

# Superconductivity in a low-density two-band model with a repulsive interaction: extended analysis

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(Submitted 5 February 1992)

*Zh. Eksp. Teor. Fiz.* **102**, 313–325 (July 1992)

A complete solution is derived for the problem of the appearance of superconductivity in 2D and 3D low-density two-band models with a repulsive interaction. The analysis is carried out in the limit of a slight one-particle hybridization. The case of two electron bands and the case of one electron band and one hole band are examined. The tendency toward *s* pairing which arises in the two-band model with greatly different masses is discussed. The role played by off-diagonal matrix elements of the Coulomb interaction is also analyzed.

## 1. INTRODUCTION

Research on superconductivity in highly correlated electron systems, such as the high  $T_c$  superconductors, heavy-fermion systems, and  $C_{60}$ , has recently diverted the interest of many researchers from the one-band model to the two-band model. In the case of 3D heavy-fermion systems, this shift of interest was spurred by experimental data and band-theory calculations which showed that two bands are present at the Fermi level: an *s-p* band of light electrons with masses of (1–10)  $m_e$  and an *f-d* band of heavy electrons with (50–200)  $m_e$ . In the case of the quasi-2D high  $T_c$  superconductors, the interest in the two-band model stems from Emery's idea<sup>1</sup> that a superconducting pairing is implemented by holes of an oxygen band through the exchange of spin excitations of a localized copper band.

The switch to a multiband analysis of superconductivity in quasi-2D systems of the  $C_{60}$  type was recently made in Ref. 2. In the case of strongly correlated systems, one of the bands (the "heavier" one) usually has a larger electron density and is analyzed in the limit of a strong Hubbard repulsion at a site,  $U_2 > t$ . The superconductivity problem can be solved in this limit only by the mean-field approach (as in the technique of slave bosons, for example). It was asserted in Refs. 3 and 4 that if the number density of particles in the heavy band is small ( $n_2 \ll 1$ ) then even in the case of a strong Hubbard repulsion there exists a small perturbation-theory parameter,  $U_2 n_2^{1/3}/8t \ll 1$  in the 3D case and  $\frac{1}{2} \ln(n_2 a^2) \ll 1$  in the 2D case, and the one-band superconductivity problem can be solved exactly (in the sense that the diagrams can be controlled). This circumstance, combined with the possible increase in  $T_c$  in the 2D two-band model (pointed out in Ref. 5), convinced us of the need to derive an exact solution in the two-band, low-density problem (with a one-particle hybridization and with all the matrix elements of the Coulomb interaction). The idea is to work from this solution to attempt to move on to the more pertinent situation in which the particle density in the heavy band is on the order of unity. We derive this comprehensive solution in the present paper. We show that in the 3D two-band model with greatly different masses and with a slight one-particle hybridization,  $f < w_h < w_l$  ( $w$  is the energy "filling" of the band), a pairing of heavy-band electrons through polarization of the same (heavy) band is the most effective pairing. In other words, the one-band model is sufficient for the heavy mass in this case. In the limit of a low-density heavy band, the pairing

corresponds to *p* symmetry,<sup>3</sup> and the transition temperature  $T_c \sim \epsilon_F \exp\{-1/U_2^2\}$  is determined by second-order perturbation theory for the effective interaction  $\tilde{\Gamma} = U_2 + U_2^2 \Pi(\tilde{q})$ . As the heavy band becomes nearly half-filled, a *d*-pairing becomes preferred.<sup>6</sup> An *s* pairing in a nonphonon model is of course impossible, because of the direct Coulomb repulsion (hard-core repulsion) at a site. The light band in this model and the increase in  $T_c$  due to the two-band nature of the model can be important only in the limit of a strong hybridization,  $f > w_h$ .

In the 2D case the situation is totally different. As was shown in Ref. 7, the 2D polarization operator calculated for a quadratic electron spectrum is of such a nature that no superconducting pairing arises in the one-band model. It was shown in Ref. 5 that a pairing is possible only if a second band is taken into account through an interband Coulomb interaction  $U_3 \hat{n}_1 \hat{n}_2 = U_3 a_\alpha^+ a_\alpha b_\beta^+ b_\beta$  ( $a$  and  $b$  are the species of particles). The pairing may be sharply intensified when the densities of the two bands form the optimum ratio.

In this paper we compare the effectiveness of superconducting pairing by this mechanism with that by other mechanisms involving off-diagonal matrix elements, such as  $K a^+ a^+ b b$ . The role of the element  $K$  was first discussed in Refs. 8. In those papers and also in a more recent paper,<sup>9</sup> it was shown that  $K$  leads to the appearance of superconductivity in the two bands simultaneously (at the same value of  $T_c$ ), although the value of  $T_c$  itself is determined primarily by the heavy band. The superconducting gaps in the two bands,  $\Delta_1(T)$  and  $\Delta_2(T)$ , behave differently.

It was demonstrated by Yamaji<sup>10</sup> that an *s*-pairing is possible even in a purely Coulomb, nonphonon situation if the diagonal elements of the Coulomb interaction ( $U_1$  and  $U_2$ ) are small ( $U_1 U_2 < K^2$ ). It was stated in the same paper that even in the case  $K^2 < U_1 U_2$  a superconductivity could appear and could even be strengthened in the *s*-channel, by virtue of an interaction of the superconducting and insulating channels,<sup>11</sup> if one of the bands is an electron band, while the other is a hole band, and the particle densities in the two bands are approximately the same (ideal nesting).

We show below that the assertion in Ref. 10 regarding the possibility of *s*-pairing is erroneous in the case of small  $K$ . An *s*-pairing due to an interaction between superconducting and insulating channels (the parquet situation) does not arise, and the dominant mechanism for superconductivity is the interband Coulomb interaction  $U_3$ , even near nesting. A *p*-pairing arises below the temperature

$T_c \sim \varepsilon_F \exp\{-1/U_3^2\}$ . In the case of exact nesting ( $p_{F1} = p_{F2}$ ), an insulating pairing comes into play first (at  $T_c \sim \varepsilon_F \exp\{-1/U_3^2\}$ ), and there is no superconductivity. If both bands are electron bands or both hole bands, there is no intensification of the off-diagonal elements of the Coulomb interaction by nesting, so the element  $U_3$  is even more dominant in the appearance of superconductivity. As in the 3D case, a one-particle hybridization  $f$  can be ignored if it is smaller than the energy "filling" of the heavy band,  $w_h$ :  $f < w_h$ .

