Spin fluctuation induced $d_{x^2-y^2}$-wave superconductivity in the three-band Hubbard model: A self-consistent fluctuation-exchange-approximation approach

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Using the fluctuation exchange approximation of the three-band Hubbard Hamiltonian we find spin fluctuation induced $d_{x^2-y^2}$-wave superconductivity with correct order of magnitude of the superconducting transition temperature. This result is obtained for model parameters and for an effective Coulomb interaction which yields normal state scattering rates in agreement with experiments. The chosen parameters of our model give results for the low energy excitations which are similar to those obtained within the effective one-band Hubbard Hamiltonian. We present results for the **k** dependence of the anomalous self-energy, the spectral density, and for the reduced quasiparticle scattering rate in the superconducting state, where both the copper and oxygen states contribute to superconductivity. Our results are a further strong support for spin fluctuation induced superconductivity and confirm previous effective one-band calculations. [S0163-1829(98)06142-6]

There is by now a large consensus about the importance of strong electronic correlations in high temperature CuO_2 superconductors.[1] A favorite theory which includes the pronounced short ranged antiferromagnetic correlations caused by strong electronic interactions is the spin fluctuation model.[2–4] In this model the dynamical spin susceptibility which is peaked near the antiferromagnetic wave vector $\mathbf{Q}=(\pi,\pi)$ and which is deduced from NMR experiments[5,6] or determined self-consistently within the fluctuation exchange approximation[7] (FLEX) causes a pairing interaction for singlet Cooper pairs with $d_{x^2-y^2}$ symmetry. Interestingly, these strong coupling Eliashberg-type calculations yield critical temperatures T_c in good agreement with experiment.[6,8,9] Furthermore, these theories are also able to describe properly a variety of further experimental observations in the normal as well as in the superconducting state. It should be noted that these studies are performed within an effective single band description of the low energetical charge carriers. As shown by Zhang and Rice the charge carrier states of the high-T_c superconductors are composed of hybridized copper (Cu) and oxygen (O) states.[10] Hence, it has been argued that the explicit consideration of these Cu and O states might be essential for a proper description of the short range spin dynamics of the cuprates.[11–14]

Consequently a variety of investigations of the three-band Hubbard model taking Cu $3d_{x^2-y^2}$ and O $2p_{x,y}$ states into account have been performed.[15–24] Using quantum Monte Carlo (QMC) techniques intensive investigation to find superconductivity in this model has been performed.[16–18,20,24–26] However, no conclusive results indicating superconductivity in terms of off-diagonal long range order were obtained. This might be due to the limitations of this method to rather high temperatures such that important characteristics of the spin fluctuations responsible for the pairing state are not yet visible by analyzing the high temperature pairing vertex.[27]

Therefore, it is of great interest to investigate the occurrence of superconductivity in the three-band Hubbard Hamiltonian within the FLEX approximation by extending our one-band calculations for the normal state as well as the superconducting pairing state and by using model parameters corresponding to those used so far for the one-band model. This could provide a further support for the spin fluctuation pairing mechanism in the high T_c superconductors.

To fulfill the requirement of a charge transfer gap observed in optical measurements[28] at half filling a set of parameters for the local Coulomb repulsion $U_d^0=6t_{pd}$ and the charge transfer energy $\Delta_{pd}=\epsilon_p-\epsilon_d=4t_{pd}$ was obtained using QMC.[20] In the following these parameters are referred to as the *bare* parameters. Putz *et al.*[23] investigated the spectral density within the three-band Hubbard model using the above bare parameters and the FLEX approximation. They found in the whole Brillouin zone (BZ) maxima of the spectral density at low excitation energies ($\omega<0.25$ eV). This was interpreted in terms of the experimentally observed[29,30] flat quasiparticle bands.[31]

