}{2}$ corresponds to an empty site and $T_i^z=+\frac{1}{2}$ corresponds to a site occupied by a pair with opposite spins. Then,

$$H=-2\sum_{\langle ij\rangle} V_{ij}(T_i^xT_j^x+T_i^yT_j^y)$$

is of the form of a XY model. For finite V_{ij} and t_{ij}, H interpolates between these two extremes. The degree of pairing can be measured by the on-site spin-up—spin-down correlation function $g_i=\langle 0\,|\,n_{i\uparrow}n_{i\downarrow}\,|\,0\rangle$, which, for temperature $T=0$ and $V_{ij}=0$, takes its uncorrelated value $\frac{1}{4}$, whereas for $t_{ij}=0$ is equal to $\frac{1}{2}$ (half-filled band).

We now proceed to study the properties of (1) in 1D. The Hamiltonian (1) can be transformed by a generalized Jordan-Wigner transformation for a chain of N sites[16]

$$
\begin{aligned}
c_{m\downarrow}^{\dagger} &= \left[\prod_{l=1}^{m-1}(-2S_l^z)\right] S_m^+ , \\
c_{m\downarrow} &= \left[\prod_{l=1}^{m-1}(-2S_l^z)\right] S_m^- , \\
c_{m\uparrow}^{\dagger} &= \left[\prod_{l=1}^{m-1}(-2\tau_l^z)\right]\left[\prod_{k=1}^{N}(-2S_k^z)\right]\tau_m^+ , \\
c_{m\uparrow} &= \left[\prod_{l=1}^{m-1}(-2\tau_l^z)\right]\left[\prod_{k=1}^{N}(-2S_k^z)\right]\tau_m^- ,
\end{aligned}
\tag{2}
$$

to a system of two coupled $S=\frac{1}{2}$ chains $\mathbf{S}_m$ and $\boldsymbol{\tau}_m$:

$$
\begin{aligned}
H = t\sum_{m=1}^{N} &(\tau_m^+\tau_{m+1}^- + \tau_{m+1}^+\tau_m^- + S_m^+S_{m+1}^- + S_{m+1}^+S_m^-) \\
&- V\sum_{m=1}^{N}(\tau_m^+\tau_{m+1}^- S_m^+S_{m+1}^- + \tau_{m+1}^+\tau_m^- S_{m+1}^+S_m^-) ,
\end{aligned}
\tag{3}
$$

where we set $t_{m,m+1}=t$, $V_{m,m+1}=V$, with $V,t>0$, and $V_{m,m'}=t_{m,m'}=0$, if $m'\neq m+1$.[17] From (2) it follows that $S_m^z=\frac{1}{2}-n_{m\downarrow}$ and $\tau_m^z=\frac{1}{2}-n_{m\uparrow}$, so for the half-filled band $\sum_m (S_m^z+\tau_m^z)=0$. The two limiting cases $V=0$ and $V=\infty$ are two uncoupled, exactly soluble XY chains and the XY chain of *pairs* $(\mathbf{S}_m,\boldsymbol{\tau}_m)$, respectively. It is clear from this representation that the transition, if it exists, is from a XY (planar) state to another planar state, and thus is hard to detect by the standard methods. The following observations may give us a way to identify this transition. For $V=0$ the ground state is a product ground state of two-independent planar states. For $N\to\infty$ there is no gap in the spectrum, i.e., if we add an extra particle the energy does not change due to the planar character of the system. On the other hand, for $V=\infty$, an extra particle drastically modifies the system as it cannot pair up! This contrasts the excitations by injecting a pair with spin up and spin down (or increasing *both* $\sum_m S_m^z$ and $\sum_m \tau_m^z$ by one). The gap for two-particle excitations for $N\to\infty$ and $V\to\infty$ is vanishing since it amounts to adding an extra particle in the $V=\infty$ planar model. So if a transition exists we expect a single-particle excitation spectrum with the energy gap opening above a certain $(V/t)_c$. One would, in analogy with other transitions into a planar phase,[18] expect the transition to be of essential singularity type.

