$d_{x^2-y^2}$ superconductivity in a generalized Hubbard model

Liliana Arrachea
PUC-Rio, Departamento de Fisica, Caixa Postal 38071, Cep: 22452-970-RJ, Rio de Janeiro, Brazil

A. A. Aligia
Centro Atómico Bariloche and Instituto Balseiro, Comisión Nacional de Energía Atómica, 8400 Bariloche, Argentina
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We consider an extended Hubbard model with nearest-neighbor correlated hopping and next-nearest-neighbor hopping t' obtained as an effective model for cuprate superconductors. Using a generalized Hartree-Fock BCS approximation, we find that for high enough t' and doping, antiferromagnetism is destroyed and the system exhibits *d*-wave superconductivity. Near optimal doping we consider the effect of antiferromagnetic spin fluctuations on the normal self-energy using a phenomenological susceptibility. The resulting superconducting critical temperature as a function of doping is in good agreement with experiment. [S0163-1829(99)06101-9]

I. INTRODUCTION

One of the most challenging properties that any effective one-band model for the high superconducting critical temperature (high-T_c) superconducting materials should explain is the experimentally observed dependence of T_c on doping (x). Extended t-J models seem to be successful in interpreting several important properties of these materials.[1–3] They were derived as effective Hamiltonians in the strong-coupling limit (very large U),[4–7] while in generalized Hubbard models obtained by similar derivations, U is of the order of the unperturbed band width $8t \sim 3$ eV.[8,9] While numerical studies in t-J-like models unambiguously indicate that they exhibit sizable superconducting correlations with *d*-wave symmetry, in agreement with experiments,[2] this is not the case of the usual Hubbard model.[10] Apart from quantitative reasons concerning the strength of the local Coulomb repulsion, it is of interest to study an accurate enough effective model amenable to weak-coupling many-body treatments. In particular, the observed pseudogap behavior for temperatures $T_c < T < T^*$ in angle-resolved photoemission spectroscopy (ARPES) experiments[11] has been interpreted as a precursor effect of the antiferromagnetic[12] (AF) as well as the superconducting state[13,14] among other possible scenarios.[15,16] For the attractive (negative-U) Hubbard model, a good deal of research helped to elucidate the nature of the superconducting transition[17] and most of this work is based on one appealing feature of this model: its explicit attractive interaction leading to a superconducting state in the Bardeen-Cooper-Schrieffer (BCS) approximation. Thus, even though the symmetry of the BCS gap is *s* wave, this model has been used for a qualitative understanding of ARPES experiments.[13] Due to the lack of genuine microscopic *d*-wave superconducting analogous to that of the negative-U Hubbard model, some phenomenological models with BCS-like interactions were studied.[14,18,19] While the model proposed in Ref. 18 is built up by pure phenomenological interactions with several free parameters, in order to fit the experimentally observed T_c vs x curve, the AF and van Hove picture[19] has been proposed on the basis of a simplification of the t-J model in which holes are constrained to move only in one sublattice (up or down) in a Néel spin background. Nevertheless, this is an oversimplification for realistic $J < t$.[20] The assumption of pairing coexisting with long-range AF order is shared with the strong-coupling polaron picture,[3] which also reproduces qualitatively the observed T_c vs x curve. However, nuclear magnetic resonance experiments indicate that the coherence length of the AF correlations ξ is of only a few lattice sites in the optimally doped materials.[21] An effective attractive separable potential has also been considered to study the *d*-wave superconducting pseudogap evolution.[14] In this case, however, the AF correlations are not taken into account at all, while they play a relevant role in underdoped and optimally doped materials.[12,22]

