Superconductivity within the t-t' Hubbard model of a bilayer

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Making use of a variational approach to Kohn-Luttinger superconductivity, we study the superconducting state of two coupled CuO_2 planes. The bilayer is described in terms of a t-t' Hubbard model with weak interplane hopping. For parameters relevant to overdoped cuprates, we find a substantial increase of the mean field transition temperature T_c, when compared with the single layer model. This increase is driven by the enhanced density of states of the bilayer.

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High temperature superconductivity occurs in a large class of layered compounds, whose common structural elements are the CuO_2 layers. The compounds differ in the chemical composition of the layers separating these basic structural elements. Materials with similar chemistry of the separating layers are usually grouped into families. The compounds within a given family may be further classified according to the number n of closely spaced CuO_2 layers. Within a given family, the transition temperature T_c for optimally chosen doping is an increasing function of n for $n<3$, the function $T_c(n)$ acquires a maximum for $n=3$, and for $n>3$ it decreases.[1]

Recent experiments[2] indicate that for $n\geqslant 3$ the doping levels of the CuO_2 planes are not equal: the inner layers are underdoped, while the outer layers are overdoped. Since the function $T_c(n)$ for $n\geqslant 3$ depends on the precise magnitude of the charge disproportionation, in this paper we do not consider this region and concentrate only on $n=1$ and 2. We just note in passing that only phenomenological theories have been proposed for differently doped CuO_2 planes: Kivelson has predicted an increase of T_c in such a situation, based on the picture that the overdoped layers provide an increased phase stiffness, while the underdoped layers exhibit an enhanced pairing scale.[3] On the other hand, Chakravarty *et al.* have explained the observed shape of $T_c(n)$ within a phenomenological picture[4] with three assumptions: (i) different doping levels of the CuO_2 planes, (ii) competing order parameters within a plane, and (iii) the contribution of interlayer tunneling to the energy is negligible in the normal state.

The last assumption of Chakravarty *et al.* which guarantees the increase of T_c between $n=1$ and 2 is in fact the basic assumption of Anderson's interlayer tunneling theory,[5] which stimulated a large body of experimental and theoretical work on the coupling between the CuO_2 planes.[6] In its original formulation, Anderson's theory described the superconducting transition as being driven by kinetic energy gain in the c axis direction. However, it has been shown later that the interlayer contribution is only a small part of the condensation energy in single layer compounds.[7] Therefore interlayer tunneling cannot be regarded as the main driving force for T_c, but nevertheless it does contribute to an enhancement of T_c.

As a first step towards a fully microscopic theory of $T_c(n)$, we will study in this paper the T_c of a bilayer system as a function of the bilayer coupling. We have chosen to study overdoped systems, which have long been suspected to behave as Fermi liquids in their normal state. Recent experiments put this hypothesis on a much more solid basis. In particular, it has been shown that the Wiedemann-Franz law is obeyed in the overdoped state of Tl2201,[8] and also the T^2 scaling of the resistivity (both in plane and out of plane) has been established in overdoped $La_{2-x}Sr_xCuO_4$.[9] Moreover, very recently the angular dependence of the c-axis magnetoresistance has been shown to agree with the assumption of coherent c-axis transport in overdoped Tl2201.[10] This latter conclusion is consistent with the recent results of angle-resolved photoemission spectroscopy in Bi2212, which also provide evidence for a coherent bilayer splitting.[11]

On the theoretical side, the old prediction that the superconducting instability is a generic property of Fermi liquids at low temperatures[12] has been recently reformulated in a way enabling quantitative characterization of the properties of Kohn-Luttinger superconductors within a well-controlled approximation which becomes essentially exact in the weak-coupling limit.[13] In the present paper we apply this technique to the study of superconductivity in a bilayer system.

Based on the results of angle-resolved photoemission spectroscopy,[11] it is well established by now that the minimal model reproducing the experimentally observed shape of the Fermi surface in the cuprates is a two-dimensional t-t' Hubbard model with the in-plane dispersion $\varepsilon_{\mathbf{k}}=-2t(\cos k_x+\cos k_y)+4t'\cos k_x \cos k_y$. As pointed out recently, the ratio t'/t is family dependent.[14] A reasonable estimate for Bi-based cuprates we are interested in here is $t'/t=0.3$.