We have performed numerically exact calculations on finite chains with $N\leq 10$ sites to obtain the low-lying spectrum of (1). We used finite-size scaling[19] to extract the critical behavior. In practice, the two $S=\frac{1}{2}$ chains of Eq. (3) have been represented by an equivalent $S=\frac{3}{2}$ chain with an interaction that corresponds exactly to (3). The following symmetries have been used to reduce the size of the subspaces to be diagonalized: The total z component of spin $\mathbf{S}$ and $\boldsymbol{\tau}$,

$$
\frac{1}{N}(S^z+\tau^z)=\frac{1}{N}\sum_{m=1}^{N}(S_m^z+\tau_m^z)=1-\rho ,
$$

where ρ the filling of the band $(0\leq\rho\leq 2)$ is held fixed; the wave vector is chosen fixed at $(2\pi/N)m$, $m=0,\ldots,N$; the left-right parity of the periodic chain and the reflection parity of inversion, $\mathbf{S}_m\to-\mathbf{S}_m$ and $\boldsymbol{\tau}_m\to-\boldsymbol{\tau}_m$ (when it applies, $S^z=\tau^z=0$), respectively, are used as good quantum numbers. The calculations are done by direct diagonalization for $N\leq 6$, and for $6<N\leq 10$ we use the Lanczos tridiagonalization scheme which yields the ground-state wave function $|0\rangle$ and the lowest part of the spectrum.

Here we present the results, primarily for even N, $N\leq 10$. From now on we use the representation in which $\tau_i^z=S_i^z=\left(\begin{smallmatrix}\frac{1}{2} & 0\\ 0 & -\frac{1}{2}\end{smallmatrix}\right)$. First, the absolute ground-state energy per site e_0 has been determined, and it is verified that it reproduces the exactly known value for the soluble cases $V=0$ and $t=0$: $(1/t)e_0(V=0)=2e_0(t=0)/V=-4/\pi$, $N\to\infty$.[20] Then we calculate the different energy gaps in the spectrum. Denoting $E_0(S^z,\tau^z)$, the ground-state energy in a subspace with given S^z and τ^z, we define the single particle and the pair gaps as $\Delta_1=E_0(2,0)-E_0(0,0)$ and $\Delta_2=E_0(2,2)-E_0(0,0)$, respectively, where $E_0(0,0)$ is the absolute ground-state energy for the half-filled band, $\rho=1$. In order to illustrate that it takes a finite energy to break a pair in the pair-hopping regime, V/t large, we show in Fig. 1 the values of $\Delta_1^{(N)}/t$ for $V/t=20$. The odd-N and even-N sequences are different, but they both extrapolate towards a common finite value $\Delta_1^{(\infty)}/t\sim 0.93\pm 0.01$. In contrast, the energy gap for pair excitations $\Delta_2^{(N)}$ always tends to zero no matter how

