Superconductivity and excitonic state in a two-band model

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We study the interplay between superconductivity and excitonic correlations in a two-band model, in the presence of hybridization and local repulsion between electrons of different bands. The ground-state phase diagram as a function of the hybridization V and the interband Coulomb repulsion G is constructed. There is a critical value of hybridization V_c to destroy superconductivity, which decreases as G is increased. For values of G above a critical strength G_c, superconductivity is suppressed even for zero hybridization. We have obtained this result within a self-consistent mean-field treatment and using the Hubbard-I approximation. The valence transition in a mixed valence superconducting compound is considered.

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I. INTRODUCTION

Theoretical descriptions of superconducting phases usually are based on two-band models for a large variety of systems, such as heavy fermions,[1] transition metals,[2] or cuprate compounds.[3] The influence of the hybridization on superconductivity in the two-band model has recently been studied.[4,5] However, the influence of the Coulomb repulsion between electrons of different bands was not considered in these earlier studies. This interaction can be described by the so-called Falicov-Kimball term,[6,7] which has been extensively used to study valence and metal-nonmetal transitions in mixed valent compounds and heavy fermions systems. In these works, the importance of the inclusion of excitonic correlations in the description[8] of the referred systems has been shown. Excitonic correlations were also used to explain lattice deformation in Kondo insulators[9] and more recently were taken into account to study superconductivity in a mixed-valent system.[10] Due to the fact that the importance of excitons is well established by these findings, it is desirable to study the competition between excitons and superconducting pairs for all values of the hybridization and interband repulsion. Let us point out that a mechanism of superconducting pairing for high-temperature superconductors cuprates (HTSC) based on excitons was proposed by Varma *et al.*[11] However, in the present study we assume a phenomenological potential pairing without any reference to a particular pairing mechanism. We will contrast our results with those obtained in the *excitonic pairing* mechanism model.

II. THE MODEL HAMILTONIAN

In this work we study the interplay between exciton correlation and superconductivity in a two-band model, which considers on-site hybridization and local Coulomb repulsion between electrons of different bands. The model Hamiltonian is given by

$$H=\sum_{\langle ij\rangle\sigma} t^f_{ij} f^\dagger_{i\sigma} f_{j\sigma}+\sum_{\langle ij\rangle\sigma} t^d_{ij} d^\dagger_{i\sigma} d_{j\sigma}-U\sum_i n^f_{i\uparrow}n^f_{i\downarrow}+V\sum_{i\sigma}(f^\dagger_{i\sigma}d_{i\sigma}+d^\dagger_{i\sigma}f_{i\sigma})+G\sum_{i\sigma} n^f_{i\sigma}n^d_{i\sigma}-N\mu, \quad (1)$$

where $f^\dagger_{i\sigma}$ ($f_{i\sigma}$) and $d^\dagger_{i\sigma}$ ($d_{i\sigma}$) create (annihilate) electrons on site i in the narrow and wide bands, respectively, $n^f_{i\sigma}=f^\dagger_{i\sigma}f_{i\sigma}$ and $n^d_{i\sigma}=d^\dagger_{i\sigma}d_{i\sigma}$, U is an attractive interaction between f electrons, V is the hybridization, G is the Coulomb repulsion between f and d electrons, N is the total number of electrons, and μ is the chemical potential. The Hamiltonian (1), is equivalent to the spinless fermion version of the Falicov-Kimball model when $U=0$, which has been extensively used to study valence transitions.[7,8,10] With the use of a Hartree-Fock factorization in Eq. (1), and performing a Fourier transformation, we obtain Green's functions for the electrons of the two bands:

$$\langle\langle f^\dagger_{-k-\sigma};f^\dagger_{k\sigma}\rangle\rangle_\omega=\frac{1}{2\pi}\Delta(\omega^2-\zeta_k'^2)P(\omega)^{-1}, \quad (2)$$

$$\langle\langle d_{k\sigma};f^\dagger_{k\sigma}\rangle\rangle_\omega=\frac{1}{2\pi}\tilde{V}[(\omega+\epsilon'_k)(\omega+\zeta'_k)-\tilde{V}^2]P(\omega)^{-1}, \quad (3)$$

$$\langle\langle f_{k\sigma}f^\dagger_{k\sigma}\rangle\rangle_\omega=\frac{1}{2\pi}(\omega-\zeta'_k)[(\omega+\epsilon'_k)(\omega+\zeta'_k)-\tilde{V}^2]P(\omega)^{-1}, \quad (4)$$

with

$$P(\omega)=[(\omega-\epsilon'_k)(\omega-\zeta'_k)-\tilde{V}^2][(\omega+\epsilon'_k)(\omega+\zeta'_k)-\tilde{V}^2]-\Delta^2(\omega^2-\zeta_k'^2),$$

