MAGNETISM AND FERROELECTRICITY

Influence of Two-Particle Excited States on the Interatomic Exchange Interaction in La$_2$CuO$_4$

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Abstract—The effective spin Hamiltonian for undoped cuprates is constructed in the framework of the realistic multiband p–d model with the parameters calculated from first principles. The exchange interaction parameter is defined as the sum of the antiferromagnetic and ferromagnetic contributions, which are determined by the two-hole triplet terms. The ferromagnetic and antiferromagnetic contributions of the excited terms compensate each other to a large extent. It is shown that the antiferromagnetic contribution of the two-hole ground singlet $^1A_{1g}$ to the exchange interaction is dominant.

1. INTRODUCTION

The the exchange mechanism of pairing is considered to be one of the main mechanisms of superconduction in cuprates. In this respect, the reliable calculation of the effective exchange parameter J is an important problem. It is known that, in the undoped case, the Hubbard model in the strong-correlation limit $U \gg t$ can be reduced to the effective Heisenberg model with the antiferromagnetic exchange parameter $J = 2t^2/U$ [1, 2]. The Hubbard model itself can be constructed as the effective low-energy model from the more general three-band p–d model [3] or the multiband p–d model [4]. The localized spin is predominantly formed by the d^9p^6 single-hole term, whereas the addition of the second hole upon doping leads to the formation of the two-hole Zhang–Rice singlet [5] in the three-band model or a more general singlet $^1A_{1g}$ [4] in the multiband p–d model. Excitations with the addition of an electron $d^9p^6 \longrightarrow d^{10}p^6$ form the bottom of the empty conduction band, whereas excitations with the addition of a hole $d^9p^6 \longrightarrow {}^1A_{1g}$ form the top of the valence band; as a result, there exists a charge-transfer gap E_g between the bottom of the conduction band and top of the valence band. In [6], the interatomic exchange interaction was calculated from the low-energy limit of the multiband p–d model. In all previous works, the exchange interaction parameter J was calculated without regard for excited two-hole terms. Although each contribution of an excited term is smaller than that of the ground term due to an increase in the energy denominator, the number of these contributions is not very small and amounts to several tens. Therefore, their total (large or small) contribution to the exchange integral is not obvious in advance.

The purpose of this study was to calculate the exchange interaction parameter with allowance made for all excited two-particle states. In the Hubbard X-operator representation, we constructed the projection operators and obtained the general relationship for the interatomic exchange interaction in the second order of the perturbation theory in the parameter $t/E_g \ll 1$. It was demonstrated that the two-hole singlet and two-hole triplet terms make the antiferromagnetic (J_A) and ferromagnetic (J_B) contributions to the total exchange interaction parameter $J = J_A - J_B$, respectively. The matrix elements of interatomic hoppings were calculated with the parameters obtained for the La$_2$CuO$_4$ compound within the multiband p–d model in the framework of the ab initio local density approximation in combination with the generalized tight-binding method [7]. It turned out that the antiferromagnetic and ferromagnetic contributions of the excited terms partially compensate each other and the main contribution $J_0 = 2t^2/E_g$ is determined by the excitations from the top of the valence band.

2. MULTIBAND p–d MODEL WITH ALLOWANCE MADE FOR ALL EXCITED STATES

In the multiband p–d model [8], the Hamiltonian includes the local energies of holes for oxygen and copper in different orbitals ($d_{x^2-y^2}$, $d_{3z^2-r^2}$), the intraatomic Coulomb and exchange interactions for copper
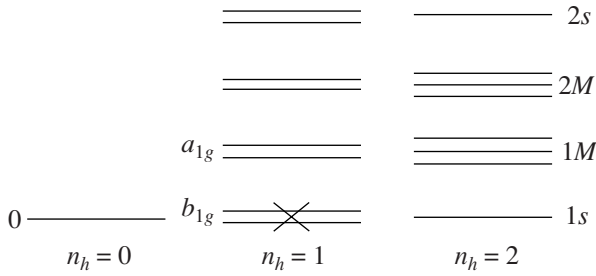
Fig. 1. Energy-level scheme of the Hilbert space of the terms of the CuO$_6$ unit cell with the numbers of holes n_h = 0, 1, and 2. The cross indicates the filled ground state $|b_{1g, \sigma}\rangle$ of the $d^9 p^6 + d^{10} p^5$ configuration in the undoped case.

