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Effects of the Correlated Hopping on the *d*-Wave Superconductivity

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A $d_{x^2-y^2}$ superconducting ground state has been obtained within a two-dimensional (2D) generalized Hubbard model, in which a next-nearest-neighbor correlated-hopping interaction is included. In spite of its smaller strength in comparison with other terms of the model, we found its key participation in the *d*-channel hole pairing. The hole singlet ground-state phase diagram shows a large *d*-symmetry pairing region that is enhanced by the on-site repulsive Coulomb interaction. For finite density of holes (n_h), the mean-field BCS theory is applied to the model. The results show a maximum *d*-wave critical temperature (T_c) around n_h = 0.35, and this T_c is favored by the presence of an antiferromagnetic background.

KEY WORDS: *d*-wave superconductivity; generalized Hubbard model; two-hole bound states.

1. INTRODUCTION

The two-dimensional (2D) Hubbard model has attracted much attention since the discovery of anisotropic cuprate superconductors. Features like the short coherence length and the bidimensional behavior of the carriers can be addressed properly by this locally correlated electronic model. In order to describe the electron and hole dynamics on the CuO planes, three-band Hubbard models have been proposed [1], and these models can be reduced into single-band Hubbard models [2] in which a next-nearest-neighbor hopping (t'_0) is included [3]. In spite of no general consensus on the high-T_c superconducting mechanism, important features have been well established, such as the singlet pairing between holes (instead between electrons) and clear $d_{x^2-y^2}$ symmetry gaps in several superconducting compounds [4,5]. However, no *d*-symmetry pairing indication has been found within the usual generalized Hubbard models [6].

In this paper, we consider a generalized single-band Hubbard model in which hopping (t'_0) and correlated hopping interaction (Δt_3) between next-nearest neighbors are included. We analyze the importance of the correlated hopping interaction Δt_3 in the formation of $d_{x^2-y^2}$ pairing ground state, in spite of its apparently small strength in comparison with direct Coulomb interactions. In Section 2, the Hamiltonian and the mapping method are briefly discussed. The hole singlet ground-state phase diagram for the case $t'_0 = 4\Delta t_3$ is analyzed in Section 3. In Section 4, we present the $d_{x^2-y^2}$ symmetry solution of the BCS mean-field equations and examine the dependence of critical temperature on hole density, including the case of an antiferromagnetic background. Finally, conclusions are given in Section 5.

2. THE MODEL

The extended Hubbard model considers only the on-site (U) and nearest neighbor (V) Coulomb interactions. The inclusion of a nearest-neighbor correlated-hopping (Δt) leads to an extended *s*-wave superconductivity, without negative U and V [7]. In this paper, we consider a generalized Hubbard model that also includes a next-nearest-neighbor hopping (t') and correlated hopping interaction (Δt_3). In general, the contribution of these interactions are very different; for example, for 3d electrons in transition metals

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U, V, Δt, and Δt_3 are typically about 20, 3, 0.5, and 0.1 eV, respectively [8,9].

The single-band generalized Hubbard Hamiltonian can be written as

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

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. When an electron-hole transformation is made in equation (1), i.e., electron operators are mapped onto hole's via $c^+_{i,\sigma} \to h_{i,\sigma}$, the Hamiltonian becomes:

$$H = (U + 2ZV)\left(N_s - \sum_{i,\sigma} n^h_{i,\sigma}\right) + (t_0 - 2\Delta t) \sum_{\langle i,j \rangle} h^+_{i,\sigma} h_{j,\sigma} + (t'_0 - 4\Delta t_3) \sum_{\langle\langle i,j \rangle\rangle,\sigma} h^+_{i,\sigma} h_{j,\sigma} + U \sum_i n^h_{i,\uparrow} n^h_{i,\downarrow} + \frac{V}{2} \sum_{\langle i,j \rangle} n^h_i n^h_j + \Delta t \sum_{\langle i,j \rangle} h^+_{i,\sigma} h_{j,\sigma} (n^h_{i,-\sigma} + n^h_{j,-\sigma}) + \Delta t_3 \sum_{\langle i,l \rangle,\langle j,l \rangle,\langle\langle i,j \rangle\rangle,\sigma} h^+_{i,\sigma} h_{j,\sigma} n^h_l, \quad (2)$$

where $n^h_{i,\sigma} = h^+_{i,\sigma} h_{i,\sigma}$, $n^h_i = n^h_{i,\uparrow} + n^h_{i,\downarrow}$, N_s is the total number of sites, and Z is the lattice coordination number. The first term in equation (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 $t_h = t_0 - 2\Delta t$ and $t'_h = t'_0 - 4\Delta t_3$, instead of $-t_0$ and $-t'_0$ for electrons.

When the correlated hopping interactions are introduced, the previously developed mapping method [10] should be extended. This method allows to map the problem of electronic correlation into a tight-binding one with impurities and therefore, the correlated states correspond to those impurity states with negative self-energies U and V [11]. In our case, for a generalized Hubbard model, the correlated electronic states are originated from the enhanced bonds (bond-impurities), with *or* without negative U or V. Therefore, the two-particle wavefunction will be localized around these impurity bonds [12]. The main features of the two-particle correlated states will be analyzed in section 3.

