Two \textit{s-wave} solutions for superconductivity in the extended Hubbard model

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The existence of more than one solution for \textit{s-wave} pairing in the extended Hubbard model is not often realized. This possibility was noted by Friedberg et al. [Phys. Rev. B50, 10190 (1994)] in the case of two electrons on a lattice, without further analysis. In the present paper, the second solution is found also in the case of superconductivity of extended \textit{s-wave} symmetry in the extended Hubbard model. The properties of both \textit{s-wave} solutions are examined by mean-field methods and thresholds for their appearance are given. A possibility of the first-order transition is discovered and modifications of the phase diagram are calculated. Results of this paper in the limit of low electron density are also applicable to the bound, two-electron pairs.

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I. INTRODUCTION

The discovery of high-temperature superconductivity (HTS) has triggered an intensive effort to reveal its mechanisms. This aim has not been attained yet but the amount of knowledge concerning HTS is substantial. From this wealth of data certain key issues emerge, which must be addressed by the eventual microscopic theory. One of them is question of the symmetry of the order parameter. Instead of originally accepted \textit{s-wave}, nowadays it is believed that the hole-doped HTS materials are predominantly of the \textit{d_{xy}}-\textit{s-wave} symmetry. Nevertheless the research concerning the \textit{d_{xy}}-\textit{s-wave} symmetry is not to be abandoned. The \textit{s-wave} symmetry is found in fullerides\cite{6,7,8} perovskites\cite{9} and MgB$_2$\cite{10} not from the HTS group but very interesting materials though. The \textit{d-wave} symmetry in electron-doped materials\cite{11,12,13} and possibility of the \textit{s} to \textit{d} change of the symmetry of the order parameter with increasing doping in the hole-doped materials\cite{11,12,13,14}. Another scenario with \textit{s-wave} symmetry includes the possibility of different order parameters in the bulk and on the surface of HTS superconductor\cite{15}. As there are reports of different mechanisms responsible for pairing and phase coherence there is possibility of pseudogap having \textit{s} symmetry, different from the \textit{d} symmetry of the order parameter\cite{16,17}. Of other possibilities we can not exclude possibility of finding an \textit{s-wave} symmetry pairing in heavy fermions, which are notorious for multiplicity of phases.

There are few rigorous results concerning \textit{s-wave} superconductivity or BCS in general. We know that in the dilute limit BCS mean-field equations go over to the Schrödinger equation for the bound two-electron pair\cite{18,19} i.e. in this limit the BCS equations become exact. Another result was given by Randeria \textit{et al.}\cite{20} stating that creating two-electron bound state of \textit{s-wave} symmetry is a necessary and sufficient condition for BCS-type superconductivity to exist in two dimensions in a dilute limit. The results of applying mean-field approximations to the Hubbard-type Hamiltonians as well as the properties of the bound pairs are well known (e.g. Refs\cite{13,16,21,22,23,24,25}). One of the seldom noticed aspects of mean-field treatment of the extended \textit{s-wave} pairing and bound pairs of this symmetry is subject of this paper.

