Hole superconductivity in a generalized two-band model

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We study superconductivity in a two-band model that generalizes the model introduced by Suhl, Matthias, and Walker: All possible interaction terms coupling both bands are included. The pairing interaction is assumed to originate in the momentum dependence of the intraband interactions that arises in the model of hole superconductivity. The model generically displays a single critical temperature and two gaps, with the larger gap associated with the band with strongest holelike character to the carriers. The dependence of the critical temperature and of the magnitudes of the gaps on the various parameters in the Hamiltonian is studied.

Suhl, Matthias, and Walker[1] introduced many years ago a simple two-band model for superconductivity with an interaction term coupling both bands. Various interesting features were found by Suhl, Matthias, and Walker, in particular, that the model displays a single critical temperature but two different gaps, and that superconductivity can be induced solely by the interaction term coupling both bands irrespective of its sign. This model was later applied to explain the specific-heat data of high-purity superconducting transition metals,[2,3] and recently was used to study the properties of some of the high-T_c oxides.[4–7] In this model the interactions were assumed to be momentum independent, presumably arising from both Coulomb and electron-phonon processes.

There are, in principle, several different interaction terms that can exist for coupling two bands, and Suhl, Matthias, and Walker restricted their attention to a single one. Some posterior theoretical work discussed the relevance of different two-band interactions to superconductivity.[8–12] However, the weak-coupling treatments of the BCS reduced Hamiltonian in the two-band model in the past have been limited to include only Suhl, Matthias, and Walker's interband interaction term.[4–7,13,14] One of the purposes of this paper is to generalize the theory to include all other possible combinations of four fermion operators coupling two bands within the BCS reduced Hamiltonian.

The second purpose of this paper is to explore the generalization of the model of hole superconductivity[15,16] to the case of two bands. In this model, a term that modulates the hopping amplitude of electrons by the presence of other electrons in the band,

$$\Delta t \sum_{i,\sigma} (c^{\dagger}_{i\sigma} c_{j\sigma} + \text{H.c.})(n_{i-\sigma} + n_{j-\sigma}) , \tag{1}$$

is included in the tight-binding Hamiltonian, which gives rise to an attractive (repulsive) interaction when the carriers are holelike (electronlike). Since a superconducting metal generically will have both holelike and electronlike pieces of the Fermi surface, it is particularly important in this model, where the sign of the interaction depends on the character of the carriers to study its generalization to a multiband situation. In a recent paper[17] an initial study of this problem in the context of a two-band model for high-T_c oxides was reported, including only the interband coupling term of Suhl, Matthias, and Walker. It was found that the gap in the electronlike band was typically 2 orders of magnitude smaller than in the holelike band when a repulsive on-site interaction of the same magnitude existed in both bands. This is somewhat disturbing as experimental evidence for two gaps in the high-T_c oxides[18] suggests a ratio between both gaps of only a factor of 3. We examine in this paper how the inclusion of other interaction terms in the Hamiltonian can modify these results.

We consider a reduced Hamiltonian of the form

$$H = \sum_{\substack{k,\sigma,\\ i}} (e^{i}_{k\sigma} - \mu) c^{\dagger}_{i,k\sigma} c_{i,k\sigma} + \frac{1}{N} \sum_{\substack{k,k',\\ i_1,i_2,\\ j_1,j_2}} V^{j_1 j_2}_{i_1 i_2}(k,k') c^{\dagger}_{i_1,k\uparrow} c^{\dagger}_{i_2,-k\downarrow} c_{j_1,-k'\downarrow} c_{j_2,k'\uparrow} , \tag{2}$$

where $c_{i,k\sigma}$, $i=1,2$, correspond to annihilation operators for bands 1 and 2, respectively, and i, i_1, i_2, j_1, j_2 are summed over 1 and 2. We use the convention that the operators describe holes in the bands. There are a total of 16 reduced interaction terms in the Hamiltonian Eq. (2). In the treatment of Suhl, Matthias, and Walker, only the interband interaction term corresponding to $i_1 = i_2$ and $j_1 = j_2$ in Eq. (2) was considered.

