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Phase Transitions in Electron Systems with Short-Range Pairing Interactions: Ground State

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We propose a real-space, tight-binding model of electrons with short-range pairing interactions. The model involves a competition between the ordinary single particle hopping t and an attractive interaction V between the singlet electronic pairs formed on neighboring lattice sites. The Hamiltonian effectively describes a mechanism for pair formation. We study the ground-state properties of its one-dimensional version using numerically exact finite chain calculations for up to $N=10$ sites. The ground-state wave functions, the energy spectrum, and various ground-state correlation functions are calculated with the help of an exactly equivalent system of two coupled $S=\frac{1}{2}$ spin chains. The results indicate the existence of a transition between the band and the localized pairs situation. The transition takes place for $V/t=1.4\pm0.1$ and appears to be of essential singularity type. Comparison with other models used for pairing phenomena, like the negative U-Hubbard model is made.

KEY WORDS: Cooper pairs; pairing in real-space; finite-size scaling; quantum ground-state phase transitions; localized electron pairs; XY model; Hubbard model; essential singularity of correlations.

1. INTRODUCTION

The Bardeen–Cooper–Schrieffer (BCS) theory of superconductivity has been highly successful in explaining the properties of a large number of isotropic metals and alloys. The BCS reduced Hamiltonian reads

$$H_{\mathrm{BCS}}=\sum_{\mathbf{k},\sigma}\varepsilon(\mathbf{k})\,c^{+}_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}-V_s\sum'_{\substack{\mathbf{k},\mathbf{k}'\\ \sigma,\sigma'}}c^{+}_{\mathbf{k},\sigma}c^{+}_{-\mathbf{k},-\sigma}c_{-\mathbf{k}',-\sigma'}c_{\mathbf{k}',\sigma'} \tag{1}$$

where $c^{+}_{\mathbf{k}\sigma}$ is the creation operator of the electron in the Bloch-wave state

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with the wave vector $\mathbf{k}$ and the spin σ, $\varepsilon(\mathbf{k})$ is the single-particle spectrum of Bloch states, $V_s > 0$ is the effective attractive interaction, which acts only between pairs of electrons with opposite $\mathbf{k}$ and σ. The prime over the second summation in (1) means that only certain values of $\mathbf{k}$ and $\mathbf{k}'$ participate in the interaction. The interaction V_s originates from the electron–phonon interactions, and the elastic properties of the lattice impose the cutoff: only those values of $\mathbf{k}$ and $\mathbf{k}'$ satisfying $|\varepsilon(\mathbf{k}) - \varepsilon_F| = |\varepsilon(\mathbf{k}') - \varepsilon_F| < 2\omega_D$, where ω_D is the Debye energy of the underlying lattice, contribute to the second term of (1), (ε_F is the Fermi energy). The term reduced in connection with (1) means that the complete Hamiltonian of electrons in a superconductor contains many other terms, but they are not of great relevance to superconductivity. The Hamiltonian (1) then singles out the terms that behave differently on both sides of the transition point. The BCS solution consists in applying the molecular-field theory (MFT) decoupling scheme to (1). This is usually justified by noting that (1) leads to the creation of Cooper pairs with a very large radius.

Furthermore, there is an intrinsic assumption about the weakness of interaction, $V_s \ll W$, where W is a certain averaged bandwidth, closely related to the existence of a bound state of two electrons with an infinitesimally small attractive interaction (Cooper effect). Thus, from the point of view of critical phenomena, the BCS treatment of three-dimensional (3D), isotropic superconductors leads (through eq. 1) to a second-order phase transition with MFT critical exponents. It can be shown using the Ginzburg criterion[2,3] that for normal superconductors this behavior persits up to $(T - T_c)/T_c \approx 10^{-10}$, which means that the critical region cannot be attained experimentally.

In practice, some of the above assumptions may, some other may not, be fulfilled, and a problem arises then as to what extent the validity and predictions of the BCS theory should be questioned. With decreasing dimensionality the role of fluctuations becomes dominant and the molecular-field BCS-like theories cease to be reliable. In addition, in low-dimensional, especially organic compounds serious complications arise in the reciprocal space[4] and the use of the real-space formulation appears to be more secure.

Real-space formulations, using localized, atomic-like orbitals, have been used in several contexts. The superconductivity in narrow d bands was studied in the "contact" approximation,[5] which consists in assuming that the components of a Cooper pair are on the same lattice site. The real-space pairing has been analyzed with the negative U Hubbard model, i.e.

$$H_H = \sum_{\substack{\langle ij \rangle \\ \sigma}} t_{ij} c_{i\sigma}^{+} c_{j\sigma} - U \sum_i n_{i\uparrow} n_{i\downarrow}, \qquad (U > 0) \tag{2}$$

where $n_{i\sigma} = c_{i\sigma}^{+} c_{i\sigma}$ and $\langle ij \rangle$ denotes a nearest-neighbor pair.[6] It is clear that with increasing U/t in (2) the probability of local pairing increases, but the mobility of pairs appears only in the second order in the transfer integral t. The Hamiltonian (2) has been microscopically derived by Anderson[7] in connection with amorphous materials and has been invoked to explain the bipolaron transition.[8,9] The Hartree–Fock (HF) analysis of (2) has been carried through[10] and 1D exact wave functions are also available.[11] Also, (2) has been called on in several experimental contexts.[12] Very recently, Nozières et al.[13] have analyzed the transition between the weak (BCS-type) and strong (negative U) coupling superconductivity. They emphasize that within an extended HF-approximation the Hamiltonian (2) does not give a right U/t dependence of T_c (for $U/t \gg 1$). They advocate the use of a nonlocal pairing interaction, which should provide a better link between the weak and strong coupling regimes in superconductivity.

In this paper we introduce a real-space model with an effective attraction of singlet electron pairs formed on different lattice sites and discuss the ground-state properties of its 1D version using the finite-size scaling (FSS) method. (A complete review of this method is given in Ref. 14.) The FSS has the distinct advantage of not being limited to particular values of the coupling constants. It utilizes exact solutions of finite systems. The paper is organized as follows: in Section 2 we define the fermionic model and discuss its invariance properties; in Section 3 the Jordan–Wigner transformation is used to obtain an exact representation of the model in terms of two coupled spin chains; in Section 4 we describe the finite-size scaling method applied to the spin representation; in Section 5 we present the results for various ground-state properties, like the ground-state energy, different energy gaps in the spectrum and various correlation functions in the ground state. The results suggest the existence of a transition at $T = 0$. In Section 6 the discussion and conclusions are given.

2. THE MODEL AND ITS SYMMETRY PROPERTIES

As mentioned in the Introduction, the BCS Hamiltonian (1) is defined in the reciprocal space and the radius of the Cooper pairs is large. Here, we attempt to construct a pairing interaction in real space which is short-ranged.

