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Doping-dependent superconducting symmetry in Hubbard systems

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The d-wave superconducting state is studied by using a generalized Hubbard model, in which a next-nearest-neighbor correlated-hopping interaction (Δt_3) is included. The results obtained within the BCS framework suggest the existence of a critical hole concentration, below which a $d_{x^2-y^2}$-wave superconducting gap is observed. However, above this critical concentration the maxima of the single-particle excitation energy gap are rotated by $\pi/4$ and no real nodes exist, as observed in tunneling experiments. In this study, the parameters estimated by first-principle calculations for cuprate superconductors are used.

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1. INTRODUCTION

During the last ten years a considerable number of experiments, including phase-sensitive ones and angle-resolved photoemission spectroscopy (ARPES), have suggested a $d_{x^2-y^2}$ symmetry superconducting gap in many cuprate superconductors.[1] However, the scanning tunneling microscope spectroscopy reveals controversial results. In particular, Kane and Ng observed[2] a gap minimum of 20 meV along the Cu-Cu direction and a gap maximum of 35 meV along the Cu-O direction indicating a d_{xy}-like symmetry with non-zero nodes, in contrast with what has been observed in ARPES experiments.[3] Although some explanations have been considered no consensus has emerged about this $\pi/4$ difference.[4]

On the other hand, it is widely accepted[5] that the single-band Hubbard model is an appropriate starting point to describe the electronic correlations on the CuO_2 planes, although the nonexistence 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 in the low density limit.[7] Recently, we have analyzed the two-hole problem,[8] finding an important participation of the second-neighbor correlated-hopping interaction (Δt_3) in the formation of $d_{x^2-y^2}$ symmetry hole singlets, in spite of its small strength in comparison with direct Coulomb repulsions. Moreover, for finite densities of holes, the transition temperature and the superconducting gap are analyzed within the BCS framework.[9] In this paper, we start directly from a generalized Hubbard model for holes and use parameters obtained from first principles calculations. The results of the single-particle excitation energy gap are compared with the experimental data.

2. THE MODEL

The on-site (U), nearest-neighbor (V) Coulomb interactions, and a nearest-neighbor correlated-hopping interaction (Δt) are considered in the usual generalized Hubbard model.[7] In this work, we include additionally a second-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.[10,11] The band structure of several high-Tc superconductors, observed by using ARPES[12] and reproduced by LDA-density functional theory,[13] can be reasonably well described by a square-lattice single-band tight-binding model with a next-nearest-neighbor hopping parameter t_0', which value is t_0'=$0.45t_0$ for YBaCuO,[14] and t_0'=$0.30t_0$ for BiSrCaCuO,[13] being the nearest-neighbor hopping (t_0) along the Cu-O bonds.

A single-band generalized Hubbard Hamiltonian for holes in a square lattice with lattice parameter a can be written as

$$H = -t_0 \sum_{<i,j>,\sigma} c_{i,\sigma}^{+} c_{j,\sigma} + t_0' \sum_{<<i,j>>,\sigma} c_{i,\sigma}^{+} c_{j,\sigma} + U \sum_i n_{i,\uparrow} n_{i,\downarrow} + \frac{V}{2} \sum_{<i,j>} n_i n_j$$

$$+\Delta t \sum_{<i,j>,\sigma} c_{i,\sigma}^{+} c_{j,\sigma} (n_{i,-\sigma} + n_{j,-\sigma}) + \Delta t_3 \sum_{<i,l>,<j,l>,\ll i,j \gg,\sigma} c_{i,\sigma}^{+} c_{j,\sigma} n_l, \quad (1)$$

where $c_{i,\sigma}^{+}$ ($c_{i,\sigma}$) is the creation (annihilation) operator of holes with spin σ=$\downarrow$ or $\uparrow$ at site i, $n_{i,\sigma}$=$c_{i,\sigma}^{+} c_{i,\sigma}$, n_i=$n_{i,\uparrow}$+$n_{i,\downarrow}$, $< i,j >$ and $\ll i,j \gg$ denote respectively the nearest-neighbor and the next-nearest-neighbor sites.

At a finite temperature T, the equations for determining the d-wave superconducting gap ($\Delta_{\mathbf{k}} = \Delta_d\,[\cos(k_x a) - \cos(k_y a)]$) and the chemical potential (μ) are[9]

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

$$n - 1 = -\frac{1}{N_s}\sum_{\mathbf{k}} \frac{\varepsilon(\mathbf{k}) - \mu}{E_{\mathbf{k}}} \tanh\left(\frac{E_{\mathbf{k}}}{2k_B T}\right), \quad (3)$$

where n is the density of holes per site, N_s is the total number of sites, the single-particle excitation energy ($E_{\mathbf{k}}$) is given by

$$E_{\mathbf{k}} = \sqrt{[\varepsilon(\mathbf{k})-\mu]^2 + \Delta_d^2\,[\cos(k_x a) - \cos(k_y a)]^2}. \quad (4)$$

and

$$\begin{aligned}\varepsilon(\mathbf{k}) &= \left(\frac{U}{2} + ZV\right) n + 2(-t_0 + n\Delta t)\,[\cos(k_x a) + \cos(k_y a)] \\ &\quad +4(t_0' + 2n\Delta t_3)\cos(k_x a)\cos(k_y a). \quad (5)\end{aligned}$$

Notice that given n and T, equations (2) and (3) should be solved simultaneously for μ and Δ_d. In particular, the critical temperature T_c is determined by the condition $\Delta_d(T_c) = 0$.

