OCCURRENCE OF LOCAL BOUND STATES IN A SUPERCONDUCTOR WITH MAGNETIC IMPURITY

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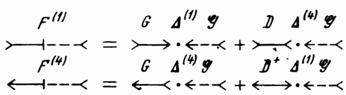
It is shown that in the case when the impurity spin is S = 1 and the impurity concentration is sufficiently small, then the condition for the occurrence of bound states is $T_K > T_{c0}$, where T_K is the Kondo temperature, at which the bound states occurs, and T_{c0} is the critical temperature of the superconducting transition of the pure metal. It is also shown that under these conditions the magnetic impurities decrease the transition temperature.

It was shown in[1] that in the case when the impurity spin is S = 1 it is possible to calculate a large number of quantities, such as the specific heat, the magnetic moment, and others. We shall employ here this technique to analyze the possible coexistence of superconductivity and bound states. We shall assume that the impurity concentration is so low, that the superconductor is practically "pure," To this end, as we shall verify later, it suffices to satisfy the condition

$$c\varepsilon_F \ll T_K, \tag{1}$$

where c—atomic concentration of the impurity, ϵ_F—Fermi energy, and T_K—Kondo temperature.



To ascertain the possibility of appearance of bound states in a superconductors, let us determine the Kondo temperature T_K, at which the formation of the bound states begins. In the vicinity of this temperature, all the $\Delta^{(i)}_{\alpha\beta}$ (see[1]) are small, and we can find the functions $F^{(i)}_{\alpha\beta}$ accurate to terms of first order in $\Delta^{(i)}_{\alpha\beta}$. The expressions for $F^{(1)}_{\alpha\beta}$ and $F^{(4)}_{\alpha\beta}$ are represented schematically by the diagrams shown in the figure. The quantities $D_{\alpha\alpha'}$ and $D^{+}_{\alpha\alpha'}$ are none other than the Gor'kov F-functions[2]. We changed the notation in order to avoid confusion.

From the conditions

$$\Delta^{(1)}_{\alpha\beta} = \frac{J}{N}\sigma^i_{\alpha\alpha_1}S^i_{\beta\beta_1}F^{(1)}_{\alpha_1\beta_1}(0) = \frac{J}{N}(\sigma S)_{\alpha\beta,\alpha_1\beta_1}T\sum_\omega F^{(1)}_{\alpha_1\beta_1}(\omega), \tag{2}$$

$$\Delta^{(4)}_{\alpha\beta} = \frac{J}{N}(\sigma S)_{\alpha_1\beta,\alpha\beta_1}T\sum_\omega F^{(4)}_{\alpha_1\beta_1}(\omega),$$

with account of the fact that

$$G_{\alpha\alpha'}(\omega) = \delta_{\alpha\alpha'}G(\omega),$$
$$D_{\alpha\alpha'}(\omega) = -g_{\alpha\alpha'}D(\omega), \quad D^{+}_{\alpha\alpha'}(\omega) = g_{\alpha\alpha'}D(\omega),$$
$$g_{\alpha\alpha'} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix},$$

we obtain a homogeneous system of equations for $\Delta^{(i)}_{\alpha\beta}$:

$$\Delta^{(1)}_{\alpha\beta} = \frac{J}{N}T\sum_\omega[G(\omega)(\sigma S)_{\alpha\beta,\alpha_1\beta_1}\Delta^{(1)}_{\alpha_1\beta_1}$$
$$-D(\omega)(\sigma S)_{\alpha\beta,\alpha_1\beta_1}g_{\alpha_1\alpha_2}\Delta^{(4)}_{\alpha_2\beta_1}]\mathcal{G}(-\omega),$$
$$\Delta^{(4)}_{\alpha\beta} = \frac{J}{N}T\sum_\omega[-D(\omega)(\sigma S)_{\alpha_1\beta,\alpha\beta_1}g_{\alpha_1\alpha_2}\Delta^{(1)}_{\alpha_2\beta_1}$$
$$+G(-\omega)(\sigma S)_{\alpha_1\beta,\alpha\beta_1}\Delta^{(4)}_{\alpha_1\beta_1}]\mathcal{G}(-\omega). \tag{3}$$

(For the notation see[1].)