In this work, we calculate T_c vs x of an effective one-band model for the high-T_c cuprates using weak-coupling techniques. We obtain beyond a certain doping, a stable paramagnetic phase with *d*-wave superconductivity (DWS). The mechanism for superconductivity is the electron-hole symmetric correlated hopping studied previously in one and two dimensions (2D).[23,24] However, previously in 2D, the next-nearest-neighbor hopping t' was neglected and only *s*-wave superconductivity was found for doping high enough to inhibit long-range antiferromagnetism. In simplified terms, this can be understood as follows: on-site Coulomb repulsion U inhibits on-site pairs, but nearest-neighbor singlet pairs are favored by the correlated hopping. In mean field, the dependence of this effective attraction in reciprocal space is proportional to $(\cos k_x - \cos k_y)^2$ for *d* symmetry and to $(\cos k_x + \cos k_y)^2$ for extended *s* symmetry (see Sec. III or Ref. 24). This implies that *d*-wave superconductivity is favored with respect to the *s*-wave one, for doping x at which the points $X[(0,\pi)$ and equivalent] lie near the Fermi surface. However, when $t' = 0$, this happens for $x \simeq 0$ and for these dopings, due to the perfect nesting of the Fermi surface, the antiferromagnetic instability is the dominant one and inhibits superconductivity. When t' is included, the perfect nesting is destroyed and the X points lie at the Fermi surface for finite doping, stabilizing the *d*-wave solution.

In Sec. II we briefly describe the derivation of the effective model and explain the meaning of the different terms. In Sec. III we calculate T_c vs x using a generalized Hartree-Fock (HF) BCS decoupling. Since the above-mentioned decoupling exaggerates the range of stability of the AF phase, in Sec. IV we include the effect of the AF spin fluctuations (AFSF) for dopings at which long-range AF order is destroyed, by evaluating the normal self-energy in the one-loop approximation with the phenomenological susceptibility of Ref. 21. Section V contains a discussion.

II. THE EFFECTIVE MODEL

The model used is obtained from the mapping of the low-energy part of the Hilbert space of the three-band Hubbard model H_{3b}.[8,9] As first suggested by Zhang and Rice,[4] and later confirmed by analytical and numerical work of several groups,[5–7] when insulating cuprates are doped, the added holes form local singlets involving a Cu $3d_{x^2-y^2}$ hole at a given site i (with creation operator $d^\dagger_{i\sigma}$) and a hole in the linear combination $\alpha^\dagger_{i\sigma}$ of the four nearest-neighbor oxygen $2p_\sigma$ orbitals with x^2-y^2 symmetry. This Zhang-Rice singlet has the form $[A(\alpha^\dagger_{i\uparrow}d^\dagger_{i\downarrow}-\alpha^\dagger_{i\uparrow}d^\dagger_{i\downarrow})+Bd^\dagger_{i\uparrow}d^\dagger_{i\downarrow}+C\alpha^\dagger_{i\uparrow}\alpha^\dagger_{i\downarrow}]|0\rangle$ and is mapped into the vacuum $|0\rangle$ at site i in the effective one-band model H. Similarly, the ground state of H_{3b} for one hole at cell i [which has the form $(Dd^\dagger_{i\sigma}+E\alpha^\dagger_{i\sigma})|0\rangle$] is mapped onto $c^\dagger_{i-\sigma}|0\rangle$ of H, where $c^\dagger_{i\sigma}$ is an effective electron creation operator. The vacuum of H_{3b} at cell i (which corresponds to full $3d$ and $2p$ shells) is mapped onto $c^\dagger_{i\uparrow}c^\dagger_{i\downarrow}|0\rangle$ in H. Calculating the matrix elements in the reduced Hilbert space, and retaining only the most important terms, the following effective Hamiltonian results:

$$H=U\sum_i n_{i\uparrow}n_{i\downarrow}-\mu\sum_i (n_{i\uparrow}+n_{i\downarrow})-\sum_{\langle ij\rangle\sigma}(c^\dagger_{i\sigma}c_{j\sigma}+h.c)$$
$$\times\{t_{AA}(1-n_{i\sigma})(1-n_{j\sigma})+t_{BB}n_{i\sigma}n_{j\sigma}+t_{AB}[n_{i\sigma}(1-n_{j\sigma})$$
$$+n_{j\sigma}(1-n_{i\sigma})]\}-t'\sum_{\langle ij'\rangle\sigma}c^\dagger_{i\sigma}c_{j'\sigma}, \quad (1)$$