3. HOLE PAIRING

The hole-singlet ground-state phase diagrams shown in Fig. 2 are calculated for $U = 0$ (Fig. 1A) and $U = 10|t_0|$ (Fig. 1B), both with $V = 0$ and $t'_0 = 4\Delta t_3$. The numeric calculations are performed in a truncated square lattice of 2401 mapped states [11]. Notice that for $U = 0$, there is no d-symmetry pairing for small Δt_3, and as the on-site Coulomb repulsion U increases, the $d_{x^2-y^2}$ pairing zone is enlarged. For $U = 10|t_0|$, the s-wave pairing is essentially avoided for positive Δt_3. It is somewhat expected because the on-site repulsion U inhibits the formation of s-symmetry pairs and does not affect the d ones; therefore, it favors the formation of $d_{x^2-y^2}$ pairing ground state. Furthermore, the $d_{x^2-y^2}$ pairing requires $\Delta t_3 > 0$, regardless of how small it is, in the large U limit. This

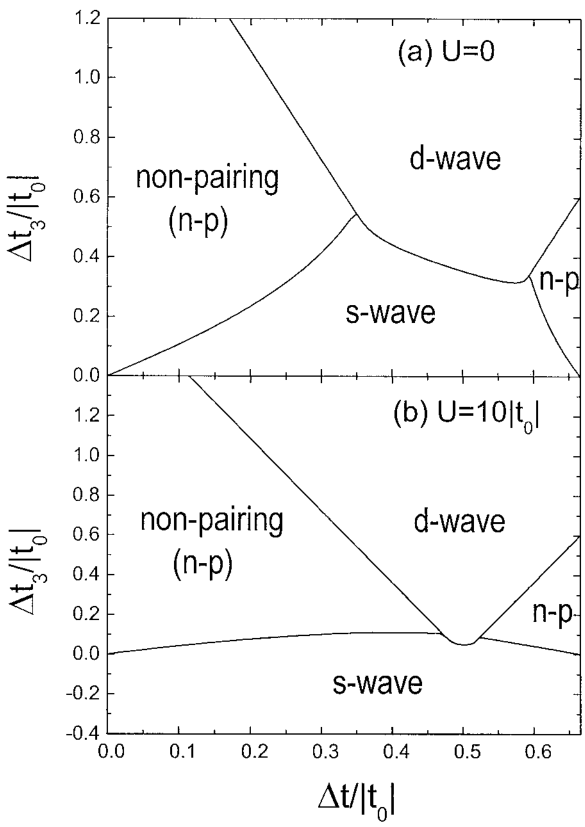

Fig. 1. Hole-singlet ground-state phase diagrams of the generalized Hubbard model with $V = 0$, $t'_0 = 4\Delta t_3$, and (a) $U = 0$ and (b) $U = 10\,|t_0|$.

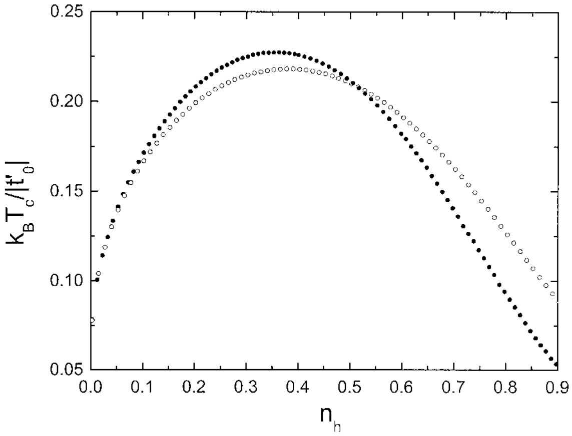

Fig. 2. Dependence of the critical temperature (T_c) on the hole density (n_h) for systems with (solid circles) and without (open circles) an antiferromagnetic background, both characterized by $\Delta t = 0.5|t_0|$, $\Delta t_3 = 0.25|t'_0|$, $|t'_0| = 0.25|t_0|$, $U = 10|t_0|$, and $V = 0$.

result confirms the fact that the correlated hopping Δt alone can give rise only to extended s-wave pairing [6]. Finally, the phase-transition lines between d wave and nonpairing can be obtained analytically, and are given by $\Delta t_3 = 1.83|t_0 - 2\Delta t|$.

