# Renormalized band structure of $CuO_2$ layers in superconducting compounds: A mean-field approach

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We have analyzed the band structure of a $CuO_2$ plane including two copper orbitals ($d_{x^2-y^2}$ and $d_{3z^2-r^2}$) and two oxygen orbitals ($p_x$,$p_y$) in a tight-binding approximation. A Hubbard interaction between copper $d$ holes has been considered with use of a slave-boson technique, while oxygen and copper holes interact via a nearest-neighbors Coulombic repulsion treated in the Hartree-Fock approximation. The resulting band structure opens the way to a comparison with the experiments and to some theoretical implications on the pairing mechanism of high-$T_c$ superconductors.

The electronic structure of the high-temperature superconductors has been a controversial issue ever since their discovery by Bednorz and Müller.[1] There is a general agreement in the scientific community in assigning a major role to the $CuO_2$ layers in determining the normal and superconducting properties of these materials.[2] At zero doping the $CuO_2$ system has one hole per unit cell residing on Cu sites with $d_{x^2-y^2}(b_1)$ symmetry. The additional holes introduced by doping in the superconducting samples reside on oxygen sites because of the large Hubbard repulsion on Cu sites $U_d$ (of the order of 8–10 eV). Experiments[3] suggest that they occupy the in-plane $p_x$,$p_y$ orbitals, while the full identification of their symmetry is still controversial. Limiting the discussion to the oxygen $2p$ orbitals pointing towards the nearest Cu site, a molecular analysis would indicate the occupation of the $b_1$ combination[4] $(1/\sqrt{4})(p_{x_1}-p_{y_2}-p_{x_3}+p_{y_4})$ which strongly hybridizes with the $3d_{x^2-y^2}$ Cu orbital. The associated hopping-matrix element is $t_{pd}\sim 1.3$ eV. The $a_1$ combination $(1/\sqrt{4})(p_{x_1}+p_{y_2}-p_{x_3}-p_{y_4})$ would instead combine with the $3d_{3z^2-r^2}$ Cu orbital, through a hopping of size $t_{pd}/\sqrt{3}$ leading to a higher energy level for the holes. This scenario favors the effective single-band spin-singlet picture proposed by Rice and Zhang.[5] However recent x-ray-absorption spectroscopy (XAS) experiments[6] with polarized light have shown a non-negligible occupation of the $3d_{3z^2-r^2}$ Cu orbitals varying from a few percent in the insulating sample up to 30–40% in some high-temperature superconducting Bi compounds. This raises the question of determining to what extent a one-band or two-band picture is suitable to describe the normal-state properties of these superconducting oxides.

In this paper we have addressed this topic of controversy in the literature and tested the relevance of the $3d_{3z^2-r^2}$ orbitals (and of the related $a_1$ symmetric $p$ combination) by a mean-field analysis of a four-band-model system. Because of the large $U_d$, we have adopted a slave-boson approach to describe the $d$-$d$ correlation. The other interactions here considered, i.e., the $p$-$d$ repulsions, are instead treated within a standard Hartree-Fock decoupling scheme. We have found that the resulting scenario critically depends on the sign of the direct oxygen-oxygen hopping integral leading to a renormalized band structure with one or two band crossing the Fermi energy.

The model that we consider here is a generalized version of a tight-binding Hubbard model in two dimensions. The Hamiltonian for the $CuO_2$ layers is written as

