Coexistence of ferromagnetism and superconductivity in semimetals

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The possibility of coexistence of ferromagnetic ordering and superconductivity in a two-band model of semimetal with an isotropic current-carrier spectrum is investigated in detail. It is shown that triplet electron-hole and Cooper pairing with weak electron coupling can coexist at unequal electron and hole densities. A nonzero mean magnetic moment appears in this case.

1. INTRODUCTION

The coexistence of superconductivity and magnetism is of great interest because the interaction of these two competing order parameters leads to the appearance of new states in which magnetic ordering and superconducting pairing are transformed in such a manner that they can coexist. In most theoretical papers, however, the investigations concern mainly materials either with magnetic impurities or made up of magnetic elements.[1] The question of coexistence of magnetism and superconductivity in substances without magnetic impurities or made up of nonmagnetic elements has been attracting attention in connection with the observed abrupt increase of the magnetic susceptibility and of the nonlinear field dependence of the magnetic moment in superconducting ternary molybdenum chacogenides to which Al and Ga are added.[2] In such cases the magnetic ordering can be due to collectivized electrons, in analogy with the Stoner band ferromagnetism[3] and the excitonic ferromagnetism.[4] In the present paper is investigated, for a simple two-band model of a semimetal with an isotropic spectrum, the possibility of existence, in a superconductor, of the nonzero magnetic moment that is produced by interference between spin-density waves and Cooper pairs. It is known that in the case of triplet pairing of electrons and holes from different bands, an excitonic dielectric is antiferromagnetic and a spin-density wave is produced in it.[5] At unequal electron and hole densities, the system is unstable to Cooper pairings. Simultaneous existence of triplet electron-hole and intraband Cooper pairings leads automatically to the existence of triplet pairing of electrons from different bands [see Eq. (8)]. Since the functions $F^{ii}_{-\sigma\sigma}$ that describe the intraband Cooper pairing [see Eq. (7)] are antisymmetric in spin, the interaction between the dielectric and superconducting order parameters lifts the spin degeneracy. By virtue of the triplet pairing of electrons from different bands, the redistributions of the spins in two bands are not canceled out and a nonzero magnetic moment exists in the system at arbitrarily small interaction constants. The Stoner criterion that the interaction constants must satisfy actually becomes weaker in the present paper because account is taken of the valence band (the extra electrons below the gap) in addition to the conduction band (extra electrons above the gap). Since the spin splitting takes place in both bands, the kinetic-energy loss that is due to the redistribution of the carriers above the gap and prevents the existence of a ferromagnetic state at weak interaction in the case of one band[3] is offset by the energy gain on account of the states below the gap.

2. THE MODEL HAMILTONIAN

The single-particle spectrum of electrons of an isotropic semimetal is described by the Hamiltonian

$$H_0=\sum_{p\sigma i}\varepsilon_i(\mathbf{p})a_{i\sigma}^+(\mathbf{p})a_{i\sigma}(\mathbf{p}), \qquad (1)$$

where p is the electron quasimomentum; $i=1$ and 2 label respectively the electron and hole bands; $a_{i\sigma}(\mathbf{p})$, $a_{i\sigma}^+(\mathbf{p})$ are the Fermi operators of annihilation and creation of electrons with spin $\sigma/2=\pm 1/2$ in the ith band, and

$$\varepsilon_{1,2}(\mathbf{p})=\delta\mu\pm\varepsilon(\mathbf{p}),\quad \varepsilon(\mathbf{p})=p^2/2m-\varepsilon_F. \qquad (2)$$

Here ε_F is the Fermi energy, m is the effective mass which is assumed for simplicity to be the same for an electron and a hole, $\delta\mu$ is the Fermi-level shift produced in each of the bands by the doping. Neglecting local impurity levels, it can be assumed that the difference between the hole and electron densities is given. This condition enables us to determine $\delta\mu$.

