Heavy-fermion superconductivity in the two-band model

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The thermodynamic and electrodynamic properties of heavy-fermion superconductors are analyzed in a model with interband singlet pairing. The general expression for the electron-electron interaction is analyzed. It is shown in particular that spin fluctuations, both ferromagnetic and (especially) antiferromagnetic, promote such a pairing. An expression is derived for the free-energy functional. The behavior of the coherence length, the upper critical field, and the London penetration depth in the limits $T = 0$ and $T \to T_c$ is analyzed. This model leads to a good qualitative agreement with the properties of heavy-fermion superconductors.

1. INTRODUCTION

Heavy-fermion superconductors[1,2]—compounds of rare earth metals and actinides in which there are electrons with huge effective masses $m_f \approx (10^2–10^3) m_0$ at the Fermi surface at low temperatures—have recently attracted much interest. So far, research has unraveled neither the nature of the heavy fermions themselves nor that of the superconductivity in them. It has been suggested[3–5] that the pairing which occurs in these substances is anisotropic and possibly of a triplet nature, as in ^{3}He. On the other hand, there are arguments in favor of the more common singlet superconductivity, especially in the case of the first superconductor of this class, $CeCu_2Si_2$ (Refs. 2 and 6).

Discussions of the superconductivity of these systems usually deal with the pairing of heavy f electrons. However, there are strong arguments[7,8] for the case that these systems contain, in addition to the heavy electrons, some comparatively light d electrons with $m_d \geqslant m_0$. A question which naturally arises is that of the relative roles played by these two components in the superconductivity. It is clear from experimental data, in particular, on the jump in the heat capacity $\Delta C/\gamma T_c$ and the value of $\partial H_{c2}/\partial T$, that the heavy component participates in the pairing.[1,2] At the same time, there are data which may be evidence that electrons with small masses are participating in the superconductivity.[2] There are furthermore indications that some of the electrons (heavy electrons in UPt_3 and light electrons in $CeCu_2Si_2$) may possibly remain normal down to temperatures $T \ll T_c$ (Ref. 6). This possibility follows from the behavior of the heat capacity $C_S(T)$ and of the thermal conductivity $K_S(R)$ for $T \ll T_c$.

In the present paper we analyze one possibility, which leads to a qualitative explanation of the basic experimental results on superconductivity in heavy-fermion compounds. Specifically, we suggest that in these systems, which we will deal with phenomenologically as two-component systems, there may be a singlet pairing of electrons from different bands, of the type $\langle a_{f\uparrow}^{+} a_{d\downarrow}^{+} - a_{f\downarrow}^{+} a_{d\uparrow}^{+} \rangle$. This possibility was examined a fairly long time ago.[9–11] It was discussed in connection with heavy-fermion systems in Refs. 12–15.

We should first mention that a tendency toward an interband singlet pairing of this sort can be seen even in the very simple model of an Anderson or Kondo lattice, which is widely used today to analyze the properties of heavy-fermion systems. Specifically, the Kondo interaction

$$H_{int} = -J a_{fs}^{+} \hat{\mathbf{s}} a_{fs'} a_{d\sigma}^{+} \hat{\boldsymbol{\sigma}} a_{d\sigma} \quad (1)$$

naturally arises in these models and leads in particular to the possibility that a singlet pair of an f electron and a d electron will form. Although the situation is actually more complicated[16] (strictly speaking, we cannot restrict the analysis to the ladder approximation here; in addition to the electron-electron mechanism, it is necessary to consider the electron-hole mechanism, etc.), it is useful, as a first step, to analyze the conditions for and the possible consequences of an interband pairing of this sort in a very simple model analogous to the BCS model. A generalization will be made at the end of this paper.

In this paper we analyze in its general form the nature of the electron-electron interaction in systems of this sort, and we examine the effective electron-electron interaction in various channels (intraband and interband). We then analyze in detail the various thermodynamic and electrodynamic properties of superconductors with an interband pairing. Analyzing the results, and comparing them with experimental data, we can draw conclusions about the plausibility of this proposed explanation of the superconductivity in heavy-fermion systems.

2. ELECTRON-ELECTRON INTERACTION IN A TWO-COMPONENT SYSTEM

To determine which types of pairing are most probable in a two-component system, we consider the general structure of the electron-electron interaction. For the most part, we will assume interband interactions of the form (1), which are specific to systems of this type, as the starting point, although we will also briefly discuss the consequences of other interactions (the electron-phonon interaction and the long-range Coulomb interaction).

To study the effective electron-electron interaction, we need to construct a two-particle vertex function which is irreducible in the particle-particle channel:

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$$\Gamma^{ijkl}_{\alpha_3\alpha_4\alpha_1\alpha_2}(p_3, p_4, p_1, p_2),$$

where $i, j, k, l = d, l$ are band indices; α_i are spin indices; and $p_i = (\mathbf{p}_i, \varepsilon_i)$ are the 4-momenta of the particles. The momentum transfer is $q = p_3 - p_1$. This quantity can be written as a sum (Refs. 17–19; see Fig. 1 of the present paper):

$$\Gamma = W + \Gamma^{dir} + \Gamma^{ex}, \tag{2}$$

where Γ^{dir} is a vertex function which is irreducible in the particle-particle channel but reducible in the direct $(q = p_3 - p_1)$ particle-hole channel, Γ^{ex} is the corresponding function which is reducible in the particle-hole exchange channel $(\tilde{q} = p_4 - p_1)$, and the block W is irreducible in any channel.