Substituting here the expressions (see[1,2] 1))

$$G(\omega) = -\frac{i\omega+\xi}{\omega^2+\xi^2+\Delta^2}, \quad D(\omega) = \frac{\Delta}{\omega^2+\xi^2+\Delta^2}, \quad \mathcal{G} = \frac{1}{i\omega}; \tag{4}$$

$$\Delta^{(1)}_{1/2,-1} = \Delta^{(3)}_{1/2\,1} = \Delta^{(1)}_{-1/2\,1} = -\Delta^{(3)}_{-1/2,-1} = \delta_1,$$
$$\Delta^{(1)}_{1/2\,0} = \Delta^{(3)}_{1/2\,0} = \Delta^{(1)}_{-1/2\,0} = -\Delta^{(3)}_{-1/2\,0} = \delta_0,$$
$$\Delta^{(2)}_{\alpha\beta} = -\Delta^{(1)}_{\alpha\beta}, \quad \Delta^{(4)}_{\alpha\beta} = -\Delta^{(3)}_{\alpha\beta}, \tag{5}$$

we obtain the equations for δ_0 and δ_1. It should be noted that inasmuch as D is an even function in ω, and $\mathcal{G}$ is odd, all the sums over ω containing D vanish. Therefore the equations for δ_0 and δ_1 coincide formally with the results obtained for the normal metal[1] (albeit with another G-function):

$$\delta_1 = \mathcal{A}\delta_1 - \sqrt{2}\mathcal{A}\delta_0, \qquad \delta_0 = -\sqrt{2}\mathcal{A}\delta_1, \tag{6}$$

where

$$\mathcal{A} = -\left|\frac{J}{N}\right| T\sum_\omega \alpha\int d\xi G(\omega,\xi)\mathcal{G}(\omega). \tag{7}$$

The homogeneous system (6) has a solution when $\mathcal{A} = 1/2$.

There are two possibilities. If the sought temperature T_K exceeds the critical temperature of the superconducting transition (which coincides with T_{c0}—the

1) An error in the choice of the signs of $\Delta^{(3)}_{\alpha\beta}$ has crept into [1] and has led to a number of inaccuracies in the result. If the sign is properly chosen (as in formula (5) of the present paper, all the $\mathcal{D}_{\beta\beta^1}$ vanish, and formula (A.3) of [1] is replaced by

$$Q = 3/4 + 1/36\,\mathrm{th}^2(\mu gH/2T),$$

and formula (49) by

$$M_i = \frac{3}{7}N_i g\mu + \frac{8N_i g^2\mu^2 H}{21\pi^2\alpha\delta_1^2}\left(\ln\frac{9\alpha\pi\delta_1^2}{g\mu H} + \frac{1}{2}\right).$$

The remaining results stay the same.

value for the pure metal—if condition (1) is satisfied), then Eq. (7) contains the function $G(\omega)$ for the normal metal, i.e., the superconductivity does not come into play. On the other hand, if $T_K < T_{c0}$, then there are two regions in the sum (7). When $\omega < \omega_D$ it is necessary to substitute G for the superconductor, and when $\omega > \omega_D$—for the normal metal. This takes into account, in a somewhat simplified form, the dependence of the superconducting gap Δ on the frequency. Thus, taking the foregoing into account, we get

$$\frac{1}{2}=\left|\frac{J}{N}\right|\alpha\pi T\left(\sum_{|\omega|<\omega_D}\frac{1}{(\omega^2+\Delta^2)^{1/2}}+\sum_{\omega_D<|\omega|<\Lambda}\frac{1}{|\omega|}\right). \quad (8)$$

The equation for the determination of Δ is

$$\Delta=|g|T\sum_{|\omega|<\omega_D}\alpha\int d\xi D(\omega,\xi)$$

or, after integrating with respect to $d\xi$

$$1=|g|\pi\alpha T\sum_{|\omega|<\omega_D}\frac{1}{\sqrt{\omega^2+\Delta^2}}. \quad (9)$$

From the condition (8) we get

$$\frac{1}{2|J/N|\alpha}-\frac{1}{|g|\alpha}=2\pi T\sum_{\omega_D<\omega<\Lambda}\frac{1}{\omega} \quad (10)$$

