

## SUPERCONDUCTIVITY OF AN ELECTRON SYSTEM WITH SINGLET OR TRIPLET PAIRS

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The effect of the type of symmetry of the coordinate part of the electron (Cooper) pair wave function on the establishment of a superconducting state is investigated. The "exchange" parts of the matrix elements, characterizing the conduction-electron interactions induced by phonons, Coulomb forces, and also by spin waves of a ferro- or antiferromagnet, are determined. The effect which the "exchange" part of the interaction exerts on the establishment of a superconducting state with singlet or triplet pairs is discussed. The appropriate modifications in the theory, making it possible to include triplet pairs in the BCS,<sup>[15]</sup> Bogolyubov's canonical transformation,<sup>[16]</sup> and the double-time temperature-dependent Green's function<sup>[17]</sup> methods are considered.

1. The question of realization of a superconducting state with singlet or triplet (Cooper) pairs of conduction electrons has important significance for the problem of the coexistence of superconductivity and ferromagnetism,<sup>[1-3]</sup> antiferromagnetism,<sup>[4-6]</sup> paramagnetism,<sup>[7-9]</sup> and also the formation of Cooper pairs with nonzero angular momentum.<sup>[10-14]</sup> In this connection, it is of interest to investigate those properties of the superconducting state which only depend on the type of symmetry of the coordinate part of the singlet or triplet electron pair wave function.<sup>1)</sup>

In the present article, it is shown that the type of symmetry of the coordinate part of the electron pair wave function manifests itself, first of all, in the appearance of an "exchange" part of the matrix element, characterizing the transitions of these pairs and having different signs in the singlet and triplet states. In this lies the specific nature of the manifestation, in the superconducting region, of the singlet or triplet nature of the state of the electron pairs which, in other quantized two-electron systems (for example, in the helium atom or in the hydrogen molecules), leads to the appearance of an additional energy term of the type  $\pm A$ ,

usually interpreted as the exchange energy. In the case of the theory of superconductivity, the result indicated above turns out to be general and does not depend on whether the interaction of the conduction electrons is induced by virtual phonons, Coulomb forces, or virtual spin waves.<sup>2)</sup> In addition, trial wave functions corresponding to the BCS<sup>[15]</sup> method are constructed in the present article for a superconductor with singlet or triplet pairs, and the corresponding variational problem is solved. At the same time, we indicate those modifications which enable us to include triplet pairs in the method of Bogolyubov<sup>[16]</sup> and in the method of double-time temperature-dependent Green's functions.<sup>[17]</sup>

2. First let us consider the interaction of conduction electrons induced by virtual phonons. According to<sup>[15]</sup> the energy operator for this interaction has the following form:

$$H''_{ph} = \sum_{\mathbf{k}, \mathbf{k}'; \sigma, \sigma'; \mathbf{x}} V_{\mathbf{k}, \mathbf{k}', \mathbf{x}} c_{\mathbf{k}' - \mathbf{x}, \sigma'}^* c_{\mathbf{k}, \sigma}^* c_{\mathbf{k} + \mathbf{x}, \sigma} c_{\mathbf{k}, \sigma}, \quad (1)$$

where the matrix element

$$V_{\mathbf{k}, \mathbf{k}', \mathbf{x}} = \hbar \omega_{\mathbf{x}} |M_{\mathbf{x}}|^2 / [(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k} + \mathbf{x}})^2 - (\hbar \omega_{\mathbf{x}})^2] \quad (2)$$

has a negative sign for  $|\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k} + \mathbf{x}}| < \hbar \omega_{\mathbf{x}}$ , which corresponds to attraction between conduction electrons near the Fermi surface;  $c_{\mathbf{k}\sigma}^*$  and  $c_{\mathbf{k}\sigma}$  are the creation and annihilation operators for an elec-

<sup>1)</sup>These properties are not related, for example, to the assumption employed in a number of articles (for example,<sup>[3,5,8-12]</sup> and others) that the matrix element  $V_{\mathbf{k}, \mathbf{k}'}$  defining the interaction of conduction electrons, depends only on the angle between the wave vectors  $\mathbf{k}$  and  $\mathbf{k}'$ , but not on their magnitudes; neither are they related to the corresponding harmonic expansion of  $V_{\mathbf{k}, \mathbf{k}'}$  nor, finally, to the separation from this series of one or several terms with a definite orbital quantum number.

<sup>2)</sup>In spite of the assertion<sup>[1,3]</sup> that a change of sign of the entire matrix element, induced by virtual spin waves of a ferromagnet, occurs during the transition from singlet pairs to triplets, and not a change of sign of only the "exchange" part of this element.

tron with wave vector  $\mathbf{k}$  and spin projection  $\sigma$ ;  $\kappa$  and  $\omega_\kappa$  are the wave vector and spin frequency of the phonon;  $\epsilon_{\mathbf{k}}$  is the electron energy measured from the Fermi surface, and  $M_\kappa$  is the matrix element describing the electron-phonon interaction.

For pairing of electrons with opposite momenta, it follows from (1) that

$$H_{ph}'' = \sum_{\mathbf{k}, \mathbf{k}_1} V_{\mathbf{k}, \mathbf{k}_1} (c_{\mathbf{k}_1 \uparrow}^* c_{-\mathbf{k}_1 \uparrow}^* c_{-\mathbf{k} \uparrow} c_{\mathbf{k} \uparrow} + c_{\mathbf{k}_1 \downarrow}^* c_{-\mathbf{k}_1 \downarrow}^* c_{-\mathbf{k} \downarrow} c_{\mathbf{k} \downarrow} + c_{\mathbf{k}_1 \uparrow}^* c_{-\mathbf{k}_1 \downarrow}^* c_{-\mathbf{k} \downarrow} c_{\mathbf{k} \uparrow} + c_{\mathbf{k}_1 \downarrow}^* c_{-\mathbf{k}_1 \uparrow}^* c_{-\mathbf{k} \uparrow} c_{\mathbf{k} \downarrow}), \quad (3)$$

where, in contrast to [15], we retain along with transitions of pairs of electrons having opposite spin projections also the transitions of pairs of electrons whose components have the same spin projections. Accordingly, along with the usual operators

$$b_{\mathbf{k}} = c_{-\mathbf{k} \downarrow} c_{\mathbf{k} \uparrow}, \quad b_{\mathbf{k}}^* = c_{\mathbf{k} \uparrow}^* c_{-\mathbf{k} \downarrow}^*, \quad (4)$$

which describe the annihilation and creation of BCS pairs, [15] we also introduce the operators

$$b_{\mathbf{k}\sigma} = c_{-\mathbf{k}\sigma} c_{\mathbf{k}\sigma}, \quad b_{\mathbf{k}\sigma}^* = c_{\mathbf{k}\sigma}^* c_{-\mathbf{k}\sigma}^*, \quad (5)$$

where  $b_{\mathbf{k}\sigma}$  ( $b_{\mathbf{k}\sigma}^*$ ) describe the annihilation (creation) of an electron pair in the state  $(\mathbf{k}\sigma, -\mathbf{k}\sigma)$ . Then it follows from (3) that

$$H_{ph}'' = \sum_{\mathbf{k}, \mathbf{k}_1} V_{\mathbf{k}, \mathbf{k}_1} (b_{\mathbf{k}_1 \uparrow}^* b_{\mathbf{k} \uparrow} + b_{\mathbf{k}_1 \downarrow}^* b_{\mathbf{k} \downarrow} + b_{\mathbf{k}_1}^* b_{\mathbf{k}} + b_{-\mathbf{k}_1}^* b_{-\mathbf{k}}). \quad (6)$$

In this expression the operators  $b_{\mathbf{k}\sigma}$  describe pairs in the triplet state with spin projection  $s_z = \pm 1$ , which is evident from the definition (5), from which, in particular, it follows that

$$b_{-\mathbf{k}\sigma} = -b_{\mathbf{k}\sigma}, \quad (7)$$

as must also occur in the case of the antisymmetric coordinate part of the wave function of a pair whose components have opposite momenta.

