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# A three-dimensional tight-binding model for single-layer La-based cuprates

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## Introduction

In 1986, Bednorz and Müller discovered high- $T_c$  superconductivity in La-based cuprate compounds (e.g.  $\text{La}_{2-x}\text{Ba}_x\text{Sr}_x\text{CuO}_4$ ) [1]. These materials have a layered body-centered tetragonal structure (BCT) consisting of  $\text{CuO}_2$  planes separated by charge reservoir layers which may dope electrons or holes into the  $\text{CuO}_2$  layers rendering them conducting. Early, in order to understand the underlying mechanism of unconventional superconductivity, P. W. Anderson [2] proposed that essential physics of cuprates would be captured by a one-band 2D Hubbard-like model in which the kinetic part is described by the nearest neighbor and the next-nearest neighbor in-plane hopping amplitudes ( $t$  and  $t'$ ), in addition to the Hubbard on-site  $U$  repulsive interaction that favors electron localization. However, recent density functional theory (DFT) calculations [3] and experimental (ARPES) investigations [4] have evidenced the three-dimensional character of the electronic structure and the Fermi surface. Therefore, a 3D model accounting for the dispersion in the direction perpendicular to the  $\text{CuO}_2$  layers is needed, and the subject of this work [9].

## 3D eight-band tight-binding model

Our goal is to establish an effective tight-binding model for the  $\text{Cu}: 3d_{x^2-y^2}$  orbital that is expected to be at the heart of high- $T_c$  superconductivity. Since this orbital possesses very little dispersion on its own but only via oxygen ions we consider the O-sublattice in more detail. We hence start the construction of our model by considering the four inequivalent oxygen ions building octahedron surrounding a given copper atom: there are two in-plane oxygen ions  $\text{O}^{(X)}$  and  $\text{O}^{(Y)}$  along the  $x$  and  $y$  directions respectively and two apical oxygens  $\text{O}^{(a)}$  and  $\text{O}^{(b)}$ , located above and below each copper ion, respectively. The position of the copper site and the oxygen sites in a unit-cell  $i$  are given by  $\mathbf{R}_{\text{Cu}} = \mathbf{R}_i$ ,  $\mathbf{R}_{\text{O}^{(X)}} = \mathbf{R}_i + a\mathbf{e}_x/2$ ,  $\mathbf{R}_{\text{O}^{(Y)}} = \mathbf{R}_i + a\mathbf{e}_y/2$ ,  $\mathbf{R}_{\text{O}^{(a)}} = \mathbf{R}_i + r\mathbf{e}_z$  and  $\mathbf{R}_{\text{O}^{(b)}} = \mathbf{R}_i - r\mathbf{e}_z$  where  $r \equiv d_{\text{Cu-O}_{\text{ap}}}$ . According to arguments given in Ref. [5] we consider the eight orbitals:  $\text{Cu}:3d_{x^2-y^2}$ ,  $\text{Cu}:4s$ ,  $\text{O}^{(X)}:2p_x^{(X)}$ ,  $\text{O}^{(Y)}:2p_y^{(Y)}$ ,  $\text{O}^{(X)}:2p_y^{(X)}$ ,  $\text{O}^{(Y)}:2p_x^{(Y)}$ ,  $\text{O}^{(a)}:2p_z^{(a)}$ ,  $\text{O}^{(b)}:2p_z^{(b)}$ , in this order. In Fourier space, our eight-band tight-binding Hamiltonian may be expressed as:

$$\hat{H}_{\text{S band}} = \hat{H}_0 + \hat{T} + \hat{H}_d, \quad (1)$$

where  $\hat{H}_0$  stands for the on-site orbital energies and  $\hat{T}$  is the kinetic energy term.  $\hat{H}_0$  reads:

$$\hat{H}_0 = \sum_{\mathbf{k}, \sigma} \left[ -\Delta_{pd} \sum_{\kappa} \hat{n}_{\mathbf{k}, \sigma, \kappa}^p - \Delta_{zd} \sum_{\rho} \hat{n}_{\mathbf{k}, \sigma, \rho}^z + \Delta_{sd} \hat{n}_{\mathbf{k}, \sigma}^s \right]; \quad \hat{H}_d = \epsilon_d \sum_{\mathbf{k}, \sigma, \mu} \hat{\Psi}_{\mathbf{k}, \sigma, \mu}^\dagger \hat{\Psi}_{\mathbf{k}, \sigma, \mu}. \quad (2)$$

