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TRIPLET STATES IN A SUPERCONDUCTOR CONTAINING MAGNETIC IMPURITIES

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Triplet states in a superconductor containing magnetic impurities are considered both in the paramagnetic and in the ferromagnetic phases. For the paramagnetic phase, the correction of second order to the energy of the electron system and the indirect interaction of impurity spins are determined. In the case of a ferromagnetic superconductor, it is shown that the energy spectrum is determined by a cubic equation. It is shown that this is related to the complete removal of degeneracy with respect to the direction of the pair spin.

1. INTRODUCTION

IN connection with difficulties arising in the theory of superconductivity (Knight shift, ferromagnetic superconductors), in recent times a number of articles have appeared in which the triplet states in a superconductor containing magnetic impurities are investigated.[1-3]

The purpose of the present article is a further consideration of this problem according to one scheme. We are, however, compelled for the present to omit such questions as taking account of the multiplicity of the shells of the impurity ions, the possibility of pairing with nonzero pair momentum, and other questions. The scheme of Gor'kov and Galitskiĭ[4] is assumed as a basis for calculations. In this scheme the Green's functions

$$G_{\alpha\beta}(x-x') = -i\langle T(\psi_\alpha(x)\psi_\beta^+(x'))\rangle,$$

$$F_{m\alpha\beta}{}^+(x-x') = \langle N+2,\ l,\ m|T(\psi_\alpha^+(x)\psi_\beta^+(x'))|N,0\rangle$$

(and the functions conjugate to them) are introduced; in the momentum representation they are determined by the equations ($G_{\beta\alpha} = G_\alpha\delta_{\beta\alpha}$)

$$\Big[\eta-\xi(\mathbf{p}\alpha)-\sum_m\Delta_{m\alpha\alpha}(p)\Delta^+_{m\alpha\alpha}(p)/(\eta+\xi(\mathbf{p}\alpha)) - \sum_m\Delta_{m\alpha,-\alpha}(p)\Delta^+_{m-\alpha\alpha}(p)/(\eta+\xi(\mathbf{p},-\alpha))\Big]G_\alpha(p)=1,$$

$$F^+_{m\beta\alpha}(p) = -i\frac{\Delta^+_{m\beta\alpha}(p)}{\eta+\xi(\mathbf{p}\beta)}G_\alpha(p). \tag{1}$$

Now let us consider the state of a superconductor with disordered impurity ion spins (we shall call such a state the paramagnetic phase).

2. PARAMAGNETIC PHASE

1. Let us determine the energy of the exchange interaction of conduction electron spins with the spins s_n of the magnetic ions

$$H_{sd} = \sum_n\int\psi^+(x)I(\mathbf{x}-\mathbf{R}_n)(\sigma\mathbf{s}_n)\psi(x)\,dx \tag{2}$$

for $T=0$ in the approximation corresponding to second-order perturbation theory. For this, it is necessary to evaluate

$$\langle(\sigma_{\alpha\alpha'}\mathbf{s}_n)\psi_\alpha{}^+(x)\psi_{\alpha'}(x)\rangle = \lim_{x'\to x-0}\langle T(\sigma_{\alpha\alpha'}\mathbf{s}_n)\psi_\alpha{}^+(x)\psi_{\alpha'}(x')S(\infty)\rangle, \tag{3}$$

to the corresponding approximation, where the operators to the right are written in the interaction representation and

$$S(\infty) = T\exp\Big(-i\int_{-\infty}H_{sd}\,dt\Big).$$

We describe the average with respect to the ground state of the product of operators encountered upon expansion of the S-matrix in the following way:[4]

$$\langle T(\sigma_{\alpha\alpha'}\mathbf{s}_n)(\sigma_{\beta\beta'}\mathbf{s}_{n'})\psi_\alpha{}^+(x)\psi_{\alpha'}(x')\psi_\beta{}^+(y)\psi_{\beta'}(y)\rangle = \langle(\sigma_{\alpha\alpha'}\mathbf{s}_n)(\sigma_{\beta\beta'}\mathbf{s}_{n'})\rangle\Big[G_{\beta'\alpha}(y,x)G_{\alpha'\beta}(x',y) + \sum_m F^+_{m\beta\alpha}(y,x)F_{m\alpha'\beta'}(x',y)\Big]. \tag{4}$$