The quantum chemistry of the cuprates dictates that the hopping of electrons between the planes of a bilayer is described in real space by the Hamiltonian[15] $H_\perp=-t_\perp\Sigma_{i\sigma}\Sigma_{\delta\tau}s_\delta s_\tau\,(a^\dagger_{i\sigma}b_{i+\delta+\tau,\sigma}+\text{h.c.})$, where $a_{i\sigma}$ and $b_{i\sigma}$ annihilate an electron at the lattice site i with spin σ in the upper and lower layer, respectively. The indices δ,τ denote nearest neighbor directions on the two-dimensional square lattice, $(\pm1,0)$ and $(0,\pm1)$, and the function $s_{(\pm1,0)}=-s_{(0,\pm1)}=1$ respects the $d_{x^2-y^2}$ symmetry of the Zhang-Rice orbital. Introducing bonding and antibonding combinations $c^0_{i\sigma}=(a_{i\sigma}+b_{i\sigma})/\sqrt{2}$ and $c^\pi_{i\sigma}=(a_{i\sigma}-b_{i\sigma})/\sqrt{2}$, and performing the in-plane Fourier transformation one finds that

the bonding and antibonding energies are $\varepsilon_{\mathbf{k}}^{0}=\varepsilon_{\mathbf{k}}-\Omega_{\mathbf{k}}$ and $\varepsilon_{\mathbf{k}}^{\pi}=\varepsilon_{\mathbf{k}}+\Omega_{\mathbf{k}}$, respectively, where $\Omega_{\mathbf{k}}=4t_{\perp}(\cos k_x-\cos k_y)^2$. Thus the splitting between the bonding and antibonding bands at $\mathbf{k}=(\pi,0)$ is $32t_{\perp}$, which should be compared with the experimental value, 88 meV.[11] If we take $t\sim 500$ meV, this leads to the estimate $t_{\perp}/t\sim 0.005$, a value to be used in most of our calculations. More generally, within the t-t' Hubbard model with $t'/t=0.3$ and $\rho=0.8$, the correct topology of the antibonding Fermi surface is obtained for $t_{\perp}/t<0.0065$.

Before starting the full calculation, let us first present a simple argument for the condensation energy gain due to bilayer splitting, $\Delta E_{\mathrm{cond}}=E_{\mathrm{cond}}(t_{\perp})-E_{\mathrm{cond}}(0)$, where $E_{\mathrm{cond}}(t_{\perp})=E_S(t_{\perp},\mu_4)-E_N(t_{\perp},\mu_2)$ and $E_{\mathrm{cond}}(0)=E_S(0,\mu_3)-E_N(0,\mu_1)$. Note that in general the chemical potentials μ_i of the superconducting (S) and normal (N) states with or without bilayer coupling are different. For the sake of simplicity, let us for the moment consider a featureless s-wave superconductor with an isotropic bilayer splitting $t_{\perp}$. Let us furthermore assume that the system is particle-hole symmetric, i.e. the density of states $N(\omega)$ is an even function of the deviation ω from the Fermi level. In that case all chemical potentials are equal, $\mu_i=\mu$, and $E_{\mathrm{cond}}(t_{\perp})$ is given by

$$-\int d\omega[N(\omega+t_{\perp})+N(\omega-t_{\perp})]\frac{(\sqrt{\omega^2+\Delta^2}-|\omega|)^2}{2\sqrt{\omega^2+\Delta^2}}.$$

Expanding to second order in $t_{\perp}$, we find from here that $\Delta E_{\mathrm{cond}}=-N''(0)t_{\perp}^2\Delta^2/2$. This means that for a featureless density of states, the bilayer coupling does not lead to a gain of condensation energy and $\Delta E_{\mathrm{cond}}=0$, as pointed out already by Chakravarty (see Ref. 16 and references therein). However, for a nontrivial density of states, this is not true anymore. Remarkably, our weak-coupling result is consistent with the strong-coupling point of view[4] according to which it is the normal state pseudogap [compatible with $N''(0)>0$] which leads to a suppression of $|\Delta E_N|$ with respect to $|\Delta E_S|$.

