Parameters of the Effective Singlet-Triplet Model for Band Structure of High-$T_c$ Cuprates by Different Approaches

M.M. Korshunov, V.A. Gavrichkov, and S.G. Ovchinnikov  
L.V. Kirensky Institute of Physics, Siberian Branch of Russian Academy of Sciences, 660036 Krasnoyarsk, Russia

Z.V. Pchelkina, I.A. Nekrasov, M.A. Korotin, and V.I. Anisimov  
Institute of Metal Physics, Ural Branch of Russian Academy of Sciences, 620219 Ekaterinburg GSP-170, Russia
(Dated: November 2, 2018)

The present paper covers the problem of parameters determination for High-$T_c$ superconductive copper oxides. Different approaches, ab initio LDA and LDA+U calculations and Generalized Tight-Binding (GTB) method for strongly correlated electron systems, are used to calculate hopping and exchange parameters of the effective singlet-triplet model for $CuO_2$-layer. The resulting parameters are in remarkably good agreement with each other and with parameters extracted from experiment. This set of parameters is proposed for proper quantitative description of physics of hole doped High-$T_c$ cuprates in the framework of effective models.

PACS numbers: 74.72.h; 74.20.z; 74.25.Jb; 31.15.Ar

I. INTRODUCTION

High-$T_c$ superconductive cuprates (HTSC) belong to the class of substances where the strong electron correlations are important. This circumstance and also the fact that these substances have non-trivial phase diagrams (see e.g. review [1]) lead to the difficulties in description of HTSC in framework of first principles (ab initio) methods, especially in the low doping region. So at present moment the most adequate method of HTSC theoretical investigations is the model approach. Effective models of HTSC (e.g. $t-J$ model) usually contain free parameters that could be fitted to experimental data (comparison of calculated and experimental Fermi surfaces, dispersion curves, etc.) but as soon as one uses model approach the question concerning correctness of these parameters arises. One of the possible ways to answer this question is to obtain relations between parameters of some effective model and microscopic parameters of the underlying crystal structure. The underlying crystal structure of HTSC could be described either by the 3-band Emery model [2, 3] or by the multiband $p-d$ model [4]. One can compare parameters bound to these models with parameters obtained by very different approach, e.g. with ab initio calculated parameters. It does not mean that the ab initio band structure is correct. Due to the strong electron correlations it is for sure incorrect in the low doping region where these correlations are most significant. Nevertheless, the single electron parameters are of interest and may be compared with the appropriate parameters obtained by fitting to the experimental ARPES data.

In the present paper we obtain relations between microscopic parameters of the multiband $p-d$ model and parameters of the effective singlet-triplet $t-J$ model for hole doped HTSC. Then we compare these parameters and the $t-J$ model parameters obtained in the ab initio calculations. In Section II the details of ab initio calculation within density functional theory are presented. In Section III formulation of the effective singlet-triplet model as the low-energy Hamiltonian for the multiband $p-d$ model with generalized tight-binding (GTB) method applied are described. In both methods the parent insulating compound $La_2CuO_4$ is investigated. Parameters are obtained at zero doping because within the GTB method the evolution of the band structure with doping is described only by changes in the occupation numbers of zero-hole, single-hole, and two-hole local terms, while all parameters are fitted in undoped case and therefore fixed for all doping levels. The resulting parameters of both approaches (GTB and ab initio) are in very good qualitative and quantitative agreement with each other and parameters extracted from experiment. Also, these parameters are in reasonable agreement with $t-J$ model parameters used in the literature. We conclude that the obtained set of model parameters should be used in effective models for proper quantitative description of HTSC in the whole doping region.

II. AB INITIO PARAMETERS CALCULATION

The band structure of $La_2CuO_4$ was obtained in frames of the linear muffin-tin orbital method [5] in tight-binding approach [6] (TB-LMTO) withing the local density approximation (LDA). The crystal structure data [7] corresponds to tetragonal $La_2CuO_4$. The effective hopping parameters $t_p$ were calculated by the least square fit procedure to the bands obtained in LDA calculation [8]. The effective exchange interaction parameters $J_p$ were calculated using the formula derived in [9], where the Green function method was used to calculate $J_{p}$ as second derivative of the ground state energy with respect to
the magnetic moment rotation angle via eigenvalues and eigenfunctions obtained in LDA+U calculation\cite{10}. The LDA+U approach allows to obtain the experimental antiferromagnetic insulating ground state for the undoped cuprate in contrast to the LDA approach which gives a nonmagnetic metallic ground state\cite{10}. The Coulomb parameters $U = 10$ eV and $J = 1$ eV used in LDA+U calculation were obtained in constrained LSDA supercell calculations\cite{11}.

