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Multi-band effective tight-binding model for the CuO_2 plane and hole dispersion in $Sr_2CuO_2Cl_2$

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Abstract

To interpret recent polarization dependent, *k*-resolved valence band photoemission measurements for $Sr_2CuO_2Cl_2$, a model substance for cuprates, LDA + U bandstructure calculations are performed and presented in terms of a multi-band effective model for the CuO_2 plane with strong on-site Coulomb (Hubbard's U) repulsion involved. As the second step the basic set of electronic orbitals is subdivided into two subsets depending on the energy positions and occupancy of orbitals of different symmetry. For the first subset (in-plane copper $d_{x^2-y^2}$ and oxygen p_σ orbitals) the effects of strong U_d and U_p interactions are taken into account explicitly. That leads to an effective $t - t' - t'' - J$ model and a photohole created in the photoemission process is considered as the Zhang – Rice singlet. For the second subset (the out-of-plane and the rest of in-plane orbitals) the predicted LDA + U bandstructure is sufficient to describe a photohole as a one-particle state with higher binding energy.

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Recent ARPES measurements [1–3] of the insulating compound $Sr_2CuO_2Cl_2$ provide a good test for several theories of the electronic structure of cuprates. In Ref. [1] the lowest energy electron removal state was measured and interpreted in terms of the Zhang–Rice singlet (ZRS). Photohole states with higher binding energy (BE) were found and discussed [2] with complementary polarization dependent study of the experimental spectra [3]. To describe the collected ARPES data for $Sr_2CuO_2Cl_2$ a theoretical approach is developed and presented in main features below. The approach is based on the (LDA and LDA + U) bandstructure calculations supplemented with analysis of a symmetry of different band states.

The electronic valence band (VB) structure is derived from O 2p and Cu 3d orbitals, that means on 11 band manifold for CuO_2 plane. First, we found that the VB structure resulted from the LDA is incompatible with the experimental spectra in the whole VB energy range. Therefore, we developed a more sophisticated LDA + U calculation taking into account explicitly effects of strong electron correlations (SEC). As a preliminary step we formulate an effective tight-binding (TB) model which incorporates the symmetry properties of the VB states from the beginning. Afterwards, the TB parameters are fitted to the LDA + U results and used to interpret the ARPES VB spectra.

Starting from the in-plane oxygen group orbitals of b_{1g} and a_{1g} symmetry, σ-subset, as well as b_{2g} and a_{2g} symmetry, π-subset, we define in the *q*-representation two subsets of band orbitals: $p_\sigma(q)$, $\tilde{p}_\sigma(q)$ and $p_\pi(q)$, $\tilde{p}_\pi(q)$. The in-plane part of the TB-model, which is 7×7 matrix, has 11 parameters: the on-site energies ε_d (for $d_{x^2-y^2}$), ε_D (for d_{xy}) and $\varepsilon_{\bar{d}}$ (for $d_{3z^2-r^2}$) as well as ε_p (for σ-orbitals) and ε_π (for π-orbitals); the nearest-neighbor hopping

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matrix elements t_{pd}, t_{pD}, $t_{p\tilde{d}}$, t_{pp}, $t_{\pi\pi}$ and $t_{p\pi}$. The out of plane O2p_z and Cu3d_{xz} and d_{yz} orbitals are presented by two 2×2 matrices with on-site energies ε_{pz} and ε_{dz} and the hopping matrix element t_{pdz}. The 11-band TB-Hamiltonian H_t should be completed by an interaction term $H = H_t + H_U$. This multi-band Hubbard model (MBHM) is just a direct extension of the three-band Emery model. The one-electron parameters entering into MBHM are "bare" ones while the results of the band structure calculations should be interpreted in terms of screened parameters which are mean-field solutions of MBHM.

To adopt SEC effects we use the ferromagnetic solution of MBHM as a starting point for the LDA + U calculation. Namely, $d_{x^2-y^2}$-orbital energy level is splitted into one for spin up, $\bar{\varepsilon}_d\uparrow$, shifted up and $\bar{\varepsilon}_d\downarrow$ level which is shifted down together with the remaining d-levels with both spin directions. Although being somewhat awkward, the ferromagnetic solution provides a better description of the strong electron correlations, giving a more reasonable energy position and occupancy of the different orbitals. Just this approach is taken by us to carry out the LDA + U calculation. The details of the procedure and some results of these calculation will be presented in the forthcoming publication. We found pronounced rearrangement of level ordering in the whole VB resulted from LDA + U as against LDA bandstructure.