We retain in the electron–electron interaction Hamiltonian $H_{\rm int}$ only the direct-interaction terms

$$H_{int}^{(1)}=\frac{1}{2}\sum\lambda_{ij}a_{i\sigma_1}^+(\mathbf{p}_1+\mathbf{q})a_{j\sigma_2}^+(\mathbf{p}_2-\mathbf{q})a_{j\sigma_2}(\mathbf{p}_2)a_{i\sigma_1}(\mathbf{p}_1) \qquad (3)$$

(the summation is over $i,j,\sigma_1,\sigma_2,\mathbf{p}_1,\mathbf{p}_2,\mathbf{q}$), so that the Hamiltonian of the system is

$$H=H_0+H_{int}^{(1)}. \qquad (4)$$

Allowance for the interaction terms

$$H_{int}^{(2)}=\sum{}' g[a_{i\sigma_1}^+(\mathbf{p}_1+\mathbf{q})a_{i\sigma_2}^+(\mathbf{p}_2-\mathbf{q})a_{j\sigma_2}(\mathbf{p}_2)a_{j\sigma_1}(\mathbf{p}_1)$$
$$+a_{i\sigma_1}^+(\mathbf{p}_1+\mathbf{q})a_{j\sigma_2}^+(\mathbf{p}_2-\mathbf{q})a_{i\sigma_2}(\mathbf{p}_2)a_{j\sigma_1}(\mathbf{p}_1)], \qquad (5)$$

(the summation is over $i,j,\sigma_1,\sigma_2,\mathbf{p}_1,\mathbf{p}_2,\mathbf{q}$ $(i\neq j)$) corresponding to electron transitions from one band to another leads only to a renormalization of the interaction constants λ_{ij}.

We continue the analysis in the high-density approximation, when the following inequalities hold:

$$\varepsilon_F\gg e^2\varkappa/\varepsilon_L,\ \delta\mu, \qquad (6)$$

where e is the electron charge, ε_L is the lattice dielectric constant, and $\varkappa$ is the reciprocal of the screening radius. In this case the potentials λ_{ij} and g can be regarded as indepen-

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dent of the momentum. This is permissible for the potential λ_{ij} because of the screening, while the potential g is short-range by its very definition. Its matrix elements are calculated with Bloch functions of different bands, and the latter are practically mutually orthogonal. We assume next that the constants λ_{ij} and g are real. They can be made real in the case of simple bands (that are degenerate only in spin) by a gauge transformation.

3. BASIC DEFINITIONS AND EQUATIONS

Our problem of coexistence of ferromagnetism and superconductivity, as stated in the Introduction, reduces to ascertaining the conditions under which coexistence of a triplet-dielectric parameter and a superconducting order parameter with nonzero magnetic moment is possible. We shall use a diagram technique for temperature Green's functions[6] which are defined, as usual:

$$G^{ij}_{\sigma_1\sigma_2}(x-x')=\langle T\psi_{i\sigma_1}(x)\psi^+_{j\sigma_2}(x')\rangle, \tag{7}$$

$$F^{ij}_{\sigma_1\sigma_2}(x-x')=-\langle T\psi_{i\sigma_1}(x)\psi_{j\sigma_2}(x')\rangle. \tag{8}$$

Here ψ and ψ^+ are the electron annihilation and creation operators in the Heisenberg representation. In the Schrödinger representation these operators can be expressed in terms of the annihilation and creation operators of band electrons with quasimomentum $\mathbf{p}$:

$$\psi_{i\sigma}(x)=\sum_{\mathbf{p}}\varphi_{i\mathbf{p}}(x)a_{i\sigma}(\mathbf{p}),$$

where $\varphi_{ip}(x)$ is a Bloch function with electron qausimomentum $\mathbf{p}$ in the ith band.

We shall consider, besides the normal Green's functions G_σ also the anomalous Green's functions that characterize the triplet dielectric pairing $G^{ij}_{-\sigma\sigma}$ $(i\neq j)$, and the intraband superconducting pairing, $F^{ii}_{-\sigma\sigma}$. Writing down the equations for these functions, we can verify right away that the simultaneous existence of the anomalous functions $G^{ij}_{-\sigma\sigma}$ $(i\neq j)$ and $F^{ii}_{-\sigma\sigma}$ leads automatically to the existence of anomalous Green's functions $F^{ij}_{\sigma\sigma}$ $(i\neq j)$, which characterize the triplet superconducting pairing. Indeed, the equations for these functions contain, on top of the diagrams shown in Fig. 1, four analogous ones with the indices 1 and 2 interchanged.