III. GTB METHOD AND FORMULATION OF THE EFFECTIVE SINGLET-TRIPLET MODEL

The $t - J$\cite{12} and Hubbard\cite{13} models are widely used to investigate HTSC compounds. While using these models one, in principle, can catch up qualitatively essential physics. The parameters in these models (i.e. the hopping integral $t$, antiferromagnetic exchange $J$, Hubbard repulsion $U$) are typically extracted from experimental data. Thus, these parameters do not have a direct microscopical meaning. More consequent approach is to write down the multiband Hamiltonian for the real crystal structure (which now includes parameters of this real structure) and map this Hamiltonian onto some low-energy model (like $t - J$ model). In this case parameters of real structure could be taken from the\textit{ab initio} calculations or fitted to experimental data.

As the starting model that properly describes crystal structure of the cuprates it is convenient to use 3-band Emery $p - d$ model\cite{14,15} or the multiband $p - d$ model\cite{16}. The set of microscopic parameters for the first one was calculated in\cite{14,15}. While this model is simpler then the multiband $p - d$ model it lacks for some significant features, namely importance of $d_{z^2}$ orbitals on copper and $p_z$ orbitals on apical oxygen. Non-zero occupancy of $d_{z^2}$ orbitals pointed out in XAS and EELS experiments which shows 2-10% occupancy of $d_{z^2}$ orbitals\cite{16,17,18} and 15% doping dependent occupancy of $p_z$ orbitals\cite{19} in all HTSC of p-type (hole doped). In order to take into account these facts the multi-band $p - d$ model should be used:

$$H_{pd} = \sum_{f,\lambda,\sigma} (\epsilon_{\lambda} - \mu) n_{f\lambda\sigma} + \sum_{<f,g>\lambda,\lambda',\sigma} T^{\lambda\lambda'}_{fg} c_{f\lambda\sigma}^{\dagger} c_{g\lambda'\sigma}$$

where $c_{f\lambda\sigma}$ is the annihilation operator in Wannier representation of the hole at site $f$ (copper or oxygen) at orbital $\lambda$ with spin $\sigma$, $n_{f\lambda\sigma} = c_{f\lambda\sigma}^{\dagger} c_{f\lambda\sigma}$. Indexes $\lambda$ run through $d_{z^2}$ and $d_{x^2-y^2}$ orbitals on copper, $p_x$ and $p_y$ atomic orbitals on the plane oxygen sites and $p_z$ orbital on the apical oxygen; $\epsilon_{\lambda}$ - single-electron energy of the atomic orbital $\lambda$. $T^{\lambda\lambda'}_{fg}$ includes matrix elements of hoppings between copper and oxygen ($t_{pd}$ for hopping $d_z \leftrightarrow p_x, p_y$; $t_{pd}/\sqrt{3}$ for $d_z \leftrightarrow p_z$; $t'_{pd}$ for $d_z \leftrightarrow p_z$) and between oxygen and oxygen ($t_{pp}$ for hopping $p_x \leftrightarrow p_y$; $t'_{pp}$ for hopping $p_x, p_y \leftrightarrow p_z$).

The Coulomb matrix elements $V_{fg}^{\lambda\lambda'}$ includes intraatomic Hubbard repulsions of two holes with opposite spins on one copper and oxygen orbital $(U_d, U_p)$, between different orbitals of copper and oxygen $(V_d, V_p)$, Hund exchange on copper and oxygen $(J_d, J_p)$ and the nearest-neighbor copper-oxygen Coulomb repulsion $V_{pd}$.

GTB method\cite{11} consist of exact diagonalization of intracell part of $p - d$ Hamiltonian\cite{11} and perturbative account for the intercell part. For $La_{2-x}Sr_xCuO_4$ the unit cell is $CuO_4$ cluster, and a problem of nonorthogonality of the molecular orbitals of adjacent cells is solved by an explicit fashion namely by constructing the relevant Wannier functions on a five-orbitals initial basis of the atomic states\cite{20,21}. In a new symmetric basis the intracell part of the total Hamiltonian is diagonalized, allowing to classify all possible effective quasiparticle excitations in $CuO_2$-plane according to a symmetry.

Calculations\cite{20,21} of the quasiparticle dispersion and spectral intensities in the framework of multiband $p - d$ model with use of GTB method are in very good agreement with ARPES data on insulating compound $Sr_2CuO_2Cl_2$\cite{22,23} (see Fig. 1).