where Δ and A are the superconducting and excitonic order parameters, defined as

$$\Delta=U\langle f^\dagger_{k\sigma}f^\dagger_{-k-\sigma}\rangle,$$

$$A=\langle f_{k\sigma}d^\dagger_{k\sigma}\rangle.$$

We also introduced $\tilde{V}=V+AG$, $\epsilon'_k=\epsilon_k-\langle n^f_\sigma\rangle U+\langle n^d_\sigma\rangle G-\mu$, and $\zeta'_k=\zeta_k+\langle n^f_\sigma\rangle G-\mu$, where ϵ_k,ζ_k are the energies for the electrons in the f and d band, respectively. The roots of the polynomial $P(\omega)$ determine the excitation energies of the system,

$$E_{1,2k}^2=\frac{1}{2}(\Delta^2+2\tilde{V}^2+\epsilon_k'^2+\zeta_k'^2)$$
$$\pm\frac{1}{2}\sqrt{(\Delta^2+\epsilon_k'^2-\zeta_k'^2)^2+4\tilde{V}^2[\Delta^2+(\epsilon_k'+\zeta_k')^2]}.$$

We note that the excitations present a gap at the Fermi level in the following two circumstances: (a) when $\Delta>0$, for which case there is the usual superconducting gap, and (b) when $\tilde{V}$ is sufficiently strong, for which case a hybridization gap opens.

In the following, we assume that the bands are homotetic, i.e., $\epsilon_k=\alpha\zeta_k+\epsilon_0$, W and D are the bandwidths of the d and f bands, respectively, where $D=\alpha W$. The quantity α is then the ratio of effective masses, $\alpha=m_e^d/m_e^f$, of the quasiparticles in the two bands. In the present study we restrict ourselves to the half-filled case ($n^f+n^d=2$). In the main part of the work we will take the two renormalized bands ϵ_k',ζ_k' to be centered at the Fermi level (the symmetric case). In our model, this corresponds to set $\epsilon_0=U/2$ and $\mu=G/2$. Within these assumptions, the critical value to open the hybridization gap is $\tilde{V}_g=W\sqrt{\alpha}/2$.[12]

III. THE EFFECT OF HYBRIDIZATION AND INTERBAND COULOMB REPULSION ON SUPERCONDUCTIVITY

From the propagators (2)–(4), we obtain the following self-consistency equations that determine the values of Δ and A:

$$\Delta=\frac{1}{N_s}\sum_k\frac{U\Delta}{(E_{1k}^2-E_{2k}^2)}\left[\frac{(E_{1k}^2-\zeta_k'^2)}{2E_{1k}}\tanh(\beta E_{1k}/2)-\frac{(E_{2k}^2-\zeta_k'^2)}{2E_{2k}}\tanh(\beta E_{2k}/2)\right],\qquad(5)$$

$$A=\frac{1}{N_s}\sum_k\frac{\tilde{V}}{(E_{1k}^2-E_{2k}^2)}\left[\frac{(E_{1k}^2+\epsilon_k'\zeta_k'-\tilde{V}^2)}{2E_{1k}}\tanh(\beta E_{1k}/2)-\frac{(E_{2k}^2+\epsilon_k'\zeta_k'^2-\tilde{V}^2)}{2E_{2k}}\tanh(\beta E_{2k}/2)\right],\qquad(6)$$

where N_s is the number of sites in the lattice. The free energy is obtained from the trace formula

$$F=-2T\sum_k\sum_{i=1,2}\ln[2\cosh(\beta E_{ik}/2)]+N_s\Delta^2/U+2N_sGA^2-\mu N.\qquad(7)$$

It is easy to check that minimizing the free energy (7) with respect to Δ and A we obtain again the self-consistency Eq. (5) and (6). These equations admit two types of solutions. One of these is the superconducting state, for which superconductivity and excitons may coexist ($\Delta>0,A>0$). This solution is possible if V and G are less than some critical values. The other is a pure excitonic solution ($A>0,\Delta=0$), which exists for any value of V and G. However, whenever the two phases coexist, it is the superconducting state that has the lowest free energy. The pure excitonic solution becomes a true minimum of F only when the superconducting solution disappears.

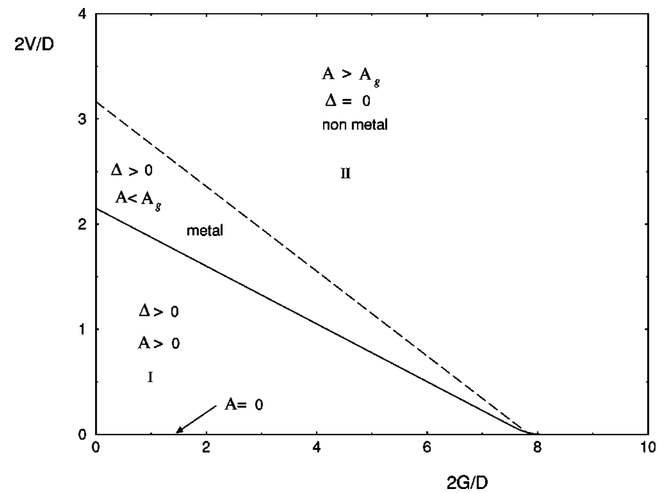

FIG. 1. Ground-state phase diagram for $U/D=0.25$ and $\alpha=0.1$. Below the thick line there is coexistence of superconductivity and excitons. In the boundary of the coexistence region the normal state is metallic, and becomes nonmetallic for the region above the dashed line (in units of half bandwidth of the narrow band).

