Effect of CuO$_2$ lattice strain on the electronic structure and properties of high-$T_c$ cuprate family

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1 Introduction

It is wide-spread believe that all hole-doped high-temperature superconducting cuprates have common generic phase diagram in the plane (concentration of doped holes $x$ per Cu site, temperature $T$). In fact, the phase diagram of cuprates is determined not only by doping degree $x$ but also by the strain of CuO$_2$ lattice. Many evidences of the influence of the strain of CuO$_2$ layer on superconducting and competing phases were obtained in the undoped and doped systems $(\text{La}_{1-y}\text{Ln}_y)_{2-x}\text{M}_x\text{CuO}_y$ (where Ln$^{3+}$ is lanthanides and M$^{2+}$ is elements Ca, Sr, Ba) in the experiments using epitaxial strain and cation substitutions in the rocksalt spacers with the same valence but different radii. It was shown that in La$_2$CuO$_4$ film compressive strain induced by the lattice mismatch with the substrate perovskite film results in significant $T_c$ increasing [1], [2]. Lattice mismatch strain between the CuO$_2$ planes and the intercalated rocksalt layers determines variation $T_c$ within family of $(\text{La}_{1-y}\text{M}_y)_2\text{CuO}_4$ superconductors [3] and different maxima of the critical temperature in the different cuprate families [4]. Two critical strains in the oxygen doped La$_2$CuO$_{4+\delta}$ and Nd doped La$_{214}$ system were discovered with EXAFS spectra [7] and x-ray diffuse scattering [8]: first critical strain determines onset of local lattice deformations and short-range striped domains formation, long-range charge ordering (insulating crystal of polaronic strings [8]) at doping $\delta = 1/8$ appears at strain above the second critical value. Critical value of buckling of CuO$_2$ layer (Cu-O-Cu angle) determines boundaries of insulating antiferromagnetic and superconducting phases inside low-temperature tetragonal striped phase in the undoped parent compound $(\text{La}_{1-y}\text{Nd}_y)_{2-x}\text{Sr}_x\text{CuO}_4$ [10].
One can imagine that all material aspects may be solved explicitly by the density functional theory (DFT) as it happens now in many condensed materials. Nevertheless cuprates and many other so called strongly correlated materials cannot be treated successfully by the DFT. That is why more simple model approaches are involved to understand the material dependent properties of cuprates. The importance of strong electron correlations in the CuO$_2$ planes was pointed out soon after the discovery of superconductivity in cuprates [11]. Following the discovery that the electronic holes in the CuO$_2$ induced by chemical doping are injected in the O(2p) orbitals [12] the microscopic analysis of the electronic orbitals of copper and oxygen with account for strong correlations results in the three-band Hubbard model, or the p-d model for CuO$_2$ square lattice [13]. The single-band Hubbard model for CuO$_2$ planes is the most known, it may be deduced from the general multielectron approach as the effective low energy model for undoped and weakly doped cuprates [14][15].

In this paper we will discuss material dependent electronic properties within the effective Hubbard model with parameters obtained from the DFT-LDA calculations. Additional material parameter will be the isotropic lattice strain of the CuO$_6$-octahedron. We start with the plane of CuO$_6$-octahedra in undoped La$_2$CuO$_4$ and calculate its lattice parameter $a_0$. For other cuprates we will considered also the CuO$_2$ planes with material specific lattice parameter $a$, and the lattice strain will be determined by $\delta a/a_0 = (a - a_0)/a_0$, and may be positive as well as negative. Similar model has been used for the analysis of the experimental data for different cuprates and construct the phase diagram in the plane (doping, strain). Here we will calculate the doping and strain dependent electronic structure in the normal state, and discuss the material dependence of the Lifshitz transitions with the change the Fermi surface topology under doping, the density of states at the Fermi level $N(\mu)$, and the interatomic exchange coupling parameter $J$. We will study later the effect of in-plane anisotropic misfit strain on the electronic structure of the CuO$_2$ plane giving an anisotropic distortion of the CuO$_6$ octahedra, with both rotation of the CuO$_4$ square planes and anisotropic compression of the Cu-O bond lengths observed at optimum doping in cuprates [16].

The paper is organized as follows: in part 2 we will discuss the ab initio calculation of strain dependent model parameters, in part 3 the doping dependent electronic structure and Fermi surface without strain are discussed, in part 4 we analyze the strain dependence of electronic structure. In part 5 the conclusion is given.

