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 $\hbar \mathbf{q}$ 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 behaviour 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 $T_c$.

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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$^1$). 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$^2$. 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.$^3$. The more radical model of Alexandrov and Mott$^4$ 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$^5$.

The concept of a bound state of two particles in medium can consistently be formulated with the reduced density matrix of the second order (2–matrix$^6$). 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 all the system of interest has a wave function. In general a subsystem is specified by the density matrix (see, e.g. Ref.$^7$). 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. 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 $\hbar \mathbf{q} = 0$, the binding energy $\varepsilon_b$ of these pairs being just the value of the superconducting gap$^8$. The bound particle pairs beyond the condensate are characterized by the continuous distribution over the total momentum of a couple$^9$. The couple like these must also have the finite binding energy $\varepsilon_b(\mathbf{q})$ that, due to the continuity argument, should tend to $\varepsilon_b$ 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 pseudogap, which manifests itself in the normal phase when the bound couples survive at $T > T_c$.

In the BCS–theory there are no bound pair states beyond the condensate absolutely$^10$ (see below) which is a consequence of the violation of the local gauge invariance (see, for example, Ref.$^11$).

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 the bound couples beyond the condensate (Schafroth’s pairs). 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, one may call these pairs 'quasi-molecules'. 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 an ordinary molecules. The proof is based on the well-known $1/N^2$ theorem of Bogoliubov for the Fermi system 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 section 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 section IV of the paper.

II. THE CONCEPT OF PAIR WAVE FUNCTIONS FOR FERMIONS

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 Gibbs ensemble:

$$\hat{\rho} = \exp\left(-\frac{\hat{H}}{k_B T}\right)/\text{Tr}\exp\left(-\frac{\hat{H}}{k_B T}\right),$$

(1)

where $\hat{H}$ is the system Hamiltonian. In this case the $2\times2$ matrix is represented in the form (see, for example)

$$\rho_2(x_1', x_2'; x_1, x_2) = \frac{1}{N(N-1)}\langle \psi^\dagger(x_1)\psi^\dagger(x_2)\psi(x_2')\psi(x_1') \rangle,$$

(2)

where $\langle \cdot \cdot \cdot \rangle$ stands for the average over the state $|\rho\rangle$. $x = (r, \sigma)$ represents the space coordinates $r$ and spin $z$-projection $\sigma = \pm 1/2$: $\psi^\dagger(x)$ and $\psi(x)$ are the field Fermi operators. The $2\times2$ matrix obeys the normalization condition

$$\int dx_1dx_2\rho_2(x_1, x_2; x_1, x_2) = 1,$$

(3)

here $\int dx_1 \cdots = \sum_{\sigma} \int d^3 r \cdots$ and integration is fulfilled over the volume $V$. Therefore, the $2\times2$ matrix has the asymptotic behaviour $1/V^2$ when $V \to \infty$, $n = N/V = \text{const}$. So, it is more convenient to deal with the pair correlation function $F_2$ differing by a norm from $\rho_2$:

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

(4)

The boundary conditions for $F_2$ follow from the principle of the correlation weakening at macroscopical separations:

$$\langle \psi^\dagger(x_1)\psi^\dagger(x_2)\psi(x_2')\psi(x_1') \rangle \to \langle \psi^\dagger(x_1)\psi^\dagger(x_2)\rangle \langle \psi(x_2')\psi(x_1') \rangle$$

(5)

when

$$r_1 - r_2 = \text{const}, r_1' - r_2' = \text{const}, |r_1' - r_1| \to \infty;$$

(6)

$$\langle \psi^\dagger(x_1)\psi^\dagger(x_2)\psi(x_2')\psi(x_1') \rangle \to \langle \psi^\dagger(x_1)\psi(x_1') \rangle \langle \psi^\dagger(x_2)\psi(x_2') \rangle$$

(7)

when

$$r_1 - r_1' = \text{const}, r_2 - r_2' = \text{const}, |r_1 - r_2| \to \infty. $$

(8)

As the kernel $\langle \cdot \cdot \cdot \rangle$ 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 (EF):

$$F_2(x_1, x_2; x_1', x_2') = \sum_\nu N_\nu \nu^\dagger(x_1, x_2)\nu(x_1', x_2'),$$

(9)

where

$$\int dx_1dx_2|\nu(x_1, x_2)|^2 = 1.$$

(10)

Therefore, the non-negative quantity $N_\nu$ can be interpreted as the mean number of the pairs in the state $\nu$, any pair being doubly taken. The ratio $w_\nu = N_\nu/(N(N-1))$ is the probability of observing a particle pair in the pure state with the wave function $\nu(x_1, x_2)$. Here, as one might expect, $\sum_\nu w_\nu = 1$.