Figure 1 shows the ground-state phase diagram for $U/D=0.25$ and $\alpha=0.1$, where a square band model is used for the f and d bands. For small and intermediate values of V and G, the ground-state solution is the coexistent phase of superconductivity and excitons (region I of the phase diagram). For sufficiently large values of V and G, the superconducting order parameter vanishes (region II). For each value of G, there is a critical value of the hybridization V_c at which superconductivity is suppressed. For values of G larger than a critical value G_c ($G>G_c$), the critical value V_c is zero. On the other hand, for any finite value of V, A is nonzero. This result is expected due to the fact that a k independent, local hybridization V acts as the conjugate field of the excitonic order parameter.[12] However, as V is reduced, the value of the excitonic correlation parameter is reduced and vanishes as $V\to0$ within the coexistence region (region I). This means that there is no coexistence of excitons and superconductivity for zero hybridization. This is caused by the competition between superconductivity and excitonic pairing, and it is in contrast with what occurs in the nonsuperconducting excitonic state solution (region II), for which the value of A approaches a nonvanishing value as V goes to zero. A very similar result was recently obtained by Czycholl[13] in a study of the competition between excitonic correlation and charge ordering in the Falicov-Kimball model, which becomes exact at $V=0$.

For the Anderson model, i.e., in which the case the f band is localized ($\epsilon_k'=0$), we can get an analytical expression that determines the critical value of the effective hybridization $\tilde{V}_c$ at zero temperature. For this purpose, we set $\Delta=0$ in Eqs. (5) and (6) and integrate the resulting expressions with a square density of states model for the d band. This gives the

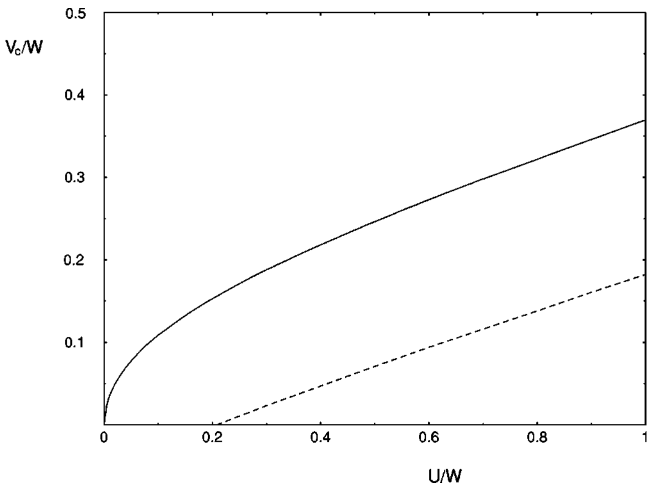

FIG. 2. The critical value of the hybridization V_c to suppress superconductivity for different values of the interband Coulomb repulsion G, for the case in which the f electrons are localized (Anderson model). The curves correspond to $G/W=0$ (solid line) and $G/W=0.4$ (dashed line). In the presence of the f-d repulsion G, the critical value V_c is zero for values of U less than a value U_{max}, which increases as G is increased.

following equations that determine $\tilde{V}_c$ and A_c:

$$1=\frac{U}{2\tilde{V}_c}\sqrt{1+\left(\frac{W}{4\tilde{V}_c}\right)^2}-\frac{U}{W}\sinh^{-1}\left(\frac{W}{4\tilde{V}_c}\right), \qquad (8)$$

$$A_c=\frac{2\tilde{V}_c}{W}\sinh^{-1}\left(\frac{W}{4\tilde{V}_c}\right), \qquad (9)$$

where A_c denotes the critical value of A for the value $\tilde{V}_c$ $[A_c=A(\tilde{V}_c,\Delta=0)]$. Using the definition of $\tilde{V}$ and Eqs. (8) and (9), we can obtain the value of V_c for a given G.

From Eq. (9) we also get the critical value of the Coulomb interband repulsion to suppress superconductivity for zero hybridization

$$G_c=\frac{W}{2}\frac{1}{\sinh^{-1}\left(\frac{W}{4\tilde{V}_c}\right)}, \qquad (10)$$

where the value of $\tilde{V}_c$ is determined by Eq. (8). In Fig. 2 we plot the results of V_c given by Eqs. (8) and (9) as a function of U/W.

We have constructed the phase diagram for the general two-band model for different values of U and α. Figures 3 and 4 show the phase diagram for $U/D=2.5$, with $\alpha=0.1$ $(U/W=0.25)$ and $\alpha=0.5(U/W=1.25)$, respectively.

