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Electronic model for superconductivity[1]

Fabian H.L. Eßler
Vladimir E. Korepin
and
Kareljan Schoutens

Institute for Theoretical Physics
State University of New York at Stony Brook
Stony Brook, NY 11794-3840, U.S.A.

Abstract

We consider a model of strongly correlated electrons that exhibits superconductivity. It differs from the Hubbard model by nearest neighbour interactions. We find the ground state wave function (in one, two or three dimensions) and show it to be superconducting for attractive and moderately repulsive on-site interaction.

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The phenomenon of high-T_c superconductivity has led to an increased interest in theoretical models for superconductivity other than the BCS theory. In [1] P.W. Anderson and F.C. Zhang and T.M. Rice proposed that superconductivity can occur in models based on purely electronic interactions. In this letter we discuss the electronic model that we introduced in [2] and show that it is superconducting. We determine the ground state structure at zero temperature and investigate under what conditions it exhibits superconductivity. We will prove that for negative U (attractive case) the model has a unique ground state which has ODLRO and is thus superconducting. This result holds for lattices of arbitrary dimension. We will also discuss the phase diagram for positive U, where we will find that superconductivity persists if the repulsion U is smaller than a certain critical value U_c. The neighbouring phases are a phase of the supersymmetric t-J model, and an insulator phase.

Electrons on a lattice are described by operators $c_{j,\sigma}$, $j = 1, \dots, L$, $\sigma = \uparrow, \downarrow$, where L is the total number of lattice sites. These are canonical Fermi operators satisfying $\{c_{i,\sigma}^\dagger, c_{j,\tau}\} = \delta_{i,j}\delta_{\sigma,\tau}$. The state $|\,0\,\rangle$ (the Fock vacuum) satisfies $c_{i,\sigma}|\,0\,\rangle = 0$. By $n_{i,\sigma} = c_{i,\sigma}^\dagger c_{i,\sigma}$ we denote the number operator for electrons with spin σ on site i and we write $n_i = n_{i,\uparrow} + n_{i,\downarrow}$.

The hamiltonian of the new model on a general d-dimensional lattice can be written as

$$H = H^0 + U \sum_{j=1}^{L} (n_{j,\uparrow} - \frac{1}{2})(n_{j,\downarrow} - \frac{1}{2}) - \mu \sum_{j=1}^{L} n_j \ , \tag{1}$$

where $H^0 = -\sum_{\langle jk \rangle} H^0_{j,k}$ ($\langle j,k \rangle$ are nearest neighbours), and

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

This hamiltonian contains kinetic terms and interaction terms that combine those of the Hubbard model and of the t-J model. It also contains a hopping term for local electron pairs (spin-down and spin-up electrons occupying the same site). The interaction terms are very similar to the ones proposed by J.E. Hirsch in his model of superconductivity, which was derived by a tight-binding analysis [3]. The second term in (1) is the on-site Hubbard interaction term and μ is the chemical potential. The Hubbard coupling U will determine the ratio of local electron pairs to single (unpaired) electrons in the ground state.

The state $\sum_{\vec{x}} \exp{(i \ \vec{k} \cdot \vec{x})} \ c^\dagger_{\vec{x},\downarrow} c^\dagger_{\vec{x},\uparrow} \mid 0 \rangle$ (where $\vec{x}$ runs over all sites of a d-dimensional lattice) is an eigenstate of the hamiltonian (1). We call this state a *localon* state of momentum $\vec{k}$.

The hamiltonian H^0 has a rich symmetry structure. It is invariant under two independent $SU(2)$ symmetries and under eight supersymmetries. Together with the number operator for local electron pairs and with the identity operator these symmetries generate the superalgebra $U(2|2)$ (see [2] for more details). The first of the two $SU(2)$ algebras corresponds to ordinary spin; the generators of the second $SU(2)$ algebra are

$$\eta = \sum_{j=1}^{L} c_{j,\uparrow} c_{j,\downarrow} \ , \qquad \eta^\dagger = \sum_{j=1}^{L} c_{j,\downarrow}^\dagger c_{j,\uparrow}^\dagger \ , \qquad \eta^z = \sum_{j=1}^{L} \frac{1}{2}(1 - n_j) \ . \tag{3}$$

It can be seen that the operator $\eta^\dagger$ creates a localon of momentum zero. The fact that it commutes with the hamiltonian H^0 and with the U-term in (1) makes it possible to construct eigenstates of the full hamiltonian H that contain a large number of zero momentum local electron pairs. Such states will play a crucial role in our discussion below.

