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d-Wave hole superconductivity in low-dimensional Hubbard systems

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Abstract

Superconducting states with d symmetry in anisotropic hole systems are investigated within a generalized Hubbard model and the BCS framework. The results reveal a key participation of the next-nearest-neighbor correlated-hopping interaction (Δt_3) in the appearance of $\cos k_x - \cos k_y$ superconducting gap, in spite of its small strength in comparison with other terms of the model. This interaction favors the superconducting state over the phase separation, which is an important obstacle when the d-wave superconducting state is originated from an attractive nearest-neighbor density–density interaction. Furthermore, the superconducting critical temperature is highly enhanced by the low-dimensionality of the system and the gap ratio exhibits a non-BCS behavior. © 2002 Elsevier Science Ltd. All rights reserved.

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1. Introduction

Low-dimensionality, short coherence length, and pairing of holes, instead of electrons, are believed to be essential to understand the properties of the cuprate high-T_c superconductors [1]. During the last years, the Hubbard model has been extensively studied due to its simplicity and emphasis on the local electron–electron correlation [2]. Three-band Hubbard models have been proposed to describe the electron and hole dynamics on the CuO_2 planes [3]. These models can be reduced into a single-band one [4] and the electronic states close to the Fermi energy can be reasonably well described by a square-lattice single-band tight-binding model with a next-nearest-neighbor hopping $t'_0 = 0.45t_0$ [5], where t_0 is the nearest-neighbor hopping parameter. Nowadays, it is widely accepted that the single-band Hubbard model is an appropriate starting point to describe the electronic correlations on the CuO_2 planes. However, the non-existence of d-wave superconductivity in the standard Hubbard model has been proved [6] and only extended s-symmetry pairing has been found within the usual generalized Hubbard models [7]. On the other hand, the experimental evidence reveals a $d_{x^2-y^2}$ symmetry superconducting gap for many cuprate superconductors [8–12]. Numerical studies performed in t–J model indicate a dominant d-superconducting channel [3], in spite of no long-range d-wave superconducting correlation has been found for $J/t \leq 0.5$ [13]. The $d_{x^2-y^2}$ pairing correlation is also observed within Hubbard-type models including a three-body interaction [14] and in a negative nearest-neighbor interaction Hubbard model [15,16]. In this attractive Hubbard model a phase separated state appears, inhibiting the formation of the superconducting ground state as the strength of the attraction grows [15]. Recently, we have analyzed the two-hole problem within a generalized Hubbard model, finding an important participation of the second-neighbor correlated-hopping interaction (Δt_3) in the formation of a $d_{x^2-y^2}$ symmetry hole singlet, in spite of its apparently small strength in comparison with direct Coulomb repulsions [17]. In this communication, we extend the previous work to study the case of finite density of holes within the well-known BCS framework [18].

The present paper is organized as follows. Section 2 contains a brief description of the Hamiltonian and the corresponding BCS equations. In Section 3, we investigate the dependence of the critical temperature on the hole density for both s- and d-channel superconducting ground

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states. The competition between d-wave superconducting ground state and phase separation is also analyzed. Finally, some conclusions are given in Section 4.

2. The model

The usual generalized Hubbard model considers only the on-site (U), nearest-neighbor (V) Coulomb interactions, and a nearest-neighbor correlated-hopping interaction (Δt), which has shown an enhanced hole-superconductivity without negative U and V [19]. In this paper, we consider a generalized Hubbard model that includes additionally a next-nearest-neighbor correlated hopping interaction (Δt_3) in the CuO_2 planes. Certainly, all these interactions are present in a real solid, even their contributions are very different, for example, for $3d$ electrons in transition metals U, V, Δt, and Δt_3 are typically about 20, 3, 0.5, and 0.1 eV, respectively [20,21].

