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CHARGE CARRIERS STATES IN A MODEL OF CuO SUPERCONDUCTIVE CERAMICS

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ABSTRACT

The translational symmetry of the distribution of atoms (ions) of the charge carriers (electrons or holes) system is broken by sputtering (doping) due to the existence of two boundary surfaces. This is a model of high-temperature superconductors in which the observed symmetry breaking orthogonal to the CuO plane is treated as a perturbation. Single-particle fermion wave functions and possible charge carrier energies were determined. The competing existence of superconducting and normal regions in such a sample is shown in agreement with experimental data. The conditions for the formation of superconducting states and the limits of the current density values in the planes parallel to the boundary surfaces (in the CuO planes) were obtained and discussed.

Keywords: ceramic oxides, charge carriers, dispersion law, energy states

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1. INTRODUCTION

High-temperature superconducting ceramics have "broken" the myth of an exclusively low-temperature effect of superconductivity [1–4]. Although they were discovered and improved at the end of the last century, the mechanism of superconductivity has not been figured out to date. The biggest difficulty is their highly anisotropic structure (Figure 1).

The answer to the question of the oxide ceramics superconductivity mechanism must be undoubtedly sought in the phonon subsystem, in the elementary charges subsystem as well as in the interaction of these subsystems. Concerning the very anisotropic structure of the superconductive ceramics [1,2], we have attempted to construct a theoretical model conveying the broken translational symmetry of atoms (molecules) arrangement along one direction in the crystal lattice, the difference in masses of these molecules, and the presence of two boundary planes along this direction [5,6].

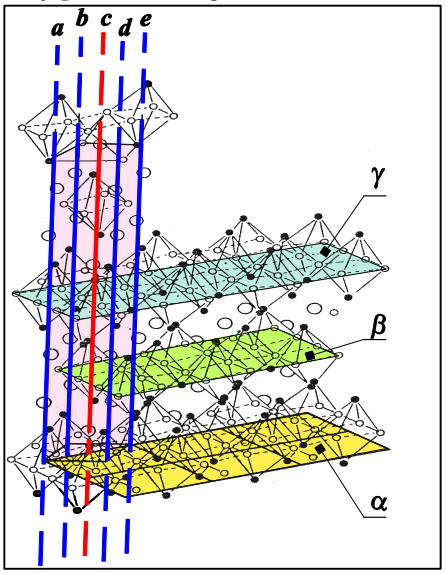

Figure 1. Model of high-temperature superconductors – CuO ceramics

The phonon system is drawn out in this model [6]. We have determined the phonon states and their energy spectra and have shown that, due to the broken crystal symmetry (actually because of deformed and tiny granular structure), the phonons of optical type owning the energy gap are present here [7]. The next task we have attempted to solve is to determine and analyse the spectra of free charge carriers (electrons or holes), the Landau criterion, and the probabilities of states and entropy within the same model. The preliminary results are already presented [8,9].

2. MODEL HAMILTONIAN

To obtain the Hamiltonian of the charge carriers in the structure with broken translational symmetry, it is most suitable to start with the standard Hamiltonian of the electron system in an ideal infinite structure [10–12]:

$$H_{id} = \sum_{\vec{k}} \frac{\hbar^2\vec{k}^2}{2m^*}\, C_{\vec{k}}^{+} C_{\vec{k}}, \qquad (1)$$

where m^* is electron effective mass, while $C_{\vec{k}}^{+}$ and $C_{\vec{k}}$ are Fermi creation and annihilation operators of electrons with momentum $\hbar\vec{k}$ and energy $\hbar^2\vec{k}^2(2m^*)^{-1}$. If we go over to the configuration space using the transformations:

$$C_{\vec{k}} = \frac{1}{\sqrt{N}}\sum_{\vec{n}} C_{\vec{n}} \mathrm{e}^{-i\vec{k}\vec{n}}; \qquad C_{\vec{k}}^{+} = \frac{1}{\sqrt{N}}\sum_{\vec{n}} C_{\vec{n}}^{+} \mathrm{e}^{i\vec{k}\vec{n}}, \quad (2)$$

where N is the number of molecules in the considered structure, we get:

$$H_{id} = \sum_{\vec{n}} \Lambda C_{\vec{n}}^{+} C_{\vec{n}} - \sum_{\vec{n},\vec{m}} W_{\vec{n}\vec{m}} C_{\vec{n}}^{+} C_{\vec{m}}. \qquad (3)$$