For band fillings slightly above the Van Hove density (the latter corresponding to the chemical potential ε_{VH}), we have $N(0)\propto\ln[\Lambda/(\mu-\varepsilon_{VH})]$ from where it follows that $N''(0)>0$ and the bilayer should gain condensation energy. Unfortunately, since $N'(0)\neq 0$, the above argument cannot be directly applied. However, we will see that the complete solution does lead to a stabilization of the superconducting state on a bilayer.

Let us proceed now with the full calculation. When written in momentum space, the Hubbard model on a bilayer with $L=l\times l\times 2$ sites, assuming periodic boundary conditions, reads as

$$H=H_{\mathrm{kin}}+\frac{U}{L}{\sum_{\mathbf{k}_1\alpha\mathbf{k}_2\beta\mathbf{k}_3\gamma}}' c^{\dagger}_{\mathbf{k}_1\alpha\uparrow}c_{\mathbf{k}_2\beta\uparrow}c^{\dagger}_{\mathbf{k}_3\gamma\downarrow}c_{\mathbf{k}_4\delta\downarrow}, \tag{1}$$

where $H_{\mathrm{kin}}=\Sigma_{\mathbf{k}\alpha\sigma}\varepsilon_{\mathbf{k}}^{\alpha}c^{\dagger}_{\mathbf{k}\alpha\sigma}c_{\mathbf{k}\alpha\sigma}$ and the indices $\alpha,\beta,\gamma,\delta$ take on the values 0 and π. The prime in the sum means that momenta $\mathbf{k}_4$ and δ are determined by momentum conservation, $\mathbf{k}_1+\mathbf{k}_2=\mathbf{k}_3+\mathbf{k}_4$ and $\alpha+\beta=\gamma+\delta$ (where we take $2\pi=0$). Note that the Hamiltonian equation (1) has the same form as for a simple square lattice, if we identify $(\mathbf{k}\alpha)$ as a three-momentum.

Since the method of Ref. 13 does not depend on the dimensionality, we can directly translate its results to the present case. In particular, the model, Eq. (1), supports superconductivity, if a nontrivial order parameter $\Delta_{\mathbf{k}}^{\alpha}$ can be found which solves the gap equation

$$\Delta_{\mathbf{k}}^{\alpha}=-\frac{1}{L}\sum_{\mathbf{p}\beta}V_{\mathbf{kp}}^{\alpha\beta}\Delta_{\mathbf{p}}^{\beta}\frac{\tanh(E_{\mathbf{p}}^{\beta}/2T)}{2E_{\mathbf{p}}^{\beta}}. \tag{2}$$

In Eq. (2) we introduced the quasiparticle enegy $E_{\mathbf{p}}^{\alpha}=[(\xi_{\mathbf{p}}^{\alpha})^2+|\Delta_{\mathbf{p}}^{\alpha}|^2]^{1/2}$, where $\xi_{\mathbf{p}}^{\alpha}=\varepsilon_{\mathbf{p}}^{\alpha}-\mu$. The effective interaction is given by $V_{\mathbf{kp}}^{\alpha\beta}=U+U^2\chi^{\alpha+\beta}(\mathbf{k}+\mathbf{p},\varepsilon_{\mathbf{p}}^{\alpha}-\varepsilon_{\mathbf{k}}^{\beta})$, where

$$\chi^{\gamma}(\mathbf{q},\omega)=\frac{1}{L}\,\mathrm{Re}\sum_{\mathbf{K}\alpha}\frac{f_{\mathbf{K}}^{\alpha}-f_{\mathbf{K}+\mathbf{q}}^{\alpha+\gamma}}{\varepsilon_{\mathbf{K}+\mathbf{q}}^{\alpha+\gamma}-\varepsilon_{\mathbf{K}}^{\alpha}-\omega-i0} \tag{3}$$

can be effectively calculated making use of the Fast Fourier Transform algorithm.[17] Note that the interaction matrix is real and symmetric, $V_{\mathbf{kp}}^{\alpha\beta}=V_{\mathbf{pk}}^{\beta\alpha}$.