We first examine the case of a short-range interaction, which reveals the basic features of the behavior of the effective interaction and yields effective coupling constants, as we will see below. In general, the Hamiltonian of the interaction of electrons from different bands can be written in the form

$$H_{int} = \sum_q \{{}^1/_4 I(q)\hat{n}_f(q) n_d(q) - J(q)(\hat{\mathbf{S}}_d \hat{\mathbf{S}}_f)\}, \tag{3}$$

where

$$\hat{n}_i(q) = \hat{\psi}_i^+(q)\hat{\psi}_i(q), \quad \hat{\mathbf{S}}_i = {}^1/_2 \hat{\psi}_i^+ \hat{\sigma} \hat{\psi}_i,$$

and I and J are assumed to be irreducible in all channels. It follows from the antisymmetry of the scattering amplitude under interchange of particles that we have

$$2I(p_3 - p_1) = I(p_4 - p_1) + J(p_4 - p_1). \tag{4}$$

If we ignore the frequency and momentum dependence of I and J, we then find the identity $I \equiv J$. In this case, I and W are the same and take the form $(i \neq j)$

$$I^{ijkl}_{\alpha_3\alpha_4\alpha_1\alpha_2} = {}^1/_4 J[\delta_{\alpha_3\alpha_1}\delta_{\alpha_4\alpha_2} - \boldsymbol{\sigma}_{\alpha_3\alpha_1}\boldsymbol{\sigma}_{\alpha_4\alpha_2}]\delta^{ik}\delta^{jl}.$$

To determine the vertex function Γ^{dir} we must solve a Bethe-Salpeter equation in the direct channel. The function Γ^{ex} is found through the interchanges $i \leftrightarrow j$, $3 \leftrightarrow 4$, $q \leftrightarrow q + p_2 - p_1$.

As a result we find

$$\Gamma^{ijkl}_{\alpha_3\alpha_4\alpha_1\alpha_2}(p_1 - q, p_2 + q, p_1, p_2)$$

$$= \mathcal{T}_{\alpha_3\alpha_1}(q)\delta^{ik}\delta^{jl} - \mathcal{T}_{\alpha_4\alpha_2}(q + p_2 - p_1)\delta^{il}\delta^{jk}, \tag{5}$$

where

$$\mathcal{T}_{\alpha_3\alpha_1}(q) = [J(q)/4d(q)]\{\delta_{\alpha_3\alpha_1}\delta_{\alpha_4\alpha_2}M^+(q) + \boldsymbol{\sigma}_{\alpha_3\alpha_1}\boldsymbol{\sigma}_{\alpha_4\alpha_2}M^-(q)\},$$
$$M^{\pm}(q) = \begin{pmatrix} -J\chi_f(q)/4 & \pm 1 \\ \pm 1 & -J\chi_d(q)/4 \end{pmatrix}.$$

Here

$$\chi_i(q) = 2i \sum_p \mathcal{G}_i(p - q/2)\mathcal{G}_i(p + q/2) \tag{6}$$

is the polarization operator for the electrons from band i, and

$$d(q) = 1 - J^2 \chi_d(q)\chi_f(q)/16. \tag{7}$$

In this model we can also derive the charge susceptibility $\chi_\rho(q)$ and the spin susceptibility $\chi_s(q)$:

$$\chi_\rho(q) = [\chi_d(q) + \chi_f(q) - J\chi_d(q)\chi_f(q)/2]/d(q), \tag{8}$$

$$\chi_s(q) = [\chi_d(q) + \chi_f(q) + J\chi_d(q)\chi_f(q)/2]/d(q). \tag{9}$$

It follows from (8) and (9) that in this model the susceptibilities χ_ρ and χ_s have singularities in the case $d(q) \equiv 0$; i.e., the magnetic transition and the structural instability occur simultaneously. The reason for this result is the condition $J = I$ in (3). If there is dispersion in the quantities J and I, the points of the instabilities in the spin and charge channels will generally not coincide.

Using a vertex function which is irreducible in the particle-particle channel, we can derive an expression for the effective interaction and the coupling constants which appear in important properties like the critical temperature of the superconducting transition. The equations for determining this quantity are[1)] (Fig. 2)

$$F^{ij}_{\alpha_3\alpha_4}(p) = i\mathcal{G}_i(p)\mathcal{G}_j(-p) \sum_{\substack{\alpha_1,\alpha_2 \\ p' \\ k,l}} \Gamma^{ijkl}_{\alpha_3\alpha_4\alpha_1\alpha_2}(p, -p, p', -p')F^{kl}_{\alpha_1\alpha_2}(p'), \tag{10}$$

where $F^{ij}_{\alpha\beta}(p) = -\langle T(\psi^j_{\beta,-p}, \psi^i_{\alpha,p})\rangle$ is the Gor'kov function. The latter can be written in the form

$$F_{\alpha\beta} = F\sigma_{\alpha\beta}{}^y$$

for singlet pairing and in the form

$$F_{\alpha\beta} = \sum_\gamma (\mathbf{F}\boldsymbol{\sigma}_{\alpha\gamma})\sigma_{\gamma\beta}{}^y$$

for triplet pairing.

In this case we find from (10)

$$F^{ij}(p) = 2i\mathcal{G}_i(p)\mathcal{G}_j(-p) \sum_{p'} V^{s,t}_{ij}(p - p')F^{ij}(p'), \tag{11}$$

where the effective singlet and triplet interactions $V^{s,t}$ depend only on the momentum transfer $p - p'$ and are given by the following expressions.

a) For the intraband interaction (e.g., $f - f$), we have

$$V^{s,t}_{ff}(q) = \pm J^2 \chi_d(q)/8d(q), \tag{12}$$

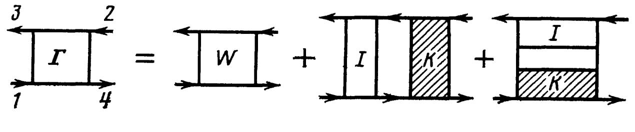

FIG. 1.