Here $\Lambda = N^{-1}\sum_{\vec{k}} \frac{\hbar^2\vec{k}^2}{2m^*}$ and $W_{\vec{n}\vec{m}} = -N^{-1}\sum_{\vec{k}} \frac{\hbar^2\vec{k}^2}{2m^*}\, \mathrm{e}^{i\vec{k}(\vec{n}-\vec{m})}$. Due to the canonicity of the transformation (2), the operators $C_{\vec{n}}^{+}$ and $C_{\vec{n}}$ are also Fermi operators.

Let us recall the most important assumptions of our model: we consider the tetragonal i.e. generalized cubic structure with very high anisotropy along the z-axis. It means that the lattice constant in this direction (a_z) is a few times larger than the lattice constant a_x, a_y in the directions x and y. The translational symmetry is fully conserved in the XY planes, while the symmetry of the masses arrangement along the z direction is broken (during the doping of the ceramic structure by the introduction of foreign atoms, the sputtered atoms located along this direction because it is energetically most convenient). We also assume here that the structure under consideration is a film (not necessarily thin!). It means that the components of lattice vector $\vec{n} \equiv (n_x, n_y, n_z)$ vary in the following way:

$$n_r \in \left(-\frac{N_r}{2}, +\frac{N_r}{2}\right), \; r = (x,y); \;\; n_z \in [0, N_z] \qquad (4)$$

The numbers of atoms N_x and N_y along the directions x and y, respectively, may be indefinitely high since we have the translational symmetry along these directions. The number of atoms along z direction (N_z) is limited. The above-described model, i.e. the highly anisotropic matrix along the z direction, necessarily doped with foreign atoms, can be used for getting some qualitative conclusions about the superconductive ceramics behaviour. It is known [1–3] that the ceramic oxides are anisotropic along one privileged direction and that the superconductive state is realised by doping. But the real structure of the ceramic oxides–perovskites is approximated by the tetragonal structure. It is also assumed in the model that the sputtering is symmetric on both boundary planes: $n_z = 0$ and $n_z = N_z$ and between the layers $n_z = 0$ and $n_z = 1$ (as well as between the layers $n_z = N_z - 1$ and $n_z = N_z$) n_0 foreign particles are placed, in such a way that the structure of the doped matrix is unchanged near the middle of the film.

If the behaviour of the quantities from (3) may be expressed by the law:

$$W_{\vec{n}\vec{m}} = \frac{W_0}{|\vec{n}-\vec{m}|^h}; \qquad W_0 > 0; \qquad h > 0, \qquad (5)$$

in the nearest neighbors approximation, we get:

$$W_{n_s;n_s\pm1} \equiv W_s = W_0\, a_s^{-h}; \qquad s = (x,y,z). \qquad (6)$$

According to the described view of the doping, it is obvious that lattice constant a_z in the doped structure becomes dependent on the position n_z, i.e. $a_z \longrightarrow a_z(n_z)$. Because of the symmetry on the boundaries: $a_z(0) = a_z(N_z) = a_z(n_0+1)^{-1}$; $a_z(N_z/2) = a_z$, we may take:

$$a_z(n_z) = a_z\left(1 - \frac{n_0}{n_0+1}\, N_z^2\right); \; N_z^2 = 2n_z N_z^{-1} - 1. \qquad (7)$$