3. RESULTS

In Fig. 1, the d-wave superconducting critical temperature (T_c) as a function of the hole concentration (n) is shown for a system with U=10t_0, V=0, and Δt=0.5t_0. Observe that there is a maximum of T_c for each pair of Δt_3 and t_0'. These maximums decrease with the diminution of Δt_3, and the optimum n shift to lower densities when t_0' grows. It is worth mentioning that in this model the gap ratio ($2\Delta_0/k_B T_c$) increases when the hole density diminishes,[9] in agreement with experimental results.[15]

The angular dependence of the single-excitation energy gap [$\Delta_0(\theta)$] is analyzed in Fig. 2(a) for U=10t_0, V=0, Δt=0.5t_0, Δt_3=0.1t_0, t_0'=0.4t_0, $t_0 = 2.2eV$ and n=0.226. The polar angle is given by θ=$\tan^{-1}(k_y/k_x)$ and Δ_0 is defined as the minimum value of $E_{\mathbf{k}}$ given by Eq. (4). The theoretical energy gap (solid line) is shown in comparison with the ARPES data (solid squares).[16] Observe that there are angular nodes in $\Delta_0(\theta)$ at θ=$\pi/4$ and θ=$3\pi/4$. The condition for the existence of these nodes is $\mu \geq -t^2/t'$, which can be obtained by minimizing Eq. (4), being t=$-t_0 + n\Delta t$ and t'=$t_0' + 2n\Delta t_3$. In other words, if $\mu < -t^2/t'$, $\Delta_0(0)$ could be smaller than

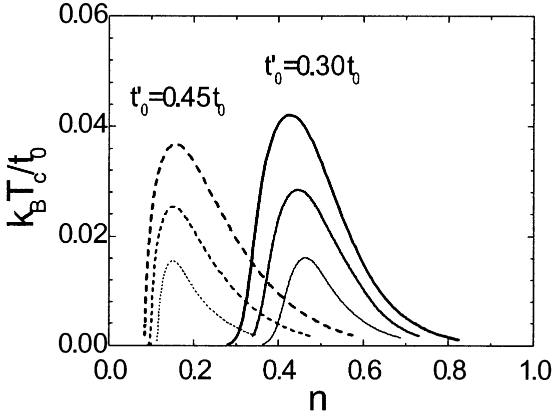

Fig. 1. The d-wave superconducting critical temperature (T_c) versus the hole concentration (n) is shown for $t'_0 = 0.3t_0$ (solid lines) and $t'_0 = 0.45t_0$ (dashed lines), where the nearest-neighbor correlated hoppings are $\Delta t_3 = 0.1t_0$ (thick lines), $0.08t_0$ (medium-width lines) and $0.06t_0$ (thin lines).

$\Delta_0(\pi/4)$, as occurred for n=0.277. This case is shown in Fig. 2(b) for the same system as in Fig. 2(a) except that n=0.277, where our results (solid line) are compared with those obtained from tunneling spectroscopy (solid circles).[2] Notice that the maxima of $\Delta_0(\theta)$ in Fig. 2(b) are rotated by $\pi/4$ with respect to those in Fig. 2(a), showing a doping-dependent energy gap symmetry, as suggested by Yeh, *et al.*[15]

4. CONCLUSIONS

We have studied the superconducting ground state 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 have found its key participation in the formation of the d-wave superconducting state. Furthermore, this model predicts the existence of both $d_{x^2-y^2}$- and d_{xy}-symmetry single-particle excitation energy gaps depending on the hole density. In particular, the d_{xy}-oriented gap has no real nodes, as observed in the tunneling spectroscopy experiments.[2,17]

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-wave superconductivity. It is worth mentioning that the three-site correlated hopping term derived from a strong coupling expansion of the U term has a negative sign,[18] which inhibits the d-wave superconductivity.[19]

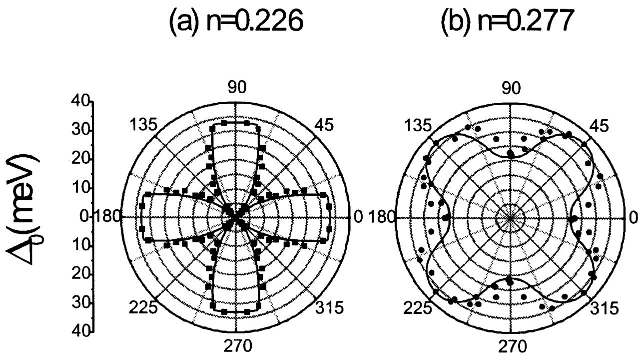

Fig. 2. Calculated single-particle excitation energy gap (Δ_0) (solid lines) as a function of the polar angle for $t'_0 = 0.4t_0$, $\Delta t_3 = 0.1t_0$, and the hole densities (a) $n = 0.224$ and (b) $n = 0.277$, in comparison with the ARPES (solid squares) and tunneling (solid circles) results.

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