(we took into account here summation with respect to ω with both signs). Recognizing that, in accord with[1],

$$T_{K0}=\frac{2\Lambda\gamma}{\pi}\exp\left(-\frac{N}{2|J|\alpha}\right)$$

(where T_{K_0} is the temperature T_K without allowance for superconductivity), and according to (9) we have

$$T_{c0}=\frac{2\omega_D\gamma}{\pi}\exp\left(-\frac{1}{|g|\alpha}\right),$$

we get from (10) $T_{c0} = T_{K_0}$. But in order to have $T_K < T_{c0}$, as we have assumed, we must have, at any rate, $T_{K_0} < T_{c0}$. Otherwise the transition will occur at T_{K_0} (the superconductivity is not felt when $T \geq T_{c0}$); this means that the equality $T_{c0} = T_{K_0}$ contradicts the initial assumption[2)].

We thus arrive at the conclusion that the condition for the occurrence of bound complexes in a superconductor is

$$T_K=T_{K0}>T_{c0}. \quad (11)$$

The same result was obtained by Fowler and Maki[3] in a study of the appearance of poles in the scattering amplitude by the Suhl method[3)].

[2)]In principle it is possible to propose one more possibility, namely, if $T_{K0} < T_{c0}$, then the transition to the bound state becomes a first-order transition. In this case it is necessary to seek not the Kondo temperature as δ and δ_0 approach 0, but to find the free energy at $\Delta \neq 0$ and $\delta_0 \neq 0$. It is possible, however, to make use of the fact that when T_{K0} is close to T_{c0}, the first-order transition should occur at a small (albeit finite) δ_1, and in this region $\Delta \ll T$. This makes it possible to show that finite δ_1 and δ_0 are incompatible with the assumption $T_{c0} > T_{K0}$.

[3)]We do not discuss here other papers dealing with this question, which contain either the incorrect conclusion that superconductivity and bound complexes are incompatible [4], or which give incorrect criteria. [5].

Let us find now the true critical temperature T_c, assuming that the bound complexes already exist. It is determined from the condition

$$1=|g|T\alpha\sum_{\omega}\int d\xi\,\overline{G(\omega,\xi)G(-\omega,\xi)} \quad (12)$$

(we are averaging over the impurity position). As shown in[1], the formation of bound complexes leads to the same effect as scattering by random impurities with a total scattering amplitude[4)]

$$V(\omega)=\frac{3\delta_1^2}{i(\omega+3\pi\alpha\delta_1^2\,\mathrm{sign}\,\omega)} \quad (13)$$

We denote $\overline{G(\omega,\xi)G(-\omega,\xi)}$ by $\Pi(\omega,\xi)$. Using the customary procedure (cf., e.g.,[6]), we obtain the equation

$$\Pi(\omega,\xi)=G(\omega)G(-\omega)+\frac{N_i}{Q}G(\omega)G(-\omega)V(\omega)V(-\omega)\int\Pi\alpha d\xi \quad (14)$$

(Q—normalization factor of the spin technique (see[1])). Taking the integral with respect to $d\xi$, we obtain directly the expression $\int\Pi\alpha d\xi$ that enters in (12). For $G(\omega)$ we use (see[1])[5)]

$$G(\omega)=(i\omega-\xi-N_iV(\omega)/Q)^{-1}. \quad (15)$$

All the manipulations lead ultimately to

$$1=|g|\alpha 2\pi T\sum_{0<\omega<\omega_D}\frac{1}{\omega}\left[1+\frac{4\delta_1^2N_i}{(\omega+3\pi\alpha\delta_1^2)^2}\right]^{-1}. \quad (16)$$

Expanding further in terms of N_i, we get

$$T_c=T_{c0}\left[1-\frac{4\delta_1^2N_i}{(3\pi\alpha\delta_1^2)^2}\left(\ln\frac{6\gamma\alpha\delta_1^2}{T_{c0}}-1\right)\right]. \quad (17)$$

We see directly from this formula that at low impurity concentration the correction to T_{c0} is of the order of

$$T_{c0}\delta_1^2N_i/(\alpha\delta_1^2)^2\sim T_{c0}c\varepsilon_F/T_K.$$

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[4)]The "non-pole" part of the scattering amplitude, which is not taken into account in (23), is of the order of $(T/T_K)^2$ and is negligibly small in the case when $T_c \ll T_K$.

[5)]The normalization of 1/Q in the expression (16) for G was not taken into account in [1]. In this case Q = ¾.

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