Bound pair states beyond the condensate for Fermi systems below T_c: The pseudogap as a necessary condition

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As is known, the $1/q^2$ theorem of Bogoliubov asserts that the mean density of the fermion pair states with the total momentum $\mathbf{q}$ obeys the inequality $n_q \geq C/q^2 (q \to 0)$ in the case of the Fermi system taken at nonzero temperature and in the superconducting state provided the interaction term of its Hamiltonian is locally gauge invariant. With the principle of correlation weakening it is proved in this paper that the reason for the mentioned singular behavior of n_q is the presence of the bound states of particle pairs with nonzero total momenta. Thus, below the temperature of the superconducting phase transition there always exist the bound states of the fermion couples beyond the pair condensate. If the pseudogap observed in the normal phase of the high-T_c superconductors is stipulated by the presence of the electron bound pairs, then the derived result suggests, in a model-independent manner, that the pseudogap survives below T_c. [S0163-1829(99)14325-X]

I. INTRODUCTION

At present the pseudogap is well established to be in the spectrum of the elementary excitations of undoped and optimally doped high-T_c superconductors (for example, see the review, Ref. 1). The presence of the pseudogap implies that the electron subsystem in the normal phase is not the Fermi liquid and, so, theoretical explanation of the pseudogap is recognized as the key point of understanding the phenomenon of the high-T_c superconductivity.[2,3] There are a great number of various theoretical approaches of investigating this problem. Two of them considered below are especially interesting in the context of this paper.

The pseudogap can be associated with the presence of the local pairing correlations without phase coherence. The idea of this approach assuming the singlet pairing of fermions without the phase coherence, as applied to the high-T_c superconductivity, has been proposed in Ref. 4. The more radical model of Alexandrov and Mott[5] operates with, say, preformed bosons (bipolarons) existing in the system above T_c, the pseudogap being treated as coming from the binding energy of a bipolaron (of the order of a few hundred K). This model dates back to the Schafroth's ideas according to which the superconductivity is a result of the Bose-Einstein condensation of the bound pairs of electrons localized in the space and appearing in the system before the condensation.[6]

The concept of a bound state of two particles in a medium can consistently be formulated with the reduced density matrix of the second order (2 matrix).[7] Indeed, the system of two particles is a subsystem of that of N particles. So, its state is not pure even in the situation when the system as a whole has a wave function. In general a subsystem is specified by the density matrix (see, e.g., Ref. 8). In particular, the reduced density matrix of the second order is of use when a noncoherent superposition of the pure states of two particles is relevant rather than any wave function. If among these states there exist bound ones, then a part of particles of the system involved form bound pair states.[9] In the superconducting phase a macroscopical number of particle pairs N_0 occupy the same bound state, i.e., there is the condensate of pairs at which the ratio $N_0/V = n_0$ is constant in the thermodynamic limit $V \to \infty$. In the space-uniform case the condensate is formed by the pairs with the zero total momentum $\mathbf{q} = 0$, the binding energy ε_b of these pairs being just the double value of the superconducting gap.[10] The bound particle pairs beyond the condensate are characterized by the continuous distribution over the total momentum of a couple.[11] The couple (like these) must also have the finite binding energy $\varepsilon_b(\mathbf{q})$ that, due to the continuity argument, should tend to ε_b when $q \to 0$. If these bound particle pairs are ''hard'' clusters, like in the theory of Alexandrov and Mott, then one may consider that the quantity $\varepsilon_b(\mathbf{q})$ is practically independent of $\mathbf{q}$. The binding energy $\varepsilon_b(\mathbf{q})$ is just the double value of the pseudogap, which manifests itself in the normal phase when the bound couples survive at $T > T_c$.

In BCS theory there are no bound pair states beyond the condensate absolutely[7,12] (see below), which is a consequence of the violation of the local gauge invariance (see, for example, Ref. 13).

In this paper we shall prove in a model-independent manner that the existence of the condensate of the bound pair states (BCS pairs) implies the presence of bound couples beyond the condensate (Schafroth's pairs). We emphasize that we do not specify the size of the pairs. If it is much more than the mean distance between particles (the condensate pairs in the BCS model), then, following Bogoliubov,[7] one may call these pairs ''quasimolecules.'' If the radius of the bound particle couples is of the order of the mean distance between particles or, even, less (the Schafroth-Alexandrov-Mott approach), then one may speak about ordinary molecules. The proof is based on the well-known $1/q^2$ theorem of Bogoliubov for the Fermi system[7] which is valid in the

space-uniform case and under the condition of the local gauge invariance of the interaction term of the system Hamiltonian.

The present article is organized as follows. In Sec. II the concept of in-medium wave functions of fermion pairs is considered. The properties of the pair condensate are discussed in the third section. At last, the proof concerning the noncondensed bound pairs of fermions is given in Sec. IV of the paper.

II. THE CONCEPT OF PAIR WAVE FUNCTIONS FOR FERMIONS

In this section we briefly discuss the concept of the pair wave functions for fermions, for details see Refs. 7,14.