where $\langle ij\rangle$ ($\langle ij'\rangle$) denotes nearest-neighbor (next-nearest-neighbor) positions of the lattice. Note that U is not directly related with a Coulomb repulsion, but represents the cost in energy of constructing a Zhang-Rice singlet from two singly occupied cells. It is lower than the difference between p and d on-site energies of H_{3b} (usually called charge-transfer energy Δ). t_{AA} represents the hopping of a Zhang-Rice singlet to a singly occupied nearest-neighbor cell. The terms with amplitude t_{AB} correspond to destruction of a Zhang-Rice singlet and a nearest-neighbor cell without holes, creating two singly occupied cells and vice versa. t_{BB} describes the movement of an isolated hole in H_{3b}. Clearly, the amplitude of these three correlated hopping processes should differ in general. The dependence of the next-nearest-neighbor hopping on the occupation of the sites involved in the hopping is neglected. Note that in the simplest strong-coupling derivation leading to the t-J model,[4] t_{AA} amounts to the only kinetic term in the model, the hopping term with amplitude t_{BB} is mapped out of the relevant Hilbert space, while the one with t_{AB} is treated in second order of perturbation theory to define the exchange term.[6] More systematic strong-coupling derivations contain other terms as well as higher-order corrections.[5–7,9]

For $t'=0$, the occurrence of metal-insulator transitions and superconductivity have been investigated for particular cases of this model,[23,24] but a stable DWS phase has not been found before. We concentrate on the parameter regime $t_{AB}>t_{AA}=t_{BB}=t$, which seems more adequate for the cuprates.[8,9,24] The effect of t' (Ref. 5) is crucial to stabilize the d-wave phase, because it removes the perfect nesting at half filling and shifts the energy of the van Hove singularity (VHS) in the unperturbed density of states (originated by the saddle points at X in the dispersion relation) away from the Fermi energy at half filling.

III. MEAN-FIELD APPROACH

The correlated hopping terms of the Hamiltonian (1) can be separated in one-, two-, and three-body contributions, with coefficients $t=t_{AA}$, $t_2=t_{AA}-t_{AB}$, and $t_3=2t_{AB}-t_{AA}-t_{BB}$, respectively.[24] We treat Eq. (1) within the generalized HF BCS approximation.[24] The term in t_3 contributes to the BCS solution in the d-wave as well as in the s-wave channels. The self-consistent parameters considered in the decoupling are $\langle n_{i\uparrow}\rangle-\langle n_{i\downarrow}\rangle=me^{i\mathbf{Q}\cdot\mathbf{R}_i}$, $\tau=\langle c^\dagger_{i+\delta\sigma}c_{i\sigma}\rangle$, $\psi=\langle c^\dagger_{i\uparrow}c^\dagger_{i\downarrow}\rangle$, and $\varphi_\delta=\langle c^\dagger_{i+\delta\uparrow}c^\dagger_{i\downarrow}\rangle$, with $\delta=\mathbf{x},\mathbf{y}$ being vectors connecting nearest neighbors and $\varphi_x=\pm\varphi_y$.[24] $n=n_\uparrow+n_\downarrow=1-x$ is the particle density, L is the number of lattice sites, $\mathbf{Q}=(\pi,\pi)$, and $\mathbf{R}_i$ indicates the lattice position. The problem is reduced to a one-particle one with three possibilities for the symmetry-breaking perturbation: (i) AF spin density wave (SDW) (with $m\neq0$ and $\psi=\varphi_x=0$), (ii) DWS (with $m=\psi=0$ and $\varphi_x=-\varphi_y\neq0$), and (iii) extended s-wave superconductivity (SWS) (with $m=0$, $\psi\neq0$ and $\varphi_x=\varphi_y\neq0$). The possibility of coexistence of SDW and superconductivity is left out here, since a previous study indicated that a sizeable superconducting gap is not possible within our model in the presence of long-range antiferromagnetism.[26] For the three cases, the renormalized dispersion relation, effective hopping, and effective chemical potential can be written in the form

$$\epsilon_k=-2t_{eff}(\cos k_x+\cos k_y)-4t'\cos k_x\cos k_y,$$
$$t_{eff}=t-t_2n+t_3[3\tau^2+\psi^2+\varphi_x^2-(n^2-m^2)/4], \quad (2)$$
$$\mu_{eff}=\mu-\{Un/2+8t_2\tau+4t_3[\tau n+\psi(\varphi_x+\varphi_y)]\}.$$

