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Superconductivity in an exactly solvable Hubbard model with bond-charge interaction

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The Hubbard model with an additional bond-charge interaction X is solved exactly in one dimension for the case $t = X$, where t is the hopping amplitude. In this case the number of doubly occupied sites is conserved. In the sector with no double occupations the model reduces to the $U = \infty$ Hubbard model. In arbitrary dimensions the qualitative form of the phase diagram is obtained. It is shown that for moderate Hubbard interactions U the model has superconducting ground states.

I. INTRODUCTION

The one-dimensional Hubbard model is long since the prototype of an exactly solvable model for correlated electrons.[1,2] However, it is difficult to include additional interactions so that the resulting model is still integrable. In this paper we present a generalized Hubbard model which, apart from the Coulomb interaction U, also contains a bond-charge interaction term X. This model has been studied extensively by Hirsch[3,4] who argued that it might be relevant for the description of high-T_c superconductors. For certain values of X and large densities of electrons (small doping) the bond-charge interaction can lead to an attractive effective interaction between the holes and the formation of Cooper pairs. Although this picture was confirmed by a BCS-type mean-field theory it is desirable to find exact results confirming this behavior. A first step in this direction was made in Ref. 5 where a simplified version of Hirsch's Hamiltonian has been studied in one dimension using Bethe-Ansatz methods. Indeed, it has been found that this model has a strong tendency towards superconductivity (see also Ref. 6).

On the other hand, there has recently been a great deal of activity in the investigation of the so-called η-pairing mechanism of superconductivity. This idea has been introduced by Yang[7] for the Hubbard model. It allows for the construction of states exhibiting off-diagonal long-range order (ODLRO). As shown in Refs. 8–10, ODLRO also implies the Meissner effect and flux quantization and can thus be regarded as definition of superconductivity. In the case of the Hubbard model it was found that the ground state is not of the η-pairing type.[7] One model with a truly superconducting ground state of the η-pairing type is the supersymmetric Hubbard model introduced by Eßler, Korepin, and Schoutens (EKS model).[11,12] The EKS model is a Hubbard model which contains additional nearest-neighbor interactions. It has some attractive features. Apart from being exactly solvable by using the Bethe Ansatz in one dimension it is possible to determine the $T = 0$ phase diagram in arbitrary dimensions. One always finds a superconducting ground state if $U < U_c$ where the critical value U_c is positive corresponding to a repulsive on-site Coulomb interaction.

In Ref. 13 it has been shown that an η-pairing ground state is not an exotic phenomenon restricted to one special model but it may be found for a large class of Hamiltonians. As a special case the Hubbard model with bond-charge interaction X is in this class, provided that $X = t$ where t is the hopping matrix element. It is this model which will be studied in this paper (A brief account of some of the results presented here can be found in Ref. 13.)

In Sec. II the symmetries of the Hamiltonian are investigated. It turns out that the model under investigation is a generalization of the $U = \infty$ Hubbard model to a model with a conserved (but in general nonzero) number of doubly occupied sites. Since the $U = \infty$ Hubbard model has attracted a great deal of interest in recent years[14–22] it seems worthwhile to study any generalization of it.

In Sec. III we present the exact solution in one dimension. It will be shown that the Hamiltonian can be mapped in certain subspaces onto a spinless free fermion model with twisted boundary conditions where the twist depends on the subspace considered. By using this fact it is easy to obtain the spectrum and the zero temperature phase diagram of the Hamiltonian. It is found that for U not too large the model contains superconducting ground states of the η-pairing type. For certain densities this is true even for moderately repulsive Coulomb interactions.

In Sec. IV we construct the qualitative form of the phase diagram in arbitrary dimensions. Basically it has the same form as the phase diagram in one dimension although the exact location of all phase boundaries cannot be determined. Section V contains a summary of the results and a discussion of the stability of the superconducting ground states. In the Appendix details of the exact solution in one dimension are given.