Thus, let us consider a homogeneous Fermi system of N particles with the spin $s=1/2$ at nonzero temperatures. Suppose that the total momentum and spin of the system are conserved quantities. Let the forces exerted by fermions on each other be described with the two-particle interaction potential depending on the relative distance between them and, may be, on the spin variables like in the case of various effective Hamiltonians. A state of the whole system is specified by the density matrix corresponding to the canonical or grand canonical Gibbs ensemble. In this case the 2 matrix is represented in the form:[15] $\rho_2(x_1',x_2';x_1,x_2) = \langle \psi^\dagger(x_1)\psi^\dagger(x_2)\psi(x_2')\psi(x_1')\rangle/\{N(N-1)\}$, where $\langle \cdots \rangle$ stands for the statistical average; $x=(\mathbf{r},s)$ represents the space coordinates $\mathbf{r}$ and spin z projection $s=\pm 1/2$; $\psi^\dagger(x),\psi(x)$ are the field Fermi operators. In order to perform the thermodynamic limit ($V\rightarrow\infty, n=N/V=$const) it is more convenient to deal with the pair-correlation function F_2 differing by a norm from ρ_2:

$$F_2(x_1,x_2;x_1',x_2') = \langle \psi^\dagger(x_1)\psi^\dagger(x_2)\psi(x_2')\psi(x_1')\rangle. \quad (1)$$

The boundary conditions for F_2 (Ref. 16) follow from the principle of the correlation weakening at macroscopical separations:[7]

$$\langle \psi^\dagger(x_1)\psi^\dagger(x_2)\psi(x_2')\psi(x_1')\rangle \rightarrow \langle \psi^\dagger(x_1)\psi^\dagger(x_2)\rangle$$
$$\times \langle \psi(x_2')\psi(x_1')\rangle \quad (2)$$

when

$$\mathbf{r}_1-\mathbf{r}_2=\text{const}, \quad \mathbf{r}_1'-\mathbf{r}_2'=\text{const}, \quad |\mathbf{r}_1'-\mathbf{r}_1|\rightarrow\infty; \quad (3)$$

$$\langle \psi^\dagger(x_1)\psi^\dagger(x_2)\psi(x_2')\psi(x_1')\rangle \rightarrow \langle \psi^\dagger(x_1)\psi(x_1')\rangle$$
$$\times \langle \psi^\dagger(x_2)\psi(x_2')\rangle, \quad (4)$$

when

$$\mathbf{r}_1-\mathbf{r}_1'=\text{const}, \quad \mathbf{r}_2-\mathbf{r}_2'=\text{const}, \quad |\mathbf{r}_1-\mathbf{r}_2|\rightarrow\infty. \quad (5)$$

As the kernel (1) is a non-negative Hermitian operator acting on the two-particle wave functions $\psi(x_1,x_2)$, we can expand it in the orthonormal set of its eigenfunctions $\psi_\nu(x_1,x_2)$ which are called the pair wave functions, or PWF. In an equilibrium state the total pair momentum $\mathbf{q}$ is a good quantum number for PWF provided that the total momentum of the whole system is a conserved quantity (see proof in

Ref. 17). The same is correct for the total spin S of a particle pair if there is no magnetic ordering.[18] So, the index ν can be represented as $\nu=(\omega,\mathbf{q},S)$, where ω stands for other quantum numbers. As to the PWF, they can be written as

$$\psi_\nu(x_1,x_2) = \psi_{\omega,\mathbf{q},S}(\mathbf{r}_1-\mathbf{r}_2,s_1,s_2)\frac{\exp\{i\mathbf{q}(\mathbf{r}_1+\mathbf{r}_2)/2\}}{\sqrt{V}}. \quad (6)$$

Then Eq. (1) can be expressed as

$$F_2(x_1,x_2;x_1',x_2') = \sum_{\omega,\mathbf{q},S} \frac{N_{\omega,\mathbf{q},S}}{V} \psi_{\omega,\mathbf{q},S}^*(\mathbf{r}_1-\mathbf{r}_2,s_1,s_2)$$
$$\times \psi_{\omega,\mathbf{q},S}(\mathbf{r}_1'-\mathbf{r}_2',s_1',s_2')$$
$$\times \exp\left\{i\frac{\mathbf{q}}{2}(\mathbf{r}_1'+\mathbf{r}_2'-\mathbf{r}_1-\mathbf{r}_2)\right\}. \quad (7)$$

If PWF are normalized as $\sum_{s_1,s_2}\int_V d^3r|\psi_{\omega,\mathbf{q},S}(\mathbf{r},s_1,s_2)|^2 =1$, then the non-negative quantity $N_{\omega,\mathbf{q},S}$ can be interpreted as the mean number of the pairs in the state $(\omega,\mathbf{q},S)$, any pair being doubly taken.

The wave function $\psi_{\omega,\mathbf{q},S}(\mathbf{r},s_1,s_2)$ which can be interpreted as the wave function of a particle pair in the center-of-mass system, is related to either discrete or continuous spectra. In the former case we define $\omega=i$, where i stands for the discrete index enumerating the bound pair states. Let us denote $\psi_{\omega,\mathbf{q},S}(\mathbf{r},s_1,s_2)=\varphi_{\mathbf{q},i}(\mathbf{r},s_1,s_2)$, thus

$$\sum_{s_1,s_2}\int_V d^3r|\varphi_{i,\mathbf{q},S}(\mathbf{r},s_1,s_2)|^2=1, \quad (8)$$

$$\varphi_{\mathbf{q},S,i}(\mathbf{r},s_1,s_2)\rightarrow 0, \quad \text{when} \quad r\rightarrow\infty. \quad (9)$$

For the states of the continuous spectra $\omega=(\mathbf{p},m_S)$. These are ''dissociated,'' or scattering, pair states corresponding to the relative motion with the momenta $\mathbf{p}$. It is convenient to set by definition $\psi_{\omega,\mathbf{q},S}(\mathbf{r},s_1,s_2)=\varphi_{\mathbf{p},\mathbf{q},S,m_S}(\mathbf{r},s_1,s_2)/\sqrt{V}$, where the following asymptotics takes place

$$\varphi_{\mathbf{p},\mathbf{q},S,m_S}(\mathbf{r},s_1,s_2)\rightarrow\chi_{S,m_S}(s_1,s_2)\varphi_{\mathbf{p},S}(\mathbf{r}) \quad (10)$$

for $r\rightarrow\infty$. Here we denote

$$\varphi_{\mathbf{p},S}(\mathbf{r})=\begin{cases} \sqrt{2}\cos(\mathbf{pr}), & S=0, \\ \sqrt{2}\sin(\mathbf{pr}), & S=1, \end{cases} \quad (11)$$

and $\chi_{S,m_S}(s_1,s_2)$ is the spin part of the pair wave function (spinor), m_S being the z projection of the total pair spin S:

$$\chi_{S,m_S}(s_1,s_2)=\begin{cases} \Delta(s_1+s_2)\text{sgn}(s_1)/\sqrt{2}, & S=0, \; m_S=0; \\ \Theta(-s_1)\Theta(-s_2), & S=1, \; m_S=-1; \\ \Delta(s_1+s_2)/\sqrt{2}, & S=1, \; m_S=0; \\ \Theta(s_1)\Theta(s_2), & S=1, \; m_S=1. \end{cases} \quad (12)$$