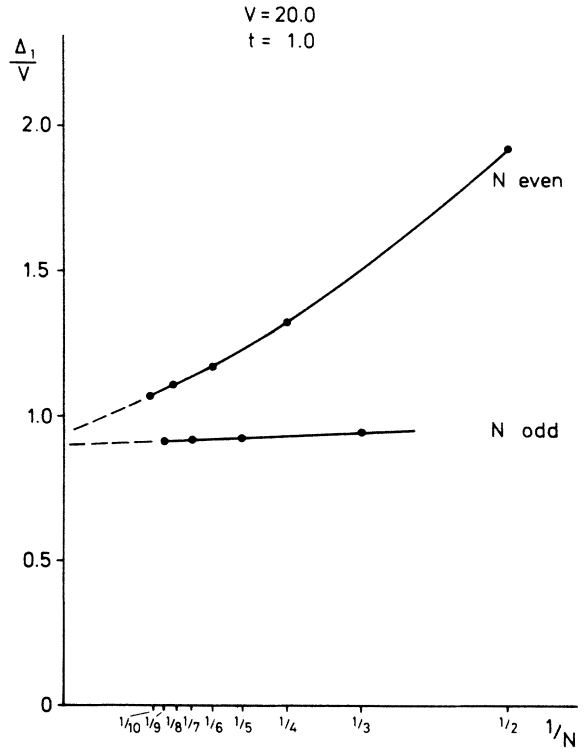

FIG. 1. Single-particle gaps $\Delta_1^{(N)}/t$ plotted as a function of N^{-1} for $V/t=20.0$ for even N and odd N. Both even-N and odd-N sequences extrapolate to a value $\Delta_1/t=0.93\pm 0.10$.

large V/t. $\Delta_1^{(\infty)}$ being zero for $V/t=0$, and finite for large V/t, implies that there must be a transition at $0 \leq (V/t)_c < \infty$. In order to locate $(V/t)_c$, we have plotted the scaled gaps $N\Delta_{1,2}^{(N)}$ as a function of V/t in Fig. 2. For single-particle scaled gaps $N\Delta_1^{(N)}$ the curves coalesce for small V/t indicating a line of fixed points.[18] For large V/t the scaled gaps for fixed V/t increase with increasing N, indicating a finite gap. In order to more precisely determine the transition point, we have calculated the crossing of $\Delta_1^{(N)}$ and $\Delta_2^{(N)}$ for a given N (even N), which necessarily gives a *lower* bound for the transition as $\Delta_2^{(N)}=2\Delta_1^{(N)}$ at $V/t=0$, but $\Delta_1^{(N)}/\Delta_2^{(N)} \to_{V/t\to\infty} \infty$. In the inset we have plotted the crossing points $(V/t)^*(N)$ as a function of N^{-1}, which extrapolate to $(V/t)_c^*=1.4\pm0.1$. The single-particle excitations for odd $N(S^z=1=\pm\tau^z)$ behave similarly to the even-N results. We have also searched for fixed points $(V/t)_c(N,N')$ of the phenomenological renormalization-group (PRG) equations,[19] $N\Delta_1^{(N)}[(V/t)^*]=N'\Delta_1^{(N')}[(V/t)^*]$, and find that