$$
\begin{aligned}
H=&-2t\sum_{k,\sigma}\sin\left(\frac{k_x}{2}\right)(d^{\dagger}_{xk,\sigma}p_{xk,\sigma}+\text{H.c.})-2t\sum_{k,\sigma}\sin\left(\frac{k_y}{2}\right)(d^{\dagger}_{xk,\sigma}p_{yk,\sigma}+\text{H.c.})-\frac{2t}{\sqrt{3}}\sum_{k,\sigma}\sin\left(\frac{k_x}{2}\right)(d^{\dagger}_{zk,\sigma}p_{xk,\sigma}+\text{H.c.})\\
&+\frac{2t}{\sqrt{3}}\sum_{k,\sigma}\sin\left(\frac{k_y}{2}\right)(d^{\dagger}_{zk,\sigma}p_{yk,\sigma}+\text{H.c.})+2t_p\sum_{k,\sigma}\alpha_k(p^{\dagger}_{xk,\sigma}p_{yk,\sigma}+\text{H.c.})+\varepsilon^0_{d_x}\sum_{i,\sigma}d^{\dagger}_{xi,\sigma}d_{xi,\sigma}+\varepsilon^0_{d_x}\sum_{i,\sigma}d^{\dagger}_{zi,\sigma}d_{zi,\sigma}\\
&+\varepsilon_p\sum_{j,\sigma}(p^{\dagger}_{xj,\sigma}p_{xj,\sigma}+p^{\dagger}_{yj,\sigma}p_{yj,\sigma})+U_d\sum_{i,\alpha,\beta=x,z}d^{\dagger}_{\alpha i\uparrow}d_{\alpha i\uparrow}d^{\dagger}_{\beta i\downarrow}d_{\beta i\downarrow}\\
&+V_x\sum_{i,j,\sigma,\sigma',\alpha=x,y}d^{\dagger}_{xi,\sigma}d_{xi,\sigma}p^{\dagger}_{\alpha j,\sigma'}p_{\alpha j,\sigma'}+V_z\sum_{i,j,\sigma,\sigma',\alpha=x,y}d^{\dagger}_{zi,\sigma}d_{zi,\sigma}p^{\dagger}_{\alpha j,\sigma'}p_{\alpha j,\sigma'}\ ,
\end{aligned}
\tag{1}
$$

 

where

$$\alpha_k \equiv \cos\left[\frac{k_x+k_y}{2}\right] - \cos\left[\frac{k_x-k_y}{2}\right] .$$

We work in the hole representation in which the vacuum state is the $3d^{10}$ configuration for the copper and the $2p^6$ for the oxygen. The $d_{xi,\sigma}$ and $d_{zi,\sigma}$ ($d^\dagger_{xi,\sigma}$ and $d^\dagger_{zi,\sigma}$) operators are annihilation (creation) operators for holes in the $3d_{x^2-y^2}$ and $3d_{3z^2-r^2}$ orbitals of the Cu atoms, while $p_{x,y,j,\sigma}$ ($p^\dagger_{x,y,j,\sigma}$) are the corresponding operators for the $2p_x$, $2p_y$ orbitals on the O sites and $\sigma$ labels the spin. $\varepsilon_p$ and $\varepsilon^0_{d_x}, \varepsilon^0_{d_z}$ are the bare atomic levels on O and Cu, respectively. Typical values considered here are $\varepsilon_p - \varepsilon^0_{d_x} = 4.7$–$6.5$ eV. The two Cu atomic levels $\varepsilon^0_{d_x}$ and $\varepsilon^0_{d_z}$ may assume slightly different values in order to consider a small ($<0.4$ eV) crystal-field splitting $\varepsilon^0_{d_z} - \varepsilon^0_{d_x}$. $t$ indicates here the $d_{x^2-y^2}-p$ hopping-matrix element $t_{pd}$ and the geometrical factor $1/\sqrt{3}$ arises in the $d_{3z^2-r^2}-p$ hopping term.

Two main ingredients are introduced in Eq. (1) to vary the relative occupation $n_{d_x}$ and $n_{d_z}$ of $d$ orbitals with different symmetries as a function of doping: (i) a direct oxygen-oxygen hopping $t_p$ and (ii) a nearest-neighbor interatomic repulsion $V$. The sign of the hopping terms should be determined by the physical requirement that the electrons tend to reside between the ions, leading to $t_p > 0$ with our choice of phases for the orbitals. The size and the sign of the hopping terms can be deduced from density-functional calculations, in particular Ref. 7 and Refs. 8 and 9 give $t_p = 0.33$ eV and $t_p = 0.65$ eV, respectively. However, although this is unexpected, it could happen that the electron-filled orbitals (such as, e.g., $d_{xy}$) overscreen the ionic potentials. This would favor electrons residing out of the oxygen-oxygen links corresponding to a different sign in the hopping term, $t_p < 0$. To cover both possibilities in the present model we assume $t_p$ to be a free parameter ranging from $-0.3$ to 0.5 eV. The repulsion $V$ is expected to depend on the symmetry of the $d$ hole and in particular $V_x \equiv V_{pd_x} > V_z \equiv V_{pd_z}$ because the $p_{x,y}$ orbitals overlap more with the $d_{x^2-y^2}$ orbitals than with the $d_{3z^2-r^2}$ ones. Typical values are $V_x \sim 1.3$ eV and $V_z \sim 0.3$–$0.9$ eV.