II. FORMALISM

Let’s consider extended Hubbard model in the standard notation:
\begin{equation}
H = \sum_{ij\sigma}(t_{ij} - \mu\delta_{ij})c_{i\sigma}^\dagger c_{j\sigma} + U\sum_i n_{i\uparrow}n_{i\downarrow} + W\sum_{ij\sigma\sigma'} n_{i\sigma}n_{j\sigma'}
\end{equation}
where we sum over nearest neighbors (n.n.), and $U$ and $W$ are on- and intersite interactions respectively, $t_{ij}$ is nearest-neighbor hopping integral and $\mu$ - chemical potential. In the mean-field approach the above Hamiltonian takes the form:
\begin{equation}
H = \sum_{k\sigma}(\varepsilon_k - \mu N) n_{k\sigma} - \sum_k (\Delta_k c_{k\uparrow}^\dagger c_{-k\downarrow} + H.c.) + \text{const.}
\end{equation}
where, using order parameter $< c_{-q\downarrow}c_{q\uparrow} >$, we introduce a gap $\Delta_k$:
\begin{equation}
\Delta_k = \frac{1}{N} \sum_q V_{kq} < c_{-q\downarrow}c_{q\uparrow} >
\end{equation}
\begin{equation}
V_{kq} = -U - W\gamma_{k-q}
\end{equation}
\begin{equation}
\gamma_k = \frac{z}{\delta} \exp(i\mathbf{k} \cdot \mathbf{\delta})
\end{equation}
\begin{equation}
\varepsilon_k = -t\gamma_k
\end{equation}
\begin{equation}
\mathbf{\Pi} = \mu - (U/2 + W\varepsilon)n
\end{equation}
z is coordination number; for the full discussion of the model the reader is referred to the Ref\cite{26} It is easy to derive the self-consistent equation for the energy gap:
\begin{equation}
\Delta_k = \frac{1}{N} \sum_q V_{kq} \frac{\Delta_q}{2E_q} \tanh \beta E_q / 2
\end{equation}
where the quasiparticle energy:
\[ E_q = \sqrt{(\varepsilon_q - \bar{\mu})^2 + |\Delta_q|^2} \]  
(9)
and \( \beta = 1/(k_B T) \) where \( T \) is temperature and \( k_B \) Boltzmann constant. To solve the model we usually make the ansatz:
\[ \Delta_k = \Delta_0 + \Delta_\gamma k^2 + \Delta_\eta \eta_k \]  
(10)
where \( \eta_k = 2(\cos k_x - \cos k_y) \) and particular terms refer to on-site s-, extended s- and d-wave pairings. Self-consistent equations for the gap separate into the s-wave and d-wave part.

Finally what is left for solving for general, non-zero \( U \) and \( W \) in the ground state is a set of three self-consistent equations for \( \Delta_0, \Delta_\gamma \) and chemical potential \( \bar{\mu} \).
\[
\Delta_0 = -U \frac{1}{N} \sum_q (\Delta_0 + \gamma_q \Delta_\gamma) \frac{1}{2E_q}  
\]  
(11)
\[
\Delta_\gamma = -W \frac{1}{z} \frac{1}{N} \sum_q \gamma_q (\Delta_0 + \gamma_q \Delta_\gamma) \frac{1}{2E_q}  
\]  
(12)
\[ n - 1 = -\frac{1}{N} \sum_q (\varepsilon_q - \bar{\mu}) \frac{1}{E_q}  
\]  
(13)
in the case of the extended s-wave pairing, and
\[
1 = -\frac{W}{z} \frac{1}{N} \sum_q \eta_q^2 \frac{1}{2E_q}  
\]  
(14)
in the case of the d-wave pairing. In the following we will focus on the s-wave pairing only. The results described in the remainder of the paper are calculated for the rectangular density of states (DOS) with \( z = 4 \), so they approximate two dimensional square lattice. For the reasons that will be explained later on the author supposes that they are of more general nature.

III. RESULTS

Equations (11)-(13) in the dilute limit yield Schrödinger equation for a bound pair, as was told in the Introduction. As is well known, in two dimensions infinitesimally small on-site attraction creates bound pair for \( W = 0 \). For \( W > 0 \) a threshold must be crossed to obtain a bound state. Analytic formula for the threshold and \( U-W \) phase diagram are given for example in Refs. 13,27. The less known facts are as follows:
(i) The threshold formula for the gap, analogical to the one given in Refs. 13,27 can be derived from BCS-MFA equations 13,19 without resorting to the limit \( n \to 0 \). Using rectangular density of states it reads:
\[
\frac{W_{\text{crit}}}{4t} = \frac{-1}{1 + \eta^2} \frac{1}{(1 + 16t/U)}  
\]  
(15)
Let’s note that the limit \( n \to 0 \) yields correct result of Refs. 13,27. The use of the exact density of states does not bring changes to the value of \( W_{\text{crit}} \) for \( n \to 0 \) but the changes appear and increase with growing \( n \), as shown in Fig. 1.
(ii) The formula (15) is valid on the entire \( U-W \) plane, both for positive and negative values of \( U \) and \( W \). The cited papers show the figure of the fourth quarter of the coordination system only. The full plot is given in Fig. 1.
As we can see in the third quarter of the coordination system, for \( U \) and \( W \) attractive enough, a second threshold line is obtained! (In the case of two-electron bound pair second solution was also noted in Ref. 27 but without further analysis).
This way the area in Fig. 1 can be divided into three main parts: Area "0" - to the right of the rightmost threshold line, mostly first quarter \( (U > 0, W > 0) \) and small parts of the second and fourth quarter of the coordination system (not exceeding asymptotic values: \( U_{\text{as}}/t = -16(n-1)^2/(1+(n-1)^2) \) and \( W_{\text{as}}/t = -4/(1+(n-1)^2) \)). There are no bound states and no gap for these parameters, the solutions describe antibonding states. Area "1" – between both threshold lines, mostly second and fourth quarter – in this area there is only one solution of