Let us consider an anisotropic cubic lattice, i.e. square lattices in the xy plane with lattice parameter a and these planes are separated by a distance $a_\perp$. A single-band generalized Hubbard Hamiltonian in this system can be written as:

$$H = -t_\perp \sum_{\langle m,n\rangle,\sigma} c^+_{m,\sigma}c_{n,\sigma} - t_0 \sum_{\langle i,j\rangle,\sigma} c^+_{i,\sigma}c_{j,\sigma} - t'_0 \sum_{\langle\langle i,j\rangle\rangle,\sigma} c^+_{i,\sigma}c_{j,\sigma} + U\sum_i n_{i,\uparrow}n_{i,\downarrow} + \frac{V}{2}\sum_{\langle i,j\rangle} n_i n_j + \Delta t \sum_{\langle i,j\rangle,\sigma} c^+_{i,\sigma}c_{j,\sigma}(n_{i,-\sigma} + n_{j,-\sigma}) + \Delta t_3 \sum_{\langle i,l\rangle,\langle j,l\rangle,\langle\langle i,j\rangle\rangle,\sigma} c^+_{i,\sigma}c_{j,\sigma}n_l, \tag{1}$$

where $c^+_{i,\sigma}(c_{i,\sigma})$ is the creation (annihilation) operator with spin $\sigma = \downarrow$ or $\uparrow$ at site i, $n_{i,\sigma} = c^+_{i,\sigma}c_{i,\sigma}$, $n_i = n_{i,\uparrow} + n_{i,\downarrow}$, $\langle i,j\rangle$ and $\langle\langle i,j\rangle\rangle$ denote, respectively, the nearest-neighbor and the next-nearest-neighbor sites in the same plane, and $\langle m,n\rangle$ denotes nearest-neighbor sites in two adjacent planes. Note that only electron–electron interactions in the same plane are considered. When an electron–hole transformation is made in Eq. (1), i.e. electron operators are mapped onto hole's via $c^+_{i,\sigma} \to h_{i,\sigma}$, the Hamiltonian becomes

$$H = t_\perp \sum_{\langle m,n\rangle,\sigma} h^+_{m,\sigma}h_{n,\sigma} + (U + 2ZV)\Big(N^{\parallel}_s - \sum_{i,\sigma} n^h_{i,\sigma}\Big) + (t_0 - 2\Delta t)\sum_{\langle i,j\rangle,\sigma} h^+_{i,\sigma}h_{j,\sigma} + (t'_0 - 2\Delta t_3)\sum_{\langle\langle i,j\rangle\rangle,\sigma} h^+_{i,\sigma}h_{j,\sigma} + U\sum_i n^h_{i,\uparrow}n^h_{i,\downarrow} + \frac{V}{2}\sum_{\langle i,j\rangle} n^h_i n^h_j + \Delta t\sum_{\langle i,j\rangle,\sigma} h^+_{i,\sigma}h_{j,\sigma}\Big(n^h_{i,-\sigma} + n^h_{j,-\sigma}\Big) + \Delta t_3 \sum_{\langle i,l\rangle,\langle j,l\rangle,\langle\langle i,j\rangle\rangle,\sigma} h^+_{i,\sigma}h_{j,\sigma}n^h_l, \tag{2}$$

where $n^h_{i,\sigma} = h^+_{i,\sigma}h_{i,\sigma}$, $n^h_i = n^h_{i,\uparrow} + n^h_{i,\downarrow}$, $N^{\parallel}_s$ is the total number of sites in each plane, and Z is the lattice coordination number in the plane. The second term in Eq. (2) only contributes to a shift of the total energy and then, the holes also interact via a generalized Hubbard model but with effective hopping parameters $t_\perp$, $t = t_0 - 2\Delta t$, and $t' = t'_0 - 2\Delta t_3$, instead of $-t_\perp$, $-t_0$, and $-t'_0$ for electrons. The Hamiltonian of holes (Eq. (2)) can be written in the momentum space as

