Superconductivity in the extended two-dimensional Hubbard model: Strong-coupling regime and hybridization effects

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In this work we have considered a two-dimensional two-band Hubbard model (extended Hubbard model) to study the effect of the nonlocal hybridization $V_{\mathbf{k}}$ on the superconductivity. In the strong-coupling regime and for a d-wave superconducting gap, we have obtained the superconducting critical temperature T_c and the zero-temperature superconducting gap Δ_0 for different hybridizations. We have adopted hopping parameters suitable to describe the high-temperature superconductor materials. The results show that for a fixed value of the hybridization and the intraband d-d attractive potential U, the gap increases for low temperatures and diminishes as the temperatures increase toward T_c. As the hybridization increases both, Δ_0 and T_c, diminish. For each hybridization, the quantity $2\Delta_0/k_BT_c$ increases and saturates in a particular value as U increases. The relation between applied pressure P and hybridization in the strong-coupling regime is also discussed.

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I. INTRODUCTION

The hybridization effects on superconductivity have been discussed in the literature in several works.[1–6] A two-band mechanism for superconductivity was proposed by Suhl *et al.*,[1] and Kondo,[2] and later investigated by several others.[3–7] In particular, in Ref. 5 it was studied the influence of an one-body hybridization on superconductivity in two-band systems through a sp-d model of overlapping bands close to the Fermi level. The physical meaning of the hybridization[5] was to create, in the normal state, new bands with mixed features, while the Hubbard potential U was treated within the Bardeen-Cooper-Schrieffer (BCS) (Ref. 8) theory, i.e., a weak correlation regime.[5]

On the other hand, with the discovery of the high-temperature superconductors (HTSC) (Ref. 9) a lot of new systems have been considered. In particular, the cuprates have been extensively studied,[10] but a great number of questions related to them remain to be answered, e.g., it is observed that the magnetic H-T phase diagram of the HTSC exhibits, in certain cases, an unusual behavior: a positive curvature for the upper critical field $H_{c2}(T)$, with no evidence of saturation at low temperatures.[11] Also, the existence of a pseudogap, i.e., a preformed gap in the density of states at temperatures above the superconducting critical temperature T_c, has been verified by several different experimental techniques[10,12] in many HTSC, but with no agreement on such basic facts as to its nature and origin. It is recognized that the electrons which move in the CuO_2 planes are the most relevant to describe the cuprate superconductivity. In particular, there is no doubt that the d electrons play a fundamental role in the onset of superconductivity:[13,14] as stressed by Beenen and Edwards,[13] much of the experimental evidence in HTSC cuprates leads inevitably to a $d_{x^2-y^2}$ pairing, which is the one considered in the present work. Moreover, a d-p hybridization between d electrons and the O uncorrelated p states should also be considered. Therefore, we adopt throughout this work a two band (p- and d-) Hubbard model, which is often associated with HTSC.[5] The simplest way to discuss strong d-electrons dynamics is the Hubbard-I approximation.[15] So we focus our attention in this work in the interplay between strong d-d attractive U and d-p hybridization V.

We stress that we consider degenerate p bands. Although p_x and p_y hybridize slightly different with the d orbital (i.e., with d-band states) and thus this simplification may miss some features in a quantitative calculation of some thermodynamic properties of high-T_c superconductors, the main point tackled here concerns the interplay of one-body d-p hybridization and d-d superconductivity. Throughout this work, it will be shown that d-p hybridization acts in detriment of d-d superconductivity. For that matter the existence of different p orbital is not specially relevant. Besides, as will be presented in the self-consistent calculation, the microscopic d-p hybridization parameter is related to macroscopic applied pressure and again, for this relation, the existence of different p orbital is not particularly relevant.

We consider a d-wave gap symmetry and the hopping parameters are those known to reproduce well HTSC phase diagrams.[16,17] To develop the calculations we consider a Green's-function method[15,18] in order to calculate the zero-temperature superconducting gap Δ_0 and the superconducting critical temperature T_c, with both, a k-dependent hybridization and a local one (a mean value over the Brillouin zone) which turns out to be constant. The paper is organized as follows: Sec. II presents the model and general formalism leading to the main equations within the Hubbard-I approximation, which is beyond the usual first-order BCS mean-field treatment.[5] In Sec. III the numerical results are presented whereas in Sec. IV the conclusions and final comments are made.

II. MODEL AND GENERAL FORMALISM

In order to study the dynamics of the carriers with correlations and the basic attractive interaction we consider a two-bandlike Hubbard Hamiltonian,

$$H=\sum_{\langle\langle ij\rangle\rangle\sigma} t_{ij}^{d} d_{i\sigma}^{\dagger} d_{j\sigma}+\sum_{\langle\langle ij\rangle\rangle\sigma} t_{ij}^{c} c_{i\sigma}^{\dagger} c_{j\sigma}-U\sum_{\langle ij\rangle\sigma} n_{i,\sigma}^{d} n_{j,-\sigma}^{d} + \sum_{\langle ij\rangle\sigma} V_{ij}(c_{i\sigma}^{\dagger} d_{j\sigma}+d_{i\sigma}^{\dagger} c_{j\sigma}), \tag{1}$$

where $c_{i\sigma}^{\dagger}(c_{i\sigma})$ and $d_{i\sigma}^{\dagger}(d_{i\sigma})$ are the fermionic creation (annihilation) operator at site $\mathbf{r}_i$ for the p and d electrons, respectively, and spin $\sigma=\{\uparrow\downarrow\}$. $n_{i\sigma}^{d}=d_{i\sigma}^{\dagger}d_{i\sigma}$ is the density operator, t_{ij}^{d} and t_{ij}^{c} are the hopping integrals between sites i and j, nearest neighbors and next-nearest neighbors, for the d and p electrons. U is the attractive potential between the d electrons, which can result from the elimination of the electron-phonon coupling through a canonical transformation or, as suggested by Hirsch and Scalapino,[19] it may be provided by the competition between on-site and nearest-neighbor sites Coulomb interaction for some range of parameters. V_{ij} is the nearest-neighbors hybridization of the p and d bands, which may be k dependent, arising from a nonlocal character of the mixing. If one considers the special case of a local hybridization, the hybridization becomes constant ($V_{\mathbf{k}}$ representing an average over the Brillouin zone).