The Hubbard $U_d$ is the largest energy scale in the model. In the following we shall take $U_d \to \infty$ so that one gets the constraint $n_{d_x} + n_{d_z} \le 1$, which is readily transformed by means of the slave-boson approach[10] leading to $b_i^\dagger b_i + n_{d_{xi}} + n_{d_{zi}} = 1$, where $b_i^\dagger$ and $b_i$ are the slave-boson operators of the standard replacement of the $d$ and $d^\dagger$ operators $d^\dagger \to d^\dagger b$, $d \to b^\dagger d$. The last condition is then implemented by a Lagrange multiplier field $\lambda_i$. The $V_{x,z}$ terms are instead decoupled via a Hubbard-Stratonovich transformation which introduces four complex-conjugate auxiliary fields $v$, $v^*$, $u$, and $u^*$.

At mean-field level we set

$$b_i = \langle b_i \rangle \equiv b_0, \quad \lambda_i = \langle \lambda_i \rangle \equiv \lambda, \quad v_i = \langle v_i \rangle \equiv v_0 ,$$
$$v_i^* = \langle v_i^* \rangle \equiv v_0, \quad u_i = \langle u_i \rangle \equiv u_0, \quad u_i^* = \langle u_i^* \rangle \equiv u_0^* .$$

In the mean-field Hamiltonian, $H_{\rm MF}$, $b_0$ renormalizes multiplicatively the hopping term and reduces the kinetic-energy gain for the coherent motion. $\lambda$ acts as a common shift of the $d$ levels ($\varepsilon_d \equiv \varepsilon^0_d + \lambda$) while the Hartree-Fock decoupled intersite Coulombic repulsion introduces two additional doping-dependent level shifts $-4v_0^*$ and $-4u_0^*$ for the $d_{x^2-y^2}$ and $d_{3z^2-r^2}$ orbitals, respectively.

The mean-field parameters must be determined via self-consistency equations which, at $T=0$, are obtained by minimizing the average mean-field energy $\langle H_{\rm MF} \rangle$ with respect to the six parameters. By solving the self-consistency equations we obtain a renormalized band structure, which is expected to describe the quasiparticle behavior of the $CuO_2$ planes. We find that the resulting band structure strongly depends on the sign of $t_p$, the main difference being that one or two bands can cross the Fermi energy for $t_p > 0$ and $t_p < 0$, respectively. This is shown in Figs. 1(a) and 1(b) for two representative sets of parameters chosen to fit the XAS data and the ir reflectivity (see below).

$t_p > 0$ lowers the $b_1$ $p$ combination favoring the mixing between $p$ and $d_{x^2-y^2}$ orbitals. The lower dispersive band has mainly $d_{x^2-y^2}$ character. The $d_{3z^2-r^2}$ band is almost flat and lays a few tenths of an eV above the Fermi energy. The $d_{3z^2-r^2}$ $\Gamma$ point, which is representative of the renormalized atomic $d_{3z^2-r^2}$ level, is displaced below the renormalized $d_{x^2-y^2}$ level by the local potential $-4u_0^* = V_z n_p < -4v_0^* = V_x n_p$. On the contrary $t_p < 0$ lowers the $a_1$ $p$ combination and favors the $p$ mixing with $d_{3z^2-r^2}$ orbitals. The $d_{3z^2-r^2}$ band becomes dispersive and, for not too small doping, can now cross the Fermi