The mean-field Hamiltonian is given by the following form:

$$H=\sum_k (c^\dagger_{1,k\uparrow}\ \ c_{1,-k\downarrow}\ \ c^\dagger_{2,k\uparrow}\ \ c_{2,-k\downarrow}) \begin{pmatrix} e^1_k-\mu & \Delta_{11}(k) & 0 & \Delta_{12}(k) \\ \Delta^\dagger_{11}(k) & -(e^1_k-\mu) & \Delta^\dagger_{21}(k) & 0 \\ 0 & \Delta_{21}(k) & e^2_k-\mu & \Delta_{22}(k) \\ \Delta^\dagger_{12}(k) & 0 & \Delta^\dagger_{22}(k) & -(e^2_k-\mu) \end{pmatrix} \begin{pmatrix} c_{1,k\uparrow} \\ c^\dagger_{1,-k\downarrow} \\ c_{2,k\uparrow} \\ c^\dagger_{2,-k\downarrow} \end{pmatrix} . \tag{3}$$

The Δ's in the above matrix are defined as

$$\Delta_{i_1 i_2}(k)=\frac{1}{N}\sum_{\substack{k' \\ j_1,j_2=1,2}} V^{j_1 j_2}_{i_1 i_2}(k,k')\langle c_{j_1,-k'\downarrow} c_{j_2,k'\uparrow}\rangle\ ,\quad i_1,i_2=1,2\ . \tag{4}$$

By generalizing the Bogoliubov transformation, we find a unitary matrix to bring the Hamiltonian into diagonal form and obtain self-consistent equations for $\Delta_{i_1 i_2}$, $i_1,i_2=1,2$ (see Ref. 19 for details).

In the following discussion, we assume

$$\langle c_{1,-k\downarrow} c_{2,k\uparrow}\rangle=\langle c_{2,-k\downarrow} c_{1,k\uparrow}\rangle \tag{5}$$

and we define

$$V^{11}_{11}(k,k')\equiv V_1(k,k')\ , \tag{6}$$

$$V^{22}_{22}(k,k')\equiv V_2(k,k')\ , \tag{7}$$

$$V^{22}_{11}(k,k')=V^{11}_{22}(k,k')\equiv V_{12}(k,k')\ , \tag{8}$$

$$\tfrac{1}{2}[V^{12}_{11}(k,k')+V^{21}_{11}(k,k')]=\tfrac{1}{2}[V^{11}_{21}(k,k')+V^{11}_{12}(k,k')]\equiv V_{13}(k,k')\ , \tag{9}$$

$$\tfrac{1}{2}[V^{12}_{22}(k,k')+V^{21}_{22}(k,k')]=\tfrac{1}{2}[V^{22}_{21}(k,k')+V^{22}_{12}(k,k')]\equiv V_{23}(k,k')\ , \tag{10}$$

$$\tfrac{1}{2}[V^{21}_{12}(k,k')+V^{12}_{12}(k,k')]=\tfrac{1}{2}[V^{12}_{21}(k,k')+V^{21}_{21}(k,k')]\equiv V_3(k,k')\ , \tag{11}$$

then we obtain $\Delta_{12}(k)=\Delta_{21}(k)$. The quasiparticle energies are given by

$$E^2_{1,2k}=\tfrac{1}{2}[(e^1_k-\mu)^2+(e^2_k-\mu)^2+\Delta^2_{11}(k)+\Delta^2_{22}(k)+2\Delta^2_{12}(k)] \pm\tfrac{1}{2}(\{[(e^1_k-\mu)^2+\Delta^2_{11}(k)-(e^2_k-\mu)^2-\Delta^2_{22}(k)]^2+4\Delta^2_{12}(k)\{(e^1_k-e^2_k)^2+[\Delta_{11}(k)+\Delta_{22}(k)]^2\}\}^{1/2}\ . \tag{12}$$