As mentioned in Sec. I, the physical meaning of one-body hybridization is to create in the normal-state new bands with mixed features, as pointed out in Ref. 5. The Hamiltonian [Eq. (1)] is used to consider the formation of the d-d Cooper pairs and to obtain the self-consistent equations for the calculation of both, the critical temperature T_c and superconducting gap Δ_0, as a function of attractive potential U and the hybridization $V_{\mathbf{k}}$. It should be noticed that in our case of mixed bands, we maintain the hybridization parameter, since external pressure can be associated to it, causing a rearrangement of the mixed states, and therefore we can discuss the effect of pressure on T_c, Δ_0, and other thermodynamical quantities. Also, in this work we assume that the main contribution for the density of states at the Fermi level E_F is due to the d electrons, and therefore we consider the d-d pairs as being the most relevant for superconductivity. Clearly, we could have also taken into account a p-d interband attractive G (described by $G\Sigma_{\langle ij\rangle\sigma} n_{i,\sigma}^{d} n_{j,-\sigma}^{d}$, $G<0$) thus obtaining also p-d pairs. However, it has been shown by Continentino and Padilha[20] that quite generally, interband pairing leads to normal first-order phase transitions, which is not the case involving the systems we are describing throughout this work.

To obtain the superconductor order parameter, we apply the Green's-function method[15,18] to calculate the equations of motion of the propagator $\langle\langle d_{i\sigma};d_{l\sigma}^{\dagger}\rangle\rangle_{\omega}$ and $\langle\langle d_{i,-\sigma}^{\dagger};d_{l\sigma}^{\dagger}\rangle\rangle_{\omega}$. Therefore, in the site (Wannier) representation

$$\omega\langle\langle d_{i\sigma};d_{l\sigma}^{\dagger}\rangle\rangle_{\omega}=\frac{i}{2\pi}\delta_{il}+\sum_{j} t_{ij}^{d}\langle\langle d_{j\sigma};d_{l\sigma}^{\dagger}\rangle\rangle_{\omega} - 2U\sum_{j}\langle\langle n_{j,-\sigma}^{d} d_{i\sigma};d_{l\sigma}^{\dagger}\rangle\rangle_{\omega}+\sum_{j} V_{ij}\langle\langle c_{j\sigma};d_{l\sigma}^{\dagger}\rangle\rangle_{\omega}, \tag{2}$$

$$\omega\langle\langle d_{i,-\sigma}^{\dagger};d_{l\sigma}^{\dagger}\rangle\rangle_{\omega}=-\sum_{j} t_{ij}^{d}\langle\langle d_{j,-\sigma}^{\dagger};d_{l\sigma}^{\dagger}\rangle\rangle_{\omega} + 2U\sum_{j}\langle\langle n_{j,\sigma}^{d} d_{i,-\sigma}^{\dagger};d_{l\sigma}^{\dagger}\rangle\rangle_{\omega} - \sum_{j} V_{ij}\langle\langle c_{j,-\sigma}^{\dagger};d_{l\sigma}^{\dagger}\rangle\rangle_{\omega}. \tag{3}$$

From the hybridization term we have

$$\omega\langle\langle c_{i\sigma};d_{l\sigma}^{\dagger}\rangle\rangle_{\omega}=\sum_{j} t_{ij}^{c}\langle\langle c_{j\sigma};d_{l\sigma}^{\dagger}\rangle\rangle_{\omega}+\sum_{j} V_{ij}\langle\langle d_{j\sigma};d_{l\sigma}^{\dagger}\rangle\rangle_{\omega}, \tag{4}$$

$$\omega\langle\langle c_{i,-\sigma}^{\dagger};d_{l\sigma}^{\dagger}\rangle\rangle_{\omega}=-\sum_{j} t_{ij}^{c}\langle\langle c_{j,-\sigma}^{\dagger};d_{l\sigma}^{\dagger}\rangle\rangle_{\omega}-\sum_{j} V_{ij}\langle\langle d_{j,-\sigma}^{\dagger};d_{l\sigma}^{\dagger}\rangle\rangle_{\omega}. \tag{5}$$

Now, following the Hubbard-I approach,[15] we calculate again the equations of motion of new generated terms $\langle\langle n_{j,-\sigma}^{d} d_{i\sigma};d_{l\sigma}^{\dagger}\rangle\rangle_{\omega}$ and $\langle\langle n_{j,\sigma}^{d} d_{i,-\sigma}^{\dagger};d_{l\sigma}^{\dagger}\rangle\rangle_{\omega}$. Therefore,