The hamiltonian density $H_{j,k}^0$ acts as a *graded permutation* $\Pi_{j,k}^g$ of the electronic states at sites j and k. By 'graded' we mean that there is an extra minus sign if the two states that are permuted are both single electron states. For example,

$$H_{j,k}^0 \, c_{j,\uparrow}^\dagger | \, 0 \, \rangle = c_{k,\uparrow}^\dagger | \, 0 \, \rangle \, , \quad H_{j,k}^0 \, c_{j,\uparrow}^\dagger c_{k,\downarrow}^\dagger | \, 0 \, \rangle = -c_{j,\downarrow}^\dagger c_{k,\uparrow}^\dagger | \, 0 \, \rangle \, , \quad \text{etc.} \tag{4}$$

This property implies that the number operators $\hat{N}_\uparrow$, $\hat{N}_\downarrow$ (the number operators of *single* electrons with given spin) and $\hat{N}_l$ (the number operator of local electron pairs), defined by

$$\hat{N}_\uparrow + \hat{N}_l = \sum_{j=1}^{L} n_{j,\uparrow} \ , \qquad \hat{N}_\downarrow + \hat{N}_l = \sum_{j=1}^{L} n_{j,\downarrow} \ , \qquad \hat{N}_l = \sum_{j=1}^{L} n_{j,\uparrow}\, n_{j,\downarrow} \ , \tag{5}$$

all commute with H^0, so that H^0 can be diagonalised within a sector with given numbers $N_\uparrow$, $N_\downarrow$ and N_l. This implies that our hamiltonian does not allow for decay of local electron pairs into two single electrons.

In the sectors without local electron pairs H^0 reduces to the hamiltonian of the supersymmetric t-J model with $t = 1$, $J = 2$ (in our discussion below we always consider this special case), and the model is isomorphic to the spin-$\frac{1}{2}$ XXX model in the sector with only vacancies and local electron pairs.

Abstract graded permutations of 2 species of bosons and 2 species of fermions were first considered as a dynamical hamiltonian by B.Sutherland in [4], where the ground state energy for the one-dimensional model was computed.

Let us now discuss physical aspects of the new model, which hold in arbitrary dimensions. We will first establish that certain eigenstates of H^0 have the property of off-diagonal long range order (ODLRO), which is characteristic of superconductivity [5]. Let us consider an eigenstate $|\psi\rangle$ of H^0 which is a highest weight state of the

η-pairing $SU(2)$ algebra (3). It has the properties

$$\eta|\psi\rangle = 0, \qquad \eta^z|\psi\rangle = \frac{1}{2}(L - N_c)|\psi\rangle \ , \tag{6}$$

where $N_c = N_\uparrow + N_\downarrow + 2N_l$ is the number of electrons in $|\psi\rangle$. We can then construct additional eigenstates of the form

$$|\psi_n\rangle = (\eta^\dagger)^n|\psi\rangle, \qquad n = 0, 1, 2, \ldots, L - N_c \ . \tag{7}$$

Following [6] we consider the following off-diagonal matrix element ($k \neq l$) of the reduced density matrix ρ_2 for the state $|\psi_n\rangle$

$$(\rho_2)_{kl} = \langle (k,\downarrow)(k,\uparrow)|\, \rho_2\, |(l,\uparrow)(l,\downarrow)\rangle = \frac{\langle\psi|\eta^n c^\dagger_{k,\downarrow} c^\dagger_{k,\uparrow} c_{l,\uparrow} c_{l,\downarrow} (\eta^\dagger)^n|\psi\rangle}{\langle\psi|\eta^n(\eta^\dagger)^n|\psi\rangle} \ . \tag{8}$$