If $c_{i\sigma}^{+}$ creates an electron with spin σ at site i of a regular lattice ($\{c_{i\sigma}, c_{j\sigma'}^{+}\} = \delta_{ij}\,\delta_{\sigma\sigma'}$) then we can define a pair creation operator $b_i^{+(l)}$

$$b_i^{+(l)} = c_{i\uparrow}^{+}\, c_{i+l\downarrow}^{+} \tag{3}$$

A general interaction between such singlet pairs can be written as

$$\mathcal{V} = -\sum_{\substack{i,j \\ l,l'}} V_{ij}(l, l')(b_i^{+(l)} \cdot b_j^{(l')} + \text{h.c.}) \tag{4}$$

For general (i, j) and (l, l') one is dealing with overlapping fermion pairs, very much like in (1). Without elaborating about the microscopic origin of interaction we simply stipulate that the dominant contributions in (4) come from nearest-neighbors i and j and, additionally, $l = l' = 0$, with $V_{ij}(0, 0) = V$, $V > 0$. The resulting Hamiltonian, including the kinetic energy and the chemical potential terms now reads

$$H - \mu \sum_{i,\sigma} n_{i\sigma} = \sum_{\langle ij \rangle, \sigma} t_{ij} c_{i\sigma}^{+} c_{j\sigma} - V \sum_{\langle ij \rangle} (c_{i\uparrow}^{+} c_{i\downarrow}^{+} c_{j\downarrow} c_{j\uparrow} + c_{j\uparrow}^{+} c_{j\downarrow}^{+} c_{i\downarrow} c_{i\uparrow}) - \mu \sum_{i,\sigma} n_{i\sigma} \tag{5}$$

Equation (5) presents a well-defined quantum mechanical problem whose solution depends on the temperature T, the dimensionality of space, and the filling of the band, defined by the electron density ρ

$$\rho = \frac{1}{N} \left\langle \sum_i (n_{i\uparrow} + n_{i\downarrow}) \right\rangle \tag{6}$$

or $\rho = \langle \hat{N}_e \rangle / N$, where $\hat{N}_e$ is the number operator of electrons and N is the number of sites in the system. Evidently, $0 \leqslant \rho \leqslant 2$ and the half-filled band corresponds to $\rho = 1$.

Some symmetry properties of the Hamiltonian of (5) can be obtained by noting that H is invariant with respect to the following transformation of electron operators

$$\begin{aligned} \tilde{c}_{m\uparrow}^{+} &\to (-1)^m c_{m\downarrow} \\ \tilde{c}_{m\downarrow}^{+} &\to (-1)^m c_{m\uparrow} \end{aligned} \tag{7}$$

The transformation (7) is canonical, i.e., it preserves the fermion commutation relations. It is a combination of a particle hole and a local gauge transformation with a gauge factor $e^{i\psi(m)}$ with $\psi(m) = m\pi$. From (7) it follows that

$$H(t, V) - \mu \hat{N}_e = \tilde{H}(t, V) + \mu \hat{\tilde{N}}_e - 2\mu N \tag{8}$$

and for the grand partition function $Z_\mu(t, V)$, one obtains $[\beta = (k_B T)^{-1}]$

$$\ln Z_\mu(t, V) = 2\beta\mu N + \ln \tilde{Z}_{-\mu}(t, V) \tag{9}$$

From this last relation one can show that for $\rho = 1$ the chemical potential $\mu = 0$. Differentiating both sides of (9) with respect to μ, we get

$$\frac{1}{\beta}\frac{\partial Z_\mu(t, V)}{\partial \mu} = 2N_s - \frac{1}{\beta}\frac{\partial \tilde{Z}_{-\mu}(t, V)}{\partial(-\mu)} \tag{10}$$

For $\rho = 1$, $\langle \hat{N}_e \rangle = N$ which implies

$$\frac{\partial Z_\mu(t, V)}{\partial \mu} = \frac{\partial \tilde{Z}_{-\mu}(t, V)}{\partial(-\mu)} \tag{11}$$

or

$$\mu = 0 \qquad (\rho = 1) \tag{12}$$

In the following we consider $\rho = 1$. The interaction V describes the nearest-neighbor hopping of singlet pairs formed on the same site. From the Pauli principle hopping from i to j can only be effective if site j is empty. Then, with increasing V/t, the energy will be lowered if singly occupied sites are eliminated from the wave function. In the limit $V = 0$, the single-particle hopping t acts the same way on singly and doubly occupied states. In fact, for $V = 0$, electrons with different spin are uncoupled and we have a system of two independent tight-binding fermions, whose properties are known. In the limit $t = 0$ there are no singly occupied sites and the two possible occupancies (empty or doubly occupied) can be described by introducing $S = \frac{1}{2}$ pseudospins $\mathbf{T}_i$ with $T_i^+ = c_{i\uparrow}^+ c_{i\downarrow}^+$ and $T_i^z = \frac{1}{2}(n_{i\uparrow} + n_{i\downarrow} - 1)$ with the eigenvalues $T_i^z = \pm\frac{1}{2}$ corresponding to doubly occupied and empty sites, respectively. The Hamiltonian for $t = 0$ can be written down as

$$H = -2V \sum_{\langle ij \rangle} (T_i^x T_j^x + T_i^y T_j^y) \tag{13}$$

i.e., is of the form of a $S = \frac{1}{2} XY$ model. Its properties are exactly known in 1D and partial information exists for higher dimensionalities, too.[15] For intermediate couplings, H interpolates between these two extremes.

Some insight into the properties of Hamiltonian (5) can be gained from the analytical solution of the simple case $N = N_e = 2$, presented in Appendix I.

As can be seen from (A7), the ground-state wave function in the absence of interaction contains empty, spin-up, spin-down, and doubly occupied sites in equal proportions. In contrast, for $t = 0$, singly occupied sites are suppressed and only empty and doubly occupied sites contribute to the wave function. This picture clearly persists for other values of N and N_e. In Fig. 1 we depict, for the half-filled band, $N = N_e = 8$, the com-

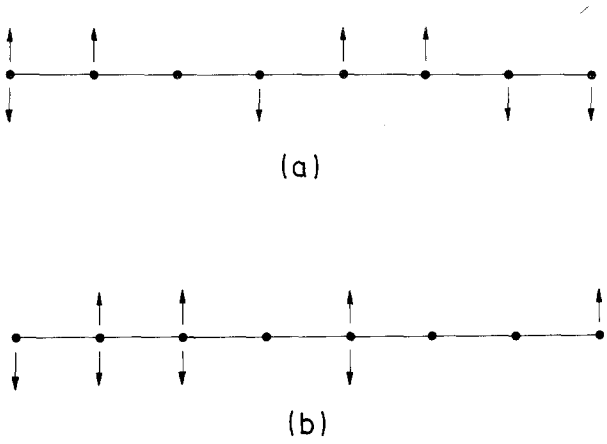

Fig. 1. Typical configurations of the ground state of a chain of $N=8$ sites: the state shown in (a) has the largest amplitude for $V/t \ll 1$ and the one in (b) for $V/t \gg 1$. In both cases $S^z = \tau^z = 0$. In the latter case the pairing induced by the interaction term is clearly visible.

ponents with the largest weight of the ground-state wave functions in the sector $\sum_{i=1}^{8} S_i^z = 0$, for V/t small (Fig. 1a) and V/t large (Fig. 1b).

One would like to understand the nature of the process of the increase of the number of paired sites in the ground state of (5), i.e., the pairing transition. As the first step we will undertake an analysis of the simplest, albeit still not exactly soluble, 1D version of Hamiltonian (5).

3. TRANSFORMATION TO THE COUPLED CHAIN SYSTEM

The Hamiltonian of (5) when rewritten in 1D takes on the following form

$$H = t \sum_{m,\sigma} (c_{m\sigma}^{+} c_{m+1\sigma} + c_{m+1\sigma}^{+} c_{m\sigma}) - V \sum_{m} (c_{m\uparrow}^{+} c_{m\downarrow}^{+} c_{m+1\downarrow} c_{m+1\uparrow} + c_{m+1\uparrow}^{+} c_{m+1\downarrow}^{+} c_{m\downarrow} c_{m\uparrow}) \tag{14}$$

The Hamiltonian (14) involves only nearest-neighbor terms and it turns our that in this case it is possible to use the generalized Jordan–Wigner transformation to map (14) into an equivalent system of $S = \frac{1}{2}$ spins.