and oxygen, hoppings, and the copper–oxygen Coulomb interaction [6]. In the framework of the local density approximation in combination with the generalized tight-binding method, the Hamiltonian parameters are calculated from first principles. Then, the cluster approach of the generalized tight-binding method [4] is used to account adequately for strong electron correlations. In this case, the crystal lattice is divided into unit cells, so that the Hamiltonian is represented as $H_0 + H_1$, where the component H_0 is the sum of intracell terms and the component H_1 takes into account the intercell hoppings and interactions. The component H_0 is exactly diagonalized, the exact electron molecular orbitals $|n, \delta\rangle$ of the unit cell and the energies $E_{n\delta}$ are determined, and these quantities are used to construct the Hubbard operators of the unit cell R_f: $X_f^{n\delta, n'\delta'} = |n\delta\rangle\langle n'\delta'|$. Thereafter, the component H_1 is exactly written in the X-operator representation and the intercell interactions are included in terms of the perturbation theory. The procedure and results of calculations for a CuO$_2$ layer are described in our previous paper [9].

In the X-operator representation of the Hamiltonian, the component H_0 is determined by the sum over the unit cells; that is,

$$H_0 = \sum_f \left\{ \varepsilon_0 X_f^{00} + \sum_{p\sigma} (\varepsilon_p - \mu) X_f^{p\sigma, p\sigma} \right.$$

$$\left. + \left[\sum_{n=1}^{N_s} (E_{ns} - 2\mu) X_f^{ns, ns} + \sum_{m=1}^{N_T} (E_{mT} - 2\mu) X_f^{mM, mM} \right] \right\},$$

where ε_0 is the energy of the vacuum term $d^9 p^6$ in the hole representation, ε_p is the energy of one-hole molecular orbitals with the spin projections $\sigma = \pm 1/2$, and the index p runs over all one-particle states of the CuO$_6$ cluster. The term in square brackets describes the two-hole terms either in the singlet state $|n, s\rangle$ or in the triplet state $|m, M\rangle$ ($M = -1, 0, +1$). The indices n ($1 \le n \le N_s$) and m ($1 \le m \le N_T$) number all two-hole spin singlets and triplets.

The condition for the completeness of the set of local Hubbard operators is represented in the form

$$X_f^{00} + \sum_{p\sigma} X_f^{p\sigma, p\sigma} + \sum_n X_f^{ns, ns} + \sum_m \sum_M X_f^{mM, mM} = 1. \quad (2)$$

The energy-level scheme of the many-electron terms determining the band structure of the La$_2$CuO$_4$ compound is depicted in Fig. 1. The creation of an electron at the bottom of the conduction band is determined by the matrix element $\gamma_{\lambda\sigma}\langle 0| = \langle 0|a_{f\lambda\sigma}|b_{1g, \sigma}\rangle$, where the index λ of the orbital corresponds either to the d orbitals $x^2 - y^2$ and $3z^2 - r^2$ or to symmetrized combinations of the $2p$ atomic orbitals centered at the copper site R_f (b_{1g}, a_{1g} orbitals [9]). The creation of a hole upon p-type doping is determined by the matrix elements with the participation of all two-hole terms; that is,

$$\gamma_{\lambda\sigma}(n) = \langle b_{1g}, -\sigma|a_{f\lambda\sigma}|ns\rangle,$$
$$\gamma_{\lambda\sigma}(m) = \langle b_{1g}, +\sigma|a_{f\lambda\sigma}|m, +2\sigma\rangle. \quad (3)$$