Most importantly we find in the analysis presented here a $d_{x^2-y^2}$ pairing symmetry and a superconducting transition temperature T_c of the correct order of magnitude. These results could only be obtained by using $\Delta_{pd}=4$ eV, $U_d\approx(1\text{ to }2)t_{pd}$ and hence by using an effective value for the Coulomb interaction $U_d<U_d^0$. Note, only the reduced Coulomb interaction properly yields the normal state scattering rate of the cuprates. U_d is different from the bare interaction, since the present theory focuses on the low energy degrees of freedom which are expected to interact with a renormalized coupling strength. In addition to finding observed T_c values we find that both Cu and O states contribute to the superconducting condensate. The dependence of the single particle excitations, quasiparticlelike versus incoherent excitations on U_d, is discussed. This supports the use of our model parameters. Note that the parameters we use for the three-band calculation, namely, $U_d/W\approx1/2$, $t_{pd}\approx1$ eV, and $U_d\approx(1-2)t_{pd}$, correspond to those commonly used in FLEX calculations of the effective one-band model ($U/W\approx1/2$, $t\approx0.25$ eV, and $U\approx4t$). Here, in both cases W is the $U=0$ bandwidth of the band crossing the Fermi level.

The three-band Hubbard model is given by

$$H=\sum_{i\sigma}(\epsilon_d-\mu)d^{\dagger}_{i\sigma}d_{i\sigma}+\sum_{j\sigma\alpha}(\epsilon_p-\mu)p^{\alpha\dagger}_{j\sigma}p^{\alpha}_{j\sigma}$$
$$+t_{pd}\sum_{ij\sigma\alpha}g^{\alpha}_{ij}(p^{\alpha\dagger}_{j\sigma}d_{i\sigma}+\text{H.c.})$$
$$+t_{pp}\sum_{lj\sigma}\tilde{g}_{lj}(p^{x\dagger}_{l\sigma}p^{y}_{j\sigma}+\text{H.c.})+U^0_d\sum_j d^{\dagger}_{j\uparrow}d_{j\uparrow}d^{\dagger}_{j\downarrow}d_{j\downarrow}. \quad (1)$$

Here, $d^{\dagger}_{i\sigma}$ creates a hole with spin σ in the Cu $3d_{x^2-y^2}$ orbital at a Cu site i. Correspondingly, $p^{\alpha\dagger}_{j\sigma}$ creates a O $2p_{\alpha}$ hole at an O site j with spin σ and $\alpha\in\{x,y\}$. t_{pd} and t_{pp} describe the p-d hybridization and p-p hybridization between nearest-neighbor Cu-O and O-O sites, respectively. g^{α}_{ij} and $\tilde{g}_{lj}$ are the corresponding phase factors reflecting the orbital symmetry of the CuO_2 planes.[10] The local orbital energy levels are given by ϵ_d and ϵ_p and the charge transfer energy is $\Delta_{pd}=\epsilon_p-\epsilon_d$. In the following we use $\Delta_{pd}=4$ eV, and $t_{pd}=1$ eV, $t_{pp}=0$ for the hopping integrals. Finally, U^0_d is the bare repulsive Coulomb interaction for two Cu holes at the same site and μ is the chemical potential. For simplicity, we neglect the Coulomb repulsion in the O $2p_{x,y}$ orbital and the interaction between Cu $3d_{x^2-y^2}$ and O $2p_{x,y}$ orbitals.[32] To investigate superconductivity we use the Nambu–Eliashberg treatment, based on the six component spinor $\Psi^{\dagger}_{\mathbf{k}}=(d^{\dagger}_{\mathbf{k}\uparrow},p^{\dagger x}_{\mathbf{k}\uparrow},p^{\dagger y}_{\mathbf{k}\uparrow},d_{-\mathbf{k}\downarrow},p^{x}_{-\mathbf{k}\downarrow},p^{y}_{-\mathbf{k}\downarrow})$. Thus, one finds the matrix Green's function

$$\hat{G}_{\mathbf{k}}(\omega)=\langle\langle\Psi_{\mathbf{k}};\Psi^{\dagger}_{\mathbf{k}}\rangle\rangle_{\omega}=\begin{pmatrix} S_{\mathbf{k}}(\omega) & T_{\mathbf{k}}(\omega)\\ T_{\mathbf{k}}(\omega) & \tilde{S}_{\mathbf{k}}(\omega)\end{pmatrix}^{-1}, \quad (2)$$

with

$$T_{\mathbf{k}}(\omega)=\begin{pmatrix} -\Phi_{\mathbf{k}}(\omega) & 0 & 0\\ 0 & 0 & 0\\ 0 & 0 & 0\end{pmatrix}, \quad (3)$$

