Electronic structure and hole-hole coupling in $YBa_2Cu_3O_{7-x}$ systems

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The electronic structure of $YBa_2Cu_3O_{7-x}$ for $x=0$, has been determined by means of an approximation to the self-energy for Hubbard systems with two channels for the localization (p and d). This self-energy contains the unrestricted Hartree-Fock terms and the dynamically screened exchange. The calculated electronic structure presents a different ionization state for the atoms of the CuO_2 sheets with respect to the CuO_3 chain. For increasing x values, electron transferences between O-O, Cu-Cu, and Cu-O atoms are produced. These electronic transferences provide holes to the CuO_2 sheets in symmetries $d_{x^2-y^2}$ of Cu(2) and p_x and p_y of O(2) and O(3). These holes suffer interatomic screening, which produces coupling for determined densities of holes and widths of the bands. The main parameter for obtaining superconductivity is the lower limit of the frequency interval for which the interatomic $W_{pd}(\omega)$ is negative. This frequency has to be sufficiently less than a critical cutoff frequency. We discuss the conditions of the electronic structure for obtaining high-T_c superconductivity.

I. INTRODUCTION

The crystal structure of the high-T_c superconductors has two subsets with different chemical coordination[1] even with different ionization degree of their component atoms: Two equivalent CuO_2 sheets composed by atoms Cu(2)-O(2)-O(3) (in the nomenclature of Yan *et al.*[1]), and a linear CuO_3 chain composed of atoms Cu(1)-O(1)-O(1)-O(4). This structure corresponds to the $YBa_2Cu_3O_7$ system, where the Y and Ba atoms have an almost irrelevant influence in the superconducting behavior. The transition occurs for a determined number of O(4) and O(1) vacancies in the linear chain. The main effect caused by the oxygen vacancies is the breaking of the $d-p$ covalent bonds between the Cu(1) and O(4) and O(1) atoms and a subsequent breaking of the linear chain. Then, the atoms Cu(1) and remaining O(4) and O(1) atoms take a larger ionic character and therefore the localization of their charge density increases.

The electronic structures of all high-T_c superconductors present a common feature which has been experimentally observed and that has a decisive influence in the appearance of the high-T_c superconductivity. This is the coexistence of strongly correlated states along with band states with large $E(\mathbf{k})$ dispersion.[2] Both of them have been detected by photoemission experiments. These experimental data can be understood by considering the different localization of the d states of Cu with respect to the p states of O. In addition, the $d_{x^2-y^2}$ orbitals of Cu(2) and p_x/p_y of O(2) and O(3) suffer a larger overlapping than those of the Cu(1) and O(4) and O(1) atoms.[3,4] On the other hand, the creation of O(4) and O(1) vacancies produces a supplementary localization of the orbitals $d_{x^2-y^2}$ and $d_{3z^2-r^2}$ of Cu(1) and the p_x/p_z ones of O(4) and O(1) atoms, respectively.[3] Then, these d and p states are involved in the Coulomb-Hubbard splitting and as a consequence, their occupations decrease in order to minimize the total energy of the crystal. This fact being the cause of the different ionization state of the atoms of the CuO_2 units with respect to those of the CuO_3 chain.

Recent experimental results have shown that the density of states (DOS) of the CuO_2 sheets of $YBa_2Cu_3O_{7-x}$ does not suffer significant modifications for light deviations of the x value.[5] However, the progressive localization of the p and d states of the CuO_3 chain, when the x value (the vacancy number) increases, causes an increase in the Coulomb correlation effects and therefore a reorganization of the conduction charge. For a determined x value, the Madelung energy per CuO_2 atom is larger than the Coulomb correlation energy for the p and d states of the linear unit. Then no electron of the CuO_3 chain is transferred to the CuO_2 sheets, leaving a determined number of holes in the planes. These hole states interatomically overlap and suffer strong dynamical screening[6] that for determined density of holes and bandwidths produces negative interactions. This hole-hole (h-h) coupling can be, in our opinion, the direct responsibility of the high-T_c superconductivity.

In this paper, we consider a band calculation method which includes different Coulomb correlation effects for the different orbitals of the different atoms according to their own occupation. The obtained electronic structure of $YBa_2Cu_3O_7$ is compatible with the photoemission experimental results.[2,4,7–9] In addition, we give an interaction model which produces coupling for determined values of the densities of holes p and d, it being necessary, moreover, that the bandwidths of these bands range between determined values.

II. BAND CALCULATION METHOD

The consideration of the different Coulomb correlation effects for each atom is based on the different localization

of each d and p symmetries. This requires a versatile model of calculation which allows us to obtain several multiband Hubbard splittings[10] in order to deduce the features of the electronic structure of the $YBa_2Cu_3O_7$. The many-body Hamiltonian considered in this work is

$$H=H_{\mathrm{LDF}}+H_p+H_d$$
$$=\sum_{\mathbf{k},\alpha}\varepsilon^0_{\mathbf{k},\alpha}n_{\mathbf{k}\alpha}+\sum_{\mu}\sum_{p\sigma<p'\sigma'}U_p n_{\mu p\sigma}n_{\mu p'\sigma'}$$
$$+\sum_{\nu}\sum_{d\sigma<d'\sigma'}U_d n_{\nu d\sigma}n_{\nu d'\sigma'}\ , \tag{1}$$

where H_{LDF} is the local-density-formalism (LDF) Hamiltonian; $\nu(\mu)$ runs over all Cu (O) atoms; U_d (U_p) stands for the totally screened Coulomb repulsion between two d (p) electrons and coincides with the energy for obtaining an electronic transference between two atoms[11] of Cu (O), i.e.,