The dependence of the lattice constant on the index n_z causes the dependence of the interaction along z direction on the index n_z, i.e.:

$$W_z \longrightarrow W_z(n_z) = W_0 a_z^{-h}(n_z) = W_0 a_z^{-h}\left(1 - N_z^2 \frac{n_0}{n_0+1}\right)^{-h} \approx W_z(1+\Phi N_z^2), \tag{8}$$

where $\Phi = hn_0(n_0+1)^{-1}$. The interactions W_x and W_y, according to the described picture, are unchanged. We must notice that the last two expressions are valid for even N_z. But, for large enough N_z ($N_z \approx N_z + 1$), or during the transition from n_z to continual variable z, the deviations from the formulas (7) and (8) for odd N_z are not essential. The values of Λ are not dependent on the index of the site, because of they are unchanged during the doping. Hence we can write the Hamiltonian of the doped structure in the form:

$$H = H_{\mathrm{B}} + H_{\mathrm{V}}, \tag{9}$$

where:

$$\begin{aligned} H_{\mathrm{B}} = \sum_{n_x,n_y} \Big\{ & C^+_{n_x n_y 0}\Big[\Lambda C_{n_x n_y 0} - W_x\left(C_{n_x+1,n_y 0} + C_{n_x-1,n_y 0}\right) - \\ & - W_y\left(C_{n_x n_y+1,0} + C_{n_x n_y-1,0}\right) - W_z(1-\Phi)C_{n_x n_y 1}\Big] + \\ & + C^+_{n_x n_y N_z}\Big[\Lambda C_{n_x n_y N_z} - W_x\left(C_{n_x+1,n_y N_z} + C_{n_x-1,n_y N_z}\right) - \\ & - W_y\left(C_{n_x n_y+1,N_z} + C_{n_x n_y-1,N_z}\right) - W_z(1-\Phi)C_{n_x n_y N_z-1}\Big]\Big\}, \end{aligned} \tag{10}$$

and, as we can see, it is related to the boundary layers ($n_z = 0$ and $n_z = N_z$), where $W_{n_x,n_y,0;n_x,n_y,-1} = W_{n_x,n_y,N_z;n_x,n_y,N_z+1} = 0$, and for H_{V} we find:

$$\begin{aligned} H_{\mathrm{V}} = \sum_{n_x,n_y} \sum_{n_z=0}^{N_z-1} \Big\{ & C^+_{n_x n_y 0}\Big[\Lambda C_{n_x n_y 0} - W_x\left(C_{n_x+1,n_y 0} + C_{n_x-1,n_y 0}\right) - \\ & - W_y\left(C_{n_x n_y+1,0} + C_{n_x n_y-1,0}\right) - W_z(1-\Phi)C_{n_x n_y 1}\Big] + \\ & + C^+_{n_x n_y N_z}\Big[\Lambda C_{n_x n_y N_z} - W_x\left(C_{n_x+1,n_y N_z} + C_{n_x-1,n_y N_z}\right) - \\ & - W_y\left(C_{n_x n_y+1,N_z} + C_{n_x n_y-1,N_z}\right) - W_z(1-\Phi)C_{n_x n_y N_z-1}\Big]\Big\}. \end{aligned} \tag{11}$$

3. SINGLE-PARTICLE STATES OF THE SYSTEM

We shall analyse the system described by Hamiltonian (9) using the orthonormalized single-electron state functions [12]:

$$|\Psi\rangle = \sum_{n_x,n_y,n_z} A_{n_x,n_y,n_z} C^+_{n_x,n_y,n_z}|0\rangle; \qquad \sum_{n_x,n_y,n_z} |A_{n_x,n_y,n_z}|^2 = 1. \tag{12}$$

We obtain the equations for finding the coefficient A_{n_x,n_y,n_z} using the equations of motion for operators C_{n_x,n_y,n_z}. From $C_{n_x,n_y,n_z}(t) = C_{n_x,n_y,n_z}(0)e^{i\omega t}$, $\omega = E/\hbar$, it follows:

$$E\, C_{n_x,n_y,n_z} - \left[C_{n_x,n_y,n_z}, H\right] \equiv O_{n_x,n_y,n_z}; \qquad O_{n_x,n_y,n_z} = O. \tag{13}$$