$$H = (U + 2ZV)N^{\parallel}_s + \sum_{\mathbf{k},\sigma} \epsilon_0(\mathbf{k})h^+_{\mathbf{k},\sigma}h_{\mathbf{k},\sigma} + \frac{1}{N_s}\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} V_{\mathbf{kk}'\mathbf{q}} h^+_{\mathbf{k}+\mathbf{q},\uparrow}h^+_{-\mathbf{k}+\mathbf{q},\downarrow}h_{-\mathbf{k}'+\mathbf{q},\downarrow}h_{\mathbf{k}'+\mathbf{q},\uparrow} + \frac{1}{N_s}\sum_{\mathbf{k},\mathbf{k}',\mathbf{q},\sigma} W_{\mathbf{kk}'\mathbf{q}} h^+_{\mathbf{k}+\mathbf{q},\sigma}h^+_{-\mathbf{k}+\mathbf{q},\sigma}h_{-\mathbf{k}'+\mathbf{q},\sigma}h_{\mathbf{k}'+\mathbf{q},\sigma}, \tag{3}$$

where N_s is the total number of sites,

$$h_{\mathbf{k},\sigma} = \frac{1}{\sqrt{N_s}}\sum_j e^{i\mathbf{k}\cdot\mathbf{R}_j}h_{j,\sigma},$$

$$\epsilon_0(\mathbf{k}) = 2t_\perp\cos(k_z a_\perp) - U - 2ZV + 2t[\cos(k_x a) + \cos(k_y a)] + 4t'\cos(k_x a)\cos(k_y a),$$

$$V_{\mathbf{kk}'\mathbf{q}} = U + V\beta(\mathbf{k}-\mathbf{k}') + \Delta t[\beta(\mathbf{k}+\mathbf{q}) + \beta(-\mathbf{k}+\mathbf{q}) + \beta(\mathbf{k}'+\mathbf{q}) + \beta(-\mathbf{k}'+\mathbf{q})] + \Delta t_3[\gamma(\mathbf{k}+\mathbf{q},\mathbf{k}'+\mathbf{q}) + \gamma(\mathbf{k}+\mathbf{q},\mathbf{k}'+\mathbf{q})], \tag{4}$$

and

$$W_{\mathbf{kk}'\mathbf{q}} = \frac{V}{2}\beta(\mathbf{k}-\mathbf{k}') + \Delta t_3[\gamma(\mathbf{k}+\mathbf{q},\mathbf{k}'+\mathbf{q}) + \gamma(-\mathbf{k}+\mathbf{q},-\mathbf{k}'+\mathbf{q})],$$

being $\beta(\mathbf{k}) = 2[\cos(k_x a) + \cos(k_y a)]$, $\gamma(\mathbf{k},\mathbf{k}') = 4\cos(k_x a)\cos(k'_y a) + 4\cos(k'_x a)\cos(k_y a)$, and $2\mathbf{q}$ is the wave vector of the pair center of mass. After a normal Hartree–Fock decoupling of the interaction terms in Eq. (3) within the standard BCS scheme, the reduced Hamiltonian can be written as [18]:

$$H - \mu N = \sum_{\mathbf{k},\sigma}(\epsilon(\mathbf{k}) - \mu)h^+_{\mathbf{k},\sigma}h_{\mathbf{k},\sigma} + \frac{1}{N_s}\sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{kk}'0}h^+_{\mathbf{k},\uparrow}h^+_{-\mathbf{k},\downarrow}h_{-\mathbf{k}',\downarrow}h_{\mathbf{k}',\uparrow}, \tag{5}$$

where μ is the chemical potential, N is the number of holes, and

$$\epsilon(\mathbf{k}) = 2t_\perp\cos(k_z a_\perp) + \left(\frac{U}{2} + ZV\right)n_h + 2(t + n_h\Delta t) \times(\cos(k_x a) + \cos(k_y a)) + 4(t' + 2n_h\Delta t_3)\cos(k_x a)\cos(k_y a), \tag{6}$$