As far as the BCS operators  $b_{\mathbf{k}}$  are concerned, they obviously do not possess an analogous property (since  $b_{-\mathbf{k}} \neq \pm b_{\mathbf{k}}$ ). This is due to the fact that the BCS operators  $b_{\mathbf{k}}^*$  create neither triplet nor singlet states, but states whose wave functions are only part of the wave function of a triplet or singlet state. Actually, for opposite momenta and opposite spins of the electrons in the pair, the wave function of the triplet or singlet states must contain the states <sup>3)</sup>  $\mathbf{k} \uparrow; -\mathbf{k} \downarrow; \mathbf{k} \uparrow; -\mathbf{k} \uparrow$ , whereas the BCS

operator  $b_{\mathbf{k}}^*$  operating on the vacuum only fills the states  $\mathbf{k} \uparrow$  and  $-\mathbf{k} \downarrow$ . In order to simultaneously fill the states  $\mathbf{k} \downarrow$  and  $-\mathbf{k} \uparrow$ , it is necessary, obviously, for the operator  $b_{-\mathbf{k}}^*$  also to act on the vacuum. This leads us to the definition of the operators  $B_{\mathbf{k}}^{*S}$ ,  $B_{\mathbf{k}}^{*T}$ ,  $B_{\mathbf{k}}^S$ ,  $B_{\mathbf{k}}^T$  for the creation and annihilation, respectively, of singlet (S) and triplet (T) electron pairs with opposite momentum components and zero projection of the total spin of the pair ( $s_z = 0$ ), in the form of the following linear combinations of BCS operators:

$$B_{\mathbf{k}}^{S,T} = (b_{\mathbf{k}} \pm b_{-\mathbf{k}})/\sqrt{2}, \quad B_{\mathbf{k}}^{*S,T} = (b_{\mathbf{k}}^* \pm b_{-\mathbf{k}}^*)/\sqrt{2}. \quad (8)$$

From (8) it follows, in the first place, that the operators for the annihilation and creation of singlet pairs introduced earlier by Cloizeaux [18] can be reduced to the same form as  $B_{\mathbf{k}}^S$  and  $B_{\mathbf{k}}^{*S}$ . As far as the triplet pair operators are concerned, they were not introduced in [18], apparently owing to the author's viewpoint that the triplet pair contributions mutually cancel (this does not always occur, as will be shown below). Second, in order to avoid misunderstandings, we immediately remark that the fact noted above, that the BCS operators  $b_{\mathbf{k}}^*$  by themselves do not create singlet pairs, does not contradict the statement repeatedly expressed in the literature that the BCS theory [15] describes the singlet state. The reason for this circumstance will be explained below as we analyze the wave function for the singlet state of a superconductor.

The following relations for the operators  $B_{\mathbf{k}}^S$  and  $B_{\mathbf{k}}^T$  follow from (8):

$$B_{-\mathbf{k}}^S = B_{\mathbf{k}}^S, \quad B_{-\mathbf{k}}^T = -B_{\mathbf{k}}^T; \quad (9)$$

$$B_{\mathbf{k}}^S B_{\mathbf{k}}^T = 0, \quad (B_{\mathbf{k}}^S)^2 = -(B_{\mathbf{k}}^T)^2 = b_{\mathbf{k}} b_{-\mathbf{k}}, \quad (10)$$

$$(B_{\mathbf{k}}^S)^3 = (B_{\mathbf{k}}^T)^3 = 0;$$

$$[B_{\mathbf{k}}^{*S}, B_{\mathbf{k}_1}^S] = \frac{1}{2} (2 - n_{\mathbf{k} \uparrow} - n_{\mathbf{k} \downarrow} - n_{-\mathbf{k} \uparrow} - n_{-\mathbf{k} \downarrow}) \times (\delta_{\mathbf{k}, \mathbf{k}_1} + \delta_{\mathbf{k}, -\mathbf{k}_1}), \quad [B_{\mathbf{k}}^S, B_{\mathbf{k}_1}^S] = 0, \quad (11)$$

$$[B_{\mathbf{k}}^{*T}, B_{\mathbf{k}_1}^T] = \frac{1}{2} (2 - n_{\mathbf{k} \uparrow} - n_{\mathbf{k} \downarrow} - n_{-\mathbf{k} \uparrow} - n_{-\mathbf{k} \downarrow}) \times (\delta_{\mathbf{k}, \mathbf{k}_1} - \delta_{\mathbf{k}, -\mathbf{k}_1}), \quad [B_{\mathbf{k}}^T, B_{\mathbf{k}_1}^T] = 0, \quad (12)$$

$$[B_{\mathbf{k}}^{*T}, B_{\mathbf{k}_1}^S] = \frac{1}{2} (n_{-\mathbf{k} \uparrow} + n_{\mathbf{k} \downarrow} - n_{\mathbf{k} \uparrow} - n_{-\mathbf{k} \downarrow}) \times (\delta_{\mathbf{k}, \mathbf{k}_1} + \delta_{\mathbf{k}, -\mathbf{k}_1}), \quad [B_{\mathbf{k}}^T, B_{\mathbf{k}_1}^S] = 0, \quad (13)$$

here  $n_{\mathbf{k}\sigma}$  is the occupation number of the state with wave vector  $\mathbf{k}$  and spin projection  $\sigma$ . It is obvious from (9) that the operators  $B_{\mathbf{k}}^S$  and  $B_{\mathbf{k}}^T$  satisfy the required symmetry properties for the coordinate part of the pair wave function (since  $B_{\mathbf{k}}^T$  changes

<sup>3)</sup>This is obvious, for example, from the expression for the wave function  $\Psi = [\psi_{\mathbf{k}}(1)\psi_{-\mathbf{k}}(2) \pm \psi_{\mathbf{k}}(2)\psi_{-\mathbf{k}}(1)][L(1)R(2) \pm L(2)R(1)]$  where the upper signs refer to the singlet state, the lower signs refer to the triplet state, and L and R denote spin functions with, respectively, "left-handed" or "right-handed" spin projections.

sign upon replacing  $\mathbf{k}$  by  $-\mathbf{k}$ , the same as, according to (7),  $b_{\mathbf{k}\sigma}$  does, whereas  $B_{\mathbf{k}}^S$  does not change sign), so that they actually describe, respectively, singlet and triplet pairs with  $s_z = 0$ .

