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# OXYGEN–OXYGEN TRANSFER IN $CuO_2$ PLANES OF WEAKLY DOPED HIGH-$T_c$ SUPERCONDUCTORS

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**Abstract.** We investigated the formation of spin polarons (spin-polarized clusters) in weakly doped antiferromagnetically ordered $CuO_2$ planes of high-$T_c$ cuprates. The influence of additional holes within a self-consistent mean-field approximation was calculated taking oxygen–oxygen hybridization (characterized by the parameter $t$) into account. The binding energy and polarization of the clusters were found to strongly depend on the value and sign of $t$, i.e., a positive $t$ promotes the spin polaron formation, while a negative $t$ suppresses it. For the common value $t \sim 0.3$–$0.6$ eV we obtained two polaron states with binding energies $\sim 0.5$ eV and $\sim 0.3$ eV.

**Key words:** high-$T_c$ superconductivity, ferrons.

## 1. INTRODUCTION

There is a general agreement that $CuO_2$ planes are of great importance for determining the normal and superconducting properties of perovskite compounds like $La_2CuO_4$ and $YBa_2Cu_3O_6$, the parent materials for the high-$T_c$ cuprates. At zero doping these materials are antiferromagnetically (AF) ordered insulators. The $CuO_2$ plane has one hole per unit cell residing on Cu sites. The copper spins are ordered antiferromagnetically. The doping or oxidation leads to the destruction of the long-range AF order. Thus the system becomes conducting and below $T_c$ superconducting. Different theoretical works show that an additional hole in

cuprate perovskites perturbs the spin structure by forming a spin polaron (spin-polarized clusters) [1–3]. According to the model developed in [1], at higher doping concentrations the clusters begin to build up a microscopic percolation network and a phase transition from an AF insulator to a conducting state takes place. Many experiments also indicate the possible existence of such clusters [4–11].

In the theoretical model the formation of ferrons was studied within the three-band Hubbard model, taking account of strong on-site energy and Cu–O hybridization [1,12,13]. It was determined that the ground state of a $CuO_2$ layer with a single defect electron (hole) is formed by a spin polaron with 5–8 parallel copper spins. The small geometrical size of the cluster leads to a size-caused quantization of the levels and to finite excitation energies. The binding energy of such a magnetic polaron is of the order of 0.4–0.5 eV. In a natural way this explains the broad in-gap excitation band centred around 0.5 eV as observed in the middle infrared (MIR) optical spectra of weakly doped La and Y cuprates [14].

Besides the chemical doping or oxidation the holes can be created via optical excitation across the insulating gap 2 eV. Such transitions are known to correspond to the charge transfer from $O^{2-}$ $p$ orbitals to $Cu^{2+}$ $d_{x^2-y^2}$ orbitals. As the mobility of the extra electron in the $Cu^{2+}$ sublattice with AF ordered spins is expected to be much lower than that of a hole in the nonmagnetic $O^{2-}$ sublattice, the optically created electron and hole should be separated and, at least for some time, exist independently. Within this time the holes tend to become self-trapped, forming ferron states. Indeed, the experimental investigations [7,9] of the photoinduced absorption in the materials under consideration display the induced broadband absorption centred around 0.5 eV (MIR absorption) with the lifetime of 1 ms, which is attributed to the optical creation of localized ingap excitations. This absorption band is analogous to the band observed for low chemical doping [14]. As the photoinduced changes of the absorption coefficient in undoped materials resemble the absorption spectrum of doped high-$T_c$ systems, it is natural to assume that the localized states responsible for the photoinduced absorption are just the ferron hole states.