II. THE MODEL AND ITS SYMMETRIES

The Hamiltonian of the Hubbard model with an additional bond-charge interaction X (or correlated hopping) on a d-dimensional lattice with L sites and periodic boundary conditions is given by

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$$\mathcal{H}(X,U) = -t\sum_{\langle jl\rangle}\sum_{\sigma=\uparrow,\downarrow}(c^\dagger_{j\sigma}c_{l\sigma}+c^\dagger_{l\sigma}c_{j\sigma}) + U\sum_{j=1}^{L} n_{j\uparrow}n_{j\downarrow}$$
$$+X\sum_{\langle jl\rangle}\sum_{\sigma=\uparrow,\downarrow}(c^\dagger_{j\sigma}c_{l\sigma}+c^\dagger_{l\sigma}c_{j\sigma})$$
$$\times(n_{j,-\sigma}+n_{l,-\sigma})\ . \tag{2.1}$$

Here $c_{j\sigma}$,$c^\dagger_{j\sigma}$ are the usual Fermi operators and $n_{j\sigma} = c^\dagger_{j\sigma}c_{j\sigma}$ is the corresponding number operator. $\langle jl\rangle$ denotes nearest-neighbor sites on the d-dimensional lattice. In the following we will be interested in the special case $\mathcal{H}(U) = \mathcal{H}(X = t, U)$. In this case it is convenient to rewrite the Hamiltonian in terms of Hubbard operators $X^{ab} = |a\rangle\langle b|$ $(a, b = 0, \pm1, 2)$ where 0 denotes an empty site, ±1 denotes a site occupied by a single electron with spin $\uparrow$ or $\downarrow$, and 2 denotes a doubly occupied site. The fact that for each site j the four states $|0\rangle$, $|-1\rangle$, $|1\rangle$, and $|2\rangle$ form a basis of the local Hilbert space leads to the local constraint $X^{00}_j + X^{22}_j + \sum_\sigma X^{\sigma\sigma}_j = 1$.

The Hubbard operators obey the following graded commutation rules

$$[X^{ab}_j, X^{cd}_l]_\pm = \left(X^{ad}_j\delta_{bc} \pm X^{cb}_j\delta_{ad}\right)\delta_{jl}\ , \tag{2.2}$$

where the anticommutator has to be taken only if both operators are fermionic, i.e., change the particle number by one (e.g., $X^{\sigma0}_j$ or $X^{2\sigma}_j$). The standard fermion operators $c_{j\sigma}$ can be expressed through the Hubbard operators

$$\begin{aligned} c^\dagger_{j\sigma} &= X^{\sigma0}_j + \sigma X^{2,-\sigma}_j,\\ c_{j\sigma} &= X^{0\sigma}_j + \sigma X^{-\sigma2}_j,\\ n_{j\sigma} &= X^{\sigma\sigma}_j + X^{22}_j \end{aligned}\tag{2.3}$$

and vice versa, e.g.,

$$\begin{aligned} X^{\sigma0}_j &= (1-n_{j,-\sigma})c^\dagger_{j\sigma}, \quad X^{2,-\sigma}_j = n_{j,-\sigma}c^\dagger_{j\sigma},\\ X^{\sigma\sigma}_j &= (1-n_{j,-\sigma})n_{j\sigma}, \quad X^{00}_j = (1-n_{j\downarrow})(1-n_{j\uparrow}). \end{aligned}\tag{2.4}$$

In terms of the Hubbard operators the Hamiltonian (2.1) takes the following form:

$$\begin{aligned}\mathcal{H}(U) &= \mathcal{H}_0 + \mathcal{H}_U\\ &= -t\sum_{\langle jl\rangle}\sum_{\sigma=\pm1}(X^{\sigma0}_jX^{0\sigma}_l + X^{\sigma0}_lX^{0\sigma}_j + X^{\sigma2}_jX^{2\sigma}_l\\ &\quad + X^{\sigma2}_lX^{2\sigma}_j) + U\sum_{j=1}^{L}X^{22}_j\ .\end{aligned}\tag{2.5}$$

The Hamiltonian $\mathcal{H}(U)$ has a lot of symmetries, since only two types of processes are allowed: (i) a particle from a singly occupied site may hop to an unoccupied neighbor site, or (ii) a particle with spin σ from a doubly occupied site may hop to a singly occupied (particle with spin $-\sigma$) neighbor site. Therefore it is clear that $\mathcal{H}(U)$ conserves not only the total number N of electrons but also the number $N^{(\sigma)}_1$ of *single* electrons with spin σ and the number $N_2 = \sum_{j=1}^{L} n_{j\uparrow}n_{j\downarrow}$ of doubly occupied sites, i.e., $[\mathcal{H}_0, \mathcal{H}_U] = 0$. In addition, $\mathcal{H}_0$ has two SU(2) symmetries: apart from the SU(2) spin symmetry, i.e., $\mathcal{H}_0$ commutes with $\mathcal{S}^+ = \sum_{j=1}^{L} c^\dagger_{j\uparrow}c_{j,\downarrow}$, $\mathcal{S}^- = (\mathcal{S}^+)^\dagger$, $\mathcal{S}^z = \frac{1}{2}(N^{(\uparrow)}_1 - N^{(\downarrow)}_1)$, and $\mathcal{H}_0$ also commutes with the following so-called η operators:

$$\eta = \sum_{j=1}^{L} c_{j\uparrow}c_{j\downarrow}, \qquad \eta^\dagger = \sum_{j=1}^{L} c^\dagger_{j\downarrow}c^\dagger_{j\uparrow}, \qquad \eta^z = \frac{1}{2}(N-L) \tag{2.6}$$

where $N = N_1 + 2N_2$ (with $N_1 = N^{(\uparrow)}_1 + N^{(\downarrow)}_1$) is the total number of particles. In terms of the Hubbard operators the η operators are given by $\eta = -\sum_{j=1}^{L} X^{02}_j$ and $\eta^\dagger = -\sum_{j=1}^{L} X^{20}_j$.

$\eta^\dagger$ creates a double occupation with momentum zero as can be seen from its form in momentum space $\eta^\dagger = \sum_k c^\dagger_{k\downarrow}c^\dagger_{-k\uparrow}$ where $c^\dagger_{k\sigma} = \frac{1}{\sqrt{L}}\sum_k e^{-ijk}c^\dagger_{j\sigma}$. Thus $\eta^\dagger$ is just the conventional s-wave pairing operator. Note that in the case of the Hubbard model the corresponding η symmetry is generated by $\eta_\pi = \sum_{j=1}^{L}(-1)^j c_{j\uparrow}c_{j\downarrow}$ corresponding to pairs with momentum π[7].

The Hamiltonian $\mathcal{H}(U = 0)$ without the Coulomb interaction is also invariant under a particle-hole transformation:

$$\mathcal{U}c_{j\sigma}\mathcal{U}^{-1} = c^\dagger_{j\sigma}, \qquad \mathcal{U}c^\dagger_{j\sigma}\mathcal{U}^{-1} = c_{j\sigma}\ , \tag{2.7}$$
$$\mathcal{U}\mathcal{H}_0\mathcal{U}^{-1} = \mathcal{H}_0\ , \tag{2.8}$$

whereas the Coulomb interaction $\mathcal{H}_U = U\sum_{j=1}^{L} n_{j\uparrow}n_{j\downarrow}$ transforms as

$$\mathcal{U}\mathcal{H}_U\mathcal{U}^{-1} = \mathcal{H}_U + U(L-N). \tag{2.9}$$

Due to this particle-hole symmetry we can restrict our investigation to the case $N \le L$.

In the following the conservation of N_2 will expecially be important. It allows us to diagonalize the Hamiltonian in subspaces with fixed N_2. For $N_2 = 0$ the Hamiltonian $\mathcal{H}_0$ reduces to the $U = \infty$ Hubbard model[14–22]

$$\begin{aligned}\mathcal{H}_\infty &= -t\sum_{\langle jl\rangle}\sum_{\sigma=\uparrow,\downarrow}(X^{\sigma0}_jX^{0\sigma}_l + X^{\sigma0}_lX^{0\sigma}_j)\\ &= -t\,\mathcal{P}\sum_{\langle jl\rangle}\sum_{\sigma=\uparrow,\downarrow}\left(c^\dagger_{l\sigma}c_{j\sigma} + c^\dagger_{j\sigma}c_{l\sigma}\right)\mathcal{P}\ ,\end{aligned}\tag{2.10}$$

where $\mathcal{P}$ is the projector onto the subspace with no doubly occupied sites. Thus the Hamiltonian (2.5) is a generalization of the the $U = \infty$ Hubbard model to a model with a conserved (but in general nonzero) number of doubly occupied sites. This is similar to the EKS model[11,12] which is a generalization of the supersymmetric t-J model[23] to a model with a conserved number of doubly occupied sites.

III. EXACT SOLUTION IN ONE DIMENSION

In the following, the Hamiltonian $\mathcal{H}_0$ [see (2.5)] is diagonalized in one dimension with periodic boundary conditions. A solution of an equivalent model with open boundary conditions has been given in Ref. 24 (see also Ref. 25).