Returning now to the interaction energy operator (6), we note that the following expressions follow from (8) [in accordance with (9)]:

$$b_{\pm\mathbf{k}} = (B_{\mathbf{k}}^S \pm B_{\mathbf{k}}^T)/\sqrt{2}. \quad (14)$$

Accordingly one can rewrite (6) in the form

$$H''_{ph} = \sum_{\mathbf{k}, \mathbf{k}_1} V_{\mathbf{k}, \mathbf{k}_1} (b_{\mathbf{k}_1\uparrow}^* b_{\mathbf{k}\uparrow} + b_{\mathbf{k}_1\downarrow}^* b_{\mathbf{k}\downarrow} + B_{\mathbf{k}_1}^{*S} B_{\mathbf{k}}^S + B_{\mathbf{k}_1}^{*T} B_{\mathbf{k}}^T). \quad (15)$$

Using (9), it is now not difficult to obtain the following expression for  $H''_{ph}$ :

$$H''_{ph} = \sum'_{\mathbf{k}, \mathbf{k}_1} [F_{\mathbf{k}, \mathbf{k}_1} B_{\mathbf{k}_1}^{*S} B_{\mathbf{k}}^S + R_{\mathbf{k}, \mathbf{k}_1} (B_{\mathbf{k}_1}^{*T} B_{\mathbf{k}}^T + b_{\mathbf{k}_1\uparrow}^* b_{\mathbf{k}\uparrow} + b_{\mathbf{k}_1\downarrow}^* b_{\mathbf{k}\downarrow})], \quad (16)$$

where

$$\left. \begin{array}{l} F_{\mathbf{k}, \mathbf{k}_1} \\ R_{\mathbf{k}, \mathbf{k}_1} \end{array} \right\} = V_{\mathbf{k}, \mathbf{k}_1} + V_{-\mathbf{k}, -\mathbf{k}_1} \pm (V_{-\mathbf{k}, \mathbf{k}_1} + V_{\mathbf{k}, -\mathbf{k}_1}); \quad (17)$$

the prime on the summation sign means that the summation is performed over all values of  $\mathbf{k}$  with  $k_z > 0$ .

It is clear from (16) and (17) that the singlet pair transitions are determined by the matrix element  $F_{\mathbf{k}, \mathbf{k}_1}$ , whereas the triplet pair transitions (both with  $s_z = 0$  as well as with  $s_z = \pm 1$ ) are determined by one and the same matrix element  $R_{\mathbf{k}, \mathbf{k}_1}$ . It is also obvious from (17) that in the present case the quantity  $V_{-\mathbf{k}, \mathbf{k}_1} + V_{\mathbf{k}, -\mathbf{k}_1}$ , which is to be added to the "nonexchange" part  $V_{\mathbf{k}, \mathbf{k}_1} + V_{-\mathbf{k}, -\mathbf{k}_1}$  in the case of singlet pairs and is subtracted from it in the case of triplet pairs, plays the role of the "exchange" part of the interaction energy matrix element, mentioned in Sec. 1. The same is obviously also true for the Coulomb interaction, whose operator, according to [15], has exactly the same form as  $H''_{ph}$ , differing from it only by the fact that the Coulomb matrix element is subtracted (near the Fermi surface) from the phonon matrix element  $V_{\mathbf{k}, \mathbf{k}_1}$ . Hence it follows that the usual statement that the interaction induced by virtual phonons leads to attraction near the Fermi surface, but the Coulomb interaction leads to repulsion of conduction electrons, is valid only for the singlet states or for the nonexchange part of the matrix element determining the triplet pair transitions. As far as the exchange part of this matrix element is concerned, in the case of the interaction induced by virtual phonons, it leads to the repulsion of electrons in triplet pair states

(near the Fermi surface), but in the case of the Coulomb interaction it leads to their mutual attraction. We also remark that the matrix element  $F_{\mathbf{k}, \mathbf{k}_1}$  determining the singlet pair transitions is even (in the sense of change of sign upon a change from  $\mathbf{k}$  to  $-\mathbf{k}$ , or from  $\mathbf{k}_1$  to  $-\mathbf{k}_1$ ), whereas the matrix element  $R_{\mathbf{k}, \mathbf{k}_1}$  determining the triplet pair transitions is (in accordance with [7] and [10]) odd and therefore, in general, alternating in sign near the Fermi surface.

3. Now let us investigate the interaction of the conduction electrons induced by the spin waves of a ferromagnet. According to [2] (or [3]) one can write the energy operator of this interaction in the form

$$H''_{fm} = \sum_{\mathbf{k}, \mathbf{k}', \mathbf{g}} 2\tilde{V}_{\mathbf{k}, \mathbf{k}', \mathbf{g}} c_{\mathbf{k}'\downarrow}^* c_{\mathbf{k}+\mathbf{g}, \uparrow} c_{\mathbf{k}\uparrow}^* c_{\mathbf{k}-\mathbf{g}, \downarrow}, \quad (18)$$

where the matrix element

$$V_{\mathbf{k}, \mathbf{k}', \mathbf{g}} = a^2 \Theta^2 / 2 (\epsilon_{\mathbf{k}\uparrow} - \epsilon_{\mathbf{k}-\mathbf{g}, \downarrow} - \hbar\tilde{\omega}_{\mathbf{g}})$$

is negative for  $\epsilon_{\mathbf{k}\uparrow} - \epsilon_{\mathbf{k}-\mathbf{g}, \downarrow} < \hbar\tilde{\omega}_{\mathbf{g}}$ ;  $a$  is the lattice constant;  $\Theta$  is the "magnetization" energy of the conduction electron ( $\epsilon_{\mathbf{k}\sigma} = \epsilon_{\mathbf{k}} + 2\sigma\Theta$ , where  $\sigma = \pm 1/2$ ), due to its exchange interaction [19] with the oriented spins of the electrons belonging to inner unfilled d- or f-shells of the ferromagnet, and  $\hbar\tilde{\omega}_{\mathbf{g}}$  is the energy of a spin wave with wave vector  $\mathbf{g}$ . In the case of electron pairs with zero momentum, [15] from (18) it follows that

$$H''_{fm} = - \sum_{\mathbf{k}, \mathbf{k}_1} 2\tilde{V}_{\mathbf{k}, \mathbf{k}_1} c_{\mathbf{k}_1\uparrow}^* c_{-\mathbf{k}_1\downarrow}^* c_{\mathbf{k}\downarrow} c_{-\mathbf{k}\uparrow}, \quad (19)$$

which, according to (5), one can express in terms of the BCS operators in the form

$$H''_{fm} = - \sum_{\mathbf{k}, \mathbf{k}_1} 2\tilde{V}_{\mathbf{k}, \mathbf{k}_1} b_{\mathbf{k}_1}^* b_{-\mathbf{k}}. \quad (20)$$