Based on equations (9 –11) and (13), we form operators $O_{n_x,n_y,0}$, O_{n_x,n_y,N_z} and O_{n_x,n_y,n_z}. After applying them to the functions (12) and using the substitution:

$$A_{n_x,n_y,n_z} = A_{n_z} e^{i(n_x a_x k_x + n_y a_y k_y)}, \tag{14}$$

where $k_j = \frac{2\pi}{N_j a_j}\nu_j$; $j = (x,y)$; $\nu_j \in \left(-\frac{N_j}{2}, +\frac{N_j}{2}\right)$ and based on the fact that $\Lambda = 2\sum_{xyz} W_j$, we find the following system of difference equations:

$$(E - 4Q - 2W_z)A_0 + W_z(1-\Phi)A_1 = 0, \qquad n_z = 0;$$

$$(E - 4Q - 2W_z)A_{N_z} + W_z(1-\Phi)A_{N_z-1} = 0, \qquad n_z = N_z; \tag{15}$$

$$(E - 4Q - 2W_z)A_{n_z} + W_z(1+\Phi N_z^2)\left(A_{n_z+1} + A_{n_z-1}\right) = 0, \quad 1 \le n_z \le N_z - 1, \tag{16}$$

where $Q \equiv Q_{k_x k_y} = W_x \sin^2\left(\frac{a_x k_x}{2}\right) + W_y \sin^2\left(\frac{a_y k_y}{2}\right)$. We shall perform further analysis in the continual approximation to avoid the complications arising during the determination of the coefficient A_n from the system of difference equations (15). Introduction of the continual variable z through $n_z \to z/a_z$ ($N_z \to L/a_z$) causes the following transformations of the expressions (7) and (8):

$$a_{z;n_z} \to a_z(z) = a_z\left[1 - \frac{n_o}{n_o+1}\left(2\frac{z}{L} - 1\right)^2\right], \quad W_{z;n_z} \to W_z(z) = W_z\left[1 + \Phi\left(2\frac{z}{L} - 1\right)^2\right]. \tag{17}$$

The coefficients A_{n_z} will be transformed in the following way:

$$A_n \to A(z)\ ; \qquad A_{n+1} + A_{n-1} \to A(z+\bar{a}_z) + A(z-\bar{a}_z), * 1.0mm$$

$$A(z \pm \bar{a}_z) \approx A(z) \pm \bar{a}_z \frac{dA}{dz} + \frac{\bar{a}_z^2}{2}\frac{d^2A}{dz^2}; \qquad \bar{a}_z \equiv \bar{a}_z(z) = \frac{1}{L}\int_0^L dz a_z(z) = a_z \frac{2n_o+3}{3(n_o+1)}.$$

The important consequence of the transition to the continuum is the fact that the first two equations from (15) vanish from the calculation at $n_z \to z$, i.e. they are merged into the last of equations from (15), which is the continual approximation has the form:

$$\frac{d^2A}{dz^2} + \frac{E-4Q-\Phi(E-4Q-2W_z)\left(2\frac{z}{L}-1\right)^2}{\bar{a}_z^2(z)\,W_z} A = 0. \qquad (18)$$

By the assumption:

$$E > 4Q + 2W_z \equiv E_z^{(0)} \qquad (19)$$

and by the substitution: $2z/L - 1 = \tau\zeta$, with $\tau^4 = W_z(\bar{a}_z L)^2\,[4\Phi\,(E-4Q-2W_z)]^{-1}$, the equation (17) becomes known Hermite-Weber equation:

$$\frac{d^2A}{d\zeta^2} + (\kappa - \zeta^2)A = 0, \qquad (20)$$

where $\kappa = \frac{L}{2\bar{a}_z}(E-4Q)\left[\Phi\,(E-E_z^{(0)})W_z\right]^{-1/2}$.