$$S_{\mathbf{k}}(\omega)=\begin{pmatrix} \omega Z_{\mathbf{k}}(\omega)-\epsilon^d_0+\mu-X_{\mathbf{k}}(\omega) & \epsilon^{pd}_{kx} & \epsilon^{pd}_{ky}\\ -\epsilon^{pd}_{kx} & \omega-\epsilon^p_0+\mu & -\epsilon^{pp}_{\mathbf{k}}\\ -\epsilon^{pd}_{kx} & -\epsilon^{pp}_{\mathbf{k}} & \omega-\epsilon^p_0+\mu\end{pmatrix}, \quad (4)$$

$$\tilde{S}_{\mathbf{k}}(\omega)=\begin{pmatrix} \omega Z_{\mathbf{k}}(\omega)+\epsilon^d_0-\mu+X_{\mathbf{k}}(\omega) & -\epsilon^{pd}_{-kx} & -\epsilon^{pd}_{-ky}\\ \epsilon^{pd}_{-kx} & \omega+\epsilon^p_0-\mu & \epsilon^{pp}_{\mathbf{k}}\\ \epsilon^{pd}_{-kx} & \epsilon^{pp}_{\mathbf{k}} & \omega+\epsilon^p_0-\mu\end{pmatrix}, \quad (5)$$

with $\epsilon^{pd}_{kx}=-i2t_{pd}\sin(k_x/2)$, $\epsilon^{pd}_{ky}=i2t_{pd}\sin(k_y/2)$, and $\epsilon^{pp}_{\mathbf{k}}=-4t_{pp}\sin(k_x/2)\sin(k_y/2)$. Here, $\omega[1-Z_{\mathbf{k}}(\omega)]$ and $X_{\mathbf{k}}(\omega)$ are the self-energy matrix elements, also present in the normal state above the superconducting transition temperature T_c, although they will be strongly affected by the pairing state below T_c. Furthermore, the anomalous self-energy $\Phi_{\mathbf{k}}(\omega)=\Delta_{\mathbf{k}}(\omega)Z_{\mathbf{k}}(\omega)$ with the superconducting gap function $\Delta_{\mathbf{k}}(\omega)$ determines the occurrence and symmetry of the superconducting state. In the normal state the usual self-energy is given by $\Sigma_{\mathbf{k}}(\omega)=\omega[1-Z_{\mathbf{k}}(\omega)]+X_{\mathbf{k}}(\omega)$, which determines the normal state scattering rate $\tau^{-1}_{\mathbf{k}}(\omega)=-\mathrm{Im}\,\Sigma_{\mathbf{k}}(\omega)$ as well as the scattering rate of the superconducting state. Within the FLEX approximation $\omega Z_{\mathbf{k}}(\omega)$, $X_{\mathbf{k}}(\omega)$, and $\Phi_{\mathbf{k}}(\omega)$ are determined by a self-consistent summation of particle-hole ladder and bubble diagrams.[8] For the rather large doping concentration discussed in this paper, the vertex corrections neglected within FLEX were shown to be of minor importance,[33] although they are expected to become relevant for underdoped systems.[34] Note, in contrast to the effective one-band model in our calculation the specific Cu and O Green's functions are taken into account. However, due to our restriction to consider only the Coulomb interaction at the Cu sites all self-energy diagrams involve only the Cu Green's function.

The spin fluctuations generate a pairing interaction and a $d_{x^2-y^2}$ pairing state.[6] The tendency for the Cooper-pair formation is reduced by the inelastic scattering of the quasiparticles.[9,35] Thus, the excitations are affected by the pronounced spin fluctuations in two different ways. The interplay of the pairing interaction and the quasiparticle lifetime is determined by the details of the Fermi surface topology and the magnitude of the effective Coulomb interaction U_d. The effective Coulomb interaction U_d for the low-lying excitations of the system is expected to be smaller than the bare interaction U^0_d, since particle-particle excitations lead to particle-hole vertex renormalization. Note, this reduction of U_d is not included in the FLEX diagrams. The reduction of any repulsive bare interaction by particle-particle excitations to a smaller value, relevant for the low energy degrees of freedom, is a very general phenomenon for systems without nesting of the Fermi surface, which certainly applies to our case if the doping concentration is not too small.[36]