Substituting (3) and (4) into (2) and going over to the momentum representation, we find

$$\langle H_{sd}\rangle = -\frac{i}{2}N_is(s+1)\int\frac{d\mathbf{p}\,d\mathbf{p}'\,d\eta}{(2\pi)^8}|I(\mathbf{q})|^2 \times\Big\{G(\mathbf{p},\eta)G(\mathbf{p}',\eta)+\sum_m[{}^1\!/_3F^+_{m\alpha\alpha}(\mathbf{p},\eta)F_{m\alpha\alpha}(\mathbf{p}',\eta) - {}^1\!/_3F^+_{m-\alpha\alpha}(\mathbf{p},\eta)F_{m\alpha,-\alpha}(\mathbf{p}',\eta) + {}^2\!/_3F^+_{m-\alpha\alpha}(\mathbf{p},\eta)F_{m-\alpha\alpha}(\mathbf{p}',\eta)]\Big\}. \tag{5}$$

Here N_i is the number of impurity atoms per unit volume, $\hbar=1$,

$$\xi(\mathbf{p}\alpha) = \xi(\mathbf{p}) = (p^2 - p_0^2)/2\mu,$$

and the Green's functions of a pure superconductor are taken as the unperturbed functions:[4]

$$G_\alpha(p) = G(p) = \frac{\eta + \xi(\mathbf{p})}{\eta^2 - \varepsilon^2(\mathbf{p})},$$

$$F^+_{m,\alpha\beta}(p) = -i\frac{\overset{+}{\Delta}_{m\alpha\beta}(\mathbf{p})}{\eta^2 - \varepsilon^2(\mathbf{p})},$$

$$F_{m\alpha\beta} = i\frac{\Delta_{m\alpha\beta}(\mathbf{p})}{\eta^2 - \varepsilon^2(\mathbf{p})}, \quad \varepsilon(\mathbf{p}) = \sqrt{\xi^2(\mathbf{p}) + \Delta^2},$$

$$\Delta_\alpha^2 = \Delta^2 = \sum_{m\beta}\Delta_{m\alpha\beta}(\mathbf{p})\overset{+}{\Delta}_{m\beta\alpha}(\mathbf{p}), \quad \beta = \alpha, -\alpha \tag{6}$$

(the indices α and β are used at this point only to indicate the relative direction of electron spins).

In order to simplify the calculations, we assume further that

$$|I(\mathbf{q})|^2 = I^2 = \text{const.}$$

In detail, this means that we are not interested in the orbital states of the pairs; electron-electron pairs interacting through an impurity atom and conduction electron-impurity electron pairs. Substituting (6) into (5) and changing to integrals over ξ and ξ', we find

$$\langle H_{sd}\rangle = -\frac{N_i s(s+1)I^2N^2(0)}{2^7\pi^3}\int d\xi\, d\xi'\, d\Omega\, d\Omega'$$
$$\times\left\{\frac{1}{\varepsilon+\varepsilon'}\left(1 - \frac{\xi\xi'}{\varepsilon\varepsilon'}\right) - \frac{1}{(\varepsilon+\varepsilon')\varepsilon\varepsilon'}\right.$$
$$\times\sum_m\left[\frac{1}{3}\overset{+}{\Delta}_{m\alpha\alpha}(\mathbf{p})\Delta_{m\alpha\alpha}(\mathbf{p}')\right.$$
$$\left.\left. -{}^1/_3\overset{+}{\Delta}_{m-\alpha\alpha}(\mathbf{p})\Delta_{m\alpha,-\alpha}(\mathbf{p}') + {}^2/_3\overset{+}{\Delta}_{m-\alpha\alpha}(\mathbf{p})\Delta_{m-\alpha\alpha}(\mathbf{p}')\right]\right\}. \tag{7}$$