In the subspace H_{N_1,N_2} with N_1 singly occupied sites and N_2 doubly occupied sites, i.e., $N = N_1 + 2N_2$ particles, we define the following basis vectors:

$$|\vec{x},\vec{\sigma},\vec{b}\rangle = \prod_{\alpha=1}^{N_1} X_{x_\alpha}^{\sigma_\alpha,0} \prod_{\beta=1}^{L-N_1} X_{y_\beta}^{b_\beta,0}|0\rangle \quad (1 \leq x_1 < \cdots < x_{N_1} \leq L). \tag{3.1}$$

$|\vec{x},\vec{\sigma},\vec{b}\rangle$ is a state in which the sites x_α are occupied by a single electron with spin σ_α. $\{y_1,\dots y_{L-N_1}\} = \{1,\dots,L\} \setminus \{x_1,\dots,x_{N_1}\}$ are the sites occupied by a boson b_α where $b_\alpha = 2$ for a doubly occupied site and $b_\alpha = 0$ for an empty site. Note that due to (2.2) all $X_{y_\beta}^{b_\beta,0}$ commute mutually and with all the $X_{x_\alpha}^{\sigma_\alpha,0}$.

Next we define the operators $\mathcal{C}$ and $\mathcal{C}'$ generating cyclic permutations of the spins and bosons, respectively,

$$\mathcal{C}\{\sigma_1,\dots,\sigma_{N_1}\} = \{\sigma_2,\dots,\sigma_{N_1},\sigma_1\}, \tag{3.2}$$

$$\mathcal{C}'\{b_1,\dots,b_{N-N_1}\} = \{b_{N-N_1},b_1,b_2,\dots,b_{N-N_1-1}\}. \tag{3.3}$$

Using these operators we can define subspaces of H_{N_1,N_2}. For every spin configuration $\{\sigma_1,\dots,\sigma_{N_1}\}$ there exists a minimal integer $K \geq 1$ such that

$$\mathcal{C}^K\{\sigma_1,\dots,\sigma_{N_1}\} = \{\sigma_1,\dots,\sigma_{N_1}\}. \tag{3.4}$$

Clearly for a fully polarized ferromagnetic state we have $K = 1$ and for a Néel state $K = 2$. In the same way we define the integer K' for the distribution of bosons.

All the states $|\vec{x},\vec{\sigma},\vec{b}\rangle$ with $\vec{\sigma}$ and $\vec{b}$ characterized by the same integers K and K' span a subspace $H_{N_1,N_2}(K,K')$ of H_{N_1,N_2}. It is now important to notice that the subspaces $H_{N_1,N_2}(K,K')$ are invariant under the action of the Hamiltonian $\mathcal{H}$. This fact is well known[14,16] for the $U = \infty$ Hubbard model, i.e., $N_2 = 0$. Since the local Hamiltonian $h_{j,j+1}$ only permutes bosons with fermions a spin $\sigma_{\alpha+1}$ will under the action of $\mathcal{H}$ always stay "to the right" of a spin σ_α except for the case where it moves "over the boundary" ($L \to L+1 \equiv 1$).

We can now restrict ourselves to the diagonalization of the Hamiltonian in the subspaces $H_{N_1,N_2}(K,K')$. In the Appendix it is shown that in each of these subspaces $\mathcal{H}$ is equivalent to a free fermion Hamiltonian $\tilde{\mathcal{H}}$ with twisted boundary conditions,

$$\tilde{\mathcal{H}} = -\sum_{j=1}^{L-1}(a_j^\dagger a_{j+1} + a_{j+1}^\dagger a_j) - (e^{iL\Delta\phi}a_L^\dagger a_1 + e^{-iL\Delta\phi}a_1^\dagger a_L)\ , \tag{3.5}$$

which now acts on the "stripped states"[14]

$$|\vec{x}\rangle = \prod_{\alpha=1}^{N} a_{x_\alpha}^\dagger|0\rangle\ . \tag{3.6}$$

The a_j are (spinless) fermion operators and the allowed values $\Delta\phi$ for the twist in the boundary conditions is different for each subspace:

$$\Delta\phi = \frac{k'-k}{L}\ , \tag{3.7}$$

$$k = \frac{2\pi}{K}\nu \qquad (\nu = 0,1,\dots,K-1), \tag{3.8}$$

$$k' = \frac{2\pi}{K'}\nu' \qquad (\nu' = 0,1,\dots,K'-1). \tag{3.9}$$

After the canonical transformation $a_j^\dagger \to e^{ij\Delta\phi}a_j^\dagger$, $a_j \to e^{-ij\Delta\phi}a_j$, the Hamiltonian (3.5) is seen to be equivalent to the following translational-invariant free fermion Hamiltonian

$$\mathcal{H}_{\text{eff}} = -\sum_{j=1}^{L}\left(e^{i\Delta\phi}a_j^\dagger a_{j+1} + e^{-i\Delta\phi}a_{j+1}^\dagger a_j\right) \tag{3.10}$$

from which the eigenvalues of $\mathcal{H}$ can be obtained easily by Fourier transformation

$$E = -2\sum_\nu \cos(q_\nu + \Delta\phi)n_{q_\nu} \tag{3.11}$$

with $\sum_\nu n_{q_\nu} = N_1$ and $n_{q_\nu} = 1$ (0) if the mode q_ν is occupied (not occupied). The wave numbers q_ν can take the values $q_\nu = \frac{2\pi}{L}\nu$ ($\nu = -\frac{L}{2}+1,\dots,\frac{L}{2}$).