To this end we first introduce a set of Paulions $a_{m\sigma}^{+}$ associated with the sites m. The Paulions anticommute on site with the same spin and commute on different sites. They satisfy the following commutation relations

$$a_{m\sigma} a_{m'\sigma'}^{+} - a_{m'\sigma'}^{+} a_{m\sigma} = \delta_{mm'} \delta_{\sigma\sigma'} (1 - 2 a_{m\sigma}^{+} a_{m\sigma}) \tag{15}$$

For a chain of N sites the generalized Jordan–Wigner (JW) transformation is[16]

$$\begin{aligned} a_{m\downarrow}^{+} &= c_{m\downarrow}^{+} \exp\left(i\pi \sum_{l=1}^{m-1} c_{l\downarrow}^{+} c_{l\downarrow} \right) \\ a_{m\uparrow}^{+} &= c_{m\uparrow}^{+} \exp\left[i\pi \left(\sum_{l=1}^{m-1} c_{l\uparrow}^{+} c_{l\uparrow} + \sum_{l=1}^{N} c_{l\downarrow}^{+} c_{l\downarrow} \right) \right] \end{aligned} \tag{16}$$

Upon observing that from (16) $c_{m\sigma}^{+} c_{m\sigma} = a_{m\sigma}^{+} a_{m\sigma}$, we can now introduce two sets of $S = \frac{1}{2}$ spin operators per site $\mathbf{s}_m$ and $\boldsymbol{\tau}_m$ by identifying

$$\begin{aligned} a_{m\downarrow}^{+} &= \mathbf{s}_m^{+} \\ a_{m\downarrow} &= \mathbf{s}_m^{-} \\ c_{m\downarrow}^{+} c_{m\downarrow} - \tfrac{1}{2} &= a_{m\downarrow}^{+} a_{m\downarrow} - \tfrac{1}{2} = \mathbf{s}_m^{z} \end{aligned} \tag{17a}$$

and

$$\begin{aligned} a_{m\uparrow}^{+} &= \tau_m^{+} \\ a_{m\uparrow} &= \tau_m^{-} \\ c_{m\uparrow}^{+} c_{m\uparrow} - \tfrac{1}{2} &= a_{m\uparrow}^{+} a_{m\uparrow} - \tfrac{1}{2} = \tau_m^{z} \end{aligned} \tag{17b}$$

With (17) we can rewrite (16) as

$$\begin{aligned} c_{m\downarrow}^{+} &= \left[\prod_{l}^{m-1} (-2s_l^z) \right] s_m^{+} \\ c_{m\downarrow} &= \left[\prod_{l=1}^{m-1} (-2s_l^z) \right] s_m^{-} \\ c_{m\uparrow}^{+} &= \left[\prod_{l=1}^{m-1} (-2s_l^z) \right] \left[\prod_{k=1}^{N} (-2s_k^z) \right] \tau_m^{+} \\ c_{m\uparrow} &= \left[\prod_{l=1}^{m-1} (-2s_l^z) \right] \left[\prod_{k=1}^{N} (-2s_k^z) \right] \tau_m^{-} \end{aligned} \tag{18}$$

The operators $\mathbf{s}_m$ and $\boldsymbol{\tau}_m$ satisfy separately the usual spin commutation relations and $[s_m^{\alpha}, \tau_{m'}^{\beta}] = 0$, for all α, β, m, m' ($\alpha, \beta = X, Y, Z$). With (18), the Hamiltonian of (14) can be rewritten as

$$\begin{aligned} H = t \sum_{m} & (\tau_m^{+} \tau_{m+1}^{-} + \tau_{m+1}^{+} \tau_m^{-} + s_m^{+} s_{m+1}^{-} + s_{m+1}^{+} s_m^{-}) \\ & - V \sum_{m} (\tau_m^{+} \tau_{m+1}^{-} s_m^{+} s_{m+1}^{-} + \tau_{m+1}^{+} \tau_m^{-} s_{m+1}^{+} s_m^{-}) \end{aligned} \tag{19}$$

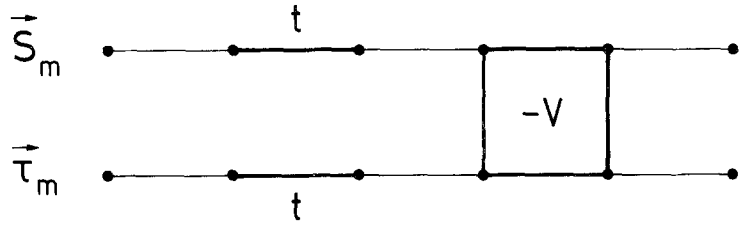

Fig. 2. Schematic representation of the coupled spin chains of (19): the kinetic energy term t acts on each chain independently; the interaction V couples them.

It represents a special case of two coupled chains with the XY symmetry. The hopping terms corresponds to two independent XY chains. The pairing term is a four-spin interaction with the XY symmetry (the equivalence between the chain of interacting fermions and two coupled spin problems have been used for the Hubbard model in Shiba, Ref. 17, and for the Kondo necklace problem in Jullien *et al.*, Ref. 17). This interaction has only nonvanishing matrix elements between the states having the same values for (s_m^z, τ_m^z) and $(s_{m\pm1}^z, \tau_{m\pm1}^z)$ separately with additional condition $s_m^z = -s_{m+1}^z$. Thus, the model can be viewed as two coupled XY chains.

Using (17a, b), the total number of electrons $\sum_m (n_{m\uparrow} + n_{m\downarrow})$ can be reexpressed as

$$\hat{N}_e = \sum_m (n_{m\uparrow} + n_{m\downarrow}) = N + S^z + \tau^z \tag{20}$$

where $S^z = \sum_m s_i^z$ and $\tau^z = \sum \tau_i^z$, with $[H, S^z] = [H, \tau^z] = 0$. The interacting system of (19) is presented schematically in Fig. 2.

4. ANALYSIS OF THE GROUND STATE THROUGH THE FINITE-SIZE SCALING METHOD

The ground state of (19) is only known exactly in the limiting situations $V = 0$ or $t = 0$. In order to gain some information about the properties of the system for intermediate values of V/t, we have chosen the use of the FSS method which, when combined with phenomenological renormalization (PRG),[18] yields reliable results for ground state of a number of different low-dimensional quantum systems. References 19 through 30 give a representative choice of work in this field.

The FSS method is based on analysis of exact solutions of the Hamiltonian problem as a function of system size N. The results are then extrapolated to the $N \to \infty$ limit with the help of appropriate scaling hypotheses. Although theoretically the quality of the extrapolation

procedure increases with increasing N, in practice FSS appears to work well even for rather small values of N. The aim of the FSS analysis of (19) is the determination of the spectrum and of the eigenfunctions of (19) as a function of V/t. For the two limiting cases $V=0$ and $V=\infty$, we have two uncoupled XY chains and the XY chain of pairs $(\mathbf{s}_m, \tau_m)$, respectively. To investigate the low-lying spectrum we study the following energy gaps: if $E_0^{(N)}(s^z, \tau^z)$ is the ground state in the sector of given s^z, τ^z, then define the single particle gaps $\Delta_1^{(N)}$ and the pair gaps $\Delta_2^{(N)}$ as (from now on we use the representation in which $(s_m^z)^2=(\tau_m^z)^2=1$)

$$\begin{aligned}\Delta_1^{(N)}(s^z, \tau^z) &= E_0^{(N)}(s^z+2, \tau^z) - E_0^{(N)}(s^z, \tau^z) \\ &= E_0^{(N)}(s^z, \tau^z+2) - E_0^{(N)}(s^z, \tau^z)\end{aligned} \tag{21}$$

and

$$\Delta_2^{(N)}(s^z, \tau^z) = E_0^{(N)}(s^z+2, \tau^z+2) - E_0^{(N)}(s^z, \tau^z) \tag{22}$$

In the following we are mainly interested in the sector of the absolute ground state with $S^z=\tau^z=0$[16] or, through (6) and (20), $\rho=1$. $\Delta_1^{(N)}$ and $\Delta_2^{(N)}$ give the energy differences by injecting a single particle and a pair of particles with opposite spins in the system.