Finally, as discussed above, it is a fairly simple matter to achieve a  $p$ -type superconductivity in 2D and 3D two-band models with a low density; it is fairly simple even to sharply strengthen the superconductivity in the 2D case. As the density increases,  $d$ -pairing may result. In these models, it is extremely difficult to find the  $s$  pairing which probably operates in the high  $T_c$  systems because of the role played by the contact Coulomb repulsion  $U$  in first-order perturbation theory for the effective interaction  $\tilde{\Gamma}$ . Furthermore, in the 2D and 3D one-band models, the second-order corrections to  $\tilde{\Gamma}(q)$ , i.e.,  $U^2\Pi(\tilde{q})$  (Refs. 5 and 12), are repulsive for  $s$  pairing. In the two-band model, with a pronounced difference between the light and heavy masses, the second-order correction for the effective interaction of two light particles,

$$\tilde{\Gamma}_1(q) = (m_1 U_1^2 - 2m_2 U_3^2) / 2\pi$$

changes sign (we are assuming  $m_2 \gg m_1$  and  $U_3 \sim U_1$ ). The appearance of an attractive correction in second-order perturbation theory for the  $s$ -channel raises the hope that it may be possible to find an  $s$ -pairing in a two-band model as we go to high densities. However, this hope could not be realized fully, because the change in the sign of  $\tilde{\Gamma}_1$  would correspond to a negative static screening  $\varepsilon(q, 0)$ , which would in turn lead to an instability. Nevertheless, a significant weakening of the direct Coulomb interaction might smooth the way for an  $s$  pairing when other degrees of freedom (an electron-phonon or electron-magnon interaction) are brought into the discussion.

## 2. 3D TWO-BAND MODEL

When the off-diagonal Coulomb matrix elements and one-particle hybridization are ignored, the 3D two-band model takes the form

$$\hat{H} = \sum_i \varepsilon_1 a_{i\alpha}^+ a_{i\alpha} + \sum_i \varepsilon_2 b_{i\beta}^+ b_{i\beta} + U_3 \sum_i a_{i\alpha}^+ a_{i\beta} b_{i\beta}^+ b_{i\alpha} + \frac{1}{2} U_1 \sum_i a_{i\alpha}^+ a_{i\beta}^+ a_{i\beta} a_{i\alpha} + \frac{1}{2} U_2 \sum_i b_{i\alpha}^+ b_{i\beta}^+ b_{i\beta} b_{i\alpha}, \quad (1)$$

where  $\varepsilon_1 = (p^2 - p_{F1}^2) / 2m_1$  and  $\varepsilon_2 = (p^2 - p_{F2}^2) / 2m_2$  are the electron spectra in the first and second bands,  $m_1$  and  $m_2$  are the electron masses,  $p_{F1}$  and  $p_{F2}$  are the Fermi momenta,  $U_1$  and  $U_2$  are the matrix elements of the intraband Coulomb interaction, and  $U_3$  is that of the interband Coulomb interaction. The effective irreducible vertices  $\tilde{\Gamma}_1$  and  $\tilde{\Gamma}_2$  of the two bands are written as follows in the Cooper channel for Hamiltonian (1) in first- and second-order perturbation theory:

$$\begin{aligned} \tilde{\Gamma}_1(q_1) &= U_1 + U_1^2 \Pi_{11}(\tilde{q}_1) - 2U_3^2 \Pi_{22}(q_1), \\ \tilde{\Gamma}_2(q_2) &= U_2 + U_2^2 \Pi_{22}(\tilde{q}_2) - 2U_3^2 \Pi_{11}(q_2), \end{aligned} \quad (2)$$

where  $q_i = p_i - p'_i$ ,  $\tilde{q}_i = p_i + p'_i$  ( $i = 1, 2$ ),  $p_i$  and  $p'_i$  are the

incoming and outgoing momenta in the Cooper channel for the first and second bands, and

$$\begin{aligned} \Pi_{11}(q_i) &= \frac{m_1 p_{F1}}{4\pi} \left[ 1 + \frac{4p_{F1}^2 - q_i^2}{2p_{F1} q_i} \ln \frac{2p_{F1} + q_i}{|2p_{F1} - q_i|} \right], \\ \Pi_{22}(q_i) &= \frac{m_2 p_{F2}}{4\pi} \left[ 1 + \frac{4p_{F2}^2 - q_i^2}{2p_{F2} q_i} \ln \frac{2p_{F2} + q_i}{|2p_{F2} - q_i|} \right] \end{aligned}$$

are the Lindhard functions. The Cooper loops for the two bands are

$$C_1 = \frac{m_1 p_{F1}}{4\pi} \ln \frac{\varepsilon_{F1}}{T}, \quad C_2 = \frac{m_2 p_{F2}}{4\pi} \ln \frac{\varepsilon_{F2}}{T}.$$

The superconducting transition temperatures are found from the equations  $\tilde{\Gamma}_1^{(l)} C_1 = 1$  and  $\tilde{\Gamma}_2^{(l)} C_2 = 1$ , where  $l$  is the orbital angular momentum of the Cooper pair. If the interband Coulomb  $b$  interaction  $U_3$  is ignored, the bands become independent, and the corresponding transition temperatures become, according to Refs. 3 and 11,

$$\begin{aligned} T_{c1} &\sim \varepsilon_{F1} \exp \left\{ - \frac{5\pi^2}{4(2 \ln 2 - 1) (m_1 p_{F1} U_1 / 4\pi)^2} \right\}, \\ T_{c2} &\sim \varepsilon_{F2} \exp \left\{ - \frac{5\pi^2}{4(2 \ln 2 - 1) (m_2 p_{F2} U_2 / 4\pi)^2} \right\}. \end{aligned} \quad (3)$$

The superconductivity in each band is of a  $p$ -pairing type. An  $s$  pairing is of course impossible because of the Coulomb repulsion  $U_1$  and  $U_2$  in first-order perturbation theory. In most cases,  $U_3$  will be of the same order of magnitude as the intraband Coulomb matrix elements  $U_1$  and  $U_2$ , so it generally cannot be ignored. In the "Hund case," i.e., when the two bands are formed by electrons of the same atom,  $U_3$  may be greater than (possibly much greater than)  $U_1$  and  $U_2$ .