![Fig. 1: Critical values for existence of extended s-wave superconductivity calculated for the rectangular DOS, for electron densities \( n = 0 \) (also \( n = 2 \), full line) and \( n = 0.2 \) (also \( n = 1.8 \), dashed line). Dot-dashed and full line with circles are thresholds for \( n = 0.2 \), calculated for the exact DOS in two dimensions (2d) and in three dimensions (3d, simple cubic lattice) respectively. Exact 2d threshold for \( n = 0 \) is the same as for rectangular DOS. Exact 3d threshold for \( n = 0 \) is given by solid line with squares. Dotted lines are the axes of coordination system. Dot-dashed lines with triangles are crossover boundaries for \( n = 0.2 \) and exact 2d DOS. Crossover boundaries for \( n = 0 \) coincide with the threshold lines in 2d. Full, flat, horizontal line is a threshold for the d-wave pairing, calculated for \( n = 0 \). Numbers "0", "1" and "2" are the names of the areas described in the text. \( U \) and \( W \) are in the half-bandwidth units \( D = 4t \) in 2d and \( D = 6t \) in 3d.](image-url)
the equations (11)-(13), which exists even for infinite on- or intersite repulsion. The further from the rightmost threshold line we are the stronger is the binding between electrons in the pairs. Points of the same binding energy form a line approximately parallel to the rightmost threshold line. Area ”2” – below the second threshold line, in the third quarter – for parameters from this area two solutions of equations (11)-(13) exist: one of the type of the ”area 1”, with large binding energy, given by a ”distance” from the first threshold line; the other, with smaller binding energy and smaller gap, given by the ”distance” from the second threshold line. We will call these solutions type 1 and type 2, respectively. Let’s note, that the range of $|U|$ is limited by a ”distance” from the first threshold line; the other, ”area 1”, with large binding energy, given by the same ”distance” from the second threshold line. The properties of both types of pairing are described in the following.

For fixed $W$, for $U \to -\infty$, type 1 solution displays what we will call here ”pure-s” type behavior: $|\Delta_0| \sim U$, $\Delta_\gamma \to 0$, $\bar{\pi} \sim U/2$ (if $W > 0$ then $\Delta_\gamma < 0$, if $W < 0$ then $\Delta_\gamma > 0$). When we move on the $U$ axis from left to right, towards smaller values of $|U|$ then, for certain intermediate value of $|U|$ (not too large if $W$ is not large and attractive) this ”pure-s” behavior disappears. If $W > W_{as}$ then with increasing $U$ we must reach threshold value $U_{crit}$ and for $U \to U_{crit} \Delta_0$ decreases non-linearly to 0, $|\Delta_\gamma|$ goes through extremum and also decreases to 0 while $\bar{\pi}$ goes to constant, non-zero value. If $W < W_{as}$ and solution of type 1 exists in the whole range of $U$ from $-\infty$ to $+\infty$, then for $U \to +\infty$ all three quantities $\Delta_0$, $\Delta_\gamma$ and $\bar{\pi}$ go to the constant values: $\Delta_0$ to a small negative one and $\Delta_\gamma$ to a larger, positive one (see Fig. 2). When $W < 0$ and $|W|$ is large enough, then ”pure-s” behavior disappears for $U \approx W$ instead of small to intermediate values of $|U|$, as shown in Fig. 2.