For $V=0$ and $N=\infty$, the spectrum is gapless and $\Delta_2^{(N)}(0,0)=2\Delta_1^{(N)}(0,0)$ and $\Delta_{1,2}^{(N)} \sim N^{-1}$ for finite N as $N\to\infty$. For $t=0$ the model can be described by a single XY interaction, so we expect that $\Delta_2^{(N)} \to_{N\to\infty} 0$. On the other hand, Δ_1 corresponds to adding a single particle (analogously, one could break a pair) and therefore remains finite. If a transition exists there should be a single particle excitation spectrum with a gap Δ_1 opening above a certain $(V/t)_c$. Note that similar considerations applied to the original version of the BCS-Hamiltonian (1), see Ref. 31.

In order to verify the picture of the transition we have performed numerically exact calculations on finite chains with $N\leqslant 10$ sites and periodic boundary conditions. To cross-check the results we carried through the calculations using both the double-chain version (19) and its equivalent $S=\frac{3}{2}$ Hamiltonian on a single chain, with interaction whose matrix elements correspond exactly to those of (19). This last representation is described in Appendix II.

We have used the following symmetries to reduce the size of matrices to be diagonalized: the total z components S^z and τ^z, the left-right parity of the periodic chain, and the wave vector $(2\pi/N)\cdot m$ with $m=0,\ldots, N-1$ are used as good quantum numbers. In addition, for $S^z=\tau^z=0$ the reflection parity $\mathbf{s}_m \to -\mathbf{s}_m$ and $\tau_m \to -\tau_m$ is utilized. The direct diagonalization is done for $N\leqslant 6$ and we use the iterative Lanczos tridiagonalization scheme for $6<N\leqslant 10$ which determines, for a given subspace, the ground state

wave function $|0\rangle$ and the lowest part of the spectrum. With the knowledge of $|0\rangle$ correlation functions of various operators $\hat{0}$, $\langle 0|\hat{0}_i^+ \hat{0}_j|0\rangle$ have been also determined.

5. RESULTS

We now present the numerical finite-chain ($N \leqslant 10$) results for the one-dimensional model (19). First the ground-state energy has been determined and its limiting values for $V \to 0$ and $t \to 0$, respectively, have been

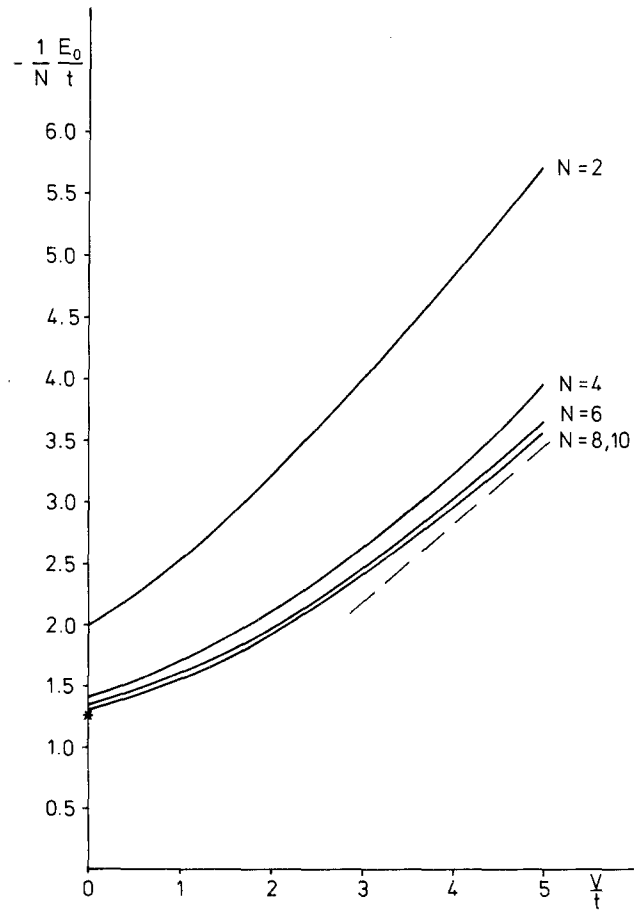

Fig. 3. The ground-state energy per site, $-E_0/(N \cdot t)$ as a function of V/t. The exact results for $V = 0$ and $N \to \infty$ is indicated by $(*)$. The limiting cases, $V \to 0$ and $t \to 0$ approach the exactly known results of the XY model as $N \to \infty$. The dashed line shows the exact slope as $V/t \to \infty$ and $N \to \infty$.

verified to reproduce the exact results for the XY chain.[32] The ground-state wave function always lies in the sector $S^z = \tau^z = 0$, has a wave vector $\mathbf{k} = 0$, and a positive parity of left-right exchange of the periodically bounded chain. In Fig. 3 the ground-state energy per site, $e_0 = E_0/N$ is shown as a function of V/t and it satisfies $(1/t)\, e_0\ (V=0) = 2e_0\ (t=0)/V = -4/\pi$ (see Ref. 32), as $N \to \infty$. As for most of the results the data are shown for N even only. We point out again that for the results we use the convention that

$$\tau_i^z = s_i^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

In order to characterise the transition from the unpaired ($V=0$) to the paired ($t=0$) state, we consider the low-lying spectrum. Notably we

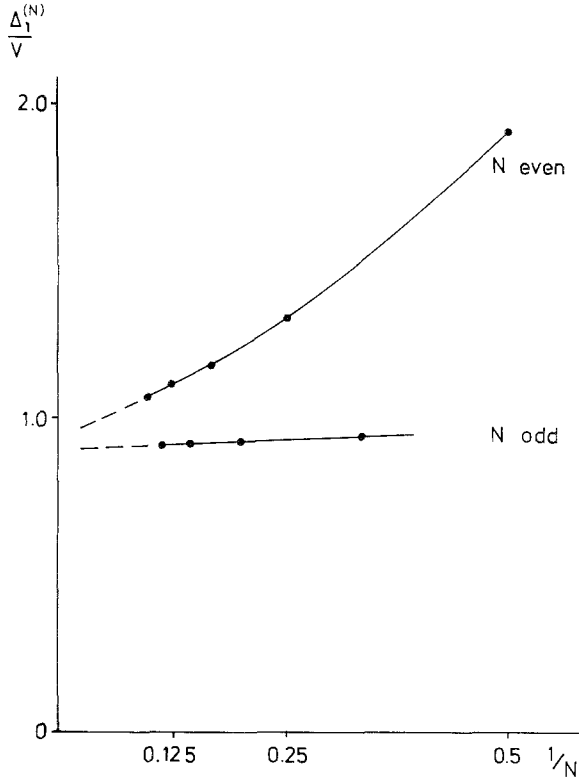

Fig. 4. Energy gap $\Delta_1^{(N)}$ of single particle excitations ($S^z = 1$, $\tau^z = 0$) for $V/t = 20$. The results plotted versus N^{-1} clearly indicate that $\Delta_1^{(N)}$ remains finite as $N \to \infty$.

calculate low-lying excitations both in the sector of the ground state and when adding an extra particle. The transition is not expected to be easily detectable in the ground-state sector, as in both limits $V \to 0$ and $t \to 0$ the model is an XY model, either of single fermions or of pairs glued together.