Then we use the representation[4]

$$\overset{+}{\Delta}_{m\alpha\beta}(\mathbf{p}) = \Delta_m^* I_{\alpha\beta} Y_{lm}(\vartheta, \varphi),$$
$$\Delta_{m\alpha\beta}(\mathbf{p}) = -\Delta_m I_{\alpha\beta} Y_{lm}(\vartheta, \varphi). \tag{8}$$

Here two cases are naturally distinguished:

$$\langle H_{sd}\rangle = -\frac{N_i s(s+1)I^2N^2(0)}{8\pi}$$
$$\times\iint_{-\infty}^{+\infty} d\xi\, d\xi' \frac{1}{\varepsilon+\varepsilon'}\left(1 - \frac{\xi\xi' + \gamma_1\Delta^2}{\varepsilon\varepsilon'}\right),$$

$$\gamma_1 = \begin{cases}1, & l = 0\\ 0, & l \neq 0\end{cases}$$

It is convenient to calculate the difference between the energies $\langle H_{sd}\rangle$ for the normal and superconducting states. For the normal state

$$\langle H_{sd}\rangle_n = -\frac{N_i s(s+1)I^2N^2(0)}{4\pi}\iint_{-\infty}^{+\infty} d\xi\, d\xi' \frac{n(\xi') - n(\xi)}{\xi - \xi'},$$

$$n(\xi) = \begin{cases}1, & \xi < 0\\ 0, & \xi > 0.\end{cases}$$

Having now carried out calculations completely analogous to those performed in [5], we obtain as a result

$$\langle H_{sd}\rangle^{(l)}{}_s - \langle H_{sd}\rangle_n = \gamma_2\varphi\Delta(l),$$

$$\varphi = \frac{\pi}{4}N_i s(s+1)I^2N^2(0), \quad \gamma_2 = \begin{cases}1, & l = 0\\ {}^1/_2, & l \neq 0.\end{cases} \tag{9}$$

Relation (9) shows that in the case when

$$N(0)[\Delta^2(0) - \Delta^2(1)]/2 < \varphi[\Delta(0) - \Delta(1)/2],$$

the state with $l = 1$ may turn out to be more favorable than the state with $l = 0$. In addition, it follows from this relation that for triplet pairing the superconducting transition temperature decreases linearly with increasing concentration of magnetic ions.[6]

2. Now let us determine the effective interaction of impurity spins, arising due to their indirect exchange by means of conduction electrons. For this, it is necessary to determine to the second approximation the average of H_{sd} over the ground state of the electron system:

$$H_{ss} = \sum_n\sum_{\alpha\alpha'}\int I(\mathbf{x} - \mathbf{R}_n)(\sigma_{\alpha\alpha'}\mathbf{s}_n)\langle\psi_\alpha^+(x)\psi_{\alpha'}(x)\rangle\, d\mathbf{x}.$$

By carrying out transformations analogous to those carried out above, in the case of singlet pairing we obtain

$$H_{ss}^{(s)} = -\frac{1}{4}\sum_{nn'}\int\frac{d\mathbf{p}\, d\mathbf{p}'}{(2\pi)^7}|I(\mathbf{q})|^2\exp(-i\mathbf{q}\mathbf{R}_{nn'})$$
$$\times(\mathbf{s}_n\mathbf{s}_{n'})\frac{1}{\varepsilon+\varepsilon'}\left\{1 - \frac{1}{\varepsilon\varepsilon'}\right.$$
$$\left.\times\left[\xi\xi' - \sum_m\overset{+}{\Delta}_{m-\alpha\alpha}(\mathbf{p})\Delta_{m\alpha-\alpha}(\mathbf{p}')\right]\right\},$$