The behavior of type 2 solution is somewhat complementary: for $U \to -\infty$, when type 1 solution shows ”pure-s” behavior, type 2 solution is constant. Moving right on the $U$ axis type 2 solution goes through a transition for the same range of $U$ as type 1 solution, and from now on it behaves in ”pure-s” way until $U$ reaches the threshold for type 2 solutions, where $\Delta_0$ and $\Delta_\gamma$ disappear and $\bar{\pi} = \text{const}$. Let’s note, that the slope of linear dependence of $\Delta_0$ vs $U$ differs just by the sign from the analogical slope of type 1 solution and that $\Delta_\gamma$ is of opposite sign to $\Delta_0$ in type 2 solution.

The constant values reached by the type 1 solution for $U \to +\infty$ are the same as the ones reached by the type 2 solution for $U \to -\infty$. These constants for small $n$ and $|W|$ large enough can be calculated as:

$$\bar{\pi} = W/2$$
$$\Delta_\gamma/\Delta_0 = -|\bar{\pi}|$$
$$\Delta_0 \approx -0.6/\sqrt{n}$$

As shown in Fig. 2 for fixed $U$, when $W$ is varied, instead of ”pure-s” behavior type 1 solution displays ”pure extended s” behavior for $U \to -\infty$: $\Delta_\gamma \sim |W|$, $\Delta_0 \to 0$, $\bar{\pi} \sim W/2$. Apart from that, the behavior of solutions vs $W$ is analogous to the behavior of the solutions vs $U$: for $W \to +\infty$ type 1 solution goes to the constant values (now $\Delta_\gamma$ to the small negative one while $\Delta_0$ to the bigger, positive one) and for $W \to -\infty$ type 2 solution goes to the same constants. For small $n$ and $|U|$ large enough these constants are:

$$\bar{\pi} = U/2$$
$$\Delta_0/\Delta_\gamma = -4|\bar{\pi}|$$
$$\Delta_\gamma \approx -\sqrt{n}/8$$

Large values of fixed parameters in Figs 2 and 3 were chosen to emphasize the characteristic behavior of the examined quantities. The plot of chemical potential $\bar{\pi}$ vs $U$ for $W/4t = -30$ is practically indistinguishable from the plot of $\bar{\pi}$ vs $W$ for $U/4t = -30$ in the scale of the picture (apart from the different critical values for which $\bar{\pi}$ in the type 2 solutions appears) so it was not shown again in Fig. 2.

A point to notice is that the gap parameter $\Delta_0$ remains finite even in the limit $U \to \infty$, despite the fact that on-site pairing amplitude $<c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger>$ must vanish in this limit.$^{28,29}$

Let’s note that the considerations above answer the unspoken question, why the equations for extended $s$-wave pairing yield formally (and numerically) the same solution in the two very different limits: infinite attraction and infinite on- or intersite repulsion. Despite they are
FIG. 3: Type 1 (full line, full line with circles) and type 2 (dashed line, dashed line with circles) solutions of the extended Hubbard model vs $W/4t$ for $U/4t = -30$ and $n = 0.01$. Dotted lines show axes of the coordination system. The dependence of $\Pi$ on $W$ is indistinguishable in the scale of the picture from the dependence of $\Pi$ on $U$ in Fig. 2 (apart from different thresholds for type 2 solutions), so it was not shown. In the inset the enlargement of the area near the origin of the coordination system is shown.

numerically the same, nevertheless they are two different solutions of two different types of pairing!