The SDW, d-wave, and s-wave BCS order parameters are

$$\Delta^{SDW}=\left(\frac{U}{2}+4t_3\tau\right)m, \quad \Delta^{BCS}_{Dk}=4t_3\tau\varphi_x(\cos k_x-\cos k_y),$$
$$\Delta^{BCS}_{Sk}=(8t_3\tau-U)\psi-4(2t_2+nt_3)\varphi_x \quad (3)$$
$$+[4t_3\tau\varphi_x-2(2t_2+nt_3)\psi](\cos k_x+\cos k_y),$$

respectively. For a given wave vector $\mathbf{k}$, they coincide with half of the corresponding energy gap. For both, d- and s-wave superconducting solutions, the dependence of T_c vs x is obtained from the linearized BCS gap equations. For the d-wave case, T_c is given by

$$1=\int \frac{d^2k}{(2\pi)^2}\tanh\left(\frac{\overline{\epsilon}_k}{2T}\right)\frac{4t_3\tau(\cos k_x-\cos k_y)}{2\overline{\epsilon}_k}\cos k_x, \tag{4}$$

where $\overline{\epsilon}_k=\epsilon_k-\mu_{eff}$ and T is the temperature. For the s-wave solution, T_c is the temperature at which λ_{max} equals one, being λ_{max} the largest eigenvalue of the matrix

$$\begin{pmatrix} \int \frac{d^2k}{(2\pi)^2}\tanh\left(\frac{\overline{\epsilon}_k}{2T}\right)\frac{\alpha_k}{2\overline{\epsilon}_k} & \int \frac{d^2k}{(2\pi)^2}\tanh\left(\frac{\overline{\epsilon}_k}{2T}\right)\frac{\beta_k}{2\overline{\epsilon}_k} \\ \int \frac{d^2k}{(2\pi)^2}\tanh\left(\frac{\overline{\epsilon}_k}{2T}\right)\frac{\alpha_k\cos k_x}{2\overline{\epsilon}_k} & \int \frac{d^2k}{(2\pi)^2}\tanh\left(\frac{\overline{\epsilon}_k}{2T}\right)\frac{\beta_k\cos k_x}{2\overline{\epsilon}_k} \end{pmatrix}, \tag{5}$$

where

$$\alpha_k=8t_3\tau-U-2(2t_2+nt_3)(\cos k_x+\cos k_y),$$
$$\beta_k=-4(2t_2+nt_3)+4t_3\tau(\cos k_x+\cos k_y), \tag{6}$$

are the coefficients of ψ and φ_x in Δ_{Sk}^{BCS}. This method of obtaining T_c in second-order phase transitions when the thermodynamic potential Ω depends on more than one parameter (here ψ and φ_x) has been used before,[27] and is equivalent to the usual one of finding the first instability (as T is lowered) of the Hessian matrix formed by the second derivatives of Ω with respect to the independent variables.[28]

In Fig. 1, we show the superconducting critical temperature as a function of doping $x=1-n$, where n is the number of electrons per site for both d-wave and s-wave solutions. Most of the pairing terms, as well as the additional contribution to the usual $U/2$ term in the expression of the SDW gap, can be generated from the mean-field decoupling of an effective two-body interaction of the form[26]