In the ground state the q_ν are as symmetric as possible around $\nu = 0$. For N_1 even we have $n_{q_\nu} = 1$ for $\nu = -\frac{N_1}{2}+1,\dots,\frac{N_1}{2}$ and thus

$$E = -2\frac{\cos\left(\frac{\pi}{L}+\Delta\phi\right)}{\sin(\pi/L)}\sin(N_1\pi/L)\ . \tag{3.12}$$

For N_1 odd we have to choose $\nu = -\frac{N_1-1}{2}+1,\dots,\frac{N_1-1}{2}$ yielding

$$E = -2\frac{\cos(\Delta\phi)}{\sin(\pi/L)}\sin(N_1\pi/L). \tag{3.13}$$

This shows that in the ground state one has

$$\Delta\phi = \begin{cases} -\pi/L & (N_1 \text{ even}) \\ 0 & (N_1 \text{ odd}), \end{cases} \tag{3.14}$$

which gives the ground-state energy

$$E_0 = -2\frac{\sin(N_1\pi/L)}{\sin(\pi/L)}. \tag{3.15}$$

The ground-state energy only depends on the number N_1 of singly occupied sites and is independent of the number N_2 of doubly occupied sites. Therefore the ground-state energy of (2.5) is $E_0(N_1,N_2,U) = E_0 + UN_2$. The mapping of the original model onto *spinless* free fermions (3.10) implies that the eigenvalues of (2.5) are highly degenerate in general.

IV. PHASE DIAGRAM AT $T = 0$

In this section we determine the phase diagram of the Hamiltonian (2.5) in the $U-D$ plane where $D = N/L$

is the particle density. First, we consider the one-dimensional case which can be treated exactly by using the results of the previous section. Then we show that the phase diagram in higher dimensions has qualitatively the same form as in one dimension. We find the same phases although we cannot determine all phase boundaries exactly. Finally we calculate correlation functions for generalized η-pairing states which appear as ground states in certain parameter regions.

A. Phase diagram in one dimension

In order to determine the phase diagram in the $U-D$ plane for the one-dimensional case we have to minimize the ground-state energy $E_0(D_1,D_2,U)/L = -\frac{2}{\pi}\sin(D_1\pi)+UD_2$ for a fixed particle density $D = D_1+2D_2$. From now on we work in the thermodynamic limit $L, N_\alpha \to \infty$ with $D_\alpha = N_\alpha/L$ fixed ($\alpha = 1,2$). A simple calculation yields

$$D_1 = \begin{cases} 0 & (U \le -4), \\ \frac{1}{\pi}\arccos(-U/4) & (-4 \le U \le U_c), \\ D & (U \ge U_c), \end{cases} \tag{4.1}$$

where $U_c(D) = -4\cos(\pi D)$.

Due to the particle-hole symmetry it is sufficient to discuss the phase diagram for $D \le 1$. We find four different phases which will be discussed separately in the following.

Regime I: $U \le -4$. From (4.1) we see that the ground state contains only doubly occupied sites and no single electrons. In this case the ground-state energy is simply $E_0(0,N/2,U)/L = UN/2$. In the absence of single electrons the double occupations are static and all states with the same number $N_2 = N/2$ of doubly occupied sites have the same energy. Among these states are the generalized η-pairing states

$$|\psi_P\rangle = \left(\eta_P^\dagger\right)^{N/2}|0\rangle, \tag{4.2}$$

$$\eta_P^\dagger = \sum_{j=1}^{L} e^{iPj} c_{j\downarrow}^\dagger c_{j\uparrow}^\dagger \tag{4.3}$$

with momentum $P = \frac{2\pi}{L}\nu$ ($\nu = 0,1,\ldots,L-1$). These states are ground states for all chain lengths L, not only in the thermodynamic limit. All of these states show ODLRO, i.e.,

$$\lim_{|l-j|\to\infty} \frac{\langle\psi_P|c_{j\downarrow}^\dagger c_{j\uparrow}^\dagger c_{l\uparrow}c_{l\downarrow}|\psi_P\rangle}{\langle\psi_P|\psi_P\rangle} \neq 0 \,. \tag{4.4}$$

