η-pairing superconductivity in generalized Hubbard models

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Abstract

We consider generalized Hubbard models in arbitrary dimensions which have additional nearest-neigbour interactions. It is shown that in a large region of the parameter space these models have ground states of the η-pairing type. These ground states exhibit off-diagonal long-range order and are thus superconducting. In special cases the complete ($T = 0$) phase diagram can be obtained.

The proposal to explain high-temperature superconductivity in the framework of strongly correlated electrons (Anderson 1987, Zhang and Rice 1988) has stimulated the search for purely electronic mechanisms of superconductivity. Unfortunately, only very few exact results are available. In this paper we will show that the so-called η-pairing mechanism can be used to construct exact ground states for generalized Hubbard models in a wide range of interaction parameters. These η-pairing states are known (Yang 1989) to exhibit off-diagonal long-range order (ODLRO) (Yang 1962). Since ODLRO implies also the Meissner effect and flux quantization (Sewell 1990, 1995, Nieh et.al. 1995) these states are superconducting. η-pairing superconductivity is closely related to local-pair superconductivity which has been reviewed in (Micnas, Ranninger and Robaszkiewicz 1990).

In the following we will be interested in generalized Hubbard models with Hamiltonian $\mathcal{H} = \sum_{\langle jl \rangle} h_{jl}$, where $\langle jl \rangle$ denotes nearest-neighbour sites on a d dimensional lattice and

$$\begin{aligned} h_{jl} = & -t \sum_\sigma (c_{j\sigma}^\dagger c_{l\sigma} + c_{l\sigma}^\dagger c_{j\sigma}) + \frac{U}{Z}\left((n_{j\uparrow} - \frac{1}{2})(n_{j\downarrow} - \frac{1}{2}) + (n_{l\uparrow} - \frac{1}{2})(n_{l\downarrow} - \frac{1}{2}) \right) \\ & + X \sum_\sigma (c_{j\sigma}^\dagger c_{l\sigma} + c_{l\sigma}^\dagger c_{j\sigma})(n_{j,-\sigma} + n_{l,-\sigma}) + R \sum_\sigma (c_{j\sigma}^\dagger c_{l\sigma} + c_{l\sigma}^\dagger c_{j\sigma}) n_{j,-\sigma} n_{l,-\sigma} \\ & + V(n_j - 1)(n_l - 1) + Y\left(c_{j\uparrow}^\dagger c_{j\downarrow}^\dagger c_{l\downarrow} c_{l\uparrow} + c_{l\uparrow}^\dagger c_{l\downarrow}^\dagger c_{j\downarrow} c_{j\uparrow} \right) \\ & + \frac{J_{xy}}{2}\left(S_j^+ S_l^- + S_l^+ S_j^- \right) + J_z S_j^z S_l^z + \frac{h}{Z}((n_{j\uparrow} - n_{j\downarrow}) + (n_{l\uparrow} - n_{l\downarrow})) \, . \end{aligned} \tag{1}$$

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Here $c_{j\sigma}$ and $c_{j\sigma}^\dagger$ are the canonical Fermi operators, $n_{j\sigma} = c_{j\sigma}^\dagger c_{j\sigma}$ and $n_j = n_{j\uparrow} + n_{j\downarrow}$ are the corresponding number operators and the $SU(2)$ spin operators 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 $S_j^+ = c_{j\uparrow}^\dagger c_{j\downarrow}$.

The first term in (1) is the single-particle hopping, X and R are known as bond-charge interaction. U and V denote the on-site and nearest-neighbor Coulomb interaction, respectively. In addition, we included a XXZ-type spin interaction with exchange constants J_{xy} and J_z between nearest neighbour sites and a pair-hopping term Y. h is a magnetic field and Z denotes the coordination number of the d-dimensional lattice.

η-pairing has first been discussed for the standard Hubbard model. Yang (1989) has shown that (on a hyper-cubic lattice with L sites) there exist exact eigenstates of the form

$$|\psi_N^{(P)}\rangle = \left(\eta_P^\dagger\right)^N |\, 0\,\rangle, \qquad \eta_p^\dagger = \sum_{\vec{j}} e^{i\vec{P}\cdot\vec{j}} c_{\vec{j}\downarrow}^\dagger c_{\vec{j}\uparrow}^\dagger. \tag{2}$$

with $\vec{P} = (\pi, \ldots, \pi)$. The operator $\eta_P^\dagger$ creates a doubly occupied site with momentum $\vec{P}$.