Another possibility to elucidate the origin of MIR absorption is the formation of a phonon polaron [9]. However, the phonon-polaron model has a difficulty with the explanation of the coexistence of free and self-trapped states as there is no energetical barrier between these two states in the case of quasi-two-dimensional charge carriers [15,16]. On the contrary, the spin-polaron (ferron) model clarifies the coexistence of free and self-trapped (polaron) hole states: in the quasi-two-dimensional case these states are separated by the energetical barrier of the order of $\sim 0.02$ eV [17]. The coexistence of free and self-trapped hole states was indeed observed in cuprate superconductors [18]. Besides, as mentioned in [7], it is difficult to explain the origin of distinct low-energy $E = 0.15$ eV electron transitions in the framework of the phonon-polaron model, while the spin-polaron model allows for such an explanation. In the present paper we continue the study of the spin polarons in $CuO_2$ planes in high-$T_c$ superconductors. It was shown in [19] that the

band structure of $CuO_2$ planes in such systems essentially depends also on direct oxygen–oxygen (O–O) hopping $t$. Besides, the O–O transfer plays an important role in hole transport which leads to the appearance of a barrier between free and self-trapped (spin-polaron) hole states [17]. The goal of this study is to establish how the binding energy and polarization of the forming clusters depends on $t$. We follow the Hartree–Fock approach of the three-band Hubbard model which neglects all fluctuations around the electronic mean-field (MF) values. For large values of the Hubbard repulsion, which are believed to be realized in the considered systems, these fluctuations are small. The incorporation of fluctuations within the scope of the slave-boson approximation shows that the MF approach yields reliable results [12].

## 2. HOLE DYNAMICS IN $CuO_2$ PLANES

Our considerations are based on the two-dimensional tight-binding Hubbard model. The model Hamiltonian for $CuO_2$ planes is written as

$$H = \sum_{\sigma} H_{0\sigma} + H_{\rm int}\,, \tag{1}$$

where

$$H_{0\sigma} = \epsilon_d \sum_{n} n^d_{n\sigma} + \epsilon_p \sum_{m} n^p_{m\sigma} + T \sum_{nm} \left( d^{\dagger}_{n\sigma} p_{m\sigma} + \text{H.c} \right)$$
$$+ t \sum_{mm\prime} \left( p^{\dagger}_{m\sigma} p_{m\prime\sigma} + \text{H.c} \right), \tag{2}$$

$$H_{\rm int} = U \sum_{n} n^d_{n\sigma} n^d_{n-\sigma}\,. \tag{3}$$

$n^d_{n\sigma}$ and $n^p_{m\sigma}$ are the electronic occupation numbers of the $d_{x^2-y^2}$ and $p_{x,y}$ orbitals, $d$ ($d^{\dagger}$) and $p$ ($p^{\dagger}$) are electronic annihilation (creation) operators on Cu and O orbitals, respectively. The spin index $\sigma$ indicates the spin direction ($\sigma = \uparrow, \downarrow$). $T$ is the transfer integral between oxygen and copper nearest neighbours, $t$ represents O–O interaction. $\epsilon_d$ and $\epsilon_p$ are on-site energies at copper and oxygen sites, respectively. The Hubbard energy $U$ describes the Coulomb repulsion between two electrons at the same copper site. Band structure calculations indicate the following parameter values: $U \approx 8$ eV, $T \approx 1$ eV, $\epsilon = \epsilon_p - \epsilon_d \approx 3$ eV [20,21]. The size of $t$ can be deduced from density-functional calculations that give $t \sim 0.3$–$0.6$ eV (in hole notation). However, some experimental results show that the choice $t < 0$ is possible [19]. Thus we assume $t$ to be a free parameter ranging from $-0.3$ to $0.6$ eV.