[See also Eq. (4.5) below]. As a consequence these ground states are superconducting since it has been shown that ODLRO also implies the Meissner effect and flux quantization.[8–10]

Regime II: $-4 < U < U_c(D) = -4\cos(\pi D)$. For $-4 < U < U_c(D)$ the ground state has both a finite density of single electrons and of double occupations. Again it is highly degenerate. Here the ground-state energy is $E_0(D_1,D_2,U)/L = -\frac{1}{2\pi}\sqrt{16-U^2}+UD_2$. Among these ground states are the η states $\left(\eta_0^\dagger\right)^{N_2}|U=\infty\rangle$ where $|U=\infty\rangle$ stands for an arbitrary ground state of the $U=\infty$ Hubbard model at particle density $D_1 = \frac{1}{\pi}\arccos(-U/4)$ and N_2 is then obtained from $D_2 = N_2/L = (D-D_1)/2$. Again these states have ODLRO (see the discussion of correlation functions below) and are thus superconducting. It is interesting that this superconducting phase extends into the region of positive U, i.e., Coulomb repulsion.

Regime III: $U \ge U_c(D) = -4\cos(\pi D)$ and $D < 1$. In regime III we have no doubly occupied sites in the ground state and every ground state of the $U=\infty$ Hubbard model is therefore also a ground state of (4). Regime III′ with $D > 1$ is obtained by using the particle-hole symmetry (2.7)–(2.9).

Regime IV: $U \ge U_c(D) = -4\cos(\pi D)$ and $D = 1$. This case is much like regime III, but now the ground states $|U=\infty\rangle$ are insulating. The point $(D=1, U=4)$ corresponds to a metal-insulator transition. The complete phase diagram for the one-dimensional case is shown in Fig. 1 (see also Refs. 13 and 25).

B. Phase diagram in arbitrary dimensions

In higher dimensions the phase diagram can be constructed along the lines of Ref. 12. In Ref. 13 it has been shown that $|\psi_0\rangle = \left(\eta_0^\dagger\right)^{N/2}|0\rangle$ will be a ground state for $U \le -2Z$ where Z is the number of nearest-neighbor sites in the d-dimensional lattice. In order to construct the full phase diagram we need the following three properties: (1) η symmetry, i.e., $[\mathcal{H}_0,\eta_0]=0$; (2) conservation of the number N_2 of doubly occupied sites; and (3) for $U=0$ the ground-state energy does not depend on the number N_2 of doubly occupied sites. The first two properties have already been demonstrated in Sec. II and property (3) can be proven by generalizing the argumentation of Ref. 26 where the analogous property for the EKS model has been derived.

Using (1)–(3) the qualitative form of the phase diagram can be established in complete analogy with Ref. 12 by first considering the grand canonical ensemble and then

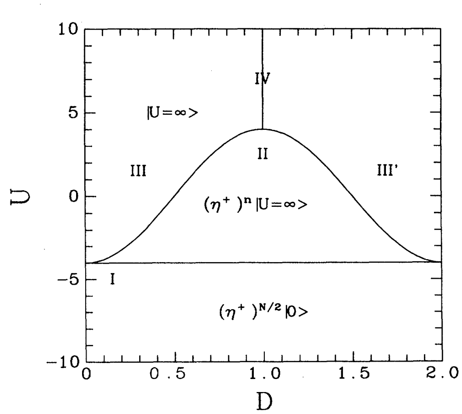

FIG. 1. $T=0$ phase diagram in one dimension. The phase diagram in higher dimensions has qualitatively the same form.

translating the results into the canonical ensemble. One finds a phase diagram which looks very similar to that of the one-dimensional case (Fig. 1). The same phases appear and only the location of the phase boundaries changes. Except for the boundary between regimes I and II (see Ref. 13) we have not been able to determine them exactly. An interesting open question is thus whether the superconducting regime II extends into the positive-U region in all dimensions.

