COEXISTENCE OF SINGLET AND TRIPLET PAIRS IN AN ANISOTROPIC SUPERCONDUCTOR

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Submitted to JETP editor July 22, 1965

J. Exptl. Theoret. Phys. (U.S.S.R.) **50**, 215–219 (January, 1966)

It is shown that, in a certain range of the coupling constants, the coexistence of singlet and triplet pairs is possible in an anisotropic superconductor.

A peculiar phenomenon is possible in an anisotropic superconductor, viz., coexistence of singlet and triplet pairs in a finite range of values of the interaction constants. This is due to the fact that in some directions the gap corresponding to a singlet pair may turn out to be larger, but in other directions it may turn out to be smaller than the triplet gap. Therefore, in certain cases the simultaneous formation of singlet and triplet pairs turns out to be energetically favorable, although the corresponding coupling constants are different. As the values of the interaction constants approach each other, coexistence obviously does not disappear, i.e., this phenomenon occurs over a whole range of values of the interaction constants.

Let us consider a model of a superconductor with account of only the interaction of electrons having opposite momenta; the Hamiltonian of this model is

$$H = \sum \xi_p a^+_{p\sigma} a_{p\sigma} + \sum U(\mathbf{p}, \mathbf{p}')\, a^+_{\mathbf{p}^{1/2}} a^+_{-\mathbf{p}-1/2} a_{-\mathbf{p}'-1/2} a_{\mathbf{p}'1/2} + \sum V(\mathbf{p}, \mathbf{p}')\, a^+_{\mathbf{p}\nu} a^+_{-\mathbf{p}\mu} a_{-\mathbf{p}'\mu} a_{\mathbf{p}'\nu}. \quad (1)$$

The quantities $a^+_{\mathbf{p}\sigma}$ and $a_{\mathbf{p}\sigma}$ are the operators for the creation and annihilation of an electron with momentum $\mathbf{p}$ and spin σ, ξ_p is the electron energy, measured from the Fermi surface. The function $U(\mathbf{p}, \mathbf{p}')$ corresponds to the interaction of electrons in the singlet state, and $V(\mathbf{p}, \mathbf{p}')$ corresponds to the triplet state (U is an even function of its arguments, V is an odd function). For simplicity we assume that these functions differ from zero only inside the shell $-\omega_D \le \xi_\mathbf{p}$, $\xi \le \omega_D$ and depend only on the normal to the Fermi surface, but not on ξ: $U(\mathbf{n}, \mathbf{n}')$, $V(\mathbf{n}, \mathbf{n}')$. The following form is assumed for U and V:

$$U(\mathbf{n}, \mathbf{n}') = -\frac{(2\pi)^3}{2p_0} g_s \varphi(\mathbf{n}) \varphi(\mathbf{n}'),$$

$$V(\mathbf{n}, \mathbf{n}') = -\frac{(2\pi)^3}{2p_0} g_t \sum_{i=1}^{f} \chi_i(\mathbf{n}) \chi_i(\mathbf{n}'). \quad (2)$$

The function $\varphi(\mathbf{n})$ transforms according to the identity representation of the symmetry group of the crystal (the analog of zero momentum in the isotropic case), and the $\chi_i(\mathbf{n})$ transform according to the f-dimensional representation. The functions φ and χ_i obey the conditions

$$[\varphi^2] = 1, \qquad [\chi_i \chi_k] = \delta_{ik}. \quad (3)$$

Here the notation

$$[\varphi^2] = \int \frac{d\sigma}{p_0 v(\mathbf{n})} \varphi^2(\mathbf{n}), \quad (4)$$

has been introduced, where $d\sigma$ is an element of the Fermi surface, $v(\mathbf{n})$ is the electron velocity on this surface, and p_0 is a constant determined by the condition $[1] = 1$.

The constant $-(2\pi)^3/2p_0$ is introduced into Eq. (2) for convenience.