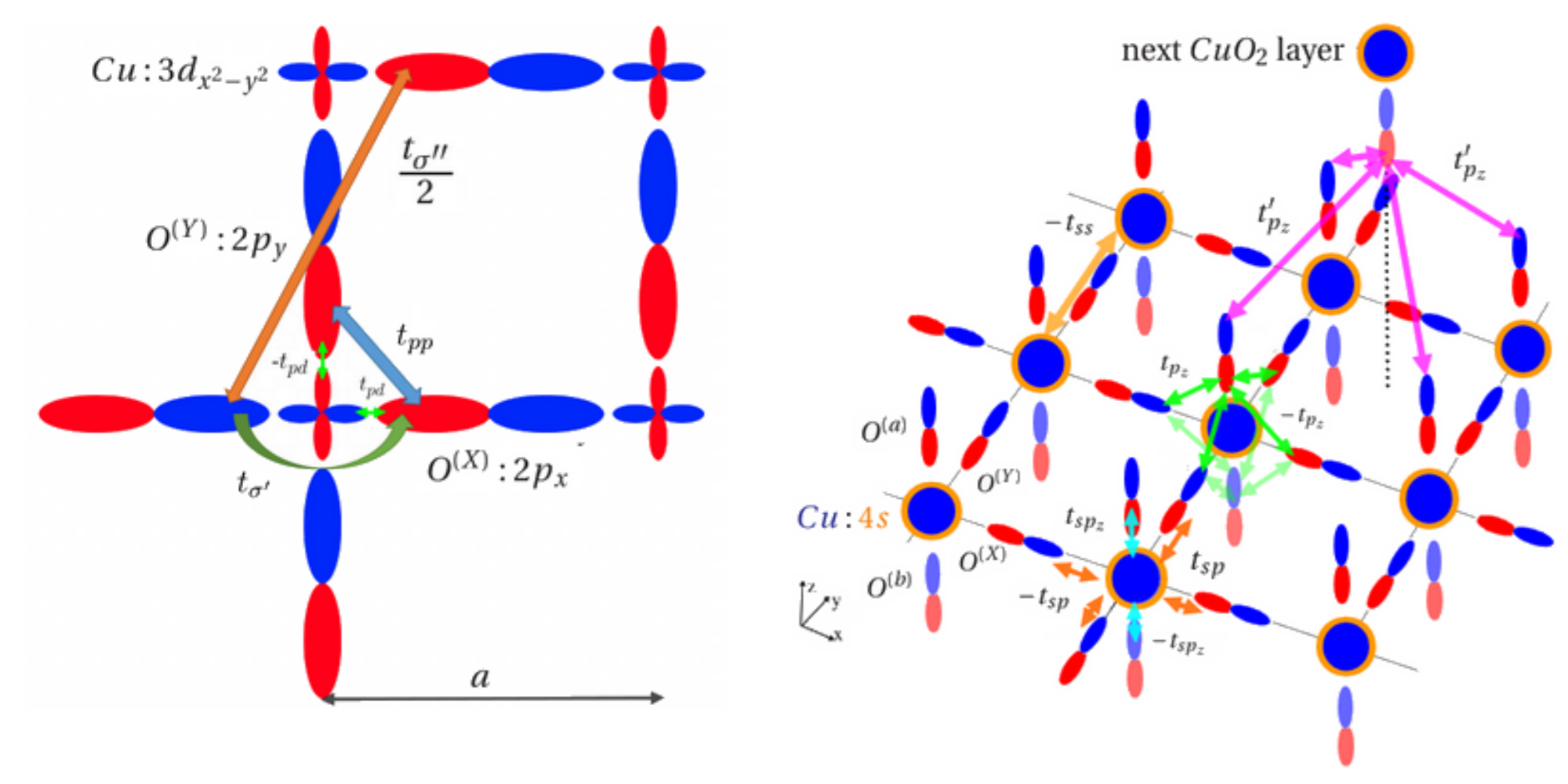
Here  $\Delta_{pd} = \epsilon_d - \epsilon_p$ ,  $\Delta_{zd} = \epsilon_d - \epsilon_z$ ,  $\Delta_{sd} = \epsilon_s - \epsilon_d$  where  $\epsilon_p$ ,  $\epsilon_d$ ,  $\epsilon_z$  and  $\epsilon_s$ , denote respectively the on-site energies of the  $2p_{x,y}^{(X,Y)}$ ,  $3d_{x^2-y^2}$ ,  $2p_z$  and  $\text{Cu}:4s$  orbitals. The various  $\hat{n}_{\mathbf{k}, \sigma, \mu}$  operators represent the occupation number operators of a given orbital with momentum  $\mathbf{k}$  and spin  $\sigma$ . Gathering all annihilation operators in the eight-component operator  $\hat{\Psi}_{\mathbf{k}, \sigma} = (\hat{d}_{\mathbf{k}, \sigma}, \hat{s}_{\mathbf{k}, \sigma}, \hat{p}_{x, \mathbf{k}, \sigma}^{(X)}, \hat{p}_{y, \mathbf{k}, \sigma}^{(Y)}, \hat{p}_{y, \mathbf{k}, \sigma}^{(X)}, \hat{p}_{x, \mathbf{k}, \sigma}^{(Y)}, \hat{p}_{z, \mathbf{k}, \sigma}^{(a)}, \hat{p}_{z, \mathbf{k}, \sigma}^{(b)})$  the kinetic energy may be written as:

$$\hat{T} = \sum_{\mathbf{k}, \sigma, \mu, \mu'} t_{\mathbf{k}}^{\mu, \mu'} \hat{\Psi}_{\mathbf{k}, \sigma, \mu}^\dagger \hat{\Psi}_{\mathbf{k}, \sigma, \mu'}. \quad (3)$$

Here  $t_{\mathbf{k}}^{\mu, \mu'}$  is the hopping integral in momentum space between the orbital  $\mu$  and the orbital  $\mu'$ . Altogether, we focus on the one-body Hamiltonian  $\hat{H} = \hat{H}_0 + \hat{T}$  expressed as:

$$\hat{H}(\mathbf{k}_{\parallel}, k_z) = \sum_{\mathbf{k}, \sigma, \mu, \mu'} \hat{\Psi}_{\mathbf{k}, \sigma, \mu}^\dagger H_{\mathbf{k}}^{\mu, \mu'} \hat{\Psi}_{\mathbf{k}, \sigma, \mu'}, \quad H_{\mathbf{k}} = \begin{pmatrix} A_{\mathbf{k}_{\parallel}} & B_{\mathbf{k}_{\parallel}} & C_{\mathbf{k}_{\parallel}} \\ B_{\mathbf{k}_{\parallel}} & D_{\mathbf{k}_{\parallel}} & E_{\mathbf{k}} \\ C_{\mathbf{k}_{\parallel}} & E_{\mathbf{k}} & F_{\mathbf{k}} \end{pmatrix} \quad (4)$$

$\mathbf{k}_{\parallel} = (k_x, k_y)$  is the in-plane momentum. The Hamiltonian is expressed in terms of the sub-matrices  $A_{\mathbf{k}_{\parallel}}$ ,  $D_{\mathbf{k}_{\parallel}}$  and  $F_{\mathbf{k}}$  entailing the tight-binding hamiltonians in the copper, in-plane oxygen, and out-of-plane oxygen orbital subspaces, respectively. The coupling between these subspaces is accounted for by the sub-matrices  $B_{\mathbf{k}_{\parallel}}$ ,  $C_{\mathbf{k}_{\parallel}}$  and  $E_{\mathbf{k}}$ . All off-diagonal matrix elements involve the hopping integrals which are defined and detailed in Ref. [9].