For simplicity, we use a flat density of states in both bands of bandwidth D_i. The energies are $e^i_{k\sigma}=\varepsilon^i_{k\sigma}-\varepsilon^0_k$, where $\varepsilon^i_{k\sigma}$ are measured from the center of each band. We take $\varepsilon^1_0=0$, so ε^2_0 is the shift of the second band relative to the first band. We take the intraband interactions V_1 and V_2 to be of the form used in Ref. 16:

$$V_i(k,k')=U_i+K_i\left[\frac{\varepsilon^i_k}{D_i/2}+\frac{\varepsilon^i_{k'}}{D_i/2}\right] +W_i\frac{\varepsilon^i_k}{D_i/2}\frac{\varepsilon^i_{k'}}{D_i/2}\ ,\quad i=1,2\ , \tag{13}$$

with the parameters U_i, W_i, K_i arising from on-site repulsion, nearest-neighbor repulsion, and modulated hopping, respectively [$K_i=2z(\Delta t)_i$, with $(\Delta t)_i$ the hopping interaction in each band as given by Eq. (1) and z the number of nearest neighbors]. All the other interaction parameters V_{12}, V_{13}, V_{23}, and V_3 are assumed momentum independent for simplicity. By choosing the parameters in this way, the Δ's will have the following forms:

$$\Delta_{ii}(k)=\Delta_{ii}(\varepsilon^i_k)=b_i-\Delta^m_i\frac{\varepsilon^i_k}{D_i/2}\ ,\quad i=1,2 \tag{14}$$

and

$$\Delta_{12}(k)=\Delta_{21}(k)=\Delta_3\ , \tag{15}$$

where b_1, b_2, Δ_3, and Δ^m_1,Δ^m_2 are parameters independent of k to be determined by the self-consistency conditions.[19] The critical temperature is determined by the single equation

$$4V_{12}V_{13}V_{23}I_0(3)X_1X_2+2I_0(3)(V^2_{13}X_1Y_2+V^2_{23}X_2Y_1) +[V_3I_0(3)+1](Y_1Y_2-V^2_{12}X_1X_2)=0\ , \tag{16}$$

where

$$X_i=W_i[I_0(i)I_2(i)-I^2_1(i)]+I_0(i)\ , \tag{17}$$

$$Y_i=-1-U_iI_0(i)-W_iI_2(i)+2K_iI_1(i) +(K^2_i-W_iU_i)[I_0(i)I_2(i)-I^2_1(i)]\ , \tag{18}$$

and

$$I_m(i)\equiv\frac{1}{N}\sum_k\left[-\frac{\varepsilon^i_k}{D_i/2}\right]^m\frac{1-2f(\varepsilon^i_k-\varepsilon^i_0-\mu)}{2(\varepsilon^i_k-\varepsilon^i_0-\mu)}\ , \quad m=0,1,2\ ,\ i=1,2\ , \tag{19}$$

$$I_0(3)\equiv\frac{1}{N}\sum_k\frac{1-f(\varepsilon^1_k-\varepsilon^1_0-\mu)-f(\varepsilon^2_k-\varepsilon^2_0-\mu)}{\varepsilon^1_k-\varepsilon^1_0+\varepsilon^2_k-\varepsilon^2_0-2\mu}\ . \tag{20}$$

To first order in the Δ's, we obtain

$$\langle c_{1,-k\downarrow}c_{1,k\uparrow}\rangle=\Delta_{11}(k)\frac{2f(e_k^1-\mu)-1}{2(e_k^1-\mu)}\ , \tag{21}$$

$$\langle c_{2,-k\downarrow}c_{2,k\uparrow}\rangle=\Delta_{22}(k)\frac{2f(e_k^2-\mu)-1}{2(e_k^2-\mu)}\ , \tag{22}$$

$$\langle c_{1,-k\downarrow}c_{2,k\uparrow}\rangle=\Delta_3\frac{f(e_k^1-\mu)+f(e_k^2-\mu)-1}{e_k^1+e_k^2-2\mu}\ . \tag{23}$$

These expressions, with the values of Δ's obtained from solving the self-consistent equations, give information on the nature of the pairs in the superconducting state. In the parameter range studied, it is found that pairs are formed mostly by particles in the same band, i.e, the expectation value Eq. (23) is very small.