The first term in (1) is diagonal over spin directions, and the Hubbard term $H_{\rm int}$ is nondiagonal. Our calculations are based on the following MF approximation:

$$n^d_{m\sigma} n^d_{m-\sigma} = (n^d_{m\sigma} - \langle n^d_{m\sigma} \rangle)(n^d_{m-\sigma} - \langle n^d_{m-\sigma} \rangle) + \langle n^d_{m-\sigma} \rangle n^d_{m\sigma}$$
$$+ \langle n^d_{m\sigma} \rangle n^d_{m-\sigma} + \langle n^d_{m-\sigma} \rangle \langle n^d_{m\sigma} \rangle\,. \tag{4}$$

By that Hartree–Fock approximation of the original Hubbard Hamiltonian reads [12]

$$H = \sum_{\sigma} H^{\sigma}_{\mathrm{MF}} + H^{\mathrm{int}}_{\mathrm{MF}}\,, \tag{5}$$

where

$$H^{\sigma}_{\mathrm{MF}} = \sum_{n}(\epsilon_d + U\langle n^d_{n-\sigma}\rangle)n^d_{n\sigma} + \epsilon_p \sum_{m} n^p_{m\sigma} + T\sum_{nm}\left(d^{\dagger}_{n\sigma}p_{m\sigma} + \mathrm{H.c}\right)$$

$$+t\sum_{mm'}\left(p^{\dagger}_{m\sigma}p_{m'\sigma} + \mathrm{H.c}\right). \tag{6}$$

As the first term of $H$ in (5) is the sum over spin directions, the corresponding wave function is the product $\Phi = \Phi_{\uparrow}\Phi_{\downarrow}$. Therefore, averaging the terms from the right-hand side of (4), not included in $H^{\sigma}_{\mathrm{MF}}$, we get

$$H^{\mathrm{int}}_{\mathrm{MF}} = -U\sum_{m}\langle n^d_{m\sigma}\rangle\langle n^d_{m-\sigma}\rangle\,. \tag{7}$$

Hamiltonian (5) is nonlinear in the wave functions. Therefore, in principle, it can describe different spin-density distributions for the same set of parameters. Because of the symmetry of the Hamiltonian with respect to the spin direction, one possible solution that should always exist is $\langle n^d_{m\uparrow}\rangle = \langle n^d_{m\downarrow}\rangle$, i.e., nonmagnetic solution. However, such state is unstable against spin-density fluctuations.

As we want to describe a hole in the AF ordered $CuO_2$ plane, we double the elementary cell (the magnetic unit cell contains two $CuO_2$ units). Owing to the renormalization, the copper on-site energies are now given by

$$\begin{aligned}\epsilon_{1\sigma} &= \epsilon_d + U\langle n^d_{1-\sigma}\rangle\,,\\ \epsilon_{2\sigma} &= \epsilon_d + U\langle n^d_{2-\sigma}\rangle.\end{aligned} \tag{8}$$

From the symmetry of the AF state one immediately obtains the following relations:

$$\begin{aligned}\langle n_{1\uparrow}\rangle &= \langle n_{2\downarrow}\rangle\,,\\ \langle n_{1\downarrow}\rangle &= \langle n_{2\uparrow}\rangle.\end{aligned} \tag{9}$$

Therefore we can use the notations $\langle n_{\uparrow}\rangle$ and $\langle n_{\downarrow}\rangle$ and consider these quantities as modulated with twice the lattice period. Two Cu sublattices with $\sigma = \uparrow$ and $\sigma = \downarrow$ are independent, only the condition (9) must be fulfilled.

Let us consider the Hamiltonian $H^{\sigma}_{\mathrm{MF}}$ for the fixed spin direction, say $\sigma = \uparrow$. In $k$-space it reads

$$\langle k\uparrow |H^{\uparrow}_{\mathrm{MF}}| k\uparrow\rangle = \begin{pmatrix} \epsilon_1 & -2Ta_x & 2Ta_y & 0 & 2Ta_x^* & -2Ta_y^* \\ -2Ta_x^* & \epsilon_p & 2tc & 2Ta_x & 0 & -2tb \\ 2Ta_y^* & 2tc & \epsilon_p & -2Ta_y & -2tb & 0 \\ 0 & 2Ta_x^* & -2Ta_y^* & \epsilon_2 & -2Ta_x & 2Ta_y \\ 2Ta_x & 0 & -2tb & -2Ta_x^* & \epsilon_p & 2tc \\ -2Ta_y & -2tb & 0 & 2Ta_y^* & 2tc & \epsilon_p \end{pmatrix}, \tag{10}$$