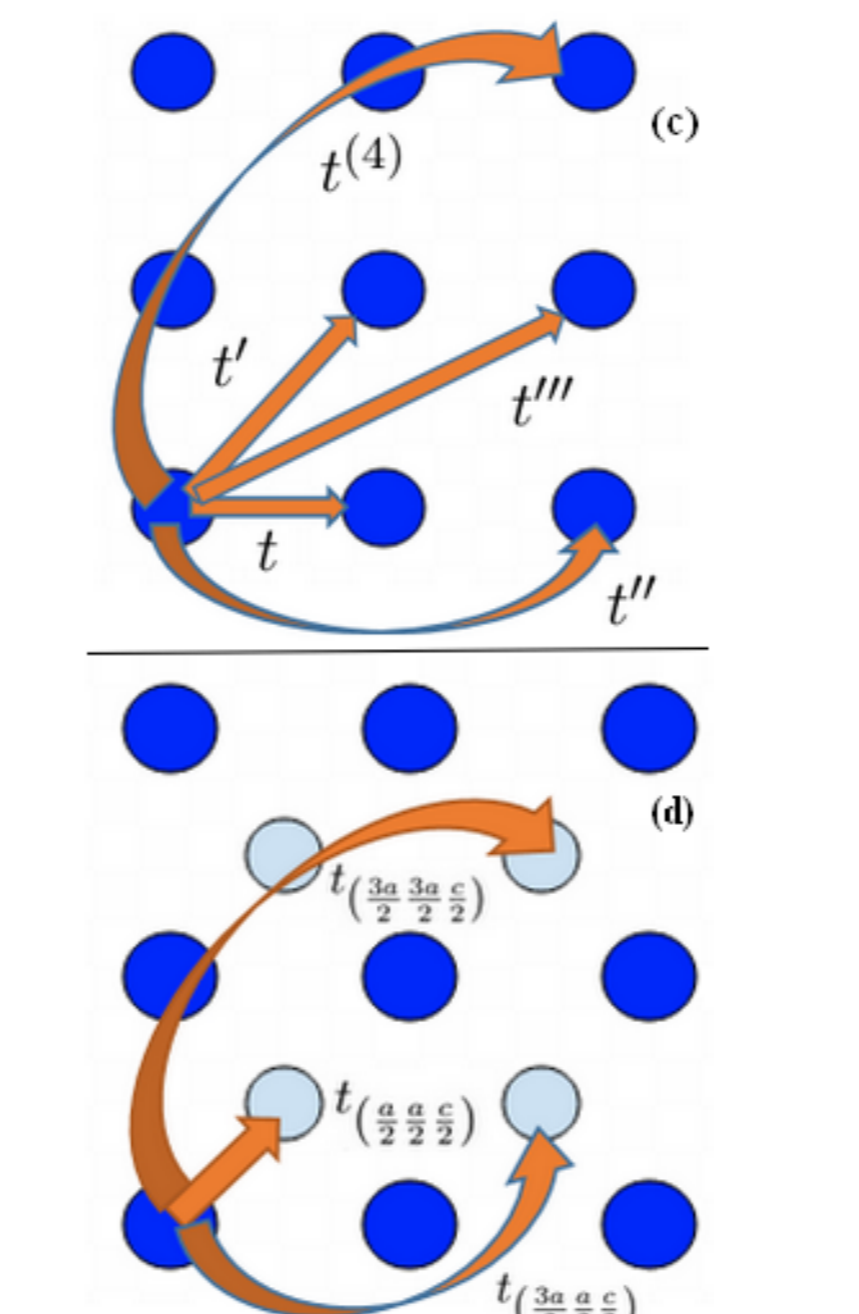
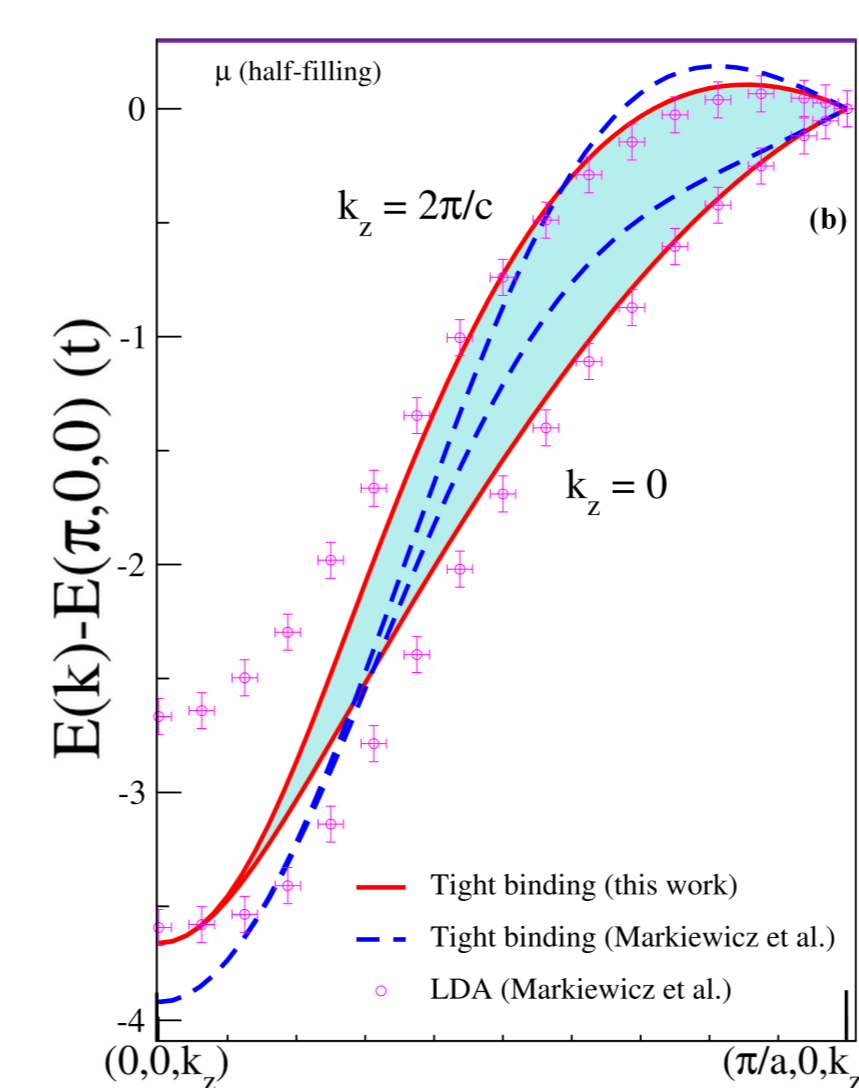
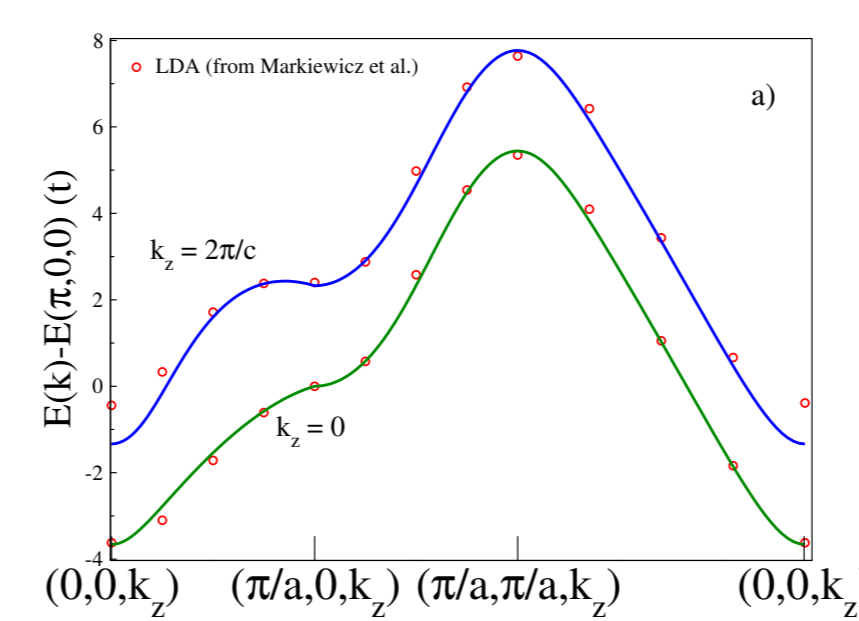
elements involve the hopping integrals which are defined and detailed in Ref. [9].