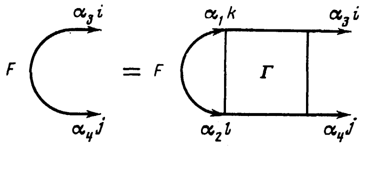

FIG. 2.

where the plus sign corresponds to singlet pairing and the minus sign to triplet pairing. For the $d-d$ interaction we need to replace χ_d by χ_f in (12).

b) For the interband pairing $(d-f)$ we have

$$V_{df}^{s}(q)=J/d(q), \quad V_{df}^{t}(q)\equiv 0. \tag{13}$$

These results can easily be generalized to the case of the long-range Coulomb and electron-phonon interactions. Without writing out the expressions for the vertex function Γ, we list the results for the effective interactions (see also Ref. 18):

$$V_{ff}^{s,t}(q)=\frac{|\Lambda_f(q)|^2}{\varepsilon_{tot}(q)}V_C(q)\pm\frac{J^2\chi_d(q)}{8d(q)}, \tag{14}$$

$$V_{df}^{s}(q)=\frac{\Lambda_d^*(q)\Lambda_f(q)}{\varepsilon_{tot}(q)}V_C(q)+J/d(q),$$

$$V_{df}^{t}(q)=\frac{\Lambda_d^*(q)\Lambda_f(q)}{\varepsilon_{tot}(q)}V_C(q), \tag{15}$$

where $V_c(q)=4\pi e^2/q^2$ is the Coulomb interaction, $\Lambda_i(q)$ is the vertex function

$$\Lambda_i(q)=\frac{1}{d(q)}\begin{pmatrix} 1-J\chi_f(q)/4 \\ 1-J\chi_d(q)/4 \end{pmatrix}_i, \tag{16}$$

and $\varepsilon_{tot}(q)$ is the total dielectric constant of the crystal, which incorporates both the electron screening and the electron-phonon interaction, and which is given by

$$1/\varepsilon_{tot}(q)=1/\varepsilon_{el}(q)+D_{ph}(q). \tag{17}$$

Here D_{ph} is the renormalized phonon Green's function, and ε_{el} is the electron dielectric constant of the nonvibrating rigid lattice, which is related to Λ_i by

$$\varepsilon_{el}(q)=1+[\Lambda_d(q)\chi_d(q)+\Lambda_f(q)\chi_f(q)]V_C(q). \tag{18}$$

To calculate the critical temperature of the superconducting transiton we need to solve Eq. (11). As in the BCS theory, we assume that the interaction is instantaneous and that the entire frequency dependence reduces to a cutoff of the interaction of the finite widths of the bands, w_d and w_f. We furthermore assume that the Fermi surfaces for the light and heavy components coincide completely (the consequences of a deviation from complete coincidence will be discussed below). If we adopt the condition $T_c \ll w_f \ll w_d$, we can easily derive expressions for T_c in the weak-coupling approximation for the cases of intraband and interband pairing.

a) For intraband (f-band) pairing we find

$$T_c\approx w_f\exp(-1/g_f^{\,l}). \tag{19}$$

b) For interband pairing (Refs. 9, 14, and 15) we have

$$T_c\approx (w_d w_f)^{1/2}\exp(-1/g_{df}^{\,l}), \tag{20}$$

where the coupling constants g^l for the various orbital angular momenta l are related to the effective interaction $V_{ij}(\mathbf{q})$ by [2)]

$$g_f^{\,l}=-N_f(0)\langle V_{ff}^{\,l}\rangle$$

$$=-N_f(0)\int_0^{2k_F}\frac{q\,dq}{(2k_F)^2}P_l\left[1-2\left(\frac{q}{2k_F}\right)^2\right]V_{ff}^{\,l}(\mathbf{q}), \tag{21}$$

$$g_{df}^{\,l}=-N_d(0)\langle V_{df}^{\,l}\rangle$$

$$=-N_d(0)\int_0^{2k_F}\frac{q\,dq}{(2k_F)^2}P_l\left[1-2\left(\frac{q}{2k_F}\right)^2\right]V_{df}^{\,l}(\mathbf{q}). \tag{22}$$

Here $\langle\ldots\rangle$ means an average over angles, and the $P_l(x)$ are the Legendre polynomials.

Substituting (12), (13) into (21), (22) we see that in the general case with $J<0$ the interaction in the singlet interband channel is the strongest. The specific values of g^l depend on the corresponding static interactions, (12), (13). If the system is nearly ferromagnetic, i.e., if $d(q)$ has a maximum at $q=0$ [see (9)], the interaction is an attraction in the singlet interband channel, and in the triplet $f-f$ channel the interaction is analogous to that in the case of ^{3}He. If the system contains highly antiferromagnetic spin fluctuations, however [if $d(q)$ goes through a maximum at some nonzero value $q_0\neq 0$], then an $f-f$ singlet pairing in the d state ($l=2$) and a $d-f$ singlet pairing will be preferable (similar conclusions were reached for the single-band case in Refs. 20–22). Figure 3 is a sketch of the various coupling constants as functions of q_0. It is not difficult to show that approaching the region of magnetic instability enhances the tendency toward interband singlet pairing, and this effect turns out to be stronger in the antiferromagnetic case. If

$$d(q)=(1-I)+\alpha(\mathbf{q}-\mathbf{q}_0)^2,$$

then it follows from relations (13) and (22) that for $q_0\equiv 0$ we have

$$g_{df}^{\,s}\sim|\ln(1-I)|,$$

while for $\mathbf{q}_0\neq 0$ we have

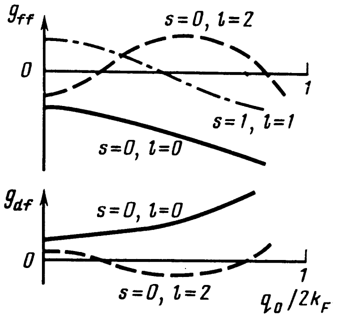

FIG. 3. Sketch of the intraband and the interband interaction constants as functions of the wave vector $\mathbf{q}_0$. Solid lines—$s=0$, $l=0$; dashed lines—$s=0$, $l=2$; dot-dashed line—$s=1$, $l=1$.

$$g_{df}^s \sim (1-I)^{-1/2}.$$

To conclude this section of the paper, we take a brief look at (1) how the result will be altered by the incorporation of long-range contributions and (2) how the constant g_{df}^s depends on the magnetic field.