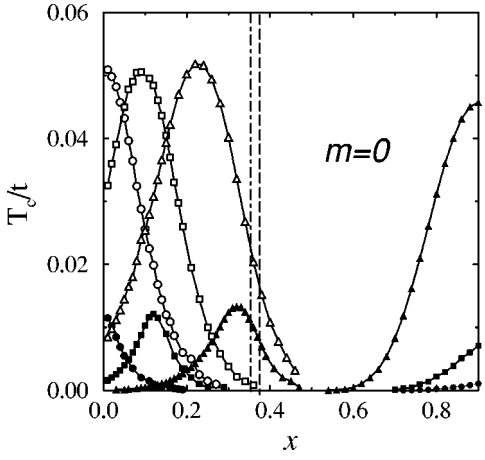

FIG. 1. d-wave BCS critical temperature T_c in units of t as a function of the doping x (for $x<0.5$), for $t_{AB}=2t$ (open symbols), and $t_{AB}=1.5t$ (filled symbols). Circles, squares, and triangles correspond to $t'=0,-0.2t,-0.45t$, respectively. The solid symbols for $x>0.5$ show T_c of the s-wave solution for $t_{AB}=1.5$ and the same values of t' as those considered for the d wave. The dotted (dot-dashed) line indicates the boundary of the SDW at $T=0$ for $U=4t(U=6t)$, $t_{AB}=1.5t(t_{AB}=2t)$, and $t'=-0.45t$.

$$V_{eff}=t_3\tau\sum_{\langle ij\rangle}(4\mathbf{S}_i\cdot\mathbf{S}_j+n_in_j). \tag{7}$$

Pairing in both d-wave and extended s-wave channels is originated by the spin-flip terms of V_{eff}. For the s-wave case, there are some additional contributions, as can be observed in Eq. (3). From mere inspection of the three possible order parameters (3), it can be seen that Δ^{SDW} and Δ_{Sk}^{BCS} depend on U in such a way that the antiferromagnetic (s-wave BCS) solution is enhanced (weakened) as U increases, whereas Δ_{Dk}^{BCS} does not depend on U. Thus, the doping region where the d-wave BCS solution exists is limited only by the difference in energy with the two other competing instabilities of the Fermi liquid. As mentioned in Sec. I, due to the wave-vector dependence of the superconducting order parameters, the shape of the Fermi surface plays an important role in defining the doping regions at which each of the two BCS solutions is possible. In Ref. 24 we have shown that for $t'=0$ and assuming a constant density of states, SWS exists for high enough x and low enough U, while DWS exists near half filling. Within this region, however, the SDW solution has lower energy than the DWS one, being the difference between the energy of both solutions small for $U\sim 0$ [as can be inferred from the form of the gaps, Eqs. (3)]. When t' is turned on, the VHS is displaced, lying at the Fermi energy for a finite doping. The increment in the density of states at finite doping enhances the critical temperature as well as the doping range associated to the s-wave solution. However, as a consequence of the vector dependence of the effective interaction, the optimal doping for SWS is always high. In Fig. 1, it is shown that for $t_{AB}=1.5$ and $U=4t$, the doping region with SWS is $x>0.6$, i.e., beyond the range of doping accessible experimentally in the cuprates. For the d-wave solution, the maximum of T_c occurs when the chemical potential coincides with the energy of the VHS. Due to the loss of perfect nesting and the closing of the indirect SDW gap for this doping, the SDW is weakened. Thus, even for large U, for sizeable t' there exists a doping range for which the d-wave BCS solution is stable and robust. We indicate in the figure the doping region for the existence of the SDW solution ($m\neq 0$) at $T=0$ for the particular values $U=4t\,(U=6t)$, $t_{AB}=1.5t\,(t_{AB}=2t)$, and $t'=-0.45t$. The Néel temperature at which m becomes zero is not calculated here since it is dominated by spin fluctuations, and the mean-field value is too large. For nearly real-

istic bare parameters, the doping range for a stable DWS (beyond the dot-dashed line in Fig. 1) corresponds to the overdoped regime of the cuprates, in agreement with experiments on Bi2212 (Ref. 11) that indicate that the superconducting state takes place in an otherwise ordinary Fermi liquid for overdoped compounds.

In the optimally doped regime, spin fluctuations not only affect directly the SDW order parameter, destroying the AF long-range order, but also affect indirectly the superconducting order parameters. Their effect should be included in a more realistic calculation of the superconducting critical temperature. This is the goal of the next section.