When  $U_3$  is taken into account, the equations for the transition temperatures of the two bands in the  $p$  channel are

$$\begin{aligned} \frac{m_1 p_{F1}}{4\pi} \ln \frac{\varepsilon_{F1}}{T} \left\{ \frac{m_1 p_{F1} U_1^2}{4\pi} \frac{4(2 \ln 2 - 1)}{5\pi^2} + 2 \frac{m_2 p_{F2} U_3^2}{4\pi} f_1 \left( \frac{p_{F1}}{p_{F2}} \right) \right\} &= 1, \\ \frac{m_2 p_{F2}}{4\pi} \ln \frac{\varepsilon_{F2}}{T} \left\{ \frac{m_2 p_{F2} U_2^2}{4\pi} \frac{4(2 \ln 2 - 1)}{5\pi^2} + 2 \frac{m_1 p_{F1} U_3^2}{4\pi} f_2 \left( \frac{p_{F1}}{p_{F2}} \right) \right\} &= 1, \end{aligned} \quad (4)$$

where

$$\begin{aligned} f_1 \left( \frac{p_{F1}}{p_{F2}} \right) &= \frac{4\pi}{m_1 p_{F1}} \int_{-1}^1 \Pi_{11}(q_2) P_1(\cos \theta) \frac{d \cos \theta}{2}, \\ f_2 \left( \frac{p_{F1}}{p_{F2}} \right) &= \frac{4\pi}{m_2 p_{F2}} \int_{-1}^1 \Pi_{22}(q_1) P_1(\cos \theta) \frac{d \cos \theta}{2} = f_1 \left( \frac{p_{F2}}{p_{F1}} \right), \\ q_{1,2}^2 &= 2p_{F1,2}^2 (1 - \cos \theta). \end{aligned}$$

It can be seen from the results of Ref. 7 that the function  $f_1(p_{F1}/p_{F2})$  goes through a maximum at  $p_{F1}/p_{F2} = 1.4$ . Its value at the maximum is approximately 1.8 times the quantity

$$f_1(1) = 4(2 \ln 2 - 1) / 5\pi^2.$$

Note that  $f_1(\infty) = 0$ . The function  $f_2(p_{F1}/p_{F2})$  falls off monotonically from the value

$$f_2(1) = 4(2 \ln 2 - 1)/5\pi^2$$

to zero.

Analyzing Eqs. (4), we easily see that the transition temperatures  $T_{c1}$  and  $T_{c2}$  depend strongly on not only the relative filling of the bands,  $p_{F1}/p_{F2} = (n_1/n_2)^{1/3}$ , but also the mass ratio of the bands. If  $m_2 \gg m_1$ , and if  $p_{F1}$  and  $p_{F2}$  are comparable in magnitude (this situation is typical of heavy-fermion systems), then we have  $T_{c2} \gg T_{c1}$ , and  $T_{c2}$  differs only slightly from  $U_3$ . In other words, a pairing of heavy particles through the polarization of (again) heavy particles occurs. The effect of the light band in the heavy-fermion situation can be seen indirectly only in the case of a strong interband interaction  $U_3$ . In this case, as was shown in Ref. 13, a pronounced additional shrinkage of the narrow band occurs. In other words, there is a pronounced increase in the heavy mass. As a result, there is a pronounced increase in  $T_c$  [see (3)].

If the masses and Fermi momenta of the bands are instead comparable in magnitude, the quantity  $U_3$  is important, and the larger of the  $T_c$ 's may rise significantly. For example, in the case with  $m_1 = m_2 = m$ ,  $U_1 = U_2 = U_3 = U$ , and  $p_{F1}/p_{F2} = 1.4$  (the optimum situation), we have  $T_{c1} > T_{c2}$ , and  $T_{c1}$  is given by

$$3,6 \left( \frac{mp_{F1}U}{4\pi} \right)^2 \frac{4}{5\pi^2} (2 \ln 2 - 1) \ln \frac{\epsilon_{F1}}{T_{c1}} = 1.$$

The argument of the exponential function for  $T_{c1}$  thus turns out to be smaller than that in the one-band case by a factor of 3.6 [see (3)].

All the results of this section of the paper were derived by ignoring the one-particle hybridization  $f$  [in Hamiltonian (1), hybridization leads to the appearance of a term  $f(a^+b + \text{H.a.})$ ], which is small in comparison with the energy separation of the level of the chemical potential and the bottom of the heavy band. In heavy-fermion systems, this condition generally may not hold; i.e., hybridization may be important.

### 3. 2D TWO-BAND MODEL

It was shown in Ref. 7 that there is no superconductivity in the one-band Coulomb problem because of the particular nature of the 2D polarization operator  $\Pi(q)$  calculated for a quadratic spectrum. On the other hand, it follows from Ref. 5 that in the two-band problem a superconductivity not only occurs in the 2D case with a repulsive interaction but may in fact be substantially strengthened. The onset of a superconductivity is related in a decisive way to the presence of an interband Coulomb interaction  $U_3$ . Another scenario for the appearance and strengthening of a superconductivity in a 2D two-band model was studied in Ref. 10. That scenario involves the presence of an off-diagonal Coulomb matrix element  $K$  (the corresponding term in the Hamiltonian is  $Ka^+a^+bb$ ). The matrix element  $U_3$  plays only an auxiliary role. It is therefore necessary to carry out a comprehensive analysis of the 2D, two-band Coulomb problem and to compare the various superconductivity mechanisms in terms of effectiveness.

The complete Hamiltonian of the 2D two-band model is

(here and below, we omit the momentum variables where we can do so without causing any confusion)

$$\begin{aligned} \hat{H} = & \sum \epsilon_1 a_\alpha^+ a_\alpha + \sum \epsilon_2 b_\beta^+ b_\beta + \frac{1}{2} U_1 \sum a_\alpha^+ a_\beta^+ a_\beta a_\alpha \\ & + \frac{1}{2} U_2 \sum b_\alpha^+ b_\beta^+ b_\beta b_\alpha + U_3 \sum a_\alpha^+ b_\beta^+ b_\beta a_\alpha \\ & + U_3 \sum a_\alpha^+ b_\beta^+ b_\beta a_\alpha + \frac{1}{2} K \sum (a_\alpha^+ a_\beta^+ b_\beta b_\alpha + \text{H.a.}) \\ & + U_4 \sum (a_\alpha^+ a_\beta^+ a_\beta b_\alpha + \text{H.a.}) + U_5 \sum (b_\alpha^+ b_\beta^+ b_\beta a_\alpha + \text{H.a.}) \end{aligned} \quad (5)$$

The quantities  $\epsilon_1$  and  $\epsilon_2$  in (5) are the spectra of the particles of species  $a$  and  $b$ ,  $U_1$  and  $U_2$  are the matrix elements of the intraband Coulomb interaction,  $U_3$  is the interband Coulomb interaction of the density-density type,  $\tilde{U}_3$  is the exchange part of this interaction, and  $K$ ,  $U_4$ , and  $U_5$  are off-diagonal (in terms of the conservation of the particles of each species) elements of the Coulomb interaction. The latter elements are generally also of an exchange nature.