In the following we consider U_d as a purely phenomenological parameter of our model Hamiltonian and which is fixed by the value of the quasiparticle relaxation rate $\tau^{-1}_{\mathbf{k}}=-2\,\mathrm{Im}\,\Sigma_{\mathbf{k}}(0)$. Here, our aim is to reproduce $\tau^{-1}_{\mathbf{k}}=(1.0\text{–}2.0)T$ estimated from the dynamical conductivity[37] and dc conductivity,[38] where T is the temperature. As will be discussed below, this requires $U_d=(1.0\text{–}1.2)t_{pd}$. In the following we use $U_d=1.2t_{pd}$. Note, the calculation of the charge transfer gap as a high energy phenomena is beyond

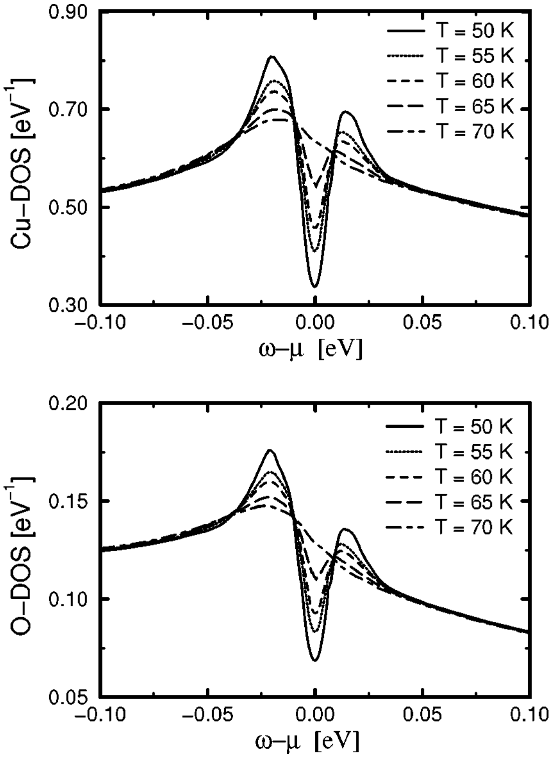

FIG. 1. The density of states at Cu and O sites for different temperatures and for $U_d = 1.2t_{pd}$ and doping $x = 0.18$. The simultaneous opening of the superconducting gap for both orbital states is clearly visible. The superconducting transition temperature is located around 70 K.

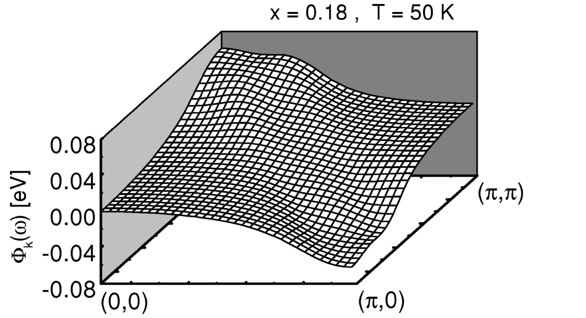

FIG. 2. Anomalous self-energy $\Phi_k(\omega=0)$ at $T=50$ K below $T_c \approx 70$ K within the first quadrant of the BZ. $\Phi_k(\omega=0)$ vanishes along the diagonal BZ and changes sign for $\mathbf{k}_x \leftrightarrow \mathbf{k}_y$, reflecting the $d_{x^2-y^2}$ symmetry of the superconducting order parameter.

the scope of the present theory. The actual calculations are performed on a (64×64) square lattice in momentum space and have a low energy resolution of $6.1\times 10^{-3}\ t_{pd} \approx 6$ meV around the Fermi energy. The method of Schmalian *et al.*[39] is used to obtain the results directly on the real frequency axis.