$$U_d=E(3d^{x+1})+E(3d^{y-1})-E(3d^x)-E(3d^y)$$

and

$$U_p=E(2p^{x+1})+E(2p^{y-1})-E(2p^x)-E(2p^y)\ ,$$

where $E(3d^y)$ [$E(2p^y)$] represents the total energy per unit cell corresponding to a $3d$ ($2p$) band with y electrons. The value for U_p is estimated as 4.7 eV (see Refs. 12 and 13) and the value of U_d depends on the localization of the d symmetry. For instance, for the orbitals d_{xz}, d_{xy}, and d_{yz} whose localizations are large, the value of U_d ranges between 5 and 7 eV. For other more extended d orbitals like $d_{x^2-y^2}$ and $d_{3z^2-r^2}$ the U value can be considered somewhat less. The calculation is performed with $U_p=4.7$ eV. The value for U_d is almost irrelevant for obtaining the electronic structure whenever $U_d\geq U_p$. For simplicity, we have calculated the band structure with a value for U_d of 4.7 eV.

In recent papers,[14] we established a procedure for systematizing the band structure calculation including many body effects from different approximations to the self-energy in strongly correlated systems. This implies solving a nonlocal Schrödinger-like equation as

$$\varepsilon_{\mathbf{k}\alpha}\varphi_{\mathbf{k}\alpha}(\mathbf{r})=[-\nabla^2+V_{\mathrm{LDF}}(\mathbf{r})]\varphi_{\mathbf{k}\alpha}(\mathbf{r})+\int\Sigma(\mathbf{r},\mathbf{r}',\varepsilon_{\mathbf{k}\alpha})\varphi_{\mathbf{k}\alpha}(\mathbf{r}')d^3r'\ . \tag{2}$$

The self-energy $\Sigma(\mathbf{r},\mathbf{r}',\omega)$ contains the unrestricted Hartree-Fock terms[14] and a dynamically screened exchange[10,15] applied to the two channels p and d and thus

$$\Sigma(\mathbf{r},\mathbf{r}',\omega)=\sum_p[U_p+M_p(\omega)]p(\mathbf{r})p(\mathbf{r}')+\sum_d[U_d+M_d(\omega)]d(\mathbf{r})d(\mathbf{r}') \tag{3}$$

with

$$M_p(\omega)=-U_p\int_{-\infty}^{E_F}\frac{N_p(x)dx}{\varepsilon_p(x-\omega)}\ , \tag{4}$$

$$M_d(\omega)=-U_d\int_{-\infty}^{E_F}\frac{N_d(x)dx}{\varepsilon_d(x-\omega)}\ , \tag{5}$$

where $d(\mathbf{r})[p(\mathbf{r})]$ are $d(p)$ orbitals defined only in the Cu (O) atoms; N_d (N_p) stands for the partial density of states corresponding to the d (p) orbital (in a first step, the DOS of the noninteracting system is considered in this expression); $\varepsilon_d(x)[\varepsilon_p(x)]$ is the intra-atomic screening function for the d (p) orbitals defined in Cu (O) atoms. The intra-atomic dielectric functions used in this work are

$$\varepsilon_{p(d)}(\omega)=1-\frac{U_{p(d)}\Pi^0_{p(d)}(\omega)}{1+\frac{1}{2}U_{p(d)}\Pi^0_{p(d)}(\omega)}\ , \tag{6}$$

where $\Pi^0_{p(d)}(\omega)$ is the polarization whose expression depends on the occupation and effective bandwidths of the p (d) orbitals of the ground state. We use in this work, the function $\Pi^0_{p(d)}(\omega)$ given in Ref. 15 and expression (6) for $\varepsilon_{p(d)}(\omega)$. Expression (6) represents the Hubbard approach to the dielectric function applied to the strongly correlated systems. It must be remembered that this dielectric function is an improvement in the random phase approximation theory for $\varepsilon(\omega)$.[16]

The electronic structure is obtained by solving Eq. (2) by means of the augmented plane wave (APW) method and the resulting matrix elements of the secular equation considering the self-energy operator are[10]

$$[M^\alpha_{ij}(E)]_\Sigma=[M^\alpha_{ij}(E)]_{\mathrm{APW}}+\sum_R X^{\alpha R}_j\sum_\nu Y^{\nu R}_{ij}Z^{\nu R}_{ij}(E)\ , \tag{7}$$

where

$$X^{\alpha R}_j=(4\pi)^2\frac{g}{n_\alpha}\Gamma^\alpha_{11}(R)\exp(i\mathbf{K}_j\cdot\mathbf{t}_R)\ , \tag{8}$$

$$Y^{\nu R}_{ij}=\frac{S_\nu^2}{\Omega}\exp[i(R^{-1}\mathbf{K}_j-\mathbf{K}_i)\cdot\mathbf{r}_\nu]\times I_m(K_iS_\nu)I_m(K_jS_\nu)\ , \tag{9}$$

$$Z^{\nu R}_{ij}=\sum_{t=1}^{2m+1}\left[\frac{d}{dr}\ln\frac{R_m(\varepsilon_t,r)}{R_m(E,r)}\right]_{r=S_\nu}\times\psi^\nu_t(\mathbf{K}_i)\psi^\nu_t(R^{-1}\mathbf{K}_j)\ , \tag{10}$$