For both $V/t \to 0$ and $V/t \to \infty$ there is no energy gap. This makes it more difficult to investigate the model with FSS methods than, for example, the Hubbard model, where there is no low-lying continuum for $U/t \to \pm\infty$. The reason is that the interaction term in our model does not bind the fermions locally but favors their hopping in pairs. Single particle

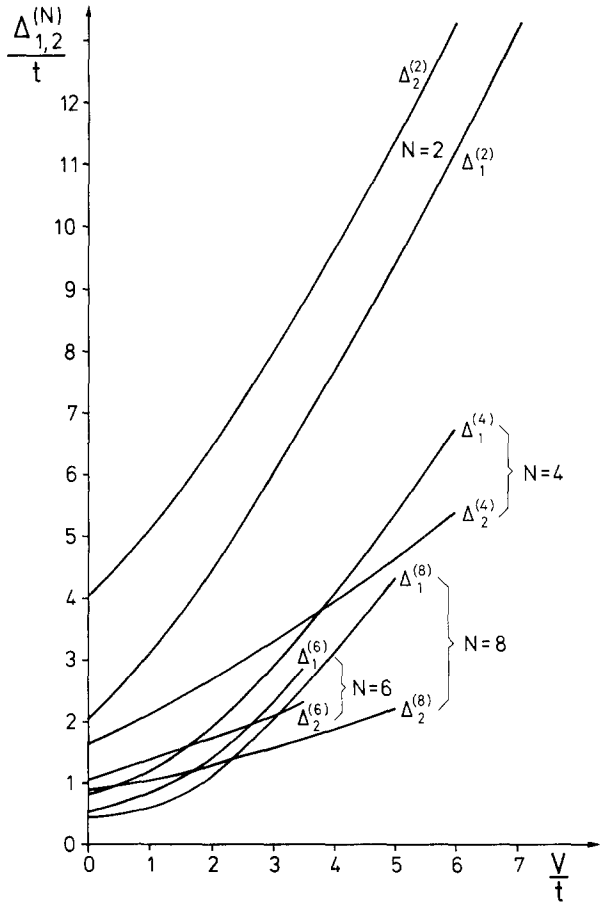

Fig. 5. Energy gaps $\Delta_1^{(N)}$ for single particle, respectively, $\Delta_2^{(N)}$ for pair excitations with opposite spin, as a function of V/t. Both $\Delta_1^{(N)}$ and $\Delta_2^{(N)}$ tend to zero for small V/t but only $\Delta_2^{(N)}$ for V/t large. $\Delta_1^{(N)} < \Delta_2^{(N)}$ for small V/t and $\Delta_1^{(N)} > \Delta_2^{(N)}$ for large V/t, which leads to a crossing of the levels.

excitations block the mobility of the pairs for V large, and hence are energetically unfavorable.

We define the single particle, respectively, pair gaps, as $\Delta_1 = E_0(2, 0) - E_0(0, 0)$ and $\Delta_2 = E_0(2, 2) - E_0(0, 0)$. $E_0(S^z, \tau^z)$ is the ground-state energy in the sector with given S^z, τ^z. Figure 4 shows Δ_1/V for $V/t = 20$ as a function of N^{-1}. This establishes quite convincingly that for large V/t there is a finite energy gap for single particle excitations. The results for even and odd N both tend toward the same value for $N \to \infty$.

In Figure 5 the gaps Δ_1 and Δ_2 are shown for different N as a function of V/t. For $V \to 0$, Δ_2 is exactly twice Δ_1 since the two chains act indepen-

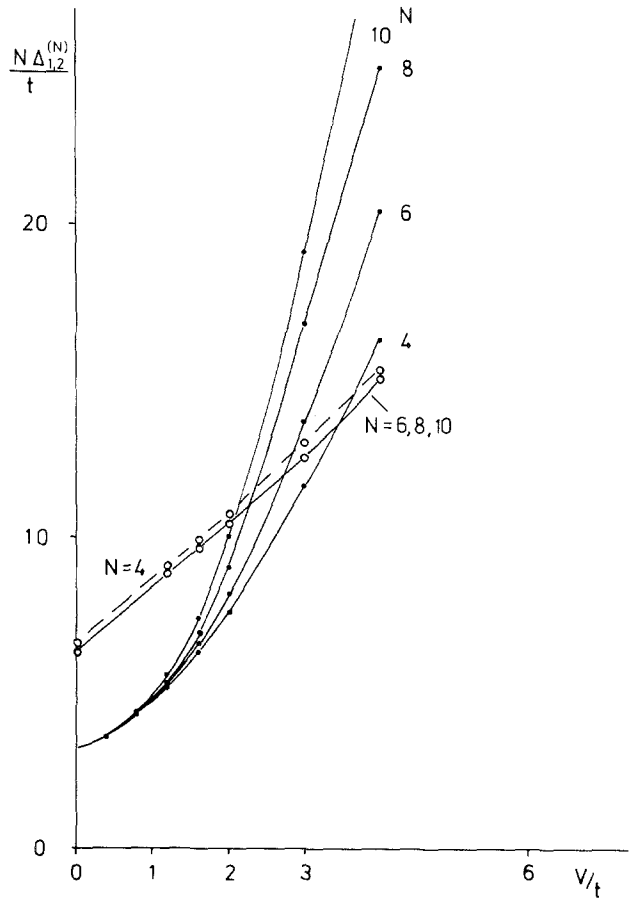

Fig. 6. Scaled gap $N\Delta_1^{(N)}$ (•) and $N\Delta_2^{(N)}$ (◦) as a function of V/t. The pair excitations converge very rapidly to a limiting value; $N = 6, 8, 10$ cases are indistinguishable. For $\Delta_1^{(N)}$ they converge well for $V/t \ll 1$ and they indicate a finite gap for $V/t \gg 1$.

dently, and both Δ_1 and Δ_2 vanish as N^{-1} when $N \to \infty$. For large V/t, Δ_1 always lies above Δ_2 since the $S^z = 2$, $\tau^z = 0$ gap is finite but the $S^z = \tau^z = 2$ gap vanishes when $N \to \infty$. Hence there is a crossing between the two gaps. It is more instructive to look at the scaled gap $N\Delta_{1,2}^{(N)}$, where gaps for different N should lie on top of each other for a continuum of excitations, i.e., for Δ_2 for any value of V/t and for Δ_1 for V/t small. In Fig. 6 the scaled gap $N\Delta_1^{(N)}$ is plotted versus V/t for different values of N. It suggests that there is a continuum of excitations up to a finite value $(V/t)^*$ above which the gap Δ_1 opens. The small V/t values are shown separately in Fig. 7, indicating that even for small N, the asymptotic form $N\Delta_1^{(N)} \to \text{const}$ (independent on N) is satisfied quite well. As is known from numerous studies,[14] it is very difficult to reliably determine from such plots at what value of V/t the gap opens if the transition is of the type essential singularity. Thus these

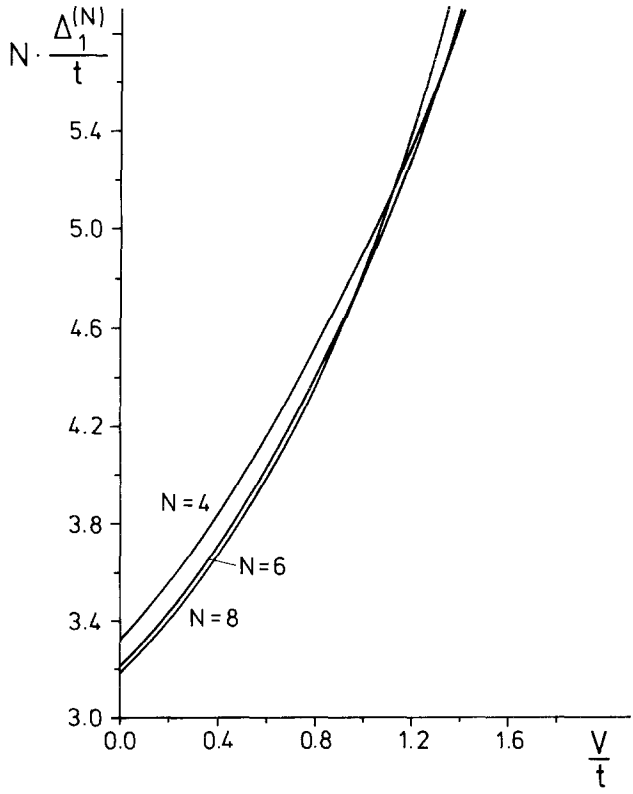

Fig. 7. Scaled gap $N \cdot \Delta_1^{(N)}$ for small V/t (from Fig. 6). The curves for $N = 4, 6, 8$ are very close, $N = 10$ coincides with $N = 8$. The curves indicate a planar region extending up to $V/t \gtrsim 1$.

curves merely serve to establish the qualitative picture. The actual determination of the transition point $(V/t)^*$ comes from comparing Δ_1 and Δ_2.