$$\begin{aligned}\omega\langle\langle n_{j,-\sigma}^{d} d_{i\sigma};d_{l\sigma}^{\dagger}\rangle\rangle_{\omega}&=\frac{i}{2\pi}\langle n_{j,-\sigma}^{d}\rangle\delta_{il}+\langle n_{j,-\sigma}^{d}\rangle\sum_{m} t_{im}^{d}\langle\langle d_{m\sigma};d_{l\sigma}^{\dagger}\rangle\rangle_{\omega}\\&+\langle n_{j,-\sigma}^{d}\rangle\sum_{m} V_{im}\langle\langle c_{m\sigma};d_{l\sigma}^{\dagger}\rangle\rangle_{\omega}\\&-\frac{\Delta_{ij}}{U}\sum_{m} V_{jm}\langle\langle c_{m,-\sigma}^{\dagger};d_{l\sigma}^{\dagger}\rangle\rangle_{\omega}\\&-2U\sum_{m}\langle\langle n_{j,-\sigma}^{d} n_{m,-\sigma}^{d} d_{i\sigma};d_{l\sigma}^{\dagger}\rangle\rangle_{\omega},\end{aligned} \tag{6}$$

$$\begin{aligned}\omega\langle\langle n_{j\sigma}^{d} d_{i,-\sigma}^{\dagger};d_{l\sigma}^{\dagger}\rangle\rangle_{\omega}&=-\frac{i}{2pi}\langle d_{j\sigma}^{\dagger} d_{i,-\sigma}^{\dagger}\rangle\delta_{jl}\\&-\langle n_{j\sigma}^{d}\rangle\sum_{m} t_{im}^{d}\langle\langle d_{m,-\sigma}^{\dagger};d_{l\sigma}^{\dagger}\rangle\rangle_{\omega}\\&-\langle n_{j\sigma}^{d}\rangle\sum_{m} V_{im}\langle\langle c_{m,-\sigma}^{\dagger};d_{l\sigma}^{\dagger}\rangle\rangle_{\omega}\\&-\frac{\Delta_{ij}}{U}\sum_{m} V_{jm}\langle\langle c_{m\sigma};d_{l\sigma}^{\dagger}\rangle\rangle_{\omega}\\&+2U\sum_{m}\langle\langle n_{j\sigma}^{d} n_{m\sigma}^{d} d_{i,-\sigma}^{\dagger};d_{l\sigma}^{\dagger}\rangle\rangle_{\omega},\end{aligned} \tag{7}$$

where $\Delta_{ij}=U\langle d_{i\sigma}^{\dagger} d_{j,-\sigma}^{\dagger}\rangle$, and we have considered the mean-field decoupling

$$\langle\langle n_{j\sigma}^{d} d_{i,-\sigma}^{\dagger};d_{l\sigma}^{\dagger}\rangle\rangle_{\omega}\approx\langle n_{j\sigma}^{d}\rangle\langle\langle d_{i,-\sigma}^{\dagger};d_{l\sigma}^{\dagger}\rangle\rangle_{\omega} \tag{8}$$

with similar equations for the operators c and $c^{\dagger}$. We have also applied the Hubbard-I approximation,[15]

$$\sum_{m} t_{jm}^{d}\langle\langle [d_{j\sigma}^{\dagger} d_{m\sigma}-d_{m\sigma}^{\dagger} d_{j,\sigma}] d_{i,-\sigma}^{\dagger};d_{l\sigma}^{\dagger}\rangle\rangle_{\omega}\approx 0. \tag{9}$$

Performing the sum in "j" in Eqs. (6) and (7), and considering the decoupling

$$2U\sum_{jm}\langle\langle n^d_{j,-\sigma}n^d_{m,-\sigma}d_{i\sigma};d^\dagger_{l\sigma}\rangle\rangle_\omega \approx \tilde{U}\sum_j\langle\langle n^d_{j,-\sigma}d_{i\sigma};d^\dagger_{l\sigma}\rangle\rangle_\omega + 2\langle n^d\rangle\sum_j \Delta_{ji}\langle\langle d^\dagger_{j,-\sigma};d^\dagger_{l\sigma}\rangle\rangle_\omega \tag{10}$$

with $\Sigma_m\langle n^d_{m\sigma}\rangle=\langle n^d_\sigma\rangle=\langle n^d\rangle$ and $\tilde{U}=2U\langle n^d\rangle$, one obtains, by the substitution of the resulting equations in Eqs. (2) and (3), the equations for the propagator in the Fourier space,

$$\left[\omega-\left(1-\frac{\tilde{U}}{\omega+\tilde{U}}\right)\left(\epsilon_{d\mathbf{k}}+\frac{V_\mathbf{k}^2}{\omega-\epsilon_{c\mathbf{k}}}\right)\right]\langle\langle d_{\mathbf{k}\sigma};d^\dagger_{\mathbf{k}\sigma}\rangle\rangle_\omega = \frac{i}{2\pi}\left[1-\frac{\tilde{U}}{\omega+\tilde{U}}\right] + \frac{2}{\omega+\tilde{U}}\left[\tilde{U}-\frac{V_\mathbf{k}^2}{\omega+\epsilon_{c\mathbf{k}}}\right]\Delta_\mathbf{k}\langle\langle d^\dagger_{-\mathbf{k},-\sigma};d^\dagger_{\mathbf{k}\sigma}\rangle\rangle_\omega, \tag{11}$$

$$\left[\omega+\left(1+\frac{\tilde{U}}{\omega-\tilde{U}}\right)\left(\epsilon_{d\mathbf{k}}-\frac{V_\mathbf{k}^2}{\omega+\epsilon_{c\mathbf{k}}}\right)\right]\langle\langle d^\dagger_{-\mathbf{k},-\sigma};d^\dagger_{\mathbf{k}\sigma}\rangle\rangle_\omega = -\frac{i}{\pi}\frac{\Delta_\mathbf{k}}{\omega-\tilde{U}} - \frac{2}{\omega-\tilde{U}}\left[\tilde{U}+\frac{V_\mathbf{k}^2}{\omega-\epsilon_{c\mathbf{k}}}\right]\Delta_\mathbf{k}\langle\langle d_{\mathbf{k}\sigma};d^\dagger_{\mathbf{k}\sigma}\rangle\rangle_\omega. \tag{12}$$