2 Strain dependence of the six-band p-d model parameters within the LDA-GTB approach

We are interested in the study of strain effect on characteristics of electronic structure related to superconducting phase therefore it is important to describe properly states with energies near chemical potential. Chemical potential is lowered approximately by 1 eV into the LHB with doping up to overdoped region. Electronic structure of La$_{2-x}$Sr$_x$CuO$_4$ compound in the interesting energy interval of the LHB will be described by six-band p-d model for one layer of CuO$_6$-octahedra. This model includes $d_{x^2-y^2}$, $d_{z^2}$-orbitals of planar Cu atoms, $p_{x,y}$-orbitals of planar O atoms and $p_z$-orbitals of two apical O atoms in each CuO$_6$-octahedron. Six-band p-d model takes into account on-site energies of all considered orbitals, hopping between them, intruderatomic Coulomb interaction and exchange interaction. Calculation of electronic structure will be realized within LDA+GTB method [15]. LDA method provides parameters of the model Hamiltonian. Generalized tight-binding (GTB) method allows to construct the effective Hamiltonian for quasiparticle excitations in the terms of the Hubbard operators, this method is actual for description of systems with strong electronic correlations.

On-site energies and hopping integrals can be calculated using the procedure of LDA eigenfunctions projection onto Wannier functions basis of the chosen model. The calculation was carried out using the Linearized Muffin-Tin Orbitals method (LMTO) [17][18][19] with some modifications [20]. The $k$-points grid is 12x12x12. The lattice parameters for undistorted La$_2$CuO$_4$ in the tetragonal phase are $a_0 = b_0 = 3.783\,\textrm{Å}$, $c_0 = 13.2883\,\textrm{Å}$. The strain effect of CuO$_6$-octahedron is simulated by the set of deformations $\delta a/a_0$. The lattice parameter $a$.
Table 1 Values of on-site energies and hopping integrals (in eV) for the tetragonal La$_2$CuO$_4$ obtained during projection on the Wannier function in the frameworks of the six-band model. Here, $x^2$, $z^2$, $p_x$, $p_y$, $p_z$ denote Cu-$d_{x^2-y^2}$, Cu-$d_{3z^2-r^2}$, O-$p_x$, O-$p_y$, O-$p_z$ electronic orbitals, respectively.

| $\delta a/a_0$ | -1% | -0.5% | 0% | 0.5% | 1.5% | 2.5% | 3.5% | 4.15% |
|----------------|-----|-------|----|------|------|------|------|-------|
| $E_{x^2}$     | -1.79 | -1.824 | -1.861 | -1.9 | -1.667 | -2.047 | -2.124 | -2.18 |
| $E_{z^2}$     | -2.056 | -2.075 | -2.097 | -2.119 | -2.182 | -2.186 | -2.227 | -2.36 |
| $E_{p_x}$     | -2.724 | -2.775 | -2.825 | -2.863 | -2.541 | -2.980 | -3.026 | -3.053 |
| $E_{p_y}$     | -1.741 | -1.727 | -1.721 | -1.720 | -1.541 | -1.690 | -1.713 | -1.729 |
| $E_{p_z}$     | 0.5170 | 0.5200 | 0.5230 | 0.5260 | 0.5340 | 0.5490 | 0.5620 | 0.5700 |
| $t(d_{x^2}, p_x(p_y))$ | 0.8930 | 0.8760 | 0.8590 | 0.8420 | 0.8090 | 0.7680 | 0.7320 | 0.7100 |
| $t(d_{p_x}, p_z)$ | 0.7790 | 0.7980 | 0.8200 | 0.8380 | 0.8600 | 0.8800 | 0.9050 | 0.9180 |
| $t(p_x(p_y), p_z)$ | 0.3790 | 0.3910 | 0.4030 | 0.4150 | 0.4280 | 0.4430 | 0.4560 | 0.4620 |

was changed by $-1\%$, $-0.5\%$, $+0.5\%$, $+1.5\%$, $+2.5\%$, $+3.5\%$, $+4.15\%$ in-plane compressing and stretching respectively. Accordingly parameter $\delta a/a_0$ was calculated under the condition of constant CuO$_6$-octahedron volume. The volume of the whole unit cell is also preserved. Table 1 below shows values of the on-site energies and hopping parameters at different strains. Since the relation between the in-plane compressing (stretching) and microscopic picture is empirical, we simulate the strain effect at $\delta a/a_0 \neq 0$ within the approach (see Fig. 1). Coulomb and exchange parameters were obtained in constrained LDA supercell calculations [21,22].