The presence in (20) of the other sign in comparison with the right side of (6) is due to the fact that upon emission or absorption of a spin wave a change of sign of the spin projection of the conduction-electron state occurs. Therefore, in order to obtain the order of the operators  $c_{\mathbf{k}\sigma}$ , in which they are arranged in (19), one additional [in comparison with (3)] permutation of the Fermi operators is required, which also leads to the appearance of the minus sign. [20, 2] Furthermore, the fact that unlike (6) the operators  $b_{\mathbf{k}\sigma}$  from (5) do not appear in (20) is due to the fact that [as is also evident from (18)] the exchange by virtual spin waves occurs only between electrons with opposite spin projections. Accordingly, in this case it is sufficient to confine our attention to the operators  $B_{\mathbf{k}}^S$  and  $B_{\mathbf{k}}^T$  which describe pairs with  $s_z = 0$ . Considering (14), we obtain from (20)

$$H''_{\text{fm}} = - \sum'_{\mathbf{k}, \mathbf{k}_1} (\tilde{F}_{\mathbf{k}, \mathbf{k}_1} B_{\mathbf{k}}^{*S} B_{\mathbf{k}}^S + \tilde{R}_{\mathbf{k}, \mathbf{k}_1} B_{\mathbf{k}}^{*T} B_{\mathbf{k}}^T), \quad (21)$$

$$\left. \begin{array}{l} \tilde{F}_{\mathbf{k}, \mathbf{k}_1} \\ \tilde{R}_{\mathbf{k}, \mathbf{k}_1} \end{array} \right\} = \tilde{V}_{\mathbf{k}, -\mathbf{k}_1} + \tilde{V}_{-\mathbf{k}, \mathbf{k}_1} \pm (\tilde{V}_{\mathbf{k}, \mathbf{k}_1} + \tilde{V}_{-\mathbf{k}, -\mathbf{k}_1}). \quad (22)$$

It is clear from (21) and (22) that in the case of exchange by virtual spin waves of a ferromagnet, the singlet pair transitions are determined by the even matrix element  $\tilde{F}_{\mathbf{k}, \mathbf{k}_1}$ , and the triplet pair transitions with  $s_z = 0$  are determined by the odd matrix element  $\tilde{R}_{\mathbf{k}, \mathbf{k}_1}$ . In this case the quantity  $\tilde{V}_{\mathbf{k}, \mathbf{k}_1} + \tilde{V}_{-\mathbf{k}, -\mathbf{k}_1}$  here plays the role of the "exchange" part indicated in Sec. 1. Thus, in the case of the interaction induced by spin waves, as also in the above-considered case of phonons, the transition from singlet to triplet pairs does not involve (in contrast to [1]) a change of sign of the entire matrix element, but leads to a change of sign of only its "exchange" part.

If we now consider the transitions of pairs with  $s_z = 0$ , induced by either virtual phonons and virtual spin waves of a ferromagnet, then from (16), (17) and (21), (22) we obtain

$$H'' = \sum'_{\mathbf{k}, \mathbf{k}_1} (F'_{\mathbf{k}, \mathbf{k}_1} B_{\mathbf{k}}^{*S} B_{\mathbf{k}}^S + R'_{\mathbf{k}, \mathbf{k}_1} B_{\mathbf{k}}^{*T} B_{\mathbf{k}}^T), \quad (23)$$

$$\left. \begin{array}{l} F'_{\mathbf{k}, \mathbf{k}_1} \\ R'_{\mathbf{k}, \mathbf{k}_1} \end{array} \right\} = (V_{\mathbf{k}, \mathbf{k}_1} \mp \tilde{V}_{\mathbf{k}, \mathbf{k}_1}) + (V_{-\mathbf{k}, -\mathbf{k}_1} \mp \tilde{V}_{-\mathbf{k}, -\mathbf{k}_1}) \\ \pm (V_{-\mathbf{k}, \mathbf{k}_1} \mp \tilde{V}_{-\mathbf{k}, \mathbf{k}_1}) \pm (V_{\mathbf{k}, -\mathbf{k}_1} \mp \tilde{V}_{\mathbf{k}, -\mathbf{k}_1}). \quad (24)$$

It is obvious from (24) that in the case of singlet pairs the "phonon" matrix elements  $V_{\mathbf{k}, \mathbf{k}_1}$  and the "spin" matrix elements  $\tilde{V}_{\mathbf{k}, \mathbf{k}_1}$  are subtracted, so that the spin waves in this case prevent (in accordance with [2]) the formation of a superconducting state. However, in the case of triplet pairs the indicated matrix elements are added to each other, so that formally one obtains the conclusion of A. Akhiezer and I. Akhiezer [3], that in this case it is necessary to take the corresponding "phonon" and "spin" matrix elements with the same signs. It is necessary, however, to emphasize that here this result has been obtained not owing to the change of sign of the matrix element  $\tilde{V}_{\mathbf{k}, \mathbf{k}_1}$  upon transition from singlet pairs to triplet pairs (as would occur in the case of a relation of the form [3]  $V_{\mathbf{k}, \mathbf{k}_1} = V_{\mathbf{k}, \mathbf{k}_1}^{\text{ph}} + (-1)^l V_{\mathbf{k}, \mathbf{k}_1}$ , where  $l = 0$  or  $1$ ), but owing to the circumstance that the electron transition is determined in the case of virtual phonon exchange by the matrix element  $V_{\mathbf{k}, \mathbf{k}_1}$ , and in the case of virtual spin wave exchange it is determined by the matrix element  $\tilde{V}_{\mathbf{k}, -\mathbf{k}_1}$ . In addition, it does not follow from (24) that spin waves necessarily lead in the triplet state to attraction

of conduction electrons near the Fermi surface, since  $R'_{\mathbf{k}, \mathbf{k}_1}$  and  $\tilde{R}_{\mathbf{k}, \mathbf{k}_1}$  are, in general, alternating in sign. Finally, it is also necessary to take into account that we obtained (24) for electron pairs with zero momentum, but not for Akhiezer-Pomeranchuk (AP) pairs [1-3] having nonzero momentum, since the ends of the momenta of the components of the pairs lie in the latter case near the different Fermi momentum spheres (displaced with respect to one another by the energy  $2\Theta$ ) for conduction electrons with different spin projections. In the latter case, it is impossible in general to investigate separately the singlet and triplet states, since the AP pairs are neither singlet nor triplet.<sup>4)</sup>

In this sense the AP pairs are similar to the BCS pairs considered above, which are likewise neither singlet nor triplet. However, while it is possible, as shown above, to construct triplet or singlet combinations from the BCS pairs, it is in general impossible to construct such combinations from AP pairs, since transitions of isolated parts of such combinations correspond in a ferromagnet to different matrix elements. This leads to the instability of the singlet or triplet combinations of AP pairs, which is manifest mathematically in the appearance in the interaction Hamiltonian, together with the already considered terms of the type  $B^{*S} B^S$  and  $B^{*T} B^T$ , of also terms of the form  $B^{*S} B^T$  and  $B^{*T} B^S$  (a more detailed account of this question is given in [21]). We also note that the displacement of the Fermi momentum surfaces for conduction electrons of a ferromagnet with opposite spin projections does not completely exclude the formation of electron pairs with zero momentum in the case of sufficiently weak  $s$ - $d$  or  $s$ - $f$  exchange, provided these pairs are formed outside the region of the shift, [22] or if the  $s$ - $d$  or  $s$ - $f$  exchange is so weak that the shift mentioned turns out to be energetically less favored. [23-25]

4. For an investigation of the interaction of conduction electrons induced by the spin waves of an antiferromagnet, one can start, for example, from the interaction Hamiltonian [5]

$$H''_{\text{afm}} = \sum_{\mathbf{k}, \mathbf{k}_1, \sigma} V_{\mathbf{k}, \mathbf{k}_1}^{\sigma} c_{\mathbf{k}_1, \sigma}^* c_{-\mathbf{k}_1, -\sigma} c_{\mathbf{k}, -\sigma}; \quad (25)$$

here the matrix element

$$V_{\mathbf{k}, \mathbf{k}_1}^{\sigma} = \frac{2I^2 \mu}{v M_0} \frac{\tilde{\omega}_{\mathbf{k}+\mathbf{k}_1}^2}{A_{\mathbf{k}+\mathbf{k}_1} + B_{\mathbf{k}+\mathbf{k}_1}} \frac{1}{(e_{\mathbf{k}} - e_{\mathbf{k}_1})^2 - \tilde{\omega}_{\mathbf{k}+\mathbf{k}_1}^2} \quad (26)$$

is negative near the Fermi surface, where

<sup>4)</sup>This is precisely why we did not make a distinction between singlet and triplet AP pairs in a previous article [2], a fact subjected to what appears to us to be unjustified criticism in [3].