Microscopically, the interactions $V_{i_1i_2}^{j_1j_2}$ can arise from intra-atomic or interatomic Coulomb interaction matrix elements. Their "bare values" are given by

$$V_{i_1i_2}^{j_1j_2}\sim e^2\int\int\frac{\phi_{i_1}^*(\mathbf{x})\phi_{i_2}^*(\mathbf{x}')\phi_{j_1}(\mathbf{x}')\phi_{j_2}(\mathbf{x})}{|\mathbf{x}-\mathbf{x}'|}d\mathbf{x}\,d\mathbf{x}'\ , \tag{24}$$

where ϕ_i, $i=1,2$, are atomic orbitals. The various interband interactions that enter the theory are associated with the following operators schematically (momentum and spin indices are omitted):

$$\begin{aligned} &V_{12}\text{:}\ \ c_1^\dagger c_1^\dagger c_2 c_2\ , \\ &V_{13}\text{:}\ \ c_1^\dagger c_1^\dagger c_1 c_2\ , \\ &V_{23}\text{:}\ \ c_2^\dagger c_2^\dagger c_2 c_1\ , \\ &V_3\text{:}\ \ c_1^\dagger c_2^\dagger c_2 c_1\ . \end{aligned} \tag{25}$$

Thus, V_3 arises from both Coulomb and exchange matrix elements involving one electron in each band, V_{13} and V_{23} arise from "hybrid" matrix elements involving the transfer of one electron from one band to the other, and V_{12} arises from exchange matrix elements involving the transfer of two electrons from one band to the other. The authors of Ref. 8 discussed the relative strength of these interactions and found that V_3 is bigger than V_{12}. From this point of view, there is no justification for including only V_{12} in the Hamiltonian as was done by Suhl, Matthias, and Walker and others. In this study, we investigate the effect of each of these interactions on the two-band model properties. We treat these interactions as phenomenological parameters, so Eq. (24) is useful only as a guideline for choosing appropriate parameter ranges.

It has been argued[8–12] that, in the presence of dynamical screening, V_3 by itself may lead to superconductivity through the acoustic plasmon mechanism. Here we do not include the effects of dynamical screening since, in the model of hole superconductivity, electron pairing mediated by bosonic excitations is of secondary importance compared with the intraband modulated hopping terms arising from the direct Coulomb interaction. In addition, the acoustic plasmon mechanism is thought to be effective only in the case where the effective mass of the carriers in both bands is very different, which is not an assumption in our model.

We consider two bands with equal bandwidth, $D_1=D_2=0.5$ eV and also choose $\varepsilon_0^1=0$, $\varepsilon_0^2=D_1/2$, so the center of band 2 coincides with the bottom of band 1. Such a case was assumed in Ref. 17 to describe a purely oxygen band (1) coupled to a copper-oxygen band (2). (We have also studied cases where the bands have different density of states, i.e., $D_1\neq D_2$.[19] Other than the usual density-of-states effects, the features of the model are unchanged.) For $\mu=-D_1/2$, at $T=0$ the pure O band is just empty of holes and the Cu-O band is half-filled. In Ref. 17, only V_{12} was included for the two-band coupling and the intraband nearest-neighbor repulsion (W_i) was set equal to zero. Following Ref. 17, we will refer to band 1 as the O band and band 2 as the Cu band and put the Fermi level around the bottom of the O band.

When the magnitude of the modulated hopping interactions K_i is significant, superconductivity is driven by the strong attractive interaction that results in the O band. From the mean-field Hamiltonian, Eqs. (3) and (4), it can be seen that, with the existence of interband interactions V_{12}, V_{13}, V_{23}, or V_3, there are several possible ways for the two bands to couple with each other. For example, if the interactions in the O band cause the development of pairing of $\langle c_{1-k\downarrow}c_{1,k\uparrow}\rangle$, when V_{13} and V_{23} exists, Δ_{12} will arise as well as the expectation value $\langle c_{1,k\uparrow}^\dagger c_{2,-k\downarrow}^\dagger\rangle$, which, in turn, can generate the Δ_{22} term and lead to paring of $\langle c_{2,k\uparrow}^\dagger c_{2,-k\downarrow}^\dagger\rangle$. However, one may intuitively expect that the pairing in the second band will be most effectively achieved by V_{12} because it does not need the "bridge" $\langle c_{1,k\uparrow}^\dagger c_{2,-k\downarrow}^\dagger\rangle$ to cause pairing in the second band. Our calculations confirm this expectation.

Below the superconducting transition temperature, order parameters $\Delta_{11}(k)$, $\Delta_{22}(k)$, and Δ_3 develop. The quasiparticle gaps, denoted by $\Delta^{01}(T)$ and $\Delta^{02}(T)$, are obtained by minimizing the energy dispersion relations $E_{1,2}(k)$ of Eq. (12). We choose the interactions in the O band and Cu band equal, let $U_1=U_2=5.0$ eV, and adjust W and K to obtain T_c in a desirable range. For some parameter sets, we found several solutions from the T_c, Eq. (16), and there are different order parameters and quasiparticle gaps corresponding to each T_c. So it is very important to calculate the free energy of the system relative to the normal state and only choose the physical solution with lowest free energy. This is discussed in detail in Ref. 19.

