Range of the t–J model parameters for CuO₂ plane: experimental data constraints.

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Abstract

The t-J model effective hopping integral is determined from the three-band Hubbard model for the charge carriers in CuO₂ plane. For this purpose the values of the superexchange constant $J$ and the charge-transfer gap $E_{\text{gap}}$ are calculated in the framework of the three-band model. Fitting values of $J$ and $E_{\text{gap}}$ to the experimental data allows to narrow the uncertainty region of the three-band model parameters. As a result, the $t/J$ ratio of the t-J model is fixed in the range $2.4 \div 2.7$ for holes and $2.5 \div 3.0$ for electrons. Formation of the Frenkel exciton is justified and the main features of the charge-transfer spectrum are correctly described in the framework of this approach.

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I. INTRODUCTION

A large amount of works dedicated to high-$T_c$ superconductors agree that an appropriate electronic model which contains all essential orbitals is the three-band Hubbard model \[1, 2\]. Some other works developing a multiband approach \[1, 4\] also support this belief.

It is also widely accepted that the low-energy physics of insulating compounds can be described by the Heisenberg Hamiltonian. According to the earlier work by Zhang and Rice \[3\] and latter studies \[4, 5\] lightly doped systems are described by the simple t-J model. Different techniques provide different exactness of the three-band model to t-J model mapping and generate a wide type of generalizations \[6, 7\].

In our previous works \[8, 10, 11\] a consistent low-energy reduction of the three-band model to the generalized t-J model in the realistic range of parameters has been performed. It has been shown \[11\] that the second-order corrections to the local energy of the carrier and its hopping integral are small ($< 5\%$). The role of the next-nearest-neighbor terms has also been discussed.

It is commonly believed that the 90\% or even higher accuracy of the t-J model as the low-energy electronic model for high-$T_c$ superconductors justifies its wider study \[12, 13\] and remains this model the main pretender in describing of the superconductivity in cuprates \[14, 15\]. Recent angle-resolved photoemission experiments \[16\] can be interpreted as a direct support of some t-J model properties \[17\]. Some other anomalous behaviors of systems in normal state as well as superconductivity itself seem to be described in the framework of the t-J model \[18, 19\].

The reasonable question from this point of view is: what is the role of either the three-band or more complex first-principles models? There are several answers: (i) calculating parameters for the t-J model for real systems; (ii) giving insight into the experiments including not only the simple t-J model degrees of freedom.

In this paper we mainly address the question of the t-J model parameters. Superexchange constant $J$ for the t-J model is directly measured \[20, 21\]. Hence, the parameter to be
determined is the effective nearest-neighbor hopping integral. The problem of its calculation is not connected with the accuracy of low-energy mapping from the three-band model, which is always very high, but results from uncertainty in the three-band model parameters. The three-band model in conventional formulation contains as inner parameters two on-site and one inter-site Coulomb repulsions, two hopping integrals, and split of the levels [1] which are not directly measurable. Some of them are fairly bad determined. This makes the calculation of the hopping integral for real systems questionable and even controversial.

We develop an obvious idea of fixing the three-band model parameters by using experimental data. This idea has already been exploited in the cluster calculations for spectroscopic data [6] and for the superexchange $J$ in our previous work [15]. Now, on the basis of better understanding of the low-energy model of the electronic system and magnetic polaron nature of the t-J model carriers [18,26,27], we calculate quite accurately the charge-transfer gap. Selfconsistent calculation provides a narrow range of possible values of $t/J$. Also, an excitonic feature of the charge-transfer spectrum is obtained in agreement with resent experiments [28].

Paper organized as follows. In Sec. II we discuss the low-energy limit of the three-band model and experimentally observable quantities. In Sec. III the calculation of the superexchange constant $J$ and the charge-transfer gap $E\text{gap}$ is produced. In Sec. IV we discuss the dependence $J$ and $E\text{gap}$ on the parameters of the three-band model and determine the range of the hopping parameter $t$ for electrons and holes. In Sec. V the properties of the excitonic state is considered. Sec. VI presents our results and discussions. The technical aspects of work are given in Appendix.