We introduced the functions

$$\Delta(s)=\begin{cases} 0, & s\neq 0, \\ 1, & s=0, \end{cases} \quad \Theta(s)=\begin{cases} 1, & s\geq 0, \\ 0, & s<0, \end{cases}$$

$$\text{sgn}(S)=\Theta(S)-\Theta(-S).$$

We remark that in the situation when the fermion interaction does not depend on spin variables, the spin and space parts of the PWF can be separated from one another not only when $r \to \infty$ but also for any $\mathbf{r}$.

Now, with the variables

$$\mathbf{R} = (\mathbf{r}_1 + \mathbf{r}_2)/2, \quad \mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2 \qquad (13)$$

and, respectively, $\mathbf{R}'$ and $\mathbf{r}'$, expression (7) is rewritten as

$$
\begin{aligned}
F_2(x_1, x_2; x_1', x_2') = & \sum_{\mathbf{q},S,i} \frac{N_{\mathbf{q},S,i}}{V} \varphi_{\mathbf{q},S,i}^*(\mathbf{r}, s_1, s_2) \\
& \times \varphi_{\mathbf{q},S,i}(\mathbf{r}', s_1', s_2') \exp\{i\mathbf{q}(\mathbf{R}' - \mathbf{R})\} \\
& + \sum_{\mathbf{p},\mathbf{q},S,m_S} \frac{N_{\mathbf{p},\mathbf{q},S,m_S}}{V^2} \varphi_{\mathbf{p},\mathbf{q},S,m_S}^*(\mathbf{r}, s_1, s_2) \\
& \times \varphi_{\mathbf{p},\mathbf{q},S,m_S}(\mathbf{r}', s_1', s_2') \exp\{i\mathbf{q}(\mathbf{R}' - \mathbf{R})\}.
\end{aligned}
\qquad (14)
$$

In the thermodynamic limit all the summations over momenta can be replaced by the corresponding integrals:

$$
\begin{aligned}
F_2(x_1, x_2; x_1', x_2') = & \sum_{S,i} \int d^3q \, w_{S,i}(\mathbf{q}) \varphi_{\mathbf{q},S,i}^*(\mathbf{r}, s_1, s_2) \\
& \times \varphi_{\mathbf{q},S,i}(\mathbf{r}', s_1', s_2') \exp\{i\mathbf{q}(\mathbf{R}' - \mathbf{R})\} \\
& + \sum_{S,m_S} \int d^3p \, d^3q \, w_{S,m_S}(\mathbf{p}, \mathbf{q}) \\
& \times \varphi_{\mathbf{p},\mathbf{q},S,m_S}^*(\mathbf{r}, s_1, s_2) \varphi_{\mathbf{p},\mathbf{q},S,m_S}(\mathbf{r}', s_1', s_2') \\
& \times \exp\{i\mathbf{q}(\mathbf{R}' - \mathbf{R})\}.
\end{aligned}
\qquad (15)
$$

Thus, from Eqs. (14) and (15) we can see that $V w_{S,i}(\mathbf{q}) d^3q$ is the number of the bound particle pairs with the spin S, in the state i and with the total couple momentum $\mathbf{q}$ located in the infinitesimal volume d^3q. Respectively, $V^2 w_{S,m_S}(\mathbf{p}, \mathbf{q}) d^3p \, d^3q$ stands for the number of the ''dissociated'' particle pairs in the state (S, m_S) with the relative momentum $\mathbf{p}$ and total momentum $\mathbf{q}$ located in the infinitely small volumes d^3p and d^3q.

In the center-of-mass system the replacement $\mathbf{p} \to -\mathbf{p}, s_1 \to s_2, s_2 \to s_1$ corresponds to the permutation of particles. So, the following symmetric relation takes place:

$$w_{S,m_S}(\mathbf{p}, \mathbf{q}) = w_{S,m_S}(-\mathbf{p}, \mathbf{q}). \qquad (16)$$

As an example, let us consider the expansion of F_2 in terms of PWF for the BCS model. Taken with an accuracy to the asymptotically small quantities, the Hamiltonian in the BCS approach is represented as the quadratic form of the Fermi operators[19] that can be diagonalized with the Bogoliubov transformation. Therefore, one is able to use the theorem of Wick, Bloch, and De Dominicis[20]

$$
\begin{aligned}
F_2(x_1, x_2; x_1', x_2') = & \langle \psi^\dagger(x_1) \psi^\dagger(x_2) \psi(x_2') \psi(x_1') \rangle \\
= & \langle \psi^\dagger(x_1) \psi^\dagger(x_2) \rangle \langle \psi(x_2') \psi(x_1') \rangle \\
& + \langle \psi^\dagger(x_1) \psi(x_1') \rangle \langle \psi^\dagger(x_2) \psi(x_2') \rangle \\
& - \langle \psi^\dagger(x_1) \psi(x_2') \rangle \langle \psi^\dagger(x_2) \psi(x_1') \rangle.
\end{aligned}
\qquad (17)
$$