In Eqs. (11) and (12) the superconducting gap is given by

$$\Delta_\mathbf{k}=\sum_\delta e^{i\delta\mathbf{k}}\Delta_\delta \tag{13}$$

with $\delta=\pm a\hat{\mathbf{x}}, \pm a\hat{\mathbf{y}}$ the vector which connects site i to its nearest-neighbor j in a two-dimensional lattice, with $\mathbf{r}_j=\mathbf{r}_i+\delta$ and a is the lattice parameter. Here, $\Delta_{ij}=\Delta_\delta$ for translational invariance. Equation (13) can account for a superconducting gap in an extended-s-wave symmetry ($|\Delta_{\hat{\mathbf{x}}}|=|\Delta_{\hat{\mathbf{y}}}|$), a d-wave symmetry ($|\Delta_{\hat{\mathbf{x}}}|=-|\Delta_{\hat{\mathbf{y}}}|$), as well as a mixed s-d ($|\Delta_{\hat{\mathbf{x}}}|\neq|\Delta_{\hat{\mathbf{y}}}|$) one.[21] In the d-wave channel Eq. (13) is given by[21]

$$\Delta_\mathbf{k}=2\Delta^{max}|\cos(k_x)-\cos(k_y)|, \tag{14}$$

where $\Delta^{max}=\Delta$ is the maximum gap amplitude and it is independent of momentum, and $a=1$. In the same way, the k-dependent hybridization is given by

$$V_\mathbf{k}=\sum_\delta e^{i\delta\mathbf{k}}V_\delta. \tag{15}$$

For nearest neighbors, and considering the same magnitude of hybridization in both $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ directions, Eq. (15) becomes

$$V_\mathbf{k}=2V[\cos(k_x)+\cos(k_y)]. \tag{16}$$

In this work calculations with constant hybridizations ($V_\mathbf{k}=V$) were also made in the same way as in Ref. 5.

From Eqs. (11) and (12) we find the following expression for the anomalous propagator:

$$\langle\langle d^\dagger_{-\mathbf{k},-\sigma};d^\dagger_{\mathbf{k}\sigma}\rangle\rangle_\omega = -\frac{i}{\pi}\Delta_\mathbf{k}\omega(\omega+\epsilon_{c\mathbf{k}}) \times(\omega-E'_{1\mathbf{k}})(\omega-E'_{2\mathbf{k}})P(\omega)^{-1}, \tag{17}$$

where

$$E'_{1,2\mathbf{k}}=-\frac{\tilde{\epsilon}_\mathbf{k}+\tilde{U}}{2}\pm\frac{\sqrt{(\tilde{\epsilon}_\mathbf{k}+\tilde{U})^2+4\zeta_\mathbf{k}}}{2}, \tag{18}$$

$$\zeta_\mathbf{k}=2\tilde{U}\epsilon_{c\mathbf{k}}-\epsilon_{c\mathbf{k}}\epsilon_{d\mathbf{k}}, \tag{19}$$

$$\tilde{\epsilon}_\mathbf{k}=\tilde{U}-(\epsilon_{c\mathbf{k}}+\epsilon_{d\mathbf{k}}), \tag{20}$$

and

$$P(\omega)=\omega^6+A_\mathbf{k}\omega^4+B_\mathbf{k}\omega^2+C_\mathbf{k} \tag{21}$$

with

$$A_\mathbf{k}=2\tilde{V}_\mathbf{k}-\tilde{\epsilon}_\mathbf{k}^2, \tag{22}$$

$$B_\mathbf{k}=\tilde{V}_\mathbf{k}^2+4\Delta_\mathbf{k}^2\tilde{U}^2, \tag{23}$$

$$C_\mathbf{k}=4\Delta_\mathbf{k}^2[2\tilde{U}V_\mathbf{k}^2\epsilon_{c\mathbf{k}}-(\tilde{U}^2\epsilon_{c\mathbf{k}}^2+V_\mathbf{k}^4)], \tag{24}$$

and

$$\tilde{V}_\mathbf{k}=\epsilon_{c\mathbf{k}}\epsilon_{d\mathbf{k}}-V_\mathbf{k}^2-\tilde{U}\epsilon_{c\mathbf{k}}. \tag{25}$$

The roots of the polynomial $P(\omega)$ determine the excitation energies of the system

$$E_{1\mathbf{k}}=\sqrt{-\frac{A_\mathbf{k}}{3}+2\sqrt{\frac{|p_\mathbf{k}|}{3}}\cos\frac{\phi_\mathbf{k}}{3}}, \tag{26}$$

$$E_{2,3\mathbf{k}}=\sqrt{-\frac{A_\mathbf{k}}{3}-2\sqrt{\frac{|p_\mathbf{k}|}{3}}\cos\frac{\phi_\mathbf{k}\pm\pi}{3}} \tag{27}$$

with

$$\cos\phi_\mathbf{k}=-\frac{q_\mathbf{k}}{2\sqrt{(|p_\mathbf{k}|/3)^3}}, \tag{28}$$

$$p_\mathbf{k}=\frac{3B_\mathbf{k}-A_\mathbf{k}^2}{3}, \tag{29}$$

$$q_\mathbf{k}=C_\mathbf{k}+\frac{2A_\mathbf{k}^3}{27}-\frac{A_\mathbf{k}B_\mathbf{k}}{3}. \tag{30}$$