with

$$\varepsilon_t=E-U_t-\mathrm{Re}[M_t(E)]\ , \tag{11}$$

where K_j, $\mathbf{t}_R$, g, R, n_α, I_m, and Ω have the standard meanings within the APW method; the index ν runs over the Cu and O atoms of the primitive cell; the index m corresponds either to d or p orbitals depending on whether ν index corresponds to a Cu or an O atom; S_ν is the muffin-tin radius of the ν atom whose position vector is $\mathbf{r}_\nu$; $\psi^\nu_t(\mathbf{K}_j)$ are linear combinations of $l=m$ orbitals compatible with the crystal symmetry and centered on the Cu and O atoms; $R_m(\varepsilon,r)$ is the radial part of the $l=m$ orbital calculated to the ε energy from the Schrödinger radial equation; $[M^\alpha_{ij}(E)]_{\mathrm{APW}}$ is the standard APW matrix elements corresponding to the irreducible representation α. The second term in the right-hand side of (7) is the pseudopotential arising from the self-energy operator between two ij APW bases. The energies E, which satisfy the condition

$$\det[M^\alpha_{ij}(E)]_\Sigma=0\ , \tag{12}$$

are eigenvalues which correspond to the eigenstates with a fixed $\mathbf{k}$ vector of the first Brillouin zone and α symmetry [it must be remembered that $\mathbf{k}=\mathbf{K}_j-\mathbf{G}_j$, where $\mathbf{K}_j$ ($\mathbf{G}_j$) is the vector corresponding to the j APW basis (a vector of the reciprocal lattice)].

The method for calculating (12) has been given elsewhere,[10] therefore, we give here no calculation details. However, we would like to comment that for each energy E, we determine $\Sigma(E)$ and the secular matrix whose elements are given by (7) is triangularized. In addition, it must be remembered that the dimension of the secular matrix for obtaining standard convergencies of around 0.002 Ry have to be larger than 600. This complex calculation can be simplified by using physical arguments for obtaining the Π^0 polarizations. These arguments consist in considering a determined occupation and effective bandwidths of the different p and d orbitals of the ground state which corresponds to the normal state of the $YBa_2Cu_3O_7$ system. This ground state is constructed by considering the following experimental and theoretical features: (i) The CuO_2 sheets present half-filled antibonding hybridized orbitals $d_{x^2-y^2}-p_{x,y}$ and fulfilled bonding orbitals corresponding to the same symmetries.[3,17,18] Moreover, the bands arising from these symmetries present a large $E(\mathbf{k})$ dispersion.[2,9] (ii) The localization in the linear chain is larger than in the CuO_2 sheets,[4,17] therefore, in this linear unit the $d_{x^2-y^2}$ and $p_{x,y}$ and p_z orbitals suffer larger Coulomb correlation effects than those of the same orbitals of the CuO_2 sheets. (iii) The O(4) vacancies appear in the CuO_3 chain[19] of the vacuum state of the $YBa_2Cu_3O_7$ system and produce a supplementary localization of the orbitals $d_{x^2-y^2}$ and $d_{3z^2-r^2}$ of Cu(1) and $p_{x,y}$ of the remaining O(4) and p_z of O(1).[4,17] This localization is caused by the breaking of the $d-p$ bindings and implies an increase in the Coulomb correlation effects. (iv) The electronic occupation of the atoms belonging to CuO_2 sheets is larger than that corresponding to the atoms of the CuO_3 chain.[3,4,17,20]

The above features of the noninteracting system ground state can be implemented in analytical expressions of the $\Pi^0_{p(d)}$ functions by considering the occupation state of each p (d) orbital. The most extremal features of this ground state is to consider unoccupied[20] a d orbital of Cu(1), a p orbital of O(4) and another p of O(1). This implies that the occupations of the d shell of Cu(2) and the p of O(2) and O(3) are larger than those of Cu(1) and O(4) and O(1), respectively.[17] Therefore, the Coulomb correlation effects are larger in the chain than in the planes, even when considering the same U parameters for their corresponding atoms since these effects strongly depend on the respective orbital occupations. Any intermediate situation can be considered proposing the corresponding $\Pi^0_{p(d)}$ given in Ref. 15. This requires performing some tentative DOS calculations from determined functions $\Pi^0_{p(d)}$ whose validity should be confirmed by comparison of the resulting electronic structure with the experimental results. The final results are not depending on the initial conditions due to the self-consistent process, however, a good choice of the initial conditions reduce considerably the number of iterations.

III. COMMENTS ON THE RESULTS OF THE ELECTRONIC STRUCTURE

In Fig. 1(a), we give the DOS considering only H_{LDF} (i.e., DOS calculated considering $U_p=U_d=0$). These results agree with other theoretical results performed with similar procedures and are given in this paper in order to show the Coulomb correlation effects by comparison. The resulting electronic structure of the Y-Ba-Cu-O system is characterized by the existence of hybridized bonding orbitals ($d_{x^2-y^2}-p_xp_y$) totally occupied and antibonding orbitals half-occupied.

Electronic transferences can occur between Cu-Cu, Cu-O, and O-Cu atoms and this implies the existence of holes located in $3d^{y-1}$ or $2p^{y-1}$ ions and the existence of excited electrons located in $3d^{x+1}$ or $2p^{x+1}$ ions. Therefore the transferred electrons have to occupy quasiparticle states of the upper Hubbard bands (unoccupied in the ground state). The spectrum of the interacting system including these quasiparticle states is obtained by means of the eigenvalues $\varepsilon_{\mathbf{k}\alpha}$ of (2) deduced from (12). In Fig. 1(b), we draw the total DOS considering U_p and U_d different from zero and the main features displayed by this DOS are the following: (i) The Fermi level is at ~ 1.6 eV above the giant peak of the valence band corresponding to $3d$ states of Cu(2). The shift up of E_F considering $U_p\neq 0$ and $U_d\neq 0$ is around 0.8 eV [compare Figs. 1(a) and 1(b)]. This result is a clear improvement with respect to that obtained by the LDF since the LDF calculations locate the gravity center of these $3d$ states of Cu(2) (see Fig. 2) ~ 0.7 eV below E_F, in disagreement with the photoemission spectroscopy.[2,7,8] This effect implies a tendency of the Cu(2) toward an ionization state between $+1$ and $+2$ in the ground state.[20] (ii) The width of the valence band is ~ 6 eV below E_F and 2.5 eV above E_F, this width being in a better agreement with the direct and inverse x-ray photoemission spectroscopy[8] (XPS) than those results performed without considering Coulomb correlation