In the shaded region there are three solutions for the self-consistency Eqs. (5) and (6), but one of them is an unstable solution (Figs. 4 and 5). If V or G are increased in this region, there is a first-order transition from the coexistent phase $(\Delta>0, A>0)$ to the normal excitonic phase $(A>0, \Delta=0)$. For sufficiently large values of G, the excitonic-state solution minimizes the free energy and the ground state is normal.

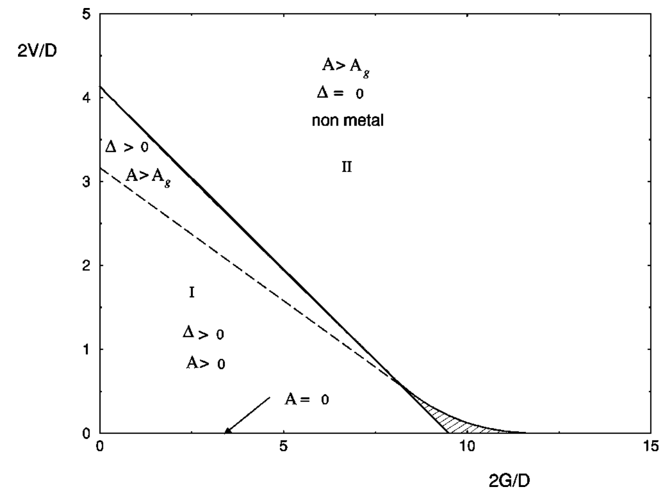

FIG. 3. Phase diagram for $U/D=2.5$ and $\alpha=0.1$ $(U/W=0.25)$. In the shaded area, there are two solutions that locally minimize the free energy and there is a first-order transition when the parameters V and G are varied.

For values of α other than those considered in Figs. 3 and 4, the phase diagram is very similar, with different critical values of V and G. In both cases of Figs. 3 and 4, the normal state is nonmetallic because $\tilde{V}>\tilde{V}_g$ at the critical line.

The shaded region (hysteresis region) is mostly reduced for weak U (Fig. 1), but it is still present. This supports the fact that the discontinuous transitions are not an artifact of Hartree-Fock approximations since they exist for small U where this approximation is expected to be valid. However, the results shown in Figs. 3–6 must be viewed as only qualitatively correct, because of the poor description given by the Hartree-Fock decoupling for large values of the interaction.

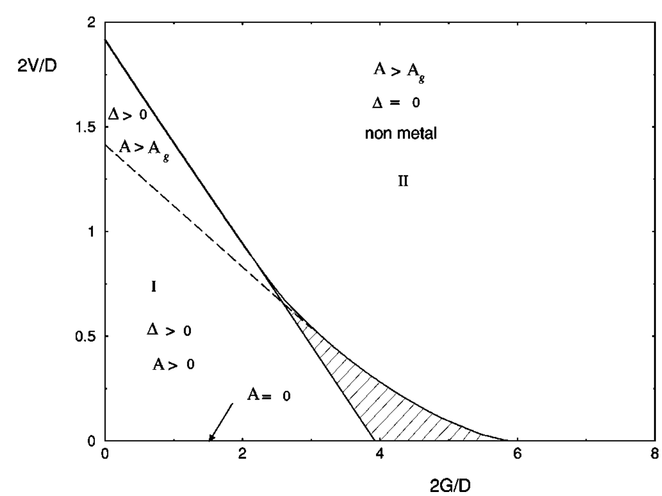

FIG. 4. Ground-state phase diagram for $U/D=2.5$ and $\alpha=0.5$ $(U/W=1.25)$. Comparison with the phase diagram of Fig. 1 shows that the critical values of V/D and G/D increase for larger values of $1/\alpha$. Note that, in both cases, the normal state is nonmetallic.

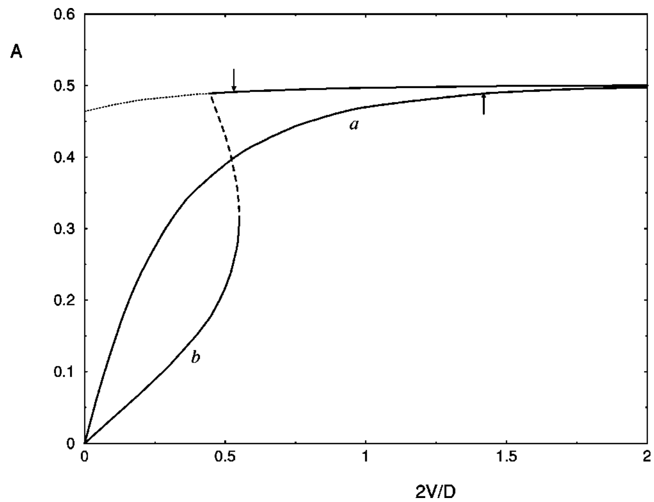

FIG. 5. Excitonic order parameter A as a function of the hybridization for (a) $G=1$, (b) $G=3$. The dashed line denotes the unstable solution and the arrows denote the values of V at which superconductivity disappears. This occurs continuously for (a) and discontinuously for (b). In the last case, the arrow indicates the point at which the excitonic state becomes energetically favorable. The dotted line denotes the solution $(A>0,\Delta=0)$ for the region in which it is unstable.