IV. THE EFFECT OF SPIN FLUCTUATIONS

Long-range antiferromagnetism is not expected to survive within the whole range of doping predicted by the mean-field approach. For doping larger than $x\sim 0.05-0.1$, the spin fluctuations are important and a Fermi liquid with strong AFSF is a more appropriate picture for this regime.[21,25] AFSF of any Hubbard-like microscopic model as the one considered here can be characterized by a spin susceptibility of the form

$$\chi(\mathbf{q},\omega)=\frac{\chi(\mathbf{Q},0)}{1+(\mathbf{q}-\mathbf{Q})^2\xi^2-i\omega/\omega_{sf}}, \tag{8}$$

where the parameters scale with the AF correlation length ξ as $\chi(\mathbf{Q},0)\sim\xi^2$, $\omega_{sf}=\Gamma_0\xi^2$, with $\Gamma_0\sim 40$ meV.[21,29] Assuming a phenomenological spin-fermion coupling, AFSF has been suggested to mediate the pairing in the cuprates.[25] This picture is supported by the observed correlation between ξ and T_c in several superconducting cuprates. Within the weak-coupling formalism, DWS due to correlated hopping, is inhibited in a background with long-range AF correlations.[26] However, the effective interaction of Eq. (7) provides an explicit channel for the coupling with collective AFSF within the doping region without AF long-range order, which has the same form as the phenomenological coupling used in Ref. 25. Thus, it might be expected that the AFSF would renormalize the bare value of t_{AB} ($<1.5t$ for realistic values of the three-band parameters[9]) to higher ones.[22,25] In what follows, we investigate how the BCS T_c vs x dependence is modified by the effect of the AFSF for the d-wave solution.

For finite t', the Fermi surface contains hot spots (for which $\epsilon_k=\epsilon_{k+Q}$). Fermions located in the neighborhood of these points are the most affected by AF correlations and exhibit a peculiar T dependence in the one-particle spectral properties, which is mainly determined by the magnitude of ξ/ξ_{th}, and ω_{sf}/T,[22,29] with $\xi_{th}=v_F/T$, v_F being the Fermi velocity. Hot spots are located at $\mathbf{k}_{hs}$ near X [$(0,\pi)$ and symmetry related points], i.e., near the antinodes of the DWS gap and with energies close to the VHS (for which $v_F\sim 0$). As T_c vs x predicted by the BCS approximation, as well as the value of the maximum T_c itself, depend on the behavior of the density of states, AFSF are expected to play some further important role apart from the eventual renormalization of the effective pairing interaction. The self-energy obtained from Eq. (8) is

$$\Sigma(\mathbf{k},i\omega_n)=T\sum_m \int \frac{d^2q}{(2\pi)^2} g(\mathbf{q})\overline{g}(\mathbf{q})\chi(\mathbf{q},i\nu_m) \times G^0(\mathbf{k}+\mathbf{q},i\omega_n+i\nu_m), \tag{9}$$

$$\chi(q,i\nu_m)=-\int_{-\omega_0}^{\omega_0}\frac{d\omega}{\pi}\frac{\mathrm{Im}\chi(\mathbf{q},\omega)}{i\nu_m-\omega},$$

where $[G^0(\mathbf{k},i\omega_n)]^{-1}=i\omega_n-\overline{\epsilon}_k$, $g(\mathbf{q})$ is an effective interaction between fermions and spin fluctuations, ω_0 is a frequency cutoff, $\nu_m=2m\pi T$, and $\omega_n=(2n+1)\pi T$. As usual, an effective coupling constant $g'\sim g(\mathbf{q})\overline{g}(\mathbf{q})\chi(\mathbf{Q},0)/\xi^2$ is defined, which in the present case should be proportional to $(U+4t_3\tau)$.[26] The ensuing spectral function is $A(\mathbf{k},\omega)=-\mathrm{Im}\,G(\mathbf{k},\omega)/\pi$, with $[G(\mathbf{k},\omega)]^{-1}=\omega-\overline{\epsilon}_k-\Sigma(\mathbf{k},\omega)$. To examine how the changes in the behavior of $A(\mathbf{k},\omega)$ affect the T_c vs x dependence, we consider the effect of AFSF using the BCS form of the anomalous self-energy Δ_{Dk}^{BCS} given by Eq. (3) and calculating the normal self-energy in the one-loop approximation [Eq. (9)]. The resulting linearized gap equation,