Yang also proved that these states cannot be ground states. It is therefore natural to asked whether there are generalized Hubbard models with additional interactions between nearest neigbours which have ground states of the form (2). The first such model has been found by Eßler, Korepin and Schoutens (1992, 1993). It correponds to the choice $t = X$, $V = -t/2$, $J_{xy} = J_z = 2t$, $Y = -t$ and $R = 0$ in (1). This so-called EKS model has an η-pairing ground state with momentum 0 for Coulomb interactions $U < U_c$. In addition it is exactly solvable by Bethe Ansatz in one dimension (Eßler, Korepin and Schoutens 1992).

In (de Boer, Korepin, Schadschneider 1995) it has been investigated whether there are further models with $\vec{P} = 0$ η-pairing ground states. The state (2) with $\vec{P} = 0$ is an eigenstate of $\mathcal{H}$ for $t = X$ and $Y = 2V$. It is easy to see that $|\psi_N^{(0)}\rangle$ can be built from the local states $|00\rangle$, $|22\rangle$ and $|20\rangle + |02\rangle$. Here 0 denotes an empty site and 2 a doubly occupied site. For $t = X$ these three states all have the energy $E_0 = \frac{U}{2Z} + V$. If we now demand that the other 13 eigenstates of h_{jl} have energies larger than E_0 we immediately see that the η-pairing state is a global ground state. This concept of an "optimal ground state" has already been applied successfully to quantum spin chains (Klümper, Schadschneider, Zittartz 1993, Zittartz 1992). In this way one finds the following conditions for the existence of an momentum-0 η-pairing ground state

$$\begin{aligned} &t = X, \qquad 2V = Y, \\ &V \leq 0, \\ &-\frac{U}{Z} \geq \max\Big(V - \frac{J_z}{4} + \frac{2|h|}{Z},\ V + \frac{J_z}{4} + \frac{|J_{xy}|}{2}, 2\max(|t|, |t+R|) + 2V + \frac{2|h|}{Z}\Big). \end{aligned} \tag{3}$$

The same reasoning can now be applied to find the interaction parameters where the momentum $(\pi, \ldots, \pi)$ η-pairing state is the ground state[1]. In this case we do not need the

[1]Similar results have been obtained in (Montorsi and Campbell 1995) by a different approach.

restriction $t = X$ since $|\psi_N^{(\pi)}\rangle$ is also an eigenstate for $t \neq X$ if only $Y = -2V$. We find the following conditions

$$\begin{aligned}
&2V = -Y, \\
&V \leq 0, \\
&-\frac{U}{Z} \geq \max\Big(2\max(|t|, |t-2X-R|) + 2V + \frac{2|h|}{Z}, V - \frac{J_z}{4} + \frac{2|h|}{Z}, \\
&\qquad\qquad V - \frac{J_{xy}}{2} + \frac{J_z}{4}, V + \frac{J_{xy}}{2} + \frac{J_z}{4} - \frac{(t-X)^2}{V}\Big).
\end{aligned} \tag{4}$$

For general $\vec{P} \neq 0, (\pi, \ldots, \pi)$ the state (2) is an eigenstate for $t = X$ and $V = Y = 0$. The bounds for this case are obtained by setting $V = 0$ in (3).

The results show that in the standard Hubbard model (all interaction constants are zero, except for t and U) $\eta-$pairing ground states exist only for $\vec{P} = (\pi, \ldots, \pi)$ and $U = -\infty$. This is consistent with the results of Singh and Scalettar (1991).

Apart from the above mentioned EKS-model there is another model with η-pairing ground states which can be solved exactly in one dimension. Here all interaction constants in (1) are zero except for $t = X$ and U. It belongs to the class of models discussed by Hirsch (1989a,b) in the context of hole superconductivity. Since for $t = X$ pairs cannot decay and the on-site Coulomb interaction merely acts as a chemical potential for the number of doubly-occupied sites. In the subspace with no double occupations the Hamiltonian reduces to that of the $U = \infty$ Hubbard model.

For the solution of this model (Schadschneider 1995, Aligia and Arrachea 1994) one makes use of the fact that the local Hamiltonian has a particular simple structure. It only permutes bosons (i.e. empty sites and doubly occupied sites) with fermions (i.e. singly occupied sites). This allows to divide the Hilbert space in certain subspaces in which the Hamiltonian can be mapped onto a system of spinless free fermions with twisted boundary conditions (Schadschneider 1995) where the twist depends on the subspace considered. In this way the complete spectrum can be obtained.