We now consider the Zubarev method[18] which relates the propagator $\langle\langle d^\dagger_{-\mathbf{k},-\sigma};d^\dagger_{\mathbf{k}\sigma}\rangle\rangle_\omega$ with the thermal average $\langle d^\dagger_{\mathbf{k},\sigma}d^\dagger_{-\mathbf{k},-\sigma}\rangle$, which defines the superconducting gap in the momentum space ($\Delta_\mathbf{k}=U\langle d^\dagger_{\mathbf{k},\sigma}d^\dagger_{-\mathbf{k},-\sigma}\rangle$). Therefore,

$$\langle d^\dagger_{\mathbf{k},\sigma}d^\dagger_{-\mathbf{k},-\sigma}\rangle=\lim_{\delta\to 0}\int_{-\infty}^{+\infty}\frac{d\omega}{1+e^{\beta\omega}}\times[\langle\langle d^\dagger_{-\mathbf{k},-\sigma};d^\dagger_{\mathbf{k}\sigma}\rangle\rangle_{\omega+i\delta} - \langle\langle d^\dagger_{-\mathbf{k},-\sigma};d^\dagger_{\mathbf{k}\sigma}\rangle\rangle_{\omega-i\delta}], \tag{31}$$

where $\beta=1/k_BT$ (k_B is the Boltzmann constant). From Eq.

(31) one obtains the self-consistent temperature-dependent gap equation within a d-wave symmetry,

$$\Delta = \frac{1}{N}\sum_{\mathbf{k}} \Delta_{\mathbf{k}} = \frac{1}{N}\sum_{\mathbf{k}} U\langle d^{\dagger}_{\mathbf{k},\sigma} d^{\dagger}_{-\mathbf{k},-\sigma}\rangle$$
$$= \frac{1}{N}2U\sum_{k}\sum_{i=1}^{3}\Delta\gamma_{\mathbf{k}}2E_{i\mathbf{k}}\frac{\Xi_{i\mathbf{k}}}{S_{i\mathbf{k}}}[F_{i\mathbf{k}} + G_{i\mathbf{k}}\tanh(\beta E_{i\mathbf{k}}/2)], \tag{32}$$

where N is the number of sites in the lattice and

$$\Xi_{1\mathbf{k}} = \frac{S_{1\mathbf{k}}}{2E_{1\mathbf{k}}(E^2_{1\mathbf{k}} - E^2_{2\mathbf{k}})(E^2_{1\mathbf{k}} - E^2_{3\mathbf{k}})}, \tag{33}$$

$$\Xi_{2\mathbf{k}} = \frac{S_{2\mathbf{k}}}{2E_{2\mathbf{k}}(E^2_{2\mathbf{k}} - E^2_{1\mathbf{k}})(E^2_{2\mathbf{k}} - E^2_{3\mathbf{k}})}, \tag{34}$$

$$\Xi_{3\mathbf{k}} = \frac{S_{3\mathbf{k}}}{2E_{3\mathbf{k}}(E^2_{3\mathbf{k}} - E^2_{1\mathbf{k}})(E^2_{3\mathbf{k}} - E^2_{2\mathbf{k}})} \tag{35}$$

with

$$\gamma_{\mathbf{k}} = |\cos(k_x) - \cos(k_y)| \tag{36}$$

for the d-wave channel. Also,

$$F_{i\mathbf{k}} = E^2_{i\mathbf{k}}[E'_{1\mathbf{k}} + E'_{2\mathbf{k}} - \epsilon_{c\mathbf{k}}] - \epsilon_{c\mathbf{k}}E'_{1\mathbf{k}}E'_{2\mathbf{k}}, \tag{37}$$

$$G_{i\mathbf{k}} = E_{i\mathbf{k}}[E^2_{i\mathbf{k}} - \epsilon_{c\mathbf{k}}[E'_{1\mathbf{k}} + E'_{2\mathbf{k}}] + E'_{1\mathbf{k}}E'_{2\mathbf{k}}]. \tag{38}$$

To obtain Δ_0 and T_c for a specific value of U and V, Eq. (32) is solved self-consistently in the first Brillouin zone of a square lattice, together with the dispersion relation

$$\epsilon_{c\mathbf{k}} = -2t[\cos(k_x) + \cos(k_y)] + 4t_2\cos(k_x)\cos(k_y) + \epsilon_0. \tag{39}$$

Here, t is the hopping integral for the nearest neighbors and t_2 the hopping integral for the next-nearest neighbors. ϵ_0 is an adjustable parameter. Also, we may introduce now the homothetic relation concerning the dispersion relation for c and d electrons,[22,23]

$$\epsilon_{d\mathbf{k}} = \alpha\epsilon_{c\mathbf{k}}, \tag{40}$$

where α is a phenomenological parameter less than unity and plays a role of an effective-mass relation between c and d electrons. In this work we will take bands $\epsilon_{c\mathbf{k}}$ and $\epsilon_{d\mathbf{k}}$ to be centered at the Fermi level (the symmetric case), which corresponds to take the chemical potential μ equal to zero.[5] In the next section we show the results of our calculations.

III. NUMERICAL RESULTS

The results shown in this work are all for half-filled bands with $\langle n^d\rangle = \langle n^c\rangle = 1.0$. In Fig. 1 we plot the gap curves for three different values of the constant α: 0.10, 0.15, and 0.20. In all curves the nearest-neighbor hopping integral t was taken as the energy unity. The attractive potential applied was $U=8.0t$ (strong-coupling limit) and hybridization strength $V=1.4t$. The next-nearest-neighbor hopping integral was $t_2=0.55t$, which is a value known to reproduce well the HTSC phase diagrams.[17,24,25] These results of Fig. 1 are for a k-dependent hybridization. We have observed the same behavior for constant hybridization ($V_{\mathbf{k}}=V$).