where

$$a_{x,y} = \frac{1}{2} e^{ik_{x,y}(a/2)}, \tag{11}$$

$$b = \cos[(k_x + k_y)(a/2)], \tag{12}$$

$$c = \cos[(k_x - k_y)(a/2)], \tag{13}$$

and $a$ is the lattice constant. $H_{kk}$ describes six bands. In the undoped case the lowest five bands are occupied with electrons. The density of states in these bands is determined by the imaginary part of local Green's function according to

$$\mathrm{ImG}^{0\sigma}_{ij} = \pi \sum_k \delta(E - E(k))\, \phi_i(k)\, \phi_j(k), \tag{14}$$

where $E(k)$ and $\phi(k)$ are eigenvalues and eigenvectors of (10) at the point $k$ of the Brillouin zone. $E(k)$ and $\phi(k)$ were calculated by the numeric diagonalization of the Hamiltonian matrix (10). Lower indices of the unperturbed Green's function $\mathrm{G}^{0\sigma}$ denote the lattice sites. The real part of Green's function can be found from the integral equation

$$\mathrm{ReG}^{0\sigma}_{ij}(E) = \mathrm{P}\frac{1}{\pi} \int_{-\infty}^{\infty} \frac{\mathrm{ImG}^{0\sigma}_{ij}(E')}{E' - E} dE', \tag{15}$$

where P is the principle value of the integral. The expectation values of polarization can be obtained from self-consistent equations

$$\langle n^d_\sigma \rangle = \frac{1}{\pi} \int_{-\infty}^{E_F} dE\, \mathrm{ImG}^{0\sigma}(E), \tag{16}$$

where the integration is extended to the filled levels.

Under doping there is a possibility that the ideal AF order remains unchanged after taking away the electron from the top of the fifth band. However, due to the nonlinear nature of the MF equations other scenarios have to be considered as well. For example, one should also consider the possibility of a spontaneous symmetry breaking that leads to the creation of a localized hole. In [12,13] it was found that in the case $t = 0$ (i.e., without taking account of the O–O transfer) the last scenario leads to lower ground state energy. We want to verify this conclusion in the case of the presence of O–O hybridization for $-0.3\ \mathrm{eV} \leq t \leq 0.6\ \mathrm{eV}$.

In the following we assume that the copper spin at the site $m = 0$ can spontaneously fluctuate, changing the spin values from $\langle n_\sigma^d \rangle$ to $\langle n_\sigma^{d\prime} \rangle$. Owing to the nonlinearity of the problem these last values have to be determined self-consistently. To find $\langle n_\sigma^{d\prime} \rangle$, we have to calculate perturbed Green's functions. For this purpose we use the Dyson equation:

$$\mathrm{G}^\sigma = \mathrm{G}^{0\sigma} + \mathrm{G}^{0\sigma}\mathrm{V}\mathrm{G}^{0\sigma}. \tag{17}$$

We assume that perturbation is localized at the site $m = 0$, so

$$\mathrm{V}_{ij} = U(\langle n_{-\sigma}^{d\prime} \rangle - \langle n_{-\sigma}^{d} \rangle)\delta_{i0}\delta_{j0}. \tag{18}$$

The perturbed Green's function can be calculated directly from the Dyson equation

$$\mathrm{G}_{00}^\sigma = \frac{\mathrm{G}^{0\sigma}}{1 - \mathrm{G}_{00}^{0\sigma} U(\langle n_{-\sigma}^{d\prime} \rangle - \langle n_{-\sigma}^{d} \rangle)}. \tag{19}$$