In the Matsubara representation, the system (Fig. 1) can be expressed after a Fourier transformation in the form

$$\begin{Vmatrix} (-i\omega+\varepsilon_1) & \Delta_{\sigma-\sigma} & {}^{11}_{-\sigma\sigma} & S^{21}_{\sigma\sigma} \\ \Delta^*_{\sigma-\sigma} & (-i\omega+\varepsilon_2) & -S^{21}_{-\sigma-\sigma} & -S^{22}_{-\sigma\sigma} \\ S^{11*}_{-\sigma\sigma} & -S^{21*}_{-\sigma-\sigma} & (-i\omega-\varepsilon_1) & -\Delta^*_{-\sigma\sigma} \\ S^{21*}_{\sigma\sigma} & -S^{22*}_{-\sigma\sigma} & -\Delta_{-\sigma\sigma} & (-i\omega-\varepsilon_2) \end{Vmatrix} \begin{Vmatrix} G^{11}_{\sigma\sigma}(\mathbf{p},\omega) \\ G^{21}_{-\sigma\sigma}(\mathbf{p},\omega) \\ F^{11+}_{-\sigma\sigma}(\mathbf{p},\omega) \\ F^{21+}_{\sigma\sigma}(\mathbf{p},\omega) \end{Vmatrix} = \begin{Vmatrix} 1 \\ 0 \\ 0 \\ 0 \end{Vmatrix}, \tag{9}$$

The gaps are defined in terms of Green's functions by the following expressions:

$$\begin{aligned} \Delta_{\sigma-\sigma}&=T\sum_{\mathbf{p},\omega}\lambda_{12}G^{12}_{\sigma-\sigma}(\mathbf{p},\omega), \\ S^{ii}_{-\sigma\sigma}&=T\sum_{\mathbf{p},\omega}\lambda_{ii}F^{ii}_{-\sigma\sigma}(\mathbf{p},\omega), \\ S_{\sigma\sigma}{}^{ij}&=T\sum_{\mathbf{p},\omega}\lambda_{ij}F_{\sigma\sigma}{}^{ij}(\mathbf{p},\omega)\quad(i\neq j), \end{aligned} \tag{10}$$

where $\omega=\pi T(2n+1)$ and n is an integer.

The solution of the system (9) is

$$\begin{aligned} DG_{\sigma\sigma}{}^{11}&=(i\omega+\varepsilon_1)(\varepsilon_2{}^2+\omega^2)-|\Delta_{-\sigma\sigma}|^2(-i\omega+\varepsilon_2) \\ &\qquad+|S^{21}_{-\sigma\sigma}|^2(i\omega+\varepsilon_2) \\ &\qquad-2\,\mathrm{Re}(S^{21*}_{-\sigma-\sigma}S^{22}_{-\sigma\sigma}\Delta_{-\sigma\sigma})+|S^{22}_{-\sigma\sigma}|^2(i\omega+\varepsilon_1), \\ DG^{21}_{-\sigma\sigma}&=-\Delta^{\cdot}_{\sigma-\sigma}(i\omega+\varepsilon_1)(i\omega+\varepsilon_2)+\Delta^{\cdot}_{\sigma-\sigma}|\Delta_{-\sigma\sigma}|^2 \\ &\qquad+S^{21}_{-\sigma-\sigma}S^{11*}_{-\sigma\sigma}(i\omega+\varepsilon_2) \\ &\qquad-S^{11*}_{-\sigma\sigma}S^{22}_{-\sigma\sigma}\Delta_{-\sigma\sigma}-S^{21*}_{\sigma\sigma}S^{21}_{-\sigma-\sigma}\Delta^{\cdot}_{-\sigma\sigma}+S^{21*}_{\sigma\sigma}S^{22}_{-\sigma\sigma}(i\omega+\varepsilon_1), \\ DF^{11+}_{-\sigma\sigma}&=S^{21*}_{-\sigma-\sigma}\Delta^{*}_{\sigma-\sigma}(i\omega+\varepsilon_2)-S^{22*}_{-\sigma\sigma}\Delta^{*}_{\sigma-\sigma}\Delta^{*}_{-\sigma\sigma} \\ &\qquad+S^{11*}_{-\sigma\sigma}(\varepsilon_2{}^2+\omega^2)+S^{11*}_{-\sigma\sigma}|S^{22}_{-\sigma\sigma}|^2 \\ &\qquad-S^{21*}_{\sigma\sigma}\Delta^{*}_{-\sigma\sigma}(-i\omega+\varepsilon_2)-S^{21*}_{\sigma\sigma}S^{21*}_{-\sigma-\sigma}S_{-\sigma\sigma}, \\ DF^{21+}_{\sigma\sigma}&=-S^{21*}_{-\sigma-\sigma}\Delta^{*}_{\sigma-\sigma}\Delta_{-\sigma\sigma}+S^{22*}_{-\sigma\sigma}\Delta^{*}_{\sigma-\sigma}(i\omega+\varepsilon_1)+S^{21*}_{\sigma\sigma}|S^{21}_{-\sigma-\sigma}|^2 \\ &\qquad-S^{11*}_{-\sigma\sigma}\Delta_{-\sigma\sigma}(-i\omega+\varepsilon_2)-S^{21}_{-\sigma-\sigma}S^{11*}_{-\sigma\sigma}S^{22*}_{-\sigma\sigma}+S^{21*}_{\sigma\sigma}(-i\omega+\varepsilon_2)(i\omega+\varepsilon_1), \end{aligned} \tag{11}$$