Compared to the single-band case, T_c is always enhanced when there are any interband interactions coupling the two bands. This had been found earlier for the case of V_{12}.[14] Figure 1 shows the effect of all the interband interactions on T_c vs n_1.

When only V_{12} exists, there are pairs $\langle c_{1,-k\downarrow}c_{1,k\uparrow}\rangle$ and $\langle c_{2,-k\downarrow}c_{2,k\uparrow}\rangle$ but no $\langle c_{1,-k\downarrow}c_{2,k\uparrow}\rangle$. When only V_{13} exists, all three pairs appear but $\langle c_{2,-k\downarrow}c_{2,k\uparrow}\rangle$ and $\langle c_{1,-k\downarrow}c_{2,k\uparrow}\rangle$ are much smaller than $\langle c_{1,-k\downarrow}c_{1,k\uparrow}\rangle$ and $\Delta^{02}(T)$ is virtually zero. Because we set the Fermi level around the bottom of the O band, V_{23} and V_3 on their own cannot lead the two bands to couple. The sign of the interband interactions V_{12}, V_{13}, and V_{23} will only affect

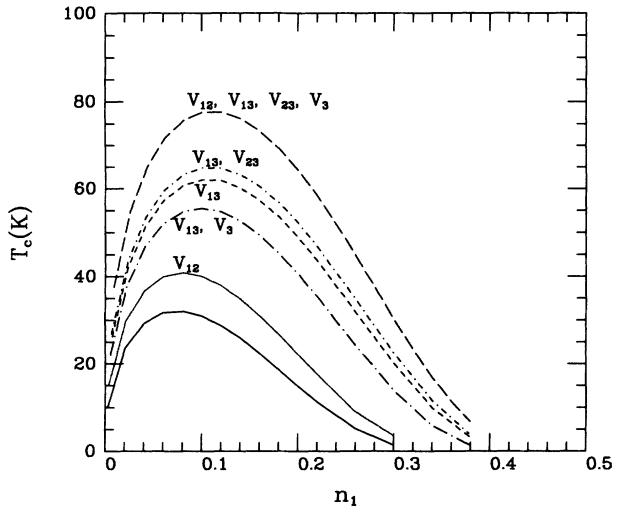

FIG. 1. T_c vs n_1 (hole concentration in the O band) for $K_1=K_2=3.8$ eV, $U_1=U_2=5.0$ eV, $W_1=W_2=2.64$ eV, $\mu=-0.22$ eV. Solid line, single-band case; dotted line, $V_{12}=0.2$ eV; short-dashed line, $V_{13}=-0.2$ eV; dot-short-dashed line, $V_{13}=V_{23}=-0.2$ eV; dot-long-dashed line, $V_{13}=-0.2$ eV, $V_3=0.2$ eV; long-dashed line, $V_{12}=V_{13}=V_{23}=-0.2$ eV, $V_3=0.2$ eV.

little, if not at all, the results. We choose V_3 to be positive since, from Eqs. (24) and (11), V_3 is related to the interband Coulomb interaction, presumably repulsive. Figure 2 shows pair expectation values versus temperature at