The equations determining spin distribution then read as follows:

$$\langle n_\sigma^{d\prime} \rangle = \frac{1}{\pi} \int_{-\infty}^{E_F} dE \, \mathrm{Im}\mathrm{G}_{00}^{0\sigma}(\langle n_{-\sigma}^{d\prime} \rangle, E). \tag{20}$$

The energies of the localized states are given by solutions of equations

$$1 - \mathrm{G}_{00}^{0\sigma} U(\langle n_{-\sigma}^{d\prime} \rangle - \langle n_{-\sigma}^{d} \rangle) = 0, \; \sigma = \uparrow, \downarrow . \tag{21}$$

Now we have to compare the energies of the AF and the locally perturbed states. The total energy change $\Delta E$, due to the local perturbation (18) of Hamiltonian (5), consists of two parts [12,13]:

$$\Delta E = \Delta E^{\mathrm{loc}} + \Delta E^{\mathrm{int}}. \tag{22}$$

Here

$$\Delta E^{\mathrm{loc}} = \sum_\sigma \int_{-\infty}^{E_F} dE \, E \, \Delta N_\sigma(E) \tag{23}$$

accounts for the change of one-electron energy, $\Delta N_\sigma(E)$ is the change in the density of states. We have to consider two contributions to $\Delta N_\sigma(E)$. The first is the change of the density of states in the bands, the second is the appearance of singularities in $\Delta N_\sigma(E)$ outside the bands due to the formation of localized levels, so

$$\begin{aligned} \Delta E^{\mathrm{loc}} &= \frac{1}{\pi} \sum_\sigma \int_{-\infty}^{E_F} E \frac{d}{dE} \mathrm{Im}[\ln \det(1 - \mathrm{G}^{0\sigma}\mathrm{V}^\sigma)] dE \\ &= \sum_i E_i^L - \frac{1}{\pi} \sum_\sigma \int_{-\infty}^{E_F} \arctan \frac{\mathrm{V}_{00} \, \mathrm{Im}\mathrm{G}_{00}^\sigma}{1 - \mathrm{V}_{00} \, \mathrm{Re}\mathrm{G}_{00}^\sigma} dE, \end{aligned} \tag{24}$$

where $E_i^L$ denotes the energies of the occupied localized states measured from band edges. The change of magnetic energy resulting from the perturbation (7) reads as

$$\Delta E^{\text{int}} = U(\langle n_\uparrow^d \rangle \langle n_\downarrow^d \rangle - \langle n_\uparrow^{d\prime} \rangle \langle n_\downarrow^{d\prime} \rangle). \tag{25}$$

Although the perturbation is localized at one site only, the spin densities on other Cu sites are changed as well. The contribution to V of also the four next neighbours in the case $t = 0$ was considered in [13]; it was found that the correction of the spin-polaron energy is rather small and the assumption (18) gives a reasonably good description of the spin polaron.

## 3. RESULTS

There are three different ways for the O–O transfer parameter $t$ to change from $-0.3$ eV to 0.6 eV.

(i) Figure 1 shows the one-particle spectrum of a spin-down polarized cluster for $-0.1 \text{ eV} \leq t < 0.1 \text{ eV}$. Only the two lowest bands are plotted. Two localized states appear in the charge-transfer gap. One of them belongs to the spin-down spectrum and splits from the lower band edge of the first oxygen band, whereas the other stems from the lower Hubbard band and belongs to the spin-up spectrum. There is one additional level appearing about $10^{-2}$ eV below the lower Hubbard band. This scenario was already obtained for $t = 0$ in [12,13]. We have shown that the same scenario takes place when $t$ lies in the range $-0.1 \text{ eV} \leq t < 0.1 \text{ eV}$.

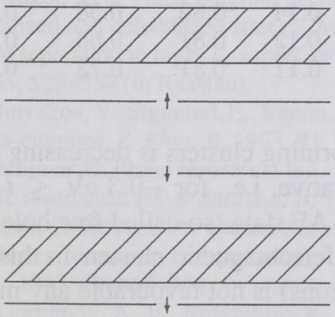


Fig. 1. The band scheme for the additional hole in the case of one turned spin which originally had mainly the spin-up direction. LHB, lower Hubbard band; LBO, lower oxygen band.