As in the 3D case, we ignore one-particle hybridization below, assuming that it is either completely absent or weak in comparison with the energy width of the filled states in each band (in comparison with the distance from the bottom of the band to the level of the chemical potential). Generally speaking, the matrix elements  $U_4$  and  $U_5$  give rise to a one-particle hybridization in second-order perturbation theory and correspondingly lead to corrections to the particle spectrum in the bands, rendering the band index a somewhat indefinite quantum number. Estimates show, however, that in the effects of interest here, within the framework of the weak-coupling approximation, those corrections can be ignored.

We also note that an analysis of the multiband problem is possible only in the clean limit, since in the opposite limit the only parameter characterizing the state of a particle is its energy. In other words, the problem effectively becomes a one-band problem.<sup>14</sup>

We thus have the following expression for the particle spectrum in (5):

$$\epsilon_1 = (p^2 - p_{F1}^2)/2m_1, \quad \epsilon_2 = (p^2 - p_{F2}^2)/2m_2$$

in the case of two electron bands or

$$\epsilon_1 = (p^2 - p_{F1}^2)/2m_1, \quad \epsilon_2 = (p_{F2}^2 - p^2)/2m_2$$

in the case of one electron band and one hole band.

The standard expression for the second-quantization interaction Hamiltonian is

$$\hat{H}_{int} = \frac{1}{2} \int \hat{\Psi}_\alpha^+(\mathbf{r}_1) \hat{\Psi}_\beta^+(\mathbf{r}_2) U(\mathbf{r}_1 - \mathbf{r}_2) \hat{\Psi}_\beta(\mathbf{r}_2) \hat{\Psi}_\alpha(\mathbf{r}_1) d\mathbf{r}_1 d\mathbf{r}_2.$$

In order to derive (5), we need to write the operator  $\Psi$  in this expression in the form of a linear combination of the operators  $a$  and  $b$ :

$$\hat{\Psi}_\alpha(\mathbf{r}) = \varphi_1(\mathbf{r}) a_\alpha + \varphi_2(\mathbf{r}) b_\alpha,$$

where  $\varphi_1(\mathbf{r})$  and  $\varphi_2(\mathbf{r})$  are Bloch functions which diagonalize the one-particle Hamiltonian

$$\hat{H}_0 = \hat{H}_{01} + \hat{H}_{02}, \quad \hat{H}_{0i} = -\frac{\hbar^2}{2m_i} \Delta_i - u_i(\mathbf{r}),$$

and  $u_i(\mathbf{r})$  is the crystal field. For the Coulomb constants in (5) we find expressions of the type

$$U_{ij,km} = \int \varphi_i^*(\mathbf{r}_1) \varphi_j^*(\mathbf{r}_2) U(\mathbf{r}_1 - \mathbf{r}_2) \varphi_k(\mathbf{r}_2) \varphi_m(\mathbf{r}_1) d\mathbf{r}_1 d\mathbf{r}_2,$$

where  $i, j, k, m$  take on the values 1, 2 (the band index). We can work from this expression to estimate the relative order of magnitude of the Coulomb constants in (5). For example, if

$$U_1 = U_{11,11} \sim U_2 = U_{22,22} \sim U_3 = U_{12,21} \sim U,$$

then

$$U_4 = U_{11,12} \sim U_5 = U_{22,21} \sim tU,$$

and

$$K = U_{11,22} \sim U_3 = U_{12,12} \sim t^2 U,$$

where  $t$  is an overlap integral.

In the typical case  $t \ll 1$ , the Hamiltonian (5) becomes the standard two-band Hamiltonian, (1). One can of course imagine a situation in which we have  $t \lesssim 1$  (if, for example, the distance between sites is small), and all terms in (5) are important. Nevertheless, even in the case  $t \ll 1$  there are several effects which cannot be understood unless we retain the exchange terms in (5). For example, it was shown in Ref. 8 that incorporating the term  $Ka^+ a^+ b b$  in the two-band Hamiltonian with an attraction between particles leads to the simultaneous opening of superconducting gaps in each of the bands, even in the case of small  $K$ . This is true even though the value of the transition temperature, which is the same for the two bands, is determined primarily by the diagonal interaction elements in this case. In light of all these ideas, we see that we must completely solve the problem of superconductivity in a two-band model with repulsion as described by Hamiltonian (5). The Bethe-Salpeter equations for the complete vertices in the Cooper channel are

$$\begin{aligned} \Gamma_{11} &= \tilde{\Gamma}_{11} - \tilde{\Gamma}_{11} C_1 \Gamma_{11} - \tilde{\Gamma}_{12} C_2 \Gamma_{21}, \\ \Gamma_{21} &= \tilde{\Gamma}_{21} - \tilde{\Gamma}_{21} C_1 \Gamma_{11} - \tilde{\Gamma}_{22} C_2 \Gamma_{21}, \\ \Gamma_{22} &= \tilde{\Gamma}_{22} - \tilde{\Gamma}_{22} C_2 \Gamma_{22} - \tilde{\Gamma}_{21} C_1 \Gamma_{12}, \\ \Gamma_{12} &= \tilde{\Gamma}_{12} - \tilde{\Gamma}_{12} C_2 \Gamma_{22} - \tilde{\Gamma}_{11} C_1 \Gamma_{12}. \end{aligned} \quad (6)$$

Here  $C_{1,2}$  are the Cooper loops for the particles of species 1 and 2;  $\Gamma_{ij}$  is the complete vertex in the Cooper channel with two incoming particles of species  $i$  with a resultant momentum of zero, and with two outgoing particles of species  $j$ ; and  $\tilde{\Gamma}_{ij}$  are the corresponding irreducible vertices, which contain a set of diagrams which are indistinguishable on the basis of the two lines representing particles of one species, which run in the same direction.