We consider the thermodynamic limit $L \longrightarrow \infty$, $N \longrightarrow \infty$, $n \longrightarrow \infty$, where the ratios $\frac{n}{L}$ (superconducting density) and $\frac{N_c}{L}$ (normal state density) are kept fixed. If the matrix element (8) approaches a nonzero value A asymptotically at large distances ($1 \ll |k-l| \ll L$), then the state $|\psi_n\rangle$ exhibits ODLRO and is superconducting. The value A can be found by averaging over k and l and then using the SU(2) structure of the generators (3)

$$A = \lim_{L\to\infty} \frac{1}{L^2} \sum_{k,l} (\rho_2)_{kl} = \frac{n}{L}\left(1 - \frac{N_c}{L} - \frac{n}{L}\right) \ . \tag{9}$$

The result establishes the property of ODLRO for the states $|\psi_n\rangle$.

We now consider the phase diagram of the hamiltonian H at zero temperature. Equation (1) defines the model in the framework of the grand canonical ensemble. We now change our point of view to the canonical ensemble, dropping the chemical potential μ from (1), fixing the magnetisation to zero and the density $D = \frac{N}{L}$ ($N = N_c + 2n$ is the complete number of electrons) to a value in the interval $0 \leq D \leq 2$. On the basis of the analysis below, we propose the phase diagram shown in figure 1.

Fig.1 : Ground states in the canonical ensemble

We claim that the ground state in the areas I and II is of the form $|\psi_n\rangle$ as in (7), implying that in these regions the model is superconducting. For the region I, corresponding to negative U, this is rigourously established by the following theorem.

Theorem. The ground state of the hamiltonian (1), with $\mu = 0$ and with $U < 0$, in the sector with an even number N of electrons and zero magnetisation is unique and is given by $|\Psi_{\frac{N}{2}}\rangle = (\eta^\dagger)^{\frac{N}{2}}|\,0\,\rangle$. The ground state energy is $E_g = U\frac{L}{4} - M$, where M is the number of nearest neighbour links on the lattice.

Proof. In the sector with N electrons the hamiltonian reads

$$H_{(N)} = H^0 + U\sum_{j=1}^{L}(n_{j,\uparrow}n_{j,\downarrow}) + (\frac{L}{4} - \frac{N}{2})U. \tag{10}$$

We first consider the term H^0. The fact that H^0 is equal to minus the sum of graded permutations shows that the energy E^0 is bounded from below by $-M$. One state which saturates this value is the empty state $|\,0\,\rangle$. Using the $U(2|2)$ symmetry of H^0 we can construct the N-particle state $|\Psi_{\frac{N}{2}}\rangle = (\eta^\dagger)^{\frac{N}{2}}|\,0\,\rangle$, which by construction has the same energy E^0. If we now take into account the remaining terms in $H_{(N)}$, we find that they are bounded from below by the value $U\frac{L}{4}$ $(U < 0)$, where the minimum is reached for states that have $\frac{N}{2}$ local electron pairs. This is precisely the case for the state $|\Psi_{\frac{N}{2}}\rangle$. This shows that $|\Psi_{\frac{N}{2}}\rangle$ is a ground state of H. To show that it is the *unique* ground state, we should check that there are no other states with $\frac{N}{2}$ local electron pairs (and no single electrons) that saturate the lower bound $-M$ of H^0. This can be proved by an elementary application of the Perron-Frobenius theorem as follows. We consider the action of $1 - H^{(0)} = 1 + \sum_{\langle jk\rangle}\Pi^g_{j,k}$, on the space of all states with $\frac{N}{2}$ local pairs and no single electrons, which can be represented as a square matrix of size $\left(\begin{array}{c} L \\ \frac{N}{2} \end{array}\right)$. It is clear that this matrix is symmetric, that its entries are non-negative and that there exists a positive power of the matrix which is such that all entries are positive. For this situation the Perron-Frobenius theorem guarantees that there is a unique state with a maximal eigenvalue for $1 - H^0$. This state, which we already identified as $|\Psi_{\frac{N}{2}}\rangle$, is the unique ground state of H^0 in the sector with $\frac{N}{2}$ local pairs and thus the unique ground state of H in the sector with a total number of N electrons. ∎