It follows from the definition (9) that

$$F_2(x_1, x_2; x_1', x_2') = -F_2(x_1, x_2; x_2', x_1').$$

(11)

So, $\psi_\nu(x_1, x_2) = -\psi_\nu(x_2, x_1)$, i.e. PWF for fermions, as usual, are antisymmetric with respect to permutations of particles.

In an equilibrium state the total pair momentum $h\mathbf{q}$ is a good quantum number for PWF provided that the total momentum of the whole system is a conserving quantity (see proof in Ref.3). The same is correct for the total
spin $S$ of a particle pair if there is no magnetic ordering. So, the index $\nu$ can be represented as

$$\nu = (\omega, q, S)$$

where $\omega$ stands for other quantum numbers. As to the PWF, they can be written as

$$\psi_\nu(x_1, x_2) = \psi_{\omega, q, S}(r_1 - r_2, \sigma_1, \sigma_2) \exp\left\{i\mathbf{q}(r_1 + r_2)\right\}. \quad (11)$$

Then expression (11) has the form

$$F_2(x_1, x_2; x'_1, x'_2) = \sum_{\omega, q, S, \sigma_1, \sigma_2} \frac{N_{\omega, q, S}}{V} \psi_{\omega, q, S}(r_1 - r_2, \sigma_1, \sigma_2) \times \psi_{\omega, q, S}(r_1 - r_2, \sigma_1, \sigma_2) \exp\left\{i\mathbf{q}(r_1 + r_2 - r_1 - r_2)\right\}. \quad (12)$$

For the wave function $\psi_{\omega, q, S}(r, \sigma_1, \sigma_2)$ which can be interpreted as the wave function of a particle pair in the center-of-mass system, from (10) and (11) we obtain

$$\sum_{\sigma_1, \sigma_2} \int d^3r |\psi_{\omega, q, S}(r, \sigma_1, \sigma_2)|^2 = 1. \quad (13)$$

It can be related to either discrete or continuous spectra. In the former case

$$\psi_{\omega, q, S}(r, \sigma_1, \sigma_2) \rightarrow 0 \quad (14)$$

when $r \rightarrow \infty$ and, so, we deal with the sector of bound states of particle pairs. The latter variant implies

$$\psi_{\omega, q, S}(r, \sigma_1, \sigma_2) \rightarrow \chi_{S, m_S}(\sigma_1, \sigma_2) \frac{\sqrt{2}}{\sqrt{V}} \left\{ \cos(pr) \sin(pr) \right\} \quad (15)$$

for $r \rightarrow \infty$. This is a 'dissociated', or scattering, pair state corresponding to the relative motion with the momentum $\hbar p$. Here $\chi_{S, m_S}(\sigma_1, \sigma_2)$ is the spin part of the pair wave function (spinor), $m_S$ being the $z$-projection of the total pair spin $S$. When $S = 0$, $m_S = 0$ (the singlet state) one should take $\cos(pr)$, for $S = 1$, $m_S = -1, 0, 1$ (the triplet state) one should use $\sin(pr)$. 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 $r \rightarrow \infty$ but also for any $r$.

In the case of (14) $\omega = i$, where $i$ stands for the discrete index enumerating the bound pair states. Let us denote $\psi_{\omega, q, S}(r, \sigma_1, \sigma_2) = \varphi_{q, S, i}(r, \sigma_1, \sigma_2)$, so that

$$\sum_{\sigma_1, \sigma_2} \int d^3r |\varphi_{q, S, i}(r, \sigma_1, \sigma_2)|^2 = 1. \quad (16)$$

In the situation of (13) $\omega = (p, m_S)$. Here it is convenient to introduce $\psi_{\omega, q, S}(r, \sigma_1, \sigma_2) = \varphi_{p, q, S, m_S}(r, \sigma_1, \sigma_2) / \sqrt{V}$. From (13) it follows that

$$\frac{1}{V} \sum_{\sigma_1, \sigma_2} \int d^3r |\varphi_{p, q, S, m_S}(r, \sigma_1, \sigma_2)|^2 = 1. \quad (17)$$

