Pairing correlations in a generalized Hubbard model for the cuprates

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Using numerical diagonalization of a 4×4 cluster, we calculate on-site *s*, extended-*s*, and $d_{x^2-y^2}$ pairing correlation functions (PCF's) in an effective generalized Hubbard model for the cuprates, with nearest-neighbor correlated hopping and next-nearest-neighbor hopping t'. The vertex contributions to the PCF's are significantly enhanced, relative to the t-t'-U model. The behavior of the PCF's and their vertex contributions, and signatures of anomalous flux quantization, indicate superconductivity in the *d*-wave channel for moderate doping and in the *s*-wave channel for high doping and small *U*.

I. INTRODUCTION

Since the discovery of high-temperature superconductivity, much effort has been devoted to studying the properties of the Hubbard model, the t-J model, and modifications of them. While these studies have helped to clarify several optical and magnetic properties of the cuprates,[1,2] the superconducting mechanism remains unclear. Studies in generalized t-J models suggest a magnetic origin of superconductivity,[3–7] but the numerical results seem to require either a superexchange J, or a three-site term,[4,7] which is beyond the realistic range for the cuprates. In addition, the constraint of no double occupancy in these models reduces the mobility of the superconducting pairs.[8,9] On the other hand, the search for signals of superconductivity in the Hubbard model have been negative so far.[1,10,11] This fact stimulates the study of modifications of the Hubbard model which represent more closely the physics of the cuprates.[12] Recently an effective modified Hubbard model for the cuprates derived earlier[13] has been studied.[12] The model includes a nearest-neighbor (NN) correlated hopping which depends on the occupation of the two sites involved and next-NN hopping t'. Within a mean-field approximation,[12] the correlated hopping has been found to originate pairing, the underlying mechanism being similar to that provided by a superexchange coupling J.[12,14] The shape of the Fermi surface and the positions of the van Hove singularities (vHS), modified with t', influence the magnitude and the symmetry of the order parameter. The expected instability for moderate dopings, is *d*-wave superconductivity in concurrence with a spin-density wave (SDW) near half-filling.

Here we report results on pairing correlation functions (PCF's) and spin-correlation functions for this effective model, obtained by numerical diagonalization of a square cluster containing $L=16$ unit cells. We find evidence of strong superconducting correlations with $d_{x^2-y^2}$ symmetry in the doping regime of interest for the cuprates. Furthermore, in contrast to the case of the ordinary Hubbard model, we find indications of anomalous flux quantization (AFQ), characteristic of superconductivity,[15] in most of the explored region of parameters. Our numerical results support the mean-field picture. The size of the cluster and the inclusion of t' made the calculation particularly difficult. To our knowledge, even with $t'=0$, no exact PCF's have been so far reported in this cluster allowing doubly occupied sites.

The model is briefly explained in Sec. II. Section III contains our main results. In Sec. IV we present spin correlations which bring useful complementary information. Section V contains a short discussion.

II. THE EFFECTIVE MODEL

The effective one-band model for the cuprates is[13]

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

where $\langle ij\rangle(\langle ij'\rangle)$ denotes NN (next-NN) positions of the lattice. The model was derived from a low-energy reduction of the three-band model for the cuprates. U represents the cost in energy of constructing a Zhang-Rice singlet from two singly occupied cells. t_{AA} represents the hopping of a Zhang-Rice singlet to a singly occupied NN cell. The terms with amplitude t_{AB} correspond to the 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. While U lies between 3 and 4 eV, the magnitude of the correlated hopping terms is ten times smaller, and $t_{AB}\sim10\%$ larger than $(t_{AA}+t_{BB})/2$ has been estimated.[13] However, for other parameters of the multiband model, this ratio can be much larger, since t_{AB} is linear in the Cu-O hopping t_{pd}, while $t_{AA},t_{BB}\sim t_{pd}^2$.[12] In the mean field, for $t_{AB}>t_{AA},t_{BB}$, superconductivity in the *s*- and *d*-wave channels is obtained.[12] Near half filling, *d*-wave superconductivity competes with the SDW. If $t'=0$, the SDW takes place at $n=1$ while finite t' destroys perfect nesting, and for doping such that vHS lie near the Fermi level, *d*-wave superconductivity coexisting with short-range antiferromagnetic fluctuations is expected. Instead, *s*-wave superconductivity develops for small U and sufficiently small particle densities n. Although vHS are not well defined in a

small cluster, t' introduces changes in the distribution of the particles in k space and conclusions concerning the tendencies in the behavior of the PCF can be extracted. We restrict to the electron-hole symmetric case $t_{AA}=t_{BB}=1$ and large $t_{AB}\geqslant 2$, in order to render more noticeably the effects of the correlated hopping. We also investigate $t'=0,-0.45$.[16]