Further, for the ''normal'' averages we have

$$
\begin{aligned}
\langle \psi^\dagger(x_1) \psi(x_1') \rangle & = \langle \psi^\dagger(\mathbf{r}_1, s_1) \psi(\mathbf{r}_1', s_1') \rangle \\
& = \int \frac{d^3k}{(2\pi)^3} n(k) \exp\{i\mathbf{k}(\mathbf{r}_1' - \mathbf{r}_1)\} \Delta(s_1 - s_1'),
\end{aligned}
\qquad (18)
$$

where $n(k) = \langle a_{\mathbf{k},s}^\dagger a_{\mathbf{k},s} \rangle$ gives the distribution of fermions over momenta. ''Anomalous'' averages are given by

$$
\begin{aligned}
\langle \psi(x_1) \psi(x_1') \rangle & = \langle \psi(\mathbf{r}_1, s_1) \psi(\mathbf{r}_1', s_1') \rangle \\
& = \int \frac{d^3k}{(2\pi)^3} \langle a_{\mathbf{k},s_1} a_{-\mathbf{k}, -s_1} \rangle \\
& \times \exp\{i\mathbf{k}(\mathbf{r}_1' - \mathbf{r}_1)\} \Delta(s_1 + s_1').
\end{aligned}
\qquad (19)
$$

In the BCS model, the quantity $\langle a_{\mathbf{k},s} a_{-\mathbf{k}, -s} \rangle$ can be represented in the following form:

$$\langle a_{\mathbf{k},s} a_{-\mathbf{k}, -s} \rangle = \sqrt{n_0} \varphi(k) \frac{\mathrm{sgn}(s)}{\sqrt{2}}, \qquad (20)$$

with $\varphi(k)$ obeying the normalization condition

$$\int \frac{d^3k}{(2\pi)^3} |\varphi(k)|^2 = 1. \qquad (21)$$

We remark that one can consider $\varphi(k)$ as a real quantity because it can be made real with the corresponding phase transformation of the operators $a_{\mathbf{k},s}$ and $a_{\mathbf{k},s}^\dagger$. Now, Eqs. (18), (19), and (20) allow us to rewrite Eq. (17) in the following form:

$$
\begin{aligned}
F_2(x_1, x_2; x_1', x_2') = & n_0 \varphi(r) \chi_{0,0}(s_1, s_2) \varphi(r') \chi_{0,0}(s_1', s_2') \\
& + \sum_{S,m_S} \int \frac{d^3p \, d^3q}{(2\pi)^6} n\left(\frac{\mathbf{q}}{2} + \mathbf{p}\right) n\left(\frac{\mathbf{q}}{2} - \mathbf{p}\right) \\
& \times \varphi_{\mathbf{p},S}(\mathbf{r}) \chi_{S,m_S}(s_1, s_2) \varphi_{\mathbf{p},S}(\mathbf{r}') \\
& \times \chi_{S,m_S}(s_1', s_2') \exp\{i\mathbf{q}(\mathbf{R}' - \mathbf{R})\},
\end{aligned}
\qquad (22)
$$

where $\varphi(r)$ is the Fourier transform of $\varphi(k)$, and we use the notations (11) and (12).

With Eq. (21) one can easily be convinced that the normalization relation (8) is satisfied. Within the BCS model $w_{S,i}(\mathbf{q}) = \Delta(S) \Delta(i) n_0 \delta(\mathbf{q}) (\delta(\mathbf{q})$ is the δ function), i.e., all the bound particle pairs are condensed.

III. PROPERTIES OF THE CONDENSATE OF PAIRS

Let us demonstrate in the most general case that if the "anomalous" average $\langle \psi(x_1)\psi(x_2)\rangle$ is not equal to zero (off-diagonal long-range order) then the distribution function $w_{S,i}(\mathbf{q})$ acquires the δ-functional singularity corresponding to some indices S_0 and i_0 or, in other words, the ratio $N_{\mathbf{q},S_0,i_0}/V$ in the first sum of Eq. (14) does not vanish in the thermodynamic limit:

$$w_{S,i}(\mathbf{q})=n_0\delta(\mathbf{q})\Delta(S-S_0)\Delta(i-i_0)+\widetilde{w}_{S,i}(\mathbf{q}), \quad (23)$$

where $\widetilde{w}_{S,i}(\mathbf{q})$ is the regular part of Eq. (23) giving the bound-pair distribution over nonzero momenta.

To do this, let us take the limit relation (2) and rewrite it with the variables (13) in the form

$$F_2(x_1,x_2;x_1',x_2')\rightarrow\langle\psi^\dagger(x_1)\psi^\dagger(x_2)\rangle\langle\psi(x_2')\psi(x_1')\rangle$$
$$=n_0\varphi^*(\mathbf{r},s_1,s_2)\varphi(\mathbf{r}',s_1',s_2'), \quad (24)$$

where the functions $\varphi^*(\mathbf{r},s_1,s_2)$ and $\varphi(\mathbf{r}',s_1',s_2')$ are introduced in such a way that the normalization condition (8) should be fulfilled. This can always be done because according to the principle of correlation weakening[7]

$$\langle\psi(x_1)\psi(x_2)\rangle\rightarrow\langle\psi(x_1)\rangle\langle\psi(x_2)\rangle=0$$

when $r\rightarrow\infty$ (see Ref. 21). Expression (24) is exactly the contribution of the first singular term of Eq. (23) into Eq. (15). The contribution of the regular part of Eq. (23) and that of the dissociated pair states into Eq. (15) are infinitely small in the situation of Eq. (3) according to the Riemann's theorem[22] because

$$|\mathbf{R}'-\mathbf{R}|=\left|\frac{\mathbf{r}_1'+\mathbf{r}_2'}{2}-\frac{\mathbf{r}_1+\mathbf{r}_2}{2}\right|\rightarrow\infty.$$

We remark that the pair distribution over the scattering states (16) does not contain δ-functional terms. Indeed, in the opposite case they would lead to the condensate of the one-particle states like in the situation of the Bose liquid,[17] which is impossible for the Fermi systems.