Other significant results of this method are\cite{21,24,25}:

i) Pinning of Fermi level in $La_{2-x}Sr_xCuO_4$ at low concentrations was obtained in agreement with experiments\cite{26,27}. This pinning appears due to the in-gap state, spectral weight of this state is proportional to doping concentration $x$ and when Fermi level comes to this in-gap band then Fermi level "stacks" there. In Fig. 2 the dop-
FIG. 2: Dependence of chemical potential shift $\Delta \mu$ on concentration of doping $x$ for $Nd_{2-x}Sr_xCuO_4$ and $La_{2-x}Sr_xCuO_4$. Straight lines are results of GTB calculations, filled circles with error bars are experimental points [26].

ing dependence of chemical potential shift $\Delta \mu$ for n-type High-$T_c$ $Nd_{2-x}Sr_xCuO_4$ (NCCO) and p-type High-$T_c$ $La_{2-x}Sr_xCuO_4$ (LSCO) is shown. The localized in-gap state exist in NCCO also for the same reason as in LSCO, but its energy is determined by the extremum of the band at $(\pi/2, \pi/2)$ point and it appears to be above the bottom of the conductivity band. Thus, the first doped electron goes into the band state at the $(\pi, 0)$ and the chemical potential for the very small concentration merges into the band. At higher $x$ it meets the in-gap state with a pinning at $0.08 < x < 0.18$ and then $\mu$ again moves into the band. The dependence $\mu(x)$ for NCCO is quite asymmetrical to the LSCO and also agrees with experimental data [26].

ii) Experimentally observed evolution of Fermi surface with doping from hole-type (centered at $(\pi, \pi)$) in the underdoped region to electron-type (centered at $(0, 0)$) in the overdoped region is qualitatively reproduced in this method.

iii) Pseudogap feature for $La_{2-x}Sr_xCuO_4$ is obtained as a lowering of density of states between the in-gap state and the states at the top of the valence band.

Above results was obtained with the following set of the microscopic parameters:

$$
\begin{align*}
\varepsilon_{d_{x^2-y^2}} &= 0, \quad \varepsilon_{d_{xz}} = 2, \quad \varepsilon_{p_x} = 1.5, \quad \varepsilon_{p_z} = 0.45, \\
 t_{pd} &= 1, \quad t_{pp} = 0.46, \quad t_{pd} = 0.58, \quad t_{pp} = 0.42, \\
 U_d &= V_d = 9, \quad J_d = 1, \quad J_p = 0, \quad U_p = V_p = 4, \quad V_{pd} = 1.5.
\end{align*}
$$

As the next step we will formulate the effective model. Simplest way to do it is to completely neglect contribution of two-particle triplet state $^3B_{1g}$. Then there will be only low-energy two-particle states - Zhang-Rice-type singlet $^1A_{1g}$ - and the effective model will be the usual $t - J$ model. But in the multiband $p - d$ model the difference $\epsilon_T - \epsilon_S$ between energy of two-particle singlet and two-particle triplet depends strongly on various model parameters, particularly on distance of the apical oxygen from the planar oxygen, energy of the apical oxygen, difference between energy of $d_{x^2}$-orbitals and $d_{x^2-y^2}$-orbitals. For the realistic values of model parameters $\epsilon_T - \epsilon_S$ is close to 0.5 eV [21, 22] contrary to the 3-band model with this value being about 2 eV (this case was considered in [24, 32]). To take into account triplet states we will derive the effective Hamiltonian for multiband $p - d$ model by exclusion of the intersubband hopping between low (LHB) and upper (UHB) Hubbard subbands, similar to [12].

As the Hubbard X-operators $X_f^q \equiv |p\rangle \langle q|$ on site $f$ represents natural language to describe strongly correlated electron systems in the rest of the paper we will use these operators. The X-operators are constructed in the Hilbert space that consists of a vacuum $H^0 = 0$, single-hole $|\sigma\rangle = \{|\uparrow\rangle, |\downarrow\rangle\}$ state of $b_{1g}$ symmetry, two-hole singlet state $|S\rangle$ of $^1A_{1g}$ symmetry and two-hole triplet state $|^TM\rangle$ (where $M = +1, 0, -1$) of $^3B_{1g}$ symmetry.