and in the case of triplet pairing

$$H_{ss}^{(t)} = -\frac{1}{4}\sum_{nn'}\int\frac{d\mathbf{p}\, d\mathbf{p}'}{(2\pi)^7}|I(\mathbf{q})|^2\exp\{-i\mathbf{q}\mathbf{R}_{nn'}\}\left\{(\mathbf{s}_n\mathbf{s}_{n'})\right.$$
$$\times\frac{1}{\varepsilon+\varepsilon'}\left\{1 - \frac{1}{\varepsilon\varepsilon'}\left[\xi\xi' + \sum_{m\beta}\overset{+}{\Delta}_{m\alpha\beta}(\mathbf{p})\Delta_{m\beta\alpha}(\mathbf{p}')\right]\right\}$$
$$+\frac{2}{(\varepsilon+\varepsilon')\varepsilon\varepsilon'}(s_n^y s_{n'}^y\sum_m\overset{+}{\Delta}_{m\alpha\alpha}(\mathbf{p})\Delta_{m\alpha\alpha}(\mathbf{p}')$$
$$\left.+ s_n^z s_{n'}^z\sum_m\overset{+}{\Delta}_{m\alpha,-\alpha}(\mathbf{p})\Delta_{m-\alpha\alpha}(\mathbf{p}')\right)\Big\},$$

where $\mathbf{q} = \mathbf{p} - \mathbf{p}'$, $\mathbf{R}_{nn'} = \mathbf{R}_n - \mathbf{R}_{n'}$. Then we again assume $|I(\mathbf{q})|^2 = I^2 = \text{const}$ and use the representation (8). Changing to integrals over ξ and ξ' and having carried out the integration over angles, for $l = 0$ we obtain

$$H_{ss}^{(0)} = -\frac{I^2N^2(0)}{16\pi}\sum_{nn'}\int\frac{d\xi\,d\xi'}{p_0^2R_{nn'}^2}(\mathbf{s}_n\mathbf{s}_{n'})\frac{1}{\varepsilon+\varepsilon'}$$

$$\times\left(1-\frac{\xi\xi'+\Delta^2}{\varepsilon\varepsilon'}\right)\cos\left[\frac{R_{nn'}}{v_0}(\xi-\xi')\right], \qquad (10)$$

for $l = 1$ we obtain

$$H_{ss}^{(1)} = -\frac{I^2N^2(0)}{16\pi}\sum_{nn'}\int\frac{d\xi\,d\xi'}{p_0^2R_{nn'}^2}\cos\left[\frac{R_{nn'}}{v_0}(\xi-\xi')\right]$$

$$\times\left[(\mathbf{s}_n\mathbf{s}_{n'})\frac{1}{\varepsilon+\varepsilon'}\left(1-\frac{\xi\xi'}{\varepsilon\varepsilon'}\right)+s_n^x s_{n'}^x\frac{{}^1/_3\Delta^2}{(\varepsilon+\varepsilon')\varepsilon\varepsilon'}\right],$$

where v_0 is the electron velocity at the Fermi surface; it is considered that distances $p_0R_{nn'} \gg 1$ are essential in the present problem. With the aid of Eq. (10), it is now not difficult to obtain the relations

$$H_{ss}^{(0)} - H_{ss}^{n} = \Delta\frac{I^2N^2(0)\pi}{8}\sum_{nn'}\frac{J(R_{nn'},0)}{p_0^2R_{nn'}^2}(\mathbf{s}_n\mathbf{s}_{n'}),$$

$$H_{ss}^{(1)} - H_{ss}^{n} = \Delta\frac{I^2N^2(0)\pi}{16}\sum_{nn'}\frac{J(R_{nn'},0)}{p_0^2R_{nn'}^2}$$

$$\times\left[(\mathbf{s}_n\mathbf{s}_{n'})-\frac{1}{3}s_n^x s_{n'}^x\right], \qquad (11)$$

where J(R, 0) is the BCS function.[5] As the right hand sides of Eqs. (11) show, superconductivity does not favor ferromagnetic ordering. (Here we shall not consider effects of the "cryptoferromagnetism" type discussed by Anderson and Suhl[7]).