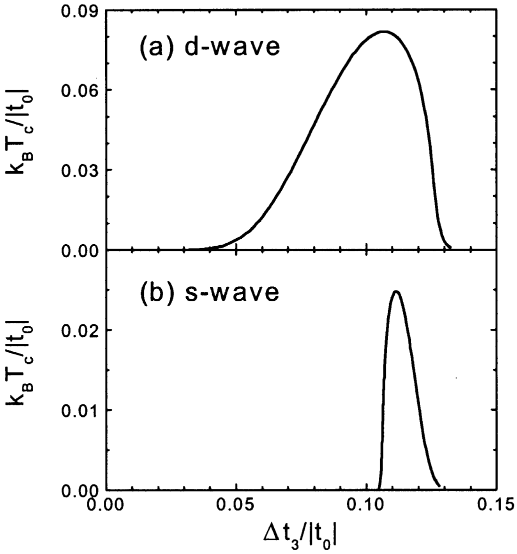

Fig. 1. (a) The d-wave and (b) s-wave superconducting critical temperatures (T_c) are plotted as functions of the second-neighbor correlated hopping (Δt_3), for a square lattice with $U = 6|t_0|$, $V = 0$, $t'_0 = 0.45t_0$, $\Delta t = 0.5|t_0|$, and $n_h = 0.2$.

being n_h the density of holes per site. Notice that the dispersion relation $\epsilon(\mathbf{k})$ is now modified by adding terms $n_h\Delta t$, $2n_h\Delta t_3$ and $(U/2 + 4V)n_h$ to the single hole hoppings t, t' and the self-energy, respectively. On the other hand, the term $W_{\mathbf{kk'q}}$ in Eq. (3) is ignored since it has no contribution on the singlets. At a finite temperature T, the equations for determining the superconducting gap and the chemical potential are [22],

$$\Delta_{\mathbf{k}} = -\frac{1}{N_s}\sum_{\mathbf{k}'} V_{\mathbf{kk}'0}\frac{\Delta_{\mathbf{k}'}}{2E_{\mathbf{k}'}}\tanh\left(\frac{E_{\mathbf{k}'}}{2k_BT}\right), \tag{7}$$

$$n_h - 1 = -\frac{1}{N_s}\sum_{\mathbf{k}'} \frac{\epsilon(\mathbf{k}') - \mu}{E_{\mathbf{k}'}}\tanh\left(\frac{E_{\mathbf{k}'}}{2k_BT}\right), \tag{8}$$

where the single excitation energy ($E_{\mathbf{k}}$) is given by:

$$E_{\mathbf{k}} = \sqrt{(\epsilon(\mathbf{k}) - \mu)^2 + \Delta_{\mathbf{k}}^2}. \tag{9}$$

For a negative-U Hubbard model analyzed within the BCS scheme [2], $V_{\mathbf{kk}'0} = -U$, in consequence only an isotropic s-wave superconducting gap is obtained. However, in our case, due to the nature of $V_{\mathbf{kk}'0}$, the last two equations admit solutions in both the extended s- and the d-channels, whose superconducting gaps are, respectively, given by $\Delta_{\mathbf{k}} = \Delta_s + \Delta_{s^*}[\cos(k_xa) + \cos(k_ya)]$ and $\Delta_{\mathbf{k}} = \Delta_d[\cos(k_xa) - \cos(k_ya)]$, where Δ_s is the standard s-channel contribution. Therefore, for the d-channel Eq. (7) can be written as,

$$1 = -\frac{(V - 4\Delta t_3)}{N_s}\sum_{\mathbf{k}} \frac{\cos(k_xa)[\cos(k_xa) - \cos(k_ya)]}{E_{\mathbf{k}}} \times\tanh\left(\frac{E_{\mathbf{k}}}{2k_BT}\right), \tag{10}$$

and for the s-channel, Eq. (7) becomes two simultaneous equations,

$$\Delta_{s^*} = -(V + 4\Delta t_3)(I_2\Delta_{s^*} + I_1\Delta_s) - 4\Delta t(I_1\Delta_{s^*} + I_0\Delta_s), \tag{11}$$

and

$$\Delta_s = -U(I_1\Delta_{s^*} + I_0\Delta_s) - 4\Delta t(I_2\Delta_{s^*} + I_1\Delta_s), \tag{12}$$

where

$$I_l \equiv \frac{1}{N_s}\sum_{\mathbf{k}} \frac{[\cos(k_xa) + \cos(k_ya)]^l}{2E_{\mathbf{k}}}\tanh\left(\frac{E_{\mathbf{k}}}{2k_BT}\right).$$