It is worth pointing out that, since we are constructing a theory for the weak coupling limit of Eq. (1), we have assumed that Cooper pairing occurs only between states related by time reversal symmetry. In particular, this means that no pairing is allowed between bonding and antibonding states. A gap equation of the same form as Eq. (2) has been derived previously by O'Donovan and Carbotte,[18] but these authors used a phenomenological $V_{\mathbf{kp}}^{\alpha\beta}$ based on the spin fluctuation exchange mechanism.

In Fig. 1 we plot the superconducting transition temperature T_c (obtained numerically following Ref. 13) as a function of $t_{\perp}$. In order to reduce the finite size effects, in Fig. 1 we also plot the fit to $T_c(t_{\perp})=T_c(0)+\omega(t_{\perp}/t)^2$. This expression is obtained by noting that $T_c(t_{\perp})$ should be an even analytic function of $t_{\perp}$. We find $\omega>0$ and therefore we conclude that T_c is an increasing function of $t_{\perp}$, in qualitative agreement with experiment.

In Fig. 1 we also plot the zero temperature condensation energy per lattice site, $E_{\mathrm{cond}}=-L^{-1}\Sigma_{\mathbf{k}\alpha}(E_{\mathbf{k}}^{\alpha}-|\xi_{\mathbf{k}}^{\alpha}|)^2/2E_{\mathbf{k}}^{\alpha}$. It is worth pointing out that in the presence of a finite $t_{\perp}$ the superconducting state gains more energy with respect to the normal state, in agreement with the result for $T_c(t_{\perp})$. Note that the contribution of the antibonding band to E_{cond} is larger than that of the bonding band and that its relative weight grows with $t_{\perp}$. This raises the question whether the gaps in the two bands are equal or not. In Fig. 2 we plot the density of states,

$$N(\omega)=L^{-1}\sum_{\mathbf{k}\alpha}[(u_{\mathbf{k}}^{\alpha})^2\delta(\omega-E_{\mathbf{k}}^{\alpha})+(v_{\mathbf{k}}^{\alpha})^2\delta(\omega+E_{\mathbf{k}}^{\alpha})],$$

where $(u_{\mathbf{k}}^{\alpha})^2$, $(v_{\mathbf{k}}^{\alpha})^2=(1\pm\xi_{\mathbf{k}}^{\alpha}/E_{\mathbf{k}}^{\alpha})$ are the usual coherence factors. Figure 2 shows that the gaps in the bonding and antibonding bands are of a very similar magnitude. This means that the difference of the contributions of the two bands to E_{cond} is caused dominantly by the different normal state densities of states (see the inset in Fig. 1), in accord with the fact that the antibonding Fermi surface is closer to the saddle point at $(\pi,0)$. The fact that $E_{\mathrm{cond}}^{\pi}/E_{\mathrm{cond}}^{0}$ grows faster with $t_{\perp}$