Now, with the variables

$$R = (r_1 + r_2)/2, \quad r = r_1 - r_2 \quad (18)$$

and, respectively, $R'$ and $r'$, the expression (12) is rewritten as

$$F_2(x_1, x_2; x'_1, x'_2) = \sum_{q, S, \sigma_1, \sigma_2} \frac{N_{q, S}}{V} \varphi_{q, S, i}(r, \sigma_1, \sigma_2) \times \varphi_{q, S, i}(r', \sigma'_1, \sigma'_2) \exp\left\{i\mathbf{q}(R' - R)\right\} + \sum_{p, q, m_S} \frac{N_{p, q, S, m_S}}{V^2} \varphi^*_{p, q, S, m_S}(r, \sigma_1, \sigma_2) \times \varphi_{p, q, S, m_S}(r', \sigma'_1, \sigma'_2) \exp\left\{i\mathbf{q}(R' - R)\right\}. \quad (19)$$

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

$$F_2(x_1, x_2; x'_1, x'_2) = \int d^3q w_{S, i}(q) \varphi_{q, S, i}(r, \sigma_1, \sigma_2) \times \varphi_{q, S, i}(r', \sigma'_1, \sigma'_2) \exp\left\{i\mathbf{q}(R' - R)\right\} + \int d^3p d^3q w_{S, m_S}(p, q) \varphi^*_{p, q, S, m_S}(r, \sigma_1, \sigma_2) \times \varphi_{p, q, S, m_S}(r', \sigma'_1, \sigma'_2) \exp\left\{i\mathbf{q}(R' - R)\right\}. \quad (20)$$

Thus, from equations (19) and (20) we can see that $V w_{S, i}(q) d^3q$ is the number of the bound particle pairs with the spin $S$, in the state $i$ and with the total couple momentum $\hbar \mathbf{q}$ located in the infinitesimal volume $d^3q$. Respectively, $V^2 w_{S, m_S}(p, q) d^3p d^3q$ stands for the number of the 'dissociated' particle pairs in the state $(S, m_S)$ with the relative momentum $\hbar \mathbf{p}$ and total momentum $\hbar \mathbf{q}$ located in the infinitely small volumes $d^3p$ and $d^3q$.

In the center-of-mass system the replacement $\mathbf{p} \rightarrow -\mathbf{p}, \sigma_1 \rightarrow \sigma_2, \sigma_2 \rightarrow \sigma_1$ corresponds to the permutation of particles. So, the following symmetric relations take place:

$$w_{S, m_S}(p, q) = w_{S, m_S}(-p, q), \quad (21)$$

$$\varphi_{p, q, S, m_S}(r, \sigma_1, \sigma_2) = -\varphi_{p, q, S, m_S}(-r, \sigma_2, \sigma_1) = -\varphi_{-p, q, S, m_S}(r, \sigma_2, \sigma_1). \quad (22)$$

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 that can be diagonalized with the Bogoliubov transformation. Therefore, one is able to use the theorem of Wick, Bloch and De Dominicis

$$F_2(x_1, x_2; x'_1, x'_2) = \langle \psi^\dagger(x_1) \psi^\dagger(x_2) \psi(x'_2) \psi(x'_1) \rangle
\quad = \langle \psi^\dagger(x_1) \psi^\dagger(x_2) \rangle \langle \psi(x'_2) \psi(x'_1) \rangle
\quad + \langle \psi^\dagger(x_1) \psi(x_1) \rangle \langle \psi^\dagger(x_2) \psi(x'_2) \rangle - \langle \psi^\dagger(x_1) \psi(x'_2) \rangle \langle \psi^\dagger(x_2) \psi(x'_1) \rangle. \quad (23)$$
Further, for the 'normal' averages we have
\[
\langle \psi^\dagger(x_1)\psi(x'_1) \rangle = \langle \psi^\dagger(r_1, \sigma_1)\psi(r'_1, \sigma'_1) \rangle = \int \frac{d^3k}{(2\pi)^3} n(k) \exp\{ik(r'_1 - r_1)\} \Delta(\sigma_1 - \sigma'_1),
\]
(24)
where \( n(k) = \langle a^\dagger_{k,\sigma}a_{k,\sigma} \rangle \) gives the distribution of fermions over momenta, and we introduced the function
\[
\Delta(\sigma) = \begin{cases} 
0, & \sigma \neq 0, \\
1, & \sigma = 0.
\end{cases}
\]