To answer the first of these questions, we must combine relations (15)–(18) and (22). As a result, we can write g_{df}^s in standard form (we are ignoring the pronounced difference between the typical phonon and electron energies):

$$g=\lambda_{ph}-\mu+\lambda_m,$$

where $\lambda_{\rm ph} = N_d(0)\langle \Lambda_d^* D_{\rm ph}\Lambda_f\rangle$ is the electron-phonon coupling constant,

$$\lambda_m=-N_d(0)J\langle 1/d(q)\rangle \tag{23}$$

is the magnon coupling constant, whole sign in this case corresponds to an attraction, and μ is the Coulomb coupling constant, to which the Kondo interaction also contributes through the dielectric constant. This coupling constant is given by

$$\mu=-N_d(0)J\langle 1/d(q)\rangle/4+O(N_d(0)/N_f(0)). \tag{24}$$

It follows from this expression that incorporating the Coulomb interaction reduces by a fourth the effective attraction due to the exchange of spin excitations, but it does not change the sign of the interaction.

The effect of a magnetic field is determined by the change in the polarization operators. The increment in the effective interaction is

$$\delta V_{df}^s(q)\approx\frac{J^3}{32d^2(q)}\chi_d(q)\delta\chi_f^{\uparrow\downarrow}(q), \tag{25}$$

where $\delta\chi^{\uparrow\downarrow}$ is the change in the polarization operator

$$\chi_i^{\uparrow\downarrow}(q)=2i\sum_p \mathcal{G}_i^{\uparrow}(p-q/2)\mathcal{G}_i^{\downarrow}(p+q/2), \tag{26}$$

which is quadratic in the field **H**. In the case of quadratic dispersion laws, this effect leads to an increase in the coupling constant g_{df}^s by an amount

$$\delta g_{df}^s\approx(g_{df}^s)^3(\mu_B H/w_f)^2 w_d/w_f, \tag{27}$$

i.e., to an increase in the coupling constant when an external field is applied. This result may prove important in interpreting the functional dependence $H_{c2}(T)$. It may be determined to a large extent in these systems by the particular way in which the normal properties of the substance, in particular, the coupling constant, depends on the magnetic field.

In summary, in some typical cases, in particular, in an interaction of the type in (1), which is the most characteristic interaction for heavy-fermion systems, and for the proximity to antiferromagnetism which is typical to these system, interband singlet s-wave pairing is predominant (possibly along with an intraband singlet d-wave pairing).

3. PROPERTIES OF SUPERCONDUCTORS WITH INTERBAND PAIRING

We turn now to a more detailed study of the properties of superconductors with a singlet interband (hybrid) pair-

$$\Delta_{\mathbf k}=|J|/2(f_{\mathbf k\uparrow}d_{-\mathbf k\downarrow}-f_{\mathbf k\downarrow}d_{-\mathbf k\uparrow})$$

[here $|J| = g_{fd}$ is to be understood as the effective constant in the $d-f$ channel given by relations (15) and (22)]. For simplicity, we assume that the Fermi surfaces for the f and d bands with the dispersion laws

$$\varepsilon_f(\mathbf p)=p^2/2m_f-\mu_f, \qquad \varepsilon_d(\mathbf p)=p^2/2m_d-\mu_d$$

coincide, and we assume that the coupling is weak (T_c is much smaller than the band widths w_f, w_d). In this case the critical temperature is given by expression (20).

To verify that the hybrid-pairing model is a good approximation for describing heavy-fermion superconductors, we will analyze various physical consequences of the model and compare them with the actual properties of the corresponding systems.

For this purpose we first find an expression for the free-energy functional which holds for all temperatures:

$$\delta\mathcal{F}=\int d^3r\left\{a|\Delta(\mathbf r)|^2+\frac{b}{2}|\Delta(\mathbf r)|^4 + c\left|\left(\nabla-\frac{2ie}{c}\mathbf A(r)\right)\Delta(\mathbf r)\right|^2\right\}, \tag{28}$$

where the coefficients a, b, and c depend on Δ and T. In this calculation we used the method proposed in Ref. 23 (see the Appendix).

We use the assumptions that the magnetic field is weak and that the nonuniformity of the order parameter is likewise weak:

$$|\Delta(\mathbf r)-\Delta_0|\ll\Delta_0.$$

Here is the final result:

$$b=\frac{4\pi\lambda N_d(0)}{(1+\lambda)^3}T\sum_{\omega_n=-\infty}^{\infty}[\omega_n^2+\tilde\Delta_0^2(T)]^{-3/2}, \tag{29}$$

$$c=\frac{2\pi k_F^2 N_d(0)}{3m_f^2(1+\lambda)^3}T\sum_{\omega_n=-\infty}^{\infty}[\omega_n^2+\tilde\Delta_0^2(T)]^{-3/2} \tag{30}$$

and $a=-b\Delta_0^2$. Here $\lambda = w_j/w_d = m_d/m_j \ll 1$, Δ_0 is the equilibrium value of the order parameter; and $\tilde\Delta_0 = [2\lambda^{1/2}/(1+\lambda)]\Delta_0$ is the actual gap in the energy spectrum,[3)] which is related to the critical temperature by the customary relation of the BCS theory: $\tilde\Delta_0=(\pi/\gamma)T_c$. Here are expressions for the corresponding coefficients: in the limit $T\to 0$,

$$b=\frac{N_d(0)}{(1+\lambda)\Delta_0^2},\qquad c=\frac{k_F^2N_d(0)}{12\lambda m_f^2(1+\lambda)\Delta_0^2},$$

and in the limit $T\to T_c$, (31)

$$b=\frac{7\zeta(3)\lambda N_d(0)}{2(\pi T_c)^2(1+\lambda)^3},\qquad c=\frac{7\zeta(3)k_F^2N_d(0)}{12m_f^2(\pi T_c)^2(1+\lambda)^3}.$$

In the latter case we find the usual Ginzburg-Landau functional.