Notice that given n_h and T, Eqs. (8) and (10) have to be solved together for μ and Δ_d. Analogously, Eqs. (8), (11), and (12) should be solved simultaneously for μ, Δ_s and Δ_{s^*}. In particular, the critical temperature T_c is determined by $\Delta_s(T_c) = \Delta_{s^*}(T_c) = 0$, or $\Delta_d(T_c) = 0$. It is worth mentioning that within the generalized Hubbard model the condition for d-channel gap can be obtained by rewriting conveniently Eq. (10) as

$$1 = -\frac{(V - 4\Delta t_3)}{2N_s}\sum_{\mathbf{k}} \frac{[\cos(k_xa) - \cos(k_ya)]^2}{\sqrt{(\epsilon(\mathbf{k}) - \mu)^2 + \Delta_d^2(\cos k_xa - \cos k_ya)^2}} \times\tanh\left(\frac{E_{\mathbf{k}}}{2k_BT}\right), \tag{13}$$

where the fact that k_x and k_y are dummy variables has been used. Notice that the sum in Eq. (13) is always positive since $E_{\mathbf{k}}/(2k_BT) > 0$. Therefore, the necessary condition for a solution of Δ_d is $4\Delta t_3 - V > 0$, which coincides with that for a single pair [17].

3. The results

In this communication, the s- and d-wave superconducting states are analyzed by looking at their critical temperature (T_c), the superconducting gaps (Δ_s,Δ_{s^*}, or Δ_d), and the single-excitation energy gap (Δ_0) that is defined as the minimum value of $E_{\mathbf{k}}$, given by Eq. (9), with $\Delta_d[\cos(k_xa) - \cos(k_ya)]$ evaluated at the antinode [23]. In Fig. 1(a) T_c of the d-channel and Fig. 1(b) T_c of the s-channel, both as functions of Δt_3, are shown for a system with $U = 6|t_0|$, $V = 0$, $t'_0 = 0.45t_0$, $\Delta t = 0.5|t_0|$, $t_\perp = 0$, and $n_h = 0.2$. A logarithmic analysis of Fig. 1(a) suggests the non-existence of a