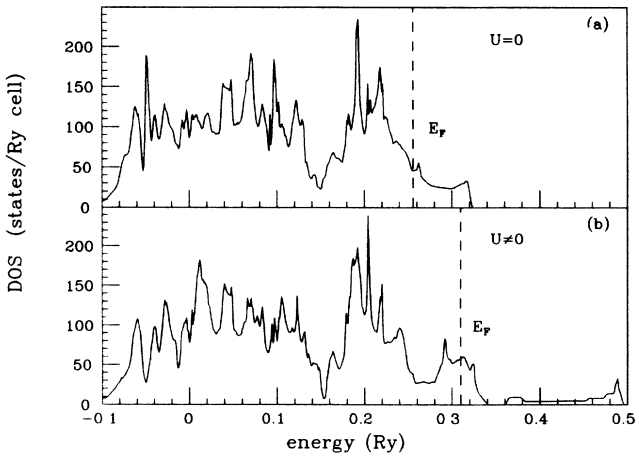

FIG. 1. Total density of states of $YBa_2Cu_3O_7$ (a) calculated within the LDF, i.e., without considering Coulomb correlation effects and (b) considering Coulomb correlation effects through Eq. (2).

effects (i.e., considering $U_p = U_d = 0$ [Fig. 1(a)]). (iii) E_F is located close to ($\sim$0.4 eV) a gap in the DOS. This gap is produced by the strong correlation effects. The existence of the gap has been schematically proposed in other recent theoretical works[21–23] and implies that a semiconducting phase is close to the superconducting transition. (iv) The structures in the DOS above the gap (in Fig. 1) are an admixture of 3*d* Cu(1) and 2*d* O(4) and O(1) states in the symmetries $d_{x^2-y^2}$ and $d_{3z^2-r^2}$ and $p_{x,y}$ and p_z, respectively. At E_F, there is an admixture of all orbitals although the p_z symmetry of O(1) and the $d_{x^2-y^2}$ and $d_{3z^2-r^2}$ symmetries of Cu(1) are dominant.

In Fig. 2 we show the partial DOS corresponding to the *d* orbitals of the Cu(2) and Cu(1) atoms. The occupations of the Cu(2) *d* orbitals are larger than those of the Cu(1) ones and this implies that the Coulomb correlation effects are larger in Cu(1) than in Cu(2). This leads to a tendency in the valence of the Cu(2) to be closer to +1 than to +2 ($\approx +1.2$), however, the valence of Cu(1) is somewhat larger than +2 ($\approx +2.1$). These different valences of Cu(2) and Cu(1) have been experimentally deduced by the ion substitution method by Xiao *et al.*[20] In Fig. 3, we give the partial DOS corresponding to *p* states of the different oxygen atoms. The occupation of the *p* orbitals of O(2) and O(3) implies an ionization state close to -2 (≈ -1.8), while the ionization of the O(4) and O(1) atoms is closer to -1 (≈ -1.1 and -1.0, respectively). However, the evaluation of the valence cannot be unambiguously determined since this depends on the volume in which is normalized the charge.

It is necessary to remark the large localization of the states with d_{xz}, d_{xy}, and d_{yz} symmetries corresponding to Cu(1) since 94% of their charge density is located within the muffin-tin sphere. These states are strongly correlated and the gravity centers of the corresponding bands are at $\sim$3 eV below E_F and this forces their total occupation. The existence of strongly correlated states below E_F is a common feature of the high-T_c superconductors[2] and this fact can originate unstabilities since the large Coulomb repulsion energies of these states can cause dynamic interchange between the occupation of the more localized symmetries with other more extended orbitals[24] (this point is used in Ref. 24 for explaining some characteristics of the electronic structure of Y-Ba-Cu-O systems). On the other hand, the orbitals $d_{x^2-y^2}$ of Cu(2) suffer large *pd* hybridizations and the respective bands have a large $E(\mathbf{k})$ dispersion. E_F cuts off these bands and this implies the existence of a Fermi surface which has been detected by Takahashi *et al.*[2] and Arko *et al.*[9]

IV. COUPLING MECHANISM

The CuO_2 sheets have an excess of negative charge with respect to the CuO_3 chain in the normal state of the $YBa_2Cu_3O_{7-x}$ system for $x=0$. This can be deduced from our results of Figs. 2 and 3 and is in agreement with other theoretical[17] and experimental[5] works. When neutral O(4) vacancies are produced approximately an electron per each O(4) vacancy is added to the conduction band. In addition, further localization of the charge of

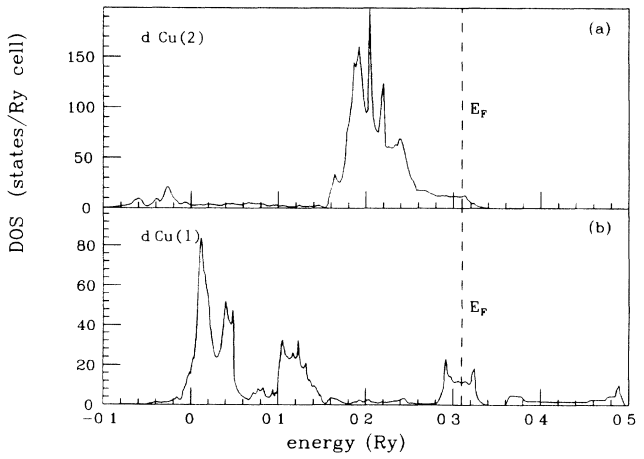

FIG. 2. Partial density of states of the 3*d* states corresponding to (a) Cu(2), (b) Cu(1), considering U_p and U_d different from zero.