'Anomalous' averages are given by
\[
\langle \psi(x_1)\psi(x'_1) \rangle = \langle \psi(r_1, \sigma_1)\psi(r'_1, \sigma'_1) \rangle = \int \frac{d^3k}{(2\pi)^3} (a_{k,\sigma}a_{k,-\sigma}) \exp\{ik(r'_1 - r_1)\} \Delta(\sigma_1 + \sigma'_1). 
\]
(25)
In the BCS–model, the quantity \( (a_{k,\sigma}a_{k,-\sigma}) \) can be represented in the following form
\[
(a_{k,\sigma}a_{k,-\sigma}) = \sqrt{m_0} \varphi(k) \frac{\text{sign}(\sigma)}{\sqrt{2}},
\]
(26)
with \( \varphi(k) \) obeying the normalization condition
\[
\int \frac{d^3k}{(2\pi)^3} |\varphi(k)|^2 = 1.
\]
(27)
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 \( a_k \) and \( a^\dagger_k \). Now, Eqs. (24), (25) and (26) allow us to rewrite (23) in the following form:
\[
F_2(x_1, x_2; x'_1, x'_2) = n_0\varphi(r)\chi_{0,0}(\sigma_1, \sigma_2)\varphi(r')\chi_{0,0}(\sigma'_1, \sigma'_2) + \sum_{S,m_S} \int \frac{d^3pd^3q}{(2\pi)^6} \left[ \frac{q}{2} + p \right] n\left[ \frac{q}{2} - p \right] \varphi_{p,S}(r)\chi_{S,m_S}(\sigma_1, \sigma_2) \times \varphi_{p,S}(r')\chi_{S,m_S}(\sigma'_1, \sigma'_2) \exp\{iq(R' - R)\}. 
\]
(28)
Here \( \varphi(r) \) is the Fourier transform of \( \varphi(k) \), for \( \varphi_{p,S}(r) \) we have
\[
\varphi_{p,S}(r) = \begin{cases} 
\sqrt{2}\cos(pr), & S = 0, \\
\sqrt{2}\sin(pr), & S = 1.
\end{cases}
\]
(29)
Respectively, the spinor \( \chi_{S,m_S}(\sigma_1, \sigma_2) \) stands for
\[
\chi_{S,m_S}(\sigma_1, \sigma_2) = \begin{cases} 
\Delta(\sigma_1 + \sigma_2)\text{sign}(\sigma_1)/\sqrt{2}, & S = 0, m_S = 0; \\
\Theta(-\sigma_1)\Theta(-\sigma_2), & S = 1, m_S = -1; \\
\Delta(\sigma_1 + \sigma_2)/\sqrt{2}, & S = 1, m_S = 0; \\
\Theta(\sigma_1)\Theta(\sigma_2), & S = 1, m_S = 1.
\end{cases}
\]
(30)
Here
\[
\Theta(\sigma) = \begin{cases} 
1, & \sigma \geq 0, \\
0, & \sigma < 0.
\end{cases}
\]
With (27), (29) and (30) one can easily be convinced that the normalization relations (16) and (17) are satisfied. Within the BCS–model \( w_{S,i}(q) = \Delta(S)|\Delta(i)| n_0 \delta(q) \) (\( \delta(q) \) is the \( \delta \)-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 \( w_{S,i}(q) \) acquires the \( \delta \)-functional singularity corresponding to some indices \( S_0 \) and \( i_0 \) or, in other words, the ratio \( N_{q,S_0,i_0}/V \) in the first sum of (19) does not vanish in the thermodynamic limit:
\[
w_{S,i}(q) = n_0\delta(q)\Delta(S - S_0)\Delta(\hat{i} - i_0) + w_{S,i}(q),
\]
(31)
where \( w_{S,i}(q) \) is the regular part of (31) giving the bound–pair distribution over nonzero momenta.