We write the Hamiltonian in the form $H = H_0 + H_1$, where the excitations via the charge transfer gap $E_{ct}$ are included in $H_1$. Then we define an operator $H(\epsilon) = H_0 + \epsilon H_1$ and make the unitary transformation $\hat{H}(\epsilon) = \exp(-i \epsilon S) H(\epsilon) \exp(i \epsilon S)$. Vanishing linear in $\epsilon$ component of $\hat{H}(\epsilon)$ gives the equation for matrix $\hat{S}$: $H_1 + i \left[ H_0, \hat{S} \right] = 0$. The effective Hamiltonian is obtained in second order in $\epsilon$ and at $\epsilon = 1$ is given by:

$$
\hat{H} = H_0 + \frac{1}{2} \left[ H_1, \hat{S} \right].
$$

Thus, for the multiband $p - d$ model [11] in case of electron doping (n-type systems) we obtain the usual $t - J$ model:

$$
H_{t-J} = \sum_{f, \sigma} \varepsilon_f X_f^\sigma + \sum_{< f, g >, \sigma} \sum_{\alpha, \beta} t_{f\alpha}^g X_f^\sigma X_g^\alpha + \sum_{< f, g >} J_{fg} \left( \hat{S}_f \hat{S}_g - \frac{1}{4} n_f n_g \right),
$$

where $\hat{S}_f$ are spin operators and $n_f$ are number of particles operators. The $J_{fg} = 2 \left( \langle \rho_{fg}^z \rangle \right)^2 / E_{ct}$ is the exchange integral, $E_{ct}$ is the energy of charge-transfer gap (similar to $U$ in the Hubbard model, $E_{ct} \approx 2$ eV for cuprates). Chemical potential $\mu$ is included in $\varepsilon_f$.

For p-type systems effective Hamiltonian has the form of a singlet-triplet $t - J$ model [31]:

$$
H = H_0 + H_1 + \sum_{< f, g >} J_{fg} \left( \hat{S}_f \hat{S}_g - \frac{1}{4} n_f n_g \right),
$$

where $H_0$ (unperturbed part of the Hamiltonian) and
TABLE I: Parameters of the effective singlet-triplet model for p-type cuprates obtained in the framework of GTB method (all values in eV).

| ρ | \( t_{00}^{ss} \) | \( t_{00}^{ps} \) | \( t_{00}^{pp} \) | \( t_{00}^{mT} \) | \( t_{00}^{sT} \) | \( J_\rho \) |
|---|---|---|---|---|---|---|
| (0.1) | 0.373 | 0.587 | -0.479 | 0.034 | 0.156 | 0.115 |
| (1.1) | 0.002 | -0.050 | 0.015 | -0.011 | 0 | 0.0001 |
| (0.2) | 0.050 | 0.090 | -0.068 | 0.015 | 0.033 | 0.0023 |
| (2.1) | 0.007 | 0.001 | -0.006 | -0.004 | 0.001 | 0 |

H_{t} (kinetic part of \( H \)) are given by the expressions:

\[
H_0 = \sum_f \left[ \varepsilon_1 \sum_{\sigma} X_{f}^{\sigma \sigma} + \varepsilon_2 S X_{f}^{SS} + \varepsilon_{2T} \sum_{M} X_{f}^{TMTM} \right],
\]

\[
H_t = \sum_{f g, \sigma} \left\{ i t_{fg}^{SS} X_{f}^{SS} X_{g}^{\bar{SS}}
+ i t_{fg}^{TT} \left( \sigma \sqrt{2} X_{f}^{TT0} - X_{f}^{T220} \right) \left( \sigma \sqrt{2} X_{g}^{T20} - X_{g}^{TT0} \right)
+ i t_{fg}^{ST} 2\sigma \gamma_b \left[ X_{f}^{\bar{S}0} \left( \sigma \sqrt{2} X_{g}^{T0} - X_{g}^{TT0} \right) + H.c. \right] \right\}.
\]

Upper indexes of hopping integrals \((0,S,T)\) corresponds to excitations which accompanied by hopping from site \( f \) to \( g \), i.e. in Hamiltonian one have the following terms: \( \sum_{f g, \sigma} i t_{fg}^{MN} X_{f}^{M \sigma} X_{g}^{N \sigma} \). The relation between these effective hoppings and microscopic parameters of multiband \( p-d \) model is as follows:

\[
t_{00}^{SS} = -2t_{pp}v_{fg}v_{ub}^2 - 2t_{pp}v_{fg}v_{ub}^2,
\]

\[
t_{00}^{ps} = -2t_{pp}v_{fg}v_{ub}^2 - 2t_{pp}v_{fg}v_{ub}^2,
\]

\[
t_{00}^{ps} = -2t_{pp}v_{fg}v_{ub}^2 - 2t_{pp}v_{fg}v_{ub}^2,
\]

\[
t_{00}^{mT} = \frac{2t_{pp}}{\sqrt{3}} \lambda_f^\rho \gamma_z \gamma_a + 2t_{pp}v_{fg}^2 \gamma_a - 2t'_{pp} \lambda_f^\gamma \gamma_p \gamma_a,
\]

\[
t_{00}^{sT} = \frac{2t_{pp}}{\sqrt{3}} \xi_f^\gamma \gamma_a + 2t_{pp} \lambda_f \gamma_a - 2t'_{pp} \lambda_f \gamma_a,
\]