As $\Delta_1 < \Delta_2$ for V/t small and a finite gap for Δ_1 implies $\Delta_1 > \Delta_2$ for V/t large, the crossing of Δ_1 and Δ_2 certainly occurs for $(V/t) \leqslant (V/t)^*$. Hence, this crossing serves as a lower bound for the transition point $(V/t)^*$. Figure 8 shows the values of $(V/t)^*$ where $\Delta_1^{(N)} = \Delta_2^{(N)}$ for increasing values of N. It suggests $(V/t)^* = 1.4 \pm 0.1$. As Δ_1 opens at about this value in Fig. 6, $(V/t)^* = 1.4$ seems to be the actual transition point. Let us mention that the odd N values behave similarly to the ones presented.

We have also applied the PRG, i.e., we have searched for solutions of $N \cdot \Delta_1^{(N)}[(V/t)_c] = N' \cdot \Delta_1^{(N')}[(V/t)_c]$. As is observed frequently for XY-like systems,[14] the values $(V/t)_c(N, N')$ do not agree with $(V/t)^*$. Describing the region $0 < V/t < (V/t)^*$ with a line of fixed points, $(V/t)_c(N, N')$ can tend toward any of these fixed points. In the present model

$$\lim_{N, N' \to \infty} (V/t)_c(N, N') = 0$$

An indication that there is a region of fixed points is the behavior of the

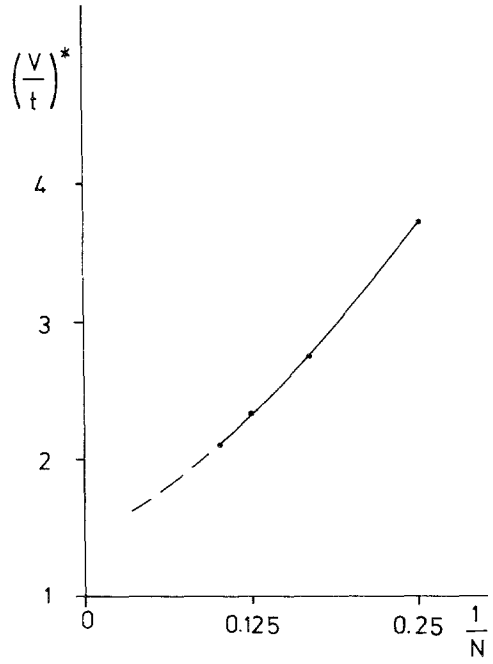

Fig. 8. Crossing of gaps $\Delta_1^{(N)}(V/t)$ and $\Delta_2^{(N)}(V/t)$ plotted versus N^{-1}. It gives an estimate (lower bound) of the transition $(V/t)^* = 1.4 \pm 0.1$.

critical exponent $\nu(N, N')$ calculated at fixed points of PRG. The values $\nu(N, N')$ diverge in the PRG analysis.

As additional evidence for a gapless region up to a finite value of V/t we have plotted in Fig. 9 the gap $\Delta_1^{(N)}$ as a function of N with V/t as a parameter. If in the whole gapless region $\Delta_1^{(N)} \sim [A(V/t)/N]^z$, where the amplitude $A(V/t)$ does not depend on N and $z = 1$ is the dynamical critical exponent, then the gapless region on a $\log \Delta_1^{(N)}$–$\log N$ plot should be seen as a set of straight lines for different V/t. Indeed on Fig. 9 the straight lines are observed up to $V/t = 1.4$. For $V/t \gg 1$ no such behavior is found. (There are slight oscillations for $N/2$ even and odd.) The ground-state correlations have been evaluated and their behavior is consistent with the above con-

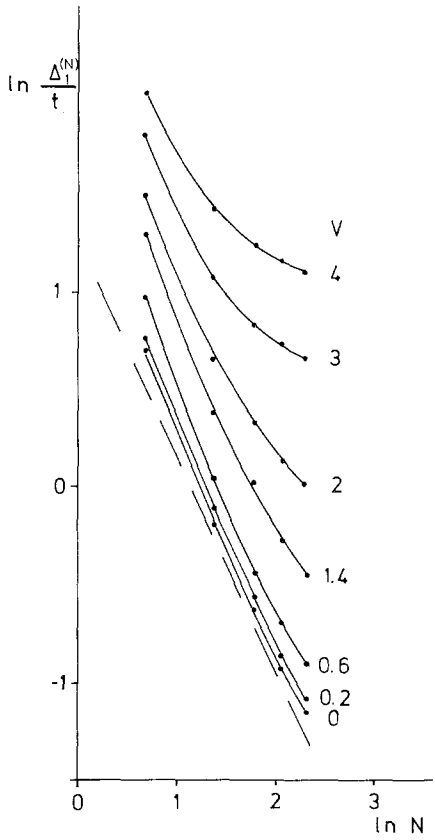

Fig. 9. Log–Log plot of the energy gap $\Delta_1^{(N)}$ versus N. The dotted line corresponds to a dynamical critical exponent $z = 1$. For $V/t < 1.4$ the points follow the expected straight line; for $V/t \gg 1$ they turn upward: there is no scaling. Even and odd values of $N/2$ oscillate slightly. The parameter is the coupling $V(t = 1)$.

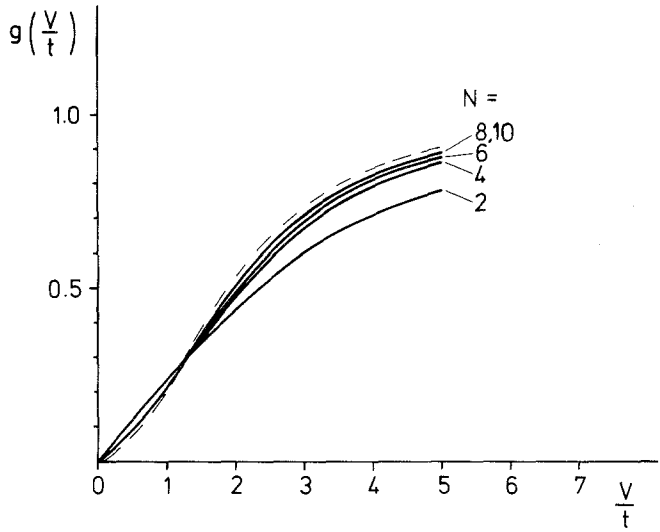

Fig. 10. On-site $s^z - \tau^z$ correlations $g = \langle 0 | s_i^z \tau_i^z | 0 \rangle$ versus V/t. The unpaired value $g = 0$ at $V = 0$ gradually increases toward the fully paired value $g = 1$ at $V = \infty$. The crossing of the curves and the inflection points occur around $V/t = (V/t)^* = 1.4$.

