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η-pairing as a mechanism of superconductivity in models of strongly correlated electrons

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Abstract

We consider extended versions of the Hubbard model which contain additional interactions between nearest neighbours. In this letter we show that a large class of these models has a superconducting ground state in arbitrary dimensions. In some special cases we are able to find the complete phase diagram. The superconducting phase exist even for moderate repulsive values of the Hubbard interaction U.

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In this letter we consider extensions of the Hubbard model. We shall show that they are superconducting. The idea to explain superconductivity in the framework of strongly correlated electrons was proposed in [1] and has subsequently been studied in numerous publications. Most of these investigations used approximate or numerical methods and so only a few exact results are known. One of these exact results is an algebraic approach based on so-called η-pairs [2]. It allows for the construction of states exhibiting off-diagonal-long-range-order (ODLRO). This important concept has been developed in [3]. ODLRO is an adequate definition of superconductivity in arbitrary dimensions since it implies also the Meissner effect and flux quantisation [3–5].

Let us first consider the Hamiltonian of the Hubbard model

$$\mathcal{H}_0(U) = -t \sum_{\langle jl \rangle} \sum_{\sigma=\uparrow\downarrow} \left(c_{j\sigma}^\dagger c_{l\sigma} + c_{l\sigma}^\dagger c_{j\sigma} \right) + U \sum_{j=1}^{L} (n_{j\uparrow} - \frac{1}{2})(n_{j\downarrow} - \frac{1}{2}) \ . \tag{1}$$

Here $c_{j\sigma}$ are canonical Fermi operators which describe electrons on a d-dimensional lattice, i.e. $\{c_{j\sigma}^\dagger, c_{l\tau}\} = \delta_{jl}\delta_{\sigma\tau}$ and $c_{j\sigma}|\,0\,\rangle = 0$ where $|\,0\,\rangle$ denotes the Fock vacuum.

In (1) j runs through all L sites of the d-dimensional lattice, $\langle jl \rangle$ denotes nearest-neighbour sites and U is the Hubbard coupling. $n_{j\sigma} = c_{j\sigma}^\dagger c_{j\sigma}$ denotes the number operator for electrons with spin σ on site j and we write $n_j = n_{j\uparrow} + n_{j\downarrow}$.

This letter consists of two parts. In the first part we shall add general nearest-neighbour interactions to the Hubbard Hamiltonian (1) and analyze the three following questions:

- When does this new Hamiltonian commute with the η-operators

$$\eta = \sum_j c_{j\uparrow} c_{j\downarrow} \ , \quad \eta^\dagger = \sum_j c_{j\downarrow}^\dagger c_{j\uparrow}^\dagger \ . \tag{2}$$

- When will $\left(\eta^\dagger\right)^N |\,0\,\rangle$ be an exact eigenstate of this Hamiltonian?
- When will $\left(\eta^\dagger\right)^N |\,0\,\rangle$ be a ground state of this Hamiltonian?

We shall answer all these questions for the general multiparametric Hamiltonian. For example, $|\,\psi_N\,\rangle = \left(\eta^\dagger\right)^N |\,0\,\rangle$ will be a ground state in a 9-parametric region (subject to some inequality).

What makes the state $|\,\psi_N\,\rangle$ special is the fact that it has been shown to have ODLRO (and thus is superconducting),

$$\langle \psi_N | c_{j\downarrow}^\dagger c_{j\uparrow}^\dagger c_{l\uparrow} c_{l\downarrow} | \psi_N \rangle \quad \stackrel{|l-j|\to\infty}{\longrightarrow} \quad \frac{N}{L}(1 - \frac{N}{L}) \ , \tag{3}$$

where we have also taken the thermodynamic limit ($N, L \to \infty$ with N/L fixed).

The results of the first part show that superconductivity based on η-pairs is a rather typical phenomenon. To see the relation between η-pairs and the usual order parameter of BCS theory we express the $\eta^\dagger$-operator in terms of electronic operators $c_{k\sigma}^\dagger$ in momentum space , $c_{j\sigma}^\dagger = \frac{1}{\sqrt{L}} \sum_k e^{ijk} c_{k\sigma}^\dagger$, which yields $\eta^\dagger = \sum_k c_{k\downarrow}^\dagger c_{-k\uparrow}^\dagger$. This is just the BCS order parameter.

In the second part of this letter we will consider two special cases of the general Hamiltonian discussed in the first part. Both of these models are exactly solvable in one dimension and have η-pairs in the ground state (and thus are superconducting) even for moderate repulsive values of U. These results are valid in any dimension.