Equations (6) must of course be understood as a symbolic form of the corresponding Bethe-Salpeter integral equations. The order of the integrations over the intermediate momenta in (6) is obvious. If the particle spectrum is isotropic, these integral equations reduce to algebraic equations for the corresponding partial harmonics  $\Gamma^{(m)}$ , where  $m$  is the magnetic quantum number. We recall that in  $D = 2$  the role of the Legendre polynomials  $P_l(\cos\theta)$ , which factorize the Bethe-Salpeter equation in the 3D case, is played by the functions  $\cos m\varphi$ . The system of equations found after the factorization is of the form of (6), with

$$C_{1,2} = \frac{m_{1,2}}{2\pi} \ln \frac{\varepsilon_{F1,2}}{T},$$

and  $\Gamma$  and  $\tilde{\Gamma}$  are the corresponding partial vertices  $\Gamma^{(m)}$  and  $\tilde{\Gamma}^{(m)}$ .

The expressions for the seed vertices  $\tilde{\Gamma}$  in the first two perturbation-theory orders are

$$\begin{aligned} \tilde{\Gamma}_{11} &= \tilde{\Gamma}_{11}(p_1, p_1') = U_1 + U_1^2 \Pi_{11}(\tilde{q}_{11}) - 2U_3^2 \Pi_{22}(q_{11}) \\ &\quad + U_4^2 [C_{12}(0) + \Pi_{12}(\tilde{q}_{11}) \\ &\quad + \Pi_{21}(\tilde{q}_{11})] + 2U_3 \tilde{U}_3 \Pi_{22}(q_{11}) + \tilde{U}_3^2 \Pi_{22}(\tilde{q}_{11}), \end{aligned} \quad (7)$$

$$\begin{aligned} \tilde{\Gamma}_{12} &= \tilde{\Gamma}_{12}(p_1, p_2') = K + KU_3 [2\Pi_{12}(q_{12}) + \Pi_{12}(\tilde{q}_{12}) + \Pi_{21}(\tilde{q}_{12})] \\ &\quad + U_4 U_5 C_{12}(0) + U_4^2 \Pi_{11}(\tilde{q}_{12}) + U_5^2 \Pi_{22}(\tilde{q}_{12}) - 2K \tilde{U}_3 \Pi_{12}(q_{12}), \end{aligned}$$

and expressions for  $\tilde{\Gamma}_{22}$  and  $\tilde{\Gamma}_{21}$  are found from (7) by making the interchanges  $1 \leftrightarrow 2$ ,  $U_4 \leftrightarrow U_5$ . In (7) (in the equations given below, the values,  $p_1, p_1', p_2, p_2'$  are the vector values) we have

$$\begin{aligned} q_{11}^2 &= 2p_{F1}^2 (1 - \cos \varphi) = (p_1 - p_1')^2, \\ \tilde{q}_{11}^2 &= 2p_{F1}^2 (1 + \cos \varphi) = (p_1 + p_1')^2, \\ q_{12}^2 &= p_{F1}^2 + p_{F2}^2 - 2p_{F1} p_{F2} \cos \varphi = (p_1 - p_2')^2, \\ \tilde{q}_{12}^2 &= p_{F1}^2 + p_{F2}^2 + 2p_{F1} p_{F2} \cos \varphi = (p_1 + p_2')^2, \end{aligned}$$

and

$$\Pi_{ij}(q) = - \sum_p \frac{n(\varepsilon_i(p+q)) - n(\varepsilon_i(p))}{\varepsilon_i(p+q) - \varepsilon_i(p)}$$

are the static polarization operators, and

$$C_{12}(0) = \sum_p \frac{1 - n(\varepsilon_1(p)) - n(\varepsilon_2(-p))}{\varepsilon_1(p) + \varepsilon_2(-p)}$$

is the Cooper loop formed by particles of different species. [It does not contain a logarithmic singularity  $\ln(1/T)$ , so it should be incorporated in the seed vertex.]

Analysis of Eqs. (6) reveals that for nonzero  $\tilde{\Gamma}_{12}$  (and thus  $\tilde{\Gamma}_{21}$ ) a pole appears in all the total vertices  $\Gamma_{ij}$  at the same transition temperature, which is found from the equation

$$1 + \tilde{\Gamma}_{11} C_1 + \tilde{\Gamma}_{22} C_2 + (\tilde{\Gamma}_{11} \tilde{\Gamma}_{22} - \tilde{\Gamma}_{12} \tilde{\Gamma}_{21}) C_1 C_2 = 0. \quad (8)$$

We thus find that the transition temperature is<sup>8,9</sup>

$$T_c \sim \tilde{\varepsilon} \exp \left\{ - \frac{1}{\lambda} \right\}, \quad \lambda = \frac{-(\lambda_1 + \lambda_2) + [(\lambda_1 - \lambda_2)^2 + 4\lambda_{12}\lambda_{21}]^{1/2}}{2}, \quad (9)$$

where the coupling constants  $\lambda$  are

$$\begin{aligned} \lambda_1 &= \tilde{\Gamma}_{11} g_1, \quad \lambda_2 = \tilde{\Gamma}_{22} g_2, \\ \lambda_{12} &= \tilde{\Gamma}_{12} g_1, \quad \lambda_{21} = \tilde{\Gamma}_{21} g_2, \end{aligned}$$

$g_i = m_i/2\pi$  is the density of states; and  $\tilde{\varepsilon}$  is a rather complex function of  $\varepsilon_{F1}, \varepsilon_{F2}, m_1$ , and  $m_2$ . Under the conditions  $\lambda_{12}, \lambda_{21} \ll \lambda_1, \lambda_2$ , the energy  $\tilde{\varepsilon}$  is close to that Fermi energy which corresponds to the larger of  $\lambda_1, \lambda_2$ , and  $T_c$  itself is close to the larger of the two temperatures  $T_{c1} \sim \varepsilon_{F1} \exp\{-1/\lambda_1\}$  and  $T_{c2} \sim \varepsilon_{F2} \exp\{-1/\lambda_2\}$ . A superconductivity is possible, of course, only if  $\lambda$  is positive.