In Fig. 1 we show the density of states (DOS) at the Cu and O sites for a hole doping of $x_h = 0.18$ and for various temperatures. For lower temperatures the superconducting gap is clearly visible and vanishes for temperatures above $T=70$ K. The opening of the superconducting gap in the DOS behaves similarly for the Cu and O states. This shows that both $3d_{x^2-y^2}$ and $2p_{x,y}$ orbitals contribute to the superconducting state. From these results we obtain a value $\Delta = 23$ meV for the superconducting gap and estimate $2\Delta/T_c = 7.63$ by assuming that Δ does not change considerably below $T=50$ K. This is the lowest temperature we could reach numerically. Furthermore, we estimated $T_c \approx 70$ K. The fact that the states at the Fermi surface are dominantly Cu states is not in disagreement with the observation of a charge transfer system at half filling with an oxygen-dominated band on the hole side of the spectrum. The observed transfer of spectral weight from high to low energies[40] is expected to generate a much larger amount of Cu states near the Fermi energy upon doping.[41,42]

In order to demonstrate that the pairing state is indeed of $d_{x^2-y^2}$ symmetry, one has to investigate the anomalous self-energy $\Phi_{\mathbf{k}}(\omega)$. In Fig. 2 we present our results for the $\mathbf{k}$ dependence of $\Phi_{\mathbf{k}}(\omega=0)$, which within the BZ vanishes along the diagonal and changes its sign for $k_x \leftrightarrow k_y$ reflecting the $d_{x^2-y^2}$ symmetry. Hence, in agreement with results obtained for the one-band Hubbard Hamiltonian,[8,9] the three-band Hubbard Hamiltonian with Cu $3d_{x^2-y^2}$ and O $2p_{x,y}$ orbitals yields a spin fluctuation induced pairing state with $d_{x^2-y^2}$ symmetry. The ratio between $\Phi_{\mathbf{k}}(\omega=0)$ and $\Delta_{\mathbf{k}}$ for $\mathbf{k}=(\pi,0)$ can basically be understood in terms of the effective mass ratio $m^*/m = Z_{\mathbf{k}}(\omega=0) = 5.4$ at $T=50$ K. At $T=75$ K we find $m^*/m=4$.

The quasiparticle scattering rate below the superconducting transition temperature of the cuprates exhibits new and anomalous features characteristic of spin fluctuation induced Cooper pairing. In Fig. 3 we show the spectral density $\rho_{\mathbf{k}}(\omega)$ and the quasiparticle scattering rate $\tau_{\mathbf{k}}^{-1}(\omega)$ for different temperatures. These results are similar to those obtained within the effective one-band Hubbard model FLEX calculations. Due to the opening of the gap in the spectral density and simultaneously in the spin excitation spectrum, the quasiparticle scattering rate $\tau_{\mathbf{k}}^{-1}(\omega)$ is suppressed for $|\omega| < 2.5\Delta$ as observed experimentally.[43] Furthermore, for $|\omega|$

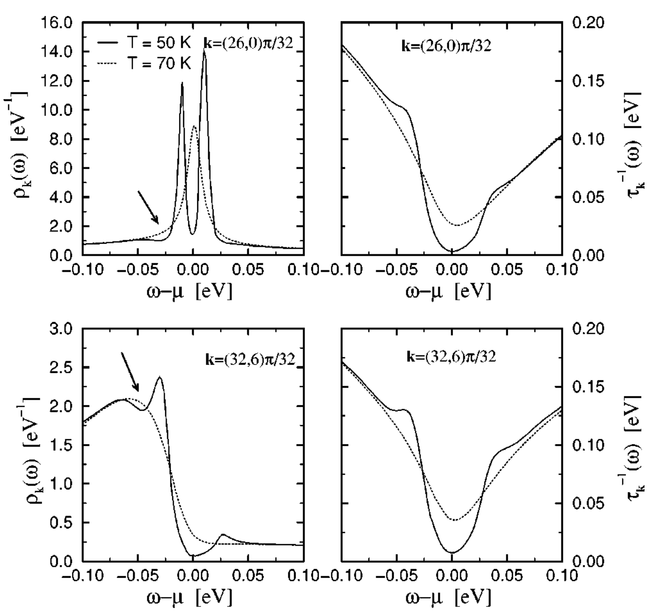

FIG. 3. Spectral density $\rho_k(\omega)$ and the scattering rate $\tau_{\mathbf{k}}^{-1}(\omega)$ in the superconducting $(T=50$ K) and normal state $(T=70$ K) for different momenta. The opening of the gap $\Delta = 23$ meV and in particular the suppression of the scattering rate for $|\omega| < 2.5\Delta$ at the FS are shown.