The factors \( \mu, \nu, \lambda, \xi, \chi \) are the coefficients of Wannier transformation made in GTB method and \( u, v, \gamma_a, \gamma_b, \gamma_z, \gamma_p \) are the matrix elements of annihilation-creation operators in the Hubbard X-operators representation.

The resulting Hamiltonian \( H_t \) is the generalization of the \( t-J \) model to account for two-particle triplet state. Significant feature of effective singlet-triplet model is the asymmetry for \( n \)- and \( p \)-type systems which is known experimentally. So, we can conclude that for \( n \)-type systems the usual \( t-J \) model takes place while for \( p \)-type superconductors with complicated structure on the top of the valence band the singlet-triplet transitions plays an important role.

Using set of microscopic parameters \( \{ \} \) in the Table \( III \) we present numerical values of the hopping and exchange parameters calculated according to \( \{ \} \).

TABLE II: Comparison of \textit{ab initio} parameters \( \{ \} \) and parameters, obtained in the framework of GTB method (all values in eV).

| ρ | \( t_\rho \) | \( J_\rho \) | \( t_\rho \) | \( J_\rho \) |
|---|---|---|---|---|
| (0.1) | 0.486 | 0.109 | 0.587 | 0.115 |
| (1.1) | -0.086 | 0.016 | -0.050 | 0.0001 |
| (0.2) | -0.006 | 0 | 0.090 | 0.0023 |
| (2.1) | 0 | 0 | 0.001 | 0 |

IV. COMPARISON OF PARAMETERS

The resulting parameters from \textit{ab initio} \( \{ \} \) and GTB calculations are presented in Table \( III \). Here \( \rho \) is the connecting vector between two copper centers, \( t_\rho \) is the hopping parameter (in the effective singlet-triplet model it is equal to \( t_\rho^{ss} \), see \( \{ \} \)), \( J_\rho \) is the antiferromagnetic exchange integral.

As one can see, despite slight differences, parameters of both methods are very close and show similar dependence on distance. It is worth to mention that both methods give disproportionality between \( t_\rho \) and \( J_\rho \). In the usual \( t-J \) model proportionality \((J_\rho = 2t_\rho^2/U)\) takes place as soon as this \( t-J \) model obtained from the Hubbard model with Hubbard repulsion \( U \). In case of the singlet-triplet model the intersubband hoppings \( t_\rho^{ss} \) which determines value of \( J_\rho \) is different \( \{ \} \) from the intrasubband hoppings \( t_\rho^{SS} \) which determines \( t_\rho \). This fact resulted in more complicated relation between \( t_\rho \) and \( J_\rho \).

In the framework of LDA band structure of \( YBa_2Cu_3O_7+x \) and whiting orbital projection approach it was shown \( \{ \} \) that the 1-band Hamiltonian reduced from eight-band Hamiltonian should include not only the nearest-neighbor hopping terms \((t)\), but also second \((t')\) and third \((t'')\) nearest-neighbors hoppings. In GTB method the dependence of hoppings \( t_\rho \) on distance automatically results from the distance dependence of coefficients of Wannier transformation made in this method (see Eq. \( \{ \} \) ). In order to show correspondence between results of various authors, we present comparison of our parameters and parameters, widely used by different groups in Table \( III \).

The parameters extracted from experimental data are listed in columns I-VI of Table \( III \) LDA calculated parameters are presented in columns VII and VIII. Our results for hoppings are in the best agreement with columns III, VII and VIII. This similarity is not surprising. In LDA calculations the bandwidth of strongly correlated electron systems are usually overestimated due to the lack of proper account of strong Coulomb repulsion of electrons. But it is well known that the Fermi surface obtained by this method is in very good agreement with experiments. The main contribution to the shape of the Fermi surface comes from kinetic energy of the electrons (hopping parameters), so values of hoppings should be properly estimated by LDA calculations (columns VII,
In works by Tohayama and Maekawa [35, 38] (column III) the parameters was obtained by fitting the LSCO tight-binding Fermi surface to the experimental one. This procedure should give the same values as an LDA calculations and, as one can see, it does. By the same technique the parameters for Bi$_2$Sr$_2$CaCu$_2$O$_{8+x}$ (Bi2212, column IV) was obtained [37, 38]. These parameters are different from LSCO case and present paper and the most straightforward explanation is the more complicated structure of the Fermi surface of Bi2212 compound. In the present paper the single-layer (LSCO-like) compounds are considered and effects of multiple CuO$_2$-planes (i.e. bi-layer splitting) are neglected. The difference between our hoppings and hoppings in column V appeared due to the same reason (in Ref. [41] the YBa$_2$Cu$_3$O$_6$ insulating compound was investigated).