In the X-operator representation, the hole annihilation operator has the form

$$a_{f\lambda\sigma} = \gamma_{\lambda\sigma}(0) X_f^{0, \sigma} + \sum_n \gamma_{\lambda\sigma}(n) X_f^{-\sigma, ns}$$

$$+ \sum_n \gamma_{\lambda\sigma}(m) \left(X_f^{\sigma, m2\sigma} + \frac{1}{\sqrt{2}} X_f^{-\sigma, m0} \right). \quad (4)$$

Some matrix elements $\gamma_{\lambda\sigma}(n)$ and $\gamma_{\lambda\sigma}(m)$ are equal to zero, and the corresponding two-hole singlets and two-hole triplets do not contribute to one-particle excitations. The two-hole states with nonzero matrix elements are involved in the formation of a complex energy structure of the valence band and form singlet and triplet Hubbard subbands between which there is a hybridization. It should be noted that the singlet (triplet) band is a conventional name for the designation of the electronic band with the spin $S = 1/2$ but with the participation of final singlet (triplet) terms (see relationship (4)).

The representation of the off-diagonal operators X can be simplified by introducing the root vectors $\alpha_r(p, q)$ corresponding to a pair of the initial and final states of the operator $X^{pq} = |p\rangle\langle q|$. In this notation, relationship (4) takes the form

$$a_{f\lambda\sigma} = \sum_r \gamma_{\lambda\sigma}(r) X_f^r, \quad (5)$$

where the integer index r numbers all one-particle excitations in relationship (4); that is,

$$\{r\} = \{(0, \sigma); (\sigma; ns); (\sigma; m, 2\sigma); (-\sigma; m0)\}.$$

Moreover, in this notation, the Hamiltonian of the intercluster hopping has the simple form

$$H_1 = \sum_{fg}\sum_{\lambda\lambda'\sigma} t^{\lambda\lambda'}_{fg} a^+_{g\lambda\sigma} a_{g\lambda\sigma} = \sum_{fg}\sum_{rr'\sigma} t^{rr'}_{fg} X^{r+}_f X^{r'}_g, \quad (6)$$

where $t^{\lambda\lambda'}_{fg}$ is the matrix of hopping integrals of a hole from the gth site (in the orbital state λ') to the fth site (in the orbital state λ) and

$$t^{rr'}_{fg} = \sum_{\lambda\lambda'} t^{\lambda\lambda'}_{fg}\gamma_\lambda(r)\gamma_{\lambda'}(r').$$

Since each index r characterizes the band of quasiparticles in a strongly correlated system (the band index of the Hubbard band), the diagonal terms t^{rr} in expression (6) describe the dispersion of the rth band and the off-diagonal terms $t^{rr'}$ describe the hybridization of the rth and r'th bands.

3. CONSTRUCTION OF THE EFFECTIVE EXCHANGE HAMILTONIAN

The exchange interaction appears in the second order of the perturbation theory with respect to hoppings. This corresponds to virtual excitations from the filled singlet and triplet bands through the insulating gap to the conduction band ($r = 0$, $\alpha_0 = (0, \sigma)$) and back. These perturbations are described by the off-diagonal elements t^{0r}_{fg} with $r \geq 1$ in expression (6). In the Hubbard model, there is only one such element t^{01}, which describes the hoppings between the lower and upper Hubbard bands. In our case, the set of nonzero matrix elements $\gamma_{\lambda\sigma}(r)$ with $r \geq 1$ determines the interband hoppings. In order to eliminate them, we generalize the projection operator method proposed by Chao et al. [2] to the Hubbard model. Since the diagonal Hubbard operators are projection operators, the X-operator representation allows us to construct this generalization. In our case, the total number of diagonal two-hole operators $X^{\mu\mu}_f$ is $N = N_s + 3N_T$. By disregarding the exponentially low temperature filling of excited one-hole terms in the absence of doping when none of the two-hole terms is filled, we can retain only one lower one-hole term marked by the cross in Fig. 1. In this case, the conditions for the completeness of the system of X operators is simplified and can be written in the form

$$X^{00}_f + \sum_\sigma X^{\sigma\sigma}_f + \sum_\mu X^{\mu\mu}_f = 1. \quad (7)$$