We now consider another approach that is more appropriate to deal with the case of strong correlations between electrons. This is the so-called Hubbard-I method,[14] which allows to study the effect of G on superconductivity, for zero hybridization, in the case of large values of this interaction. The Hubbard-I approximation is expected to give reliable results in the strong coupling case in the absence of magnetic ordering.[15] For simplicity, we shall take $\alpha=1$. We also assume that the attractive interaction U can be treated at the mean-field level, as done previously. The Hamiltonian to be considered now is

$$H=\sum_{\langle ij\rangle\sigma} t_{ij}^{f} f_{i\sigma}^{\dagger} f_{j\sigma}+\sum_{\langle ij\rangle\sigma} t_{ij}^{d} d_{i\sigma}^{\dagger} d_{j\sigma}-U\sum_{i} n_{i\uparrow}^{f} n_{i\downarrow}^{f} +G\sum_{i\sigma\sigma'} n_{i\sigma'}^{f} n_{i\sigma}^{d}. \quad (11)$$

Notice that the Hamiltonian above differs from Eq. (1) not only for the fact that hybridization is absent, but also because the interband repulsion G acts between f and d electrons with the same and opposite spins. If a mean-field treatment is applied to Eq. (11) and we neglect magnetic solutions, we obtain results similar to those obtained for Eq. (1), with the difference that now, $\tilde{V}=\sqrt{2}AG$.

The frequency dependent Green's functions obeys the following equations of motion:

$$\omega\langle\langle f_{i\sigma};f_{l\sigma}^{\dagger}\rangle\rangle_{\omega}=\frac{1}{2\pi}\delta_{il}+\sum_{j} t_{ij}^{f}\langle\langle f_{j\sigma};f_{l\sigma}^{\dagger}\rangle\rangle_{\omega} +G\langle\langle n_{i}^{d} f_{i\sigma};f_{l\sigma}^{\dagger}\rangle\rangle_{\omega}-\Delta\langle\langle f_{i-\sigma}^{\dagger};f_{l\sigma}^{\dagger}\rangle\rangle_{\omega}, \quad (12)$$

$$\omega\langle\langle f_{i-\sigma}^{\dagger};f_{l\sigma}^{\dagger}\rangle\rangle_{\omega}=-\sum_{j} t_{ij}^{f}\langle\langle f_{j-\sigma}^{\dagger};f_{l\sigma}^{\dagger}\rangle\rangle_{\omega} -G\langle\langle n_{i}^{d} f_{i-\sigma}^{\dagger};f_{l\sigma}^{\dagger}\rangle\rangle_{\omega}-\Delta\langle\langle f_{i-\sigma};f_{l\sigma}^{\dagger}\rangle\rangle_{\omega}, \quad (13)$$

where $n_{i}^{d}=n_{i\uparrow}^{d}+n_{i\downarrow}^{d}$. We now calculate the equations of motion for the new generated Green's functions $\langle\langle n_{i}^{d} f_{i\sigma};f_{l\sigma}^{\dagger}\rangle\rangle_{\omega}$ and $\langle\langle n_{i}^{d} f_{i-\sigma}^{\dagger};f_{l\sigma}^{\dagger}\rangle\rangle_{\omega}$,

$$(\omega-G)\langle\langle n_{i}^{d} f_{i\sigma};f_{l\sigma}^{\dagger}\rangle\rangle_{\omega}=\frac{1}{2\pi}\langle n^{d}\rangle\delta_{il} +\langle n^{d}\rangle\sum_{j} t_{ij}^{f}\langle\langle f_{j\sigma};f_{l\sigma}^{\dagger}\rangle\rangle_{\omega} -\langle n^{d}\rangle\Delta\langle\langle f_{i-\sigma}^{\dagger};f_{l\sigma}^{\dagger}\rangle\rangle_{\omega}, \quad (14)$$

$$(\omega-G)\langle\langle n_{i}^{d} f_{-i\sigma}^{\dagger};f_{l\sigma}^{\dagger}\rangle\rangle_{\omega}=-\langle n^{d}\rangle\sum_{j} t_{ij}^{f}\langle\langle f_{j-\sigma}^{\dagger};f_{l\sigma}^{\dagger}\rangle\rangle_{\omega} -\langle n^{d}\rangle\Delta\langle\langle f_{i\sigma};f_{l\sigma}^{\dagger}\rangle\rangle_{\omega}. \quad (15)$$

Equation (14) was obtained using the approximation that characterizes the Hubbard-I approach

$$\sum_{j} t_{ij}^{f}\langle\langle[d_{i\sigma'}^{\dagger}d_{j\sigma'}-d_{j\sigma'}^{\dagger}d_{i\sigma'}]f_{i\sigma};f_{l\sigma}^{\dagger}\rangle\rangle\approx 0.$$