where the determinant of the system (9) is

$$D=(\omega^2+\omega_+{}^2)(\omega^2+\omega_-{}^2). \tag{12}$$

Substituting the expressions (11) for the Green's functions in (10) we obtain a system of self-consistent equations for the gaps.

4. CONDITIONS FOR THE COEXISTENCE OF ELECTRON-HOLE AND COOPER PAIRINGS

Denoting the phases of the gaps by α_1 for $\Delta_{\sigma-\sigma}$; α_2 for $\Delta_{-\sigma\sigma}$; α_3 for $S^{11}_{-\sigma\sigma}$; α_4 for $S^{22}_{-\sigma\sigma}$; α_5 for $S^{21}_{-\sigma-\sigma}$; α_6 for $S^{21}_{\sigma\sigma}$, we obtain the conditions for the existence of a solution of the

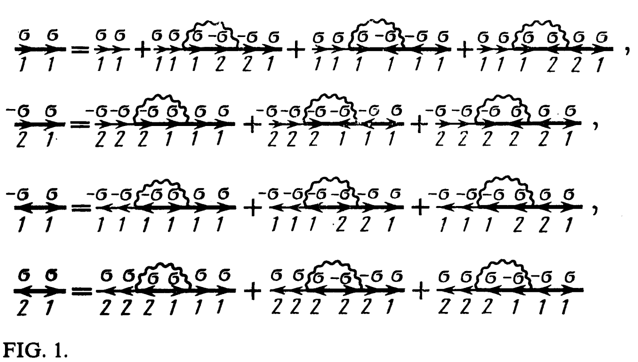

FIG. 1.

system of equations (10) for the gaps:

$$\alpha_1-\alpha_3+\alpha_5=k_1\pi,\quad \alpha_1+\alpha_4-\alpha_6=k_2\pi,$$
$$\alpha_1-\alpha_2+\alpha_5-\alpha_6=k_3\pi, \tag{13}$$

where k_1, k_2, and k_3 are integers. An investigation of these conditions yields readily the following physical solutions:

a) a solution corresponding to a spectrum of elementary excitations of the form

$$\omega_\pm^2=(E\pm\delta\tilde{\mu})^2+\tilde{S}^2,$$
$$E^2=\varepsilon^2+\tilde{\Delta}^2,\quad \delta\tilde{\mu}^2=\delta\mu^2+S_2^2, \tag{14}$$
$$\tilde{\Delta}^2=(\delta\mu\Delta\pm S_1S_2)^2/\delta\tilde{\mu}^2,\quad \tilde{S}^2=(\delta\mu S_1\mp S_2\Delta)^2/\delta\tilde{\mu}^2;$$

b) a solution corresponding to a spectrum of elementary excitations of the form (14) with $S_2=0$;

c) a solution corresponding to a spectrum of elementary excitations of the form

$$\omega_\pm^2=(E\pm\delta\tilde{\mu})^2+S_1^2,\quad E^2=\varepsilon+\Delta^2. \tag{15}$$

These solutions were obtained under the assumption that the gaps $\Delta_{\sigma-\sigma}$ and $\Delta_{-\sigma\sigma}$, $S^{11}_{-\sigma\sigma}$ and $S^{22}_{-\sigma\sigma}$, and $S^{21}_{\sigma\sigma}$ and $S^{21}_{-\sigma-\sigma}$ have pairwise identical moduli, which were designated Δ, S_1, and S_2 respectively. We are not interested in solutions a) and b), which yield a zero magnetic moment and coincide with the solutions investigated in Ref. 7 for singlet dielectric pairing.