To do this, let us take the limit relation (5) and rewrite it with the variables (18) in the form
\[
F_2(x_1, x_2; x'_1, x'_2) \rightarrow \langle \psi^\dagger(x_1)\psi^\dagger(x_2) \rangle \times \langle \psi(x_2)\psi(x'_1) \rangle = n_0\varphi^*(r, \sigma_1, \sigma_2)\varphi(r', \sigma'_1, \sigma'_2). 
\]
(32)
where the functions \( \varphi^*(r, \sigma_1, \sigma_2) \) and \( \varphi(r', \sigma'_1, \sigma'_2) \) are introduced in such a way that the normalization condition (14) should be fulfilled. This can always be done because according to the principle of correlation weakening in
\[
\langle \psi(x_1)\psi(x_2) \rangle \rightarrow \langle \psi(x_1) \rangle \langle \psi(x_2) \rangle = 0
\]
when \( r \rightarrow \infty \) (see Ref. [1]). Expression (32) is exactly the contribution of the first singular term of (31) into (20). The contribution of the regular part of (11) and that of the 'dissociated' pair states into (20) are infinitely small in the situation of (1) according to the Riemann's theorem because
\[
|R' - R| = \left| \frac{r'_1 + r'_2}{2} - \frac{r_1 + r_2}{2} \right| \rightarrow \infty.
\]
Remark that the pair distribution over the scattering states (23) does not contain \( \delta \)-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 which is impossible for the Fermi systems.

Eq. (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 Eq. (16) and (30) gives
\[
n_0 = \frac{N_q=0,S_0,i_0}{V} = \sum_{\sigma_1,\sigma_2} \int d^3r |\langle \psi(r,\sigma_1)|\psi(0,\sigma_2)\rangle|^2 = \sum_{\sigma} \int \frac{d^3k}{(2\pi)^3} |\langle a_{k,\sigma}a_{-k,-\sigma} \rangle|^2,
\]

(33)

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

\[
\varphi(r,\sigma_1,\sigma_2) = \frac{1}{\sqrt{n_0}} (\psi(r,\sigma_1)|\psi(0,\sigma_2))
\]

\[
= \int \frac{d^3k}{(2\pi)^3} \langle a_{k,\sigma}a_{-k,-\sigma} \rangle \Delta(\sigma_1 + \sigma_2) \sqrt{n_0} \exp(ikr) = \frac{1}{\sqrt{n_0}} \Delta(\sigma_1 + \sigma_2) \varphi_s(r) \varphi_t(r),
\]

(34)

where \(\varphi_s(r) = \varphi_s(-r)\) and \(\varphi_t(r) = -\varphi_t(-r)\). According to Eq. (33) the first term in (33) corresponds to the singlet and the second, to the triplet components of the wave function of the condensed fermions. However, (34) 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 (34) one should select either \(\varphi_s(r) \neq 0, \varphi_t(r) = 0\) or \(\varphi_s(r) = 0, \varphi_t(r) \neq 0\). So, we have:

\[
\varphi(r,\sigma_1,\sigma_2) = \left\{ \begin{array}{l}
\varphi_s(r)\chi_{0,0}(\sigma_1,\sigma_2)/\sqrt{n_0}, \\
\varphi_t(r)\chi_{1,0}(\sigma_1,\sigma_2)/\sqrt{n_0}.
\end{array} \right.
\]

(35)

The phase coherence takes place for the condensed bound pairs due to the uncertainty relation \(\Delta \varphi \Delta N \approx 1\) for the phase \(\varphi\) and number of the bound fermion pairs \(N_0 = N_q=0,S_0,i_0\) in the state \((q = 0, S_0, i_0)\). In the thermodynamic limit the macroscopical occupation of this state results in \(\Delta N \approx \sqrt{N_0} \rightarrow \infty\) and, therefore, \(\Delta \varphi \rightarrow 0\). For the bound pair states beyond the condensate \(N_q,S,i\) is limited above even for \(V \rightarrow \infty\). Thus these states are not correlated with respect to the phase.