$$\varphi_x=T\int\frac{d^2k}{(2\pi)^2}\Delta_{Dk}^{BCS}\cos k_x\sum_n e^{i\omega_n 0^+}G(\mathbf{k},i\omega_n) \times G(-\mathbf{k},-i\omega_n), \tag{10}$$

can be cast in real frequency as

$$\varphi_x=-\int\frac{d^2k}{(2\pi)^2}\Delta_{Dk}^{BCS}\cos k_x \times\int d\omega d\omega'\frac{A(\mathbf{k},\omega)A(-\mathbf{k},\omega')}{\omega+\omega'}\tanh\left(\frac{\omega}{2T}\right), \tag{11}$$

where $n_F(\omega)=1/\{1+\exp[(\omega-\mu_{\mathrm{eff}})/T]\}$. Equation (11) reduces to the linearized version of the usual BCS Eq. (4) when $A(\mathbf{k},\omega)=\delta(\omega-\overline{\epsilon}_k)$. As discussed in previous works, assuming ξ approximately constant or with a weak T dependence, two different regimes due to the AFSF can be distinguished as a function of T in the behavior of $A(\mathbf{k},\omega)$:[22,29] (i) For $T\ll\omega_{sf}$, quantum contributions dominate the behavior of the self-energy (9) and $A(\mathbf{k},\omega)$ exhibits Fermi liquidlike quasiparticle peaks, even for Fermi points near $\mathbf{k}_{hs}$. Within this regime, no relevant qualitative changes in comparison with the BCS description are expected in the solution of the gap equation (11). (ii) For $T\gg\omega_{sf}$, and for $\mathbf{k}$ points satisfying $\xi\gg\xi_{th}$, classical effects [introduced by the $m=0$-Matsubara frequency in Eq. (9)] dominate. The AFSF can be considered as quasistatic and $A(\mathbf{k}_{hs},\omega)$ exhibits a shadow-band structure for large enough values of g'.[22,29] This implies a transfer of spectral weight from low to high frequencies, and we expect an effective blurring of the large density of states near the VHS with a concomitant decrease of T_c.

The above qualitative issues are confirmed by our numerical calculations, as illustrated in Fig. 2. We restrict ourselves to the case with finite $t'=-0.45t$, which reproduces the observed Fermi surface of $YBa_2Cu_3O_7$ (YBCO) and B2212 and to the case of $t_{AB}=2t$, for which the optimal doping and the maximum T_c predicted by the BCS approximation are in

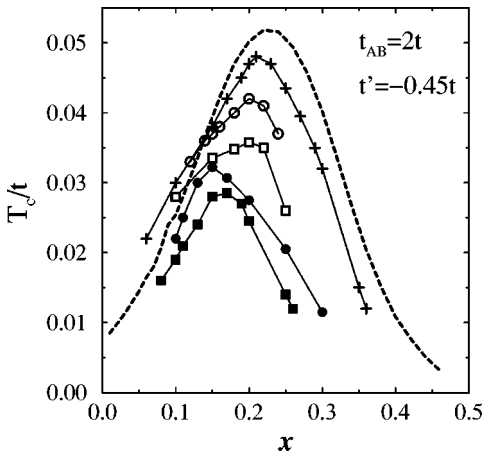

FIG. 2. Critical temperatures T_c in units of t as a function of the doping x, for $t_{AB}=2t$ and $t'=-0.45t$, considering AFSF. The dashed line (crosses) corresponds to the BCS solution in the thermodynamic limit (using k discretization). Circles correspond to $g'=3t$, and $\xi=2.5$ (open circles) and $\xi=10$ (filled circles). Squares correspond to $g'=10t$ and $\xi=2.5$ (open squares) and $\xi=4$ (filled squares).