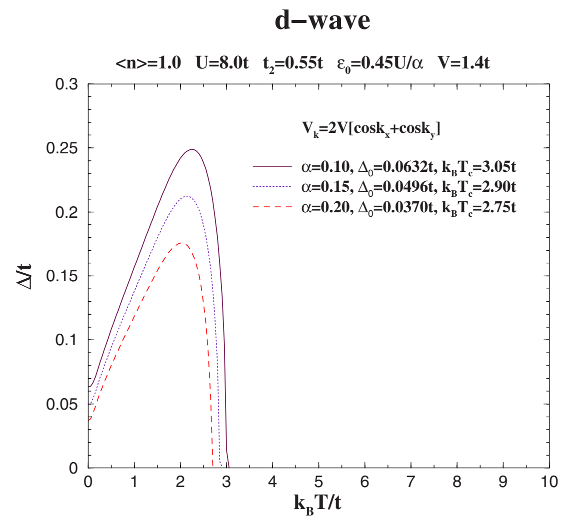

FIG. 1. (Color online) The gap curves for three different values of the constant α: 0.10, 0.15, and 0.20. We see that, as α increases both, Δ_0 and T_c, diminish.

From Fig. 1 we see that as α increases both Δ_0 and T_c diminish. Also, we observe for low temperatures the gap raises and, by further increasing T, the gap begins to shrink due to the destruction of superconductivity, until it entirely vanishes at a certain value, which we define as the superconducting critical temperature T_c. This is an unexpected result and is independent of the hybridization since we have a gap for $V_{\mathbf{k}}=0$ [see Eqs. (30) and (31)]. This behavior is a direct consequence of the Hubbard-I approximation employed in the correlation U term. A similar behavior was obtained recently by Aryanpour *et al.*:[26] they have considered a negative-U Hubbard model approach with real-space Bogoliubov-de Gennes (BdG) local equations, to obtain the superconducting phase diagram in an inhomogeneous two-dimensional medium. In their analysis they concluded that the anomalous increase in the gap curve was an actual feature and was believed to be related to the gradual destruction of the charge-ordered phase due to temperature, leading to an intermediate superconducting phase. Also, in a earlier work[27] they have employed a Monte Carlo mean-field technique as an independent examination for the validity of their BdG approach and the agreement between the two techniques was clearly confirmed. On the other hand, from experimental results[28] one can observe the same anomalous behavior for the gap curve for an overdoped Bi2212 HTSC sample, obtained from angle-resolved photoemission spectroscopy (ARPES), one of the most experimental direct probes of the electronic structure. Also in Ref. 29 the gap curve exhibits the anomalous behavior on an ARPES study of the electronic structure of the trilayer HTSC Bi2223. We should mention that in all the above cited articles,[28,29] the superconducting gaps are all consistent with a d-wave gap symmetry.

In Fig. 2 we can see the effect of changing the hybridization strength V for a k-dependent hybridization. From the

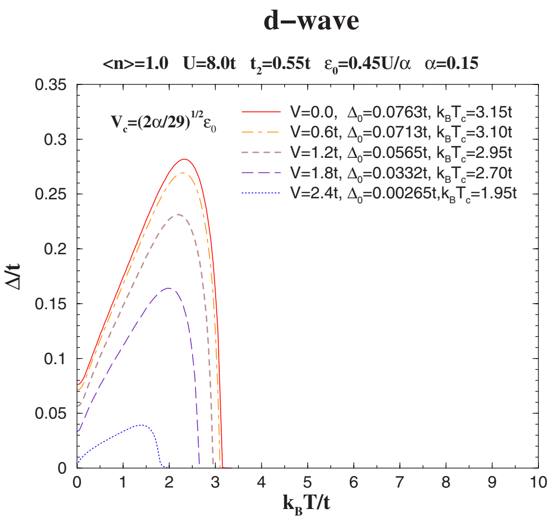

FIG. 2. (Color online) In this figure we can see the effect of changing the hybridization strength V for a k-dependent hybridization. For increasing V, each superconducting gap Δ_0, and critical temperature T_c, diminishes.

figure we observe that as V increases, each superconducting gap Δ_0, and critical temperatures T_c, diminishes, indicating a destruction of the superconductivity of the system. The same behavior is observed for a constant hybridization. The constant α is the same employed in earlier works.[5,22,30] Also, from inspection of Fig. 2 we have found that a critical hybridization V_c, above which there is no more superconductivity, is proportional to the square root of α ($V_c \propto \alpha^{1/2}$). This behavior was observed earlier by Ramunni *et al.*[30] and Japiassu *et al.*,[22] indicating a common behavior between our present approach and the previous BCS calculations.[22,30] In Fig. 3 one can see the results of Fig. 2 for the quantity $2\Delta_0/k_BT_c$, and also the same for a constant hybridization (open symbols). Figure 3 shows that when V increases, $2\Delta_0/k_BT_c$ diminishes and goes to zero.

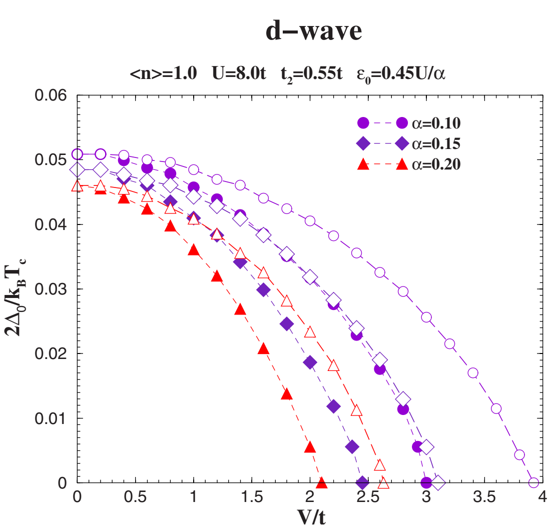

FIG. 3. (Color online) The change in $2\Delta_0/k_BT_c$ for a k dependent and a constant hybridization (open symbols). The figure shows that for increasing V, $2\Delta_0/k_BT_c$ diminishes, and goes to zero at different values of α.