A similar term was neglected to obtain Eq. (15). We have also used the decouplings

$$\langle\langle n_{i}^{d} f_{j\sigma};f_{l\sigma}^{\dagger}\rangle\rangle\approx\langle n^{d}\rangle\langle\langle f_{j\sigma};f_{l\sigma}^{\dagger}\rangle\rangle$$

and

$$\langle\langle n_{i}^{d} f_{j-\sigma}^{\dagger};f_{l\sigma}^{\dagger}\rangle\rangle\approx\langle n^{d}\rangle\langle\langle f_{j-\sigma}^{\dagger};f_{l\sigma}^{\dagger}\rangle\rangle.$$

Substituting the equalities (14) and (15) in Eqs. (12) and (13), and going to Fourier space, we get the following set of equations for the regular and anomalous Green's functions:

$$[(\omega-\epsilon_{k})(\omega-G)-\langle n^{d}\rangle G\epsilon_{k}]\langle\langle f_{k\sigma};f_{k\sigma}^{\dagger}\rangle\rangle_{\omega} =\frac{1}{2\pi}[\omega-(1-\langle n^{d}\rangle)G] -\Delta[\omega-(1-\langle n^{d}\rangle)G]\langle\langle f_{-k-\sigma}^{\dagger};f_{k\sigma}^{\dagger}\rangle\rangle_{\omega},$$

$$[(\omega+\epsilon_{k})(\omega+G)-\langle n^{d}\rangle G\epsilon_{k}]\langle\langle f_{-k-\sigma}^{\dagger};f_{k\sigma}^{\dagger}\rangle\rangle_{\omega} =-\Delta[\omega+(1-\langle n^{d}\rangle)G)\langle\langle f_{k\sigma};f_{k\sigma}^{\dagger}\rangle\rangle_{\omega}.$$

Consistently with the previous calculations, we assume half-filled bands, with $\langle n^{d}\rangle=1$ and $\langle n^{f}\rangle=1$. In the following equations, the chemical potential is taken to be zero. This is because the Hubbard-I approximation gives two subbands located at both sides of the zero energy level. Each band can accommodate one electron and, thus, the half-filled condition is consistent with taking $\mu=0$. In this case, we find the following expression for the anomalous propagator

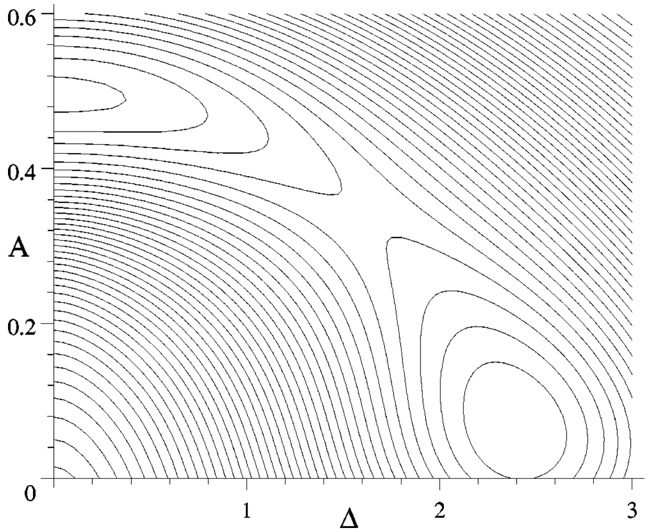

FIG. 6. Contour plot of the free energy for $G=3.8$, $V=0.2$, $\alpha=0.5$, and $U/D=2.5$. There are three stationary points of F, one of them being a saddle point and, thus, an unstable physical solution. The other two are the excitonic and coexistent solutions. Depending on the values of V and G, one or the other is the solution with lowest free energy.

$$\langle\langle f^{\dagger}_{-k-\sigma};f^{\dagger}_{k\sigma}\rangle\rangle_{\omega}=\frac{1}{2\pi}\frac{\Delta}{(\omega+\epsilon_k+G)(\omega-\epsilon_k-G)-\Delta^2}. \tag{16}$$

From which we get the BCS-like equation that determines Δ,

$$\Delta=\frac{1}{N_s}\sum_k \frac{U\Delta}{2\eta_k}\tanh(\beta\eta_k/2), \tag{17}$$

where $\eta_k=\sqrt{(\epsilon_k+G)^2+\Delta^2}$. Integration of Eq. (17) with a constant density of states, yields the critical value G_c for zero temperature

$$G_c=\frac{1}{2}W\left[\tanh\left(\frac{W}{U}\right)\right]^{-1} \tag{18}$$

This result agrees with that derived in the mean-field approximation, in the sense that it confirms that the interband repulsion G may destroy superconductivity even in the absence of hybridization. In the intermediate regime, the results for G_c obtained from the two approximations agree very well. We have calculated the value of G_c [from Eq. (11)] in the mean-field approximation for $\alpha=1$ and $U/W=0.2$, obtaining the value $G_c/W=\frac{1}{2}$, which practically coincides with the value obtained from the relation (18) for the same values of the parameters α,U.

Thus, the two used approximations provide complementary results for the weak and strong coupling cases with a smooth interpolation between them (see Fig. 7).