good agreement with experiments (for these parameters, the ratio $t'/t_{eff}\sim 0.27$). To compute T_c we evaluate μ_{eff} and τ from

$$n=1+T\int \frac{d^2k}{(2\pi)^2}\sum_n e^{i\omega_n 0^+}\mathrm{Re}\,G(\mathbf{k},i\omega_n),$$
$$\tau=T\int \frac{d^2k}{(2\pi)^2}\sum_n e^{i\omega_n 0^+}\cos k_x \mathrm{Re}\,G(\mathbf{k},i\omega_n), \tag{12}$$

and afterwards check if there exists (or not) a solution of the linearized gap equation (10). A cutoff $\Omega_m=432\omega_{sf}$ was chosen for the ν_m-Matsubara summation in Eq. (9) while another one $\Omega_n=46t$, assuming $t=250$ meV, was used for the ω_n-Matsubara summation in Eqs. (10) and (12). The sum over the tails was approximated by a Euler–Mc Laurin formula. The k integral in Eq. (9) is calculated with a relative precision of 10^{-6}, while a fixed finite mesh was used to evaluate the k integrals in Eqs. (10) and (12). In the latter step, some precision is lost and the BCS T_c vs x, calculated in the thermodynamic limit, is not exactly recovered as indicated in Fig. 2. We considered $\xi=2.5\,(\omega_{sf}=0.0256t)$ and $\xi=4\,(\omega_{sf}=0.01t)$, which are supposed to be representative of YBCO and LaSrCuO, respectively,[21] near optimal doping, and $\xi=10\,(\omega_{sf}=0.0016t)$ which could be realistic only for strongly underdoped materials. Taking $g'=3t$ a weak effect on T_c is observed. For $g'=10t$, which is expected to be representative of the cuprates,[25,29] a decrease in T_c is observed as ξ increases. For the case of $\xi=10$, $g'=10t$ (not shown in the figure) the maximum T_c is below $0.012t$.

V. DISCUSSION

We have shown that for high enough next-nearest-neighbor hopping t', d-wave superconductivity is stabilized for doping $x\sim 0.35$ at the mean-field level in the correlated hopping model (1). The corresponding critical temperature T_c has the right order of magnitude (~ 70–100 K). Our calculations are in 2D and this result may be, of course, affected by the fluctuations of the superconducting state, which have not been taken into account in the present work. However, within the optimally doped to overdoped regime, the superfluid density is large and the critical temperature corrected by these latter fluctuations is expected to be close to the mean-field BCS one, even when the transition is Kosterlitz-Thouless-like rather than BCS-like.[15] For dopings accessible experimentally in the cuprates ($x<0.5$) the s-wave superconducting instability is suppressed. Including the effect of antiferromagnetic spin fluctuations (AFSF), we find that three different regimes remain as a function of doping in the realistic range: (i) long-range antiferromagnetism near half filling, (ii) d-wave superconductivity in a pure Fermi liquid (usual BCS) scenario within the overdoped regime, (iii) d-wave superconductivity in the presence of AFSF within the underdoped to optimally doped regime. The maximum T_c within our BCS treatment depends on the strength of the interaction and the position of the VHS. The effect of the spin fluctuations, however, modifies the BCS picture within this regime. The effective pairing interaction of Eq. (1) has the form of an exchange coupling, being ineffective in the Néel state,[26] but provides an explicit coupling in the regime of doping for which the AF correlations are short ranged. We considered particular values of the model parameters for which optimal doping, T_c, and shape of the Fermi surface are in agreement with experiments and further examined the effect of the nontrivial temperature behavior induced by the existence of hot spots in the Fermi surface in the presence of AFSF. We found that T_c decreases as the correlation length increases in correspondence with experiments. For optimally doped materials, we expect that the magnitude of T_c is dominated by the effect of spin fluctuations rather than by phase fluctuations of the superconducting order parameter. Details of the coupling with AFSF, renormalizations of the bare interactions, and eventual consequences upon the pseudogap behavior requires a treatment of the full T matrix of the effective pairing interaction on equal footing with the spin susceptibility and is left for future studies.

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