In the last two columns of Table III the antiferromagnetic exchange parameter $J$ obtained from two-magnon Raman scattering analysis by moment expansion (LSCO, column VII) and spin-wave theory (YBCO, column X) are presented (for details see review [43] and references therein). Our values of $J$ (column 0) are in good agreement with values extracted from experiments and similar to listed in columns I-VI.

In the paper [44] the Heisenberg Hamiltonian on the square lattice with plaquette ring exchange was investigated. The fitted exchange interactions $J = 0.151$ eV, $J' = J'' = 0.025 J$ gave values for the spin stiffness and the Neel temperature in excellent agreement with experimental data for insulating compound La$_2$CuO$_4$. In GTB calculations $J = 0.115$ eV, $J' = 0.009 J$ and $J'' = 0.034 J$. The values of $J$ are close to each other but different. This difference could be explained by the fact that authors of [44] used the Heisenberg Hamiltonian and inclusion of hopping term should renormalize presented values of exchange interactions. Agreement between $J''$ in GTB calculations and Ref. [44] is good but values of $J'$ is completely different. The last issue could be addressed to oversimplification of calculations in [44] – the authors put $J' = J''$ by hand to restrict number of fitting parameters.

Now we will discuss the difference between our parameters and parameters in columns I,II,VI and column IV (SCOC). The hoppings in mentioned papers were obtained by fitting $t - t' - t'' - J$ model results to experimental ARPES spectra [22, 39] for insulating Sr$_2$CuO$_2$Cl$_2$. We claim that the discrepancy between GTB method results and $t - t' - t'' - J$ model results stems from absence of singlet-triplet hybridization in latter model. This statement can be proved by comparison of "bare" $t - t' - J$ model [4] dispersion and dispersion of singlet-triplet $t - t' - J$ model [57]. The paramagnetic non-superconductive phase was investigated in Hubbard-I approximation both in the singlet-triplet and $t - t' - J$ models. Results for optimal doping (concentration of holes $x = 0.15$) are presented in Fig. 3.

There is strong mixture of singlet and triplet bands along $(0,0) - (\pi, \pi)$ and $(\pi, 0) - (0, 0)$ directions due to the $t^{ST}$ matrix element (see [4]) in both paramagnetic (Fig. 3) and in antiferromagnetic phases (Fig. 1). It is exactly the admixture of the triplet states that deter-

### Table III: Comparison of calculated parameters and parameters, used in the literature.

| Quantity | $0^\circ$ | $0^\circ$ | I$^\circ$ | II$^\circ$ | III$^\circ$ | IV$^\circ$ | V$^\circ$ | VI$^\circ$ | VII$^d$ | VIII$^d$ | IX$^c$ | X$^c$ |
|----------|-----------|-----------|-----------|-----------|-----------|-----------|----------|-----------|-----------|-----------|---------|--------|
| LSCO     | here      | here      | LSCO      | LSCO      | B2212     | YBCO      | SCOC     | YBCO      | LSCO      | LSCO      | YBCO    | YBCO   |
| $t$, eV  | 0.587     | 0.486     | 0.416     | 0.35      | 0.35      | 0.35      | 0.40     | 0.40      | 0.349     | 0.43      | –       | –      |
| $t'/t$   | -0.085    | -0.154    | -0.350    | -0.20     | -0.12     | -0.34     | -0.42    | -0.35     | -0.028    | -0.17     | –       | –      |
| $t''/t$  | 0.154     | 0.15      | 0.08      | 0.23      | 0.17      | 0.12      | 0.17     | 0.25      | 0.25      | 0.178     | –       | –      |
| $J$, eV  | 0.115     | 0.196     | 0.109     | 0.125     | 0.14      | 0.14      | 0.17     | 0.12      | 0.126     | 0.125     | 0.150   |        |
| $J/|t|$   | 0.196     | 0.224     | 0.300     | 0.40      | 0.40      | 0.40      | 0.43     | 0.30      | –         | –         | –       | –      |