Substituting the expressions for the Green's functions (11) with spectrum (15) in (10), we obtain a system of equations for the gaps:

$$1=\frac{1}{2}\int_0^{\omega_c}N(0)\lambda_{12}\frac{d\varepsilon}{E}\left[\frac{E-\delta\tilde{\mu}}{\omega_-}\operatorname{th}\frac{\omega_-}{2T}+\frac{E+\delta\tilde{\mu}}{\omega_+}\operatorname{th}\frac{\omega_+}{2T}\right],$$
$$1=-\frac{1}{2}\int_0^{\omega_D}N(0)\lambda_{11}d\varepsilon\left[\frac{1}{\omega_+}\operatorname{th}\frac{\omega_+}{2T}+\frac{1}{\omega_-}\operatorname{th}\frac{\omega_-}{2T}\right], \tag{16}$$
$$1=\frac{1}{2}\int_0^{\infty}N(0)\lambda_{12}\frac{d\varepsilon}{\delta\tilde{\mu}}\left[\left(\frac{E+\delta\tilde{\mu}}{\omega_+}\operatorname{th}\frac{\omega_+}{2T}-\frac{E-\delta\tilde{\mu}}{\omega_-}\operatorname{th}\frac{\omega_-}{2T}\right)+\frac{S_1\Delta\delta\mu}{S_2E}\left(\frac{1}{\omega_-}\operatorname{th}\frac{\omega_-}{2T}-\frac{1}{\omega_+}\operatorname{th}\frac{\omega_+}{2T}\right)\right],$$

where $N(0)$ is the density of states on the Fermi level, and ω_c and ω_D are the cutoff frequencies for λ_{ij} $(i\neq j)$ and λ_{ii}, respectively.

It can be seen from (16) that the equations for the gaps have a solution when $\lambda_{11}<0$ and $\lambda_{12}>0$, corresponding to attraction of the electrons in one band and of an electron to a hole from different bands, just as when the dielectric and superconducting pairings exist separately.

For $T=0$ (we can obtain analytically the interaction-constants region in which electron-hole and Cooper pairings coexist (mixed *S-D* state). This region is shown in Fig. 2 in the coordinates (Δ_0, S_0), where Δ_0 and S_0 are respectively the dielectric and superconducting gaps when they exist separately:

$$\Delta_0=2\omega_c\exp\left(-\frac{1}{\lambda_{12}N(0)}\right),\quad S_0=2\omega_D\exp\left(-\frac{1}{|\lambda_{12}|N(0)}\right). \tag{17}$$

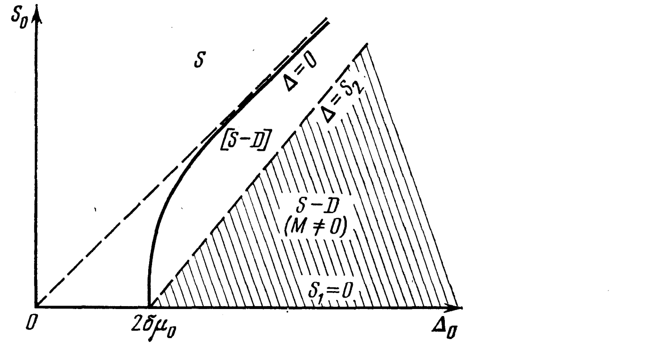

FIG. 2. *S*—region of existence of superconducting state; [*S-D*]—region of metastable mixed state. *S-D* ($M\neq 0$)—region of existence of mixed state with nonzero magnetic moment.