We can now study the thermodynamic and electromagnetic properties of our state in the limit of low temperatures and near T_c. If we ignore possible interband terms in the Hamiltonian and retain only the intraband contribution to the current operator (more on this below), we find the following expression for the current density [see (A7)]:

$$\mathbf{j}=-\frac{n_s(T)e^2}{m_f(1+\lambda)c}\mathbf{A} \quad (n_s(T=0)=n_d+n_f). \tag{32}$$

Correspondingly, the London penetration depth λ_L is given by

$$\lambda_L{}^2(T)=\frac{m_f(1+\lambda)c}{4\pi n_s(T)e^2}. \tag{33}$$

This is precisely the expression which we would expect for a hybrid superconducting state: The mass of the Cooper pair in the BCS relation has been replaced by the resultant mass of the hybrid pair, $m_d+m_f=m_f(1+\lambda)$.

The correlation length $\xi(T)$ is given by the expressions

$$\xi(T)=\left(\frac{2}{3}\right)^{1/2}\frac{k_F}{m_f+m_d}\frac{1}{\tilde\Delta_0}, \quad T\to 0, \tag{34}$$

$$\xi(T)=\left[\frac{7\zeta(3)}{12}\frac{T_c}{T_c-T}\right]^{1/2}\frac{k_F}{m_f+m_d}\frac{1}{\pi T_c}, \quad T\to T_c. \tag{35}$$

The Ginzburg-Landau parameter $\varkappa$ is given by

$$\varkappa=\frac{2^{1/2}}{12\cdot 7\zeta(3)}(\pi T_c)^2\frac{m_f{}^{3/2}}{k_F{}^{5/2}}(1+\lambda)^{3/2}. \tag{36}$$

Finally, we can estimate the upper critical field $H_{c2}\approx\Phi_0/\xi^2(T)$:

$$H_{c2}(T)=\begin{cases}\dfrac{(1+\lambda)^2}{8c}\dfrac{m_f{}^2}{k_F{}^2}\tilde\Delta_0{}^2, & T\to 0\\ \dfrac{3(1+\lambda)^2}{7e\zeta(3)}(\pi T_c)^2\dfrac{m_f{}^2}{k_F{}^2}\dfrac{T_c-T}{T_c}, & T\to T_c\end{cases} \tag{37}$$

In this model, the basic properties of superconductors with hybrid pairing are thus actually determined by the mass of the heavy component. Specifically, the correlation length is small, $\xi(T)\sim m_f^{-1}$, and the critical field $H_{c2}\sim m_f^2$ and also $\varkappa\sim m_f^{3/2}$ are large. These results correspond to experimental results on heavy-fermion superconductors. The thermodynamic properties, e.g., the jump in the heat capacity, also correspond to experimental data.[14,15] These consequences are obvious from the physical standpoint: In the superconducting phase, the pair moves as a whole with a mass $m_p=m_f+m_d\approx m_f$.

Less clear is the question of which mass determines the penetration depth λ_L. Expression (33) yields $\lambda_L^2\sim m_f$, which does not agree completely with the experimental results. In Ref. 24, for example, it was asserted that we have $\lambda_L^2\sim m_f$, in UBe_{13} compounds, while it was mentioned in Ref. 2 that in the compounds UBe_{13} and $ZrBe_{13}$ the values of λ_L are of the same order of magnitude. The meaning may be that it is the mass of the light component, m_d, which determines the penetration depth.

It can be shown that incorporating in our model a factor which has previously been omitted—interband transitions—leads to a more complicated dependence of λ_L on the masses of the components. This question is taken up in the following section.

4. ELECTROMAGNETIC RESPONSE WITH INTERBAND TRANSITIONS

In the analysis above we used a Hamiltonian in which it was assumed that the f and d bands are orthogonal, and interband terms arise only to the extent that there is a hybrid superconducting pairing. Actually, there are usually some direct interband contributions, also. To discuss this problem, we will generalize our model a bit and make it more realistic. Taking the standard approach, similar to the well-known (**kp**) method in semiconductor physics, we write the Hamiltonian of the two noninteracting bands as follows (cf. Ref. 25):

$$H_0=\begin{pmatrix}\varepsilon_d\left\{\dfrac{\nabla}{i}-\dfrac{e}{c}\mathbf{A}\right\} & \dfrac{\mathbf{P}_{12}}{m_0}\left(\dfrac{\nabla}{i}-\dfrac{e}{c}\mathbf{A}\right)\\ \dfrac{\mathbf{P}_{12}^*}{m_0}\left(-\dfrac{\nabla}{i}-\dfrac{e}{c}\mathbf{A}\right) & \varepsilon_f\left\{\dfrac{\nabla}{i}-\dfrac{e}{c}\mathbf{A}\right\}\end{pmatrix}. \tag{38}$$

Here the $\{\ldots\}$ means the argument of the quantities $\varepsilon_{d,f}$, not their product, m_0 is the electron mass, and

$$\mathbf{P}_{12}=\int d^3r\,\psi_f{}^*(\mathbf{r})\left(\frac{\nabla}{i}\right)\psi_d(\mathbf{r}) \tag{39}$$

is the interband matrix element of the momentum operator, which depends on the symmetry of the crystal lattice and the symmetry of the corresponding energy bands. As a result, we find the following system of equations for the Green's functions G_{dd}, G_{fd}, F^+_{dd}, F^+_{fd}:

$$(\hat A+\hat B)\overline{G}=\overline{I}, \tag{40}$$

where we are using the vectors $\overline{G}=(G_{dd},G_{fd},F_{dd},F_{fd})$, $\overline{I}=(1,0,0,0)$. The matrices $\hat A$ and $\hat B$ are given by

$$\hat A=\begin{pmatrix}i\omega-\varepsilon_d & 0 & 0 & \Delta\\ 0 & i\omega-\varepsilon_f & \Delta & 0\\ 0 & \Delta^* & i\omega+\varepsilon_d & 0\\ \Delta^* & 0 & 0 & i\omega+\varepsilon_f\end{pmatrix}, \tag{41}$$

$$\hat B=\begin{pmatrix}-\mathbf{k}\nabla/im_d & -\mathbf{P}_{12}\mathbf{k}/m_0 & 0 & 0\\ -\mathbf{P}_{12}^*\mathbf{k}/m_0 & -\mathbf{k}\nabla/im_f & 0 & 0\\ 0 & 0 & \mathbf{k}\hat{\mathbf{O}}/md & -\mathbf{P}_{12}^*\hat{\mathbf{k}}/m_0\\ 0 & 0 & -\mathbf{P}_{12}\hat{\mathbf{k}}/m_0 & \mathbf{k}\hat{\mathbf{O}}/m_0\end{pmatrix}. \tag{42}$$

Here $\varepsilon_{d,f}$ is the energy of the electrons in the bands, $\mathbf{k}$ is a wave vector, and

$$\hat{\mathbf{O}}=-i\nabla-e\mathbf{A}/c, \quad \hat{\mathbf{k}}=\mathbf{k}-i\nabla+2e\mathbf{A}/c.$$

There is a corresponding system of equations for the quantities G_{ff}, etc.