*aGTB method parameters

*bab initio parameters obtained in present paper

*cparameters obtained by fitting to experimental data

*dab initio parameters

*parameters obtained from two-magnon Raman scattering

---

![FIG. 3: Dispersion curves on top of the valence band for effective singlet-triplet model (singlet subband - solid line, triplet subbands - dotted lines) and $t - t' - J$ model (dashed line) at optimal doping $x = 0.15$, dashed line denotes self-consistently obtained chemical potential $\mu$.](image-url)
mines in our approach the dispersion and the ARPES data in the undoped SCOC at the energies 0.3 ± 0.4 eV below the top of the valence band, where the $t - t' - J$ model failed, and the additional $t''$ parameter have been involved in the $t - t' - t'' - J$ model [25, 37]. In our approach this parameter is not as necessary as in "bare" $t - t' - J$ model since the singlet-triplet hybridization is included explicitly.

In Ref. [15] the $t - t' - t'' - J$ model was also used to describe dispersion of insulating $Sr_2CuO_2Cl_2$ and the set of parameters was the same as in Refs. [25, 37]. But the authors of Ref. [15] used completely different definition of hopping parameters: in their paper the $t'$ term stands for hopping between two nearest neighboring oxygens and the $t''$ term stands for the hopping between two oxygens on the two sides of Cu. Such definition is completely different from used in other cited papers where $t$, $t'$, $t''$ terms stands for hoppings between plaquettes centered on copper sides and we can’t make comparison with their results.

The analysis of Table [1] data gives the following ranges for different parameters: $0.350 \pm 0.587$ eV for $t$, $-0.420 \pm -0.028$ eV for $t'/t$, $0.012 \pm 0.250$ for $t''/t$ with the exception of value in Ref. [16] and $0.115 \pm 0.150$ eV for $J$. In general one can see close similarity in the first neighbor hopping $t$ and interaction $J$ for the different methods and materials, and more discrepancy in such subtle parameters as $t'$ and $t''$.

V. CONCLUSION

One of the significant results of this paper is the relationship between microscopic parameters and parameters of the effective singlet-triplet model. Thus the effective model parameters are not free any more and have a direct physical meaning coming from the dependence on microscopic parameters. The parameters of the effective singlet-triplet model were obtained both from ab initio and model calculations. Model calculations were performed in the framework of GTB method for insulating single-layer copper oxide superconductor. The ab initio calculations for $La_2CuO_4$ were done by conventional LDA TB-LMTO method. The agreement between parameters is remarkably good. Obtained parameters are also in good agreement with widely used parameters of the $t - t' - t'' - J$ model but some difference exists. This difference is attributed to the neglect of triplet excitations in simple $t - t' - t'' - J$ model. After careful analysis we proposed the set of parameters for effective models (e.g. $t - t' - t'' - J$ model or effective singlet-triplet model) for proper quantitative description of physics of hole doped High-$T_c$ cuprates.

Acknowledgments

M.M.K., V.A.G., and S.G.O. thank the Free University of Berlin for hospitality during their stay. This work has been supported by INTAS grant 01-0654, Joint Integration Program of Siberian and Ural Branches of Russian Academy of Science, Russian Foundation for Basic Research grant 03-02-16112, Russian Federal Program “Integratsia” grant B0017, Program of the Russian Academy of Science “Quantum Macrophysics”, and Siberian Branch of Russian Academy of Science (Lavrent’yev Contest for Youth Projects), RFFI-01-02-17063 (VIA, IAN, MAK), RFFI (MAS)-03-02-06126 (IAN), Ural Branch of Russian Academy of Science for Young Scientists (IAN, ZVP), Grant of the President of Russia MK-95.2003.02 (IAN).