Equation (24) allows us to treat the anomalous averages as the wave functions of the condensed pairs of fermions, (of course, with an accuracy to the normalizing factor). For the density of the pairs like these, Eqs. (8) and (24) gives

$$n_0=\frac{N_{\mathbf{q}=0,S_0,i_0}}{V}=\sum_{s_1,s_2}\int d^3r|\langle\psi(\mathbf{r},s_1)\psi(0,s_2)\rangle|^2$$
$$=\sum_s\int\frac{d^3k}{(2\pi)^3}|\langle a_{\mathbf{k},s}a_{-\mathbf{k},-s}\rangle|^2, \quad (25)$$

where it has been taken into account that the total momentum of the system and z component of its spin are conserved quantities. Keeping in mind these integrals of the motion, one could expect that in the most general case the wave function of the condensed pairs should be written as

$$\varphi(\mathbf{r},s_1,s_2)=\frac{1}{\sqrt{n_0}}\langle\psi(\mathbf{r}_1,s_1)\psi(\mathbf{r}_2,s_2)\rangle$$
$$=\frac{1}{\sqrt{n_0}}\int\frac{d^3k}{(2\pi)^3}\langle a_{\mathbf{k},s_1}a_{-\mathbf{k},-s_1}\rangle\Delta(s_1+s_2)\exp(i\mathbf{k}\mathbf{r})$$
$$=\frac{1}{\sqrt{n_0}}\frac{\Delta(s_1+s_2)}{\sqrt{2}}\{\varphi_s(\mathbf{r})\mathrm{sgn}(s_1)+\varphi_t(\mathbf{r})\}, \quad (26)$$

where $\varphi_s(\mathbf{r})=\varphi_s(-\mathbf{r})$ and $\varphi_t(\mathbf{r})=-\varphi_t(-\mathbf{r})$. According to Eq. (12) the first term in Eq. (26) corresponds to the singlet and the second, to the triplet components of the wave function of the condensed fermions. However, Eq. (26) is not quite correct because the total pair spin should be an integral of the motion, even in the situation with the spin-dependent interaction between fermions. Therefore, we are not able to obtain a superposition of the singlet and triplet states. Instead, in Eq. (26) one should select either $\varphi_s(\mathbf{r})\neq0$, $\varphi_t(\mathbf{r})=0$ or $\varphi_s(\mathbf{r})=0$, $\varphi_t(\mathbf{r})\neq0$. So, we have

$$\varphi(\mathbf{r},s_1,s_2)=\begin{cases}\varphi_s(\mathbf{r})\chi_{0,0}(s_1,s_2)/\sqrt{n_0},\\\varphi_t(\mathbf{r})\chi_{1,0}(s_1,s_2)/\sqrt{n_0}.\end{cases} \quad (27)$$

The spinors (12) can be expressed with the help of the Pauli matrices: $\chi_{0,0}=i\sigma_y/\sqrt{2}$, $\chi_{1,0}=i\sigma_z\sigma_y/\sqrt{2}$. Thus, the expression (27) can be rewritten in the standard form[23] proposed first in Ref. 24,

$$\varphi(\mathbf{r},s_1,s_2)=\begin{cases}\Delta(\mathbf{r})i\sigma_y, & S=0,\\(\mathbf{d}(\mathbf{r})\cdot\boldsymbol{\sigma})i\sigma_y, & S=1,\end{cases} \quad (28)$$

where we introduce the notations $\boldsymbol{\sigma}=(\sigma_x,\sigma_y,\sigma_z)$, $\Delta(\mathbf{r})=\Delta(-\mathbf{r})=\varphi_s(\mathbf{r})/\sqrt{2n_0}$, $\mathbf{d}(\mathbf{r})=-\mathbf{d}(-\mathbf{r})=(0,0,\varphi_t(\mathbf{r})/\sqrt{2n_0})$. We get Eq. (28) in the z representation for the spinors. An arbitrary representation can be obtained from Eq. (27) with the unitary transformation of the spinors (12). It is not difficult to verify that in the general case all the three components of $\mathbf{d}(\mathbf{r})$ are not zero, and $\mathbf{d}(\mathbf{r})$ is transformed as a spin–space vector.

The phase coherence takes place for the condensed bound pairs due to the uncertainty relation $\Delta\varphi\Delta N_0\simeq1$ for the phase φ and number of the bound fermion pairs $N_0=N_{\mathbf{q}=0,S_0,i_0}$ in the state $(\mathbf{q}=0,S_0,i_0)$. In the thermodynamic limit the macroscopical occupation of this state results in $\Delta N_0\propto\sqrt{N_0}\rightarrow\infty$ and, therefore, $\Delta\varphi\rightarrow0$. For the bound pair states beyond the condensate $N_{\mathbf{q},S,i}$ is limited above even for $V\rightarrow\infty$. Thus these states are not correlated with respect to the phase.

We remark that the total number of the bound particle pairs (condensed and not)

$$N_b=V\sum_{S,i}\int d^3q\,w_{S,i}(\mathbf{q})$$

is proportional to the total number of particles N. In particular, there is the inequality for the number of the condensed bound pair states[25]

$$N_0\leqslant N. \quad (29)$$

It should be emphasized that the inequality (29) is not trivial. One can consider, for example, a dilute gas of m-particle molecules. In this case we have $N_b=(m-1)N$, thus, one can obtain $N_b>N$ provided $m\geq 3$.