We choose a pair of neighboring sites (i, j) and construct the set of projection operators p_μ:

$$p_0 = \left(X^{00}_i + \sum_\sigma X^{\sigma\sigma}_i\right)\left(X^{00}_j + \sum_\sigma X^{\sigma\sigma}_j\right), \quad (8)$$

$$p_\mu = X^{\mu\mu}_i + X^{\mu\mu}_j - X^{\mu\mu}_i \sum_{n'} X^{n'n'}_j, \quad q \leq \mu \leq N. \quad (9)$$

It is easy to check that each operator p_μ is a projection operator,

$$p^2_\mu = p_\mu \quad (10)$$

and that these operators form a complete system and are orthogonal,

$$p_\mu p_\nu = \delta_{\mu\nu} p_\mu, \quad \sum_{\mu=0}^{N} p_\mu = 1.$$

By using the identity

$$H = \sum_{\mu\nu} p_\mu H p_\nu, \quad (11)$$

we calculate the diagonal and off-diagonal elements of matrices (11). In this case, the term $p_0 H p_0$ corresponds to the Hamiltonian component acting in the lower Hubbard band $\alpha_0 = (0, \sigma)$, etc. It is easy to show that the equality

$$\sum_\mu p_\mu H_0 p_\mu = H_0$$

is satisfied and that the diagonal elements $p_\mu H_1 p_\mu$ describe the hoppings in the band μ and the off-diagonal elements $p_\mu H_1 p_\nu$ correspond to the hybridization of the bands μ and ν; that is,

$$p_\mu H_1 p_\nu = \sum_{ij} t^{\mu\nu}_{ij} X^{\mu+}_i X^\nu_j.$$

We choose the off-diagonal matrix elements

$$\tilde{H}(\varepsilon) = \tilde{H}_0 + \varepsilon\tilde{H}_1,$$

$$\tilde{H}_0 = \sum_\mu p_\mu H p_\mu,$$

$$\tilde{H}_1 = \sum_{\mu \pm \nu} p_\mu H p_\nu \quad (12)$$

as a perturbation and perform the standard unitary transformation

$$H'_{(\varepsilon)} = e^{-i\varepsilon\tilde{S}} H(\varepsilon) e^{i\varepsilon\tilde{S}}$$

in such a way as to eliminate the linear (in ε) contributions of $\tilde{H}_1$. If the matrix $\tilde{S}$ satisfies the equation

$$\tilde{H}_1 + i[\tilde{H}_0, \tilde{S}] = 0, \tag{13}$$

the transformed Hamiltonian has the form

$$H'(\varepsilon) = \tilde{H}_0 + i\varepsilon^2[\tilde{H}_1, \tilde{S}]_-/2. \tag{14}$$

In order to solve Eq. (13), we multiply each term by p_μ from the left and by p_ν from the right. As a result, we obtain

$$p_\mu H p_\nu (1 - \delta_{\mu\nu}) + i(p_\mu H p_\mu)(p_\mu \tilde{S} p_\nu)$$
$$- i(p_\mu \tilde{S} p_\nu)(p_\nu H p_\nu) = 0. \tag{15}$$

This equation coincides in form with the corresponding equation in [2] and differs from it only in the dimension of matrices. Therefore, our derivation of the system of operators p_μ in the multidimensional case is actually a generalization of the method proposed in [2].

It follows from Eq. (15) that the diagonal matrix elements have the form $p_\mu \tilde{S} p_\mu = \gamma p_\mu$, where γ is a constant. In order to solve the equation with respect to the off-diagonal elements $p_\mu \tilde{S} p_\nu$, according to [2], we make the approximation $p_\mu H p_\mu \longrightarrow \varepsilon_\mu$. As a result, the solution has the form

$$p_\mu \tilde{S} p_\nu = i p_\mu H p_\nu / \Delta_{\mu\nu}, \quad \Delta_{\mu\nu} = \varepsilon_\mu - \varepsilon_\nu \tag{16}$$