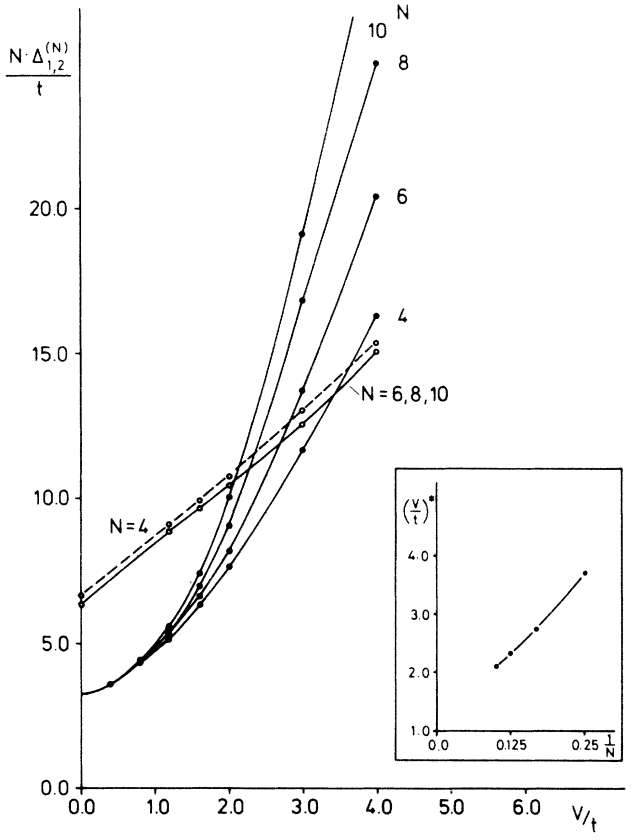

FIG. 2. Scaled gaps for single-particle excitations $N\Delta_1^{(N)}/t$ and for pair excitations $N\Delta_2^{(N)}/t$ plotted versus V/t for different sizes N. While the pair excitation gaps (open circles) are finite for all V/t, the single-particle gaps (solid circles) tend to coalesce for $0 < V/t \lesssim 1.4$, signaling a line of fixed points. For large values of V/t, the $N\Delta_1^{(N)}/t$ scaled gaps diverge with increasing N. In the inset the crossing points of $\Delta_{1,2}^{(N)}$, i.e., the solutions of $\Delta_1^{(N)}[(V/t)^*]=\Delta_2^{(N)}[(V/t)^*]$ are plotted as a function of N^{-1}. $(V/t)_N^*$ extrapolates to $(V/t)_\infty^*=1.40\pm0.10$ for $N\to\infty$, suggesting that the line of fixed points terminates at this value.

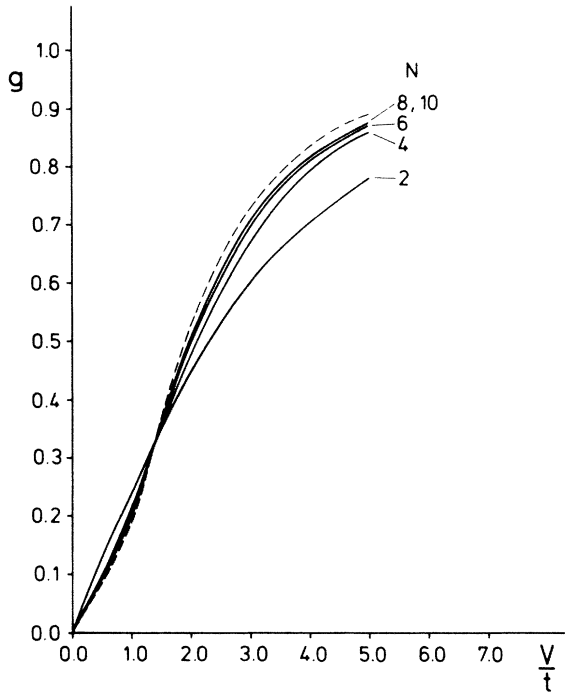

FIG. 3. Local on-site correlation function $g_i=\langle 0 | S_i^z\cdot\tau_i^z | 0\rangle$ as a function of V/t for different sizes N. The curves all have an inflection point near $V/t\approx1.4$, where the transition occurs.

for odd N, $(V/t)_c=0$ for all N, and for even N, $(V/t)_c(N,N')$ extrapolates to zero with increasing N,N'. The critical exponent ν calculated from the PRG increases dramatically with increasing N,N'. This is typical for behavior observed at transitions of essential singularity type.[18] The results from PRG combined with the results from Fig. 2, then suggest a whole *line* of critical points extending from $V/t=0$ to $V/t\approx1.40$.

The knowledge of the ground state $|0\rangle$ allows one to calculate the correlation functions. We present the local spin-up–spin-down correlations $g_i=\langle 0 | S_i^z\cdot\tau_i^z | 0\rangle$ for $\rho=1$, which measure the degree of local spin pairing. In Fig. 3, $g_i(N)$ are plotted as a function of V/t. One observes that g_i approaches its limiting value like $1/N$ (indicated by the dashed line). Note that the curves have an inflection point at about the value of the transition, $V/t\sim1.4$.

In conclusion, we have presented an analysis of a real-space model which describes the hopping of highly localized electron pairs. The single-particle hopping acts against the pairing, and a transition results for a finite $V/t\sim1.4$ of an essential singularity type. Several extensions of this approach are being considered. Among them the inclusion of the Hubbard term, the extensions to finite temperatures and higher dimensions should provide a clue to what extent (1) may be a model of real-space superconductivity.

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