[1] Z.-X. Shen and D.S. Dessau, Phys. Rep. 253, 1 (1995); E. Dagotto, Rev. Mod. Phys. 66, 763 (1994); A.P. Kampf, Phys. Rep. 249, 219 (1994)
[2] V.J. Emery, Phys. Rev. Lett. 58, 2794 (1987)
[3] C.M. Varma et al., Solid State Commun. 62, 681 (1987)
[4] Yu. Gaididei and V. Loktev, Phys. Status Solidi B 147, 307 (1988)
[5] O.K. Andersen and O. Jepsen, Phys. Rev. Lett. 53, 2571 (1984)
[6] O.K. Andersen, Z. Pawlowska and O. Jepsen, Phys. Rev. B 34, 5253 (1986)
[7] J.D. Axe and M.K. Crawford, J. Low Temp. Phys. 95, 271 (1994)
[8] V.I. Anisimov et al., Phys. Rev. 66, 100502 (2002)
[9] A.I. Lichtenstein et al., J. Magn. Mag. Matter 67, 65 (1987); A.I. Lichtenstein, V.I. Anisimov and J. Zaanen, Phys. Rev. B 52, R5467 (1995)
[10] V.I. Anisimov, J. Zaanen and O. Andersen, Phys. Rev. B 44, 943 (1991); V.I. Anisimov et al., J. Phys.: Condens. Matter 9, 767 (1997)
[11] O. Gunnarsson et al., Phys. Rev. B 39, 1708 (1989); V.I. Anisimov and O. Gunnarsson, ibid. 43, 7570 (1991)
[12] K.A. Chao, J. Spalek and A.M. Oles, J. Phys. C: Sol. Stat. Phys. 10, 271 (1977)
[13] J.C. Hubbard, Proc. Roy. Soc. A 286, 238 (1963)
[14] M.S. Hybertsen, M. Schluter and N.E. Christensen, Phys. Rev. B 39, 9028 (1989)
[15] A.K. McMahan, J.F. Annett and R.M. Martin, Phys. Rev. B 42, 6268 (1990)
[16] A. Bianconi et al., Phys. Rev. B 38, 7196 (1988); H. Romberg et al., Phys. Rev. B 41, 2609 (1990)
[17] C.H. Chen et al., Phys. Rev. Lett. 68, 2543 (1992)
[18] S.G. Ovchinnicov and I.S. Sandalov, Physica C 161, 607 (1989)
[19] V.A. Gavrichkov and S.G. Ovchinnikov, Phys. Rev. B 64, 235124 (2001)
[20] V.A. Gavrichkov et al., Zh. Eksp. Teor. Fiz. 118, 422 (2000); [JETP 91, 369 (2000)]
[21] B.O. Wells et al., Phys. Rev. Lett. 74, 964 (1995)
[22] C. Dürr et al., Phys. Rev. B 63, 014505 (2000)
[23] A.A. Borisov, V.A. Gavrichkov and S.G. Ovchinnikov, Mod. Phys. Lett. B 17, 479 (2003)
[24] A.A. Borisov, V.A. Gavrichkov and S.G. Ovchinnikov, ibid. 43, 7570 (1991)
[26] N. Harima et al., Phys. Rev. B 64, 220507(R) (2001)
[27] A. Ino et al., Phys. Rev. Lett. 79, 2101 (1997)
[28] A. Ino et al., Phys. Rev. B 65, 094504 (2002)
[29] J. Zaanen, A.M. Oles, P. Horsch, Phys. Rev. B 46, 5798 (1992)
[30] R. Hayn et al., Phys. Rev. B 47, 5253 (1993)
[31] M. Korshunov and S. Ovchinnikov, Fiz. Tv. Tela 43, 399 (2001) [Phys. Sol. State 43, 416 (2001)]
[32] R. Raimondi et al., Phys. Rev. B 53, 8774 (1996)
[33] O.K. Andersen et al., J. Phys. Chem. Solids 56, 1573 (1995)
[34] A. Nazarenko et al., Phys. Rev. B 51, 8676 (1995)
[35] V.I. Belinicher, A.I. Chernyshev and V.A. Shubin, Phys. Rev. B 53, 335 (1996)
[36] V.I. Belinicher, A.I. Chernyshev and V.A. Shubin, Phys. Rev. B 54, 14914 (1996)
[37] T. Tohayama and S. Maekawa, Supercond. Sci. Technol. 13, R17 (2000)
[38] T. Tohayama and S. Maekawa, Phys. Rev. B 67, 092509 (2003)
[39] C. Kim et al., Phys. Rev. Lett. 80, 4245 (1998)
[40] F.P. Onufrieva, V.P. Kushnir and B.P. Toperverg, Phys. Rev. B 50, 12935 (1994)
[41] R. Eder, Y. Ohta, G.A. Sawatzky, Phys. Rev. B 55, R3414 (1997)
[42] E. Pavarini et al., Phys. Rev. Lett. 87, 047003 (2001)
[43] W. Brenig, Phys. Rep. 251, 153 (1995)
[44] A.A. Katanin and A.P. Kampf, Phys. Rev. B 66, 100403(R) (2003)
[45] T. Xiang and J.M. Wheatley, Phys. Rev. B 54, R12653 (1996)