$|\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}_1}| < \tilde{\omega}_{\mathbf{k}+\mathbf{k}_1}$ , and the quantities  $I, \mu, \nu, M_0, \tilde{\omega}, A_{\mathbf{k}+\mathbf{k}_1}, B_{\mathbf{k}+\mathbf{k}_1}$  have the same meaning as in the article by Privorotskii.<sup>[5]</sup>

Only electrons with opposite spins interact in (25), the same as in (18). Accordingly, one can express (25) in terms of the BCS operators (4) in the form

$$H''_{\text{afm}} = - \sum_{\mathbf{k}, \mathbf{k}_1} V_{\mathbf{k}, -\mathbf{k}_1}^a (b_{\mathbf{k}_1}^* b_{\mathbf{k}} + b_{-\mathbf{k}_1}^* b_{-\mathbf{k}}), \quad (27)$$

where the minus sign in front of the sum has the same origin as in the right side of (20). Now transforming to the operators  $B_{\mathbf{k}}^S$  and  $B_{\mathbf{k}}^T$  in (27), according to (14) we obtain

$$H''_{\text{afm}} = - \sum'_{\mathbf{k}, \mathbf{k}_1} (F_{\mathbf{k}, \mathbf{k}_1}^a B_{\mathbf{k}_1}^{*S} B_{\mathbf{k}}^S + R_{\mathbf{k}, \mathbf{k}_1}^a B_{\mathbf{k}_1}^{*T} B_{\mathbf{k}}^T), \quad (28)$$

where

$$\left. \begin{matrix} F_{\mathbf{k}, \mathbf{k}_1}^a \\ R_{\mathbf{k}, \mathbf{k}_1}^a \end{matrix} \right\} = V_{\mathbf{k}, -\mathbf{k}_1}^a + V_{-\mathbf{k}, \mathbf{k}_1}^a \pm (V_{\mathbf{k}, \mathbf{k}_1}^a + V_{-\mathbf{k}, -\mathbf{k}_1}^a). \quad (29)$$

Thus, in the case of conduction-electron interaction induced by virtual spin waves of an antiferromagnet, the role of the exchange part is played by the quantity  $V_{\mathbf{k}, \mathbf{k}_1}^a + V_{-\mathbf{k}, -\mathbf{k}_1}^a$ , which enters with a plus sign in the even matrix element  $F_{\mathbf{k}, \mathbf{k}_1}^a$  determining the singlet pair transitions, and enters with a minus sign into the odd matrix element  $R_{\mathbf{k}, \mathbf{k}_1}^a$  determining the triplet-pair transitions. In this connection, in accordance with<sup>[4-6]</sup>, the spin waves of an antiferromagnet lead, near the Fermi surface, to the repulsion of conduction electrons whose pairs are in the singlet state. According to the estimates of Baltensperger and Strässler,<sup>[6]</sup> however, this circumstance does not exclude the possibility of coexistence of superconductivity and antiferromagnetism, in view of the quite possible predominance of the stronger attraction due to virtual phonons. As far as the triplet state is concerned, here, according to (29), only the nonexchange part of the matrix element  $R_{\mathbf{k}, \mathbf{k}_1}^a$  leads, near the Fermi surface, to the mutual repulsion of the conduction electrons in an antiferromagnet, whereas the exchange part leads to their mutual attraction.

5. Now let us consider trial wave functions describing singlet or triplet electron pair states of a superconductor. According to (10) (with account of the fact that  $(B_{\mathbf{k}}^S)^3 = (B_{\mathbf{k}}^T)^3 = 0$ ), these functions may contain the operators  $B_{\mathbf{k}}^S$  and  $B_{\mathbf{k}}^T$  in powers not higher than the second. Therefore, it is natural to write these functions in the form

$$\Psi^S = \prod'_{\mathbf{k}} [(1 - \alpha_{\mathbf{k}} - \beta_{\mathbf{k}})^{1/2} + \beta_{\mathbf{k}}^{1/2} B_{\mathbf{k}}^{*S}] + \alpha_{\mathbf{k}}^{1/2} (B_{\mathbf{k}}^{*S})^2 \Psi_v, \quad (30)$$

$$\Psi^T = \prod'_{\mathbf{k}} [(1 - \gamma_{\mathbf{k}} - \delta_{\mathbf{k}})^{1/2} + \delta_{\mathbf{k}}^{1/2} B_{\mathbf{k}}^{*T}] + \gamma_{\mathbf{k}}^{1/2} (B_{\mathbf{k}}^{*T})^2 \Psi_v, \quad (31)$$

where the primes on the product sign have the same meaning as the prime on the summation sign in Eq. (16);  $\Psi_v$  is the wave function of the vacuum, and  $\beta_{\mathbf{k}}, \alpha_{\mathbf{k}}, \delta_{\mathbf{k}}$ , and  $\gamma_{\mathbf{k}}$  are the desired occupation probabilities, respectively, of the states  $B_{\mathbf{k}}^{*S} \Psi_v, (B_{\mathbf{k}}^{*S})^2 \Psi_v, B_{\mathbf{k}}^{*T} \Psi_v$ , and  $(B_{\mathbf{k}}^{*T})^2 \Psi_v$ . In this connection, desiring to investigate simultaneously the effect of both phonons and spin waves, we include in Eqs. (30) and (31) only the singlet and triplet states with  $s_z = 0$ .

Taking this limitation into account, it is not difficult to also obtain the functions (30), (31) by means of a generalization of the unitary transformation of Yosida's article,<sup>[26]</sup> where it was shown that the transition from the variational method of BCS<sup>[15]</sup> to the canonical transformation method of Bogolyubov<sup>[16]</sup> can be accomplished by means of the unitary operator  $e^{iU}$ , where

$$U = -i \sum_{\mathbf{k}} \theta_{\mathbf{k}} (b_{\mathbf{k}}^* - b_{\mathbf{k}}). \quad (32)$$

For this we take<sup>[27]</sup>

$$\begin{aligned} U_S &= -i \sum_{\mathbf{k}} V \sqrt{2} \theta_{\mathbf{k}} (B_{\mathbf{k}}^{*S} - B_{\mathbf{k}}^S), \\ U_T &= -i \sum_{\mathbf{k}} V \sqrt{2} \varphi_{\mathbf{k}} (B_{\mathbf{k}}^{*T} - B_{\mathbf{k}}^T), \end{aligned} \quad (33)$$

where  $U_S$  and  $U_T$  are written for singlet and triplet states, respectively. Then we obtain

$$\begin{aligned} \alpha_{\pm \mathbf{k}}^S &= e^{iU_S} c_{\pm \mathbf{k} \uparrow} e^{-iU_S} = \cos \theta_{\mathbf{k}} c_{\pm \mathbf{k} \uparrow} - \sin \theta_{\mathbf{k}} c_{\mp \mathbf{k} \downarrow}^*, \\ \alpha_{\pm \mathbf{k}}^T &= e^{iU_T} c_{\mp \mathbf{k} \downarrow} e^{-iU_T} = \cos \theta_{\mathbf{k}} c_{\mp \mathbf{k} \downarrow} + \sin \theta_{\mathbf{k}} c_{\pm \mathbf{k} \uparrow}^*, \end{aligned} \quad (34)$$

which, after introducing the notation

$$\cos \theta_{\mathbf{k}} = u_{\mathbf{k}}, \quad \sin \theta_{\mathbf{k}} = v_{\mathbf{k}}, \quad u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2 = 1, \quad (35)$$

coincides with the canonical transformation of<sup>[16]</sup> which thus remains unchanged for singlet pairs.