Here we introduce the requirement that the amplitudes A are finite for arbitrary structure thickness (it means even for $L \to \infty$ too). To satisfy this requirement we must take the known condition of the finiteness for the solutions for the Hermite-Weber equation: $\kappa = 2\mu + 1; \quad \mu = 0,1,2,\ldots$ Based on this we find:

$$E_{1,2} = 4Q + 2b^2(2\mu+1)^2\Phi W_z\left\{1 \pm \left[1 - \frac{2}{(2\mu+1)^2 b^2 \Phi}\right]^{1/2}\right\}, \qquad (21)$$

were $b = \bar{a}_z/L$. The expression for energies (20) indicates that index μ must be limited from below (the energies must be real):

$$2\,\mu \;\geq\; b^{-1}\sqrt{2/\Phi} - 1. \qquad (22)$$

It means that the minimal allowed value of the index μ is the minimal integer which is bigger than the final term in (20). As we can see, the lower boundary of quantum number μ depends on the number of structural layers (through N_z), on the way of sputtering (through n_0), and on the type of ion-ion interaction (through h). If the thickness of the structure increases, the lower value of μ increases too.

For simplification, instead of the expression (20), we will use the approximate expressions for energies, which we obtain by the expansion of the square root up to the quadratic terms:

$$E_1 = E_z^{(0)} + 4b^2(2\mu+1)^2\Phi W_z - \frac{W_z}{2(2\mu+1)^2 b^2 \Phi} \qquad (23)$$

and

$$E_2 = E_z^{(0)} + \frac{W_z}{2(2\mu+1)^2 b^2 \Phi}. \qquad (24)$$

It is very easy to notice that both obtained expressions for energies satisfy the necessary condition (18). However, by the analysis of (22) and (23), we can conclude the following.

- Since $E_2 < E_1$, the states with energy E_2 are more stable and more populated and so they essentialy define the normal behavior of the system.
- From the expressions (21) and (23) it follows that the increase of film thickness (the increase of N_z) causes the increase of the lower boundary of the index μ, and the correction of E_2, which depends on sputtering, decreases. This is in complete agreement with the conclusions that we can accomplish without going over to continuum, i.e. directly analysing discrete eq.s (15).

We can see in expressions defining ζ – text under (18), that the boundaries of the interval for ζ are proportional to $L/\bar{a}_z = b^{-1}$ and so we can approximately take: $\zeta \in [-\infty, +\infty]$, where the approximation is better if the film is thicker. We can then express the solutions of equation (19) using Hermite polynomials:

$$A_\mu(\zeta) = \frac{e^{-\zeta^2/2}}{\left(2^\mu \mu!\sqrt{\pi}\right)^{1/2}} H_\mu(\zeta)\;; \quad H_\mu(\zeta) = (-1)^\mu e^{\zeta^2}\frac{d^\mu}{d\zeta^\mu}(e^{-\zeta^2}) \quad \mu = 0,1,2,\ldots \qquad (25)$$

In this way we have defined single-particle degenerate states of the system: for the wave functions – by the equations (12), (14), and (24) and for energies – by (20).

4. CHARGE CARRIERS DISPERSION LAW

We shall perform the diagonalization of the electron Hamiltonian in the following stages.

1. In the framework of the continual approximation, Hamiltonian H_B "melted" in Hamiltonian H_V using the formulas for transition to continuum

$$C_{n_xn_yn_z} \to C_{n_xn_y}(\zeta); \qquad W_z\left[1+\frac{4\Phi}{L^2}\left(z-\frac{L}{2}\right)^2\right] \to W_z\left(1+\frac{4\Phi\tau_\mu}{L^2}\zeta^2\right).$$

(Because of the transformation $n_z \to z \to \tau\zeta$, it is obvious that the sum over n_z must be changed by integral over ζ: $\sum_{n_xn_yn_z} \longrightarrow \tau\bar{a}_z^{-1}\sum_{n_xn_y}\int_{-\infty}^{\infty}d\zeta$).