II. THE LOW-ENERGY LIMIT OF THE THREE-BAND MODEL AND OBSERVABLE QUANTITIES

Previously, it was suggested that the three-band Hubbard model is an appropriate starting point for describing the electronic structure of CuO$_2$ planes [1,4]. The Cu $d_{x^2−y^2}$ orbital
and \( p\sigma(x,y) \) orbitals are strongly hybridized. These orbitals are explicitly treated in the three-band model with the justifiable assumption that other orbitals does not directly participate in the low-energy dynamics. The full Hamiltonian of the model is defined by

\[
H = H_0 + H_t + \Delta H
\]

\[
H_0 = \epsilon_d \sum_{l,\alpha} n_{l\alpha}^d + \epsilon_p \sum_{m,\alpha} n_{m\alpha}^p + U_d \sum_l n_{l\uparrow}^d n_{l\downarrow}^d,
\]

\[
H_t = t_{pd} \sum_{<lm>,\alpha} (d_{l\alpha}^+ p_{m\alpha} + H.c.)
\]

\[
- t_{pp} \sum_{<mm'>,\alpha} (p_{m\alpha}^+ p_{m'\alpha} + H.c.) ,
\]

\[
\Delta H = U_p \sum_m n_{m\uparrow}^p n_{m\downarrow}^p + V_{pd} \sum_{<lm>,\alpha\beta} n_{l\alpha}^d n_{m\beta}^p,
\]

in standard notation of holes at O(\( p \)) and Cu(\( d \)) sites. The sign convention for oxygen orbitals in \( H_t \) [15,29] is accepted. Our approach to description of low-energy properties of the above model [15] is based on taking into account the main Coulomb (\( U_d \)) interaction exactly and the others as perturbations.

In order to justify this method we briefly describe here the magnitudes of the three-band model’s parameters. Different experimental [6,7,30], atomic [31], and band calculations [4,32,33] show that: \( U_d = 5 \div 7 \) eV [31], \( 7 \div 11 \) eV [4,31], \( U_p = 3 \div 8 \) eV [4], \( V_{pd} = 0 \div 1.7 \) eV. \( U_p \) is always less than \( U_d \). There is a general agreement for the Cu-O system that \( \Delta = \epsilon_p - \epsilon_d \) is always \( > 0 \) and \( < U_d \) [30]. It reflects the facts that the first hole in the unit cell is predominantly at the Cu site and the added hole has an oxygen’s character. \( t_{pd} = 1 \div 1.6 \) eV (and it is unlikely that it is less than 1 eV) , \( t_{pp} = 0.5 \div 0.7 \) eV [4,32,33]. This set of magnitudes will be called hereafter the realistic region of parameters.

The consistent low-energy reduction of the three-band model to the generalized t-J model has been performed in previous works [12,13,15]. Our method of the low-energy reduction has been based on construction of a set of local states with different number of holes over the filled atomic orbitals. The most essential states are:

1. The vacuum state or the vacancy which is simply

\[
|v> = |0>,
\]
2. The one-hole states which represent the ground state of CuO$_2$ plane

\[ |f\alpha> \equiv |\alpha> = U|d\alpha> - V|p\alpha>, \]  

where $|d\alpha>$ and $|q\alpha>$ are the copper and symmetrical oxygen hole states with spin projection $\alpha$, respectively.

3. The two-hole states which are the Zhang-Rice singlets:

\[ |c> = U_1|d \uparrow d \downarrow> + V_1|q \uparrow q \downarrow> \\
+ W_1(|d \uparrow q \downarrow> - |d \downarrow q \uparrow>)/\sqrt{2}. \]  

The coefficients $U, V, U_1, V_1, W_1$ are functions of the parameters of the three-band model [13].

At half filling Hamiltonian (1,2) is reduced to the Heisenberg Hamiltonian with spin-1/2 which are antiferromagnetically ordered due to the second-order virtual transitions through the set of two-hole states. Note, that the above named spins-1/2 are exactly states $|f\alpha>$ (Eq. (4)).

It has been shown [13,15] that for the case near to half filling the Hamiltonian of the three-band model is reduced to the Hamiltonian of the t-J like model of singlets, vacancies and spins:

\[ H_{t-J} = (E_v - \mu) \sum_l X_{l\alpha\alpha}^v + (E_c + \mu) \sum_l X_{l\alpha\alpha}^c \\
+ t_e \sum_{<ll'>,\alpha} X_{l\alpha\alpha}^v X_{l'\alpha\alpha}^v + t_h \sum_{<ll'>,\alpha} X_{l\alpha\alpha}^c X_{l'\alpha\alpha}^c \\
+ J \sum_{<ll'>} S_l S_{l'}. \]  

Where $X_{l\alpha\beta}^{ab} \equiv |al><lb|$ are the Hubbard operators at the site $l$, $S_l = \sigma_{\alpha\beta}X_{l\alpha\beta}^\alpha/2$. The constants $E_v$ and $E_c$ are the local energies of the vacancy and singlet; $\mu$ is the chemical potential; $t_e$ and $t_h$ are the hopping integrals for the vacancy and singlet (electron and hole), respectively; $J$ is the exchange constant. All five parameters $E_v, E_c, t_e, t_h$ and $J$ are functions of the three-band model parameters. It has been shown that relative magnitudes
of the omitted terms in the Hamiltonian $H_{t-J}$ (Eq. (6)) are of the order of ten percent [13,15].