Coulomb repulsion on one site results in the dependence of electron (or hole) energy on occupation of the site on which this electron is located. In this case there are two types of particles on each site: (i) electron added to the empty site and (ii) electron added to the site that is occupied by electron with the opposite spin projection. Description of such system can be performed using representation of electron as superposition of Fermi-type excitations between different multielectron initial and final states. Generalized tight-binding (GTB) method [23,24] is realization of this representation of quasiparticle excitations. Each quasiparticle excitation is defined as transition between multielectron initial and final states of the single cluster, it acquires dispersion due to intercell hopping. Electronic structure in the crystal lattice is formed by bands of quasiparticle excitations. Thus GTB method is the cluster form of perturbation theory in the terms of quasiparticle excitations. In this work cluster is chosen as single CuO$_6$-octahedron. First step of GTB method is representation of full Hamiltonian in the form of sum of Hamiltonian of intracluster interactions and Hamiltonian of intercluster interactions $H = \sum f H^c_f + \sum_{f,g} H^c_{fg}$. Second step is exact diagonalization of Hamiltonian $H^c_f$ of the cluster $f$ with different number of carriers (in cuprates of p-type carriers are holes). The result of exact diagonalization is a set of multihole local cluster eigenstates.

To reproduce electronic structure in the upper part of the valence band and the lower part of the conductivity band it is sufficient to consider cluster with number of holes $n_h = 0, 1, 2$ and to take into account only ground cluster eigenstates. Eventually we come to basis of the effective Hubbard model: zero-hole state $|0\rangle$ (hole vacuum, electronic configuration $d^{10}p^6$), single-hole states $|\sigma\rangle$ and $|\bar{\sigma}\rangle$ (superpositions of the configurations $d^9p^6$ and $d^{10}p^5$) degenerate in the paramagnetic phase, and two-hole singlet state $|S\rangle$ (mix of the configurations $d^9p^8$, $d^9p^7$ and $d^{10}p^6$). Doping by holes increases occupation of two-hole cluster eigenstate $|S\rangle$ and decreases occupation of single-hole cluster eigenstates $|\sigma\rangle$ and $|\bar{\sigma}\rangle$.

Third step is the construction of the quasiparticle excitations which are transitions between multihole cluster eigenstates with the number of holes differs by one. These Fermi-type quasiparticle excitations are called Hubbard fermions. There are four quasiparticle excitations in the Hubbard model: excitations between zero-hole state $|0\rangle$ and single-hole states ($|\sigma\rangle$, $|\bar{\sigma}\rangle$) form upper Hubbard band (UHB) of electrons or the conductivity band (CB). Excitations between states $|\sigma\rangle$, $|\bar{\sigma}\rangle$ and two-hole states ($|S\rangle$) form lower Hubbard band (LHB) of electrons or the valence band (VB). Each excitation is described by the Hubbard operator $X^{pq} = |p\rangle \langle q|$. At the last step the total Hamiltonian is rewritten in the terms of Hubbard operators. To obtain dispersion of Hubbard fermions we use equation of motion for the matrix Green function $\hat{D}(f,g; t, t')$ with elements

$D_{mn}(f,g; t, t') = \left\langle \left\langle X^m_f(t) X^n_{g}(t') \right\rangle \right\rangle$, where $m, n$ are indexes of the quasiparticle excitations, each index is uniquely defined by initial and final states of excitation $m \equiv (p, q)$. Equation of motion is decoupled by applying the Mori-type projection technique to the matrix Green function $\hat{D}(f,g; t, t')$ [25]. The Dyson equation
Fig. 2  (Color online) (a)-(f) Reconstruction of the Hubbard fermions bands with hole doping at zero strain $\delta a/a_0 = 0\%$. Color of the each point of the dispersion curve indicates quasiparticle spectral weight at given $k$-point. Dashed line indicates the Fermi level

for matrix Green function $\hat{D}(\mathbf{k}; \omega)$ in the momentum space looks like [26]:

$$
\hat{D}(\mathbf{k}; \omega) = \left[ \omega \hat{E} - \hat{\Omega} - \hat{F}(\mathbf{k}) - \hat{\Sigma}(\mathbf{k}; \omega) \right]^{-1} \hat{F} \tag{1}
$$