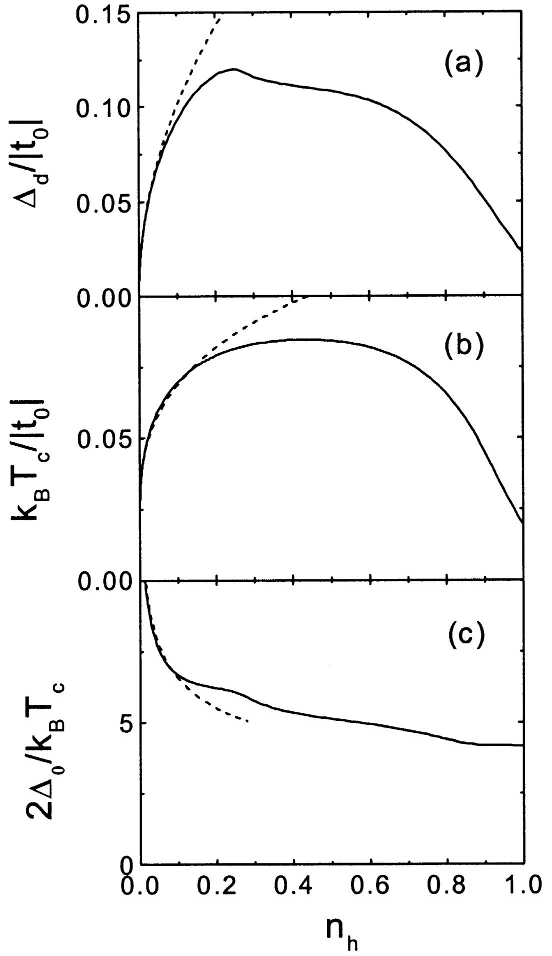

Fig. 2. The d-channel (a) superconducting gap (Δ_d), (b) superconducting critical temperature (T_c) and (c) gap ratio $[2\Delta_0/(k_BT_c)]$ versus the hole concentration (n_h) are shown for the same system as in Fig.1 with a fixed $\Delta t_3 = t_0'/4$.

minimum value of Δt_3 in the d-channel. Nevertheless, the maximum negative value of $\partial T_c/\partial(\Delta t_3)$ occurs at $\Delta t_3 = t_0'/(4-2n_h) = 0.125|t_0|$, which corresponds to the change of sign of t'. On the other hand, for a given value of T_c, the required Δt_3 is much smaller for the d-channel than that for the s one. This fact is relevant since small values of Δt_3 are expected in real systems as discussed previously. It is worth mentioning that the maximum value of the s-channel's T_c depends strongly on the value of U, while the d-channel's one does not.

In Fig. 2(a)–(c), the d-channel superconducting gap (Δ_d), the critical temperature (T_c) and the gap ratio $[2\Delta_0/(k_BT_c)]$ versus the hole concentration (n_h) are, respectively, shown for the same system as in Fig. 1 with a fixed $\Delta t_3 = t_0'/4$. The values of Δt and Δt_3 are chosen to minimize the kinetic energy of the pairs. In this case, for the low density regime ($n_h \ll 1$) analytical results can be obtained, since $\epsilon(\mathbf{k}) \to 0$, and they are

$$\Delta_d = 2\left(\Delta t_3 - \frac{V}{4}\right)\sqrt{2n_h}, \tag{14}$$

$$k_BT_c = \frac{(4\Delta t_3 - V)(1-n_h)}{4\tanh^{-1}(1-n_h)}, \tag{15}$$

$$\frac{2\Delta_0}{k_BT_c} = \frac{2\ln\left(\frac{2-n_h}{n_h}\right)}{1-n_h}, \tag{16}$$

as indicated by dashed lines in Fig. 2. Indeed, for $n_h = 0$, the chemical potential at zero temperature is half of the hole-singlet binding energy [17]. Note that the gap ratio in the dilute limit is independent of the parameters as found in Ref. [24]. In general, T_c and Δ_d rise initially as n_h increases, because the attractive interaction grows with the Fermi surface size. However, for high hole densities, the decreasing of the Δt_3 term in Eq. (4) together with the nearest-neighbor and next-nearest-neighbor hoppings renormalization, causes superconductivity to disappear. Also, notice that in the low density limit the gap ratio reaches very high values in comparison with 3.57 predicted by the BCS theory [25], and it decreases as hole density grows in concordance with experimental data [26]. Furthermore, around $n_h = 0.25$ a slight change of behavior is observed in Fig. 2(a) and (c), since below this density of holes the chemical potential is lower than the minimum of the single-hole band, as found in Ref. [24]. For a Δt_3 lower than $t_0'/4$ the general behavior of T_c versus n_h is sharper than that shown in Fig. 2. Moreover, the maximum of T_c diminishes and shifts to lower densities when Δt_3 decreases.

The effects of the dimensionality on the superconducting state are shown in Fig. 3(a)–(c), corresponding to the same quantities as in Fig. 2(a)–(c), respectively, except they are versus the interplane hopping strength ($t_{0\perp}$). Two cases are considered: isotropic $t_\perp = t_{0\perp}$ (open circles) and anisotropic $t_\perp = t_\perp(\mathbf{k})$ (open squares) ones. For high-T_c materials, band structure calculations yield $t_\perp(\mathbf{k}) = (t_{0\perp}/4)[\cos(k_xa_\perp) - \cos(k_ya_\perp)]^2$ so that interplane coupling is dominated by states near the $(\pm\pi,0)$ and $(0,\pm\pi)$ points of the Brillouin zone at which the superconducting gap is maximal [27]. It is observed that in general the superconducting state is weakened by increasing $t_{0\perp}$, being the effects more pronounced for the isotropic case.