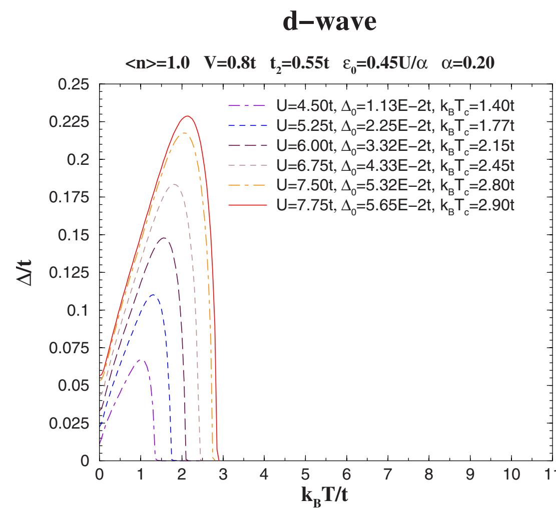

FIG. 4. (Color online) The same as in Fig. 2 but changing the attractive potential U. The figure shows that as U increases, both Δ_0 ant T_c increase.

At this point let us make a comment about the effect of applied pressure in the HTSC system. It is generally claimed that the hybridization V increases with applied pressure P. So, our results (see Fig. 2) show that both Δ_0 and T_c decrease with P (at least in the range where electronic effects dominate) since as V increases both Δ_0 and T_c also diminishes. In fact, experiments in HTSC materials have shown that they present a complicate dependence on P, e.g., they can exhibit positive or negative slope $\frac{dT_c}{dP}$ due to the competing effects associated with the lattice vibrations, which gives $\frac{dT_c}{dP}>0$ and the electronic dependence, which gives $\frac{dT_c}{dP}<0$.[31]

The d-p hybridization can be viewed also as an effective d-p hopping and since the d electronic states in our model constitute a degenerate d band, it is natural in this framework to consider also the p states as being degenerate. Besides the variation in the hybridization, it is important to see the behavior of Δ_0 and T_c when the attractive Hubbard potential U changes. Figure 4 shows the gap curves for different U values, for a k-dependent hybridization. When U decreases, Δ_0 and T_c also decrease, which is correct since U originates the superconductivity of the system. Notice that the anomalous behavior of the gap curves does not disappear when U diminishes, and there is a different value of Δ_0 and T_c for each U, in the same way of V in Fig. 2. The same behavior was observed for a constant hybridization. It is also important to verify the dependence of $2\Delta_0/k_BT_c$ on U for this Hubbard-I approximation. According to the BCS mean-field theory, the superconducting gap is weakly temperature dependent at low temperatures but falls off rapidly to zero around T_c. In Fig. 5 we plot the dependence of $2\Delta_0/k_BT_c$ on U for a k-dependent hybridization, for different values of the hybridization strength V. From the figure we see that for low values of U, $2\Delta_0/k_BT_c$ is quite low and, as U increases, $2\Delta_0/k_BT_c$ seems to saturate in different values, depending on V. Therefore we conclude that as U increases, one goes from a region where $2\Delta_0/k_BT_c$ varies significantly (low values of U), to a region where $2\Delta_0/k_BT_c$ saturates and becomes a constant. We should mention that for HTSC it is known that $2\Delta_0/k_BT_c$ varies widely.[32]

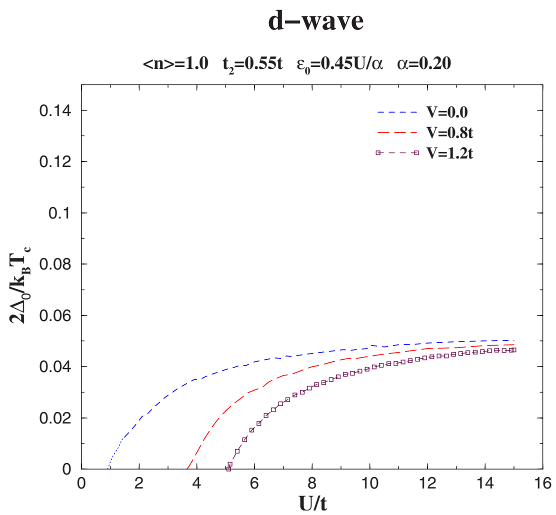

FIG. 5. (Color online) The dependence of $2\Delta_0/k_BT_c$ on U for a k-dependent hybridization, for different V values. From the curve we observe that as U increases $2\Delta_0/k_BT_c$ seams to saturate. Again one can see that as the hybridization strength V increases, the superconductivity diminishes.

From all the results above, we may conclude that both Δ_0 and T_c depend on α, and also on U. Figure 6 shows the dependence of Δ_0 on U. The results show that for a k dependent there is an almost linear dependence of Δ_0 on U, although the gap curves of Figs. 1, 2, and 4 exhibit an anomalous behavior. Therefore, we may conclude that the anomalous behavior of the gap curves do not affect Δ_0. Moreover, one sees that it is needed a higher value of U to obtain superconductivity as long as hybridization increases.

Figure 7 shows the behavior of the critical temperature T_c renormalized to zero hybridization temperature $T_c(0)$ $[T_c(V=0)=T_c(0)]$. One has initially a small decrease in $T_c/T_c(0)$ with hybridization and a pronounced decrease when $T_c/T_c(0)$ approaches V_c, where T_c goes to zero. Finally, Fig. 8 shows the behavior of the renormalized gap $\Delta_0/\Delta_0(0)$, where $\Delta_0(V=0)=\Delta_0(0)$. From the figure one sees an almost monotonic decrease in the renormalized gap for increasing hybridization until the V_c value, in the similar way of Fig. 3.