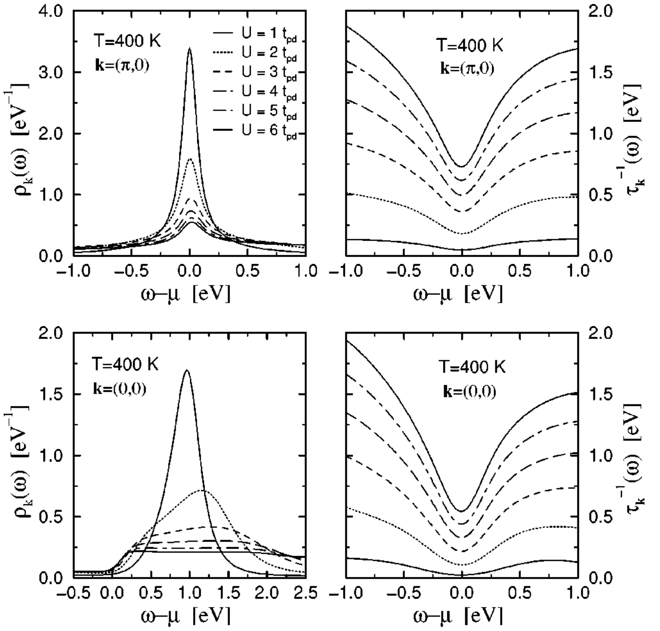

FIG. 4. Normal state spectral density $\rho_k(\omega)$ and scattering rate $\tau_{\mathbf{k}}^{-1}(\omega)$ for $\mathbf{k}=(\pi,0)$ near the FS and for $\mathbf{k}=(0,0)$ for different values of the Coulomb repulsion U_d. Note the huge scattering rates for larger values of U_d which totally destroy the coherent character of states away from the FS. The resulting weak maxima at $\mathbf{k}=(0,0)$ for $\omega-\mu=0.25$ eV are only of incoherent character inhibiting superconductivity for larger values of U_d due to scattering processes.

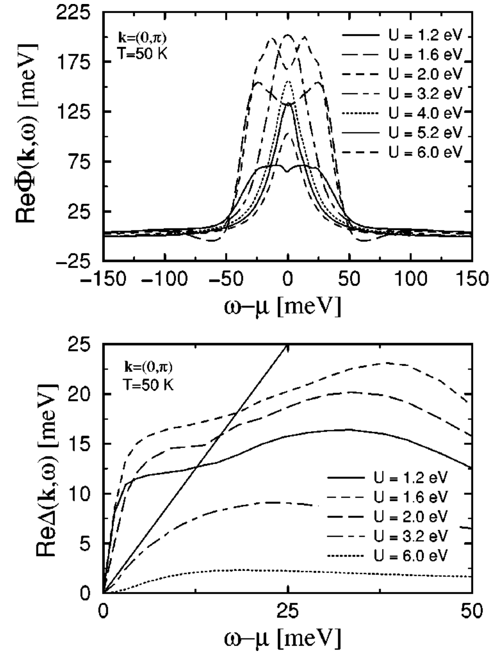

FIG. 5. Results for Re $\Phi(\mathbf{k},\omega)$ and Re $\Delta(\mathbf{k},\omega)$ of the superconducting gap function at the point $\mathbf{k}=(0,\pi)$ as a function of frequency for various values of the Coulomb repulsion U. Note, even though there is a finite value of the anomalous self-energy $\Phi(\mathbf{k},\omega)$ for all shown values of U, a finite solution of $\Delta_{\mathbf{k}}^0=\mathrm{Re}\,\Delta(\mathbf{k},\omega=\Delta_{\mathbf{k}}^0)$ exists only for small values of the Coulomb repulsion.