2. From the operators $C_{n_xn_y}(\zeta)$ we go over to new operators $C_{k_xk_y\mu}$ using the canonical transformations:

$$C_{n_xn_y}(\zeta) = \sum_{k_xk_y\mu} A_{n_xn_y}^{k_xk_y}(\mu,\zeta)C_{k_xk_y\mu}. \tag{26}$$

Therefore we can write Hamiltonian H_V in the continual approximation in the form:

$$\begin{aligned} H_V \longrightarrow H = \frac{\tau}{a_z}\sum_{n_xn_y}\int_{-\infty}^{\infty}d\zeta C_{n_xn_y}^{+}(\zeta)\Big\{\Lambda C_{n_xn_y}(\zeta) - \\ -W_x\left[C_{n_x+1,n_y}(\zeta)+C_{n_x-1,n_y}(\zeta)\right] - W_y\left[C_{n_xn_y+1}(\zeta)+C_{n_xn_y-1}(\zeta)\right] - \\ -W_z\left(1+\frac{4\Phi\tau^2}{L^2}\zeta^2\right)\left[2C_{n_xn_y}(\zeta)+\frac{\bar{a}_z^2}{\tau^2}\frac{d^2C_{n_xn_y}(\zeta)}{d\zeta^2}\right]\Big\}. \end{aligned} \tag{27}$$

We can now perform the diagonalization of Hamiltonian. After the substitutions (26) into (27) we have:

$$\begin{aligned} H = \frac{\tau}{\bar{a}_z}\sum_{k_xk_y\mu}\sum_{q_xq_y\nu}C_{q_xq_y\nu}^{+}C_{k_xk_y\mu}\sum_{n_xn_y}\int_{-\infty}^{\infty}d\zeta\left[A_{n_xn_y}^{q_xq_y}(\nu;\zeta)\right]^*\Big\{\Lambda A_{n_xn_y}^{k_xk_y}(\mu;\zeta) - \\ -2W_x\left[A_{n_x+1,n_y}^{k_xk_y}(\mu;\zeta)+A_{n_x-1,n_y}^{k_xk_y}(\mu;\zeta)\right] - 2W_y\left[A_{n_xn_y+1}^{k_xk_y}(\mu;\zeta)+A_{n_xn_y-1}^{k_xk_y}(\mu;\zeta)\right] - \\ -2W_z\left(1+\frac{4\Phi^{\ 2}}{L^2}\zeta^2\right)\left[2A_{n_xn_y}^{k_xk_y}(\mu;\zeta)+\frac{\bar{a}_z^2}{\tau^2}\frac{d^2A_{n_xn_y}^{k_xk_y}(\mu;\zeta)}{d\zeta^2}\right]\Big\}. \end{aligned} \tag{28}$$

Based on (14) one can write: $A_{n_j+1}^{k_xk_y}(\mu;\zeta)+A_{n_j-1}^{k_xk_y}(\mu;\zeta) = 2\,A_{n_xn_y}^{k_xk_y}(\mu;\zeta)\cos(a_jk_j), \quad j=(x,y)$. If we substitute E with $E_{k_xk_y\mu}$ and z with ζ in the last of (15), we find $W_z(1+\frac{4\Phi\tau^2}{L^2}\zeta^2)\left[2A_\mu(\zeta)+\frac{\bar{a}_z^2}{\tau^2}\frac{d^2A_\mu(\zeta)}{d\zeta^2}\right] = \left(E_z^{(0)}-E_{k_xk_y\mu}\right)A_\mu(\zeta)$, which yields

$$W_z\left(1+\frac{4\Phi\tau^2}{L^2}\zeta^2\right)\left[2A_{n_xn_y}^{k_xk_y}(\mu;\zeta)+\frac{\bar{a}_z^2}{\tau^2}\frac{d^2A_{n_xn_y}^{k_xk_y}(\mu;\zeta)}{d\zeta^2}\right] = \left(E_z^{(0)}-E_{k_xk_y\mu}\right)A_{n_xn_y}^{k_xk_y}(\mu;\zeta).$$