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

\[
N_0 = V \sum_{S,i} \int d^3q w_{S,i}(q)
\]

is proportional to the total number of particles \(N\). In particular, there is the inequality for the number of the condensed bound pair states

\[
N_0 \leq N.
\]

(36)

It should be emphasized that the inequality (36) 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 (36) with the inequality of Cauchy–Schwarz–Bogoliubov

\[
\langle \hat{A}\hat{B} \rangle^2 \leq \langle \hat{A}\hat{A}^\dagger \rangle\langle \hat{B}\hat{B}^\dagger \rangle.
\]

Indeed, assuming \(A = a_{k,\sigma}\) and \(B = a_{-k,-\sigma}\) we arrive at

\[
\langle a_{k,\sigma}a_{-k,-\sigma} \rangle^2 = \langle a_{k,\sigma}^\dagger a_{k,\sigma} \rangle \langle a_{-k,-\sigma}^\dagger a_{-k,-\sigma} \rangle \equiv (1 - n(k)) n(k).
\]

Then, from (33) we derive

\[
n_0 = \frac{N_0}{V} = \frac{1}{V} \sum_k \langle a_{k,\sigma}a_{-k,-\sigma} \rangle^2 \leq \frac{2}{V} \sum_k n(k) - n^2(k) \leq \frac{2}{V} \sum_k n(k) = \frac{N}{V} = n.
\]

(37)

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

\[
n_0 \leq \frac{2}{V} \sum_k D(n(k))
\]

demonstrates that the number of the condensed pairs is tightly connected with the ‘wash–out’ 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 BOGLIUBOV 1/Q² 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 \(w_{S,m}(p,q)\) is expressed in terms of the occupation numbers of the one–particle states \(n(k) = \langle a_{k,\sigma}^\dagger a_{k,\sigma} \rangle\). Indeed, on the one hand, in the limiting situation of (36) we have the relation (36), which can be written as

\[
F_2(x_1, x_2; x_1', x_2') = \int \frac{d^3p_1}{(2\pi)^3} \frac{n(p_1)}{n(p_1)} \exp(i p_1(r'_1 - r_1)) \Delta(\sigma_1 - \sigma_1')
\]

\[
\times \int \frac{d^3p_2}{(2\pi)^3} \frac{n(p_2)}{n(p_2)} \exp(i p_2(r'_2 - r_2)) \Delta(\sigma_2 - \sigma_2')
\]

\[
= \int d^3q d^3p \frac{n(q/2 + p)}{(2\pi)^3} \frac{n(q/2 - p)}{(2\pi)^3} \exp(i p(r' - r))
\]

\[
\times \exp(i q(R' - R)) \Delta(\sigma_1 - \sigma_1') \Delta(\sigma_2 - \sigma_2'),
\]

(38)
where, passing to the last equality, we introduced the new variables \( q = p_1 + p_2 \) and \( p = (p_1 - p_2)/2 \) and used notations (18). On the other hand, when (8) is true, we have

\[
    r = |r_2 - r_1| \to \infty, \quad r' = |r_2' - r_1'| \to \infty,
\]

\[
    |r + r'| \to \infty, \quad R' - R = \text{const}, \quad r' - r = \text{const}.
\]

Therefore, it follows from (14), (17) and (27) that in the limiting case (8) we have

\[
    F_2(x_1, x_2; x_1', x_2') \to
    \sum_{S, m_S} d^3 q d^3 p w_{S, m_S}(p, q) \varphi_{p, S}(r) \varphi_{p, S}(r')
    \times \chi_{S, m_S}(\sigma_1, \sigma_2) \chi_{S, m_S}(\sigma_1', \sigma_2') \exp(i(q(R' - R))),
\]

where we used notations (29) and (30). Further, the Riemann’s theorem is used while integrating over \( p \) and relation (21) allow us to rewrite (39) as

\[
    \chi_{S, m_S}(\sigma_1, \sigma_2) \chi_{S, m_S}(\sigma_1', \sigma_2') \exp(i(p(r' - r)) \exp(i(q(R' - R))). (40)
\]

The right–hand side of Eq. (38) is equal to that of (41) at all the values of the spin variables and space ones \( \bar{r} = r' - r \) and \( \bar{R} = R' - R \). Taking into account the completeness of the set of the spin functions (31) and we derive the following equality:

\[
    w_{S, m_S}(p, q) = \frac{n(q/2 + p) n(q/2 - p)}{(2\pi)^6}. (41)
\]

Thus, in the thermodynamic limit one can write

\[
    N_{p, q, S, m_S} = n(q/2 + p) n(q/2 - p). (42)
\]