Here $\hat{E}$ is the unit matrix, $\hat{\Omega}$ is diagonal matrix of local quasiparticle energies with matrix elements $\Omega(m) = \Omega(pq) = \varepsilon_p - \varepsilon_q$, where $\varepsilon_p$ is the energy of the cluster eigenstate $p$. $\hat{F}$ is diagonal matrix of the filling factors of the quasiparticles, its diagonal matrix elements are $F(m) = F(pq) = \langle X^{pp} \rangle = \langle X^{pp} \rangle$. Filling numbers of cluster eigenstates $\langle X^{pp} \rangle$ is determined self-consistently from the condition of local basis completeness $\sum_{n_k=0}^2 \sum_{p} X^{pp} = 1$ and the chemical potential equation $n = 1 + x = \sum_{n_k=0}^2 \sum_{p} n_k \langle X^{pp} \rangle$ (here $n = 1 + x$ is the hole concentration for La$_{2-x}$Sr$_x$CuO$_4$). $\hat{\Sigma}(\mathbf{k}; \omega)$ is the matrix of intercluster hoppings, its matrix elements
are defined in work [15]. ˆΣ(k; ω) is the self-energy matrix which contains spin-spin and kinematic correlation functions. In a static limit of the self-energy we obtain the generalized mean field approximation as has been described in [27]. Spin-spin correlation functions were taken from work [28]. Kinematic correlation functions are calculated self-consistently with filling numbers and chemical potential.

3 Doping dependence of the electronic structure in the system without strain

Wide valence band with homogeneous distribution of the spectral weight over all k-points with minimum at \( k = (0, 0) \) and maximum at \( k = (\pi, \pi) \) obtained in LDA calculations is described by dispersion of single electron within tight-binding (TB) model. In the system with strong Coulomb correlations single electron band is splitted into two Hubbard subbands, width of each subband is smaller than of the free electron band in TB model. Without interband hopping the spectral weight of electrons in these subbands is homogeneous at all k-points and twice smaller than of electron band in TB model. Interband hoppings mix two types of electrons (i) and (ii), VB (and CB) is formed by superposition of low-intensity parts which are connected at points \( k = (\pi/2, \pi/2) \) and at k-point in the direction \( k = (\pi, 0) - k = (\pi, \pi) \). The general structure of bands can be presented as result of hybridization of high-intensity single band of free electrons in antiferromagnetic lattice and shadow low-intensity band [30,31]. It is seen that band structures at \( x = 0 \) and at \( x = 0.03 \) are identical except for slight difference in quasiparticle energy at the points \( k = (0, 0) \) and \( k = (\pi, \pi) \). Note band structure of quasiparticle excitations with spin projection "up" (+1/2) and spin projection "down" (-1/2) coincides.

At small concentration of doped holes \( (x = 0.03) \) the Fermi contour (FC) is a small hole pocket centered around \( k = (\pi/2, \pi/2) \) (Fig. 3a). Spectral weight is inhomogeneously distributed over FC for all doping levels (Fig. 3a)-(f). Maximal spectral weight is in the nodal direction on the one side of hole pocket close to \( k = (\pi/2, \pi/2) \), on the opposite side of pocket spectral weight is suppressed. This is well seen on the angular profile of spectral weight distribution over high-intensity \( A^+ \) (Fig. 3a, black line) and low-intensity \( A^- \) (Fig. 3b, black line) sides of the hole pocket. The intensity of the quasiparticle excitations monotonically decreases when traversing from maximum to minimum of the spectral weight. Inhomogeneity of spectral weight distribution can be characterized by ratio \( \Delta A = A^-_{\text{min}}/A^+_{\text{max}} \). Parameter of inhomogeneity for the hole concentration \( x = 0.03 \) is equal to \( \Delta A (x = 0.03) = 0.381 \) (Fig. 3).

Increasing hole concentration shifts chemical potential deeper to VB, reconstructs band structure and redistributes spectral weight. VB is modified stronger than CB. In the CB doping results in the flat band formation at point \( k = (\pi, 0) \). VB transformation is associated with increase of quasiparticle energy at \( k = (\pi, \pi) \) (Fig. 3) which is consequence of spin-spin correlation function damping with doping. Formation of local en-
energy maximum in the direction \( k = (\pi, 0) \). Hole pocket becomes larger with doping \((\text{Fig. 3b}),\) spectral weight inhomogeneity increases \((\text{Fig. 4b}),\) red line\), parameter \( \Delta A(x = 0.1) = 0.215\). Reduced intensity of quasiparticle excitations at low-intensity FC may be a reason of its absence in the ARPES measured Fermi surfaces.