$>2.5\Delta$ the scattering rate increases in the superconducting state, where $\Delta=23$ meV is the gap amplitude. This has been observed in the corresponding scattering rate of optical measurements, which is expected to behave similarly to the single particle scattering rate discussed here.[44] This phenomenon was shown to be responsible for the observed dip structures in the spectral density $\rho_{\mathbf{k}}(\omega)$ within one-band model calculations[9] and which we also find in the spectral density of the present treatment.

It is important to state that all our results are obtained for an effective Coulomb interaction $U_d=1.2t_{pd}$, which is considerably smaller than the value $U_d=6t_{pd}$ used previously.[23,45] In order to demonstrate that our choice of U_d is the reasonable one for our FLEX treatment of the three-band Hubbard model, we have investigated the U_d dependence of the quasiparticle scattering rate $\tau_{\mathbf{k}}^{-1}(\omega)$. Results are shown in Fig. 4. Obviously, the experimentally observed order of magnitude of the scattering rate[37,38] is obtained if we use $U_d=(1.0–1.2)t_{pd}$, but not for $U_d=6t_{pd}$. Since the direct oxygen-oxygen hopping t_{pp} is expected to decrease the scattering rate, we show our results for $t_{pp}=-0.6t_{pd}$. Even in this case, values such as $U_d=6t_{pd}$ generate much too large scattering rates. Thus, on the average we find $\mathrm{Im}\,\Sigma_{\mathbf{k}}(\omega=0)=-0.06$ eV for $T=400$ K. In contrast, using $U_d=6t_{pd}$ the scattering rate is approximately 50 times too large.

This rapidly increasing scattering rate has a drastic influence on the Cooper pairing, since it reduces the lifetime of the quasiparticles and therefore the possibility of coherent Cooper pair formation. Hence, we will now discuss the U dependency of the superconducting state and make a connection to the recent paper by Esirgen and Bickers.[46] They presented results for FLEX calculations within the three-band model and found $d_{x^2-y^2}$ superconductivity for $U=8.0t_{pd}$ ($t_{pd}=1.3$ eV) by calculating the singlet pair eigenvalues in the particle-particle channel. If this eigenvalue reaches unity this indicates a superconducting phase transition and thus determines T_c and the symmetry of the order parameter. Within a self-consistent theory such as FLEX the crossing of unity by the eigenvalue corresponds to getting a finite value of the anomalous self-energy. Using FLEX and the three-band model we also get a finite value for $\Phi(\mathbf{k},\omega)$ with U/t_{pd} up to 6.0 (see Fig. 5) in fair agreement with the results of Esirgen and Bickers. However, in the DOS a significant superconducting gap opens up only for U/t_{pd} of the order 1.2 to 2.0. Note, $\Phi(\mathbf{k},\omega)$ as a function of U is, in our calculation largest for intermediate values of about $U/t_{pd}\approx 3.0$. As can also be seen from Fig. 5 the gap function $\Delta(\mathbf{k},\omega)=\Phi(\mathbf{k},\omega)/Z(\mathbf{k},\omega)$ itself is strongly affected by the drastically increasing scattering rates for larger values of the Coulomb repulsion. Therefore, the largest gap amplitude is obtained for smaller values of U.

It is also of interest to note in Fig. 5 that $\Delta_{\mathbf{k}}^0=\mathrm{Re}\,\Delta(\mathbf{k},\omega=\Delta_{\mathbf{k}}^0)$ only has solutions for $U/t_{pd}\leqslant 2.0$ and that only then the superconducting state is expected to be stable against phase fluctuations of the order parameter.[47] In accordance with our one-band calculations we expect that we get for the three-band model from the requirement $\Phi(\mathbf{k},\omega)=0$ for all ω a transition temperature T_c^* reflecting only an onset of phase-disordered Cooper pairing and yielding furthermore no maximal T_c^* as a function of doping. A phase coherent Cooper-pair state is only obtained at T_c resulting from $\Delta_{\mathbf{k}}^0$ having a finite value.[47] Note that only for this can one get a maximal T_c for optimal doping in the one-band case.

It is interesting that we obtain for our reduced value of $U_d=1.2t_{pd}$ corresponding to the usually taken value $U=4t$ of the one-band FLEX calculations[8] similar results for $\mathrm{Im}\,\Sigma_{\mathbf{k}}(\omega=0)/W$. Here, W is the uncorrelated bandwidth of the band crossing the Fermi energy and U and t are the effective Coulomb repulsion and nearest-neighbor hopping element of the one-band model, respectively.