In Fig. 1 the ground state phase diagram in the $D-U$ plane where D is the particle density (Schadschneider 1995) is shown. In regime I ($U \leq -4$) all states which have no single electrons are ground states. The pairs in these states are static. Among these ground states are the η-pairing states $\left(\eta_P^\dagger\right)^{DL/2} |\,0\,\rangle$, see (3),(4). In regime II ($-4 \leq U \leq U_c(D) = -4\cos(\pi D)$) the ground state consists of both single electrons and pairs. Among those ground states are more complicated η-pairing states of the form $\left(\eta^\dagger\right)^{LD_2} |U = \infty, D_1\rangle$ where $|U = \infty, D_1\rangle$ is the ground state of the $U = \infty$ Hubbard model for a density D_1 of (single) electrons, and $D_1 + 2D_2 = D$. These states also exhibit ODLRO showing the existence of superconducting ground states even for moderately positive values of U. For $U \geq U_c(D)$ the ground state has no doubly-occupied sites and is that of the $U = \infty$ Hubbard model (for densities $D > 1$ it is the state obtained by particle-hole symmetry). In general, the ground state is highly degenerate as is already known for the $U = \infty$ Hubbard model.

The phase diagram in higher dimensions looks quite similar although we cannot give an explicit expression for $U_c(D)$. From (3) we know that $\left(\eta^\dagger\right)^{DL/2} |\,0\,\rangle$ is a ground state for

$U \leq -2Z$. The rest of the phase diagram can be obtained by an argumentation analogous to that in (Eßler, Korepin and Schoutens 1993). Recently, it was shown in (Ovchinnikov 1994) that the metal-insulator at half-filling $D = 1$ in d dimensions is located at $U = 2Z$ so that the regime II also in $d > 1$ extends to the region $U > 0$.

Finally we like to mention that the ideas presented here can also be used to construct other exact ground states of generalized Hubbard models (de Boer and Schadschneider 1995), like ferromagnetic or Néel states.

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REFERENCES

[1] Aligia, A.A. and L. Arrachea (1994). Exact solution of a Hubbard chain with bond-charge interaction. Phys. Rev. Lett. **73**, 2240.

[2] Anderson, P.W. (1987). The resonating valence bond state in La_2CuO_4 and superconductivity. Science **235**, 1196.

[3] de Boer, J., V.E. Korepin and A. Schadschneider (1995). η-pairing as a mechanism of superconductivity in models of strongly correlated electrons. Phys. Rev. Lett. **74**, 789.

[4] de Boer, J. and A. Schadschneider (1995). Exact ground states of generalized Hubbard models. preprint (cond-mat/9503122).

[5] Eßler, F.H.L., V.E. Korepin and K. Schoutens (1992). New exactly solvable model of strongly correlated electrons motivated by high-T_c superconductivity. Phys. Rev. Lett. **68**, 2960.

[6] Eßler, F.H.L., V.E. Korepin and K. Schoutens (1993). Electronic model for superconductivity. Phys. Rev. Lett. **70**, 73

[7] Micnas, R., J. Ranninger, and S. Robaszkiewicz (1990). Superconductivity in narrow-band systems with local nonretarded attractive interactions. Rev. Mod. Phys. **62**, 113.

[8] Montorsi, A., and D.K. Campbell (1995). Rigorous results on superconducting ground states for attractive extended Hubbard models. preprint (cond-mat/9502027).

[9] Nieh, H.T., G. Su and B.M. Zhao (1995). Off-diagonal long range order: Meissner effect and flux quantization. Phys. Rev. **B51**, 3760

[10] Ovchinnikov, A.A. (1994). Metal-insulator transition in the generalized Hubbard model. J. Phys. **CM6**, 11057.

[11] Schadschneider, A. (1995). Superconductivity in an exactly solvable Hubbard model with bond-charge interaction. Phys. Rev. **B51** (in press)

[12] Sewell, G.L. (1990). Off-diagonal long-range order and the Meissner effect. J. Stat. Phys. **61**, 415.

[13] Sewell, G.L. (1995). Macroscopic quantum theory of superconductivity and the Higgs mechanism. in "Stochastics, Physics and Geometry", Proceedings of the Third International Conference, Ed, S. Albeverio, U. Cattaneo and D. Merlini, World Scientific, Singapore,

[14] Singh, R.R.P. and R.T. Scalettar (1991). Exact demonstration of η pairing in the ground state of an attractive-U Hubbard model. Phys. Rev. Lett. **66**, 3203.

[15] Yang, C.N. (1989). η pairing and off-diagonal long-range order in a Hubbard model. Phys. Rev. Lett. **63**, 2144.

[16] Yang, C.N. and S. Zhang (1990). SO_4 symmetry in a Hubbard model. Mod. Phys. Lett. **B4**, 759.

[17] Yang, C.N. (1962). Concept of off-diagonal long-range order and the quantum phases of liquid He and of superconductors. Rev. Mod. Phys. **34**, 694.

[18] Zhang, F.C. and T.M. Rice (1988) Phys. Rev. **B 37**, 3759.

[19] Zittartz, J. (1992). unpublished results.

FIGURES

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