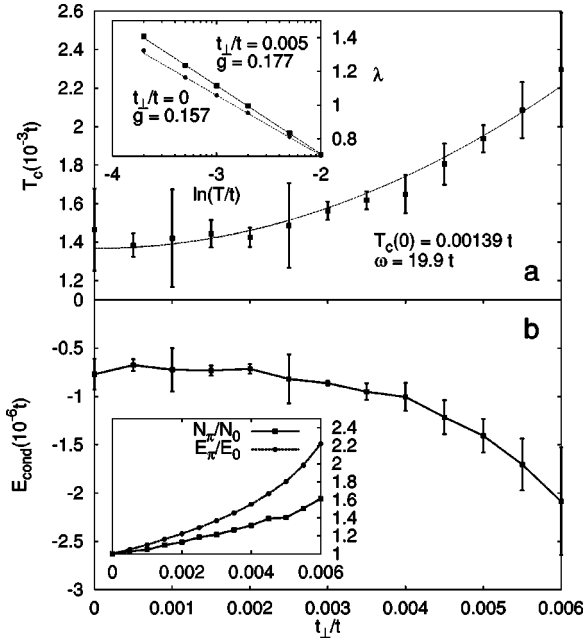

FIG. 1. (a) Superconducting transition temperature T_c and (b) condensation energy per lattice site as functions of $t_\perp/t$. The data is calculated for $\rho=0.8$, $t'/t=0.3$, and $U/t=4$ on special lattices (Ref. 13) with $L=512\times512$. The error bars are estimated from the difference with respect to the 256×256 data. The dotted line in (a) is a fit to $T_c(t_\perp)=T_c(0)+\omega(t_\perp/t)^2$. The inset in (a) shows the maximal eigenvalue $\lambda(T)$ and its fit to $g\ln(\Omega/T)$ for $t_\perp/t=0$ and 0.005. In the inset in (b) we plot the relative contributions of the bonding and antibonding bands to the condensation energy and to the normal density of states.

than $N_\pi(0)/N_0(0)$ can be explained as follows. The condensation energy can be written as a Fermi surface average $E^\alpha_{\rm cond}\approx-(16\pi^2\hbar)^{-1}\oint dk(\Delta^\alpha_{\mathbf{k}})^2/v^\alpha_{\mathbf{k}}$, whereas the density of states $N_\alpha(0)\propto\oint dk/v^\alpha_{\mathbf{k}}$. Therefore for equal and isotropic bonding and antibonding gaps we should have $E^\pi_{\rm cond}/E^0_{\rm cond}=N_\pi(0)/N_0(0)$. Now let us notice two facts: (i) the Fermi velocity $v^\alpha_{\mathbf{k}}$ is small in the antinodal region, and (ii) $v^\alpha_{\mathbf{k}}$ is more strongly modulated in the antibonding band than

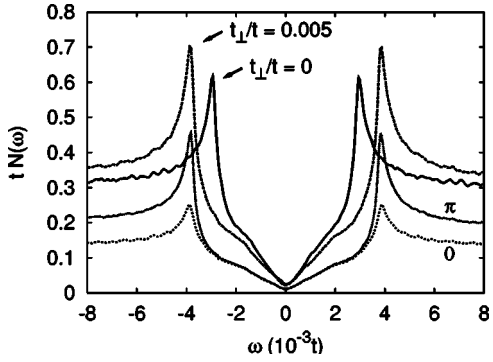

FIG. 2. Density of states per lattice site (in units of t^{-1}) at $T=0$. The bonding and antibonding contributions at $t_\perp/t=0.005$ are denoted 0 and π, respectively. The curves are calculated for $\rho=0.8$, $t'/t=0.3$, and $U/t=4$, linearly interpolating the $L=512\times512$ data to $L=8192\times8192$. The delta functions were given a finite width $\gamma/t=1\times10^{-4}$.

in the bonding band. From these facts it follows that regions with large values of Δ have a larger relative weight in the antibonding than in the bonding band, in agreement with the inset in Fig. 1.

The small difference between the gaps in the bonding and antibonding bands demonstrated by Fig. 2 is in qualitative agreement with recent ARPES experiments. In view of the large increase $\delta T_c/T_c$, this weak dependence on the band index α is a surprising feature, which can however be understood within the following simple model. Consider two featureless s-wave superconductors on a bilayer. At $T=0$, the gap equation can be written as

$$\Delta_\alpha=\frac{1}{2}\sum_\beta g_{\alpha\beta}\Delta_\beta\ln\frac{\Omega}{\Delta_\beta},\tag{4}$$

where $\Delta_{0,\pi}$ are the gaps in the bonding and antibonding bands and the coupling constants $g_{\alpha\beta}$ are estimated as