In order to argue that superconductivity based on η-pairing is a generic rather than an exotic phenomenon, we consider the Hamiltonian $\mathcal{H}(U) = \mathcal{H}_0(U) + \mathcal{H}_1$, where $\mathcal{H}_0(U)$ is the Hubbard Hamiltonian (1), and

$$
\begin{aligned}
\mathcal{H}_1 = X & \sum_{<jl>,\sigma} (c_{j\sigma}^\dagger c_{l\sigma} + c_{l\sigma}^\dagger c_{j\sigma})(n_{j,-\sigma} + n_{l,-\sigma}) \\
& + V \sum_{<jl>} (n_j - 1)(n_l - 1) + J_z \sum_{<jl>} S_j^z S_l^z \\
& + \frac{J_{xy}}{2} \sum_{<jl>} (S_j^\dagger S_l + S_l^\dagger S_j) + Y \sum_{<jl>} (c_{j\uparrow}^\dagger c_{j\downarrow}^\dagger c_{l\downarrow} c_{l\uparrow} + c_{l\uparrow}^\dagger c_{l\downarrow}^\dagger c_{j\downarrow} c_{j\uparrow}) \\
& + P \sum_{<jl>} \Big((n_{j\uparrow} - \frac{1}{2})(n_{j\downarrow} - \frac{1}{2})(n_l - 1) + (n_{l\uparrow} - \frac{1}{2})(n_{l\downarrow} - \frac{1}{2})(n_j - 1) \Big) \\
& + Q \sum_{<jl>} (n_{j\uparrow} - \frac{1}{2})(n_{j\downarrow} - \frac{1}{2})(n_{l\uparrow} - \frac{1}{2})(n_{l\downarrow} - \frac{1}{2}), \\
& + \mu \sum_j n_j + h \sum_j (n_{j\uparrow} - n_{j\downarrow})
\end{aligned} \tag{4}
$$

where the $SU(2)$ spin operators S_j^a are given by $S_j^z = \frac{1}{2}(n_{j\uparrow} - n_{j\downarrow})$, $S_j = c_{j\downarrow}^\dagger c_{j\uparrow}$ and $S_j^\dagger = c_{j\uparrow}^\dagger c_{j\downarrow}$. The first term in (4) is known as the bond-charge interaction, the second one is the nearest-neighbour Coulomb interaction. In addition we included a XXZ-type spin interaction with exchange constants J_{xy} and J_z between nearest neighbour sites. The relevance of the pair-hopping term Y for high-temperature superconductivity has recently been discussed in [8]. Apart from a chemical potential μ and a magnetic field h we also added a three- and four-particle density interaction P and Q, respectively.

The Hamiltonian (4) with $t = X$ and zero magnetic field $h = 0$ is the most general Hamiltonian that one can write down that is hermitian, symmetric under spinflip ($\sigma \to -\sigma$) and conserves the total number $N_\sigma = \sum_{j=1}^L n_{j\sigma}$ of electrons with spin σ and the number of doubly occupied sites. The last requirement is quite natural if we consider exact η-pairing ground states, since these are eigenstates of the number operator for doubly occupied sites $N_2 = \sum_j n_{j\uparrow} n_{j\downarrow}$. To include the Hubbard model itself we allow $t \neq X$ and have for convenience also included a chemical potential μ and allowed for nonzero magnetic field h.

The conditions under which $\mathcal{H}(U)$ commutes with $\eta^\dagger$ can be read of from the identity

$$
[\mathcal{H}(U), \eta^\dagger] = 2(t - X) \sum_{<jl>} (c_{l\uparrow}^\dagger c_{j\downarrow}^\dagger + c_{j\uparrow}^\dagger c_{l\downarrow}^\dagger)
$$

$$+(2V-Y)\sum_{<jl>}(\eta_j^\dagger(n_l-1)+\eta_l^\dagger(n_j-1))$$

$$+2P\sum_{<jl>}(\eta_j^\dagger(n_{l\uparrow}-\frac{1}{2})(n_{l\downarrow}-\frac{1}{2})+\eta_l^\dagger(n_{j\uparrow}-\frac{1}{2})(n_{j\downarrow}-\frac{1}{2}))$$

$$+2\mu\sum_j\eta_j^\dagger\ . \tag{5}$$

Therefore, the condition for η-symmetry is that $t=X$, $2V-Y=0$, $P=0$ and $\mu=0$. Using (5) one finds that $(\eta^\dagger)^N|\,0\,\rangle$ is an eigenstate of $\mathcal{H}(U)$ if $t=X$ and $2V=Y$. The corresponding eigenvalue is

$$E_N=\frac{UL}{4}+\frac{ZL}{2}\left(V+\frac{P}{2}+\frac{Q}{16}\right)+N\left(2\mu+\frac{PZ}{2}\right), \tag{6}$$

where Z is the number of nearest neighbours of a lattice site.