We believe that the Hamiltonian (6) describes many important properties of the cuprates. Therefore, the real values of its parameters are of great interest. As was noted above, the parameters of the primary model (1,2) are known with low precision. In this situation calculation of the observable quantities is an urgent issue since it provides a way to fix parameters of Hamiltonians (1,2) and (6). The best-defined experimental values which we can describe quite accurately are the superexchange constant $J$ and the charge-transfer gap $E_{gap}$. The experimental values of $J$ are 0.14 eV and 0.17 eV for the lantan and yttrium systems, respectively [24,25]. These values of $J$ follow from measurement of the velocity of sound for magnons. The value of the charge-transfer gap is known from a variety of optical measurements [28,30,33,34] and is near to 2.0 eV. Observation of photoconductivity at the same energies shows that the excitations result in separated electrons and holes [28,34]. We have taken most of clear experimental features of the charge-transfer spectrum from Ref. [28] where photoconductivity as well as reflectivity data for La$_2$CuO$_4$ are presented.

### III. CALCULATION OF THE OBSERVABLE QUANTITIES

The expression for the AF coupling constant $J$ in the framework of our approach is

$$J = -2h_1 V^4 U_p + \sum_n x_n \frac{|D_n|^2}{\Delta E_n}. \tag{7}$$

The first term in Eq. (7) represents the exchange energy between two holes (spins) due to the repulsion at an oxygen. This contribution has the ferromagnetic sign and arises as an exchange interaction between the hole states (4) due to their nonlocal nature. The constant $V$ is defined in Eq. (4), $h_1$ is in Appendix. The second term in Eq. (7) represents the correction to the energy due to the virtual transition of hole from the state Eq. (4) into the two-hole states and back [15]. Here $n$ numerates the two-hole states; matrix elements of transitions $D_n$ were calculated in Ref. [15]. $\Delta E_n$ are differences in energies between the
energy of the vacancy and two-hole states at neighbor sites and the ground state energy (see Fig. 4); the coefficients $x_n = 4$ for the singlet and $x_n = -2$ for triplet two-hole states.

The most general expression for the charge-transfer energy is:

$$E_{\text{gap}} = E_{\text{min}}^{N-1} - E_g^N + E_{\text{min}}^{N+1} - E_g^N,$$

where $N$ refers to the total number of electrons, $E_g^N$ is the ground state energy, $E_{\text{min}}^{N+1}$ is the minimal energy of a system with one removed and added electron. For our system Eq. (8) can be specified as

$$E_{\text{gap}} = E_{\text{gap}}^0 + \Delta E_e + \Delta E_h,$$

where $E_{\text{gap}}^0$ is the difference in energies between a singlet and vacancy at local states separated by large distance and the ground state (see Fig. 3); $\Delta E_e$ and $\Delta E_h$ are depths of bands for electron and hole (vacancy and singlet). $E_{\text{gap}}^0$ can be calculated in the framework of the three-band model, whereas for the calculation of $\Delta E_e$ and $\Delta E_h$ we will use the t-J model.

The expression for $E_{\text{gap}}^0$ in terms of Eq. (8) is very simple:

$$E_{\text{gap}}^0 = E_c + E_v.$$ 

The values of $\Delta E_e$ and $\Delta E_h$ can be determined from numerous analytical and numerical calculations [16]- [19], [22, 26, 27, 33, 36] of the dispersion relation $\epsilon(k)$ for one hole in the t-J model on an antiferromagnetic background. There is a general agreement that the hole (or vacancy) on the antiferromagnetic background creates a magnetic polaron of a small radius [17, 26], or, in the other words, the carriers are strongly dressed by the spin waves [23]. The influence of antiferromagnetism and strong correlations are manifested in a special form of dispersion relation $\epsilon(k)$. For our calculations we use the results from the earlier work by Sushkov Ref. [18] where hole wave function and $\epsilon(k)$ were obtained variationally:

$$\epsilon(k) = 1.32J + \frac{1}{2} \left( \tilde{\Delta} J - \sqrt{\Delta^2 J^2 + 16t^2[(1 + y) - (x + y)\gamma_k^2]} \right).$$
and
\[
\Delta E = 1.32J + \frac{1}{2} \left( \tilde{\Delta}J - \sqrt{\tilde{\Delta}^2J^2 + 16t^2(1+y)} \right),
\]