Fig. 4 shows the temperature dependence of the gap ratio $[2\Delta_0/(k_BT_c)]$ for the same system as in Fig. 2(c) (solid line), in comparison to the s-wave one obtained from a negative-U Hubbard model with $t_0' = 0.45t_0$, $U = -2|t_0|$, $V = \Delta t = \Delta t_3 = t_\perp = 0$ (dashed line), both for a hole density $n_h = 0.5$. It is worth mentioning that the gap ratio of a negative-U Hubbard model is essentially independent of U, and it is very close to the BCS prediction, even though in the former case the attractive interaction is uniform on the whole $\mathbf{k}$ space. In the inset of Fig. 4, the normalized gap ratios for the same systems as in the main plot are comparatively

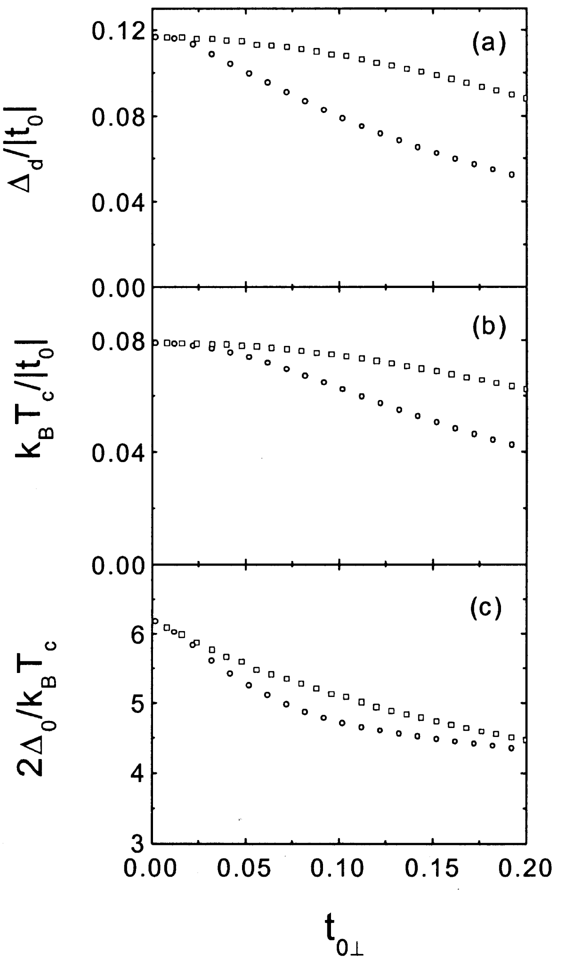

Fig. 3. The d-channel (a) superconducting gap (Δ_d), (b) superconducting transition temperature (T_c) and (c) gap ratio $[2\Delta_0/(k_B T_c)]$ versus the interplane hopping strength ($t_{0\perp}$) for both isotropic (open circles) and anisotropic (open squares) cases are shown for the same system as in Fig. 2 with a fixed $n_h = 0.2$.

shown. Observe that the temperature-dependence behavior of a d-channel superconducting state is quite different from the s-one, similar conclusions can be obtained from Ref. [28].