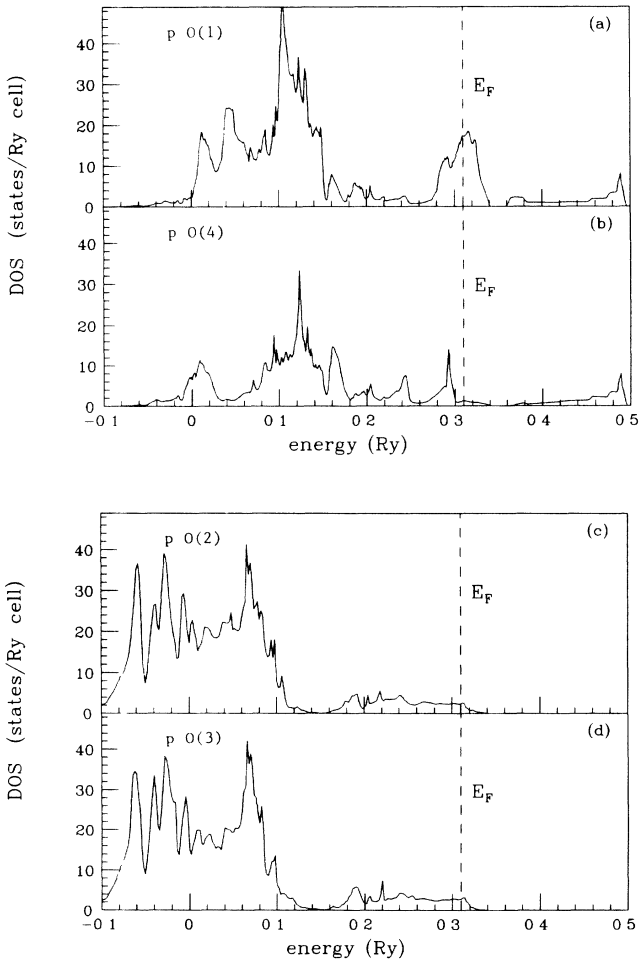

FIG. 3. Partial density of states of the 2*p* states corresponding to (a) O(1), (b) O(4), (c) O(2), and (d) O(3), considering $U_p \neq 0$ and $U_d \neq 0$.

the CuO_3 chain is produced implying a reorganization of the total charge. The free charge added to the band conduction will tend fundamentally to occupy states arising from the p_z orbital of O(1) and $d_{x^2-y^2}$ and $d_{3z^2-r^2}$ of Cu(1) since these symmetries are dominant at E_F. However, some few states arising from the orbitals $p_{x,y}$ of O(2) and O(3) and $d_{x^2-y^2}$ of Cu(2) can also be occupied by the free charge added per each O(4) vacancy (see Figs. 2 and 3) implying a light increase in the Madelung energy in the CuO_2 sheet. Therefore, for increasing values of x, the Madelung energy per ion in CuO_2 increases.[25] This energy can increase until it becomes larger than the Coulomb correlation energy in the CuO_3 unit. Then, the holes of the CuO_2 remain unaltered in the process of O(4) vacancy production. These hole states have a large interatomic overlapping and the corresponding interatomic [Cu(2)-O(2) and O(3)] h-h interaction suffers a strong dynamical screening.[26] However, only for determined DOS in symmetries $d_{x^2-y^2}$ of Cu(2) and p_x and p_y of O(2) and O(3), can the superconductivity arise. The objective of this part of our work is to analyze the conditions of the CuO_2 hole bands which are compatible with a h-h coupling caused by the dynamically screened interactions, and to compare these conditions with the results of the first part of this paper.

The dynamical screened h-h interaction is deduced from recurrent equations as

$$W_p(\mathbf{q},\omega)=U_p+U_p\Pi_p(\mathbf{q},\omega)W_p(\mathbf{q},\omega)+U_{pd}\Pi_d(\mathbf{q},\omega)W_{dp}(\mathbf{q},\omega)\ , \tag{13}$$

$$W_d(\mathbf{q},\omega)=U_d+U_d\Pi_d(\mathbf{q},\omega)W_d(\mathbf{q},\omega)+U_{dp}\Pi_p(\mathbf{q},\omega)W_{pd}(\mathbf{q},\omega)\ , \tag{14}$$

$$W_{pd}(\mathbf{q},\omega)=U_{pd}+U_p\Pi_p(\mathbf{q},\omega)W_{pd}(\mathbf{q},\omega)+U_{pd}\Pi_d(\mathbf{q},\omega)W_d(\mathbf{q},\omega)\ , \tag{15}$$

$$W_{dp}(\mathbf{q},\omega)=U_{dp}+U_{dp}\Pi_p(\mathbf{q},\omega)W_p(\mathbf{q},\omega)+U_d\Pi_d(\mathbf{q},\omega)W_{dp}(\mathbf{q},\omega)\ , \tag{16}$$

where U_{pd} is the interatomic bare interaction between p and d orbitals. The dependence of $W_d(\omega)$, $W_p(\omega)$, and $W_{pd}(\omega)$ on $\mathbf{k}$ is dropped by considering average values over the first Brillouin zone [i.e., $W_d(\omega)=(1/N)\sum_{\mathbf{k}}W_d(\mathbf{k},\omega)$]; the functions Π are defined as