$$A_{\mathbf{k}_{\parallel}} = \begin{pmatrix} |3d_{x^2-y^2}\rangle & |4s\rangle \\ 0 & 0 \\ 0 & \tilde{\Delta}_{\mathbf{k}_{\parallel}} \end{pmatrix}, \quad B_{\mathbf{k}_{\parallel}} = \begin{pmatrix} |3d_{x^2-y^2}\rangle & |4s\rangle \\ -2it_{pd}p_x & -2it_{sp}p_x \\ 2it_{pd}p_y & -2it_{sp}p_y \\ 0 & 0 \\ 0 & 0 \end{pmatrix}, \quad C_{\mathbf{k}_{\parallel}} = \begin{pmatrix} |3d_{x^2-y^2}\rangle & |4s\rangle \\ 0 & t_{sp_z}e^{-irk_z} \\ 0 & -t_{sp_z}e^{irk_z} \end{pmatrix}$$

$$D_{\mathbf{k}_{\parallel}} = \begin{pmatrix} |p_x^{(X)}\rangle & |p_y^{(Y)}\rangle & |p_y^{(X)}\rangle & |p_x^{(Y)}\rangle \\ \tilde{\Delta}_{\mathbf{k}_{\parallel}} & -4t_{pp}p_xp_y & -2t_{\sigma''}p_{2x}p_{2y} & 4t_{pp}\pi_x\pi_y \\ -4t_{pp}p_xp_y & \tilde{\Delta}'_{\mathbf{k}_{\parallel}} & 4t_{pp}^{(2)}\pi_x\pi_y & -2t_{\sigma''}p_{2x}p_{2y} \\ -2t_{\sigma''}p_{2x}p_{2y} & 4t_{pp}^{(2)}\pi_x\pi_y & \tilde{\Delta}''_{\mathbf{k}_{\parallel}} & -4t_{pp}p_xp_y \\ 4t_{pp}^{(2)}\pi_x\pi_y & -2t_{\sigma''}p_{2x}p_{2y} & -4t_{pp}p_xp_y & \tilde{\Delta}_{\mathbf{k}_{\parallel}} \end{pmatrix}, \quad E_{\mathbf{k}} = \begin{pmatrix} |p_z^{(a)}\rangle & |p_z^{(b)}\rangle \\ 2it_{p_z}p_xe^{irk_z} & -2it_{p_z}p_xe^{-irk_z} \\ 2it_{p_z}p_ye^{irk_z} & -2it_{p_z}p_ye^{-irk_z} \\ -2it_{p_z}p_ye^{-ivk_z} & 2it_{p_z}p_ye^{ivk_z} \\ -2it_{p_z}p_xe^{-ivk_z} & 2it_{p_z}p_xe^{ivk_z} \end{pmatrix}$$

$$F_{\mathbf{k}} = \begin{pmatrix} |p_z^{(a)}\rangle & |p_z^{(b)}\rangle \\ -\Delta_{zd} & 4t_{p_z}^{(2)}\pi_x\pi_y e^{iuk_z} + g^* \\ 4t_{p_z}^{(2)}\pi_x\pi_y e^{-iuk_z} + g^* & -\Delta_{zd} \end{pmatrix}, \quad \text{where } \left\{ \begin{array}{l} \tilde{\Delta}_{\mathbf{k}_{\parallel}} = -\Delta_{pd} + 2(t_{\sigma'} \cos(k_x a) - t_{\sigma'} \cos(k_y a)) \\ \quad + 2t_{\sigma''} \cos(k_x a) \cos(k_y a) \\ \tilde{\Delta}'_{\mathbf{k}_{\parallel}} = -\Delta_{pd} + 2(t_{\sigma'} \cos(k_y a) - t_{\sigma'} \cos(k_x a)) \\ \quad + 2t_{\sigma''} \cos(k_x a) \cos(k_y a) \\ \tilde{\Delta}''_{\mathbf{k}_{\parallel}} = \Delta_{sd} - 2t_{ss}(\cos(k_x a) + \cos(k_y a)) \\ \quad - 4t_{ss}' \cos(k_x a) \cos(k_y a) \\ t_{pp} = (t_{\sigma} + t_{\pi})/2; \quad t_{pp}^{(2)} = (t_{\sigma} - t_{\pi})/2 \\ p_x = \sin(k_x a/2); \quad p_y = \sin(k_y a/2) \\ p_{2x} = \sin(k_x a); \quad p_{2y} = \sin(k_y a) \\ \pi_x = \cos(k_x a/2); \quad \pi_y = \cos(k_y a/2) \\ v \equiv d_{\text{O}_{\text{ap}}^{\text{next-layer}} - \text{O}_{\text{in-plane}}} ; \quad u \equiv d_{\text{O}_{\text{ap}}^{\text{next-layer}} - \text{O}_{\text{ap}}} \\ g = t_{p_z}^{(2)} e^{2irk_z}; \quad g^* = t_{p_z}^{(2)} e^{-2irk_z} \end{array} \right.$$

## Results



**Figure 1:** (a) & (b): solid lines account for the dispersion of the conduction band of our model. Below, illustration of copper atoms positions on a BCT lattice and various hopping processes. (c) In-plane hopping integrals between Cu atoms. (d) Inter-plane hopping integrals along the  $c$ -axis across the unit cells. The stacking of  $\text{CuO}_2$  layers is staggered by  $(a/2, a/2)$ .