$$g_{00}=N_0(0)V_0=(1+\epsilon+\delta_1)g,$$

$$g_{0\pi}=N_\pi(0)V_\pi=(1-\epsilon+\delta_2)g,$$

$$g_{\pi0}=N_0(0)V_\pi=(1+\epsilon+\delta_2)g,$$

$$g_{\pi\pi}=N_\pi(0)V_0=(1-\epsilon+\delta_1)g,$$

where $V^{00}=V^{\pi\pi}=V_0$ and $V^{0\pi}=V^{\pi0}=V_\pi$ are the intraband and interband interactions, respectively. Now we assume that in the absence of bilayer splitting the coupling constant reads as $g=N(0)V$ and that in the presence of a finite $t_\perp$ the deviation of the interactions V_0 and V_π from V is $O(t_\perp^2)$, whereas the deviation of $N_{0,\pi}(0)$ from $N(0)$ also contains linear terms in $t_\perp$ (of opposite sign for the bonding and antibonding bands). From here the last equations for $g_{\alpha\beta}$ follow immediately, with $\epsilon=O(t_\perp)$ and $\delta_i=O(t_\perp^2)$.

A straightforward calculation shows that under such conditions the maximal eigenvalue of the matrix $g_{\alpha\beta}/2$ changes from g to $g+\delta g$ with $\delta g/g=(\delta_1+\delta_2)/2$ and therefore from the scaling $T_c\propto\exp(-1/g)$ we find that the relative change of T_c is $\delta T_c/T_c\approx\delta g/g^2$. Moreover, from Eq. (4) it follows that the bonding and antibonding gaps change with respect to the gap of isolated layers, Δ, but they remain equal to each other, $\Delta_0=\Delta_\pi=(1+\delta g/g^2)\Delta$. The renormalization of T_c (or, equivalently, of the gap) can be large even for small relative changes $\delta g/g$, since $g\ll1$ at weak coupling. In fact, from the fits in Fig. 1 we find $g\approx0.157$ for $t_\perp=0$ and $g\approx0.177$ for $t_\perp/t=0.005$, implying $\delta T_c/T_c\approx0.8$, in an order-of-magnitude agreement with the main panel in Fig. 1.[19]

Before proceeding it is worth pointing out that, within the present weak-coupling theory, the magnitude of the relative increase $\delta T_c/T_c$ due to finite interlayer coupling depends on the interaction strength U, the effect being most pronounced at weak coupling, since both δg and g scale with U^2. The present weak coupling theory cannot be directly compared with experiments, since for $U=4t$ the single layer transition temperature is only $T_c\approx7$ K. As an order-of- magnitude estimate, in Ref. 13 we have applied our theory outside its well-controlled range of applicability and we found that for $U=6t$ the gap is $\approx9\times10^{-2}t$, slightly larger than the experi-

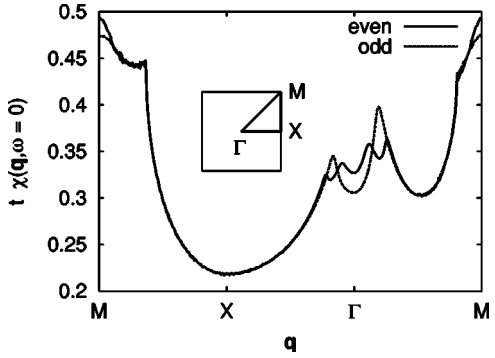

FIG. 3. Even ($\gamma=0$) and odd ($\gamma=\pi$) static susceptibilities $\chi^{\gamma}(\mathbf{q},0)$ along the symmetry lines of the Brillouin zone. The parameters are the same as in Fig. 2. The odd component at $t_{\perp}/t=0.005$ is very close to the single layer susceptibility (not shown for clarity).

mental value. From the scaling $(\delta T_c/T_c)_{U=6t} \approx (\delta T_c/T_c)_{U=4t}/1.5^2$ and from the data in Fig. 1 we thus obtain the estimate $(\delta T_c/T_c)_{U=6t}\approx 0.16$. This estimate compares well with the experimental data for the $Tl_2Ba_2Ca_{n-1}Cu_nO_{2n+4}$ and $HgBa_2Ca_{n-1}Cu_nO_{2n+2+\delta}$ families (for a compilation, see Ref. 20), where $T_{c(n=1)}=90$ K, $T_{c(n=2)}=110$ K, $\delta T_c/T_c=0.22$ and $T_{c(n=1)}=95$ K, $T_{c(n=2)}=114$ K, $\delta T_c/T_c=0.2$, respectively.