IV. MIXED VALENCE SUPERCONDUCTORS

We now consider the effect of the superconductivity on the properties of a mixed valence phase. Recently, it was suggested that discontinuous valence transitions may occur in a weak coupling superconductor described by an Anderson lattice model that includes the Falicov-Kimball term.[10] The question of whether the Falicov-Kimball model gives discontinuous transitions in the f-electron occupation number has been largely discussed (Refs. 7,8 and references therein). It has been shown by Leder,[8] that even in a Hartree-Fock treatment the discontinuous transitions disappear when the renormalization of the hybridization due to A is taken into account. Since in the superconducting state this renormalization is reduced, we could expect that discontinuous transitions could appear.

We have calculated the value of n_f as a function of the energy level of the f band, which is assumed to be localized ($\epsilon_k=\epsilon_0$), going away from the symmetric case. From Eq. (4) we obtain that

$$n_f=\frac{1}{N_s}\sum_k 1-\frac{1}{(E_{1k}^2-E_{2k}^2)}\left[\frac{1}{E_{1k}}[E_{1k}^2\epsilon_f-\zeta_k(\epsilon_f\zeta_k' -\tilde{V}^2)]\tanh(\beta E_{1k}/2)-\frac{1}{E_{2k}}[E_{2k}^2\epsilon_f-\zeta_k'(\epsilon_f\zeta_k' -\tilde{V}^2)]\tanh(\beta E_{2k}/2],\right. \tag{19}$$

where $\epsilon_f=\epsilon_0-U/2$ and ζ_k' was defined previously. This must be solved together with Eqs. (5) and (6) and the condition $n^f+n^d=2$, which fixes the chemical potential. From the Green's functions of the f and d electrons we obtain that this condition may be written in the form

$$\sum_k \frac{1}{(E_{1k}^2-E_{2k}^2)}\left[\frac{1}{E_{1k}}[E_{1k}^2(\epsilon_f+\zeta_k')-\Delta^2\zeta'-(\zeta_k'+\epsilon_f)(\epsilon_f\zeta_k' -\tilde{V}^2)]\tanh(\beta E_{1k}/2)-\frac{1}{E_{2k}}[E_{2k}^2(\epsilon_f+\zeta_k')-\Delta^2\zeta' -(\zeta_k'+\epsilon_f)(\epsilon_f\zeta_k'-\tilde{V}^2)]\tanh(\beta E_{2k}/2)\right]=0. \tag{20}$$

Figure 8 shows the value of n_f as a function of ϵ_f. We have not obtained discontinuous transitions for nonvanishing hybridization. While the value of $\tilde{V}$ is reduced by superconductivity, this reduction is not sufficient to allow for discontinuous changes in n_f. The figure corresponds to the values $U/W=0.05, V/W=0.025$ for $G/W=0.125$ and $G/W=0.2$. For these values of U and V, superconductivity is destroyed for $G/W>G_c/W=0.179$ [as can be checked from Eqs. (8) and (10)]. It cannot be excluded that discontinuous valence transitions may occur for strong values of U, but this is probably nonrealistic for mixed-valent compounds.[16]

V. THE EXCITONIC PAIRING MECHANISM

Up to now we have assumed that the pairing potential U is independent of the excitonic correlation. However, the results can be modified if U is an intrinsic function of the parameter A. As mentioned previously, a pairing mechanism based on excitons was proposed to explain superconductivity

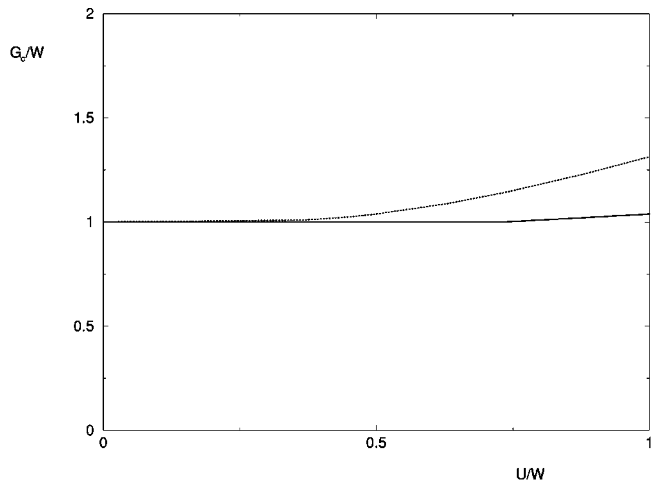

FIG. 7. The critical value G_c/W as a function of U/W obtained in the mean-field (solid curve) and Hubbard-I (dashed curve) approximations, with $\alpha=1$.