C. Correlation functions

Correlation functions with respect to the η-pairing states can be calculated in a straightforward way[27]. Let $|\phi\rangle$ be a state with $\eta_P|\phi\rangle = 0$ and $\eta^z|\phi\rangle = \frac{1}{2}(N_1 - L)|\phi\rangle$, e.g., $|\phi\rangle$ is a state with N_1 singly and no doubly occupied sites. In our case we have $|\phi\rangle = |0\rangle$ or $|\phi\rangle = |U=\infty\rangle$. For the η-pairing states $|\psi_P(N_2)\rangle = (\eta_P^\dagger)^{N_2}|\phi\rangle$ we denote the expectation value of an arbitrary operator $\mathcal{O}$ by $\langle\mathcal{O}\rangle = \frac{\langle\psi_P(N_2)|\mathcal{O}|\psi_P(N_2)\rangle}{\langle\psi_P(N_2)|\psi_P(N_2)\rangle}$. We now can express any correlation function with respect to $|\psi_P(N_2)\rangle$ through correlation functions with respect to $|\phi\rangle$. With $\langle\mathcal{O}\rangle_\phi = \frac{\langle\phi|\mathcal{O}|\phi\rangle}{\langle\phi|\phi\rangle}$ we find (for $L\to\infty$, $D_\alpha = N_\alpha/L$ and $j \neq l$):

$$\begin{aligned}\langle\eta_j^\dagger\eta_l\rangle &= \langle c_{j\downarrow}^\dagger c_{j\uparrow}^\dagger c_{l\uparrow}c_{l\downarrow}\rangle\\ &= e^{iP(l-j)}\,\frac{(1-D_1-D_2)D_2}{(1-D_1)^2}\\ &\quad\times\langle(1-n_j)(1-n_l)\rangle_\phi\ ,\end{aligned}\tag{4.5}$$

$$\begin{aligned}\langle c_{j\sigma}^\dagger c_{l\tau}\rangle &= \frac{1-D_1-D_2}{1-D_1}\,\langle c_{j\sigma}^\dagger c_{l\tau}\rangle_\phi\\ &\quad-\sigma\tau e^{iP(l-j)}\,\frac{D_2}{1-D_1}\,\langle c_{l,-\tau}^\dagger c_{j,-\sigma}\rangle_\phi\ ,\end{aligned}\tag{4.6}$$

$$\begin{aligned}\langle n_{j\sigma}n_{l\tau}\rangle &= \langle n_{j\sigma}n_{l\tau}\rangle_\phi\\ &\quad+\frac{D_2}{1-D_1}[\langle n_{j\sigma}(1-n_l)\rangle_\phi + \langle n_{l\tau}(1-n_j)\rangle_\phi]\\ &\quad+\left(\frac{D_2}{1-D_1}\right)^2\langle(1-n_l)(1-n_j)\rangle_\phi\ ,\end{aligned}\tag{4.7}$$

$$\langle S_j^\alpha S_l^\alpha\rangle = \langle S_j^\alpha S_l^\alpha\rangle_\phi \qquad (\alpha = x,y,z).\tag{4.8}$$

These results hold in all dimensions in the thermodynamic limit. Correlators for phase I (where $|\phi\rangle = |0\rangle$) are trivial. The asymptotics for the correlation functions in phase II (where $|\phi\rangle = |U=\infty\rangle$) in one dimension can be obtained using the results of Refs. 28–31. The result for the η correlator $\langle\eta_j^\dagger\eta_l\rangle$ proves the existence of ODLRO since the value of the limit in (4.4) is found to be $e^{iP(l-j)}(1-D_1-D_2)D_2 \neq 0$.

V. CONCLUSIONS

In this paper a Hubbard model with an additional bond-charge interaction X has been investigated at the special point $X = t$ where the number of doubly occupied sites is conserved. In one dimension the complete spectrum of the Hamiltonian could be determined exactly by mapping onto a system of spinless free fermions with twisted boundary conditions. In arbitrary dimensions the $T = 0$ phase diagram in the $D-U$ plane has been obtained. One finds four phases, two of them containing ground states of the η-pairing type. These states exhibit ODLRO and thus are superconducting. Therefore the model (2.1) provides an example of a purely electronic model with a superconducting phase. The Cooper pairs have zero size which might be regarded as an approximation to the small coherence length found experimentally in high-T_c superconductors. For reviews on other models of local-pair superconductors, see, e.g., Refs. 32 and 33 and references therein..

Let us finally discuss the question of stability of the superconducting phases. As in the EKS model all interaction constants (apart from the Coulomb interaction U) have to take certain values in order to allow for the η-pairing ground states. The bond-charge interaction X especially has to be equal to the hopping matrix element t in order to guarantee the conservation of local pairs. One might wonder if the superconducting properties will survive if one allows for a decay of Cooper pairs (i.e., $X \neq t$). The results obtained in Ref. 34 suggest that this is indeed the case.

For the EKS model other perturbations of coupling constants have been investigated.[35] It has been found that in one dimension these perturbations destroy superconductivity, but in higher dimensions the superconducting phase is likely to be stable under such perturbations.