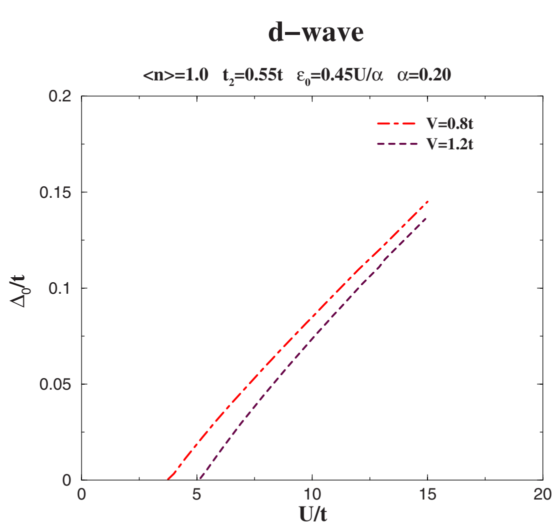

FIG. 6. (Color online) The dependence of Δ_0/t on U for a k-dependent hybridization.

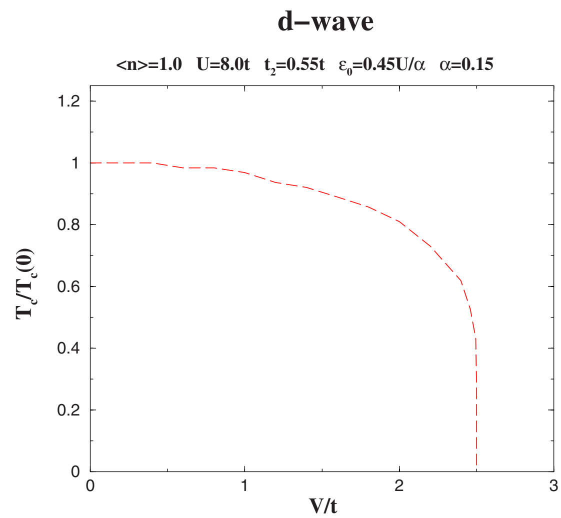

FIG. 7. (Color online) The dependence of the renormalized critical temperature $T_c/T_c(0)$ on V for a k-dependent hybridization.

IV. CONCLUSIONS AND FINAL COMMENTS

We have applied the Hubbard-I approximation[15] to study the two-dimensional two-band attractive Hubbard model, investigating some thermodynamical properties of this extended model, as well as obtaining the equations for the critical temperature T_c and the gap (order parameter) Δ, involving explicitly the d-d coupling U, the hybridization strength V, and the parameter α, which accounts for the ratio of the effective masses of the d and p bands.

We have pointed out throughout the present work the role of the one-body and nonlocal hybridization $V_{\mathbf{k}}$, which is to create in the normal state new bands with mixed features. In the case of a local hybridization the mixing turns out to be a constant one and can be interpreted as being a mean value of

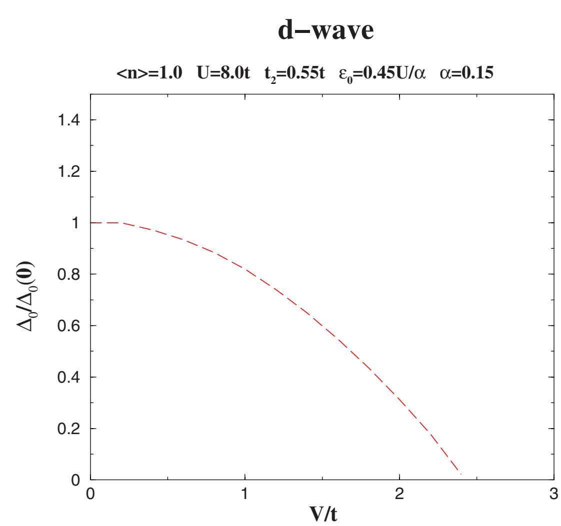

FIG. 8. (Color online) The dependence of the renormalized gap $\Delta_0/\Delta(0)$ on V for a k-dependent hybridization.

the hybridization over the Brillouin zone. The one-body hybridization can be tuned by the application of external pressure. When the hybridization is increased, we have verified from the self-consistent calculations that there is a critical value V_c, proportional to $\sqrt{a}$ for which T_c and Δ vanish.

We have focused on intraband d-d Cooper pairing since the main contribution for the density of states at the Fermi level is due to the d band. Therefore we have assumed that this pairing is the most relevant for superconductivity.

As commented in Sec. II, interband pairing could also arise. The most typical physical systems for the occurrence of this kind of pairing appear in some heavy fermions, such as $CeCu_2Si_2$. Heavy fermions are intermetallic systems containing unstable f-shell elements, mostly Yb, Ce, and U.[33] Several experiments involving Ce band compounds have shown the existence of a large density of states at the Fermi level. Band calculations have also indicated the delocalized nature of the f states in these metallic systems. It is then natural to expect the Ce $4f$ atoms to have a certain degree of itineracy and, therefore, f-d pairing may be important in the description of the $CeCu_2Si_2$ superconductivity. In fact, in Ref. 34 a mean-field BCS description with a hybrid d-f pairing was used to calculate the critical temperature of $CeCu_2Si_2$. For a set of reasonable parameters, it was obtained $T_c \approx 0.4$ K in a good agreement with the experimental value $T_c = 0.5$ K. However, a more consistent calculation using an f-d Hubbard band model considering strong attractive f-d pairing is needed. This work is now in progress.

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