At the present time, there apparently is no unanimity on how to generalize the method of F-functions[1] to the case of nonzero momenta. On the other hand, this method is generally accepted in connection with the investigation of pairs having zero momentum. Therefore, it makes sense to solve the problem of the coexistence of singlet and triplet pairs in the following way: By assuming $g_s > g_t$ and taking the existence of singlet pairs into account, find at what temperatures the 4-vertex describing the scattering of electrons in the triplet state has a purely imaginary pole, indicating an instability of the initial state.[2]

Thus, the formation of singlet pairs is taken into account by the introduction of the F-function which, in the momentum representation, has the form (see Sec. 34 of [3])

$$F(\mathbf{p}\omega_m) = \frac{\Delta(\mathbf{n})}{\omega_m^2 + \xi_\mathbf{p}^2 + \Delta^2(\mathbf{n})}, \quad (5)$$

where $\omega_m = (2m+1)\pi T$ (T is the temperature), $\Delta(\mathbf{n})$ is the energy gap, $\Delta(\mathbf{n}) = Q(T)\varphi(\mathbf{n})$.

For the one-particle Green's function we have the expression

$$G(\mathbf{p}\omega_m) = -\frac{i\omega_m + \xi_\mathbf{p}}{\omega_m^2 + \xi_\mathbf{p}^2 + \Delta^2(\mathbf{n})}. \qquad (6)$$

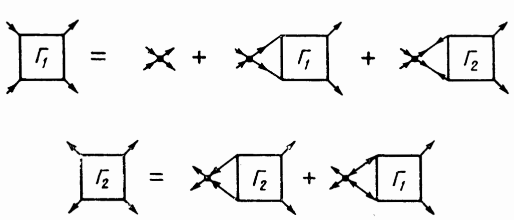
The value of Q(T) is determined by the equation

$$\int \frac{d\sigma}{p_0 v(\mathbf{n})} \varphi^2(\mathbf{n}) \int_0^{\omega_D} d\xi \frac{1}{\sqrt{\xi^2 + Q^2\varphi^2}} \operatorname{th} \frac{\sqrt{\xi^2 + Q^2\varphi^2}}{2T} = \frac{1}{g_s}. \qquad (7)^*$$

The equations for the vertex Γ_1 describing the scattering of an electron by an electron are represented graphically in the figure. Here a point corresponds to the function $V(\mathbf{n}, \mathbf{n}')$ (the scattering of electrons in the triplet state interests us), a line with two arrows corresponds to the function F, and a line with one arrow corresponds to the function G. After summing over the spins, these equations take the following form:

$$\Gamma_1(\mathbf{p}, \mathbf{q}; E) = -2T \sum_{m,k} V(\mathbf{p}, \mathbf{k}) G(\mathbf{k}\omega_m) G(-\mathbf{k}; E - \omega_n)$$
$$\times \Gamma_1(\mathbf{k}, \mathbf{q}; E) + 2T \sum_{m,k} V(\mathbf{p}, \mathbf{k}) F(\mathbf{k}\omega_m) F(-\mathbf{k}, E - \omega_m)$$
$$\times \Gamma_2(\mathbf{k}, \mathbf{q}; E),$$
$$\Gamma_2(\mathbf{p}, \mathbf{q}; E) = 2T \sum_{m,k} V(\mathbf{k}, \mathbf{p}) F(\mathbf{k}\omega_m) F(-\mathbf{k}, E - \omega_m) \Gamma_1(\mathbf{k}, \mathbf{q}; E)$$
$$-2T \sum_{m,k} V(\mathbf{k}, \mathbf{p}) G(\mathbf{k}\omega_m) G(-\mathbf{k}, -E - \omega_m) \Gamma_2(\mathbf{k}, \mathbf{q}; E). \qquad (8)$$

Here E is the total frequency, and $\mathbf{p}$ and $\mathbf{q}$ are the electron momenta before and after scattering. The free term is omitted from the first equation of (8), which is valid near a singularity of Γ_1, Γ_2.



We rewrite Eq. (8), having carried out certain transformations. Namely, we sum over m and then we analytically continue these equations from discrete points E into the upper half-plane. As a result we obtain

$$\Gamma_1(\mathbf{n}, \mathbf{n}'; \Omega) = g_t \int \frac{d\sigma''}{p_0 v(\mathbf{n}'')} \sum_i \chi_i(\mathbf{n}) \chi_i(\mathbf{n}'')$$
$$\times \{\Gamma_1(\mathbf{n}'', \mathbf{n}'; \Omega) \alpha(\mathbf{n}'') - \Gamma_2(\mathbf{n}'' \mathbf{n}'; \Omega) \beta(\mathbf{n}'')\},$$