Let us examine the possibility of  $s$ -pairing in the system described by Hamiltonian (5) in the weak-coupling approximation. In first-order perturbation theory for the vertices

$\tilde{\Gamma}_{ij}$  we have  $\lambda_1 = U_1 g_1 > 0$ , and  $\lambda_2 = U_2 g_2 > 0$ . A superconducting pairing is thus possible only under the condition  $(U_1 U_2 - K^2) g_1 g_2 < 0$ , i.e.,  $U_1 U_2 > K^2$ . In this case, a pairing with an  $s$  symmetry arises. We might note that in most cases the opposite inequality ( $U_1 U_2 < K^2$ ) holds, since there is an additional small factor in  $K$  because of the overlap integral. We thus reach the conclusion that, for the typical two-band Coulomb problem,  $s$ -pairing in weak coupling is suppressed by direct Coulomb repulsion in each of the bands. The only hope for achieving an  $s$ -pairing is to go beyond the weak-coupling approximation in evaluating the vertices  $\tilde{\Gamma}_{ij}$  and the effective "redecorated" of the repulsive first-order perturbation theory by the following orders.

For pairing of other types (with  $m > 0$ ), however, the direct Coulomb repulsion does not contribute to the partial seed vertices  $\tilde{\Gamma}^{(m)}$ , since it vanishes in the course of the integration with the functions  $\cos m\varphi$  ( $m \neq 0$ ). The expansion of  $\tilde{\Gamma}^{(m)}$  in this case thus begins with the terms of second-order perturbation theory [see (7)].

From this point on, the analysis depends strongly on whether we are considering two electron bands [ $\varepsilon_{1,2} = (p^2 - p_{F1,2}^2)/2m_{1,2}$ ] or one electron band and one hole band [ $\varepsilon_1 = (p^2 - p_{F1}^2)/2m_1, \varepsilon_2 = (p_{F2}^2 - p^2)/2m_2$ ]. In the case of two electron bands (the simpler to analyze), all the polarization operators, normalized to the corresponding densities of states, are slowly varying functions on the order of unity in the region pertinent to the superconductivity,  $q \ll 2p_F$ , as was shown in Refs. 5 and 10. When the small value of the overlap integral  $t$  is taken into account, expressions (7) for the corresponding vertices  $\tilde{\Gamma}_{11}^{(m)}$  and  $\tilde{\Gamma}_{22}^{(m)}$  can thus be simplified dramatically:

$$\begin{aligned} \tilde{\Gamma}_{11}^{(m)} &= U_1^2 \Pi_{11}^{(m)}(\tilde{q}_{11}) - 2U_3^2 \Pi_{22}^{(m)}(q_{11}), \\ \tilde{\Gamma}_{22}^{(m)} &= U_2^2 \Pi_{22}^{(m)}(\tilde{q}_{22}) - 2U_3^2 \Pi_{11}^{(m)}(q_{22}), \\ \tilde{\Gamma}_{12}^{(m)} &\sim \tilde{\Gamma}_{21}^{(m)} \sim t^2 \tilde{\Gamma}_{ii}^{(m)} \ll \tilde{\Gamma}_{ii}^{(m)}. \end{aligned} \quad (10)$$

Expressions (10) for  $\tilde{\Gamma}_{11}^{(m)}$  and  $\tilde{\Gamma}_{22}^{(m)}$  are the same as the corresponding expressions in Ref. 5. In the case  $\tilde{\Gamma}_{12}^{(m)} = \tilde{\Gamma}_{21}^{(m)} = 0$ , according to the results of that study, a superconductivity would arise in a band with a large number of particles (with larger  $p_F$ ) and would be of a  $p$ -pairing nature. The band with the fewer particles (with smaller  $p_F$ ) would remain normal down to  $T = 0$ . We recall that the quantity  $U_3$  plays a key role in the occurrence of superconductivity according to this scenario. In other words, there is a pairing of particles in one band (that with the larger  $p_F$ ) as a result of a polarization of particles in the other band (with the smaller  $p_F$ ). If  $\tilde{\Gamma}_{12}^{(m)}$  and  $\tilde{\Gamma}_{21}^{(m)}$  are small but nonzero, as in Ref. 5, both bands become superconducting, at the same temperature. We see from (9) that this temperature is close to the superconductivity transition temperature in the first band, according to Ref. 5. In other words, it is close to

$$T_c \rightarrow T_{c1} \sim \varepsilon_{F1} \exp \left\{ -\frac{16\pi^2}{m_1 m_2 U_3^2} \frac{p_{F1}^2 / p_{F2}^2}{8(p_{F1}/p_{F2} - 1)} \right\} \quad (11)$$

and is determined by the polarization operator  $\Pi_{22}^{(m=1)}(q_{11})$  if  $p_{F1} > p_{F2}$ . Naturally, a  $p$ -pairing also occurs in this case.

A more complex situation is that in which there are one electron band and one hole band. In this case, as was shown in Ref. 10, the interband polarization operator  $\Pi_{12}(q)$  has a

clearly defined maximum  $\ln(k_{\max}/|p_{F2} - p_{F1}|)$  at  $q = |p_{F2} - p_{F1}|$ . The height of this maximum increases as the Fermi momenta of the bands move closer together. It is thus necessary to retain, in expression (7) for  $\tilde{\Gamma}$ , terms which contain the product of off-diagonal elements of the Coulomb interaction ( $U_4, U_5, K$ ) and the polarization operator  $\Pi_{12}$  (the small values of the off-diagonal interaction elements are offset by the large value of  $\Pi_{12}$ ). Since  $\Pi_{12}$  is a logarithmic function of  $q$ , however, the contribution of the corresponding terms to the partial vertices  $\tilde{\Gamma}^{(m)}$  does not contain a large parameter. This contribution is thus competitive with the contribution from  $\Pi_{22}^{(m)}(q_{11})$  in (10) only if the difference  $|p_{F2} - p_{F1}|$  is small, and we have  $\Pi_{22}^{(m)}(q_{11}) \sim |p_{F2} - p_{F1}|/p_{F2}$  (and this is a small quantity). We thus reach the conclusion that, again in the case of one electron band and one hole band, provided that the Fermi momenta are not too close together, the predominant superconductivity mechanism is, as before, the mechanism of Ref. 5, which involves an interband Coulomb interaction,  $U_3$ . The terms associated with  $U_4, U_5$ , and  $K$  could be important to the occurrence of superconductivity only if  $p_{F1}$  and  $p_{F2}$  were approximately equal. In this region, however, the very possibility of a superconductivity is problematic because a transition to an insulating phase by the Keldysh-Kopaev mechanism<sup>11,15</sup> would occur faster. The reason (as was shown in those Refs. 11 and 15) is that the transition to the insulating phase is of first order in the Coulomb constants, while the superconductivity mechanism which we are discussing is of second order. If the Fermi momenta of the electron band and the hole band are strictly identical, then the polarization operator  $\Pi_{12}(q)$  has a logarithmic singularity<sup>10,11,15</sup>  $\sim \ln q$  as  $q \rightarrow 0$ . One might thus be led to believe that the exact answer to the question of the relative effects of insulating and superconducting pairing would require going beyond the second of the ladder approximation, i.e., the solution of equations of the one-logarithm parquet type.<sup>11</sup> It might be possible in principle to sharply increase the superconducting transition temperature  $T_{cs}$  in this manner—perhaps even to make it comparable to the insulating transition temperature  $T_{cd}$ .