III. PAIRING CORRELATION FUNCTIONS

The PCF's are

$$P_\alpha(i)=\langle \Delta_\alpha^\dagger(i)\Delta_\alpha(0)\rangle, \tag{2}$$

where for on-site s pairing $\Delta_{os}^\dagger(i)=c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger$, while $\Delta_\alpha^\dagger(i)=\Sigma_\delta f_\alpha(\delta)[c_{i+\delta\uparrow}^\dagger c_{i\downarrow}^\dagger - c_{i+\delta\downarrow}^\dagger c_{i\uparrow}^\dagger]/\sqrt{8}$, with $f_{es}(\delta)=1$ for extended s pairing, and $f_d(\delta)=1[f_d(\delta)=-1]$ when $\delta=\pm(1,0)$ $[\delta=\pm(0,1)]$ for $d_{x^2-y^2}$ pairing. We normalize $\Delta_\alpha^\dagger(i)$ in such a way that $|\Delta_\alpha^\dagger(i)|0\rangle|^2=1$, to facilitate comparison among the different PCF's.[17] To compute the vertex contribution to the PCF,[18] denoted as $\overline{P}_\alpha(i)$, the quantity $(\langle c_\lambda^\dagger c_\xi\rangle\langle c_\mu^\dagger c_\nu\rangle - \langle c_\lambda^\dagger c_\nu\rangle\langle c_\mu^\dagger c_\xi\rangle)$ is subtracted for every term in Eq. (2) of the form $\langle c_\lambda^\dagger c_\mu^\dagger c_\nu c_\xi\rangle$. For a BCS ground state, $\overline{P}_\alpha(i)$ is positive and proportional to the square of the order parameter. The results we show for the correlation functions correspond to ''optimum'' boundary conditions (OBC's), which could be periodic (PBC), antiperiodic, or mixed (MBC), i.e., periodic in one direction and antiperiodic in the other, according to those which lead to the minimum ground-state energy. The computation has been made possible by exploiting all symmetry operations of the space group of the square lattice[19] plus time reversal (256 operations in the cluster). Half of these operations are lost for MBC, and the reported PCF's are averages over equivalent distances in the periodic system.

To give an idea of the expected magnitude of the PCF's and in order to establish a criterion to interpret our results, we analyze the behavior of the PCF's and the vertex contribution for the usual attractive Hubbard model with a quite large attraction $U=-5$, in which case superconductivity is well supported by several calculations.[20] These quantities are displayed in Fig. 1 for $N=10$ particles and distances larger than one lattice site.[21] As in the case of previous Monte Carlo results,[11] $P_\alpha(r)$ shows oscillations with distance r, while $\overline{P}_\alpha(r)$ exhibits a smoother behavior. It is clear that $\overline{P}_{os}(r)$ dominates over the other PCF, which is in agreement with s-wave superconductivity (predominantly on-site) in the model.[20] In light of these results, we establish the following criterion to extract information from our numerical data: we conclude that superconducting correlations in the α channel are present in the model when both quantities, P_α and $\overline{P}_\alpha$, are enhanced at large distances relative to the noninteracting case.

In Fig. 2, we show the effect of t_{AB} and t' for $U=0$. The PCF $P_\alpha(r)$ (not shown) display the same qualitative behavior as those in Fig. 1(a). We conclude that for these parameters the model has strong signals of s-wave superconductivity in both on-site and NN channels. This agrees with the mean-field calculations.[12] For $N=12$ particles, the values of $\overline{P}_\alpha(r)$ (not shown) are reduced in ~ 0.01, but the qualitative behavior remains the same. For $t'=0$, the PCF's are also