Finally, we discuss the dispersion and the structure of the spectral density and compare it with the results obtained for $U=6t_{pd}$ in Ref. 23. Using these large values of the Coulomb interaction, we also find that the maximum of the spectral density is shifted considerably to lower binding energies compared to the uncorrelated case. Furthermore, we find for states $\mathbf{k}=(\pi,0)$ at the Fermi surface (FS) that large U_d values ($U_d\approx 6t_{pd}$) drastically reduce the quasiparticle weight due to the too large scattering rate, but not their energy positions. Hence, one still has a quasiparticle, i.e., a solution $E_{\mathbf{k}}$ of $E_{\mathbf{k}}=\epsilon_{\mathbf{k}}(E_{\mathbf{k}})+\mathrm{Re}\,\Sigma_{\mathbf{k}}(E_{\mathbf{k}})$, but with reduced weight. Here in the case of the three-band model $\epsilon_{\mathbf{k}}(\omega)$ is given by

$$\epsilon_{\mathbf{k}}(\omega)=\epsilon_0^d+\gamma_{\mathbf{k}}(\omega), \tag{6}$$

with

$$\gamma_{\mathbf{k}}(\omega)=-\frac{(\omega-\epsilon_0^p)(\epsilon_{kx}^{pd2}+\epsilon_{ky}^{pd2})+\epsilon_{kx}^{pd}\epsilon_{ky}^{pd}\epsilon_k^{pp}}{(\omega-\epsilon_0^p)^2-\epsilon_k^{pp2}}. \tag{7}$$

The situation is different for states far away from the FS. For example, for $\mathbf{k}=(0,0)$ one still finds a drastically reduced spectral weight for $U_d=6t_{pd}$, but additionally the now only weakly formed maxima in the spectral density are shifted by ≈ 0.6 eV towards the Fermi energy. As a consequence we analyze for the spectral density at $\mathbf{k}=(0,0)$ strongly incoherent states for the large U_d values. This follows from the determination of the energy position of the quasiparticle pole of the single particle Green's function which shifts from $\omega=0.9$ eV to $\omega=1.2$ eV as U_d changes from 1 eV to 6 eV. Besides the fact that perturbation theory becomes questionable for large U_d, this demonstrates that one must be careful in interpreting the maxima of the spectral density as quasiparticle peaks. However, even more importantly than this is the above discussed extremely large scattering rate occurring for large U_d, overestimating the incoherency of the system dramatically and being inconsistent with the normal state properties of the cuprates.

In summary, by choosing input parameters corresponding to the ones used for the effective one-band model we obtain for the three-band Hubbard model using FLEX theory normal-state properties of high T_c superconductors in good agreement with experiments. Moreover, we get spin fluctuation induced superconductivity at high temperatures ($T_c \approx 70$ K) and a d-wave symmetry order parameter. Our results are in fair agreement with those obtained previously within FLEX theory for the effective one-band Hubbard model.

Note the recently discussed suppression of the mean-field transition temperature of the Eliashberg theory in underdoped systems due a drastic reduction of the superfluid density[47] is expected to be of less importance for the doping concentration investigated in this paper. Of course, further calculations within the three-band model are necessary to show the observed doping dependence of various properties and in particular of T_c. Extensions of our theory should properly yield for underdoped cuprates the tendency for the spin-singlet state of Cu and O states and site specific spin susceptibilities. Also, extensions of the theory are needed to understand the interplay of spin and charge fluctuations and of low and high energy excitations. In view of the recent discussion that certain sum rules related to the Pauli principle are not fulfilled within FLEX,[48] it is worth noticing that in the case of the one-band model and for the doping values investigated in this paper these sum rules are quantitatively fulfilled to rather high precision (5% for $x=0.16$). There is certainly a need to develop new theoretical methods which are as self-consistent as FLEX (essential to study the superconducting state) and which are elaborated more as far as two-particle excitations are concerned.[48] This will help to better understand the limitations of FLEX and the different results obtained by various other studies.[25,45]

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