and the effective Hamiltonian is represented as

$$H'(\varepsilon = 1) = \sum_\mu p_\mu H p_\mu + \frac{1}{2}\sum_{\nu \neq \mu}(p_\mu H p_\nu \tilde{S} - \tilde{S} p_\mu H p_\nu)$$

$$= \sum_\mu p_\mu H p_\mu + \frac{1}{2}\sum_{\mu \neq \nu}\left\{\frac{[p_\mu H p_\nu p_\nu H p_\mu]_-}{\Delta_{\mu\nu}}\right.$$

$$\left. + \sum_{\substack{\alpha \neq \mu \\ \alpha \neq \nu}}\left[\frac{(p_\mu H p_\nu)(p_\nu H p_\alpha)}{\Delta_{\nu\alpha}} - \frac{(p_\alpha H p_\mu)(p_\mu H p_\nu)}{\Delta_{\alpha\mu}}\right]\right\}. \tag{17}$$

4. ANALYSIS OF THE EXCHANGE CONTRIBUTIONS TO THE EFFECTIVE HAMILTONIAN

The calculation of the terms in Hamiltonian (17) for the singlet and triplet bands leads to different results. The interband transitions through the gap are described by the commutator

$$[p_0 H p_\nu, p_\nu H p_0]_-. \tag{18}$$

For the nth singlet band $\alpha_\nu = (-\sigma, nS)$, commutator (18) is determined by the operators

$$\sum_{fgij}\sum_{\sigma\sigma'}[X_f^{\sigma 0} X_g^{-\sigma, ns}, X_i^{ns, -\sigma'} X_j^{0\sigma'}]_-.$$

The exchange contribution to the Heisenberg Hamiltonian has the form

$$H_A = \sum_{ij} J_A(\mathbf{R}_{ij})\left(\mathbf{s}_i \mathbf{s}_j - \frac{1}{4}n_i n_j\right), \tag{19}$$

where $\mathbf{s}_i$ and n_i are the spin operators for $s = 1/2$ and the number of particles at the ith site, respectively, and

$$J_A(\mathbf{R}_{ij}) = \sum_n J_A^{(n)}(\mathbf{R}_{ij}) = \sum_{n=1}^{N_s}\left|t_{ij}^{0, ns}\right|^2/\Delta_{ns},$$
$$\Delta_{ns} = E_{ns} - 2\varepsilon_1.$$

For the mth triplet band, commutator (18) is determined by the terms

$$\left[X_f^{\sigma; 0}\left(X_g^{\sigma; -m, 2\sigma} + \frac{1}{\sqrt{2}}X_g^{-\sigma; m, 0}\right)\right.$$
$$\left. \times \left(X_i^{m, 2\sigma'; \sigma'} + \frac{1}{\sqrt{2}}X_i^{m, 0; -\sigma'}\right)X_j^{0; \sigma'}\right]_-.$$

As a result, the ferromagnetic exchange contribution to the Heisenberg Hamiltonian takes the form

$$H_F = \sum_{ij} J_B(\mathbf{R}_{ij})\left(\mathbf{s}_i \mathbf{s}_j + \frac{3}{4}n_i, n_j\right), \tag{20}$$

where $J_B(\mathbf{R}_{ij}) = \sum_m J_B^{(m)}(\mathbf{R}_{ij}) = -\sum_{m=1}^{N_T}\left|t_{ij}^{0, m}\right|^2/2\Delta_m$ and $\Delta_m = E_m - 2\varepsilon_1$. By summing up over all singlet and triplet bands, we find the following expression for the effective exchange interaction parameter:

$$J_{ij}^{\text{eff}} = \sum_{n=1}^{N_s}\left|t_{ij}^{0, ns}\right|^2/\Delta_{ns} - \sum_{m=1}^{N_T}\left|t_{ij}^{0, m}\right|^2/2\Delta_m. \tag{21}$$

It can be seen from this expression that the contributions of the singlet and triplet bands to the exchange interaction parameter have different signs. The antiferromagnetic interaction with the participation of the singlet states is conventional. This contribution t^2/U in the Hubbard model describes the superexchange mechanism. In our case, the excited singlet states also result in the antiferromagnetic contribution, which decreases with an increase in the energy of the excited term at the expense of the denominator. The ferromagnetic contribution of the triplet states is associated with the fact that the spins of two holes upon triplet formation are oriented parallel to each other and then hoppings from site to site carry this parallel spin orientation.