In the limit of large $|U|$ or large $|W|$ the solutions for $\Delta_0$ and $\Delta_\gamma$ are symmetric or antisymmetric regarding to the change $n \to 2 - n$. For large, negative $U$ (or $W$) and fixed $W$ (or $U$) $\Delta_0$ ($\Delta_\gamma$) of "pure-s" (of "pure extended s") type 1 solution is symmetric, reaching maximum for the half-filled band, while $\Delta_\gamma$ ($\Delta_0$) is antisymmetric: positive (or negative) for less than half-filled band and of opposite sign for more than half-filled band, crossing through 0 for $n = 1$. In the opposite limit $U$ (or $W$) going to $+\infty$ the behavior of $\Delta_0$ and $\Delta_\gamma$ in "type 1" solutions change to the reverse: $\Delta_0$ ($\Delta_\gamma$) becomes antisymmetric and $\Delta_\gamma$ ($\Delta_0$) symmetric. The behavior vs $n$ of type 2 solutions for $U$ or $W \to -\infty$ is the same as behavior of respective "pure-s" or "pure extended s" type 1 solutions in the limit $U$ or $W \to +\infty$. This is the correct behavior if the limiting, constant values reached by the type 1 solutions are to be identical to the type 2 limiting, constant solutions for every $n$. For smaller values of the parameters $|U|$, $|W|$ there is an area in parameter space of "type 2" solution, where both $\Delta_0$ and $\Delta_\gamma$ are symmetric in the band, though of opposite sign.

A peculiarity of solutions is the existence of critical charge density $n_c$. For a given value of the fixed parameter ($U$ or $W$) there exists $n_c$ such that for $n$ in the range $(n_c, 2 - n_c)$ the transition between the "pure (extended) s" part of one solution and the "constant" part of the same solution is no longer smooth, but both parts join in an non-continuous way: we have a first-order transition, where $\Delta$'s and derivative of $\Pi$ jump. Some approximate values of $n_c(U/4t, W/4t)$ for type 1 solution, given as a function of parameters for which the jump takes place, are: $n_e(-29.1, -30) \approx 0.0475$, $n_e(-9.1, -10) \approx 0.15$, $n_e(-2.75, -3.75) \approx 0.5$, $n_e(-1.1, -2) \approx 0.8$. We can see here that for $|W|$ large enough and attractive the jump takes place for $U \approx W$, as was stated before. The values of $|U|$ and $|W|$ required to obtain any given $n_c$ are much larger in type 2 solution than in type 1 solution.

To complete the examination of the $n$-dependence let’s notice that at half-filled band solutions fully separate and we obtain true pure-s solution, with $\Delta_\gamma = 0$ and no threshold for pairing and true extended s solution with $\Delta_0 = 0$ and threshold $W = -4t$ ($W \approx -3.24t$ for exact 2d density of states).26

Another point to notice is that we can add the third and fourth solution to the two found, by changing $\Delta_0$ and $\Delta_\gamma$ to $-\Delta_0$ and $-\Delta_\gamma$. The number of nontrivially-different solutions seems to depend on the number of coupled terms from the ansatz Eq. (1) and does not depend on the lattice dimensionality. In Fig. 1 there is a plot of threshold curves for simple cubic, three dimensional (3d) lattice. Their behavior is analogous to the 2d case. In particular the threshold line for the type-1 pairing goes through the point ($U, W$) = (0, 0), even for small electron densities (except from $n = 0$). This does not contradict the fact that for $U = 0$ we have critical value for $|W|$ to bound electron pair in 3d. The existence of bound pairs is prerequisite for superconductivity in a dilute limit only in 2d.25 A curve for two-electron bound pair in 3d can be obtained from Eqs. (11)–(13), by solving them for $n = 0$. This curve is also given in Fig. 1, plotted in a certain distance from other 3d curves for $n > 0$, in agreement with Refs. 13, 27.

There appears a question: which of the two solutions will be physically realized? The type 1 pairing has larger binding energy, higher critical temperature and lower free energy so this is the solution to be found even in the area of parameter space where both solutions exist. In this area care should be taken not to mix the two solutions especially for $U \approx W$, where the absolute values of solutions of type 1 become close to the respective values of solutions of type 2 and also in the limit of large negative $U$ or $W$, where equations can easily yield type 2 solution numerically.

