Available online at www.sciencedirect.com
SCIENCE DIRECT®
Physica B 359–361 (2005) 1168–1170
PHYSICA B
www.elsevier.com/locate/physb

# Electronic structure and its evolution with doping in cuprates with account for strong electron correlations ☆

S.G. Ovchinnikov*, V.A. Gavrichkov, M.M. Korshunov

*LV Kirensky Institute of Physics, Siberian Branch of RAS, Krasnoyarsk 660036, Russian Federation*

Received 30 December 2004

**Abstract**

The electronic structure of the undoped and p- and n-type doped cuprates is studied in the framework of the multiband p–d model using the generalized tight binding method. With hole doping, an unusual in-gap state appears just at the top of the valence band with the spectral weight proportional to the doping concentration. The chemical potential dependence on the hole and electron concentration is asymmetrical and in good agreement with the experimental data. The in-gap bands have spin-polaron origin and the spectral function of this band has a form of small low-energy satellite that can be detected in ARPES measurements.


*PACS:* 79.60.−i; 74.25.−q

*Keywords:* Strong electron correlations; Multiband p–d model; Spin-polaron effect

The key issue to understand the nature of high-temperature superconductivity in the cuprates is the evolution of the electronic structure from an antiferromagnetic insulator to a superconductor with hole doping. The adequate model for high-$T_c$ cuprates is the multiband p–d model [1]. At small doping, we have to treat the strong electronic correlations explicitly and therefore we use the generalized tight-binding (GTB) method [2] that consists of exact diagonalization of the intracell part of p–d Hamiltonian and perturbative treatment of the intercell part. The model parameters are determined by fitting the ARPES data for the undoped $Sr_2CuO_2Cl_2$. The minimal energy in the single-hole sector of the Hilbert space has the $b_{1g}$ molecular orbital, and in the two-hole sector besides the Zhang–Rice $^1A_{1g}$ singlet a significant contribution of the triplet $^3B_{1g}$ state is found at the

☆This work was supported by RFBR Grant 03-02-16124, Program of Physical Branch of Russian Academy of Science "Strongly correlated electron systems", INTAS Grant 01-0654, Siberian Branch of RAS (Lavrent'yev Contest for Young Scientists), The Dynasty Foundation and ICFPM.

*Corresponding author. Tel.: +7 3912 432906; fax: +7 3912 438923.

*E-mail address:* sgo@iph.krasn.ru (S.G. Ovchinnikov).

0921-4526/$ - see front matter © 2005 Elsevier B.V. All rights reserved.
doi:10.1016/j.physb.2005.01.311

upper part of the valence band. A staggered magnetic field $h$ split $b_{1g}$ levels by spin: $\varepsilon_{A\sigma} = \varepsilon_1 - \sigma h$, $\varepsilon_{B\sigma} = \varepsilon_1 + \sigma h$. Our calculations [3,4] of the quasiparticle dispersion and spectral functions using the GTB method are in very good agreement with ARPES data on $Sr_2CuO_2Cl_2$ [5].

The top of the valence band is given by the quasiparticles with $m = 1$: $X^1_A = |b_{1g,\uparrow}\rangle\langle {}^1A_{1g}|$ and $X^1_B = |b_{1g,\downarrow}\rangle\langle {}^1A_{1g}|$, as usually there is spin degeneracy of the band in the antiferromagnetic state. The occupation number $n_p \equiv \langle X^{pp}\rangle$ is calculated self-consistently via the chemical potential equation. In the mean-field Hubbard I approximation, the solution of this equation for the hole-doped cuprates with hole concentration $n_h = 1 + x$ is given by

$$n_{1\uparrow} \equiv n_{A\uparrow}(b_{1g}) = 1 - x, \quad n_{1\downarrow} = 0,$$
$$n_2 \equiv n({}^1A_{1g}) = x. \tag{1}$$

For the band $m = 1$, we get $F_{A\uparrow}(1) = 1$, while for the band $m = 2$ with $X^2_A = |b_{1g,\downarrow}\rangle\langle {}^1A_{1g}|$, the filling factor is $F_{A\downarrow}(2) = x$. The quasiparticle spectral weight is proportional to the filling factor; thus it is the band $m = 2$ that forms the in-gap state. In the limit $x \to 0$, its spectral weight is zero, when $x \neq 0$ this band acquires both dispersion and nonzero spectral weight proportional to doping concentration $x$. The observed pinning of the Fermi level in $La_{2-x}Sr_xCuO_4$ at low concentrations is due to the in-gap state, when Fermi level comes to this in-gap band it "stacks" there. In Fig. 1 the doping 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 exists 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 conduction band. Thus, the first doped electron goes into the band state at $(\pi, 0)$ 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 that of LSCO and also agrees with experimental data [7].

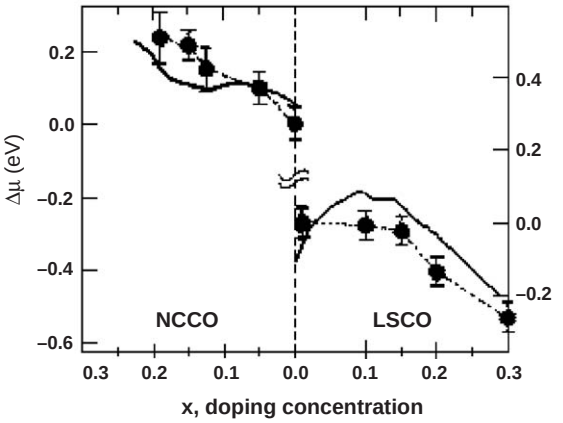


Fig. 1. Dependence of chemical potential shift $\Delta\mu$ on concentration of doping $x$ for NCCO and LSCO. Straight lines are results of GTB calculations [4,6], filled circles with error bars are experimental data points [7].