Table 1. Spectral weights of the initial two-hole configurations in the singlet states

| $\lvert ns\rangle$	E_{ns}, eV	$A^2_{1n}(d_x b)$	$A^2_{2n}(bb)$	$A^2_{3n}(d_x d_x)$	$A^2_{4n}(ap_z)$	$A^2_{5n}(ad_z)$	$A^2_{6n}(d_z p_z)$	$A^2_{7n}(aa)$	$A^2_{8n}(p_z p_z)$	$A^2_{9n}(d_z d_z)$
$\lvert 1s\rangle$	−3.528	0.506	0.456	0.037	0	0	0	0	0	0
$\lvert 2s\rangle$	−0.360	0	0	0	0.008	0.001	0.389	0.000	0.598	0.004
$\lvert 3s\rangle$	1.0733	0	0	0	0.373	0.026	0.314	0.000	0.277	0.009
$\lvert 4s\rangle$	2.230	0	0	0	0.016	0.693	0.047	0.192	0.034	0.019
$\lvert 5s\rangle$	3.349	0.361	0.529	0.109	0	0	0	0	0	0
$\lvert 6s\rangle$	3.664	0	0	0	0.529	0.009	0.229	0.1323	0.090	0.011
$\lvert 7s\rangle$	6.299	0	0	0	0.071	0.215	0.004	0.670	0.001	0.040
$\lvert 8s\rangle$	11.018	0	0	0	0.002	0.058	0.017	0.005	0.000	0.917
$\lvert 9s\rangle$	11.439	0.132	0.014	0.854	0	0	0	0	0	0

Table 2. Spectral weights of the initial two-hole configurations in the triplet states

$\lvert mM\rangle$	E_{mM}, eV	$B^2_{1m}(d_x a)$	$B^2_{2m}(ba)$	$B^2_{3m}(d_x d_z)$	$B^2_{4m}(bd_z)$	$B^2_{5m}(d_x p_z)$	$B^2_{6m}(bp_z)$
$\lvert 1M\rangle$	−2.085	0.001	0.000	0.013	0.073	0.382	0.531
$\lvert 2M\rangle$	−0.661	0.196	0.316	0.052	0.398	0.026	0.013
$\lvert 3M\rangle$	1.552	0.274	0.215	0.018	0.430	0.057	0.007
$\lvert 4M\rangle$	3.289	0.021	0.002	0.015	0.006	0.518	0.438
$\lvert 5M\rangle$	5.433	0.452	0.445	0.094	0.000	0.003	0.006
$\lvert 6M\rangle$	9.520	0.057	0.022	0.809	0.093	0.014	0.001

5. NUMERICAL CALCULATIONS OF THE EFFECTIVE EXCHANGE PARAMETER

The eigenstates in the A_{1g} and $^3B_{1g}$ bands can be represented in the form $\lvert ns\rangle = \sum_{i=1}^{9} A_{ni}\lvert A_i\rangle$ and $\lvert mM\rangle = \sum_{i=1}^{6} B_{mi}\lvert B_i\rangle$ [9]. The spectral weights of the initial hole configurations $\lvert A_i\rangle$ and $\lvert B_i\rangle$ are listed in Tables 1 and 2, respectively. The distinguishing feature of the states with symmetry A_{1g} (Table 1) is that the spectral weight of the initial configurations in the ground state amounts to 95%. The contribution of the polar configuration distinguishes our ground state from the Zhang–Rice state. Moreover, the dominant hopping integrals t_{pd} and t_{pp} contribute to the exchange interaction parameter (21) with the same weight (Fig. 2a). For states in the band with symmetry $^3B_{1g}$, there are also preferred configurations (Table 2). For example, this is the initial configuration $(b_{1g}p_z)$ in the ground state with a spectral weight of 53%. However, since the corresponding hopping integrals are considerably smaller, the band of the triplet states is narrower than the band of the singlet states and the antiferromagnetic contribution to the exchange interaction parameter (21) is dominant. Indeed, for the Hamiltonian parameters calculated in the framework of the local density approximation in combination with the generalized tight-binding method, the calculations performed according to