Assuming that all quantities vary slowly in space, and retaining interband terms proportional to $\mathbf{P}_{12}$, we have the inequality $\hat B\ll\hat A$, which means that we can invert the matrix $\hat A+\hat B$.

As a result we find the following expression for $\delta\overline{G}$, the correction to the Green's functions:

$$\delta\overline{G}=(\hat A^{-1}\hat B\hat A^{-1})\overline{I}=d_1{}^{-1}d_2{}^{-1}\overline{M}, \tag{43}$$

where

$$\overline{M}=\begin{pmatrix} -(i\omega+\varepsilon_f)^2\dfrac{d_2\mathbf{k}\nabla}{d_1 i m_d}+\Delta^* d_2\mathbf{k}\hat{\mathrm{O}}\Delta/d_1 m_f \\ -(i\omega+\varepsilon_d)(i\omega+\varepsilon_f)\mathbf{P}_{12}\mathbf{k}/m_0-m_0^{-1}\Delta^* d_1\mathbf{P}_{12}\nabla(\Delta/d_1) \\ \Delta m_0^{-1}\mathbf{P}_{12}^*\mathbf{k}(i\omega+\varepsilon_f)+(i\omega-\varepsilon_f)d_1\mathbf{P}_{12}^*\mathbf{k}\Delta/d_1 \\ \Delta d_2\mathbf{k}\nabla(i\omega+\varepsilon_f)/m_d i d_1-(i\omega-\varepsilon_d)d_2\mathbf{k}\hat{\mathrm{O}}(\Delta/d_1) \end{pmatrix}. \tag{44}$$

Here $d_1=-\omega^2+i\omega(\varepsilon_f-\varepsilon_d)-\varepsilon_f\varepsilon_d-|\Delta|^2$, $d_2=d_1^*$.

We can find an expression for the current density by convolving the current density operator $\hat{j}$, given by

$$\hat{\mathbf{j}}=\begin{pmatrix} e\dfrac{\partial\varepsilon_d}{\partial\mathbf{k}} & \dfrac{e}{m_0}\mathbf{P}_{12} \\ \dfrac{e}{m_0}\mathbf{P}_{12}^* & e\dfrac{\partial\varepsilon_f}{\partial\mathbf{k}} \end{pmatrix}, \tag{45}$$

with the Green's function $\overline{G}$ found above:

$$\mathbf{j}=\mathrm{Sp}(\hat{\mathbf{j}}G)=\sum_i \mathbf{j}_{ii}+\delta\mathbf{j}_{ij}. \tag{46}$$

The contribution in which we are interested, which is nondiagonal with respect to the bands, is

$$\delta\mathbf{j}_{ij}=-\frac{2e}{m_0}\sum_{\mathbf{k}}\mathrm{Sp}\,T\sum_{\omega_n}\left\{\frac{|\Delta|^2(\mathbf{A}\mathbf{P}_{12}^*)\mathbf{P}_{12}}{d_1 d_2}+(1\leftrightarrow 2)\right\}. \tag{47}$$

We thus see that the anisotropic nature, $\delta j\sim\mathbf{P}_{12}(\mathbf{A}\mathbf{P}_{12})$, generally makes a nondiagonal contribution to the current. Summing over $\mathbf{k}$, we finally find

$$\delta\mathbf{j}_{12}=\mathbf{P}_{12}(\mathbf{A}\mathbf{P}_{12}^*)\frac{2\pi N_d(0)}{(1+\lambda)^2}T|\Delta|^2\sum_{\omega_n}\frac{1}{(\Delta^2+\omega_n^2)[\omega_n^2+\Delta^2]^{1/2}}. \tag{48}$$

The corresponding contribution to the penetration depth, $\delta(1/\lambda_L^2)$, is

$$\delta(1/\lambda_L^2)\sim\begin{cases} N_d(0)(|\mathbf{P}_{12}|^2/m_0^2)\ln\lambda, & T\to 0, \\ N_f(0)(|\mathbf{P}_{12}|^2/m_0^2)[(T_c-T)/T_c]^2, & T\to T_c. \end{cases} \tag{49}$$

Combining this result with (33), we easily see that very different situations may prevail, depending on the relations among m_f, m_d, and $\mathbf{P}_{12}/m_0$. For example, if $\mathbf{P}_{12}$ and $m_f\gg m_d\sim m_0$ are not too small, we find $\lambda_L^2\sim m_0/\ln(m_f/m_d)$ in the limit $T\to 0$ and $\lambda_L^2\sim m_0^2/m_f$ in the limit $T\to T_c$. We thus see that if the interband terms in the current are important, the London depth λ_L is determined primarily by the light mass. The reason is that incorporating the nondiagonal terms in Hamiltonian (38) leads to the induction of an intraband pairing in addition to the interband pairing.[26] In this case, not only the $f-d$ pairs with mass $m_p=m_f+m_d$ but also the intraband pairs, in particular, $d-d$ pairs with a mass $m_p=2m_d\sim 2m_0$, participate in the screening.

5. EFFECT OF DIELECTRIC (EXCITON) PAIRING

It follows from the analysis above that incorporating the interband matrix elements, in particular, $\mathbf{P}_{12}$, leads to nontrivial consequences, e.g., the induction of intraband pairing, F_{dd}, F_{ff}. We would thus naturally ask whether a more detailed consideration of the specific features of the two-band model is necessary. In particular, in addition to the interband pairing in the electron-electron channel there might also be a singularity in the electron-hole (exciton) channel and in the Cooper channel.