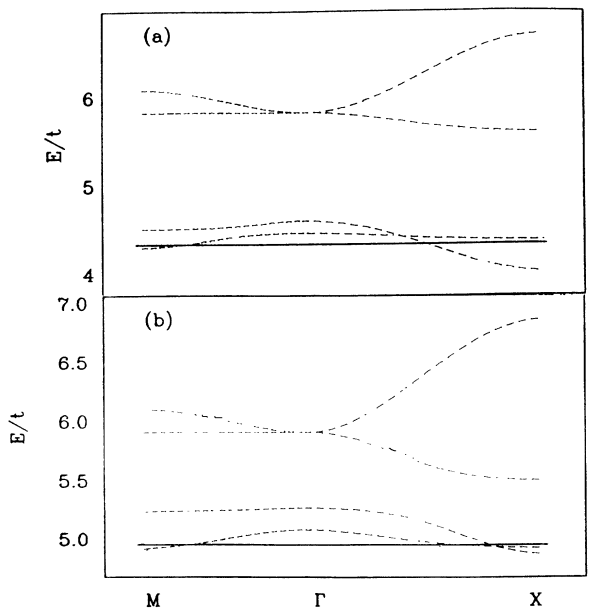


FIG. 1. Renormalized band structure for $t=1.3$, $V_x=1.3$, $V_z=0.75$, $\varepsilon_p - \varepsilon^0_{d_x} = 6.5$. Case (a) corresponds to $\varepsilon^0_{d_z} - \varepsilon^0_{d_x} = 0$, $t_p = 0.26$, and case (b) to $\varepsilon^0_{d_z} - \varepsilon^0_{d_x} = 0.4$, $t_p = -0.26$.

level around the $X$ point. In the present case a sizable $d_{3z^2-r^2}$ occupation is compatible with a local crystal-field shift of the order of 0.4 eV. Indications of the presence of two dispersive bands in the vicinity of the Fermi level in a $Bi_2Sr_2CaCu_2O_8$ single crystal were given by angle-resolved photoemission spectroscopy (ARPES) in Ref. 11. One of the bands ($A$) apparently crosses the Fermi level midway along the high-symmetry line $\Gamma X$; also the other band ($B$) approaches the Fermi level suggesting a crossing which, however, was not stated because of the finite-energy resolution. More recent ARPES analysis[12] confirms the presence of band $A$ leaving open the problem of the presence of the crossing of band $B$, which could also be assigned to the bismuth. In our model bands $A$ and $B$ would correspond to the two hole bands which at the $\Gamma$ point lay 0.2–0.8, 0.4–1 eV above the Fermi level (to be compared with the experimental finding $\sim$0.2, 0.5 eV) for $\varepsilon_p-\varepsilon_{d_x}^0$ varying in the range 6.5–4.7 eV. Notice that in our model the crossing of the Fermi level by two hybridized oxygen-copper bands, if confirmed, will be properly described by the (unlikely) choice $t_p<0$.

Photoemission experiments usually indicate an overwhelming $p$ character of the holes near the Fermi surface. This is well accounted for in the present model if one keeps in mind that the coherence factor $b_0^2$ is directly related to the residuum of the pole in the single-particle Green function of the physical fermions. Therefore the correspondence between the calculated weight $W_d^{\rm MF}$ and the measured weight $W_d^{\rm expt}$ is established via the factor $b_0^2\sim0.1$, $W_d^{\rm expt}\sim b_0^2 W_d^{\rm MF}$. On the other hand, $W_p^{\rm expt}=W_p^{\rm MF}$. Since we find $W_p^{\rm MF}/W_d^{\rm MF}\sim0.6$, it is readily seen that our model gives $W_p^{\rm expt}/W_d^{\rm expt}\sim6$, which is compatible with the observed ($\sim80\%$) $p$ character. We also emphasize that the smallness of $b_0^2$ is a signature of the relevant strength of the interaction which reduces the relative weight of the coherent pole with respect to the incoherent background.

Aside from the photoemission experiments our mean-field band structure has other important implications, both experimental and theoretical, which we are now going to discuss.