To establish the phase diagram in figure 1 for positive coupling U it is more convenient to work in the grand canonical ensemble first, and then translate the results to the D-U plane in the canonical ensemble. The phase diagram at zero temperature in the grand canonical ensemble is given in figure 2. In order to derive this diagram we rewrite the hamiltonian (1) as a function of μ and U as

$$H(\mu, U) = H^0 - (\mu + \frac{1}{2}U)\,(N_\uparrow + N_\downarrow) - 2\mu\, N_l + U\frac{L}{4}\ . \tag{11}$$

We first note that (up to a constant) under the particle-hole transformation $c^\dagger_{j,\sigma} \leftrightarrow c_{j,\sigma}$ the hamiltonian transforms according to $H(\mu, U) \longrightarrow H(-\mu, U) - 2\mu\ L$. Therefore it is sufficient to determine the ground states for $\mu \leq 0$; the ones for $\mu > 0$ can then be obtained by a particle-hole transformation. We also note that all eigenstates of the (supersymmetric) t-J model are eigenstates of the hamiltonian (1) as well. Using this fact we will be able to express the ground state wave function $|\Psi_g\rangle$ of the hamiltonian (11) in terms of the ground state wave function $|t-J\rangle$ of the t-J submodel (in the grand canonical ensemble) and the $U(2|2)$ generators. In one dimension the t-J ground state wave function is known exactly [7] and our results become explicit.

Fig.2 : Ground states in the grand canonical ensemble

It was proved by B. Sutherland in [4] that the ground state energy of H^0, which is minus the sum over graded permutations on four states (two bosons and two fermions), will be equal to that of the t-J submodel, which is minus the sum over graded permutations on three states. Here the numbers of the two species of fermions and the total number of bosons is fixed but arbitrary. This theorem can be used as follows : If no local electron pairs are present in the ground states, the hamiltonian reduces to the t-J hamiltonian with effective chemical potential $\mu_{tJ} = \mu + \frac{1}{2}U$. Whether it is energetically favourable to have local electron pairs in the ground state is then determined exclusively by the term $-2\mu\ N_l$ in the hamiltonian.

We recall the following results for the ground-state of the t-J model at zero temperature as a function of μ_{tJ} (see, for example [7]). For $\mu_{tJ} < 0$ the ground state is the empty state. Once μ_{tJ} becomes positive the ground state starts filling up, with the density monotonically increasing as a function of μ_{tJ} until it reaches half-filling for a finite value $\mu_{tJ} = \mu_c$. In one dimension the Bethe Ansatz solution gives $\mu_c = 2\log 2$. The equations $\mu + \frac{1}{2}U = 0$ and $\mu + \frac{1}{2}U = \mu_c$ define two critical lines in the μ-U plane for our model (see figure 2).

Let us now consider the regions II, III, IV and V in figure 2. The ground states in the regions III' and V' will follow from the ones in III and V by particle-hole correspondence. Note that below we use the term "t-J submodel" in the context of the grand canonical ensemble (*i.e.* including the $\mu_{tJ}(N_\uparrow + N_\downarrow)$ -term).

In region V the ground state of the t-J submodel is empty. Furthermore, since $\mu < 0$ Sutherland's result tells us that it is not favourable for local electron pairs to enter the ground state. We conclude that the ground state in region V is the empty state, *i.e.* $|\Psi_g\rangle = |\,0\,\rangle$.

If we now cross the line $\mu + \frac{1}{2}U = 0$ to enter the region III ($-2\mu \leq U \leq 2(\mu_c - \mu)$, $\mu < 0$), there are single electrons present in the ground state of the t-J model. Since μ is still negative, it is not energetically favourable to have local electron pairs in the ground state. We conclude that in region III the ground state is that of the t-J model (which is presumably metallic) without any local electron pairs, *i.e.* $|\Psi_g\rangle = |t - J\rangle$.