However, that is not what happens in the problem at hand, since one of the channels (e.g., the Cooper channel) does not select "favorable" momenta for the appearance of a logarithmic singularity in the second (zero-sound) channel. The singularity of the zero-sound channel is thus integrated, and there is no mutual intensification of singularities: The parquet "crumbles." In other words, in the temperature technique we have  $C \sim \ln(1/T)$  and  $\Pi_{12} \sim \ln(1/T)$ , but the integral of the product of  $C$  and  $\Pi_{12}$  over the intermediate momenta is not  $\ln^2(1/T)$  but again only  $\ln(1/T)$ . If we wish to prevent the parquet from crumbling, we need either (as in Refs. 11) a one-dimensional situation, in which there is no integration over angles, or a two-dimensional situation in which a discrete set of momenta are prominent near a half filling by Van Hove singularities in the density of states. Again in this second case, the integration over angles would effectively be eliminated.

#### 4. CASE OF TWO 2D BANDS WITH VERY DIFFERENT MASSES

We now consider the case of two 2D bands with very different masses  $m_2 \gg m_1$ . Again in this case, generally

speaking, it may be necessary to go beyond the weak-coupling approximation for the effective interaction  $\tilde{\Gamma}$ . We are interested in the *a priori* possibility of obtaining an *s* pairing in a repulsive 2D problem.

A situation of this sort is realized in the 2D case with  $m_2 > m_1$  and  $f_1 = m_1 U_3 / 4\pi \ll 1$  but  $f_2 = m_2 U_3 / 4\pi \lesssim 1$ . If both  $f_1$  and  $f_2$  are much smaller than one (but the condition  $m_2 \gg m_1$  still held), the expressions of the partial vertices  $\tilde{\Gamma}^{(m=0)}$  corresponding to *s* pairing would be, according to the results of Ref. 5 and Eq. (10),

$$\begin{aligned}\tilde{\Gamma}_{11} &= U_1 + \frac{m_1 U_1^2}{2\pi} - 2 \frac{m_2 U_3^2}{2\pi} \approx U_1 - \frac{m_2 U_3^2}{\pi}, \\ \tilde{\Gamma}_{22} &= U_2 + \frac{m_2 U_2^2}{2\pi} - 2 \frac{m_1 U_3^2}{2\pi} \approx U_2 + \frac{m_2 U_2^2}{2\pi}.\end{aligned}\quad (12)$$

(As was mentioned above, the diagonal elements of the Coulomb interaction— $U_1$ ,  $U_2$ , and  $U_3$ —are of the same order of magnitude.) If  $f_1 \ll 1$  but  $f_2 \lesssim 1$ , expression (12) should be modified. Specifically, in the customary approach for Coulomb systems, we should sum the RPA diagrams containing loops of particles of species 2. As a result we find

$$\begin{aligned}\Gamma_{11} &= U_1 - \frac{m_2 U_3^2 / \pi}{1 + m_2 U_2 / \pi}, \\ \Gamma_{22} &= \frac{U_2}{1 + m_2 U_2 / \pi} + 3 \frac{m_2 U_2^2 / 2\pi}{(1 + m_2 U_2 / \pi)^2}.\end{aligned}\quad (13)$$

We see from expression (13) that  $\tilde{\Gamma}_{22}$  is always positive, so it is of no interest from the standpoint of superconductivity. The vertex  $\tilde{\Gamma}_{11}$  is

$$\tilde{\Gamma}_{11} = \frac{U_1 + m_2 (U_1 U_2 - U_3^2) / \pi}{1 + m_2 U_2 / \pi}.\quad (14)$$

In other words, under the condition  $U_3^2 > U_1 U_2$  the second term in the numerator is generally negative and may “redecorate” the seed Coulomb repulsion  $U_1$  (we recall that we are considering the case  $m_2 U \sim 1$ ). A superconductivity would result. A similar possibility in the 3D case was pointed out in Ref. 16. However, we find this superconductivity scenario dubious, since the entire expression for  $\tilde{\Gamma}_{11}$  can be reduced to the form  $\tilde{\Gamma}_{11} = U_1 \epsilon_{\text{eff}} = U_1 / \epsilon(q, 0)$ , where the function

$$\epsilon(q, 0) = \frac{1 + m_2 U_2 / \pi}{1 + m_2 (U_2 - U_3^2 / U_1) / \pi}$$

is the same as the static dielectric constant if  $U_1$ ,  $U_2$ , and  $U_3$  are understood as representing the real Coulomb interaction  $2\pi e^2 / q$ . A change in the sign of  $\tilde{\Gamma}_{11}$  is thus dubious, since for the real long-range Coulomb interaction it would correspond to a negative value of  $\epsilon$  at a zero frequency. This negative value would imply an instability of the system—a negative value of the square of phonon frequencies—according to the standard ideas (but see Ref. 17). The result found for  $\tilde{\Gamma}_{11}$  should thus probably be regarded as an indication that there may be a pronounced suppression of the seed intraband Coulomb repulsion  $U_1$ . This effect might smooth the way for an *s* pairing when other degrees of freedom (e.g., phonon or magnon degrees of freedom) are taken into account.