In the space–uniform case we can readily find relation (29) with the inequality of Cauchy-Schwarz-Bogoliubov[7]

$$|\langle \hat{A}\hat{B}\rangle|^2 \leq \langle \hat{A}\hat{A}^\dagger\rangle\langle \hat{B}^\dagger\hat{B}\rangle.$$

Indeed, assuming $A=a_{\mathbf{k},s}$ and $B=a_{-\mathbf{k},-s}$ we arrive at

$$|\langle a_{\mathbf{k},s}a_{-\mathbf{k},-s}\rangle|^2 \leq \langle a_{\mathbf{k},s}a_{\mathbf{k},s}^\dagger\rangle\langle a_{-\mathbf{k},-s}^\dagger a_{-\mathbf{k},-s}\rangle$$
$$=[1-n(k)]n(k).$$

Then, from Eq. (25) we derive

$$n_0=\frac{N_0}{V}=\frac{1}{V}\sum_{\mathbf{k},s}|\langle a_{\mathbf{k},s}a_{-\mathbf{k},-s}\rangle|^2 \leq \frac{2}{V}\sum_{\mathbf{k}}(n(k)-n^2(k))$$

$$\leq \frac{2}{V}\sum_{\mathbf{k}}n(k)=\frac{N}{V}=n.$$

It is interesting to note that $n(k)-n^2(k)=\langle(a_{\mathbf{k},s}^\dagger a_{\mathbf{k},s})^2\rangle - \langle a_{\mathbf{k},s}^\dagger a_{\mathbf{k},s}\rangle^2=D(n(k))$ is nothing else but the mean-square deviation of the occupation number of the $(\mathbf{k},s)$ one-particle state. So, the stronger inequality

$$n_0 \leq \frac{2}{V}\sum_{\mathbf{k}}D(n(k)) \tag{30}$$

demonstrates that the number of the condensed pairs is tightly connected with the washout of the Fermi surface. In the BCS model at zero temperature

$$\frac{n_0}{n}\propto \frac{k_B T_c}{E_F}\ll 1$$

because the bound pairs are formed by the particles located near the Fermi surface only. In general, n_0 is the most "reliable" order parameter of the superconducting phase transition.

IV. THE BOGOLIUBOV $1/Q^2$ THEOREM AND BOUND PAIR STATES BEYOND THE CONDENSATE

Let us now prove with the principle of the correlation weakening that the distribution of the particle pairs over the "scattering" states $w_{S,m_S}(\mathbf{p},\mathbf{q})$ is expressed in terms of the occupation numbers of the one-particle states $n(k)=\langle a_{\mathbf{k},s}^\dagger a_{\mathbf{k},s}\rangle$. Indeed, on the one hand, in the limiting situation of Eq. (5) we have the relation (4), which can be written as

$$F_2(x_1,x_2;x_1',x_2')$$

$$\rightarrow \int \frac{d^3 p_1}{(2\pi)^3}n(p_1)\exp(i\mathbf{p}_1(\mathbf{r}_1'-\mathbf{r}_1))\Delta(s_1-s_1')$$

$$\times \int \frac{d^3 p_2}{(2\pi)^3}n(p_2)\exp(i\mathbf{p}_2(\mathbf{r}_2'-\mathbf{r}_2))\Delta(s_2-s_2')$$

$$=\int d^3q\, d^3p\frac{n(\mathbf{q}/2+\mathbf{p})n(\mathbf{q}/2-\mathbf{p})}{(2\pi)^6}\exp(i\mathbf{p}(\mathbf{r}'-\mathbf{r}))$$

$$\times \exp(i\mathbf{q}(\mathbf{R}'-\mathbf{R}))\Delta(s_1-s_1')\Delta(s_2-s_2'), \tag{31}$$

where, passing to the last equality, we introduced the new variables $\mathbf{q}=\mathbf{p}_1+\mathbf{p}_2$ and $\mathbf{p}=(\mathbf{p}_1-\mathbf{p}_2)/2$ and used notations (13). On the other hand, when Eq. (5) is true, we have

$$r=|\mathbf{r}_2-\mathbf{r}_1|\rightarrow\infty, \quad r'=|\mathbf{r}_2'-\mathbf{r}_1'|\rightarrow\infty,$$

$$|\mathbf{r}+\mathbf{r}'|\rightarrow\infty, \quad \mathbf{R}'-\mathbf{R}=\text{const}, \quad \mathbf{r}'-\mathbf{r}=\text{const}.$$

Therefore, it follows from Eqs. (9), (10), and (15) that in the limiting case (5) we have

$$F_2(x_1,x_2;x_1',x_2')\rightarrow \sum_{S,m_S}\int d^3q\, d^3p\, w_{S,m_S}(\mathbf{p},\mathbf{q})\varphi_{\mathbf{p},S}(\mathbf{r})$$

$$\times \varphi_{\mathbf{p},S}(\mathbf{r}')\chi_{S,m_S}(s_1,s_2)\chi_{S,m_S}(s_1',s_2')$$

$$\times \exp(i\mathbf{q}(\mathbf{R}'-\mathbf{R})), \tag{32}$$

where we used notations (11) and (12). Further, Riemann's theorem[22] used while integrating over $\mathbf{p}$ and relation (16) allow us to rewrite Eq. (32) as

$$F_2(x_1,x_2;x_1',x_2')\rightarrow \int d^3q\, d^3p \sum_{S,m_S}w_{S,m_S}(\mathbf{p},\mathbf{q})\chi_{S,m_S}(s_1,s_2)$$

$$\times \chi_{S,m_S}(s_1',s_2')\exp(i\mathbf{p}(\mathbf{r}'-\mathbf{r}))$$

$$\times \exp(i\mathbf{q}(\mathbf{R}'-\mathbf{R})). \tag{33}$$

The right-hand side of Eq. (31) is equal to that of Eq. (33) at all the values of the spin variables and space ones $\tilde{\mathbf{r}}=\mathbf{r}'-\mathbf{r}$ and $\tilde{\mathbf{R}}=\mathbf{R}'-\mathbf{R}$. Taking into account the completeness of the set of the spin functions (12)

$$\sum_{S,m_S}\chi_{S,m_S}(s_1,s_2)\chi_{S,m_S}(s_1',s_2')=\Delta(s_1-s_1')\Delta(s_2-s_2'),$$

we derive the following equality:

$$w_{S,m_S}(\mathbf{p},\mathbf{q})=\frac{n(\mathbf{q}/2+\mathbf{p})n(\mathbf{q}/2-\mathbf{p})}{(2\pi)^6}. \tag{34}$$

Thus, in the thermodynamic limit one can write

$$N_{\mathbf{p},\mathbf{q},S,m_S}=n(\mathbf{q}/2+\mathbf{p})n(\mathbf{q}/2-\mathbf{p}). \tag{35}$$

As it is seen, when there is no magnetic ordering (it is obviously true for the superconducting phase), the function of the pair distribution over the dissociated states is independent of the quantum numbers S,m_S.