$$\Pi_{p(d)}(\omega)=F_{p(d)}(\omega)+F_{p(d)}(-\omega) \tag{17}$$

being

$$F_{p(d)}=\sum_{p(d)}\int_{-a}^{E_F}\int_{E_F}^{b}\frac{N_{p(d)}(\varepsilon)N_{p(d)}(\varepsilon')d\varepsilon\,d\varepsilon'}{\omega+\varepsilon-\varepsilon'+i\theta}\ , \tag{18}$$

where $N_{p(d)}(\varepsilon)$ is the DOS corresponding to the p (d) orbitals calculated by the method described in Sec. II of this paper [Eq. (12)]. In our case, as in Emery and Reiter's model,[27] we have only the DOS corresponding to the symmetries $d_{x^2-y^2}$ of Cu(2) and p_x and p_y of O(2) and O(3). In expression (17) $a+b=\delta_{p(d)}$, $\delta_{p(d)}$ being the effective width of the band in which the paired holes are located. Takahashi *et al.*[2] detected this band which is cut by E_F and its width is between 0.1 and 0.3 eV.

Then, the screened interactions are given by[28] $\mathbf{W}(\omega)=[\mathbf{I}-\mathbf{U}\boldsymbol{\Pi}(\omega)]^{-1}\mathbf{U}$; where $\mathbf{W}$, $\mathbf{U}$, and $\boldsymbol{\Pi}$ are matrices defined in the $p\otimes d$ space. $\boldsymbol{\Pi}$ is considered diagonal and is calculated from the spectrum of the interacting system. The dependence on $\mathbf{k}$ of the $\mathbf{W}$ interaction could proportionate the evaluation of the anisotropy of the superconducting gap, however, we only analyze in this work the possibility for the coupling through the pd interaction. For the DOS of the superconducting phase of $YBa_2Cu_3O_{7-x}$ this screened produces attractive interaction at frequencies less than the critical frequency[18,26,28] (the models for the pairing proposed in Refs. 6 and 12 can be classified within the same group). The critical frequency ω_c for high-T_c systems can be estimated from experimental results like those given in Ref. 29. The value of ω_c is between 0.08 and 0.11 eV [other estimations give a value for ω_c of around 0.5 eV (Ref. 6)] and the energy interval for which $W_{pd}(\omega)$ is negative ranges between $\simeq$0.03 eV and $\simeq$0.2 eV (see Fig. 4). Therefore, $W_{pd}(\omega)$ can produce coupling between holes of Cu(2) ($d_{x^2-y^2}$) and O(2) and O(3) (p_x and p_y). This coupling is sufficiently intensive for obtaining high-T_c superconductivity. However, the main parameters which determine the h-h coupling are the frequency interval for which W_{pd} is negative and above all the lower limit of this interval.

The origin of the coupling is the dynamical screening and this effects $W_{pp}(\omega)$, $W_{dd}(\omega)$, and $W_{pd}(\omega)$ effective interatomic interactions which have identical dynamics, although different expressions for each of them. We have performed an analysis of the tendencies of $W_{pd}(\omega)$ for different band parameters. This $W_{pd}(\omega)$ interaction is given by

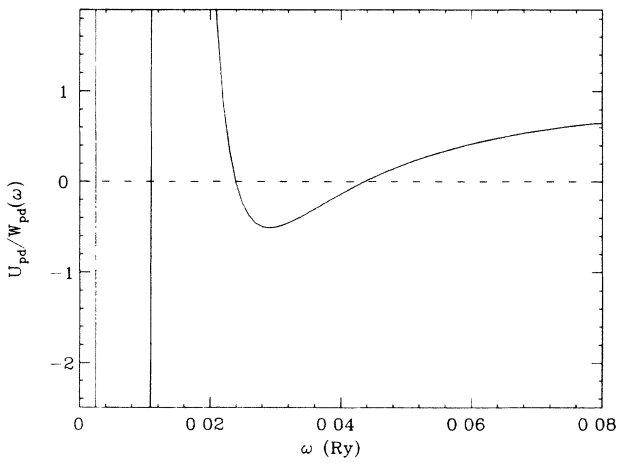

FIG. 4. An example of the real part of the function $U_{pd}/W_{pd}(\omega)$ which implies h-h coupling. This function is obtained with the following band parameters: $\delta_d=0.1$ eV, $\delta_p=0.3$ eV, $n_d=0.5$, and $n_p=0.5$. n_d and n_p in all figures have the meaning of the number of electrons in the orbitals $d_{x^2-y^2}$ of CuO_2 and p_x and p_y of O(2) and O(3), respectively.