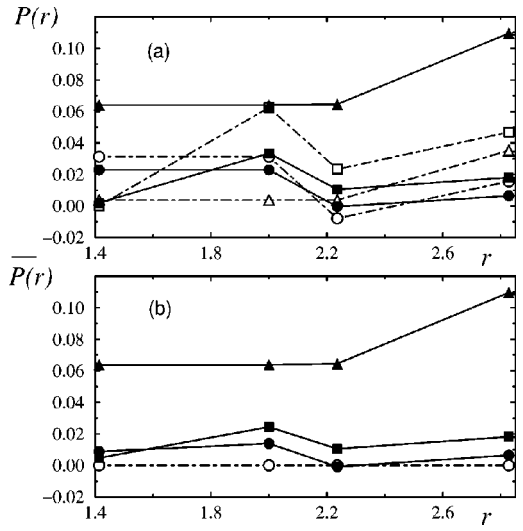

FIG. 1. (a) Pairing correlation functions and (b) vertex contributions to them as functions of distance for $U=0$ (open symbols) and $U=-5$ (solid symbols), with $t_{AB}=1$, $t'=0$, $N=10$, and PBC. Triangles, circles, and squares correspond to on-site s, extended-s, and $d_{x^2-y^2}$ PCF, respectively. Open symbols coincide in (b).

strongest in the s channel. For $N=12$, $\overline{P}_{es}(\sqrt{8})$ is approximately one half of the corresponding value for $N=10$. For both densities, a negative t' enhances $\overline{P}_{es,os}(r)$ relative to the case with $t'=0$. According to Ref. 12 when U overcomes a certain value, s-wave superconductivity is replaced by a SDW when $t'=0$ and by d-wave superconductivity for finite t'. Keeping $t'=-0.45$, $t_{AB}=2$, and increasing U, we find a decrease in the s-wave PCF's and an increase in the d-wave ones. The latter dominate already for $U=4$ and $N=10$, with $\overline{P}_d(r)\sim 0.015$ and values significantly larger than those for $t_{AB}=1$.

For $U=10$, with $t_{AB}=2$, the PCF's are much larger in the d-wave channel. The behavior of $P_d(r)$ and $\overline{P}_d(r)$ for different densities ($N/L=0.625$, 0.75, and 0.875), is shown in Fig. 3, for $t'=0,-0.45$. To simplify the figure, we do not show the values of $P_d(r)$ for $t_{AB}=1$ and for the noninteracting case. For $N=10,12$, with $t_{AB}=2$ and $t'=-0.45$, the values $\overline{P}_d(r)\sim 0.02,0.03$ [Fig. 3(d)] at distances $\sqrt{2}\leqslant r\leqslant\sqrt{8}$ are roughly half of the values of $\overline{P}_{os}(r)$ for the Hubbard model with strong on-site attraction (Fig. 1), and very

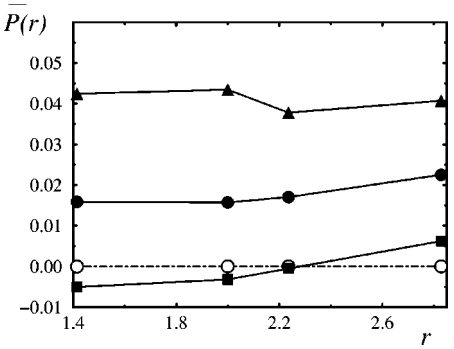

FIG. 2. Vertex contribution to the PCF for $t_{AB}=2$, $t'=-0.45t$, $U=0$, $N=10$, and PBC. For $t_{AB}=1$ (open circles) $\overline{P}_\alpha(r)=0$. Symbols are the same as in Fig. 1.

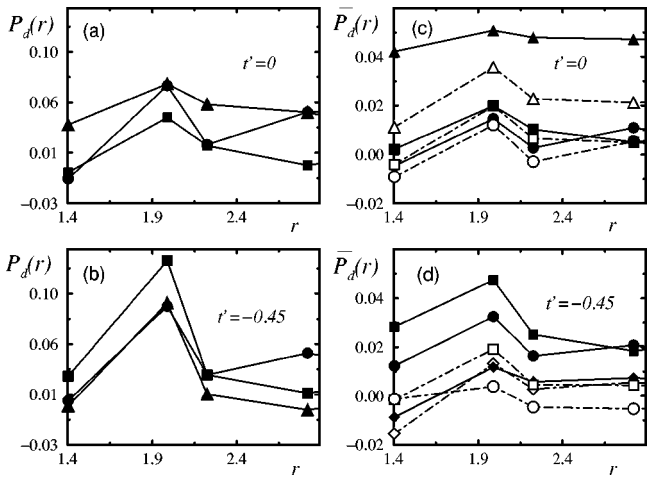

FIG. 3. $P_d(r)$ and $\overline{P}_d(r)$ for $U=10$ and $t_{AB}=1$ (open symbols) and $t_{AB}=2$ (solid symbols). Circles, squares, and triangles correspond to $N=10,12,14$, respectively.