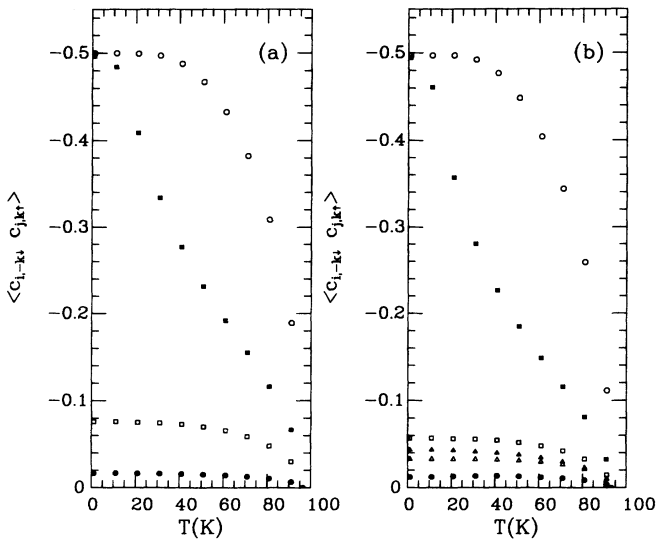

FIG. 2. Expectation values $\langle c_{1,-k\downarrow}c_{1,k\uparrow}\rangle$, $\langle c_{2,-k\downarrow}c_{2,k\uparrow}\rangle$ and $\langle c_{1,-k\downarrow}c_{2,k\uparrow}\rangle$ vs temperature at k values where $E_{1k}=\Delta^{01}$, $E_{2k}=\Delta^{02}$. $K_1=K_2=6.99$ eV, $W_1=W_2=10.0$ eV, $\mu=-0.22$ eV. Open points for k values corresponding to Δ^{01}; solid points for k values corresponding to Δ^{02}. (a) $V_{12}=-0.5$ eV, $V_{13}=V_{23}=V_3=0$, circles for $\langle c_{1,-k\downarrow}c_{1,k\uparrow}\rangle$, squares for $\langle c_{2,-k\downarrow}c_{2,k\uparrow}\rangle$. No $\langle c_{1,-k\downarrow}c_{2,k\uparrow}\rangle$ pairing exists in this case. (b) $V_{12}=-0.24$ eV, $V_{13}=V_{23}=0-.25$ eV, $V_3=0.25$ eV. Circles for $\langle c_{1,-k\downarrow}c_{1,k\uparrow}\rangle$, squares for $\langle c_{2,-k\downarrow}c_{2,k\uparrow}\rangle$, triangles for $\langle c_{1,-k\downarrow}c_{2,k\uparrow}\rangle$.

k values minimizing the quasiparticle energies. Because the Fermi energy corresponds to very different k values in both bands, we find that, when the pair expectation value is large in one band (which is for the k value that minimizes the quasiparticle energy in that band), it is small in the other. In Fig. 2(a), with the only interband interaction being V_{12}, only intraband pairs $\langle c_{i,-k\downarrow}c_{i,k\uparrow}\rangle$ exist. In Fig. 2(b), we consider all interband interactions of similar magnitude and find that here interband pairs $\langle c_{i,-k\downarrow}c_{j,k\uparrow}\rangle$, $i\neq j$, do exist, but with an amplitude substantially smaller than that of the dominant intraband pair. These interband pair expectation values show only weak dependence on k.

Figure 2 suggests that inclusion of the new interactions V_{13}, V_{23}, and V_3 does not qualitatively change the results from the case studied by Suhl, Matthias, and Walker, with only V_{12}, despite the fact that the new interactions do have a substantial effect on T_c, as was shown in Fig. 1. Although V_{12} may not always be the most effective interband interaction to enhance T_c, we find that V_{12} is the most important interband interaction which promotes pairing in the second band and the appearance of the second gap. Figure 3 shows T_c, $\Delta^{01}(0)$, and $\Delta^{02}(0)$ as a function of V_{12} and V_{13}. Note that V_{13} has a negligible effect on the second gap despite the fact that it strongly enhances the transition temperature.

In Ref. 17, where $W_1=W_2=0$, it was found that U_2 drives Δ^{02} rapidly to zero. Here we have found through an extensive parameter search that even including all possible other interband interactions, $\Delta^{02}(0)$ remains much smaller than $\Delta^{01}(0)$ if $W_i=0$. However, when we include W in the intraband interactions and increase K and W to keep the T_c in the same range, we find that the second gap $\Delta^{02}(0)$ can increase to reach comparable magnitude as the first gap $\Delta^{01}(0)$. Figure 4 shows cases for different parameter sets. Thus, we find that the appearance of the second gap is caused by the interband interaction V_{12},