4. FINITE HOLE DENSITY

In this section, the d-wave superconductivity is analyzed within the generalized Hubbard model by using the BCS theory, in which the reduced Hamiltonian [13] can be written as

$$H - \mu N = \sum_{\mathbf{k},\sigma} (\varepsilon(\mathbf{k}) - \mu)\, h^+_{\mathbf{k},\sigma} h_{\mathbf{k},\sigma} + \frac{1}{N_s} \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{kk}'\mathbf{0}}\, h^+_{\mathbf{k},\uparrow} h^+_{-\mathbf{k},\downarrow} h_{-\mathbf{k}',\downarrow} h_{\mathbf{k}',\uparrow}, \quad (3)$$

where μ is the chemical potential. In particular, for the generalized Hubbard model we have

$$\varepsilon(\mathbf{k}) = \left(\frac{U}{2} + ZV\right) n_h - U - 2ZV + 2(t_h + n_h \Delta t)(\cos(k_x a) + \cos(k_y a)) + 4(t'_h + 2n_h \Delta t_3) \cos(k_x a) \cos(k_y a),$$

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

where $\beta(\mathbf{k}) = 2(\cos(k_x a) + \cos(k_y a))$, $\gamma(\mathbf{k}, \mathbf{k}') = 4\cos(k_x a)\cos(k'_y a) + 4\cos(k'_x a)\cos(k_y a)$ and $2\mathbf{q}$ is the wave-vector of the pair center of mass. Notice that the dispersion relation $\varepsilon(\mathbf{k})$ 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_h, t'_h and the self-energy, respectively. These terms are obtained from a normal Hartree–Fock decoupling of the interaction terms in Eq. (2). At a finite temperature T, the equations for determining the superconducting gap and the chemical potential [14] are

$$\Delta_{\mathbf{k}} = -\frac{1}{N_s}\sum_{\mathbf{k}'} V_{\mathbf{kk}'\mathbf{0}} \frac{\Delta_{\mathbf{k}'}}{2E_{\mathbf{k}'}} \tanh\left(\frac{E_{\mathbf{k}'}}{2k_B T}\right) \quad (5)$$

$$n_h - 1 = -\frac{1}{N_s}\sum_{\mathbf{k}'} \frac{\varepsilon(\mathbf{k}') - \mu}{E_{\mathbf{k}'}}[1 - 2f(E_{\mathbf{k}'})] \quad (6)$$

where $E_{\mathbf{k}} = \sqrt{(\varepsilon(\mathbf{k}) - \mu)^2 + \Delta^2_{\mathbf{k}}}$ and $f(E)$ is the Fermi–Dirac distribution. In our case, the d-wave superconducting gap is given by $\Delta_{\mathbf{k}} = \Delta_d(\cos(k_x a) - \cos(k_y a))$. Therefore, after some algebra, Eq. (5) becomes

$$1 = -\frac{(V - 4\Delta t_3)}{N_s}\sum_{\mathbf{k}} \frac{\cos(k_x)[\cos(k_x) - \cos(k_y)]}{E_{\mathbf{k}}} \tanh\left(\frac{E_{\mathbf{k}}}{2k_B T}\right). \quad (7)$$

Observe that Eqs. (6) and (7) are coupled integral equations and have been solved numerically for both cases with and without an antiferromagnetic background.

Let us consider a half-filled single-band generalized Hubbard square-lattice system (i.e., one electron per site). Due to the presence of an effective Coulomb repulsion U_{eff}, a charge-transfer gap appears and the system becomes an antiferromagnet [1]. When a hole singlet is introduced in the fully filled lower Hubbard band (i.e., two holes with opposite spins in a quantum antiferromagnet), each hole can move only in one of the two sublattices of the system [15]. Therefore, the terms of $(t_0 - 2\Delta t)$, U and Δt in Eq. (2) have no effects on the pairing process.

In Fig. 2, the critical temperature T_c, determined by $\Delta_d(T_c) = 0$, as a function of the hole density (n_h) is shown for $\Delta t = 0.5|t_0|$, $\Delta t_3 = 0.25|t'_0|$, $|t'_0| = 0.25|t_0|$, and $U = 10|t_0|$. The values of Δt and Δt_3 are chosen to minimize the kinetic energy of the pairs. Notice that T_c is expressed in units of t'_0, instead of t_0 because t_0 is absent in the case of an antiferromagnet. Furthermore, T_c rises initially as n_h increases, because the attractive interaction grows with the Fermi surface size. However, for high hole densities, the decreasing of Δt_3 term in Eq. (4) dominates. Observe also that the maximum T_c corresponds to those with an antiferromagnetic background (solid circles) (i.e., antiferromagnets enhance the d-wave superconductivity), and their changes are more drastic due to the absence of the Δt term in the effective Hamiltonian.

5. CONCLUSIONS

In summary, we studied the hole-pairing symmetry within the 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 found its key participation in the *d*-channel hole pairing. Furthermore, a mean-field BCS analysis of the *d*-wave superconducting state within the generalized Hubbard model has shown essentially the same results that the second-neighbor correlated-hopping enhances the *d*-symmetry pairing. The maxima T_c observed around $n_h = 0.35$ in Fig. 2 is close to those obtained from the experimental data [1], considering the simplicity of the model. Moreover, the importance of an antiferromagnetic background has been also evident. Finally, the present study has shown that terms usually ignored in the Hubbard model could be relevant in certain phenomena, such as the *d*-wave superconductivity.

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