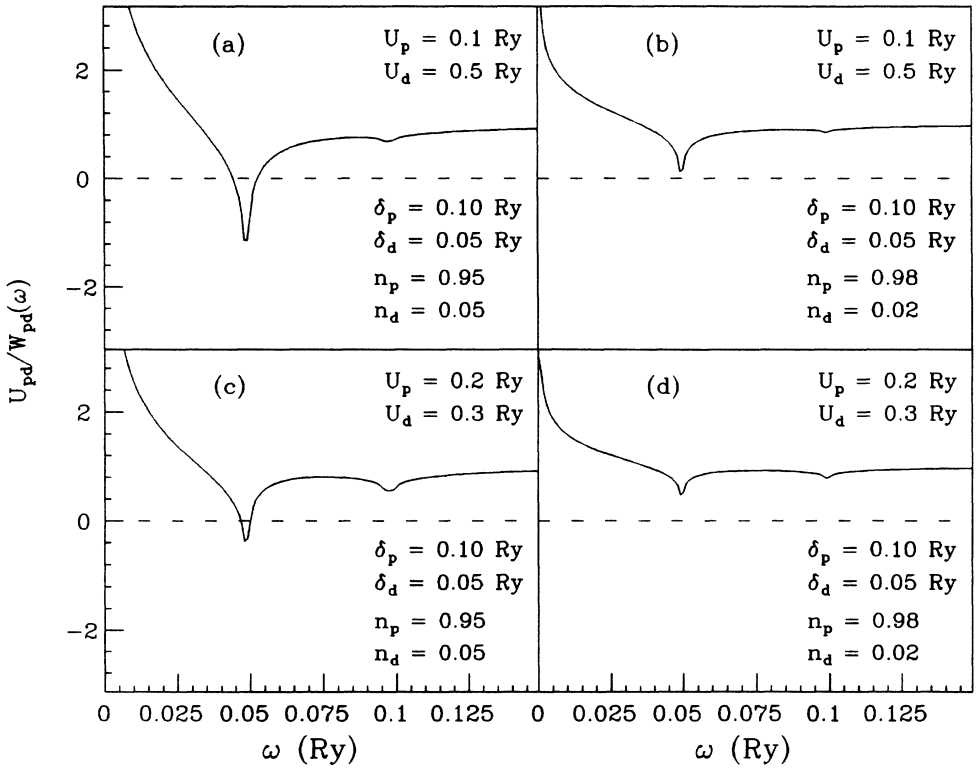

FIG. 5. Examples of the function $\mathrm{Re}[U_{pd}/W_{pd}(\omega)]$ which does not imply h-h coupling. This function is obtained with the parameters given in the figure.

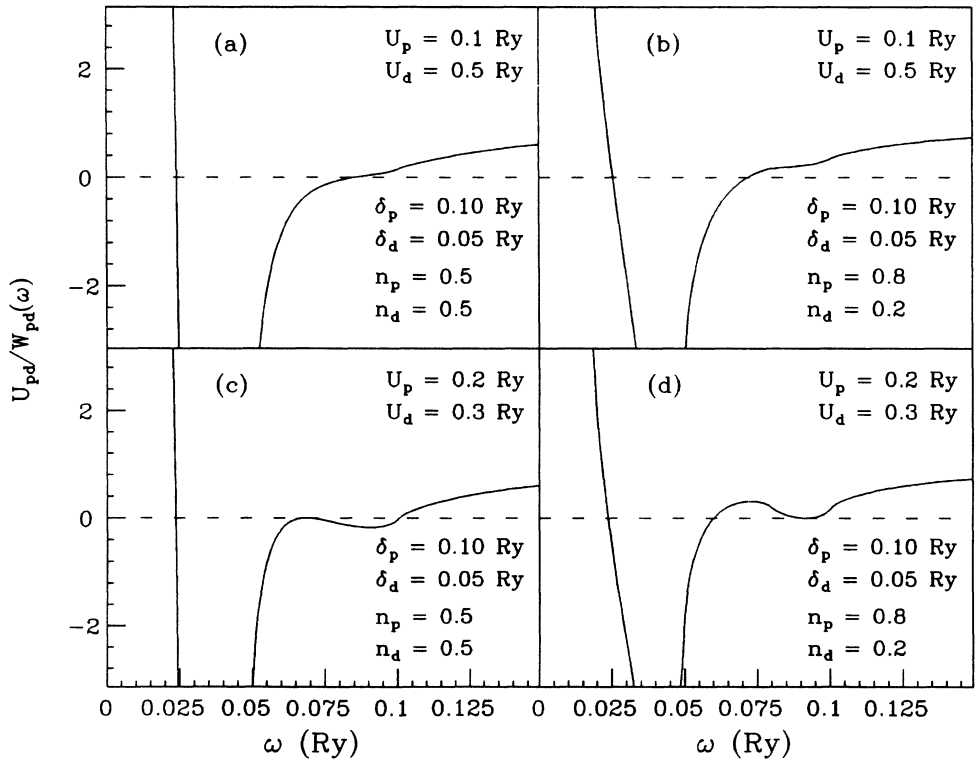

FIG. 6. Examples of the function $\mathrm{Re}[U_{pd}/W_{pd}(\omega)]$ for which it is dubious whether the screening implies h-h coupling or not. This function is obtained with the parameters given in the figure.

$$W_{pd}(\omega)=U_{pd}[1-U_p\Pi_p(\omega)-U_d\Pi_d(\omega)+(U_pU_d-U_{pd}^2)\Pi_p(\omega)\Pi_d(\omega)]^{-1}, \quad (19)$$

where Π is calculated from the spectrum of the interacting system. The analysis of the other interatomic interactions can be performed in a similar way and the evolutions versus the band parameters present similar behaviors. Both $W_{pp}(\omega)$ and $W_{dd}(\omega)$ can produce coupling and superconductivity for determined band parameters and, perhaps, the high-T_c superconductivity could be a combination of the three W interactions.

In Figs. 4–6 we represent the dielectric response corresponding to interatomic U_{pd}, for different values of the occupation of the orbitals and the widths of the partially occupied bands. An important characteristic feature of this dielectric response is that for $\omega=0$ the interaction W_{pd} is positive, assuring the stability[26] and $\varepsilon_{pd}(\omega)$ is negative at low frequencies, which implies a h-h coupling. The first zero of $\varepsilon_{pd}(\omega)$ comes closer to $\omega=0$ as the width of the band arising from the $d_{x^2-y^2}$ orbital decreases (in Fig. 4 this zero is around 0.004 Ry). Therefore, the energy interval where W_{pd} is attractive is smaller for an increasing localization of the $d_{x^2-y^2}$ states. However, this localization implies a decrease of the bare interatomic interaction U_{pd}.