The Hamiltonian of our model (Eq. 4) is numerically diagonalized in order to obtain the dispersion of the energy bands. We attempt to reproduce the dispersion of the band crossing the Fermi level and based on the  $\text{Cu}:3d_{x^2-y^2}$  orbital along the main symmetry lines of the Brillouin zone (the high-symmetry points are  $\Gamma(0,0,0)$ - $X(\pi/a,0,0)$ - $M(\pi/a,\pi/a,0)$ - $\Gamma(0,0,0)$ ), including the out-of-plane ones, as obtained by DFT calculations from Markiewicz *et al.* [3]. This comparison is shown in Fig. 1(a) & (b) where we have fixed a set of realistic optimal tight-binding parameters [9]. The dispersion of the conduction band of our model is in good agreement with LDA especially near the Fermi level. As experimentally observed [4], there is no  $k_z$ -dispersion along the high-symmetry line  $\Gamma$ - $M$  but only along the anti-nodal direction  $\Gamma$ - $X$ . Our tight-binding dispersion for  $k_z=0$  and  $k_z=2\pi/c$  is in better agreement with LDA than the phenomenological 3D one-band effective tight-binding dispersion proposed by Markiewicz *et al.* [3]. In order to simplify our multiband model, we also describe the conduction band by means of a one-band tight-binding effective dispersion, which, up to a constant ensuring  $E(0) = 0$ , reads:

$$E(\mathbf{k}_{\parallel}, k_z) = E_{\parallel}(k_x, k_y) + E_z(k_x, k_y, k_z) = \frac{1}{L} \sum_{i,j} t_{i,j} e^{i\mathbf{k} \cdot (\mathbf{R}_i - \mathbf{R}_j)} \quad (5)$$

where the 2D in-plane dispersion reads:

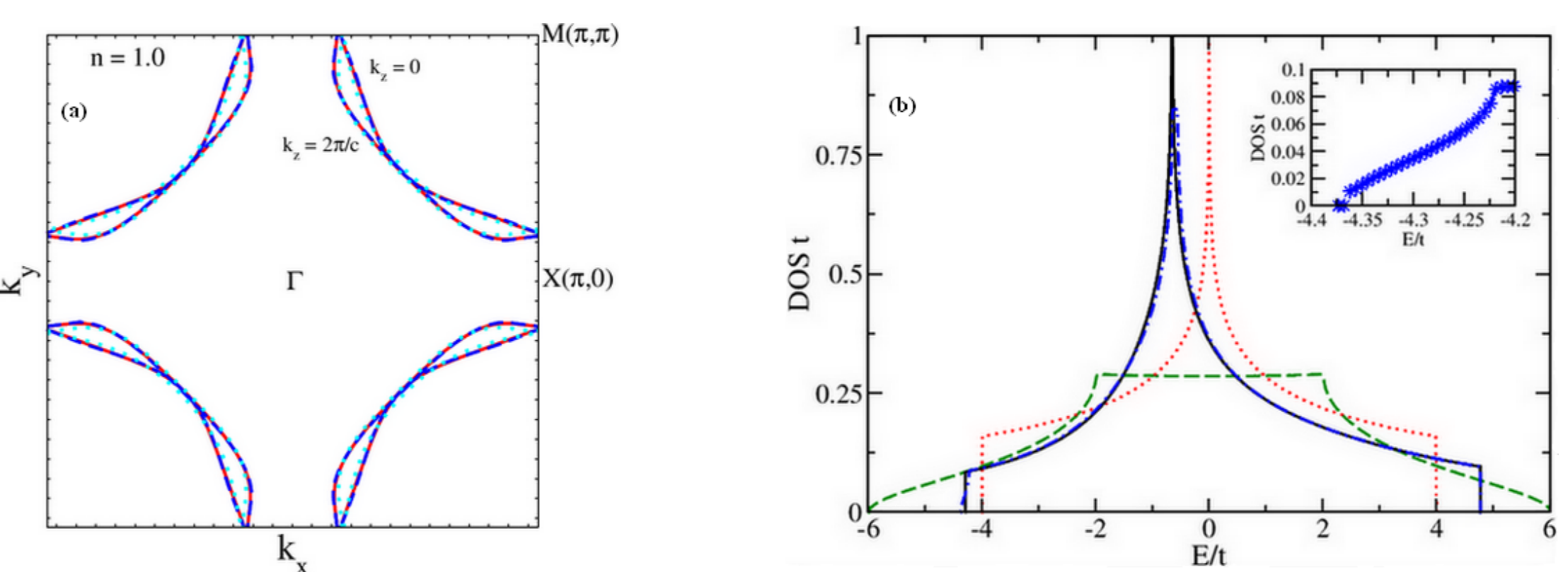
$$E_{\parallel}(k_x, k_y) = -2t [\cos(k_x a) + \cos(k_y a)] - 4t' \cos(k_x a) \cos(k_y a) - 2t'' [\cos(2k_x a) + \cos(2k_y a)] - 4t''' [\cos(2k_x a) \cos(k_y a) + \cos(2k_y a) \cos(k_x a)] \quad (6)$$