(11)

where for Néel background \( \tilde{\Delta} = 1.33, x = 0.56, y = 0.14 \). Loss of energy due to the broken AF bonds (four per carrier) is included. Result for the bottom of the band at \( t/J = 2.5 \) from Eq. (11) \( \Delta E = -1.2t \) coincides almost exactly with the recent results of the Green function Monte Carlo calculation by Dagotto, Nazarenko, and Boninsegni \[23\] \( \Delta E = -1.255t \). Formula (11) is quite good up to \( t/J \approx 5 \) \[18\].

Let us discuss the characteristic values of all essential parameters which determine the observable quantities \( J \) and \( E_{\text{gap}} \) (8), (9). In the realistic region of parameters of the three-band model one can easily obtain the experimental values \( J = 0.14 \) eV and \( J = 0.17 \) eV for lanthan and yttrium systems. The value for \( E_{\text{gap}}^0 \) (10) was obtained in Ref. \[15\] and is equal to 3.2 eV in the same region of parameters. The characteristic values of \( \Delta E_e \) and \( \Delta E_h \) (11) depend on ratios \( t/J \) for electrons and holes. These ratios weakly differ and for a typical value of \( t/J = 2.5 \) we have \( \Delta E_e \approx \Delta E_h \approx 0.42 \) eV. Thus, the overall gain in energy due to magnetic polaron formation is of the order of 1 eV, which is comparable with the experimentally observed \( E_{\text{gap}} \approx 2.0 \pm 0.1 \) eV. Therefore, the magnetopolaron effect gives essential contribution in the value of the charge-transfer gap.

In the paper \[28\] it was proposed that the usual phonon polaron effect contributes in the observable values of the charge-transfer spectrum. The corresponding gain in energy was estimated as 0.5 eV. However, we suppose that due to the Frank-Condon principle the usual polaronic effect does not contribute in the optical transition. Magnetopolaron effect has no such restriction since it involves electronic degrees of freedom only. We will return to this question in Discussions.

IV. PARAMETERS SENSITIVITY

Thus, we find superexchange constant \( J \) (7) and charge-transfer gap \( E_{\text{gap}} \) (8) \( \[24, 27\] \) as functions of the three-band model parameters:
\[ J = J(t_{pd}, t_{pp}, \Delta, U_d, U_p, V_{pd}) \]
\[ E_{gap} = E_{gap}(t_{pd}, t_{pp}, \Delta, U_d, U_p, V_{pd}) \]

Both observable quantities are strongly depend on hopping integrals and \( \Delta = \epsilon_p - \epsilon_d \), that provides the way of fixing these latter by the experimental values of the first.

As was discussed earlier, abundance of the parameters makes questionable the calculation of the effective hopping integral for the t-J model from the three-band model for real CuO\(_2\) planes. While Coulomb repulsions are known with a fair precision (30\%−50\%), the situation is complicated due to a very low precision of the direct determination of \( t_{pd}, t_{pp} \) and \( \Delta \), which mostly affect all effective parameters. Previously, the above parameters have been determined from the analysis of spectroscopic data [6,7]. In our recent work we fitted \( \Delta \) to experimental value of \( J \) [15].

Now, on the basis of a better understanding of the charge-transfer process and more accurate calculations, fixing of the worse known parameters using experimental values of \( J \) and \( E_{gap} \) suggests itself. We will show that this procedure keeps effective \( t_h \) inside a narrow enough region.

Firstly, for further discussion we define O-O hopping as \( t_{pp} = \gamma t_{pd} \). In order to characterize the above mentioned strong dependence of the parameters (12) one can calculate \( \Delta(t_{pd}) \) at fixed \( J \) or at fixed \( E_{gap} \), with other parameters (Coulomb repulsions and \( \gamma \)) as constants in the realistic region. We evaluate \( \Delta \) vs \( t_{pd} \) at \( J = 140 \) meV and 170 meV, \( E_{gap} = 2.0 \) eV and 2.5 eV (see Fig. 3). Note that the profiles of the curves resemble those at the diagram of \( U(t) \) for the simple one-band Hubbard model where \( E_{gap} = U + 2W, W = -\alpha t, J = 4t^2/U \), and the crossing point uniquely determines \( U \) and \( t \).