$$\Gamma_2(\mathbf{n}, \mathbf{n}'; \Omega) = -g_t \int \frac{d\sigma''}{p_0 v(\mathbf{n}'')} \sum_i \chi_i(\mathbf{n}) \chi_i(\mathbf{n}'')$$
$$\times \{\Gamma_1(\mathbf{n}'', \mathbf{n}'; \Omega) \beta(\mathbf{n}'') - \Gamma_2(\mathbf{n}'', \mathbf{n}'; \Omega) \alpha(\mathbf{n}'')\}, \qquad (9)$$

where

$$\alpha(\mathbf{n}) = 2 \int_0^{\omega_D} d\xi \frac{\varepsilon^2 + \xi^2}{4\varepsilon^2 + \Omega^2} \frac{1}{\varepsilon} \operatorname{th} \frac{\varepsilon}{2T},$$

$$\beta(\mathbf{n}) = 2 \int_0^{\omega_D} d\xi \frac{\Delta^2}{4\varepsilon^2 + \Omega^2} \frac{1}{\varepsilon} \operatorname{th} \frac{\varepsilon}{2T}, \quad \varepsilon^2 = \xi^2 + \Delta^2. \qquad (10)$$

The real quantity Ω characterizes the degree of instability ($E = i\Omega$).

We seek the solution of Eqs. (9) in the form

$$\Gamma_1, \Gamma_2 \sim \sum_i \chi_i(\mathbf{n}) \chi_i(\mathbf{n}').$$

The condition for solvability of Eqs. (9) has the form

$$\int \frac{d\sigma}{p_0 v(\mathbf{n})} \chi^2(\mathbf{n}) \int_0^{\omega_D} d\xi \frac{\varepsilon^2}{\varepsilon^2 + \Omega^2/4} \frac{1}{\varepsilon} \operatorname{th} \frac{\varepsilon}{2T} = \frac{1}{g_t},$$

$$\chi^2(\mathbf{n}) = \frac{1}{f} \sum_{i=1}^{f} \chi_i^2(\mathbf{n}). \qquad (11)$$

Equation (11) for $\Omega = 0$ gives the temperature at which the system becomes unstable with respect to the formation of triplet pairs. In the general case, for arbitrary φ and χ, g_s and g_t, this question cannot be solved. Therefore, we consider Eqs. (7) and (11) in certain limiting cases.

If $\varphi(\mathbf{n})$ is an isotropic function, then (11) has a solution only for $g_t = g_s$ (and $\Omega = 0$). This stems from the fact that for $g_t < g_s$ the triplet pair binding energy is always less than the singlet pair binding energy.

The situation is different in the case of an anisotropic φ. The function φ plays the role of the singlet pair wave function, and χ (more precisely χ_i) plays the role of the triplet pair wave function. The gap is minimal at the minimum of φ^2, and the triplet pair binding energy may exceed the magnitude of the gap at this place. It is clear that this is still insufficient for instability. In addition, it is necessary that χ^2 be as large as possible there where the triplet pair binding energy is larger than the gap, and as small as possible in the remaining regions; only in this case may the formation of a triplet pair turn out to be advantageous. As an illustration, let us consider the case when χ^2 is a δ-function at the minimum of φ^2. From Eq. (11) we find that an instability for $T = 0$ appears at the following value of g_t:

*th ≡ tanh.

$$g_t = \left(\ln \frac{2\omega_D}{\Delta_m^{(0)}}\right)^{-1} \quad (\Delta \ll \omega_D), \tag{12}$$

where $\Delta_m^{(0)}$ is the minimum value of the gap for $T = 0$. On the other hand, for $T = 0$ and $\Delta = 0$ (no singlet pairs), from (11) we obtain the following result for the binding energy Ω of a triplet pair:

$$g_t = \left(\ln \frac{2\omega_D}{\Omega}\right)^{-1} \quad (\Omega \ll \omega_D). \tag{13}$$

By comparing (12) and (13) we see that the instability with respect to the formation of triplet pairs in the presence of singlet pairs appears when the binding energy Ω of the triplet pair is comparable with $\Delta_m^{(0)}$.

If $\Delta_m^{(0)} = 0$, and χ^2 is a δ-function at the minimum of Δ, then the temperature of the instability naturally coincides with the temperature of the transition for $g_s = 0$ (since singlet pairs do not change the states of the electrons at the point $\Delta_m^{(0)} = 0$).