*Fermi surface.* The Fermi surface has a different shape and curvature depending on the sign of $t_p$. In particular the choice $t_p>0$ leads to an electronlike Fermi surface. This feature derives from the introduction of the $d_{3z^2-r^2}$ orbitals and reverses the conclusions drawn in Ref. 13. On the other hand, the $t_p<0$ case present holelike "pockets" in the Fermi surface whose sizes depend on the doping. If this were the real situation interesting consequences in the Hall coefficient would appear. Even more interesting in this latter case is the nearly squared shape of the Fermi surface that would drive strong instabilities of the incommensurate charge- and spin-density-wave type for momenta $q\sim2k_F$ in the $\Gamma M$ directions. This characteristic is mainly due to the quasi-one-dimensional character of the bands along those directions.

*XAS experiments.* X-ray-absorption experiments with polarized light[6] have revealed a substantial $d_{3z^2-r^2}$ character in the conduction hole band. The absorption of x rays with the electric field along the direction perpendicular to the $CuO_2$ planes shows in fact a peak whose integrated area is proportional to the amount of $z$-symmetric $d$ holes in the sample. In our model the ratio of $d_{3z^2-r^2}$- versus planar-($d_{x^2-y^2}$-) symmetric holes $n_z/n_x$ depends on the doping both in the $t_p>0$ and in the $t_p<0$ case. However, the dependence on doping is stronger in the second case as is apparent from Fig. 2, where we report the ratio $n_z/n_x$ as a function of doping together with experimental data of Ref. 6. We have (arbitrarily) assumed a proportionality relation between $\delta$ and $T_c$ to make a comparison between the two sets of data possible. Although a qualitative agreement with experiments is found in the increasing tendency of $n_z/n_x$ versus $\delta$, an unambigous choice of the sign of $t_p$ on the basis of the behavior of $n_z/n_x$ from XAS experiments is still not possible. This is mainly due to the large error bars in the experimental values of $n_z/n_x$ and to the difficulty in connecting the doping with $T_c$, the most commonly accessible quantity. The inset in Fig. 2 shows the occupation number of $d_{3z^2-r^2}$ that we obtain for different values of doping.

Our results partially contrast with the results of Eskes *et al.*[14] where an exact numerical diagonalization of the full many-body Hamiltonian was carried out for two clusters with $Cu_2O_7$ and $Cu_2O_8$ structure. Their set of parameters was $\varepsilon_p-\varepsilon_d^0=3.5$ eV, $t=1.3$ eV, $t_p=0.65$ eV, $U_d=8.8$ eV, $U_p=6$ eV. In the case of three holes in the cluster the occupation of the $d_{3z^2-r^2}$ orbital was never

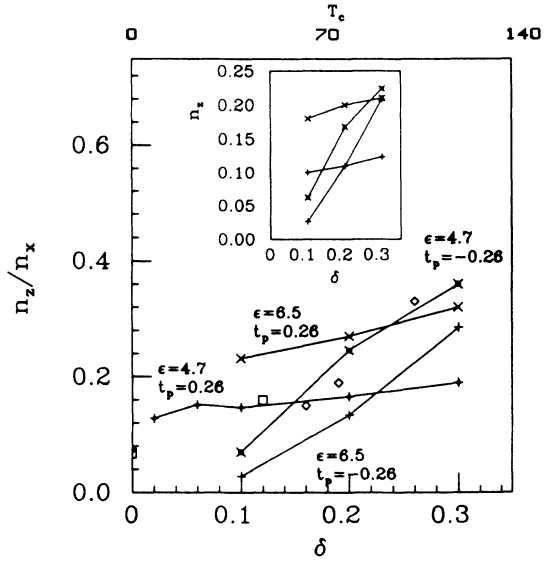


FIG. 2. Ratio of the average $d_{3z^2-r^2}$ density vs the average $d_{x^2-y^2}$ density, $n_z/n_x$, as a function of doping for various values of $t_p$ and $\varepsilon_p-\varepsilon_{d_x}^0$. In the $t_p=0.26$ eV cases the crystal-field splitting is $\varepsilon_{d_z}^0-\varepsilon_{d_x}^0=0$, while, for $t_p=-0.26$ eV, $\varepsilon_{d_z}^0-\varepsilon_{d_x}^0=0.4$ eV. Experimental XAS values are shown for comparison: squares for La-Sr-Cu-O as a function of $\delta$ (lower axis) and diamonds for Bi-Sr-Ca-Cu-O as a function of $T_c$ (upper axis). The inset shows the dependence of $n_z$ on the doping.