A similar analysis is also desirable for the model presented here. It would be interesting to find a perturbation by allowing for (small) additional nearest-neighbor interactions which lifts the large ground-state degeneracy in such a way that only (some) of the η-pairing states remain as ground states. In Refs. 36 and 37 the ground state for the model (2.1) has been obtained in the presence of an additional nearest-neighbor Coloumb interaction V at half-filling in arbitrary dimensions. In that case the ground state is unique (apart from a trivial twofold degeneracy) for $U < 2ZV - Z\max(2t, V)$, but not superconducting.

These questions are currently under investigation using perturbation theory and exact diagonalizations of small systems. Results will be presented in the future.

Note added in proof. In Ref. 38 it has recently been shown that the metal-insulator transition at half-filling in d dimensions is located at $U = 2Z$. This implies that even for $d > 1$ the regime II extends to positive values of U.

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APPENDIX

In this appendix we extend the method used in Ref. 14 to map the $U = \infty$ Hubbard model onto a free fermion Hamiltonian with twisted boundary conditions to our case. First we investigate the action of the local Hamiltonian (we set $t = 1$ from now on)

$$h_{j,j+1} = h^{(+)}_{j,j+1} + h^{(-)}_{j,j+1}, \qquad h^{(-)}_{j,j+1} = \left(h^{(+)}_{j,j+1}\right)^\dagger ,$$
$$h^{(+)}_{j,j+1} = -\sum_{\sigma=\uparrow,\downarrow}\sum_{\delta=0,2} X_j^{\sigma\delta} X_{j+1}^{\delta\sigma} \tag{A1}$$

on the states $|\vec{x},\vec{\sigma},\vec{b}\rangle$. We restrict ourselves to the investigation of $h^{(+)}_{j,j+1}$ since $h^{(-)}_{j,j+1}$ can be treated analogously.

It is easy to see that $h^{(+)}_{j,j+1}|\vec{x},\vec{\sigma},\vec{b}\rangle = 0$ if either $j \in \{x_1,\ldots,x_{N_1}\}$ or $j+1 \notin \{x_1,\ldots,x_{N_1}\}$. Therefore it is sufficient to consider the case $j+1 = x_\gamma \in \{x_\alpha\}$, $j = y_{\gamma'} \in \{y_\beta\}$. A straightforward calculation yields for $1 \le j \le L-1$

$$h^{(+)}_{j,j+1}|\vec{x},\vec{\sigma},\vec{b}\rangle = -|\vec{x'},\vec{\sigma},\vec{b}\rangle \tag{A2}$$

with

$$x'_\alpha = \begin{cases} x_\alpha & (\alpha \neq \gamma) \\ j & (\alpha = \gamma) \end{cases} \tag{A3}$$

and for $j = L$

$$h^{(+)}_{L,1}|\vec{x},\vec{\sigma},\vec{b}\rangle = (-1)^{N_1}|\vec{x''},\mathcal{C}\{\sigma_\alpha\},\mathcal{C}'\{b_\beta\}\rangle \tag{A4}$$

with

$$x''_\alpha = \begin{cases} x_{\alpha+1} & (\alpha = 1,\ldots,N_1-1) \\ L & (\alpha = N_1). \end{cases} \tag{A5}$$

In the subspace $H_{N_1,N_2}(K,K')$ we introduce the following states

$$|\vec{x},k,k'\rangle = \sum_{l=0}^{K-1}\sum_{m=0}^{K'-1} e^{ikl}e^{-ik'm}|\vec{x},\mathcal{C}^l\{\sigma_\alpha\},\mathcal{C}'^m\{b_\beta\}\rangle \tag{A6}$$

where k and k' are given by (3.8) and (3.9), respectively. $h^{(+)}_{j,j+1}$ acts on these spaces in a simple manner:

$$h^{(+)}_{j,j+1}|\vec{x},k,k'\rangle = \begin{cases} -|\vec{x'},k,k'\rangle & (j = 1,\ldots,L-1) \\ (-1)^{N_1}e^{-ik}e^{ik'}|\vec{x''},k,k'\rangle & (j = L) \end{cases} \tag{A7}$$

in the case $j+1 \in \{x_\alpha\}$ and $j \in \{y_\beta\}$ and is zero otherwise. Thus $\sum_{j=1}^{L} h^{(+)}_{j,j+1}$ acts on the states $|\vec{x},k,k'\rangle$ in the same way as $-\sum_{j=1}^{L-1} a_j^\dagger a_{j+1} - e^{iL\Delta\phi}a_L^\dagger a_1$ acts on the stripped states (3.6) where the a_j, $a_j^\dagger$ are spinless fermion operators and $\Delta\phi$ is given by (3.7).

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