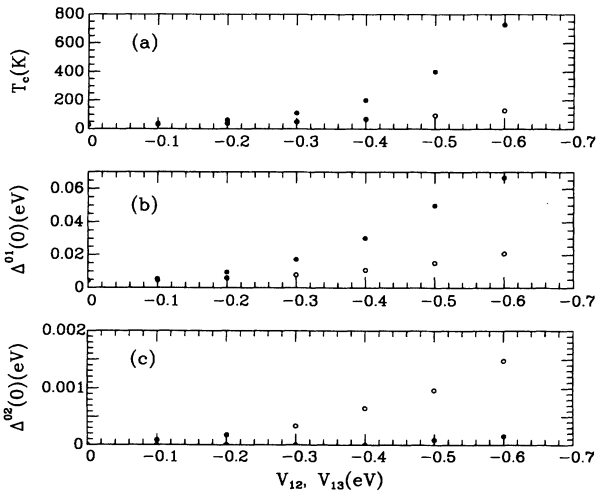

FIG. 3. T_c and $\Delta^{01}(0)$, $\Delta^{02}(0)$ vs V_{12} and V_{13} for $K_1=K_2=3.8$ eV, $U_1=U_2=5.0$ eV, $W_1=W_2=2.64$ eV, $\mu=-0.22$ eV. Open points for V_{12} (with $V_{13}=0$), solid points for V_{13} (with $V_{12}=0$).

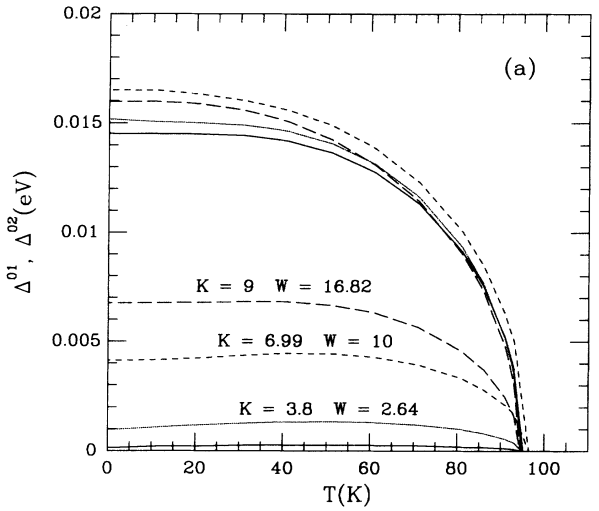

FIG. 4. $\Delta^{01}(T),\Delta^{02}(T)$ vs T for various K and W values at $V_{12}=-0.5$ eV, $U_1=U_2=5.0$ eV, $K=K_1=K_2$, $W=W_1=W_2$, $\mu=-0.22$ eV. Solid line, $K=1.63$ eV, $W=0$; dotted line, $K=3.8$ eV, $W=2.64$ eV; short-dashed line, $K=6.99$ eV, $W=10.0$ eV; long-dashed line, $K=9.0$ eV, $W=16.82$ eV.

but the size of the second gap is mainly determined by the intraband interactions in the two bands.

We also examined the effect of the relative position of the two bands on T_c and gaps, while keeping the Fermi level around the bottom of the O band.[19] The essential features of the model are preserved as the relative position of the two bands is changed. The magnitude of T_c and gaps will decrease when the Fermi level approaches the top of the Cu band, due to the stronger repulsive interaction between electronlike carriers of the Cu band.

In summary, we have generalized the treatment of Suhl, Matthias, and Walker to include all possible interactions between two bands and considered the behavior of a hole band coupled with an electron band with intraband interactions as in the model of hole superconductivity. Our conclusions can be summarized as follows: (1) The generalized two-band model exhibits the same qualitative dependence of T_c on carrier concentration as well as the linear energy dependence of gap functions found in the single-band model of hole superconductivity. (2) The magnitude of the "mixed pair" order parameter is much smaller than that of the intraband pairs. (3) The new interband interactions included here have an appreciable effect on the magnitude of T_c but not on the relative magnitude of the two gaps; the interaction V_{12} of Suhl, Matthias, and Walker is by far the most effective one in inducing a gap in the band that does not have strong holelike character. (4) When intraband nearest-neighbor repulsive interactions W are included, the gap in the electronlike band can become comparable to the one in the holelike band, in parameter ranges that do not appear unrealsitic. Although for certain materials it has been argued that evidence exists for two gaps of very different magnitude,[2] in other cases it appears that there are two gaps of comparable magnitude.[20] It is therefore satisfying that the model discussed here can encompass both regimes.

ACKNOWLEDGMENT

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