larger than 0.01. The evaluation of the effective doping introduced by three holes in the cluster is somewhat ambiguous. We have estimated $\delta \sim 0.3$ for $Cu_2O_7$ and $\delta \sim 0.2$ for $Cu_2O_8$. This would suggest a comparison of their result for $n_z$ with our $\delta = 0.2, 0.3$, $t_p > 0$ case revealing a sizable discrepancy. Besides their higher value of $t_p$ we single out two main sources for this discrepancy: (i) even when they consider an intersite repulsion they do not assume different values for $V_x$ and $V_z$; (ii) our model is carried out on a lattice. Since $V_z < V_x$ the effective local level for $d_{3z^2-r^2}$ is below the corresponding $d_{x^2-y^2}$ level; the almost flat $d_{3z^2-r^2}$ band along the $\Gamma M$ direction mixes with a dispersive $d_{x^2-y^2}$ band as in a heavy-fermion system. The two bands repel each other resulting in a crossing of the Fermi level of the $d_{x^2-y^2}$ band around the $M$ point. In that region, as it is pointed out in Ref. 14, there is a strong $d_{3z^2-r^2}$-$d_{x^2-y^2}$ mixing leading to a sizable value for $n_z$. This possibility was suggested by Eskes *et al.* as a consequence of the lattice structure; we have found that $V_x > V_z$ enhances this effect.

*Optical absorption.* Infrared reflectivity experiments also provide a valid source of data for the understanding of the electronic structure of the high-$T_c$ materials. In order to compare these data with the predictions of our model we have calculated the frequency-dependent conductivity estimating the current matrix element in the $x$ direction from the continuity equation. The conductivity $\sigma^{xx}(\omega)$ in the $xx$ direction is evaluated according to the golden rule and satisfies the following sum rule:

$$\int_0^{+\infty} \sigma^{xx}(\omega) d\omega = -\frac{\pi}{16}(\langle T_{pd_x} \rangle + \langle T_{pd_z} \rangle + 2\langle T_{pp} \rangle) , \tag{2}$$

where the $T$'s are the kinetic-energy contributions coming from the various hybridizations. The results for the interband $\sigma$ in the low-energy region are shown in Figs. 3(a) and 3(b). Figure 3(a), corresponding to a positive $t_p$, shows a small absorption edge of the order of 0.05–0.1 eV, which increases with doping while the absorption peaks move from 0.1 to 0.3 eV. On the other hand, the absorption edge is absent in the $t_p < 0$ case [Fig. 3(b)] and correspondingly the peaks are shifted at lower frequency.[15] In both cases the area below the curves increases with doping showing a dependence on the number of carriers. Conductivity data coming from reflectivity measurements[16–19] show broad peaks in the mid-ir low-frequency region. The presence of an absorption at low frequency ($\sim 0.1$ eV) is a common feature of experiments and has often been interpreted as due to some frequency-dependent scattering mechanism.[20] Recent mid-ir absorption experiments on $YBa_2Cu_3O_{7-\delta}$ films[18] have been interpreted in terms of a direct electronic excitation. In the same mid-ir region our analysis predicts an interband optical transition between the two low-lying hybridized $p$-$d$ bands. Rather surprisingly our results for $t_p < 0$ seem to represent rather well the experimental findings of Ref. 17. The linewidths of the oscillators used to fit the measured reflectivity of Bi-Sr-Ca-Cu-O films[17] are larger than