It is now easy to prove that the pair condensate must always be accompanied by the presence of the noncondensed fermion pairs: $\tilde{w}_{S,i}(\mathbf{q}) \neq 0$ in Eq. (23) if $n_0 \neq 0$. Let the interaction energy of the system be invariant with respect to the local gauge transformation of the field Fermi operators[26]

$$\psi(\mathbf{r},s) \rightarrow \psi(\mathbf{r},s)\exp(i\chi(\mathbf{r})),$$

$$\psi^\dagger(\mathbf{r},s) \rightarrow \psi^\dagger(\mathbf{r},s)\exp(-i\chi(\mathbf{r})). \qquad (36)$$

In this case the $1/q^2$ theorem of Bogoliubov for the Fermi systems[7] is valid which asserts that in the presence of the pair condensate we have the inequality for sufficiently small q

$$\max_{\omega,S} N_{\omega,\mathbf{q},S} \geq \frac{C}{q^2},$$

where $N_{\omega,\mathbf{q},S}$ appears in Eq. (7) and ω is the set of the quantum numbers corresponding to both the continuous spectrum $[\omega=(\mathbf{p},m_S)]$ and the discrete one $(\omega=i)$.[27] However, Eq. (35) results in

$$N_{\mathbf{p},\mathbf{q},S,m_S} \leq 1$$

because $n(k) \leq 1$ for fermions. Therefore, we have the only possibility at which the singularity $1/q^2$ appears due to the noncondensed bound pairs. It is reasonable to expect that these pairs have the quantum numbers of the condensate couples S_0, i_0:

$$\tilde{w}_{S_0,i_0}(\mathbf{q}) \geq \frac{C'}{q^2}. \qquad (37)$$

The BCS model is not locally gauge invariant which results in absence of the noncondensed bound pairs: $\tilde{w}_{S,i}(\mathbf{q}) = 0$. It is important to note in this connection that the bound pair states beyond the condensate may play a noticeable role in calculating the gauge-invariant response of the system to the electromagnetic fields.

We have proved that the noncondensed bound pairs coexist with the condensed ones at $T < T_c$. So, any theory ignoring the noncondensed bound pairs of fermions is not fully consistent. We remark that the distribution of the bound fermion pairs over the center-of-mass momenta obeys the inequality (37) with $C' \propto k_B T n_0$ (see Ref. 7). The distribution of the particles over momenta in the Bose gas $w(q) = n(q)/(2\pi)^3$ answers, at small q, the similar relation $w(q) \geq C''/q^2$ with $C'' \propto k_B T n_0$ (here n_0 denotes the density of the condensed bosons).[7] Therefore, there are fundamental parallels between the Bose gas and the considered subsystem of the fermion bound pairs. These parallels are not only reduced to agreement between the fermion-pair statistics and the Bose one. Following this analogy, we can expect that the bound fermion pairs exist even at $T > T_c$ (apparently, in some temperature interval $T_c < T < T^*$, in spite of the disappearance of the $1/q^2$ singularity). Thus, it looks as if any superconducting phase transition is a particular case of the Bose-Einstein condensation. This conclusion can be of interest in the context of the discussion concerning different approaches of investigating the high-T_c superconductivity (see Refs. 28, 29). We remark that possible experimental consequences of the existence of fermion bound pairs beyond the condensate can be found in paper[12] in the case of neutral Fermi systems.

The space-uniform character of the Fermi system is of use in the proof given above. Electrons in the crystalline field, of course, cannot be treated on the same level. However, for $q \rightarrow 0$ (large wavelengths) a crystalline lattice can be considered as the continuum. Therefore, the derived result remains correct in this case.

We emphasize that the bound pair states can fully be a result of the collective effects. Indeed, as it was demonstrated by Cooper,[30] an arbitrary small attraction between electrons leads to forming the condensate of the bound electron pairs. Hence, if we considered a sufficiently shallow well as the two-fermion interaction potential, we would observe formation of the condensed and, according to the obtained result, noncondensed pairs at low temperatures. However, the well can be chosen in such a way as to prevent the bound states of two ''bare'' fermions from appearing within the ordinary two-particle problem.

It is important to make one more remark on the connection between the $1/q^2$ theorem of Bogoliubov and the Goldstone theorem.[31] As it has been demonstrated in Ref. 7, the existence of the Goldstone mode in the Bose system results from the Bogoliubov theorem provided the mass operator $\Sigma(\omega,k)$ is regular in the vicinity of the point $\omega=0$, $k=0$. Let us emphasize that there are situations when the Bogoliubov theorem is valid while this is not the case for the Goldstone one. For example, in the case of a neutral weakly interacting Bose gas the condition mentioned above for the mass operator is correct, and the Goldstone mode exists. On the contrary, for the charged Bose gas the mass operator is not regular at $k=0$, and, thus, there is no Goldstone mode. A similar situation is realized for the Fermi systems (see, e.g., Ref. 32).