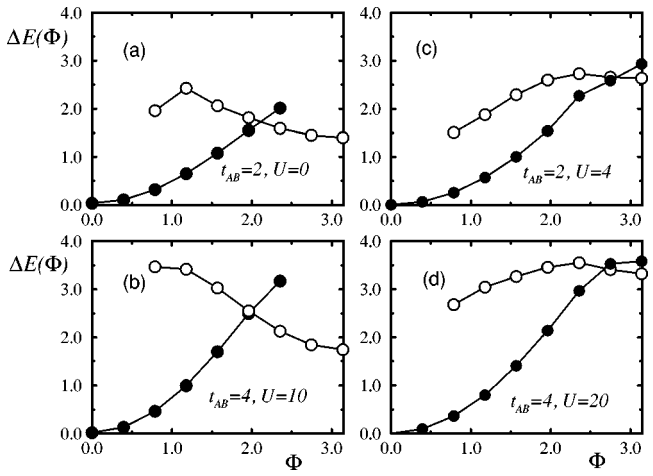

FIG. 4. Lowest relevant energies as a function of flux for $t'=-0.45t$, $N=10$ and several values of U and t_{AB}. The value $E(0)$ is subtracted. Only half of the interval $[0,2\pi)$ is shown because $E(\Phi)=E(-\Phi)=E(2\pi-\Phi)$.

similar to those of $P_d(r)$ for a short-range resonance-valence-bond wave function which by construction has superconducting off-diagonal long-range order.[4,17] These results are strong indications of *d*-wave superconductivity. We should also note that the superconducting *d*-wave pairs in the model, have an internal structure which extends beyond NN and with only a partial overlap with $\Delta_d^\dagger(i)$. Thus, our *d*-wave PCF's are reduced with respect to the optimum normalized PCF's by the square of this overlap.[8]

For $N=10,12$, the effect of a negative t' is to enhance the vertex contribution $\overline{P}_d(r)$. Instead, for $N=14$, both $P_d(r)$ and $\overline{P}_d(r)$ are large for the case with $t'=0$, while they are very small for $t'=-0.45$. Note that in all the cases with sizable pairing correlations, the values of $\overline{P}_d(r)$ corresponding to $t_{AB}=2$ are significantly larger than those corresponding to $t_{AB}=1$, with the same values of t' and U. In addition, in these cases, the noninteracting $P_d(r)$ lie below the displayed ones for $t_{AB}=2$ in Fig. 3(a). The remarkable large values of $\overline{P}_d(r)$ observed in Fig. 3(c) for the case with $N=14$ particles could be somewhat exaggerated due to particular finite-size effects.[22] In fact, when $t_{AB}=1$,$\overline{P}_d(r)$ in Fig. 3(c) is large while the values of $P_d(r)$ are smaller than those of the noninteracting case. The mean-field treatment[12] predicts a maximum of the superconducting gap with *d*-wave symmetry at half-filling for $t'=0$, when the SDW is not taken into account. The concurrence between superconductivity and the SDW near half-filling manifests itself in this cluster when different BC are used. For $N=14$, $t'=0$, $t_{AB}=2$, $U=10$, spin-spin correlations (not shown) are much stronger for PBC than for MBC, while in the first (latter) case $P_d(r)$ is weaker (stronger) than in the noninteracting case. In any case, as expected,[6,7,12] the maximum of the PCF with doping shifts to higher doping as t' increases.