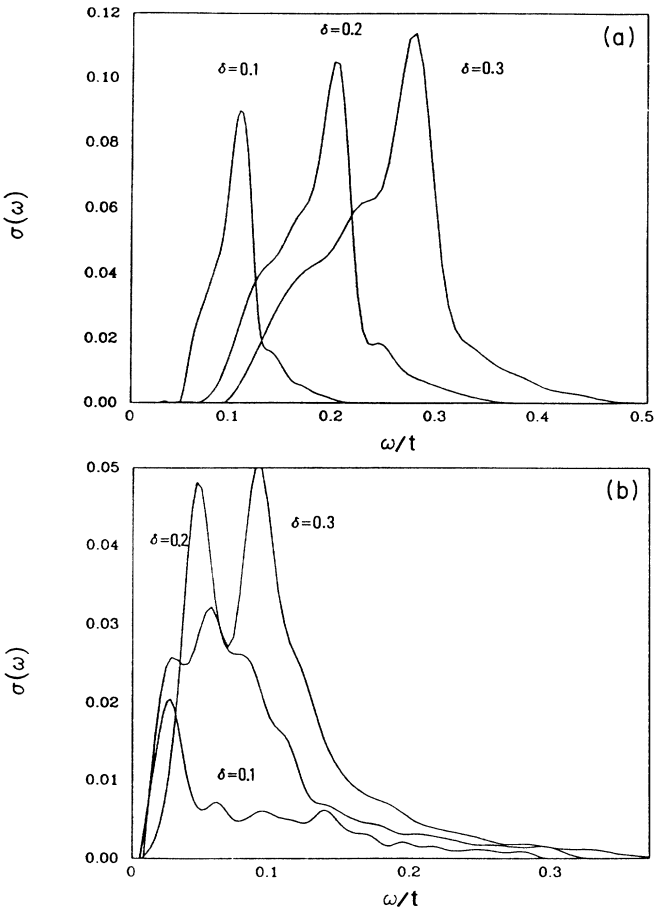


FIG. 3. Frequency-dependent conductivity from direct electronic transitions in units of $e^2/\hbar$. Cases (a) and (b) correspond to the same parameters of Fig. 1. For (a) the weight of the Drude term $W_{\sigma_D}$ and the weight of the interband term $W_{\sigma_{12}}$ are $W_{\sigma_D} = 0.021$, 0.034, 0.044, and $W_{\sigma_{12}} = 0.013$, 0.026, 0.038 for doping $\delta = 0.1$, 0.2, 0.3, respectively; in case (b) $W_{\sigma_D} = 0.020$, 0.049, 0.077 and $W_{\sigma_{12}} = 0.004$, 0.004, 0.014.

the peaks of Fig. 3, but this discrepancy can be easily understood because in the framework of the present mean-field slave-boson formalism, only the coherent (quasiparticle) contribution to the optical conductivity is obtained. A noncoherent part is expected as a background and at higher energy as well. This noncoherent background will show up beyond our mean-field approximation as it occurs in the photoemission spectra calculated in Ref. 21 by introduction of Gaussian fluctuations in a related approximate model.

So far only the normal-state properties have been discussed. The above-described band structure, however, has important consequences for the pairing mechanism leading to high-temperature superconductivity. In fact the closeness of the two lowest bands suggests that isovalent excitonic effects of the type described in Ref. 22 could be a relevant source of pairing. Apart from excitonic effects our analysis shows that, with $t_p > 0$, only one band is crossing the Fermi level and the presence of up to

$\sim 35\%$ of $3d_{3z^2-r^2}$ holes is still compatible with an effective single-band $t(t')J$ model,[23] even though the Fermi-liquid vs non-Fermi-liquid nature of the system still remains an open problem.[24] On the other hand, the $t_p < 0$ case, with two bands crossing the Fermi level, opens the way to another possibility: the holes in the upper band could interact via a Kondo-like interaction with the spins of the antiferromagnetically correlated holes in the lowest band. This would introduce a pairing mechanism (possibly cooperative with the excitonic one) on the lines described in Refs. 25–28.

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[15]In Fig. 3 $\varepsilon_p - \varepsilon^0_{d_x} = 6.5$ eV has been chosen to fit the ir data of Ref. 17. For the smaller value $\varepsilon_p - \varepsilon^0_{d_x} = 4.7$ eV the doping dependence of $\sigma_{12}(\omega)$ shows a different trend. The absorption peaks move towards lower frequencies starting from the crystal-field value ($\sim 0.4$ eV) at very low doping as soon as the $d_{3z^2-r^2}$ band acquires a $p$ character and becomes optically active. A similar feature for the optical conductivity in La-Sr-Cu-O has been reported in Ref. 19.

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