In fact arc can be high-intensity part of hole pocket. Wherein with doping absolute value of maximal spectral weight in the high-intensity FC becomes larger and absolute value of minimal spectral weight in the low-intensity FC becomes smaller \((\text{Fig. 4a,b})\).

When chemical potential at \( x_{c1} = 0.1601\) touches local maximum of dispersion surface at \( k\)-point in the directions \((\pi, 0) - (\pi, \pi)\) and \((0, \pi) - (\pi, \pi)\) first quantum phase transition \((\text{QPT})\) of the Lifshits type occurs. This QPT is accompanied by closing of hole pockets \((\text{Fig. 3b})\) and their transformation into two large contours, bigger one is hole contour, smaller one is electron type \((\text{Fig. 3b})\).

Spectral weight is very different in the hole and electron contours, parameter of inhomogeneity \( \Delta A(x = 0.2) = 0.177\). However intensity gradient along each contour individually begins to decrease with doping after first QPT \((\text{Fig. 4b,b, green and purple lines})\). It is seen from \( \text{Fig. 4b} \) that spectral weight of the low-intensity FC is almost angle and momentum independent at \( x = 0.2 \) and \( x = 0.25\). Small ratio \( \Delta A\) may be the reason why small sectors of the FC cannot be found in the ARPES \([32,33]\), while quantum oscillation experiments can determine the area of a closed contour \([34,35]\). Further doping leads to expansion of the hole contour and the reduction of electron contour. Second QPT occurs when chemical potential crosses local minimum of VB at point \( k = (\pi, \pi)\) at \( x_{c2} \approx 0.283\) \((\text{Fig. 4})\): electron contour disappears and only hole contour remains \((\text{Fig. 4})\). Thus Fermi surface of the overdoped system \( (x = 0.3)\) is slightly inhomogeneous hole contour around \( k = (\pi, \pi)\) \((\text{Fig. 4f})\). Similar transformations of the electronic structure was obtained within t-J-model in the work \([36]\) and the Hubbard model \([37,38]\). The critical values for the Lifshitz transition obtained in \([28]\) for t-J model are \( x_{c1} = 0.15 \) and \( x_{c2} = 0.24\). The inhomogeneous distribution of the spectral weight over dispersion surface has been obtained also in the Hubbard model \([37,38]\).

4 Strain dependence of the electronic structure

There are two main effects of lattice parameter increasing on band structure: (I) energy shift of the VB and CB; (II) their bandwidths decrease. Bands are shifted to lower energies \((\text{Fig. 5})\). This shift is not rigid, its value depends on wave vector \( k\). Transformation of the band structure with lattice parameter changing has the same character for entire range of hole concentrations under study \((\text{from 0.03 to 0.3})\).

Evolution of the Fermi contour with doping at different lattice parameters is qualitatively the same as at \( \Delta a/a_0 = 0\). But concentrations of doped holes at which two QPTs occur are slightly shifted to smaller values with lattice parameter increasing \((\text{Table 2})\). Chemical potential is in the maximum of density of states (DOS) at hole concentration \( x_{c1} \) of the first QPT. Therefore it is believed that \( T_c\) maximum is determined by the critical concentration \( x_{c1}\). The magnitude of DOS maximum \( N_{\text{max}}(\mu_{\text{c1}})\) increases with lattice parameter increasing \((\text{Fig. 6, Table 2})\). Moreover the larger lattice parameter the higher DOS at all energy regions. This fact results from that fixed number of states \((n_h = 1 + x)\) is distributed over smaller energy interval for the larger lattice parameter since bandwidth decreases with strain increasing \((\text{Fig. 5})\). Strain dependence of superexchange interaction \( J\) demonstrates behavior inverted to \( N_{\text{max}}(\mu_{\text{c1}})\): \( J\) noticeably increases with a de-
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| Compound                  | $T_c$ max, K | $\delta a/a_0$, % | $x_{c1}$ | $x_{c2}$ | $J$ (eV) | $N_{max}(\mu_c)$ | $JN_{max}(\mu_c)$ |
|--------------------------|--------------|------------------|----------|----------|----------|------------------|-------------------|
| La$_{2+x}$Sr$_x$CuO$_4$  | 40           | 0                | 0.1604   | 0.285    | 0.168    | 3.3296           | 0.5594            |
| Bi$_2$Sr$_2$CaCu$_2$O$_{8+x}$ | 82           | 1.5              | 0.1599   | 0.28    | 0.14     | 3.7355           | 0.5230            |
| HgBa$_2$Ca$_2$Cu$_4$O$_{8+x}$ | 135          | 2.5              | 0.1594   | 0.277    | 0.127    | 3.9886           | 0.5066            |
| HgBa$_2$CaCuO$_{4+x}$     | 97           | 3.1              | 0.1589   | 0.2735   | 0.112    | 4.3413           | 0.4862            |
| HgBa$_2$CuO$_{4+x}$       | –            | –                | 0.1589   | 0.2735   | 0.112    | 4.3413           | 0.4862            |
| HgBa$_2$CaCuO$_{6+x}$     | 97           | 3.1              | 0.1589   | 0.2735   | 0.112    | 4.3413           | 0.4862            |
| HgBa$_2$CuO$_{4+x}$       | –            | –                | 0.1589   | 0.2735   | 0.112    | 4.3413           | 0.4862            |
| HgBa$_2$CuO$_{4+x}$       | –            | –                | 0.1589   | 0.2735   | 0.112    | 4.3413           | 0.4862            |