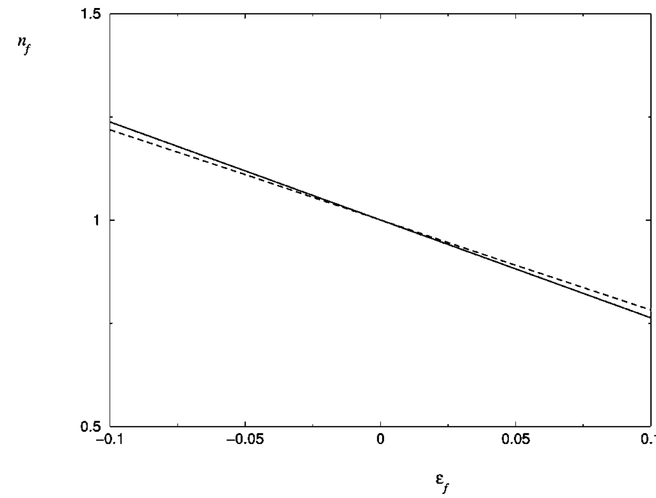

FIG. 8. Average number of f electrons n_f as a function of ϵ_f, for $U=0.1$, $V=0.05$, and $G=0.25$ (solid line, superconducting state), $G=0.4$ (dashed line, normal state).

in HTSC. Several works have suggested this as a plausible source of electron pairing.[17–19] We now compare our results with those found in these previous works. In the region in which we have obtained a coexistence between superconductivity and excitonic correlation, a pairing mechanism based on excitons is suitable. In fact as shown in Refs. 17–19, close to regions of charge-transfer instabilities as well as phase separation, superconductivity may appear by taking advantage of collective charge-transfer excitations as a source of pairing. Notice, however, that as we go away from these regions of instability, as in the case $V\rightarrow 0$, such that A tends to zero, this mechanism cannot hold. Since a finite value of V is required, and large values of V act in detriment to superconductivity, there is a range of intermediate values of V for which pairing is optimized and T_c will have a maximum in this range.[20]

In Refs. 18,19 it was shown that a minimum value of G is required to make negative the binding energy of electrons pairs. Particularly, in Ref. 19 it was shown that the binding energy approaches a constant value as $G\rightarrow\infty$, which makes appropriate our approximation of constant U. In this approximation, our results show that G acts in detriment to superconductivity, and, as a consequence, similarly to what occurs for V, there is an intermediate value of G for which the pairing is optimized. This means that there are optimum values of V and G, for which superconductivity is mostly favored. An experimental consequence of this is to give rise to negative or positive values of dT_c/dP. When pressure P is applied, the hybridization and Coulomb repulsion will be renormalized causing an increment or decrement of T_c, if the values V and G are approached or departed from the optimal values. This also shows that high values of T_c require *fine tuning* of these parameters.

We now consider briefly the effect of finite temperature in the different regions of the phase diagram. In the superconducting region (excluding the shaded area) as T is increased, Δ diminishes and becomes zero continuously. In the region where $A>A_g\equiv(\tilde{V}_g-V)/G$ (which means that $\tilde{V}>\tilde{V}_g$), the system goes to a nonmetallic state when T reaches the critical temperature T_c at which superconductivity disappears. If temperature is further increased, there is a metal-nonmetal transition associated with the vanishing of the hybridization gap. This transition will be studied elsewhere, where its possible relevance for high-T_c superconductor cuprates will be considered.

VI. CONCLUSIONS

In summary, we have constructed the ground-state phase diagram for the model (1), showing the regions of parameter space for the pure superconducting, coexistent, and normal states. For each value of G, there is a critical value of the hybridization for destroying superconductivity, which decreases as G increases. This critical value becomes zero ($V_c=0$) if G is greater than a critical value G_c.

We have shown that the presence of hybridization is required in order to occur a coexistence between superconductivity and excitonic correlation. For the particular case of vanishing hybridization, $V=0$, these two correlations compete strongly and only one of the two remains finite.

The fact that hybridization acts in detriment of superconductivity is well known and is often used to explain the absence of superconductivity.[21,22] We have shown here the importance of the interband repulsion G to enhance this effect and even to suppress superconductivity solely by itself in systems in which hybridization is negligible. This result was obtained within a self-consistent mean-field and Hubbard-I approximations, which provide a good interpolation for all values of G.

For the particular case in which the mechanism for superconductivity is the excitonic pairing, we have shown that the model gives rise to negative or positive values of dT_c/dP. This is because there are optimum values of the hybridization and the repulsive interaction that maximizes the critical temperature T_c. Pressure application can then approximate or depart the values of V or G of the system from these optimal values.

The effect of superconductivity on valence transitions in weak coupling mixed valence superconductors was considered. We did not find discontinuous valence transitions in the superconducting state. Although the renormalization of the hybridization is smaller in the superconducting state, the influence of this reduction on the shape of the occupation number curve n_f, as a function of ϵ_f, is very small.

We note that the results for the mean-field and Hubbard-I approximations are in agreement in the intermediate coupling case because the excitonic correlation was taken into account. If this were not the case, the results from the two decoupling schemes would be very different, as occurs in valence transitions.[8] We conclude that the interplay between superconductivity and excitonic correlation can be relevant and must be included in an adequate description of superconductivity in a two-band system for any kind of pairing mechanism.

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