3. FERROMAGNETIC PHASE

In this case the electron energy depends on its spin projection and, to the first approximation, has the form

$$\xi(\mathbf{p}\alpha) = \xi(\mathbf{p}) + \alpha\tilde{I}.$$

$\tilde{I}$ is the parameter of the s – d or s – f exchange interaction. The excitation spectrum is now determined from the cubic equation

$$\eta - \xi(\mathbf{p}\alpha) - \frac{\Delta_{\alpha\alpha}^2}{\eta+\xi(\mathbf{p}\alpha)} - \frac{\Delta_{\alpha,-\alpha}^2}{\eta+\xi(\mathbf{p},-\alpha)} = 0,$$

$$\Delta_{\alpha\alpha}^2 = \sum_m \Delta_{m\alpha\alpha}(\mathbf{p})\Delta_{m\alpha\alpha}^{+}(\mathbf{p}),\ \Delta_{\alpha,-\alpha}^2$$

$$= \sum_m \Delta_{m\alpha,-\alpha}(\mathbf{p})\Delta_{m-\alpha,\alpha}^{+}(\mathbf{p}). \qquad (12)$$

Neglecting relativistic effects (the spin-orbit interaction), one can use the representation (8) and consequently $\Delta_{\alpha\alpha}^2$ and $\Delta_{\alpha,-\alpha}^2$ [4] will be isotropic. The form of Eq. (12), which is unusual for the theory, characterizes the instability of the superconducting state, representing a superposition of energetically nonequivalent states $(\alpha, -\alpha)$ and (α, α). Actually, the energy of these states is, respectively, given by

$$E_1 = E_0 - N(0)\Delta^2/2,\quad \tilde{I} \leqslant 0.707\,\Delta,$$
$$E_2 = E_0 - N(0)\tilde{I}^2 - N(0)\Delta^2/2$$

(for $\tilde{I} > 0.707\,\Delta$ the nonsuperconducting state turns out to be more favorable[8]). Here E_0 denotes the energy of the normal paramagnetic state, and in both cases

$$\Delta = 2\tilde{\omega}\exp\left(-\frac{1}{\rho_l}\right),\quad \rho_l = N(0)\frac{|V_l|}{2l+1},$$

(l is odd); V is the matrix element of the electron-electron interaction due to exchange of virtual phonons (we neglected the scattering by spin waves which exists in the first case; in real ferromagnetic superconductors it is too weak[1)] to compensate for the term $N(0)\tilde{I}^2$). Thus, the solution $\Delta_{\alpha,-\alpha}^2 = 0$, $\Delta_{\alpha\alpha}^2 \neq 0$ is energetically lower. The superconducting transition temperature for this state is equal to $T_c = \gamma\Delta/\pi$ ($\ln\gamma = C = 0.577$),[1] i.e., it does not depend on $\tilde{I}$, and ordinary and magnetic[9] scattering by impurities, modification of the lattice (for example, a reduction of the Debye temperature due to the presence of impurities[10]) and other effects may contribute to its reduction. At the same time, as one can easily verify, in this case the spin polarization of the electrons is given by

$$\langle\sigma\rangle = \frac{1}{4}N(0)\left\{2\tilde{I} + \int_{\xi_0-\tilde{I}}^{\xi_0+\tilde{I}}[1-2f(\varepsilon)]\frac{\xi\,d\xi}{\varepsilon}\right\},$$

$$\varepsilon = \sqrt{\xi^2+\Delta^2(T)},\quad f(\varepsilon) = (e^{\varepsilon/T}+1)^{-1}.$$

Here ξ_0 is the Fermi energy. Thus, $\langle\sigma\rangle$ differs appreciably from the normal case. According to [11], this means that the Curie temperature curve does not undergo any substantial modification in the superconducting phase which, apparently, is also observed experimentally.[6] In this sense the triplet model is attractive for a theory of a ferromagnetic superconductor. It is necessary, however, to note that Eq. (12) apparently may give an even lower state if a superposition of singlet and triplet pairings is introduced into consideration. Such an investigation is being carried out at the present time.

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1)Although many people hold the same point of view, we know of no rigorous investigation of this question.

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