On the other hand, operating on the vacuum wave function (with respect to the initial  $c$ -particles)  $\Psi_v$  with the operator  $e^{iU_S}$ , we obtain

$$\begin{aligned} e^{iU_S} \Psi_v &= \prod'_{\mathbf{k}} [\cos^2 \theta_{\mathbf{k}} + \sqrt{2} \sin \theta_{\mathbf{k}} \cos \theta_{\mathbf{k}} B_{\mathbf{k}}^{*S}] \\ &+ \sin^2 \theta_{\mathbf{k}} (B_{\mathbf{k}}^{*S})^2 \Psi_v, \end{aligned} \quad (36)$$

which coincides with the wave function (30) after introduction of the notation

$$\begin{aligned} \cos^2 \theta_{\mathbf{k}} &= (1 - \alpha_{\mathbf{k}} - \beta_{\mathbf{k}})^{1/2}, \quad \sqrt{2} \sin \theta_{\mathbf{k}} \cos \theta_{\mathbf{k}} = \beta_{\mathbf{k}}^{1/2}, \\ \sin^2 \theta_{\mathbf{k}} &= \alpha_{\mathbf{k}}^{1/2} \end{aligned} \quad (37)$$

Further, it is not difficult to see that (30) in turn coincides with the trial wave function (2.13) of the BCS article:<sup>[15]</sup>

$$\begin{aligned}\Psi_{\text{BCS}} &= \prod_{\mathbf{k}} [(1 - h_{\mathbf{k}})^{1/2} + h_{\mathbf{k}}^{1/2} b_{\mathbf{k}}^*] \Psi_{\nu} \\ &= \prod'_{\mathbf{k}} [(1 - h_{\mathbf{k}}) + h_{\mathbf{k}}^{1/2} (1 - h_{\mathbf{k}})^{1/2} (b_{\mathbf{k}}^* + b_{-\mathbf{k}}^*) \\ &\quad + h_{\mathbf{k}} b_{\mathbf{k}}^* b_{-\mathbf{k}}^*] \Psi_{\nu},\end{aligned}\quad (38)$$

where the fact that  $h_{-\mathbf{k}} = h_{\mathbf{k}}$  has been taken into account. Furthermore, taking account of (8) and (10) and introducing the notation

$$\begin{aligned}1 - h_{\mathbf{k}} &= (1 - \alpha_{\mathbf{k}} - \beta_{\mathbf{k}})^{1/2}, & \sqrt{2} h_{\mathbf{k}}^{1/2} (1 - h_{\mathbf{k}})^{1/2} &= \beta_{\mathbf{k}}^{1/2}, \\ h_{\mathbf{k}} &= \alpha_{\mathbf{k}}^{1/2},\end{aligned}\quad (39)$$

it is easy to see that the BCS function (38) actually coincides with (30). This also explains the fact mentioned above in Sec. 2 that, although the BCS operators  $b_{\mathbf{k}}^*$  do not create singlet or triplet pairs, nevertheless the BCS wave function (2.13) describes just the singlet state.

In the case of triplet pairs we have

$$\begin{aligned}\alpha_{\pm\mathbf{k}}^T &= e^{iU_T} c_{\pm\mathbf{k}\uparrow} e^{-iU_T} = \cos \varphi_{\mathbf{k}} c_{\pm\mathbf{k}\uparrow} \mp \sin \varphi_{\mathbf{k}} c_{\mp\mathbf{k}\downarrow}^*, \\ \alpha_{\mp\mathbf{k}}^T &= e^{iU_T} c_{\mp\mathbf{k}\downarrow} e^{-iU_T} = \cos \varphi_{\mathbf{k}} c_{\mp\mathbf{k}\downarrow} \pm \sin \varphi_{\mathbf{k}} c_{\pm\mathbf{k}\uparrow}^*.\end{aligned}\quad (40)$$

On the other hand, acting on  $\Psi_{\nu}$  with the operator  $e^{iU_T}$  and introducing the notation

$$\begin{aligned}\cos^2 \varphi_{\mathbf{k}} &= (1 - \gamma_{\mathbf{k}} - \delta_{\mathbf{k}})^{1/2}, & \sqrt{2} \sin \varphi_{\mathbf{k}} \cos \varphi_{\mathbf{k}} &= \delta_{\mathbf{k}}^{1/2}, \\ \sin^2 \varphi_{\mathbf{k}} &= \gamma_{\mathbf{k}}^{1/2},\end{aligned}\quad (41)$$

we return to the trial wave function (31).

It follows from (34) and (40) that for both singlet and triplet pairs (with  $s_Z = 0$ ) one can write the canonical transformation<sup>[16]</sup> in the same form:

$$u_{\mathbf{k}} = u_{\mathbf{k}} c_{\mathbf{k}\uparrow} - v_{\mathbf{k}} c_{-\mathbf{k}\downarrow}^*, \quad \alpha_{\mathbf{k}_i} = u_{\mathbf{k}} c_{-\mathbf{k}\downarrow} + v_{\mathbf{k}} c_{\mathbf{k}\uparrow}^*, \quad (42)$$

imposing, however, different conditions on  $v_{\mathbf{k}}$  in this connection. Namely, in the case of singlet pairs it is necessary to put

$$u_{-\mathbf{k}} = u_{\mathbf{k}}, \quad v_{-\mathbf{k}} = v_{\mathbf{k}}, \quad (43)$$

and in the case of triplet pairs it is necessary to require

$$u_{-\mathbf{k}} = u_{\mathbf{k}}, \quad v_{-\mathbf{k}} = -v_{\mathbf{k}}. \quad (44)$$

Triplet pairs (with  $s_Z = 0$ ) may also be included in similar fashion in the double-time Green's function method, where for the average values of the type  $A_{\mathbf{k}} = \langle c_{\mathbf{k}\uparrow}^* c_{-\mathbf{k}\downarrow}^* \rangle$  it is necessary in the case of singlet states, in accordance with<sup>[17]</sup>, to set

$$A_{-\mathbf{k}}^S = A_{\mathbf{k}}^S. \quad (45)$$

However, in the case of triplet pairs it is necessary to require

$$A_{-\mathbf{k}}^T = -A_{\mathbf{k}}^T \quad (46)$$

in place of (45). The latter requirement is connec-

ted, as it is not difficult to see, with the circumstance that  $A_{-\mathbf{k}}$  represents the average value of the operator  $b_{-\mathbf{k}}^*$ , which has the same sign as the average value of the operator  $b_{\mathbf{k}}^*$  in the singlet state, and the opposite sign—in the triplet state.