To be more specific, we firstly determined \( \Delta \) for constant \( J \) at an arbitrary \( t_{pd} \) and further moved up or down along the curve \( J = \text{const} \) to fix the value of \( E_{gap} \). We used the data for \( \text{La}_2\text{CuO}_4 \) \( J = 140 \) meV [25] and \( E_{gap} = 2.1 \) eV (photoconductivity) [28]. Figures 4,5,6 show the parameter of our prime interest: the effective integral for hole in the t-J model. Parameter \( \gamma = t_{pp}/t_{pd} \) is 0.5, 0.7, 0.3 for Figs. 4,5,6 respectively. In all figures simple dotted
curve corresponds to $V_{pd} = U_p = 0$, dotted ones with crosses $V_{pd} = 0$, $U_p = 3$ eV, $6$ eV, dotted ones with triangles $V_{pd} = 0.5$ eV, $1$ eV, $U_p = 0$, and full curves correspond to including both Coulombs $V_{pd} = 0.5$ eV, $U_p = 3$ eV (upper), $V_{pd} = 1$ eV, $U_p = 6$ eV (lower). The maximum on the first three curves is due to transition from $\Delta > U_d$ (unrealistic range) to $\Delta < U_d$. All variations of $\theta(U_d, V_{pd}, U_p, \gamma)$ actually show only weak dependence, and in the most preferential region, when all Coulombs are included, $\theta$ lies between $(2.4 \div 2.7)J$. We believe, that our consideration is quite accurate and well justified. Hence, one can hope that the interval for $t/J$ obtained above provides the basis for quantitatively correct calculations in the framework of the t-J model. For example, for the recently proposed mechanism of superconductivity in the t-J model which provides a very $t/J$-sensitive (exponentially) gap value [20].

Also some other features can be achieved. Figures [4],[5] represent effective hopping $|t_e|$ for vacancy, $t_{pd}$ and $\Delta$ respectively, vs other parameters. Here always $\gamma = 0.5$. Strong support of our fixing procedure is that selfconsistently determined $t_{pd}$ and $\Delta$ (Figs. [4],[5]) lie in the most appropriate region. From our calculation $t_{pd} = 1.2 \div 1.4$ eV, $\Delta = 2.5 \div 4.5$ eV, that is really close to cluster calculation of Eskes and Sawatzky [7] and to the results of other groups [4,32,33].

V. EXCITONIC STATE

The problem of consistently taking into account the Coulomb interaction of the carriers in the framework of the t-J-like model remains open. Several recent works are devoted to this problem [38].

As was suggested earlier [4], the short-range part of this Coulomb interaction may be kept by inclusion of the nearest-neighbour Cu-O repulsion. Since $V_{pd}$ is included in our effective model, one can expect that some effects will be caught.

In the recent work [28] a kink in the optical reflectivity somewhere below the charge-transfer peak (at 1.75 eV) was observed. Since it had no associated photoconductivity, it
was related to creation of exciton. An essential role of the short-range Coulomb interaction was also discussed in Ref. [28]. In our way of reasoning the exciton state, if it exists, is the Frenkel exciton, because of short-range nature of interactions.

Now it is evident that an effective attraction can result from pure magnetopolaron effect in the t-J model [18,36]. As was shown in works [35,36], ”contact” interaction of two holes (without charge) dressed by spin fluctuations is attractive for a special symmetry of the wave-function. However, the associated energy is very small ($\lesssim J/3 \approx 0.04$ eV).

It is possible to combine the ideas of the short-range Coulomb and magnetopolaron effects. The difference between $E_{\text{gap}}^0$ (10) when hole and electron are separated and $\Delta E_n$ (Fig. 4) (where $n$ denotes the lowest singlet) when they are close, is the effective Coulomb attraction of the ”bare” hole and electron (singlet and vacancy). We write an addition to Eq. (6) as

$$\Delta H_c = -V_c \sum_{<\ell^\prime>,\alpha\beta} n^e_{\ell\alpha} n^h_{\ell^\prime\beta}, \quad (13)$$

where $n^e$ is the electron number operator, $n^h$ is the hole number operator. We have found that $V_c$ is really almost independent from $U_d$ and $U_p$, and $V_c \approx 0.4V_{pd}$. ”Bare” electron-hole attraction itself does not mean Frenkel’s exciton effect. One has to show that ”dressed” electron and hole placed closely possess the lower energy than the mobile ones. In order to specify the magnetopolaronic language we reproduce here the wave function of the magnetic polaron from the Ref. [18]. For the Ising background it has the more simple form:

$$\psi_{n^+,k}^+ = \frac{1}{\sqrt{N/2}} \sum_n d_{n^+}^+ \exp(i\mathbf{k}r_n),$$

$$d_{n^+}^+ = \nu h_{n^+}^+ + \mu S_{n^+}^\uparrow \sum_{n^\prime < n} h_{n^\prime}^\downarrow, \quad (14)$$

where $n \in$ sublattice with the spin $s = -1/2$, $h_{n^+}^+$ primarily hole operators; at $t/J > 1$, $\nu^2 \approx 1/2$, $\mu^2 \approx 1/8$. Thus, ansatz consist of mixture of ”bare” hole and holes with one overturned spin. Contact interaction of these polarons with opposite spins was considered in Ref. [36] (see Fig. 10). The gain in energy for ”attracting polarons” arises from the pure t-J model effects [36] and effective Coulomb attraction [13]. The loss in energy is
from restriction of the mobility. Competition of these evident effects (without Coulomb interaction) provides bound states up to $t/J = 2 \div 3$ [35,36]. Simply acting in a spirit of magnetic polaron interaction [36] we obtain $\Delta E_{exc} \approx 0.35V_c$. Thus, at $V_{pd} = 1$ eV, $\Delta E_{exc} = 0.14$ eV.

More accurate variational construction of the exciton-magnetopolaron wave-function (on the Ising background) yields $\Delta E_{exc} \approx 0.5V_c$ (at $t/J = 2.5 \div 3$). This wave-function consists of the mixture of "bare" hole and electron at neighbor sites and hole and electron with overturned spins. It is schematically shown in Fig. 11a. Thus, at $V_{pd} = 1$ eV, $\Delta E_{exc} \simeq 0.2$ eV, that is slightly less than the observed $\Delta E_{exc}^{exp} = 0.25 \div 0.35$ eV [28]. In our calculations the interaction between next-nearest-neighbor magnetic polaron was neglected, which produced small effect for the pure t-J model [36] but may be essential for the problem with attraction. (These configurations are shown in Figs. 11b,c). Also, the answer may partly lie in the rest of the long-range Coulomb interaction.

VI. DISCUSSIONS

The detailed quantitative consideration of some of the effective parameters of the low-energy models related to description of the high - $T_c$ superconductors presented in this work relies heavily on our earlier works. In these works consistent mapping of the three-band Hubbard model onto the effective t-J model ( [2,3,5]) has been produced. Taking into account all essential interactions enables us to correctly calculate local energies of various set of states with different number of particles and matrix elements of interesting transitions. Combination of properties of the local "bare" hole and electron (ZR-singlet and vacancy) and their magnetic polaron nature as the carriers allows us to approach the calculation of some observable quantities adequately.

We have calculated the superexchange $J$ and charge-transfer gap $E_{gap}$. Their experimental values strongly constrict a possible variation interval for the quantity of great interest: the $t/J$ ratio in the t-J model. Selfconsistent calculation of this ratio for a wide range of pa-
rameters places it into the region $t/J = 2.4 \pm 2.7$. Narrowed ranges for the three-band model parameters have also been determined: $t_{pd} = 1.2 \pm 1.4$ eV, $\Delta = 2.5 \div 4.5$ eV. They coincide quite well with earlier cluster calculations, that supports our selfconsistent procedure. An excitonic state of the Frenkel type induced by the short-range Coulomb interaction with the energy lower than the charge-transfer transition approximately by 0.2 eV is found.

We have also compared the width of the peak in the $\epsilon_2(\omega)$ at 2.3 eV from Ref. [28] which is of the order of 0.5 eV with the total width of the charge-transfer spectrum. This total width is equal to the combined width of the vacancy and singlet bands. According to Eq. (11), the width of the hole band is $W_h = 2.0J$ at $t_h = 2.55J$ and width of the electron band is $W_e = 2.2J$ at $t_e = 2.75J$. Resulting total width of the charge-transfer spectrum is about 0.6 eV. Thus, the narrowness of the $\epsilon_2(\omega)$ spectrum can also be easily reproduced by magnetic polaron language.