expression (21) lead to $J_A = 0.149$ eV and $J_B = 0.003$ eV for the nearest neighbors and $J^{\rm eff} = 0.146$ eV for the total exchange interaction parameter. The largest contribution (~73%) to the ferromagnetic interaction is made by the excited ($m = 3$) triplet state with the largest
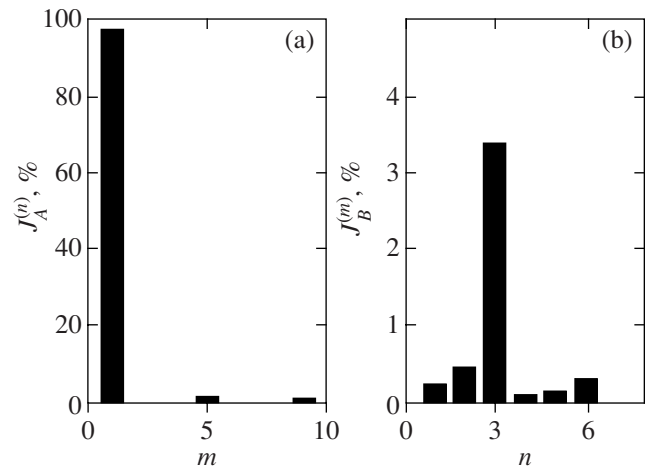
Fig. 2. Partial contributions (a) $J_A^{(n)}$ of the singlet states and (b) $J_B^{(m)}$ of the triplet states to the exchange interaction parameter (in percent with respect to the quantity $J_A + J_B$).

contribution from the initial (bd_z) configuration (Fig. 2b). This ratio between the antiferromagnetic and ferromagnetic components is explained by the fact that the contribution of the initial configurations to the exchange interaction parameter $J_A(\mathbf{R}_{ij})$ is proportional to the dominant hopping integrals t_{pd} and t_{pp}. In combination with the high spectral weights of the configurations ($d_x b$) and $(b)^2$ in the ground state, this leads to a ratio $|J_A/J_B| \gg 1$. The contributions of the two-hole ground states to the exchange interaction parameters are estimated to be 97.2 and 3.7% for J_A and J_B, respectively.

Together with small and comparable ferromagnetic and antiferromagnetic contributions of the excited states, this indicates that the constraint imposed in [9] on the configurational space for high-temperature superconducting materials results in an error smaller than 1% in the calculation of the exchange interaction.

In the A_{1g} band, the contribution of the ground state is such large that the crossover of the singlet and triplet states does not lead to a change in the sign of the exchange interaction parameter and this interaction remains antiferromagnetic. This inference can be made from the analysis of the exchange interaction in high-temperature superconducting materials with an unusual electronic structure [11, 12]. In the structures investigated in both works, the $^3B_{1g}$ states are located at the top of the valence band. This effect is associated with the chemical pressure upon replacement of Ca by Y in $Bi_2Sr_2Ca_{1-x}Y_xCu_2O_{8+\delta}$ ($0.55 < x < 0.92$) compounds in [11] and with the external uniaxial pressure in the structure of $La_{1-x}Sr_xCuO_4$ compounds in [12]. We calculated the exchange interaction parameter with the use of the characteristics taken from [12]. It was revealed that, at the hypothetical crossover point, the exchange interaction remains antiferromagnetic in character but decreases in magnitude: $J^{\mathrm{eff}} \approx 0.078$ eV.

Therefore, despite the competition between the singlet and triplet states for the ground state, the antiferromagnetic character of the exchange interaction is governed by the specific features of the crystal structure of high-temperature superconducting materials and by the chemical nature of their constituent elements.

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