In Fig. 5, a ground-state phase diagram for a system with $U = \Delta t = 0$, $t_0' = 4\Delta t_3$, and $n_h = 1$ is presented in order to analyze the competition between the superconducting state and the phase separation, where holes doubly occupy a macroscopic region of the system to minimize the energy, when a negative-V is considered. The energy of the phase-separated state has been calculated as it is done in Ref. [29]. In particular, this system has been chosen for analysis since the starting point, i.e. $\Delta t_3 = 0$, reproduces part of fig. 8 of Ref. [29]. We can observe that the presence of Δt_3 enhances the d-wave superconductivity and enlarges the d-channel superconducting zone, which could be important since the

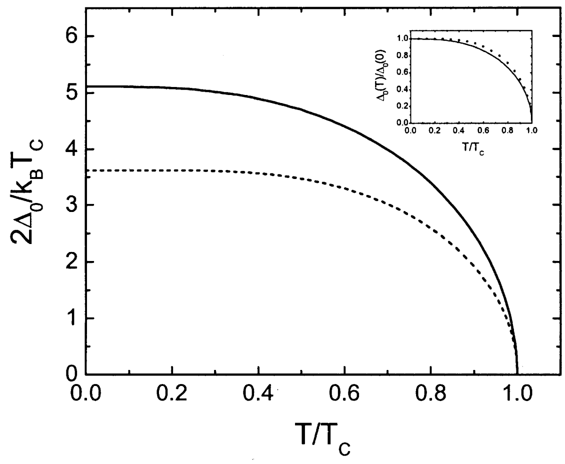

Fig. 4. The temperature dependence of the gap ratio $[2\Delta_0/(k_B T_c)]$ for the same system as in Fig. 2(c) (solid line), in comparison to the s-wave one obtained from a negative-U Hubbard model with $t_0' = 0.45 t_0$, $U = -2|t_0|$, $V = \Delta t = \Delta t_3 = t_\perp = 0$ (dashed line), both for a hole density $n_h = 0.5$. In the inset, the corresponding normalized gap ratios are shown.

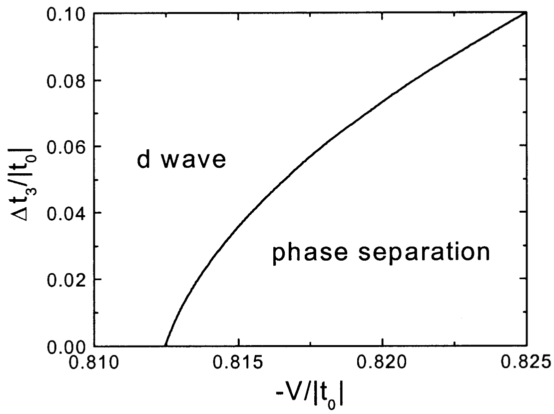

Fig. 5. Ground-state phase diagram for a system with $U = \Delta t = 0$, $t_0' = 4\Delta t_3$, and $n_h = 1$.

phase separation would dominate over the superconducting phase as V grows (Fig. 5).

4. Conclusions

We have studied the principal features of the superconducting ground state within a generalized Hubbard model, in which a second-neighbor correlated-hopping term is included. In spite of its smaller strength in comparison with other terms of the model, we have found its key participation in the formation of the d-channel superconducting state. In particular, we have shown that, within this model, a d-symmetry superconducting ground state with relatively high T_c is suitable for small values Δt_3, in contrast to the higher values required in the *s*-channel. Furthermore, the *d*-wave superconducting state is not sensitive to the on-site repulsion as occurs for the *s*-wave one.

In comparison with the negative-V Hubbard model, the second-neighbor correlated hopping extends the *d*-wave superconduction to the low hole-density region, in agreement with that observed in experiments [26]. Furthermore, Δt_3 enhances the *d*-channel superconductivity in the competition with the phase separation. On the other hand, the *d*-wave superconducting state has a normalized gap ratio $[\Delta_0(T)/\Delta_0(0)]$ differing from that of the BCS theory. Moreover the superconductivity is in general favored by the low dimensionality of the system, and the *d*-channel one is not an exception.

In summary, the present study has shown that terms usually ignored in the Hubbard model could be relevant in certain phenomena, such as the *d*-channel superconductivity. Finally, this study is suitable to analyze real materials by including specific parameters and then compare closely with the experimental data, which is currently in progress.

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