$t^{(n)} = t_{i,j}$  are the hopping integrals to the  $(n+1)^{\text{th}}$  nearest neighbors on the copper lattice as illustrated in Fig. 1(c). Furthermore, according to the BCT structure considered here, inter-plane hopping amplitudes between two  $\text{CuO}_2$  layers lead to the dispersion relation:

$$E_z(k_x, k_y, k_z) = -8t \left( \frac{a}{2}, \frac{a}{2}, \frac{c}{2} \right) \cos(k_x a/2) \cos(k_y a/2) c_z - 8t \left( \frac{3a}{2}, \frac{a}{2}, \frac{c}{2} \right) [\cos(3k_x a/2) \cos(k_y a/2) + \cos(3k_y a/2) \cos(k_x a/2)] c_z - 8t \left( \frac{3a}{2}, \frac{3a}{2}, \frac{c}{2} \right) \cos(3k_x a/2) \cos(3k_y a/2) c_z \quad (7)$$

where  $c_z = \cos(k_z c/2)$  and  $t \left( \frac{a}{2}, \frac{a}{2}, \frac{c}{2} \right)$ ,  $t \left( \frac{3a}{2}, \frac{a}{2}, \frac{c}{2} \right)$ ,  $t \left( \frac{3a}{2}, \frac{3a}{2}, \frac{c}{2} \right)$  are the inter-plane integrals between copper sites (Fig. 1(d)). Performing the Fourier transform of the numerically obtained conduction band yields a set of in-plane and out-of-plane effective hopping parameters that exactly characterize it (see the table below). These parameters differ from those reported in Ref. [3]. It is well accepted that  $t'/t \sim -0.1$  in case of La-based cuprates [5] and experimental ARPES investigations widely assume that  $-t''/t \sim 1/2$  in order to correctly fit the Fermi surface [7]. Furthermore, we have found that  $t'''/t$  is as robust as  $t''/t$  and  $t'''/t$  has already been invoked in order to fit ARPES or LDA results [3, 6]. While it is often neglected in theoretical studies as well as inter-plane hopping parameters, the density of states and the Fermi surface are shown here to be significantly modified (Fig. 2).

Hopping parameters	$t'/t$	$t''/t$	$t'''/t$	$t \left( \frac{a}{2}, \frac{a}{2}, \frac{c}{2} \right) / t$	$t \left( \frac{3a}{2}, \frac{a}{2}, \frac{c}{2} \right) / t$	$t \left( \frac{3a}{2}, \frac{3a}{2}, \frac{c}{2} \right) / t$
Markiewicz <i>et al.</i> (Ref. [3])	-0.09	0.07	0.08	0.015	-0.007	-0.015
This work	-0.136	0.068	0.061	0.028	-0.007	-0.022



**Figure 2:** (a) Comparison of the projected Fermi surface map of our model (red solid line) with those from one-band effective model using the parameters given in the table (cyan dotted line) and by adding - so far neglected - longer neglected others (blue dashed-dotted line). The fit is very good at half-filling ( $n=1$ ) as well as for lower densities. (b) Density of states (DOS) of our model (blue dashed-dotted line) compared to the one obtained for the 2D model (black solid line). The density of states for the dispersion including only the nearest-neighbor hopping  $t$  is also plotted for the 2D square (red dotted line) and the 3D cubic (green dashed line) lattice. The DOS of our 3D model exhibits a plateau surrounded by two Van Hove singularities in the vicinity of the middle of the band as similar to the cubic lattice. However, the plateau is far narrower, as a consequence of the anisotropy of the model. Clearly, the 3D case remains strikingly close to the 2D one. While the logarithmic singularity vanishes when going to 3D, striking similarities, such as jumps at the band edges, remain.

## Conclusions

A three-dimensional tight-binding model for La-based cuprate superconductors is presented [9]. Unfortunately attempts with simpler models lead us to consider an eight-band model. In-plane and inter-plane dispersions of the conduction band are reproduced as obtained by DFT calculations from Markiewicz *et al.* [3]. We have also provided an accurate one-band effective description. In particular, we obtain  $(|t'| + |t''|)/t \sim 0.2$  as reported for overdoped  $\text{La}_{1.78}\text{Sr}_{0.22}\text{CuO}_4$  [7, 8]. Finally, we have shown that the Fermi surface and the density of states are substantially modified by the dispersion perpendicular to the  $\text{CuO}_2$  layers. Such an observation should be taken into account for further theoretical studies.

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