At the line $\mu + \frac{1}{2}U = \frac{1}{2}U_c$ the t-J ground state reaches half filling and in the entire region IV the t-J half-filled ground state is the ground state of our model.

Let us finally look at region II, where $0 \leq U \leq U_c = 2\mu_c$ and $\mu = 0$ ($U_c = 4\log 2$ in one dimension). Let us first consider the ground state $|t - J\rangle$ of the t-J submodel, which is also an eigenstate of the hamiltonian (1) of energy E. It has a certain filling, which varies from zero for $U = 0$ to one for $U = U_c$. As $\mu = 0$ it follows from Sutherland's theorem that the ground state energy of the hamiltonian (11) is equal to E, and thus that $|t - J\rangle$ is a state of lowest energy of $H(0, U)$.

Using the fact that $[\eta^\dagger, H_0] = 0$, we can construct additional states with energy E of the form $(\eta^\dagger)^n|t - J\rangle$. In figure 2 the segment under consideration is thus singular, representing a large number of possible ground states. However, if we pass to the D-U plane in figure 1 this singularity is resolved because the number n of local electron pairs adjusts itself to the density that is imposed. Thus a non-zero number of local electron pairs will enter the ground state in the region II in figure 1. The resulting ground state wave function is of the form $|\Psi_g\rangle = (\eta^\dagger)^n|t-J\rangle$ and we already showed that it is superconducting (note that $\eta|t-J\rangle = 0$). The ground state consists of a condensate of zero-momentum local pairs, and single non-paired electrons in a Fermi sphere. Due to the (superconducting) condensation, the volume of the Fermi sphere of the unpaired electrons is smaller than the volume of the Fermi sphere for a free electron gas (Luttinger's theorem is not applicable [12]).

In sector III in figure 1 the ground state is that of the t-J submodel (no local electron pairs). In sector III' the ground state is that of the particle-hole transformed t-J model. It can be shown to be of the form $(\eta^\dagger)^{L-N}|t-J\rangle$, where $|t-J\rangle$ is the ground state of the t-J submodel for the opposite value μ (in sector III). Sectors III and III' are separated by an energy gap of H that exists at half filling, $D=1$, for $U > U_c$. This situation is similar to the the one in the repulsive 1-d Hubbard model, where a gap arises at half filling [8]. In regions I and II (dotted line in fig 2) the compressibility is infinite, which is intimately connected to the presence of the superconducting condensate. The situation is quite similar to Bose condensation in a free Bose gas, and can be 'regularised' by a perturbation of the hamiltonian.

For the attractive case we also determined the wavefunction of the supercurrent in a circular wire, threaded by a magnetic field [9] (see also [10]). We found it to be a bound state of all local electron pairs . Its wave function is equal to the one of a string solution in the one dimensional spin-$\frac{1}{2}$ Heisenberg XXX ferromagnet.

In conclusion, we have shown that the model that we introduced in [2] provides a particularly simple example of a superconducting system. The mechanism of superconductivity is similar to the one of the strongly attractive Hubbard model. At zero temperature, the superconductivity already exists in one dimension and we have seen that it persists if the on-site interaction becomes weakly repulsive. We expect that in three dimensions the superconductivity will persist at finite temperature. In a future publication we will further clarify the physics of the model in one dimension by using the Bethe Ansatz solution [9].

Due to the experimentally established fact that Cooper pairs in high-T_c superconductors are rather small, our model (with "zero-size" pairs) might have applications in this field. In order to make contact with experiment it is necessary to perturb the model (change the coefficients of the various interactions in our hamiltonian). If this is done the most important newly occuring phenomenon is the decay of local electron pairs into two single electrons. The physics of this process has been studied by T.D.Lee and R.Friedberg in their field theoretical model of superconductivity

[11]. In their model electron pairs are described by a scalar Bose field interacting with fermionic fields (representing the single electrons) *via* the above mentioned decay process. Their results (obtained in perturbation theory) show the existence of superconductivity and thus indicate that the decay of local electron pairs would not destroy the superconducting properties of our model.

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