This question has been analyzed in detail elsewhere.[26] To round out the present discussion, we will simply summarize that analysis briefly and discuss the basic conclusions.

For the analysis we start from the model Hamiltonian

$$H=\sum_{\mathbf{k},\sigma}\{\varepsilon_d(\mathbf{k})f^+_{\mathbf{k}\sigma}f_{\mathbf{k}\sigma}+\varepsilon_f(\mathbf{k})d^+_{\mathbf{k}\sigma}d_{\mathbf{k}\sigma}+V(f^+_{\mathbf{k}\sigma}d_{\mathbf{k}\sigma}+\mathrm{H.a.})\}$$
$$-\frac{|J|}{2}\sum_{\mathbf{k},\mathbf{p},\mathbf{q}}(f^+_{\mathbf{k}\uparrow}d^+_{\mathbf{p}\downarrow}-f^+_{\mathbf{k}\downarrow}d^+_{\mathbf{p}\uparrow})(d_{\mathbf{p}-\mathbf{q}\uparrow}f_{\mathbf{k}+\mathbf{q}\downarrow}-d_{\mathbf{p}-\mathbf{q}\downarrow}f_{\mathbf{k}+\mathbf{q}\uparrow}), \tag{50}$$

in which an $f-d$ hybridization V has been added to the customary terms. In addition to the superconducting channel, there is also a singularity in the electron-hole channel in the case of completely coincident Fermi surfaces. This singularity can be dealt with by introducing anomalous averages of the form[27] $\langle f_{\mathbf{k}\sigma}d^+_{\mathbf{k}\sigma}\rangle$. Incorporating them leads to a renormalization of the hybridization:

$$V\to\tilde{V}=V+(|J|/2)\sum_{\mathbf{k}}\langle f_{\mathbf{k}\sigma}d_{\mathbf{k}\sigma}^+\rangle.$$

Introducing the corresponding Green's functions, we find a system of four equations which are similar in structure to (40). From this system we can find the energy spectrum and also expressions for the Green's functions and self-consistent equations for the superconducting and exciton order parameters Δ and $\tilde{V}$ (Refs. 27 and 26). Using them, we can analyze the mutual effects of interband superconducting and exciton pairings. It can be verified that the hybridization and the exciton pairing in our case suppressed the superconductivity, lowering T_c:

$$\frac{\delta T_c}{T_c}=-\frac{\lambda}{(1+\lambda)}\frac{7\zeta(3)}{4\pi^2T_c^2}|\tilde{V}|^2. \tag{51}$$

This effect is easy to understand at a qualitative level: In the case of completely coincident Fermi surfaces, the hybridization mixes states near ε_F, which are participating in the interband pairing, with states which are not involved in the interaction (1). In other words, some of the averages $\langle f^+d^+\rangle$ are replaced by intraband averages $\langle f^+f^+\rangle$ and $\langle d^+d^+\rangle$.

The equations found above become more transparent when we use the Landau functional:

$$\mathscr{F}=a|\Delta|^2+{}^1\!/_2 b|\Delta|^4+a'|\tilde{V}|^2+{}^1\!/_2 b'|\tilde{V}|^4+v|\Delta|^2|\tilde{V}|^2-dV\tilde{V}. \tag{52}$$

Minimization yields the following expressions for Δ and $\tilde{V}$:

$$|\Delta|^2=-\frac{a(T)+c|\tilde{V}|^2}{b},\qquad |\tilde{V}|^2=\frac{1}{2}\frac{dV}{a'+c|\Delta|^2}. \tag{53}$$

The mutual effects of the parameters Δ and $\tilde{V}$ are determined by the sign of the coefficient c in (52) and (53). A microscopic calculation[26] yields $c>0$ for this sign; i.e., incorporating the exciton averages reduces Δ and T_c.

In the case of a very narrow f band, with a width $w_f \lesssim T_c$, the calculation scheme used above must be modified. The parquet approximation must be used.[16,28] Some results in this direction are reported in Ref. 29.

6. CONCLUSION

We can say in conclusion that the model with singlet interband pairing is nontrivial and is capable of explaining many aspects of the behavior of heavy-fermion superconductors. The basis thermodynamic characteristics [ΔC and $\xi(T)$] and electrodynamic characteristics (H_{c2} and λ_L) are explained in a natural way. One might attempt to use this model to generate a (slightly speculative) explanation for the most intriguing feature of these superconductors, the nonexponential dependence of various quantities at $T<T_c$. This dependence may be a consequence of incomplete "nesting" of the f and d Fermi surfaces, which would give rise, in particular, to a highly anisotropic gap, so that electrons on some part of the Fermi surface may in fact remain in a normal state (cf. the experimental results reported in Ref. 6).

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APPENDIX

We calculate the free energy of the systems by the Eilenberger method[23]:

$$\tilde{\Omega}=\Omega_0+\frac{1}{g}\int d^3r|\Delta|^2+\frac{1}{8\pi}\int d^3r[\mathbf{B}(\mathbf{r})-\mathbf{H}(\mathbf{r})]^2,$$

$$\Omega_0=\int d^3r\left\{iT\sum_{l,i}\int_{\omega_l(T)}^{\pm\infty}G_{i\omega}(\mathbf{r},\mathbf{r})d\omega+\text{c.c.}\right\},$$

$$\omega_l(T)=(2l+1)\pi T,\quad i=d,f \tag{A1}$$

where Δ is the gap, and $\mathbf{H}(\mathbf{r})$ the external magnetic field. The system of equations for the Green's function G_d, G_f, F^+_{fd}, F^+_{df} splits into two subsystems (G_d, F^+_{fd}) and (G_f, F^+_{df}), simplifying the corresponding solution.