Using this and the orthonormalization condition from (12), we diagonalize the expression (28) for the Hamiltonian of the system:

$$H = \sum_{k_xk_y\mu}E_{k_xk_y\mu}C_{k_xk_y\mu}^{+}C_{k_xk_y\mu}. \tag{29}$$

This expression represents the Hamiltonian of the electron subsystem which was the subject of this study. Together with the Hamiltonian of the phonon subsystem derived earlier [5–7], it enables the continuation of the investigation of the superconductivity mechanism in high-temperature oxide ceramics. Analyses performed until now enable us to conclude that the theoretical model of symmetrically deformed structures satisfies the basic experimental indicators of superconductive perovskite behavior. It is primarily related to the proven presence of a gap in the spectrum of elementary excitations in this system (phonons or electrons) and its behavior in the structures with different stoichiometry. The question of the interaction between the subsystem of elementary charges and the subsystem of phonons (optical type) is still open; this question is crucial for the understanding of the nature of the new superconductive state.

5. ESTIMATE OF SYSTEM ORDERING

In this section of the paper, we shall analyse the Landau superfluidity criterion and determine the probabilities of states and entropy of the system. Landau criterion for superfluid motion is $\min v > 0$, where $v = E(p)/p$. The expression for energies (20) (using the approximations: $a_x \cong a_y \equiv a$, $a_z \cong 3a$, $W_x \cong W_y \equiv W$, $W_z = W/3^h$, $\sin\alpha \simeq \alpha$, $k_x = k\sin\theta\cos\varphi$, $k_y = k\sin\theta\sin\varphi$, $k_z = k\cos\theta$) yields the following expression:

$$E_{1;2}(p) = \frac{Wa^2}{\hbar^2}\left[p^2\sin^2\theta + g_{\pm}^2(\mu)\right], \qquad (30)$$

where $g_{\pm}^2(\mu) = 2\,3^{-h}\hbar^2 a^{-2} f^2(\mu)\left[1 \pm \sqrt{1-2f^{-2}(\mu)}\right]$; $f^2(\mu) = b^2(2\mu+1)^2\Phi$. For the phase velocity, we get:

$$v_{1;2}(p) = \frac{E_{1;2}(p)}{p} = \frac{Wa^2}{\hbar^2}\left[p\,\sin^2\theta + \frac{1}{p}g_{\pm}^2(\mu)\right] \qquad .(31)$$

The condition $dv/dp = 0$ yields $p_e = g_{\pm}(\mu)\sin^{-1}\theta$. Because of $\theta \in [0,\pi] \Rightarrow v_{1,2}^2 \geq 0$, and because $g_+ \geq g_- \Rightarrow v_1^2 \geq v_2^2$. It follows that the state with the energy E_1 has a more expressive minimum than the state with the energy E_2. For the second derivative, we get:

$$\frac{d^2v_{1;2}}{dp^2}|_{p=p_e} = 2Wa^2\hbar^{-2}\,g_{\pm}^{-1}(\mu)\sin^3\theta \;\geq\; 0. \qquad (32)$$

We can see that the known − Landau criterion is satisfied for both energies, but it is "stronger" for the states with the energies E_1 ($\geq E_2$) because E_1 has a bigger gap than E_2.

We shall now determine the probability of the state of the system under consideration. If we introduce the notation

$$\epsilon_{1;2} \equiv E_{1;2} - E_z^{(0)} = 2W_z\left[3^h a^2\hbar^{-2}g_{pm}^2(\mu) - 1\right], \qquad (33)$$

we can find − see text under the (18):

$$\tau_{1;2} = \left(\frac{\bar{a}_z}{2}L\right)^{1/2}\left(\Phi\epsilon_{1;2}W_z^{-1}\right)^{-1/4} \qquad .(34)$$