6. Using the functions (30) and (31), we now investigate the corresponding variational problem.<sup>5)</sup> The Hamiltonian of the system under consideration in the case of a superconducting ferromagnet has the form

$$H = \sum_{\sigma} \sum_{\mathbf{k} > k_{F\sigma}} \varepsilon_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}^* c_{\mathbf{k}\sigma} + \sum_{\sigma} \sum_{\mathbf{k} < k_{F\sigma}} |\varepsilon_{\mathbf{k}\sigma}| c_{\mathbf{k}\sigma}^* c_{\mathbf{k}\sigma} + H'', \quad (47)$$

where  $H''$  is defined in Eqs. (23) and (24), and  $k_{F\sigma}$  is the radius of the Fermi sphere for electrons with spin projection  $\sigma$ . In the case of a superconducting antiferromagnet,  $H$  has outwardly the same form as in (47), where it is necessary, however, to replace  $\tilde{V}_{\mathbf{k},\mathbf{k}_1}$  by  $V_{\mathbf{k},\mathbf{k}_1}^a$  in  $H''$  and, in addition, to take into account that in an antiferromagnet  $\mathbf{k}_{F\uparrow} = \mathbf{k}_{F\downarrow}$ . The following values for the average energy of the system (at  $T = 0^\circ\text{K}$ ) follow from (47), (30), and (31):

$$\begin{aligned}W^S &= \sum_{\sigma} \sum'_{\mathbf{k} > k_{F\sigma}} \varepsilon_{\mathbf{k}\sigma} (\beta_{\mathbf{k}} + 2\alpha_{\mathbf{k}}) \\ &\quad + \sum_{\sigma} \sum'_{\mathbf{k} < k_{F\sigma}} |\varepsilon_{\mathbf{k}\sigma}| (2 - \beta_{\mathbf{k}} - 2\alpha_{\mathbf{k}}) + \sum'_{\mathbf{k}, \mathbf{k}_1} F'_{\mathbf{k}, \mathbf{k}_1} \beta_{\mathbf{k}}^{1/2} \beta_{\mathbf{k}_1}^{1/2} \\ &\quad \times [(1 - \alpha_{\mathbf{k}} - \beta_{\mathbf{k}})^{1/2} + \alpha_{\mathbf{k}}^{1/2}] [(1 - \alpha_{\mathbf{k}_1} - \beta_{\mathbf{k}_1})^{1/2} + \alpha_{\mathbf{k}_1}^{1/2}], \quad (48) \\ W^T &= \sum_{\sigma} \sum'_{\mathbf{k} > k_{F\sigma}} \varepsilon_{\mathbf{k}\sigma} (\delta_{\mathbf{k}} + 2\gamma_{\mathbf{k}}) + \sum_{\sigma} \sum'_{\mathbf{k} < k_{F\sigma}} |\varepsilon_{\mathbf{k}\sigma}| (2 - \delta_{\mathbf{k}} - 2\gamma_{\mathbf{k}}) \\ &\quad + \sum'_{\mathbf{k}, \mathbf{k}_1} R'_{\mathbf{k}, \mathbf{k}_1} \delta_{\mathbf{k}}^{1/2} \delta_{\mathbf{k}_1}^{1/2} [(1 - \gamma_{\mathbf{k}} - \delta_{\mathbf{k}})^{1/2} + \gamma_{\mathbf{k}}^{1/2}] \\ &\quad \times [(1 - \gamma_{\mathbf{k}_1} - \delta_{\mathbf{k}_1})^{1/2} + \gamma_{\mathbf{k}_1}^{1/2}]. \quad (49)\end{aligned}$$

Comparison of (48) and (49) indicates that it is sufficient to solve the variational problem for the singlet state (48) and after this to obtain at once the solution of the problem for the triplet state by replacing  $F'_{\mathbf{k},\mathbf{k}_1}$  by  $R'_{\mathbf{k},\mathbf{k}_1}$  in the final result. Introducing the notation  $u_{\mathbf{k}} = \beta_{\mathbf{k}} + 2\alpha_{\mathbf{k}}$ ,<sup>[18]</sup> it is not difficult to see that the derivative  $\partial W^S / \partial \alpha_{\mathbf{k}}$  vanishes for  $u_{\mathbf{k}}^2 = 4\alpha_{\mathbf{k}}$ . Correspondingly setting  $\alpha_{\mathbf{k}} = h_{\mathbf{k}}^2$ , we write (48) in the form

$$\begin{aligned}W^S &= 2 \sum_{\sigma} \sum'_{\mathbf{k} > k_{F\sigma}} \varepsilon_{\mathbf{k}\sigma} h_{\mathbf{k}} + 2 \sum_{\sigma} \sum'_{\mathbf{k} < k_{F\sigma}} |\varepsilon_{\mathbf{k}\sigma}| (1 - h_{\mathbf{k}}) \\ &\quad + 4 \sum'_{\mathbf{k}, \mathbf{k}_1} F'_{\mathbf{k}, \mathbf{k}_1} h_{\mathbf{k}}^{1/2} (1 - h_{\mathbf{k}})^{1/2} h_{\mathbf{k}_1}^{1/2} (1 - h_{\mathbf{k}_1})^{1/2}.\end{aligned}\quad (50)$$

<sup>5)</sup>We also obtained the same results by the canonical transformation method<sup>[16]</sup> with account of the modification (44), and by the method of double-time temperature-dependent Green's functions with account of the modification (46).

Minimizing (50) with respect to  $h_{\mathbf{k}}$ , we obtain in the region of  $\mathbf{k}$  space in which pairs are present:

$$h_{\mathbf{k}} = 1/2 [1 - \epsilon_{\mathbf{k}}/(\epsilon_{\mathbf{k}}^2 - \epsilon_{0\mathbf{k}}^2)^{1/2}], \quad (51)$$

$$\epsilon_{0\mathbf{k}} = -2 \sum_{\mathbf{k}_1} F'_{\mathbf{k}, \mathbf{k}_1} h_{\mathbf{k}_1}^{1/2} (1 - h_{\mathbf{k}_1})^{1/2}. \quad (52)$$

The equation for  $\epsilon_{0\mathbf{k}}$  follows from (51) and (52):

$$\epsilon_{0\mathbf{k}} = - \sum_{\mathbf{k}_1} F'_{\mathbf{k}, \mathbf{k}_1} \epsilon_{0\mathbf{k}_1} / (\epsilon_{\mathbf{k}_1}^2 + \epsilon_{0\mathbf{k}_1}^2)^{1/2}, \quad (53)$$

which we shall solve under the assumption that  $F'_{\mathbf{k}, \mathbf{k}_1} \rightarrow \bar{F}' > 0$  for  $|\epsilon_{\mathbf{k}}| < \delta$  and  $F'_{\mathbf{k}, \mathbf{k}_1} = 0$  for  $|\epsilon_{\mathbf{k}}| > \delta$ , where  $\bar{F}'$  is the positive average value<sup>6)</sup> of  $F'_{\mathbf{k}, \mathbf{k}_1}$  in the region  $|\epsilon_{\mathbf{k}}| < \delta$ , and  $\delta$  is defined as the effective phonon frequency (or the Debye temperature and accordingly gives the isotope effect) in the case when the region of the phonon-induced attraction is larger than the region of spin wave-induced attraction. In the opposite case,  $\delta$  is determined by the effective frequency of the spin wave (or Curie temperature) and correspondingly does not give an isotope effect.