V. CONCLUSION

In conclusion, let us take notice of the main results once more. The reduced density matrix of the second order is a fundamental characteristic of a many-particle system, its eigenfunctions being the pure states of two particles selected in an arbitrary way. The appearance of the condensate of the bound pair states (25) implies the occurrence of the δ-functional term in the distribution of the bound pairs over the momentum $\mathbf{q}$ of the pair center-of-mass [see Eq. (23)]. Using the space homogeneity of the system and the local gauge invariance (36) of the fermion interaction, we have proved that there is the $1/q^2$ singularity in the distribution function $\tilde{w}_{S,i}(\mathbf{q})$ provided that $n_0 \neq 0$. Thus, we refined the $1/q^2$ theorem of Bogoliubov, having proved the singularity appears in $\tilde{w}_{S,i}(\mathbf{q})$. Therefore, the presence of noncondensed bound pairs below T_c is a necessary condition of superconductivity. A new simple proof of the Yang inequality for the Fermi systems (29) and its stronger variant (30) have also been derived as results of secondary importance.

[1] M. Randeria, cond-mat/9710223 (unpublished).

[2] P. W. Anderson, Phys. World **8**, 37 (1995).

[3] N. F. Mott, Phys. World **9**, 16 (1996).

[4] G. Baskaron, Z. Zou, and P. W. Anderson, Solid State Commun. **63**, 973 (1987).

[5] A. S. Alexandrov and N. F. Mott, Rep. Prog. Phys. **57**, 1197 (1994); A. S. Alexandrov, V. V. Kabanov, and N. F. Mott, Phys. Rev. Lett. **77**, 4796 (1996).

[6] J. M. Blatt, *Theory of Superconductivity* (Academic, New York, 1964).

[7] N. N. Bogoliubov, *Lectures on Quantum Statistics* (Gordon and Breach, New York, 1970), Vol. 2, p. 1.

[8] L. D. Landau and E. M. Lifshitz, *Course of Theoretical Physics*, Vol. 3, *Quantum Mechanics–Non–Relativistic Theory* (Pergamon, New York, 1977), Sec. 14.

[9] It is more correct to speak about the bound pair states rather than about bound pairs. Indeed, a particle can form a bound state together with $M(M \geq 1)$ particles, while it forms ''dissociated'' states with the other $N - 1 - M$ particles.

[10] Strictly speaking, this is valid for the *s*-wave pairing. In the general case the gap in the single-particle spectrum becomes **k** dependent, and one usually supposes that $\Delta = \Delta(\mathbf{k})$ is proportional to ''anomalous'' averages $\langle a_{-\mathbf{k},\alpha} a_{\mathbf{k},\beta} \rangle$. We associate the anomalous averages with the wave function of pairs in the condensate [see Eq. (26)]. As to the exact relation between the binding energy ε_b and the gap $\Delta(\mathbf{k})$ in the general case, it is a rather complicated question. However, at any rate, the presence of the gap implies that $\varepsilon_b \neq 0$.

[11] The continuous distribution can only be introduced in the thermodynamic limit $N/V = \mathrm{const}, V \to \infty$.

[12] A. J. Leggett, in *Modern Trends in the Theory of Condensed Matter*, edited by A. Pekalski and J. Przystawa (Springer-Verlag, Berlin, 1980), p. 13.

[13] J. R. Schrieffer, *Theory of Superconductivity* (Benjamin, New York, 1964).

[14] A. Yu. Cherny, A. A. Shanenko, cond-mat/9901224 (unpublished).

[15] N. N. Bogoliubov, *Lectures on Quantum Statistics* (Gordon and Breach, New York, 1967), Vol. 1, p. 39.

[16] After the thermodynamic limit $V \to \infty$.

[17] A. Yu. Cherny, cond-mat/9807120, J. Phys.: Condens. Matter (to be published).

[18] Of course, there is no magnetic ordering in the superconducting state.

[19] N. N. Bogoliubov, *Lectures on Quantum Statistics* (Ref. 7), p. 76.

[20] C. Bloch and C. De Dominicis, Nucl. Phys. **7**, 459 (1958).

[21] The equation $\langle \psi(x) \rangle \neq 0$ implies that there is a condensate of the one-particle states which is impossible due to the Pauli principle.

[22] The Riemann's theorem asserts that for any regular function $f(\mathbf{q})$ [i.e., $f(\mathbf{q})$ does not contain the δ function] we have $\lim_{r \to \infty} \int d^3q f(\mathbf{q}) \exp(i\mathbf{q}\mathbf{r}) = 0$, provided the integral $\int d^3q f(\mathbf{q}) \exp(i\mathbf{q}\mathbf{r})$ exists.

[23] J. F. Annett, N. Goldenfeld, and S. N. Renn, in *Physical Properties of High Temperature Superconductors*, edited by D. M. Ginsberg (World Scientific, Singapore, 1996), Vol. 6, p. 375.

[24] P. W. Anderson and W. F. Brinkman, in *The Helium Liquids: Proceedings of the 15th Scottish Universities Summer School in Physics, 1974*, edited by J. G. M. Armitage and I. E. Farquhar (Academic, New York, 1975).

[25] C. N. Yang, Rev. Mod. Phys. **34**, 694 (1962).

[26] We emphasize that some other fields can also be included into the Hamiltonian, for example, the phonon one. Thus, the Fröhlich model is invariant with respect to the transformation (36).

[27] Bogoliubov proved the theorem in the particular case of the *s*-wave pairing, i.e., when in Eq. (27) $\varphi_s(\mathbf{r}) = \varphi(r)$, where $\varphi(r)$ is radially symmetric function. The proof can easily be extended to the more general case.

[28] B. K. Chakraverty, J. Ranninger, and D. Feinberg, Phys. Rev. Lett. **81**, 433 (1998).

[29] A. S. Alexandrov, cond-mat/9807185 (unpublished).

[30] L. N. Cooper, Phys. Rev. **104**, 1189 (1956).

[31] J. Goldstone, Nuovo Cimento **19**, 154 (1961).

[32] H. Wagner, Z. Phys. **195**, 273 (1966).