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: \( \bar{w}_{S, i}(q) \neq 0 \) in (31) 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

\[
    \psi(r, \sigma) \to \psi(r, \sigma) \exp(i\chi(r)),
    \psi^\dagger(r, \sigma) \to \psi^\dagger(r, \sigma) \exp(-i\chi(r)). (43)
\]

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

\[
    \max_{\omega, S} N_{\omega, q, S} \geq \frac{C}{q^2},
\]

where \( N_{\omega, q, S} \) appears in Eq. (12) and \( \omega \) is the set of the quantum numbers corresponding to both the continuous spectrum \( (\omega = (p, m_S)) \) and the discrete one \( (\omega = i) \). However, Eq. (42) results in

\[
    N_{p, q, S, m_S} \leq 1
\]

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 \( S_0, i_0 \):

\[
    \bar{w}_{S_0, i_0}(q) = \frac{C'}{q^2}. (44)
\]

The BCS–model is not locally gauge invariant which results in absence of the noncondensed bound pairs: \( \bar{w}_{S, i}(q) = 0 \). 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. Remark that the distribution of the bound fermion pairs over the center–of–mass momenta obeys the inequality (44) with \( C' \propto k_B T n_0 \) (see Ref. 1). 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 \( C'' \propto k_B T \) (here \( n_0 \) denote the density of the condensed bosons). Therefore, there are fundamental parallels between the Bose gas and the considered subsystem of the fermion bound pairs. And 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. 1, 2, 3). Remark that possible experimental consequences of the existence of fermion bound pairs beyond the condensate can be found in paper 1 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, can not be treated on the same level. However, for \( q \to 0 \) (large wave lengths) a crystalline
lattice can be considered as continuum. Therefore, the derived result remains correct in this case.

Emphasize that the bound pair states can fully be a result of the collective effects. Indeed, as it was demonstrated by Cooper, 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.

At last, it is important to make one more remark on the connection between the \(1/q^2\) theorem of Bogoliubov and the Goldstone theorem. As it has been demonstrated in Ref.\(^{[4]}\), existence of the Goldstone mode in the Bose system results from the Bogoliubov theorem provided that 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 it is not the case for the Goldstone one. For example, in the case of 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. The similar situation is realized for the Fermi systems (see, e.g. Ref.\(^{[13]}\)).

V. CONCLUSION

Concluding, 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. Appearance of the condensate of the bound pair states \(\langle\psi_{n}\rangle\) implies the occurrence of the \(\delta\)–functional term in the distribution of the bound pairs over the momentum of the couple center of mass \(q\) (see Eq. \(\langle\psi_{n}\rangle\)). Using the space homogeneity of the system and the local gauge invariance \(\langle\psi_{n}\rangle\) of the fermion interaction, we have proved that there is the \(1/q^2\)-singularity in the distribution function \(\tilde{w}_{S_i}(q)\) provided that \(n_0 \neq 0\). Thus, we refined the \(1/q^2\) theorem of Bogoliubov, having proved the singularity to appear in \(\tilde{w}_{S_i}(q)\). Therefore, presence of the noncondensed bound pairs below \(T_c\) is the necessary condition of superconductivity.

A new simple proof of the Yang inequality for the Fermi systems \(\langle\psi_{n}\rangle\) and its stronger variant \(\langle\psi_{n}\rangle\) have also been derived as results of secondary importance.

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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 \(N – M\) particles.
10. Strictly speaking, this is valid for the \(s\)-wave pairing. In general case the gap in the single–particle spectrum becomes \(k\)-dependent, one usually suppose that \(\Delta = \Delta(k)\) 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. \(\langle\psi_{n}\rangle\)). As to the exact relation between the binding energy \(\varepsilon_b\) and the gap \(\Delta(k)\) in general case, it is 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 \(N/V = \text{const}, V \to \infty\).
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tion $f(q)$ (i.e. $f(q)$ does not contain $\delta$–function) we have

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provided the integral $\int d^3 q f(q) \exp(iqr)$ exists.

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24 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 (43).

Bogoliubov proved the theorem in the particular case of the $s$–wave pairing, i.e. when in (43) $\varphi_s(r) = \varphi(r)$, where $\varphi(r)$ is radially symmetric function. The proof can easily be extended to the more general case.

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