To go beyond the mean-field Hubbard I approximation, one has to calculate single-loop diagrams for self-energy. In the ferromagnetic or antiferromagnetic state, the most important contribution is given by loops with spin-wave excitations (a spin-polaron effect). According to Ref. [8], the main effect of the spin excitations is given by the spin-wave renormalization of the multielectron configuration's occupation numbers, so instead of Eq. (1), one gets

$$n_{1\uparrow} = (1 - x)(1 - n_{sf}), \quad n_{1\downarrow} = (1 - x)n_{sf}, \quad n_2 = x, \tag{2}$$

where $2n_{sf}$ is the concentration of the spin fluctuations (magnons) and it determines the spin-fluctuation decrease of the sublattice magnetization $\langle S^z_A\rangle = (1 - x)(1/2 - n_{sf})$.

Thus, at small $x$ and $n_{sf}$, the filling factors for the valence band $F(1) = 1 - n_{sf}$, and for the in-gap states $F(2) = x + n_{sf}$. It means that the spin-polaron effect results in the non-zero spectral weight of the in-gap states even for undoped cuprates $La_2CuO_4$ and $Sr_2CuO_2Cl_2$. The quasiparticle band structure and the spectral functions for the undoped $La_2CuO_4$ with $n_{sf} = 0.138$ (this value was obtained both from neutron diffraction experiments and self-consistently calculated in the Heisenberg model) are given in Fig. 2 [9]. The

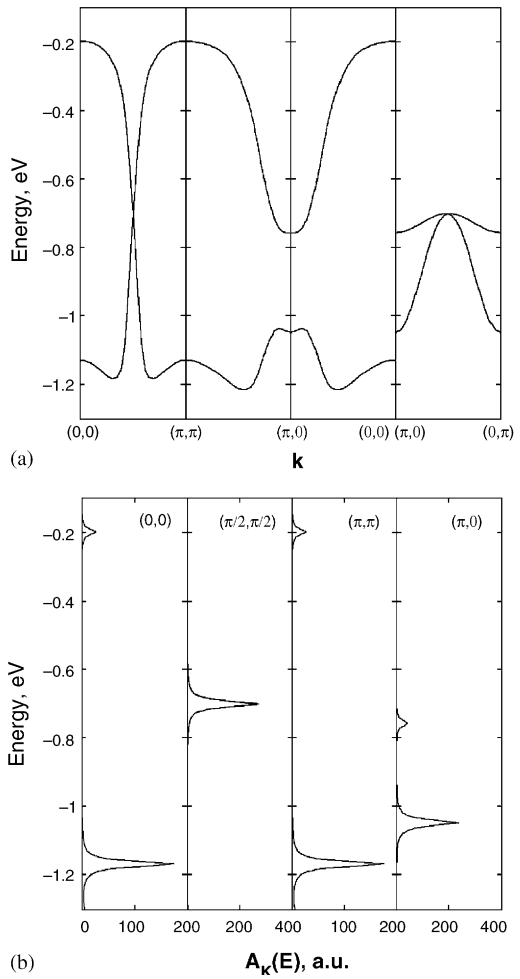


Fig. 2. The quasiparticle band structure (a) and the spectral function (b) of the undoped $La_2CuO_4$ with magnon concentration $2 \cdot n_{sf} = 2 \cdot 0.138$ calculated by the GTB method. The Fermi level is above all bands shown here.

band formed in by hole hopping via two-hole triplet $^3B_{1g}$ state lies at $\approx -1.4$ eV and is not shown here. The lowest band in Fig. 2 is the top of the valence band ($m = 1$) without spin fluctuations with a maximum at $k = (\pi/2, \pi/2)$. The upper band ($m = 2$) formed by the dispersion of the in-gap states. Despite its width, each state has a low spectral weight as seen in Fig. 2b and the total number of states in this in-gap band without doping is proportional to $n_{sf}$. The appearance of such non-Fermi liquid states is the direct effect of strong electron correlations. The maximal spectral weight of the in-gap state is near $(\pi, 0)$ point of the Brillouin zone (BZ). At the $(\pi/2, \pi/2)$ point, the two bands are degenerate, and we cannot separate the contribution of the in-gap band to the spectral function $A_k(E)$.

In conclusion, we have shown that the spin-polaron effect results in the formation of the in-gap band above the top of the valence band even in the undoped cuprates like $La_2CuO_4$, $Sr_2CuO_2Cl_2$, and $Ca_2CuO_2Cl_2$. For the hole-doped cuprates there are two contributions to the in-gap spectral weight: the mean field contribution is given by doping concentration $x$ and the spin-fluctuation contribution is given by the magnon concentration $2n_{sf}$.

## References

[1] Yu. Gaididei, V. Loktev, Phys. Stat. Sol. B 147 (1998) 307.
[2] S.G. Ovchinnicov, I.S. Sandalov, Physica C 161 (1989) 607.
[3] V.A. Gavrichkov, et al., JETP 91 (2000) 369.
[4] V.A. Gavrichkov, S.G. Ovchinnikov, JETP 98 (2004) 556.
[5] B.O. Wells, et al., Phys. Rev. Lett. 74 (1995) 964.
[6] A.A. Borisov, et al., JETP 97 (2003) 773.
[7] N. Harima, et al., Phys. Rev. B 64 (2001) 220507(R).
[8] A.N. Podmarkov, I.S. Sandalov, JETP 86 (1984) 146.
[9] S.G. Ovchinnikov, et al., J. Phys.: Condens. Matter 16 (2004) L93.