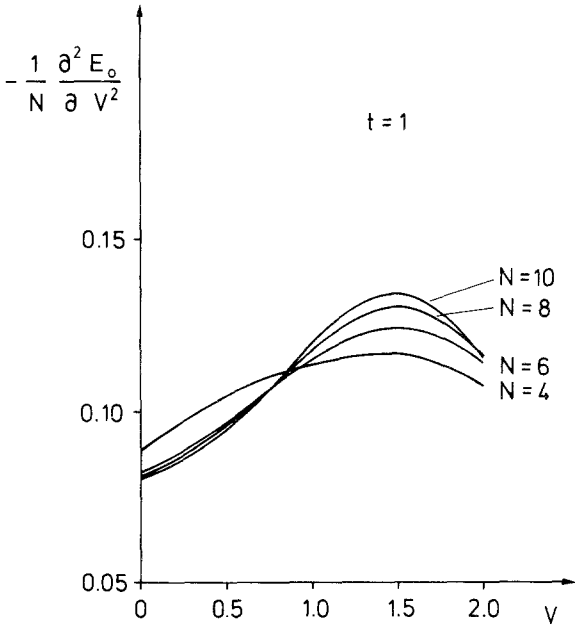

Fig. 11. Second derivative ("specific heat") of the ground-state energy as a function of V. At $(V/t) \approx 1.4$ a maximum develops. This maximum appears to remain finite as $N \to \infty$.

clusions. The local on-site correlation function $g \equiv \langle 0|s_i^z \cdot \tau_i^z|0\rangle$ measures the degree of pairing. It is shown in Fig. 10 for $\rho = 1$. For $V = 0$, $g = 0$ for all N and for $V \to \infty$, $g \to 1$ as $N \to \infty$, indicating that there is complete pairing. The extrapolated curve for $N = \infty$ has an inflection point at approximately $V/t = (V/t)^* = 1.4$. At the same point there is also a crossing of the curves for different chain lengths N.

In Fig. 11 we have presented the second derivative of the ground-state energy with respect to the coupling V/t. This quantity corresponds to the specific heat in $T \neq 0$ phase transitions. It can be seen that this quantity develops a maximum as a function of N. This maximum appears close to $(V/t) \sim 1.4$. The long-range properties of two correlation functions have also been calculated. The single-particle correlation $c(r) = \langle 0|(s_1^+ s_r^- + \text{h.c.})|0\rangle$ has been obtained for $r = N/2$ (periodic chain) as a function of V/t. In Fig. 12, $c(r = N/2)$ is shown for different N. As $N \to \infty$, $c(N/2) \to 0$ as expected. The shape of c for finite N shows the amplitude with an inflection point separating the small V/t from the large V/t behavior. In Fig. 13 the pair correlation (for $r = N/2$) $C(r) = \langle 0|(s_1^+ \tau_1^+ s_r^- \tau_r^- + \text{h.c.})|0\rangle$ is plotted versus N. An analogous behavior to the one in Fig. 12 is observed. For V/t large, the correlation for finite N is larger as V/t favors the pairs over the independent particles.

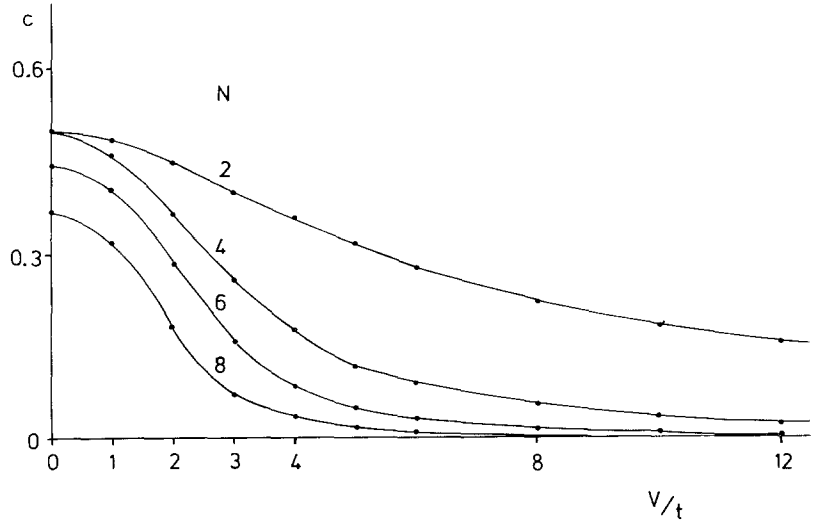

Fig. 12. Ground-state correlation function $c(N/2) = \langle 0|(s_1^+ s_{N/2}^- + \text{h.c.})|0\rangle$ versus V. $c(N/2) \to 0$ for all V as $N \to \infty$, the amplitude having a different curvature for V small and V large.

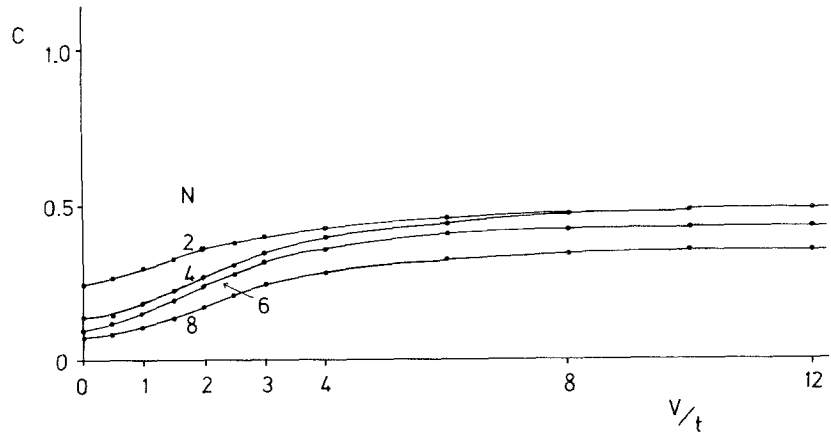

Fig. 13. Ground-state correlation function $C(N/2) = \langle 0|(s_1^+ \tau_1^+ s_{N/2}^- \tau_{N/2}^- + \text{h.c.})|0\rangle$ versus V. The correlation for V large (N finite) is stronger than for V small.

6. CONCLUSIONS

In conclusion, we have investigated a new model for electronic-pair formation in order to determine the properties of the transition from the unpaired to the paired state. The interaction induces pairing by favoring hopping of pairs of electrons with opposite spin. In a one-dimensional model we find that the transition is of type essential singularity and occurs at a finite value of the interaction. This is in marked contrast to the Hubbard model where an infinitesimal interaction already induces the transition. The important difference between these two models of local pairing is that in our model the mobility of pairs is large but the presence of single particles reduces the mobility of pairs. For the Hubbard model there is a direct local attraction between the electrons which actually hinders the mobility of pairs.