We must also remember that only the relative stability of two extended s-wave solutions was examined in the above considerations. The question of stability of another symmetry pairings, e.g. $d$- or $p$-wave, was not addressed at all. While $p$-wave pairing can be diminished by adding antiferromagnetic coupling to the Hamiltonian, $d$-wave can not. From Fig. 1 we can see that for large enough $|W|$, $d$-wave pairing can surely have bigger binding energy than second extended s-wave solution. As we know it can win the competition even with the first extended s-wave solution (with the lower free energy – see e.g. 13). In establishing the detailed phase diagram we must thus take into account the competition of pairings with other
symmetries, including $s + d$ or $s + id$.

Another question is how physical is the first order transition found, isn’t it just an artefact of the MFA, especially that it appears for larger $n$? This question could be probably answered by numerical simulations. If this effect is physical it should have influence on all superconducting properties of the superconductor with extended $s$-wave superconductivity. In particular one can ask whether the found first order transition could be an argument in favor of non-smooth crossover between BCS and local pairs limits in the models of extended $s$-wave superconductivity. It seems unlikely as we notice that $|U|$ and $|W|$ being the arguments of $n_c$ cited before in the text, decrease for growing $n_c$ while the BCS-Bose boundary (calculated form the Leggett’s criterion i.e., that chemical potential crosses the bottom of the band) moves toward larger values of $|U|$ and $|W|$ with increasing electron density, so that the two boundaries do not coincide. Crossover boundaries for $n = 0$ and $n = 0.2$ are plotted in Fig. 4. There are two branches of crossover boundary corresponding to the two threshold lines. For $n = 0$ they coincide with the threshold lines, with increasing $n$ they move left, towards larger and larger values of $|U|$ and $|W|$. Again, if other than $s$-wave symmetry pairing is realized, this problem is irrelevant.

The third issue concerns the possible phase separation for large, values of $|U|$ or $|W|$. This question was addressed by Hartree type analysis e.g. in the paper of Robaszkiewicz and Pawlowski, from where the phase boundaries shown in Fig. 4 come (solid lines). Under the lowest, horizontal line, for large n.n. attraction, we have a phase separation of normal state and electron droplets. In the area between the solid lines there is $s$-wave superconductivity (on-site only, denoted as SS) and above the upper solid line there is inhomogeneous phase separation of charge density waves (CDW) and superconductivity (CDW/SS). For the half filled band the ground state is CDW for $W > 0$ while CDW and superconductivity are degenerated for $W = 0$.

Our second superconducting $s$-wave solution does not enter this picture but for intermediate values of on-site attraction, Eq. (15) helps us to make an upper boundary for superconducting state, denoted by dashed lines in Fig. 4. Above this line no superconductivity exists. This way for small electron densities, for $W$ large enough (above the critical value) a normal state is obtained (denoted as NO in the figure). With increasing $n$ we can have a transition to SS and then to CDW/SS state. For certain larger $W$ we can have NO-CDW/SS transition and for still larger $W$ we obtain NO-CDW-CDW/SS transition. This way a phase diagram of Ref. 23 is substantially modified. Considering full extended $s$-wave superconducting solution, with order parameter depending on both on- and intersite interaction, changes phase boundaries in Fig. 4 only in negligible way.

Let’s note, that the described modification of the phase diagram takes place only for intermediate values of $|U|$. For larger values of $|U|$ or more precisely for $U < U_{as}$,

where $U_{as}$ was defined in connection with Fig. 1, $s$-wave superconductivity exists independently of $W$, and there is no normal phase area in the phase diagram.

In conclusion a mean-field criterion for existence of $s$-wave superconducting solution in the extended Hubbard model was calculated. The modified $W - n$ phase diagram was shown. A second $s$-wave solution was found and a threshold for its existence together with a full phase diagram in the $UW$ plane were calculated. The second solution helped to answer the question why limits $U$ (or $W$) = $\pm \infty$ are formally the same. (These results apply also to the two-electron bound states of the same symmetry). First-order transition in the extended $s$-wave solution was found and its possible implications on the crossover problem were discussed. The results may apply to all properties of the superconducting state of extended $s$-wave symmetry.

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