Refining expression (14) for  $\tilde{\Gamma}_{11}$  requires summing the corrections to the vertex functions and the polarization

loops which arise when the ladders from the interactions  $U_2$  are taken into account. Correspondingly, we find the following expressions for  $\tilde{\Gamma}_{11}$  and  $\tilde{\Gamma}_{22}$ :

$$\begin{aligned}\tilde{\Gamma}_{11} &= U_1 - \frac{m_2 U_3^2 / \pi}{1 + m_2 U_2 / 2\pi} = \frac{U_1 - (2U_3^2 - U_1 U_2) m_2 / 2\pi}{1 + m_2 U_2 / 2\pi}, \\ \tilde{\Gamma}_{22} &= \frac{U_2}{1 - m_2 U_2 / 2\pi - (m_2 U_2 / 2\pi)^2} \approx \frac{U_2}{1 - m_2 U_2 / 2\pi}.\end{aligned}\quad (15)$$

Comparison of (13) and (15) reveals that the occurrence of an *s*-pairing for particles of species 1 looks just a bit more plausible in the latter case, since it would require less stringent conditions on the values of the interaction constants  $U_i$ . However, again in this case [as in (13)] the quantity  $\tilde{\Gamma}_{11}$  can be written as  $U_1 / \epsilon(q, 0)$ , where  $\epsilon(q, 0)$  incorporates correlation corrections.

Let us summarize the results of this study.

Analysis of the two-band model in the three-dimensional case shows that only if the masses are approximately equal could the second band play an important role in strengthening the superconductivity beyond that in the one-band case. If the masses are instead greatly different, the heavy band plays the dominant role; i.e., the problem becomes an essentially one-band problem. At any rate, if the density of particles is small, and we can get by with a quadratic dispersion law, the superconductivity which arises is of the *p*-pairing type.

In the two-dimensional case, for either two electron bands or one electron band and one hole band, the dominant superconductivity mechanism is the pairing of particles in the band with the larger  $p_F$  through a polarization of particles in the band with the smaller  $p_F$ . The superconductivity which arises is of the *p*-pairing type, as in the three-dimensional case. In the 2D case, with greatly different masses, there is the possibility that the seed intraband Coulomb repulsion will be substantially suppressed. This effect might promote an *s*-pairing when other superconductivity mechanisms, e.g., a phonon or magnon mechanism, are brought into the picture.

Incorporating the off-diagonal matrix elements of the Coulomb interaction leads to the simultaneous opening of superconductivity gaps in the two bands, in both the 3D and 2D cases.

We thank A. F. Andreev, K. Begel<sup>1</sup>, Yu. Kagan, M. I. Kaganov, A. V. Chubukov and P. Shekter for useful discussions. We are also grateful to G. Vendin and Kh. M. Kapel for their hospitality at the last stages of the research.

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- <sup>1</sup> V. J. Emery, Phys. Rev. Lett. **58**, 2794 (1987).
- <sup>2</sup> M. Z. Rice, H. Y. Choi, and Y. R. Wang, Phys. Rev. B **44**, 10414 (1991).
- <sup>3</sup> M. A. Baranov and M. Yu. Kagan, Zh. Eksp. Teor. Fiz. **99**, 1236 (1991) [Sov. Phys. JETP **72**, 689 (1991)].
- <sup>4</sup> M. A. Baranov and M. Yu. Kagan, Z. Phys. B, 1992 (in press).
- <sup>5</sup> M. Yu. Kagan, Phys. Lett. A **152**, 303 (1991).
- <sup>6</sup> D. J. Scalapino, E. Loh, and J. E. Hirsch, Phys. Rev. B **35**, 6694 (1987); K. Miyake, S. Schmitt-Rink, and C. M. Varma, Phys. Rev. B **34**, 6554 (1986).
- <sup>7</sup> M. Yu. Kagan and A. V. Chubukov, Pis'ma Zh. Eksp. Teor. Fiz. **50**, 483 (1989) [JETP Lett. **50**, 517 (1989)].
- <sup>8</sup> V. Moskalenko, Fiz. Met. Metalloved. **8**, 503 (1959); H. Suhl, B. Matias, and L. Walker, Phys. Rev. Lett. **3**, 552 (1959).
- <sup>9</sup> V. Z. Kresin and S. A. Wolf, Physica C **169**, 476 (1990).
- <sup>10</sup> K. Yamaji, J. Phys. Soc. Jpn. **59**, 677 (1990).
- <sup>11</sup> L. V. Keldysh and Yu. V. Kopayev, Fiz. Tverd. Tela (Leningrad) **6**,

- 2791 (1964) [Sov. Phys. Solid State **6**, 2219 (1965)]; Yu. A. Bychkov, L. P. Gor'kov, and I. E. Dzyaloshchinskiĭ, Zh. Eksp. Teor. Fiz. **50**, 738 (1966) [Sov. Phys. JETP **23**, 489 (1966)]; I. E. Dzyaloshinskiĭ and E. I. Kats, Zh. Eksp. Teor. Fiz. **62**, 1104 (1972) [Sov. Phys. JETP **35**, 584 (1972)]; I. E. Dzyaloshinskiĭ and V. M. Yakovenko, Zh. Eksp. Teor. Fiz. **94**(4), 344 (1988) [Sov. Phys. JETP **67**(4), 844 (1988)].
- <sup>12</sup> M. Yu. Kagan and A. V. Chubukov, Pis'ma Zh. Eksp. Teor. Fiz. **47**, 525 (1988) [JETP Lett. **47**, 614 (1988)].
- <sup>13</sup> Yu. Kagan and I. V. Prokof'ev, Zh. Eksp. Teor. Fiz. **93**, 366 (1987) [Sov. Phys. JETP **66**, 211 (1987)].
- <sup>14</sup> P. W. Anderson, J. Phys. Chem. Solids **11**, 26 (1959).
- <sup>15</sup> A. I. Kozlov and L. A. Maksimov, Zh. Eksp. Teor. Fiz. **48**, 1184 (1965) [Sov. Phys. JETP **21**, 790 (1965)].
- <sup>16</sup> B. T. Geĭlikman, Zh. Eksp. Teor. Fiz. **48**, 1194 (1965) [Sov. Phys. JETP **21**, 796 (1965)].
- <sup>17</sup> O. V. Dolgov, D. A. Kirzhnits, and E. G. Maksimov, Rev. Mod. Phys. **53**, 81 (1981).

Translated by D. Parsons