In this connection, it is necessary to distinguish the case when the displacement of the Fermi momentum surfaces is removed on account of the energy decrease due to the increase in the number of paired electrons,<sup>[23-25]</sup> from the case when the removal of the displacement of the Fermi surfaces is energetically unfavorable.<sup>[22]</sup> For simplicity, we confine our attention to the first case. Then it follows from (53) and (50) that

$$\epsilon_0 = \delta / \text{sh}(1/N_0 \bar{F}'), \quad (54)^*$$

$$W^S \approx -1/2 N_0 \epsilon_0^2 + N_0 \Theta^2, \quad (55)$$

where  $N_0$  is the density of states near the Fermi surface for one spin projection, but the last term in (55) describes the increase of the exchange energy of the system, accompanying the removal of the displacement of the Fermi surface. It is clear from (55) that this removal is (energetically) favorable only in the case of sufficiently weak s-d or s-f exchange, when  $\epsilon_0 < \sqrt{2} \Theta$ . In this connection, the lowering of the energy will be greater, the greater  $\epsilon_0$  is, and therefore the larger  $\bar{F}'$  is. This enables us to assert, taking account of (49), that the formation of singlet pairs will be energetically advantageous upon fulfillment of the inequality

$$\bar{F}' > \bar{R}', \quad (56)$$

<sup>6)</sup>Here we prefer to use the average value of  $F'_{\mathbf{k}_1, \mathbf{k}}$  instead of the approximate expansion of  $F'_{\mathbf{k}_1, \mathbf{k}}$  in Legendre polynomials,<sup>[10,11]</sup> since the subsequent various assumptions utilized in<sup>[10,11]</sup> lead to different results (also see<sup>[12-14]</sup>).

\*sh = sinh.

where  $\bar{R}'$  is the average value of  $R_{\mathbf{k}, \mathbf{k}_1}$  in the region  $|\epsilon_{\mathbf{k}}| < \delta$ . In the opposite case, the formation of triplet pairs will be energetically more favorable. Criteria similar to (56) also hold in the case of a superconducting antiferromagnet [although in this case, of course, it is necessary to set  $\Theta = 0$  in Eq. (55)].

7. We now present, without detailed calculations, the results of an investigation of nonferromagnetic and nonantiferromagnetic superconductors, in which the phonon-induced interaction leads, according to Eq. (16), to the equivalent formation of triplet states of three possible types (both with  $s_Z = 0$  and with  $s_Z = \pm 1$ ). We chose trial wave functions for this case in the form

$$\Psi^T = \prod_{\mathbf{k}} [\alpha_{\mathbf{k}}^{1/2} + \beta_{\mathbf{k}}^{1/2} B_{\mathbf{k}}^{*T} + \gamma_{\mathbf{k}}^{1/2} (B_{\mathbf{k}}^{*T})^2 + \delta_{\mathbf{k}}^{1/2} b_{\mathbf{k}\uparrow}^* + \eta_{\mathbf{k}}^{1/2} b_{\mathbf{k}\downarrow}^*] \Psi_v. \quad (57)$$

Correspondingly, the solution of the variational problem led to an equally-probable distribution of all three types of triplet pairs with probability<sup>7)</sup>

$$\beta_{\mathbf{k}} = \delta_{\mathbf{k}} = \eta_{\mathbf{k}} = 1/3 \epsilon_0^2 / (\epsilon_{\mathbf{k}}^2 + \epsilon_0^2), \quad (58)$$

$$\epsilon_0 = \hbar\omega / \text{sh}(1/N_0 \bar{R}'), \quad (59)$$

which corresponds to an energy of the superconducting system equal to

$$W_0 = -2N_0 (\hbar\omega)^2 / [\exp(2/N_0 \bar{R}') - 1]. \quad (60)$$

The equivalence of the three types of triplet pairs vanishes, however, upon the above-considered inclusion of spin waves of a ferro- or antiferromagnet, or upon introduction into the investigation of the intensity of the external magnetic field. In the latter case a nonvanishing paramagnetic susceptibility of the superconductor may appear at  $T = 0$ , as has been shown by Fischer<sup>[7]</sup> (for "alternative" pairs with  $s_Z = \pm 1$ ), Privorotskii<sup>[8]</sup> and Balian and Werthamer<sup>[9]</sup> (in the last article for pairs in a p-state). A more detailed investigation of this question falls, however, outside the scope of the present article.

8. The account presented above indicates that the presence of the "exchange" part of the matrix element, defining the transitions of singlet or triplet pairs, actually turns out to be a general property of all the interactions considered above (induced by

<sup>7)</sup>In order to avoid a misunderstanding, which the symmetry of (58) with respect to  $\epsilon_{\mathbf{k}} = 0$  may cause, we emphasize that the occupation of electron states is determined not only by  $\beta_{\mathbf{k}}$ , but also by the quantity  $\gamma_{\mathbf{k}}$ , and that on the whole  $1/2(3\beta_{\mathbf{k}} + 2\gamma_{\mathbf{k}})$  coincides with  $h_{\mathbf{k}}$  of<sup>[15]</sup> and has the same anti-symmetric behavior with respect to  $\epsilon_{\mathbf{k}} = 0$ .

virtual phonons, Coulomb forces, or by virtual spin waves of a ferro- or antiferromagnet), which is quite natural, since this "exchange" part (having, in general, a different form for the various interactions) is a direct consequence of the type of symmetry of the coordinate part of the electron-pair wave function. In this connection, near the Fermi surface a singular change takes place in the nature of the interaction described by the exchange part, corresponding to the triplet state, namely: a change from attraction to repulsion for the interaction induced by phonons, and, conversely, a change from repulsion to attraction for the interactions induced, respectively, by Coulomb forces or by spin waves of a ferro- or antiferromagnet. The latter circumstance enables us, of course, as one of the alternatives to explain the coexistence of superconductivity and ferromagnetism, or antiferromagnetism, or paramagnetism, and also the absence of a normal isotope effect in certain systems containing transition metals, having assumed the formation in the enumerated cases of a superconducting state with triplet pairs.

It is, however, necessary to note that the odd matrix element  $\bar{R}_{\mathbf{k},\mathbf{k}_1}$ , determining the transitions of triplet pairs, apparently is usually smaller<sup>[7]</sup> than the even matrix element  $\bar{F}_{\mathbf{k},\mathbf{k}_1}$  determining the singlet pair transitions (for example, for the simplest assumption,  $V_{\mathbf{k},\mathbf{k}_1} = \text{const}$ , the element  $R_{\mathbf{k},\mathbf{k}_1}$  simply vanishes, which corresponds to the cancellation assumed by Cloizeaux<sup>[18]</sup>). In such a case, according to (56) the singlet state may turn out to be energetically more favorable. Accordingly, in order to understand the coexistence of superconductivity and ferromagnetism or superconductivity and paramagnetism and so forth, other generalizations of BCS pairs may turn out to be useful; one of these alternative versions was proposed and applied to one of these problems by Cooper in<sup>[28]</sup>, and to other problems by us.<sup>[29]</sup>

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