The line $\Delta=0$ on which $S_2=0$ is determined by the equation

$$\ln\frac{\Delta_0}{S_0}=\frac{\delta\mu}{2}(\delta\mu^2+S_0^2)^{-1/2}\ln\frac{(\delta\mu^2+S_0^2)^{1/2}+\delta\mu}{(\delta\mu^2+S_0^2)^{1/2}-\delta\mu}, \tag{18}$$

and the line S_1 on which S_2 is also equal to zero is determined by the equation

$$S_0=0. \tag{19}$$

The region of existence of mixed *S-D* state is located between the line $S_1=0$ and the line $\Delta=0$. It can be seen from (18) and (19) that the system is unstable at arbitrarily weak interaction between the electrons, when extra electrons exist ($\delta\mu\neq 0$), and the region of the dielectric pairing becomes narrower because of the existence of Cooper pairing (see Fig. 2). In fact, the region of the existence of a mixed *S-D* state is restricted also by the condition for the free energy. Indeed, a general expression for the free energy of the state in question, relative to the state of the normal semimetal,[8] is

$$\Delta\Omega_{SD}=\int\sum_{ij}\left\langle\frac{H^{ij}_{int}}{\lambda_{ij}}\right\rangle d\lambda_{ij}, \tag{20}$$

where we use the representation

$$H^{(1)}_{int}=\sum_{ij}H^{ij}_{int}.$$

From this we get

$$\Delta\Omega_{SD}=\Delta\Omega_g-2\int_0^{|\lambda_{11}|}\frac{S_1^2}{\lambda_{11}^2}d|\lambda_{11}|,$$
$$\Delta\Omega_{SD}=\Delta\Omega_s-2\int_0^{\lambda_{12}}\frac{\Delta^2-S_2^2}{\lambda_{12}^2}d\lambda_{12}, \tag{21}$$

where $\Delta\Omega_g$ and $\Delta\Omega_s$ are the free energies of the dielectric and superconducting states relative to the state of the normal semimetal when they exist separately.

It can be seen from (21) that for the mixed *S-D* state to be energywise favored over the excitonic dielectric and the superconducting states, when they exist separately, the following condition must be satisfied:

$$\Delta>S_2. \tag{22}$$

On the diagram the line $\Delta = S_2$ lies in the (Δ_0, S_0) plane, between the lines $\Delta = 0$ and $S_1 = 0$, so that the region of existence of the mixed *S-D* state lies between the line $\Delta = S_2$ and the line $S_1 = 0$ (the shaded region in Fig. 2). Since a numerical calculation is needed to plot the line $\Delta = S_2$, we show it symbolically as dashed.

5. MAGNETIC PROPERTIES OF MIXED *S-D* STATE

The average magnetic moment can be calculated in terms of the Green's functions:

$$M = T\sum_{\omega}\mu_0\int\frac{d\mathbf{p}}{(2\pi)^3}[G^{11}_{\uparrow\uparrow}(\mathbf{p}\omega) - G^{11}_{\downarrow\downarrow}(\mathbf{p}\omega) + G^{22}_{\uparrow\uparrow}(\mathbf{p}\omega) - G^{22}_{\downarrow\downarrow}(\mathbf{p}\omega)], \quad (23)$$

where μ_0 is the Bohr magneton. Substituting in (23) the expressions for the Green's functions from (11), we obtain for the considered state with spectrum (15)

$$M = 2\frac{\mu_0 S_1 S_2 \Delta}{\delta\tilde{\mu}}\int_0^\infty N(0)\frac{d\varepsilon}{E}\left(\frac{1}{\omega_-}\operatorname{th}\frac{\omega_-}{2T} - \frac{1}{\omega_+}\operatorname{th}\frac{\omega_+}{2T}\right). \quad (24)$$

The magnetic moment that results from the interaction of the dielectric and superconducting order parameters vanishes when one of these order parameters is zero. In the general case the dielectric-transition temperature T_D (at which $\Delta = 0$) differs from the superconducting-transition temperature T_s (at which $S_1 = 0$). Thus, the Curie temperature (at which $M = 0$) will be the smaller of T_D and T_s.

To conclude this section we note that in the case of an undoped semimetal the system (16) has a solution only at a finite value of λ_{12}. For weak interaction, the system (16) has a solution if $S_2 = 0$ and $S_0 = \Delta_0$. Notwithstanding so stringent a condition on the interaction constants at $S_1 = 0$, it can be seen from (24) that the average magnetic moment is also equal to zero. It is seen from the figure that the mixed *S-D* state in which a nonzero magnetic moment exists can be stable at any value of S_0, but only at $\Delta_0 > 2\delta\mu$. Thus, the conditions for the interaction constants, which, as stated in the Introduction, are weakened by spin splitting in both bands compared with the similar condition in Stoner's theory,[3] do not change for λ_{12} in this case (owing to the condition $\delta\mu \neq 0$).

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