Table 2: Concentrations of the first and second quantum phase transitions ($x_{c1}$ and $x_{c2}$), superexchange parameter ($J$), DOS maximum at chemical potential for concentration $x_{c1}$ ($N_{max}(\mu_c)$) and their product ($JN_{max}(\mu_c)$) at different values of the strain $\delta a/a_0$. First row shows HTSC compound with lattice parameter $a$ ($b$) corresponding to a given strain, experimental $T_c$ max of the related compound is in second row.

5 Conclusion

Evolution of electronic structure of CuO$_6$-octahedra layer with doping is obtained for different Cu-O distances $a$ ($b$). With hole doping Fermi contour is transformed from four small hole pockets with inhomogeneous spectral weight to large hole and electron contours and then only large hole contour with almost homogeneous spectral weight distribution remains. Inhomogeneity of the spectral weight on the opposite sides of the hole pockets relative to the boundary of the antiferromagnetic Brillouin zone increases with hole doping. Low spectral weight on the one side potentially can be reason of its
absence in the ARPES. Changes of the electronic structure with lattice parameter \( a (b) \) varying are quantitative but not qualitative. Band structure is shifted to smaller energies, width of the valence and conductivity bands shrinks, concentrations of the first and second QPT are shifted with strain increasing. We obtain strain dependence of the characteristics determining superconducting temperature \( T_c \) within the mean-field theory with magnetic mechanism of pairing, DOS and antiferromagnetic exchange constant \( J \). The singularity of the DOS at the chemical potential energy at concentration of doped holes corresponding to first QPT \( N_{\text{max}} (\mu_{\text{ct}}) \) demonstrates monotonic growth with lattice parameter \( a (b) \) increasing. Exchange constant \( J \) monotonically decreases with strain increasing as well as resulting effective exchange constant \( J N_{\text{max}} (\mu_{\text{ct}}) \) in the \( T_c \) equation. Strain dependences of both characteristics \( J \) and \( N_{\text{max}} (\mu_{\text{ct}}) \) are managed by one type of parameters, hopping integrals. Supercurrent interaction is directly determined by hopping integral and DOS depends on bandwidth which is also defined by hopping integrals. Growth of DOS and damping of \( J \) are qualitative effects of the lattice parameter \( a (b) \) increasing, in the general case behavior of the product \( J N_{\text{max}} (\mu_{\text{ct}}) \) depends on rate of change of each of the characteristics \( J \) and \( N_{\text{max}} (\mu_{\text{ct}}) \) with lattice parameter \( a (b) \) varying. For example slight increase in the growth rate of the function \( N_{\text{max}} (\mu_{\text{ct}}) \) of the lattice parameter \( a (b) \) in comparison with that shown in the Table 2 results in the nonmonotonic dependence of \( J N_{\text{max}} (\mu_{\text{ct}}) \) on lattice parameter. There is nonmonotonic dependence of experimental \( T_c \) max on the lattice parameter \( a (b) \) among all compounds of different cuprate families (Table 2 second row). Therefore one can expect that different material dependent parameters such as bilayer splitting, chemical and electronic inhomogeneity and others play important role in the formation of the electronic structure and DOS.

Finally we have discussed the effect of a variable lattice strain on the unconventional "Lifshitz transitions" appearing in the strongly correlated electronic structure of the CuO\(_2\) as a function of doping. "Lifshitz transitions" are recently becoming a hot topic in the models of high-temperature superconductivity since there is growing evidence for the emergence of the "superconducting domes" in different high-temperature superconductors tuning the chemical potential near Lifshitz transitions [45][46][47][48][49][50].

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