(ii) For $0.1 \text{ eV} \leq t \leq 0.6$ eV the MF Hamiltonian for a doped system has two solutions with local fluctuations of Cu spins. Both clusters have a lower energy than the ordered AF system. One-particle spectra of these ferron states are similar to the spectrum shown in Fig. 1. The ferron state with the highest binding energy is the ground state of the system.

The calculation of binding energy and polarization of the clusters gives the results summarized in the table. As one can see, the copper spin at the site $m = 0$ for the ground polaron state is nearly totally turned. This means that the cluster of five mainly parallel copper spins is formed (see Fig. 2). The perturbation of the AF order in the case of an excited polaron is small.

**The Cu-spin polarization for the unperturbed antiferromagnetic $\langle n_{\uparrow}^{d} \rangle$, $\langle n_{\downarrow}^{d} \rangle$ and two cases of perturbed $\langle n_{\uparrow}^{d\prime} \rangle$, $\langle n_{\downarrow}^{d\prime} \rangle$ and $\langle n_{\uparrow}^{d\prime\prime} \rangle$, $\langle n_{\downarrow}^{d\prime\prime} \rangle$, and the binding energy of two perturbed states $-\Delta E'/T$ and $-\Delta E''/T$ in dependence of the O–O transfer parameter $t/T$, given for a Hubbard repulsion $U/T = 8$ and for the values of $\epsilon/T = 3$ and 5. All values are presented in hole notation**

| $t$ | $U$ | $\epsilon$ | $\langle n_{\uparrow}^{d} \rangle$ | $\langle n_{\downarrow}^{d} \rangle$ | $\langle n_{\uparrow}^{d\prime} \rangle$ | $\langle n_{\downarrow}^{d\prime} \rangle$ | $-\Delta E'$ | $\langle n_{\uparrow}^{d\prime\prime} \rangle$ | $\langle n_{\downarrow}^{d\prime\prime} \rangle$ | $-\Delta E''$ |
|---|---|---|---|---|---|---|---|---|---|---|
| −0.1 | 8 | 3 | 0.80 | $4E-3$ | 0.19 | 0.70 | 0.05 | – | – | – |
| 0.0 | 8 | 3 | 0.79 | $4E-3$ | 0.16 | 0.71 | 0.18 | – | – | – |
| 0.1 | 8 | 3 | 0.77 | $6E-3$ | 0.14 | 0.71 | 0.23 | 0.69 | 0.11 | 0.12 |
| 0.2 | 8 | 3 | 0.75 | $7E-3$ | 0.13 | 0.70 | 0.30 | 0.63 | 0.14 | 0.19 |
| 0.3 | 8 | 3 | 0.72 | $8E-3$ | 0.12 | 0.69 | 0.36 | 0.59 | 0.16 | 0.28 |
| 0.4 | 8 | 3 | 0.70 | $10E-3$ | 0.11 | 0.68 | 0.42 | 0.54 | 0.17 | 0.36 |
| 0.5 | 8 | 3 | 0.67 | $12E-3$ | 0.10 | 0.67 | 0.48 | 0.50 | 0.17 | 0.44 |
| 0.6 | 8 | 3 | 0.64 | $14E-3$ | 0.10 | 0.65 | 0.54 | 0.45 | 0.18 | 0.52 |
| −0.1 | 8 | 5 | 0.89 | $2E-3$ | 0.24 | 0.82 | 0.16 | – | – | – |
| 0.0 | 8 | 5 | 0.88 | $2E-3$ | 0.21 | 0.82 | 0.31 | – | – | – |
| 0.1 | 8 | 5 | 0.88 | $2E-3$ | 0.18 | 0.83 | 0.37 | 0.84 | 0.10 | 0.07 |
| 0.2 | 8 | 5 | 0.87 | $3E-3$ | 0.17 | 0.83 | 0.44 | 0.82 | 0.12 | 0.11 |
| 0.3 | 8 | 5 | 0.86 | $3E-3$ | 0.14 | 0.83 | 0.51 | 0.80 | 0.13 | 0.16 |
| 0.4 | 8 | 5 | 0.85 | $4E-3$ | 0.14 | 0.82 | 0.58 | 0.78 | 0.14 | 0.22 |
| 0.5 | 8 | 5 | 0.83 | $4E-3$ | 0.12 | 0.81 | 0.66 | 0.77 | 0.13 | 0.28 |
| 0.6 | 8 | 5 | 0.82 | $5E-3$ | 0.11 | 0.81 | 0.73 | 0.75 | 0.12 | 0.34 |