Next, we want to determine under which conditions the η-pairing state is actually the ground state of the theory. For this, we use the following lower bound for the ground state energy. Let $\{\psi_\alpha\}$ be an orthonormal basis of the Hilbert space, then the ground state energy E_0 satisfies

$$E_0\geq\min_\alpha\left(\langle\psi_\alpha|\mathcal{H}(U)|\psi_\alpha\rangle-\sum_{\beta\neq\alpha}|\langle\psi_\beta|\mathcal{H}(U)|\psi_\alpha\rangle|\right). \tag{7}$$

This lower bound has previously been used by Ovchinnikov [9] to analyze ferromagnetic ground states continuing the work of Strack and Vollhardt [10]. By requiring that this lower bound equals E_N in (6) one can prove [11] that $(\eta^\dagger)^N|\,0\,\rangle$ is a ground state of $\mathcal{H}(U)$ if $V\leq 0$ and

$$\frac{-U}{Z}\geq\max\left(|P|+2\frac{|h|}{Z}+\frac{Q}{4}+2|t|+2V,\ V-\frac{J_z}{4}+\frac{2|h|}{Z},\ V+\frac{J_z}{4}+|\frac{J_{xy}}{2}|\right). \tag{8}$$

This shows that if $t=X$ and $2V=Y\leq 0$, one can for every value of the parameters in $\mathcal{H}$ always make the ground state superconducting, by making the Hubbard coupling sufficiently small.

The results of [12] suggest that even if we relax the conditions $t=X$ and $2V=Y$, we still will have a superconducting ground state for sufficiently small U. This is much harder to prove, since the explicit form of the ground state is not known, but one might get some indications from doing perturbation theory in $t-X$ or $2V-Y$.

One might object that negative U does not represent the real physical situation, since U represents the Coulomb repulsion between electrons and that should be positive. However, we shall see in a moment that in two special cases the following happens: as soon as U becomes larger than the bound (8), the ground state becomes $(\eta^\dagger)^{N-n}|\,\psi_n\,\rangle$, where $|\,\psi_n\,\rangle$ is a $2n$-electron state without doubly occupied sites. As U increases, so does n until $n=N$. At this value of U the theory will no longer be superconducting. It is therefore quite likely that superconductivity will persist for a somewhat larger range of values of U than given by (8).

After these general considerations let us now look at two models more closely. For these models the full phase diagram in arbitrary dimensions can be obtained. Furthermore, in one dimension we are able to calculate the complete spectrum. From now on we will set $t = 1$ for convenience.

The first model is obtained by setting all parameters in (4) equal to zero except for the bond-charge interaction X,

$$\mathcal{H}(X,U) = -\sum_{\langle jl\rangle}\sum_{\sigma=\uparrow\downarrow}\left(c_{j\sigma}^\dagger c_{l\sigma} + c_{l\sigma}^\dagger c_{j\sigma}\right)\left(1 - X\left(n_{j,-\sigma} + n_{l,-\sigma}\right)\right) + U\sum_{j=1}^{L}(n_{j\uparrow} - \frac{1}{2})(n_{j\downarrow} - \frac{1}{2}) \ . \tag{9}$$

For general values of X this model has been discussed extensively by Hirsch [13]. He argued that for large densities of electrons (low doping) the bond-charge interaction leads to an attractive effective interaction between the holes which may even create Cooper-pairs of holes. Indeed, using a BCS-type mean-field theory he found a superconducting phase for small hole concentrations.

Unfortunately, up to now even in one dimension there are almost no exact results available although it has been shown that a simplified version of Hirsch's Hamiltonian in one dimension indeed has a strong tendency towards superconductivity [17].

In the following we consider the Hamiltonian for the special case $X = 1$. As mentioned above, at this point the number of doubly occupied sites is conserved. Therefore the Hubbard interaction acts as chemical potential for the doubly occupied sites. The dynamics become quite simple since the local Hamiltonian permutes bosons (i.e. empty sites and doubly occupied sites) with fermions (i.e. singly occupied sites) on neighbouring sites but not bosons with bosons or fermions with fermions. In the sector with no double-occupations the Hamiltonian reduces to the well-known $U = \infty$ Hubbard model.

In one dimension this Hamiltonian can be solved exactly [14] by generalising the method applied in [15,16] to the $U = \infty$ Hubbard model. The Hilbert space is divided into certain subspaces in which the Hamiltonian can be mapped onto spinless fermions with twisted boundary conditions. The twisting angle depends on the subspace considered. In this way the complete spectrum can be obtained. The ground state energy for a system of N_1 (single) electrons and N_2 doubly occupied sites at $U = 0$ is given by