One of the essential questions for the CuO$_2$ - planes systems, which we only briefly touched, is the phonon polaron effect. If it does not have a projection on optics, or, as we believe, the Frank-Condon principle is applicable, our calculated $t_h/J$ ratio is the upper limit of the real parameter. This is due to mass renormalization for real carriers. There is another view on the polaron effect (see Ref. [28,39]). It is stated that electron-phonon interaction lies in an intermediate range and thus the Frank-Condon principle is not obeyed. If such is the situation, we underestimate the depth of the bands (or overestimate $E_{gap}$), and effective $t_h$ should be increased. Our estimation shows that this increasing of $t_h$ is no more than 30%. Naturally, this problem requires additional investigations.

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APPENDIX:

In this Appendix we present some details of the technical treatment of the problems discussed in the paper. According to our previous work [15], we use the following transformation from the primary oxygen $p_{lx}, p_{ly}$ operators to the operators $q_{l}, \tilde{q}_{l}$ of the symmetrical and antisymmetrical oxygen states:

\[
(q_{l}, \tilde{q}_{l}) = \sum_{k} [p_{ka} \cos(k_{x}/2) \pm p_{kb} \cos(k_{y}/2)]
\times (1 + \gamma_{k})^{-1/2} \exp(ikl),
\]

where $p_{ka}$ is the Fourier image of $p_{lx}$ for $q_{l}$ and $p_{kb}$ is the Fourier image of $p_{ly}$ for $q_{l}$; $\gamma_{k} = (\cos(k_{x}a) + \cos(k_{y}a))/2$. The summation in Eq. (A1) is produced over the Brillouin zone, and the lattice constant $a=1$.

Since the groundstates of both undoped and doped systems do not consist of antisymmetrical oxygen state [6,7,15], the reformulated Hamiltonian (1,2) where only essential degrees of freedom are kept, is conveniently expressed through the local and hopping parts [15]. The local part is:

\[
H_{loc} = \epsilon_{d} \sum_{l,\alpha} n_{l\alpha}^{d} + (\epsilon_{p} - \mu_{0}t_{pp}) \sum_{l,\alpha} n_{l\alpha}^{q}
+ U_{d} \sum_{l} n_{l\uparrow}^{d} n_{l\downarrow}^{d} + V_{pd}f_{0} \sum_{l,\alpha\beta} n_{l\alpha}^{d} n_{l\beta}^{q}
+ U_{p}h_{0} \sum_{l} n_{l\uparrow}^{q} n_{l\uparrow}^{q} + 2t_{pd} \lambda_{0} \sum_{l,\alpha}(d_{l\alpha}^{+} q_{l\alpha} + H.c.) ,
\]
\[
\Delta H_{int} = V_{pd}f_{1} \sum_{<ll'>,\alpha\beta} n_{l\alpha}^{d} n_{l'\beta}^{q}
- 2U_{p}h_{1} \sum_{<ll'>} (S_{l}^{q} S_{l'}^{q} - \frac{1}{4} n_{l\uparrow}^{q} n_{l\downarrow}^{q} ) ,
\]

with $S_{l}^{q} = \frac{1}{2} q_{l\alpha}^{+} \sigma_{\alpha\beta} q_{l\beta}$, $n^{q} = n_{l\uparrow}^{q} + n_{l\downarrow}^{q}$.  

(A2)
The hopping part is:

\[ H_{\text{hop}} = 2t_{pd}\lambda_1 \sum_{<l>.,\alpha} (d_{l\alpha}^+ q_{l\alpha} + H.c.) \]
\[ - 2t_{pp}\mu_1 \sum_{<l>.,\alpha} q_{l\alpha}^+ q_{l\alpha}, \]
\[ \Delta H_{\text{hop}} = V_{pd} f' \sum_{<l>.,\alpha\beta} n_{l\alpha}^d [q_{l\alpha}^+ q_{l\beta} + H.c.] \]
\[ + U_p h' \sum_{<l>.,\alpha} n_{l\alpha}^d [q_{l\alpha}^+ q_{l\bar{\alpha}} + H.c.]. \]  

(A4)

All constants \(\lambda, \mu, f, h\) in Eqs. (A2,A4) are of Wannier nature. Their Fourier images and magnitudes are given in Ref. [15]. In order to group them together we reproduce

\[ \lambda_0 = 0.9581 \quad \lambda_1 = 0.1401 \quad \mu_0 = 1.4567 \quad \mu_1 = 0.2678 \]
\[ f_0 = 0.9180 \quad f_1 = 0.2430 \quad h_0 = 0.211 \quad h_1 = 0.059 \]
\[ f' = 0.1342 \quad h' = 0.030. \]