(iii) The binding energy of forming clusters is decreasing with the decrease of $t$. For $t < -0.1$ it becomes negative, i.e., for $-0.3$ eV $\leq t < -0.1$ eV we get the lowest energy for the ordered AF state (so-called free hole in the AF lattice) as compared with the energy of the ferromagnetic cluster. In this case the creation of the clusters (small magnetic polarons) is not favourable any more.

In conclusion, by solving the self-consistency equations we obtained a renormalized band structure which is expected to describe the behaviour of an extra hole added to the ground state of the AF ordered $CuO_2$ plane. We found that the resulting band structure strongly depends on the O–O transfer parameter $t$. Our calculations showed that doping leads to the creation of ferromagnetic clusters (ferrons), whose polarization and binding energy rise with the increase of the O–O parameter $t$. In the hole-doped case the formation of small ferromagnetic hole clusters appeared to be favoured energetically for $-0.1$ eV $\leq t \leq 0.6$ eV. Note that for the common values of $t$ (0.3 eV $\leq t \leq$ 0.6 eV) two polaron states are formed.

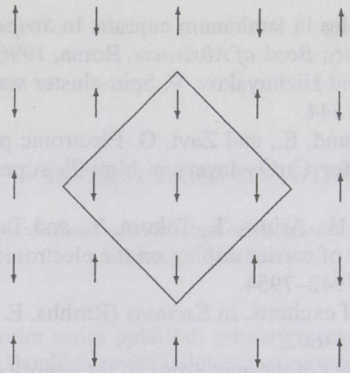

Fig. 2. The configuration of spins around an access hole. The arrows show the main direction of the copper spins.

The binding energy of the lower (ground) state of the polaron is 0.4–0.7 eV. The difference in the energy of the lower and higher polaron states is 0.1–0.3 eV. This may possibly account for $E = 0.55$ eV and $E = 0.15$ eV electron transitions which are measured in nearly all superconductors [7].

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## O–O ÜLEKANNE NÕRGALT DOPEERITUD KÕRGTEMPERATUURSETE ÜLIJUHTIDE $CuO_2$ TASANDITES

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On uuritud spinnpolaronide (spinnpolariseeritud klastrite) formeerumist kõrgtemperatuursete kupraatide nõrgalt dopeeritud antiferromagnetiliselt korrastatud $CuO_2$ tasandites. On arvutatud lisaaukude mõju enesekooskõlalise keskmise välja lähenduses, võttes arvesse O–O hübridisatsiooni, mida iseloomustab parameeter $t$. On näidatud, et klastrite seoseenergia ja polarisatsioon sõltuvad tugevasti $t$ väärtusest ja märgist, s. t. positiivne $t$ soodustab, negatiivne aga takistab spinnpolaroni formeerumist. Hariliku väärtuse $t \sim 0{,}3$–$0{,}6$ eV tarvis on saadud kaks polaronseisundit seoseenergiaga $\sim 0,5$ eV ja $\sim 0,3$ eV.