At $t_{\perp}=0.005t$ the total density of states of a bilayer increases with respect to its $t_{\perp}=0$ value by $\delta N(0)/N(0) \approx 0.07$, which is of the same order of magnitude as $\delta g/g \approx 0.13$.[19] Moreover, Fig. 3 shows explicitly that (in the most important static limit) the intraband and interband interactions change only little with respect to $t_{\perp}=0$. The largest change occurs in the even channel in the vicinity of the Γ point, again due to an increase of the density of states. Summarizing the above evidence, we conclude that the coupling constant increase is driven by the increased density of states of the bilayer. This is in agreement with our qualitative argument that condensation energy is gained for $N''(0)>0$. Let us also emphasize that the increase of T_c under interlayer coupling is a nonuniversal feature of Eq. (4) and of the microscopic model Eq. (1), which are therefore different from the case discussed previously by O'Donovan and Carbotte.[18]

In order to gain further insight into the nature of the pairing state, let us finally consider the pairing functions:[21]

$$F_{ij}^{\alpha\beta}=\sum_{\sigma}\sigma\langle c_{i-\sigma}^{\alpha}c_{j\sigma}^{\beta}\rangle=\delta_{\alpha\beta}\frac{2}{L}\sum_{\mathbf{k}}\frac{\Delta_{\mathbf{k}}^{\alpha}}{E_{\mathbf{k}}^{\alpha}}\cos\mathbf{k}\cdot\mathbf{R}_{ij}, \qquad (5)$$

where i, j are lattice sites of a single plane connected by the vector $\mathbf{R}_{ij}$, and α, β distinguish the bonding and antibonding bands. Going back to the representation in terms of the upper and lower layers, let us define $F_{ij}^{aa}=\Sigma\sigma\langle a_{i-\sigma}a_{j\sigma}\rangle$, $F_{ij}^{ab}=\Sigma\sigma\langle a_{i-\sigma}b_{j\sigma}\rangle$, and similarly also F_{ij}^{ba} and F_{ij}^{bb}. If we define in-plane and interplane pairing functions $F_{ij}^{\parallel}$ and $F_{ij}^{\perp}$, respectively, then from Eq. (5) it follows that $F_{ij}^{\parallel}=F_{ij}^{aa}=F_{ij}^{bb}=(F_{ij}^{00}+F_{ij}^{\pi\pi})/2$ and $F_{ij}^{\perp}=F_{ij}^{ab}=F_{ij}^{ba}=(F_{ij}^{00}-F_{ij}^{\pi\pi})/2$. Figure 4 shows the normalized in-plane and interplane pairing functions, $\Phi_{ij}^{\parallel,\perp}=F_{ij}^{\parallel,\perp}/\sqrt{\Sigma_j|F_{ij}^{\parallel,\perp}|^2}$. Let us discuss first the in-plane pairing function. Its tails are located close to the nodal directions and this is qualitatively consistent with a model calculation for a d-wave superconductor with a circular Fermi surface with radius k_F, Fermi velocity v_F, density of states $N(0)$, BCS cut-off ω_0, and a gap function $\Delta_{\varphi}=\Delta\cos 2\varphi$. In fact, the model calculation predicts that at intermediate distances $k_F^{-1}\ll r\ll v_F/\Delta$ the pairing function reads as

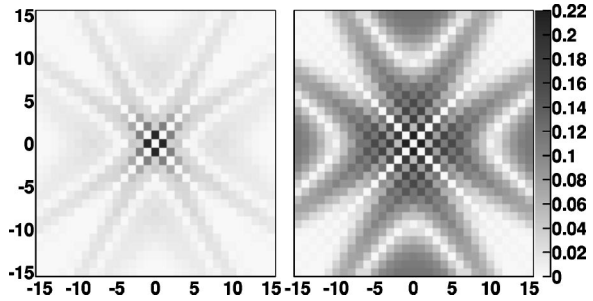

FIG. 4. Absolute values of the normalized pairing functions $|\Phi_{ij}^{\parallel}|$ (left panel) and $|\Phi_{ij}^{\perp}|$ (right panel, magnified by a factor 5) as functions of the vector $i-j$. The parameters are the same as in Fig. 2.