In contrast to the cases without correlated hopping, we find signs of AFQ in most of the explored parameter space. AFQ consists of a periodicity of half a flux quantum in the ground-state energy $E(\Phi)$ as a function of a flux Φ threading the system in a toroidal geometry, and it is a necessary but not sufficient condition for superconductivity.[15] In finite systems, a tendency to AFQ is indicated by a crossing of energy levels with different total wave vector as Φ is varied, and the presence of two relative minima in $E(\Phi)$ with a difference of Φ in π (usually at $\Phi=0$ and $\Phi=\pi$) in the interval $[0,2\pi)$. In Fig. 4 we show the dependence on Φ of the lowest energy levels of the system for several values of the parameters in which the level crossing occurs. Figure 4(a) and 4(b) correspond to dominant *s*-wave PCF's. In the other cases shown, the *d*-wave PCF's are the largest ones. For $t'=0,N=10$ we found a very similar behavior of $E(\Phi)$ to that observed in Fig. 4. Due to the fact that the introduction of a flux breaks the space-group symmetry and increases considerably the size of the irreducible subspaces, we have not constructed $E(\Phi)$ curves for $N>10$.

IV. SPIN STRUCTURE FACTOR

We have also calculated charge and spin-correlation functions. The spin structure factor $S(\mathbf{q})=\Sigma_{ij}\langle S_i^z S_j^z e^{i\mathbf{q}(\mathbf{R}_i-\mathbf{R}_j)}\rangle/L^2$ for $N=12$ is shown in Fig. 5. In the absence of correlated hopping (Hubbard model with t'), there is a peak near $(\pi/2,\pi/2)$ which is inconsistent with experiments. For $N=10$, moderate t_{AB} and some values of U, the peak is at $(\pi,\pi/2)$. This result is consistent with neutron measurements in $La_{2-x}Sr_xCuO_4$, which indicate that the

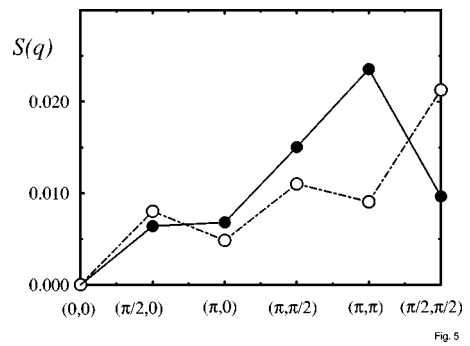

FIG. 5. Spin structure factor as a function of wave vector for $t'=-0.45t$, $U=10$, $N=12$. Open (solid) circles denote $t_{AB}=1(t_{AB}=2)$.

position of the incommensurate peak moves from (π,π) towards $(\pi,0)$ with doping x, and the magnitude of the displacement is $2\pi x$.[23] For lower dopings, the increase of t_{AB} tends to restore a peak at (π,π), which is rather broad, indicating the presence of short-range antiferromagnetism, similar to that found for a resonance-valence-bond (RVB) state with superconducting off-diagonal long-range order.[4] For the case $N=14, t'=0, t_{AB}=2, U=10$ $S(\mathbf{q})$ exhibits a broad structure at (π,π) for MBC, while large $P_d(r)$ is obtained, as discussed above. Instead, for PBC a much narrower peak, suggestive of longer-range antiferromagnetic correlations is observed in $S(\mathbf{q})$ while $P_d(r)$ are weaker than those of the noninteractive case. These results suggest that the broad peak in $S(\mathbf{q})$ and enhanced $P_d(r)$ have the same physical origin, possibly the establishment of an RVB ground state.

V. DISCUSSION

In summary, we have shown that correlated hopping, which arises naturally in a low-energy reduction of multiband models for the cuprates,[13] leads to pairing correlations of magnitude similar to that observed in the same cluster for states for which superconductivity is well established. For low to moderate doping, the favored symmetry is $d_{x^2-y^2}$ for finite U and t'.

For weak coupling, the three-site term of the effective one-band Hamiltonian reduces to the sum of three two-body interactions:[12,14,24] an exchange J, a nearest-neighbor repulsion V, and a hopping of on-site pairs W. It is the effect of J which favors singlet superconductivity.[12,14] This agrees with recent studies of pairing correlation functions in t-U-J ladders, which also obtain enhanced d-wave pairing.[9]

In one dimension (1D), there is analytical and numerical evidence that for small U and large t_{AB}, the ground state at half filling consists of singlet dimers, and singlet PCF's dominate when the system is doped.[14] The natural extension of this scenario to 2D, seems to be a short-range RVB-like state at half filling, which turns into a singlet superconductor as the dimers acquire mobility with doping. While we expect long-range antiferromagnetism in the half-filled case, our results for pairing correlation functions and spin structure factor are consistent with this scenario as the system is doped.

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