ACKNOWLEDGMENT

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APPENDIX I. SOLUTION OF HAMILTONIAN (5) FOR $N_e = N = 2$

We limit ourselves here to the subspace $\sum^z = \sum_{i=1}^2 (n_{i\uparrow} - n_{i\downarrow}) = 0$ where $\sum^z$ is the z component of the electron spin. The other subspaces are trivial,

since V has vanishing matrix elements in them. Introduce four basic functions

$$\begin{aligned} |1\rangle &= c_{1\uparrow}^{+} c_{1\downarrow}^{+} |0\rangle \qquad |2\rangle = c_{1\uparrow}^{+} c_{2\downarrow}^{+} |0\rangle \\ |3\rangle &= c_{1\downarrow}^{+} c_{2\uparrow}^{+} |0\rangle \qquad |4\rangle = c_{2\uparrow}^{+} c_{2\downarrow}^{+} |0\rangle \end{aligned} \tag{A1}$$

where the subscripts 1 and 2 refer to the sites 1 and 2, respectively. By acting with the Hamiltonian we get

$$\begin{aligned} H|1\rangle &= t(|2\rangle + |3\rangle) - V|4\rangle \\ H|2\rangle &= t(|1\rangle + |4\rangle) \\ H|3\rangle &= t(|1\rangle + |4\rangle) \\ H|4\rangle &= t(|2\rangle + |3\rangle) - V|1\rangle \end{aligned} \tag{A2}$$

or introducing normalized linear combinations

$$\begin{aligned} \psi_1 &= \frac{1}{\sqrt{2}}(|1\rangle + |4\rangle) \\ \psi_2 &= \frac{1}{\sqrt{2}}(|2\rangle + |3\rangle) \end{aligned} \tag{A3}$$

the Hamiltonian matrix in the (ψ_1, ψ_2) basis is

$$\hat{H} = \begin{pmatrix} -V & 2t \\ 2t & 0 \end{pmatrix}$$

The linear combinations with the minus sign, i.e., $|1\rangle - |4\rangle$, have matrix elements independent of t and have no influence on transition.

The ground-state energy is

$$E_0 = -\frac{V}{2} - \frac{\sqrt{V^2 + 16t^2}}{2} \tag{A4}$$

and the normalized ground-state wave function

$$|0\rangle = \frac{1}{\sqrt{2}}[a(t, V)(|1\rangle + |4\rangle) + b(t, V)(|2\rangle + |3\rangle)] \tag{A5}$$

where the coefficients of the wave function are

$$\begin{aligned} a(t, V) = \left(\frac{8t^2 + V^2 + \sqrt{V^2 + 16t^2}}{16t^2 + V^2 + \sqrt{V^2 + 16t^2}} \right)^{1/2} &= \frac{1}{\sqrt{2}} \quad \text{for} \quad V = 0 \\ &= 1 \quad \text{for} \quad t = 0 \\ b(t, V) = -\left(\frac{8t^2}{16t^2 + V^2 + \sqrt{V^2 + 16t^2}} \right)^{1/2} &= -\frac{1}{\sqrt{2}} \quad \text{for} \quad V = 0 \\ &= 0 \quad \text{for} \quad t = 0 \end{aligned} \tag{A6}$$

We observe (a) that in absence of interaction ($V=0$) the ground-state wave function is an equally weighted linear combination

$$|0\rangle = \frac{1}{2}(|1\rangle + |4\rangle - |2\rangle - |3\rangle) \tag{A7}$$

with energy $E_0 = -2t$; (b) in the absence of hopping ($t=0$) only two basic functions survive

$$|0\rangle = \frac{1}{\sqrt{2}}(|1\rangle + |4\rangle) \tag{A8}$$

with the energy $E_0 = -V$.

We proceed now to compute various averages in the ground state $|0\rangle$. The average occupation of site 1 with an electron with up spin is

$$\langle 0 | n_{1\uparrow} | 0 \rangle = \tfrac{1}{2}(a^2 + b^2) = \tfrac{1}{2} \tag{A9}$$

The total number of electrons evidently gives $\langle 0 | \sum_{i=1}^{2} (n_{i\uparrow} + n_{i\downarrow}) | 0 \rangle = 2$. The average occupation of site 1 by a pair of electrons is given by

$$\langle 0 | n_{1\uparrow} n_{1\downarrow} | 0 \rangle = \frac{a^2}{2} \tag{A10}$$

The total occupation by pairs is given by

$$\begin{aligned} \langle 0 | \sum_{i=1}^{2} n_{i\uparrow} n_{i\downarrow} | 0 \rangle = a^2 = \frac{1}{2} \quad &\text{for} \quad V = 0 \\ = 1 \quad &\text{for} \quad t = 0 \end{aligned} \tag{A11}$$

Similarily, the average value of interaction in the ground state is obtained as

$$-V \langle 0 | (c_{1\uparrow}^{+} c_{1\downarrow}^{+} c_{2\downarrow} c_{2\uparrow} + \text{h.c.}) | 0 \rangle = -Va^2 \tag{A12}$$

Last, the average of the kinetic energy in the ground state is

$$t\langle 0|\left(\sum_{\sigma} c_{1\sigma}^{+} c_{2\sigma} + \text{h.c.}\right)|0\rangle = 4tab_{V\to 0} \to -2t \tag{A13}$$

in agreement with (A7).

Note that a convenient measure of pairing in the system is provided by the (A11). It can be taken over for other values of N and N_e as it has been done in the body of this work.

APPENDIX II. REPRESENTATION OF TWO-COUPLED $S=\frac{1}{2}$ SPIN CHAINS AS A $S=\frac{3}{2}$ SPIN CHAIN

In order to numerically solve the eigenvalue problem posed by (19), we have considered the equivalent formulation in terms of a single $S=\frac{3}{2}$ spin chain with an appropriate interaction. This is suggested by the fact that both the two coupled $S=\frac{1}{2}$ spins and the single $S=\frac{3}{2}$ spin have 4 df per lattice site. First, we write down the correspondence between the $S=\frac{1}{2}$ and the $S=\frac{3}{2}$ problem. Denote the $S=\frac{3}{2}$ spin operators by (J^x, J^y, J^z), the value of J^z in terms of s^z and τ^z can be read off in the following table

τ^z \ s^z	$-\frac{1}{2}$	$\frac{1}{2}$
$-\frac{1}{2}$	$-\frac{3}{2}$	$+\frac{1}{2}$
$\frac{1}{2}$	$-\frac{1}{2}$	$+\frac{3}{2}$

The Hamiltonian (19) consists of a number of spin raising and lowering operators. To find the corresponding $S=\frac{3}{2}$ representation, we need the equivalent of, say, s^+ in terms of J^+, etc. According to the table, s^+ raises the quantum number by 2, hence s^+ is replaced by $(J^+)^2$. The proportionality factor directly follows from the coefficients in

$$s^+|m\rangle = \sqrt{\frac{3}{4} - m(m+1)}\,|m+1\rangle$$

and

$$J^+|m\rangle = \sqrt{\frac{15}{4} - m(m+1)}\,|m+1\rangle$$

and hence

$$s^+ \to (J^+)^2/(2\sqrt{3})$$

and analogously for s^-. τ^+ in the representation J^z raises the m quantum number by 1, hence τ^+ is proportional to J^+. The transition $J^+|-\frac{1}{2}\rangle = 2|\frac{1}{2}\rangle$ has to be excluded, however, as this flips both the S and τ spins. This is accomplished by including a factor $(4-J^+J^-)$. The correspondence then is $\tau^+ \to (1/\sqrt{3})\, J^+(4-J^+J^-)$ and similarly for τ^-.

The Hamiltonian (19) then reads in terms of J

$$H = \frac{t}{3}\sum_m \left[J_m^+(4-J_m^+J_m^-)\cdot J_{m+1}^-(4-J_{m+1}^-J_{m+1}^+) + \frac{1}{4}(J_m^+)^2\,(J_{m+1}^-)^2 \right]$$

$$-\frac{V}{108}\sum_m J_m^+(4-J_m^+J_m^-)\cdot J_{m+1}^-\cdot(4-J_{m+1}^-J_{m+1}^+)\cdot(J_m^+)^2\cdot(J_{m+1}^-)^2 + \text{h.c.}$$

The symmetries of the original problem manifest themselves directly in the $S=\frac{3}{2}$ representation: (1) the wave vector and the left–right parity of the chain is exactly as before, (2) the total value of J^z is conserved as a consequence of the conservation of s^z and τ^z, (3) changing J^z into $-J^z$ corresponds to $s^z \to -S^z$ and $\tau^z \to -\tau^z$.

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