Assuming that Δ is a slowly varying function, and making use of the small value of the potential $\mathbf{A}(\mathbf{r})$, we carry out an expansion $G=G^{(0)}+G^{(1)}+G^{(2)}+\ldots$ and (by analogy with F (an expansion in the small parameters to within second order, more precisely, to second order in

$$(-i\nabla_{r'},\ \hat{\mathbf{O}}=-i\nabla-2e\mathbf{A}/c)$$

and to first order in

$$-i[B\nabla_r],\quad (-i\nabla_r)^2.$$

As a result we find

$$G_i^{(0)}=\frac{\hat{\xi}_i}{d_i},\quad F_{ji}^{(0)}=-\frac{\Delta^*}{d_i},$$

$$G_i^{(1)}=-\frac{\Delta\mathbf{k}_j\hat{\mathbf{O}}\Delta^*}{d_i^4}-\frac{\mathbf{k}_i\hat{\xi}_i^2-\mathbf{k}_j|\Delta|^2}{d_i^3}\frac{\nabla_r}{i}|\Delta|^2,$$

$$F_{ji}^{(1)}=\frac{\xi_i\mathbf{k}_j\hat{\mathbf{O}}\Delta^*}{d_i}+\frac{\Delta^*(\mathbf{k}_j\xi_i+\mathbf{k}_i\hat{\xi}_i)}{d_i^3}\frac{\nabla_r}{i}|\Delta|^2,$$

$$G_i^{(2)}=d_i^{-1}\left\{\hat{\xi}_i\left[\frac{1}{2m_i}\left(\frac{\nabla_r}{i}\right)^2G_i^{(0)}+\frac{\mathbf{k}_i\nabla}{i}G_i^{(1)}\right]+\Delta\left[\frac{1}{2m_j}\hat{\mathbf{O}}^2F_{ji}^{(0)}+\mathbf{k}_j\hat{\mathbf{O}}F_{ji}^{(1)}\right]\right\}. \tag{A2}$$

Here $\xi_i=i\omega-\varepsilon_i$, $\hat{\xi}_i=-i\omega-\varepsilon_j$, $k^2-k_F^2=2m_i\varepsilon_i$, $\varepsilon_d=\varepsilon$, $\varepsilon_f=\lambda\varepsilon$, $\lambda=m_d/m_f$, $d_j=d^*_j$, and $d_i=\xi\hat{\xi}+|\Delta|^2$.

To calculate Ω_0 (and $\tilde{\Omega}$) it is sufficient to know $G_i^{(0)}$ and $G_i^{(2)}$, since the parity in $\mathbf{k}$ tells us that the function $G^{(1)}$ will not contribute to Ω_0. The term with $\mathbf{k}[\mathbf{Bk}]$ in $G^{(2)}$ is also equal to zero in this case of an isotropic gap. Finally, by virtue of the parity, only $\mathrm{Im}G_i$ makes a contribution. With an eye on a calculation of the electromagnetic response, we retain in G_i and F_i only the contributions which depend on the square of the field:

$$\delta G_d^{(2)}=-\frac{|\Delta|^2|\mathbf{A}|^2(i\omega-\varepsilon_d)}{m_f^2d_d^3},\quad \delta F_{fd}^{(2)}=-\frac{\Delta^*|\mathbf{A}|^2(i\omega-\varepsilon_d)}{m_f^2d_d^3} \tag{A3}$$

(and similarly for $\delta G_f^{(2)}$, δF_{df}).

The corresponding part of the free energy is

$$\delta\Omega_0=-2iT\int d^3r\sum_{l>0}\int_{\omega_l}^{\infty}d\omega\int d^3k\frac{|\Delta|^2}{3}|\mathbf{A}|^2\times\left\{\frac{(i\omega-\varepsilon_d)}{m_f^2d_d^3}+\frac{(i\omega-\varepsilon_f)}{m_d^2d_f^3}\right\}. \tag{A4}$$

Evaluation of the integrals in (A4) here, in contrast with the case studied in Ref. 23, requires some caution (cf. Ref. 30). Integrating over $\mathbf{k}$ and then over ω, we find

$$\delta\Omega_0=\frac{4\pi e^2T|\Delta|^2|\mathbf{A}|^2N_d(0)k_F^2}{3c^2m_f^2}\times\sum_{\omega_n>0}\{[\omega_n(1+\lambda)]^2+4\lambda\Delta^2\}^{-3/2}. \tag{A5}$$

Precisely the same result is found for $\delta\Omega_0$ if we use the well-known method of intergating over the coupling constant.

As a result, the current density $\mathbf{j}$ turns out to be

$$\mathbf{j}=-\frac{\partial\delta\Omega_0}{\partial\mathbf{A}}=-\frac{8\pi\mathbf{A}N_d(0)k_F^2\Delta^2}{3m_f^2(1+\lambda)^2}T\sum_{\omega_n>0}(\omega_n^2+\tilde{\Delta}^2)^{-3/2}, \tag{A6}$$

where $\tilde{\Delta}=2\lambda^{1/2}\Delta/(1+\lambda)$ is the real (indirect) gap.

The same result can be found by directly calculating the current in terms of the corrections of first order in the magnetic field to the Green's function. In the limit $T\to T_c$ we find

$$\mathbf{j}=-\frac{e^2}{c^2}\frac{7\xi(3)n_s\tilde{\Delta}^2}{4(\pi T_c)^2m_f(1+\lambda)^3}\mathbf{A}=\frac{n_se^2}{2m_fc^2(1+\lambda)}\mathbf{A}, \tag{A7}$$

which yields the well-known result in the case $\lambda=1$. In the case $T=0$ we find

$$\mathbf{j}=-\frac{ne^2}{(m_f+m_d)c^2}\mathbf{A}. \tag{A8}$$

[1)]We are assuming a pairing with oppositely directed momenta (more on this below).

[2)]Here and below (unless otherwise stipulated), we are considering only the short-range contribution to the effective interaction.

[3)]The gap $\tilde{\Delta}_0$ is the indirect gap in the energy spectrum. It is this gap which appears in the state density and thus in the thermodynamic characteristics. Experiments involving direct transitions might provide information on the gap Δ_0.

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