$$E_0(N_1, N_2) = -2\,\frac{\sin(N_1\pi/L)}{\sin(\pi/L)} \ . \tag{10}$$

Note that this energy is independent of N_2. In general, the ground state is highly degenerate as is known for the $U = \infty$ Hubbard model. After including the Hubbard interaction we can minimize this energy for a given total number $N = N_1 + 2N_2$ of electrons. We find the phase diagram shown in fig. **??**. For $U \leq -4$ (sector I) the η-pairing state $\left(\eta^\dagger\right)^{N/2} |\,0\,\rangle$ is a ground state in agreement with the inequality (8). In sector II where $-4 \leq U \leq U_c(N) = -4\cos(N\pi/L)$ the ground state is of the form $\left(\eta^\dagger\right)^{N/2} |U = \infty, N_1\rangle$ where $|U = \infty, N_1\rangle$ is the ground state of the $U = \infty$ Hubbard model for N_1 electrons. Both these states exhibit ODLRO showing the existence of a superconducting ground state even for moderately positive values of U. For $U \geq U_c(N)$ the ground state is that of the $U = \infty$ Hubbard model (for densities $D = N/L > 1$ it is the state obtained by particle-hole symmetry).

The phase diagram in higher dimensions looks quite similar although we can not give an explicit expression for $U_c(N)$. From (8) we know that $\left(\eta^\dagger\right)^{N/2} |\, 0\, \rangle$ is a ground state for $U \leq -2Z$. The rest of the phase diagram can be obtained by an argumentation analogous to that in [7]. The properties necessary for this argumentation to hold are

- η-symmetry,
- conservation of the number of doubly occupied sites,
- for $U = 0$ the ground state energy is independent of N_2.

Another interesting special case of the general Hamiltonian (4) is the supersymmetric Hubbard model [6,7]. The Hamiltonian of this model is given by

$$\mathcal{H}_{sH} = \mathcal{H}^0 + U \sum_{j=1}^{L} (n_{j\uparrow} - \frac{1}{2})(n_{j\downarrow} - \frac{1}{2}) \tag{11}$$

where $\mathcal{H}^0 = -\sum_{\langle jl \rangle} H^0_{j,l}$, and

$$\begin{aligned} H^0_{j,l} = {} & c^\dagger_{l\uparrow} c_{j\uparrow}(1 - n_{j\downarrow} - n_{l\downarrow}) + c^\dagger_{j\uparrow} c_{l\uparrow}(1 - n_{j\downarrow} - n_{l\downarrow}) \\ & + c^\dagger_{l\downarrow} c_{j\downarrow}(1 - n_{j\uparrow} - n_{l\uparrow}) + c^\dagger_{j\downarrow} c_{l\downarrow}(1 - n_{j\uparrow} - n_{l\uparrow}) \\ & + \frac{1}{2}(n_j - 1)(n_l - 1) + c^\dagger_{j\uparrow} c^\dagger_{j\downarrow} c_{l\downarrow} c_{l\uparrow} + c_{j\downarrow} c_{j\uparrow} c^\dagger_{l\uparrow} c^\dagger_{l\downarrow} \\ & - \frac{1}{2}(n_{j\uparrow} - n_{j\downarrow})(n_{l\uparrow} - n_{l\downarrow}) - c^\dagger_{j\downarrow} c_{j\uparrow} c^\dagger_{l\uparrow} c_{l\downarrow} - c^\dagger_{j\uparrow} c_{j\downarrow} c^\dagger_{l\downarrow} c_{l\uparrow} \\ & + (n_{j\uparrow} - \frac{1}{2})(n_{j\downarrow} - \frac{1}{2}) + (n_{l\uparrow} - \frac{1}{2})(n_{l\downarrow} - \frac{1}{2}) \; . \end{aligned} \tag{12}$$

This Hamiltonian corresponds to the choice $X = t = 1$, $V = -1/2$, $J_{xy} = J_z = 2$, $Y = -1$ and $P = Q = \mu = h = 0$ in (4). Note that $H^0_{j,l}$ also contains a Coulomb interaction term $-Z(n_{j\uparrow} - \frac{1}{2})(n_{j\downarrow} - \frac{1}{2})$. $\mathcal{H}^0$ commutes with η and $\eta^\dagger$ as defined in (2). Actually, the model has a larger set of symmetries that form the superalgebra $U(2|2)$ [6].

The ground state phase diagram has been obtained in [7]. It looks very similar to fig. **??**. The main difference is the occurence of the ground state $|t - J\rangle$ of the supersymmetric $t - J$ model [18] that replaces $|U = \infty\rangle$ in fig. **??**. In addition, the sector I exists for all $U < 0$ (in every dimension) as can also be seen from the inequality (8). A superconducting phase exist for moderate positive U in all dimensions. The additional interactions of (12) lift the degeneracies encountered in the model (9). A more detailed discussion of the phase diagram of the supersymmetric Hubbard model has been given in [7].

In conclusion, in this letter we have shown that η-pairs provide a simple and clear mechanism of superconductivity.

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