We have treated the Hamiltonian \(H_{\text{loc}} + \Delta H_{\text{int}} (A2)\) in the selfconsistent mean-field approximation [15] that enables us to solve the problem of the local states at site with different number of holes. The matrix elements of the Hamiltonian (A4) between states with a singlet or vacancy at different sites in initial and final states lead to the following expression for the hopping constants:

\[ t_h = 2t_1 (W_1 V' - \sqrt{2} U_1 U')(W_1 U' - \sqrt{2} V_1 V') \]
\[ + t_p\mu_1 (W_1 U' - \sqrt{2} V_1 V')^2/2 \]
\[ - (V_{pd} f_1 W_1 U' - \sqrt{2} U_p h_1 V_1 V')(W_1 U' - \sqrt{2} V_1 V'), \]
\[ t_e = - 4t_1 U'' V'' - t_p\mu_1 (V'')^2, \]  

(A5)

where \(U', V'\) are the coefficients of \(|f>\) - state nearest to singlet, \(U'', V''\) - those nearest to vacancy. The coefficients \(U', V'\) and \(U'', V''\) are slightly different from the ones in Eq. (4) due to a distortion of \(|f>\) - states by the nearest vacancy or singlet. This distortion has its origin in the short-range Coulomb repulsions due to \(U_p\) and \(V_{pd}\) terms in the Hamiltonian (4). Note that it changes the energy of the \(|f>\) - states nearest to a vacancy or singlet. We
take this effect into consideration when we calculate the quantity \( E_{\text{gap}}^0 \). Thus, we have for the total energies \( E_c \) and \( E_v \) for a singlet and a vacancy Eq. (10)

\[
E_c = E_s + 4E_{fs} - 5E_f,
\]

\[
E_v = E_0 + 4E_{f0} - 5E_f,
\]

(A6)

where \( E_s \) and \( E_0 \) are the local energies of singlet and vacancy; \( E_{fs} \) and \( E_{f0} \) are the energies of the \(|f>\) - states nearest to a singlet or vacancy; \( E_f \) is the energy of \(|f>\) - state in an undoped sample. These states are schematically shown in Fig. 2.

When the vacancy and the two-hole state are created at the neighbour sites (see Fig. 1) the difference in energy between this state and the ground state is determined by the relation

\[
\Delta E_n = E_n + E_0 + 3E_{fs} + 3E_{f0} - 8E_f.
\]

(A7)

These energies \( \Delta E_n \) are involved in calculation of the superexchange constant \( J \) (Eq. (7)) and in the energy of the Coulomb attraction of a singlet and vacancy in Sec. V.
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FIGURES

FIG. 1. The nearest-neighbor two-hole state and vacancy. Black circle denotes two-hole state, empty circle denotes vacancy. Crosses are one hole states (spins).

FIG. 2. The separated ZR singlet (hole) and vacancy (electron). Black circle denotes singlet, empty circle denotes vacancy. Crosses are one-hole states (spins).

FIG. 3. $\Delta$ vs $t_{pd}$ at constant $J$ or $E_{gap}$. $U_d = 7$ eV, $U_p = 3$ eV, $V_{pd} = 1$ eV, $t_{pp}/t_{pd} = 0.5$. Full curve - $J = 140$ meV, dashed curve - $J = 170$ meV, full curve with markers - $E_{gap} = 2.0$ eV, dotted curve - $E_{gap} = 2.05$ eV.

FIG. 4. Effective hopping integral for t-J model hole vs $U_d$. Dotted line - $V_{pd} = U_p = 0$, dotted with crosses - $V_{pd} = 0$, $U_p = 3$, $6$ eV, dotted with triangles - $U_p = 0$, $V_{pd} = 0.5$, $1$ eV, full curves - $V_{pd} = 0.5$ eV, $U_p = 3$ eV (upper), $V_{pd} = 1$ eV, $U_p = 6$ eV (lower), $\gamma = 0.5$.

FIG. 5. All notations as for Fig.4; $\gamma = 0.7$.

FIG. 6. All notations as for Fig.4; $\gamma = 0.3$.

FIG. 7. Effective hopping integral for electron in the t-J model vs $U_d$, curves markers as for Fig.4; $\gamma = 0.5$.

FIG. 8. Cu-O hopping integral vs $U_d$, curves markers as for Fig.4; $\gamma = 0.5$.

FIG. 9. $\Delta$ vs $U_d$; $\gamma = 0.5$.

FIG. 10. Configuration of interacting magnetic polarons from Ref. [36].

FIG. 11. (a) Exciton-magnetopolaron; (b),(c) next-nearest-neighbor magnetic polarons.