The experimental peak positions [3] are compared with the LDA + U prediction in Table 1. Pure bands are denoted by a single and the mixed bands by two orbitals, with the first one being dominant. The resulting TB-parameters obtained by fitting the LDA + U bandstructure and the VB spectra (taken from more complete measurements [3]) are the following (in eV): $\bar{\varepsilon}_d^{\uparrow} = 2.00$, $\bar{\varepsilon}_d^{\downarrow} = -4.90$, $\bar{\varepsilon}_{\tilde{d}} = -4.78$, $\bar{\varepsilon}_D = -5.22$, $\bar{\varepsilon}_{d_z} = -6.40$, $\bar{\varepsilon}_\pi = -3.88$, $\bar{\varepsilon}_{p_z} = -3.86$, $\bar{\varepsilon}_p = -4.59$, $t_{pd} = 1.33$, $t_{pp} = 0.71$, $t_{p\pi} = 0.34$, $t_{\pi\pi} = 0.37$, $t_{D\pi} = 0.84$, $t_{pdz} = 1.15$, $t_{p\tilde{d}} = 0.77$, where $\bar{\varepsilon}$-parameters are screened ones.

Together with the gap opening, the occupied band states with the lowest BE are now predominantly of oxygen character. The ordering of the energy positions and the symmetry of these states becomes compatible with experimental data except for one important feature. That is the state with the lowest BE of $(p_\sigma d_{x^2-y^2})$-character giving rise to the ZRS. In fact, the energy position and dispersion of the ZRS are very sensitive to local AFM correlations which are well pronounced in the samples measured [1–3]. To provide a correct description of the ZRS (and its triplet partner) we subtracted two orbitals, p_σ and $d_{x^2-y^2}$, from the 11-band manifold and developed supplementary calculation for this two-band Hubbard model with Coulomb-parameters standard for CuO_2 plane, $U_d = 10.5$ eV, $U_p = 4$ eV and $U_{pd} = 1.2$ eV. This development, done within the cell-perturbation method, led to a rather good account, like in [4], of the ZRS dispersion measured.

Table 1
Comparison of experimental peak positions (in eV) with LDA + U results at high-symmetry points in BZ

Orbital	LDA + U	Exp.
	Γ	
$(p_\pi p_\sigma)$	− 2.69	− 2.9
$(\tilde{p}_\pi \tilde{p}_\sigma)$		
p_z	− 3.83	− 3.9
$d^{\downarrow}_{x^2-y^2}$	− 4.92	− 5.8
d_{xy}	− 5.40	
$(p_\sigma p_\pi)$	− 5.57	
$(\tilde{p}_\sigma \tilde{p}_\pi)$		
$d_{(x,y)z}$	− 5.87	− 6.5
	(π, π)	
$(p_\sigma d^{\downarrow}_{x^2-y^2})$ (ZRS)	0.65	− 1.2
p_π	− 2.43	− 2.4
$(p_z d_{(x,y)z})$	− 2.98	− 2.7
$(\tilde{p}_\pi d_{xy})$	− 3.35	
$(p_\sigma d^{\uparrow}_{x^2-y^2})$ (ZRT)	− 4.94	− 3.8
$(d_{(x,y)z} p_z)$	− 6.62	− 5.8
$(d_{xy} \tilde{p}_\pi)$	− 7.20	
$(d^{\downarrow}_{x^2-y^2} p_\sigma)$	− 7.28	− 6.0

Remarkably, the energy position and dispersion of other band states predominantly of $\tilde{p}_\sigma(q)$, $p_\pi(q)$, $\tilde{p}_\pi(q)$ and p_z character are nearly spin independent. So, these bands to much extent are insensitive to the spin background and the presented LDA + U calculation is rather reliable for them. The occupied bands with dominant d-character are predicted to lie regularly at higher BE (near 6 eV) than their p-partners and this prediction is less accurate.

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