Let us determine the behavior of T as a function of g_t for $T \ll T_c$ (T_c is the temperature of the transition to the superconducting state). From formula (7) we obtain an expression for $Q(T)$ at low temperatures:

$$\frac{Q(T)}{Q(0)} = 1 - AT^{3/2}\varphi_m^2 \exp\left(-\frac{\Delta_m^0}{T}\right), \tag{14}$$

where φ_m^2 is the minimum value of φ^2, A is a positive constant. Substituting (14) into (11), we obtain when $\Omega = 0$

$$AT^{3/2}(\varphi_m^2 - \chi_m^2)\exp\left(-\frac{\Delta_m^0}{T}\right) + \left[\chi^2 \ln \frac{2\omega_D}{\Delta^{(0)}}\right] = \frac{1}{\sigma}. \tag{15}$$

Here χ_m is the value of χ at the minimum of Δ, and $\Delta^{(0)}$ is the gap at $T = 0$.

The temperature T of the instability, determined by formula (15), varies differently with change of g_t depending on the relation between φ_m^2 and χ_m^2. First let us consider the case $\chi_m^2 > \varphi_m^2$. From Eq. (15) it is evident that T decreases with decreasing g_t and for

$$g_t = g_0 = \left[\chi^2 \ln \frac{2\omega_D}{\Delta^{(0)}}\right]^{-1} \tag{16}$$

it tends to zero. It is assumed that $g_0 < g_s$, i.e., the condition

$$[\varphi^2 \ln \varphi^2] > [\chi^2 \ln \varphi^2] \tag{17}$$

is satisfied.

The case $\chi_m^2 < \varphi_m^2$ is of interest. Here an instability is possible even for $g_t < g_0$, where T increases with decrease of g_t. This corresponds to the fact that when $g_t < g_0$ the formation of triplet pairs is advantageous in the temperature interval, let us say, from T_1 to T_2, where $0 < T_1 < T_2 < T_c$ [Eq. (15) determines the lower limit T_1 of the interval]. Then, one can verify that this is actually so by finding the temperature dependence of the magnitude Ω of the instability for some fixed value of g_t. It turns out that Ω increases with temperature.

Such behavior of Ω (and of the temperature of the instability) lends itself to a descriptive interpretation. Let g_t be such that the formation of triplet pairs is advantageous for $T = 0$. With increasing temperature, smearing of the quasiparticle Fermi distribution takes place near the minimum $\Delta^{(0)}$. This smearing causes a decrease of the binding energy for both singlet and triplet pairs. But the wave function of a triplet pair at the minimum $\Delta^{(0)}$ is smaller than the wave function of a singlet pair: $\chi_m^2 < \varphi_m^2$, i.e., the triplet pair is less sensitive to an increase of the temperature (its binding energy decreases more weakly than the binding energy of a singlet pair). Since only the ratio of Δ to the binding energy of a triplet pair is important, the formation of a triplet pair becomes more advantageous with increasing temperature (Ω increases).

Let us consider the other limiting case, $T_c - T \ll T_c$. One can find $Q(T)$ from formula (7):[4]

$$Q^2(T) = \frac{C}{[\varphi^4]} \cdot \frac{T_c - T}{T_c}, \tag{18}$$

where C is a certain constant (independent of the form of φ). Substituting (18) into (11) (we take $\Omega = 0$), we find the temperature of the instability

$$\frac{T_c - T}{T_c}\left\{\frac{[\varphi^2\chi^2]}{[\varphi^4]} - 1\right\} = \frac{1}{g_s} - \frac{1}{g_t}. \tag{19}$$

It is obvious that T must be less than T_c for $g_t < g_s$. Therefore Eq. (19) makes sense only if the condition

$$[\varphi^4] > [\varphi^2\chi^2] \tag{20}$$

is satisfied. If this condition is not satisfied, then T does not tend to T_c as $g_t \to g_s - 0$.

From the examples considered, it is clear that under certain conditions the formation of triplet pairs is actually energetically favorable. Coexistence occurs over a certain range of values of g_t. The temperature interval in which coexistence is possible may not extend down to zero.

It is obvious that a phase transition of the second kind takes place at the temperature of the instability. At this point the heat capacity must undergo a discontinuous change. Below this temperature, the heat capacity must exhibit a more abrupt decrease. Coexistence also manifests itself in other properties of a superconductor (for example, in the paramagnetic susceptibility).

The author wishes to thank V. L. Pokrovskiĭ for a discussion of this work.

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Translated by H. H. Nickle
29