From inspection of Figs. 5–8, we can also deduce the following: (i) The coupling tends to disappear when the values of n_p and n_d are complementary and very different, for instance $n_p=0.98$ and $n_d=0.02$ (see Fig. 5). Moreover, there is no coupling if either n_d or n_p tends to 1 or 0. In contrast, the coupling is favored for similar values of n_p and n_d whenever these are clearly different from 1 and 0. (ii) The intensity of the coupling potential [i.e., $W_{pd}(\omega)$] increases when the values of n_p and n_d are different (see Fig. 6) but the frequency interval for which W_{pd} is negative tends to disappear if $|n_p-n_d|$ increases. On the other hand, the conditions $|n_p-n_d|\to 0$, $n_p\not\to 0$, and $n_d\not\to 0$, assure the coupling, but its intensity rapidly decreases. Therefore there are critical values, that we estimate around $n_p\simeq 0.7$ and $n_d\simeq 0.7$, for which the conditions for obtaining high-T_c superconductivity can be optimum. *In our results of the electronic structure, the holes in symmetries $d_{x^2-y^2}$ of Cu(2) and p_x and p_y of O(2) and O(3) imply ionization states $\approx +1.2$ for Cu(2) and ≈ -1.8 for O(2) and O(3). Therefore, the pattern offered by these results is compatible with the existence of a W_{pd} coupling.* (iii) The smallest values of the first zero of $\varepsilon_{pd}(\omega)$ are obtained for decreasing values of the bandwidths (see Fig. 8). In Fig. 7 one can see that the variations of the δ's modify substantially the frequency interval for which $\varepsilon_{pd}(\omega)\leq 0$. However, the increasing localization of the pair components implies a decrease of the intensity of the coupling potential. (iv) The value of U's is almost irrelevant whenever either U_p or U_d were clearly different from zero (see Fig. 8).

In summary, we deduce that the intensity of the pair coupling potential and the frequency range of attractive interaction are two competing variables, since an increase in the first implies a decrease in the second. Another similar conclusion can be drawn in regard to the localization since it implies an interval of attractive interaction smaller and closer to $\omega=0$ but also implies a decrease in the intensity of the coupling potential.

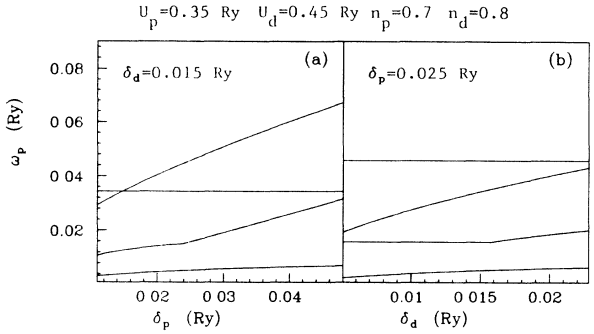

FIG. 7. Evolution of the four zeros of the function $\mathrm{Re}[U_{pd}/W_{pd}(\omega)]$ vs the effective bandwidths where the holes are located. (a) Varying δ_p and (b) varying δ_d.

V. CONCLUDING REMARKS

We have given a method for analyzing the electronic structure of the high-T_c superconductors based in an approximation to the self-energy. This self-energy has different influence in each atom of the unit cell since its effects largely depend on the occupation state of their corresponding orbitals. The results seem to be compatible with some experimental data and are characterized by the different nature of the states of the valence band, since there are strongly correlated states coexisting with band states. This implies an occupation in the external shells of the two-dimensional layers larger than that of the chain and as a consequence the Coulomb correlation effects are larger in the chain than in the planes. For a certain degree of O(4) and O(1) vacancies, electronic transferences between the atoms of the CuO_3 unit and CuO_2 sheets take place, leaving holes in the planes with large interatomic overlapping. We have deduced a

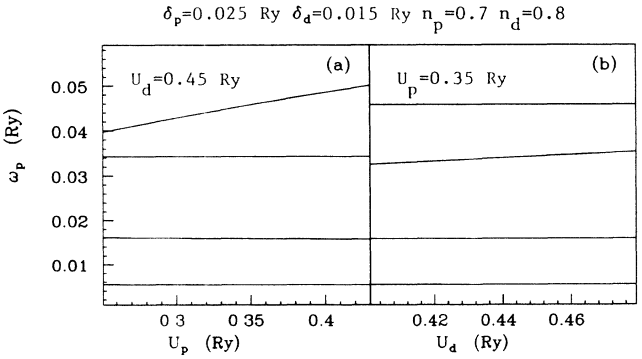

FIG. 8. Evolution of the four zeros of the function $\mathrm{Re}[U_{pd}/W_{pd}(\omega)]$ vs (a) the U_p Coulomb correlation energy and (b) the U_d Coulomb correlation energy.

dynamically screened effective interaction between d states of Cu and p states of O corresponding to the CuO_2 layer and we have proven that it is negative from a frequency value close to zero. This value decreases when the localization of the $d_{x^2-y^2}$ hole increases and the range of frequencies, in which the coupling is possible, increases when the localization of the other hole of the pair decreases. Therefore, the fermions of the pair should be of different localization character in order to assure the superconductivity. However, the localization also implies an intensity decrease of the pair potential. All these facts lead us to think that an interaction with a probability for producing coupling and superconductivity is the interatomic W_{pd}, however, the other interatomic interactions W_{dd} and W_{pp} can also yield coupling.

ACKNOWLEDGMENTS

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