$$F(r,\varphi)\approx\sqrt{\frac{8}{\pi}}N(0)\Delta_{\varphi}\frac{\cos\left(k_Fr-\frac{\pi}{4}\right)}{\sqrt{k_Fr}}\ln\left[\frac{\xi_{\varphi}}{\max\left(\frac{v_F}{2\omega_0},r\right)}\right],$$

where $\xi_{\varphi}=v_F/|\Delta_{\varphi}|$ is an angle-resolved coherence length.

Note also the large peaks of $F_{ij}^{\parallel}$ at the four nearest neighbor sites. This is a generic result close to half filling, valid also for a single plane. Both our numerical data and the model calculation for a d-wave superconductor show that the total weight of the pairing function $\Sigma_j|F_{ij}|^2=2N(0)\Delta$ is distributed in a radius $\sim v_F/\Delta$. It is remarkable, however, that ≈ 0.18 of this weight is localized at the four nearest neighbor sites, which is definitely an unexpected result at weak coupling.

The out-of-plane pairing function $F_{ij}^{\perp}$ exhibits the same overall shape as $F_{ij}^{\parallel}$, but all features are smeared with respect to the in-plane pairing function. In particular, the four sharp nearest-neighbor peaks are replaced by a checkerboard pattern of $F_{ij}^{\perp}$ at small distances. These features can be qualitatively explained within perturbation theory with respect to $t_{\perp}$. In fact, consider first-order corrections to the wavefunction. One of the electrons forming an in-plane Cooper pair can hop into the neighboring plane of the bilayer. Since the interlayer hopping is nonlocal (hopping occurs between sites with in-plane coordinates i and $i+\delta+\tau$), the delocalized form of $F_{ij}^{\perp}$ follows. Moreover, since i and $i+\delta+\tau$ belong to the same sublattice, the checkerboard pattern of the inter-plane pairing function follows from the four nearest neighbor peaks of the in-plane pairing function.

Let us estimate the region of applicability of perturbation theory in $t_{\perp}$. Assuming that the inter-plane coupling is $16t_{\perp}\cos^2 2\varphi$ and neglecting the difference between $\Delta_{\mathbf{k}}^0$ and $\Delta_{\mathbf{k}}^{\pi}$, the ratio of the total weights of the inter-plane and in-plane pairing functions can be estimated within the model

calculation for a d-wave superconductor as $\Sigma_j|F_{ij}^{\perp}|^2/\Sigma_j|F_{ij}^{\parallel}|^2 = \frac{1}{3}(8t_{\perp}/\Delta)^2$. This shows that perturbation theory is quantitatively accurate for $t_{\perp} \ll \Delta$. Let us note in passing that in the opposite limit $t_{\perp} \gg t$, only the bonding band is occupied and $F_{ij}^{\pi\pi}=0$. Therefore our weak coupling formalism predicts $F_{ij}^{\perp}=F_{ij}^{\parallel}$ in that case. The data presented in Fig. 4 correspond to the crossover region $t_{\perp} \sim \Delta$ and that is why we obtain $\Sigma_j|F_{ij}^{\parallel}|^2=0.00634$ and $\Sigma_j|F_{ij}^{\perp}|^2=0.00462$.

Before concluding let us recall that the increased density of states of the bilayer is due to the vicinity of the antibonding band to the Van Hove density. However, single layer systems close to the Van Hove density are expected to support magnetic instabilities.[22] This opens the question about the competition between superconductivity and magnetism on a bilayer which will not be addressed here.

In conclusion, we have studied the pairing transition within the Hubbard model on a bilayer. For parameters relevant to overdoped cuprates, we have found a substantial increase of the mean field transition temperature T_c, when compared with the single layer model. Within our weak coupling formalism, this increase is due to the enhanced total density of states in the presence of bilayer splitting.

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