Then the wave function (12) has the form:

$$\Psi_{1;2}(k_x,k_y,k_z) = \frac{\tau_{1;2}}{\bar{a}_z}\sum_{n_xn_y}\int_{-\infty}^{+\infty} d\zeta |A_{n_xn_y}^{k_xk_y}(\mu;\zeta)|_{1;2}\, C_{n_xn_y}^{+}\,|0\rangle \qquad (35)$$

where $|A_{n_xn_y}^{k_xk_y}(\mu;\zeta)|_{1;2} = N_{1;2}\,e^{i(n_xa_xk_x+n_ya_yk_y)}A_\mu(\zeta)$ and norm-factor is defined on the following way $N_{1;2} = \bar{a}_z\left(N_xN_y\tau_{1;2}\right)^{-1}$. The probability of finding the elementary charges with the energy E_1 (and E_2), in agreement with (35), is:

$$P_{1;2}(\mu;\zeta) = \left(\frac{\tau_{1;2}}{\bar{a}_z}\right)^2 |A_{n_xn_y}^{k_xk_y}(\mu;\zeta)|_{1;2}^2 = N_x^{-2}N_y^{-2}\,A_\mu^2(\zeta), \qquad (36)$$

wherefrom:

$$P_1(\mu;\zeta) = P_2(\mu;\zeta) \equiv P_\mu(\zeta). \qquad (37)$$

Based on the last expression we can see that both states appear with equal probabilities!

The entropy of the system under consideration is:

$$S_{1;2}(\mu) = -\frac{\tau_{1;2}}{\bar{a}_z}I(\mu), \qquad (38)$$

where the integral $I(\mu) \equiv \int_{-\infty}^{+\infty} d\zeta P_\mu(\zeta)\ln P_\mu(\zeta)$ is need not be calculated, since, from (4.9) and (34), it follows:

$$\frac{S_1(\mu)}{S_2(\mu)} = \frac{\tau_1}{\tau_2} \equiv \left(\frac{\epsilon_2}{\epsilon_1}\right)^{1/4} \leq 1 \;\Rightarrow\; S_1(\mu) \leq S_2(\mu). \qquad (39)$$

(Since $E_1 \geq E_2$, we get $\epsilon_{1;2} \geq 0$ and $\epsilon_1 \geq \epsilon_2$). This expression yields that the states Ψ_2 (with E_2) are less ordered than the states Ψ_1 (with E_1). It means that the states with E_1 (with higher energy and lower population) are probably responsible for superconductive effects in the observed system. The states with E_2 (with lower energy and higher population) are responsible for the normal behavior of this system. This is in agreement with the above comments about these two possible energies

6. CONCLUSION REMARKS

The particular features of high-temperature superconductors based on oxide ceramics are their granular structure and the anisotropy of properties. The existence of the weak isotopic effect and Cooper pairs of charge carriers is experimentally verified, similar to the conventional superconductors, but the BCS model could not explain high critical

temperature. For that reason and based on established experimental results [1–3,13–15], we have proposed the model of ceramic structure as tetragonal i.e. generalised cubic structure in which interatomic distances along one direction are a few times bigger than along the other two directions. It is, energetically, most convenient if the sputtered atoms locate themselves just along this direction.

The analysis of the phonon spectrum in our model yields that we have phonon branches of optical type only in the spectrum (there exists an energy gap). It means that for phonon excitation the energy (heat) must be bigger than the energy gap.

The analysis of the electron spectrum in these symmetrically deformed structures (concerning the planes $n_z = 0$ and $n_z = N_z$) yields that, as a consequence of the existence of the boundaries along z axes, we have two energy branches in the spectrum of charge carriers. The lower energy value is related to more populated states and contains the term depending on the sputtering. This term decreases with increasing of the film thickness. The higher energy value in the spectrum of charge carriers is not particularly analysed because these levels are low populated.

In addition to this, in the framework of the model under consideration, we have determined the orthonormalized single-particle state functions of this system, entropy, and the probabilities of possible states. The theoretical investigation in the framework of the presented model is not finished. It is necessary to form a Hamiltonian of the interaction between charge carriers and phonons and separate from it the essential part only, which describes the formation of Cooper pairs. Only after this, the thermodynamical analysis of the complete system follows.

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Conflicts of Interest

The authors declare no conflict of interest.

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