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),and 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.

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).

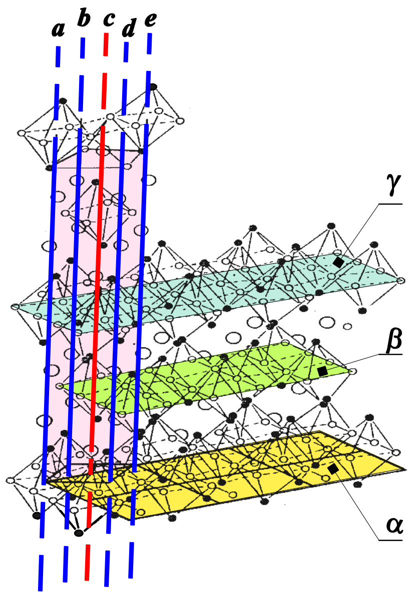

Figure 1: Model of high-temperature superconductors – CuO *ceramics*

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. With regard to 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 of masses of these molecules and the presence of two boundary planes along this direction [5,6].

The phonon system is drawn out in this model [6]. We have determined the phonon states and their energy spectra and we 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 that we have attempted to solve is to determine and analyse the spectra of free charge carriers (electrons or holes), Landau criterion, the probabilities of states, and entropy within the same model. The preliminary results are already presented [8,9].

2. MODEL HAMILTONIAN

In order to obtain 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]:

$$H_{id} = \sum_{\vec{k}} \frac{\hbar^2 \vec{k}^2}{2m^*} C_{\vec{k}}^{+} C_{\vec{k}} \tag{1}$$

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:

$$C_{\vec{k}} = \frac{1}{\sqrt{N}} \sum_{\vec{n}} C_{\vec{n}} \mathrm{e}^{-i\vec{k}\vec{n}}; \; C_{\vec{k}}^{+} = \frac{1}{\sqrt{N}} \sum_{\vec{n}} C_{\vec{n}}^{+} \mathrm{e}^{i\vec{k}\vec{n}} \tag{2}$$

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

$$H_{id} = \sum_{\vec{n}} \Lambda C_{\vec{n}}^{+} C_{\vec{n}} - \sum_{\vec{n},\vec{m}} W_{\vec{n}\vec{m}} C_{\vec{n}}^{+} C_{\vec{m}} \tag{3}$$

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 locate 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:

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

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 behaviour of the superconductive ceramic. 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:

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

in the nearest neighbors approximation we get:

$$W_{n_s;n_s\pm 1} \equiv W_s = W_0 a_s^{-h}; s = (x, y, z). \tag{6}$$

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:

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

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.:

$$W_z \longrightarrow W_z(n_z) = W_0a_z^{-h}(n_z) = W_0a_z^{-h}\left(1 - N_z^2\frac{n_0}{n_0+1}\right)^{-h} \approx W_z(1+\Phi N_z^2), \tag{8}$$

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 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:

$$\begin{aligned}H_{\mathrm{B}} = \textstyle\sum_{n_x,n_y} \Big\{&C^{+}_{n_xn_y0}\Big[\Lambda C_{n_xn_y0} - W_x\left(C_{n_x+1,n_y0} + C_{n_x-1,n_y0}\right) -\\ &- W_y\left(C_{n_xn_y+1,0} + C_{n_xn_y-1,0}\right) - W_z(1-\Phi)C_{n_xn_y1}\Big] +\\ &+C^{+}_{n_xn_yN_z}\Big[\Lambda C_{n_xn_yN_z} - W_x\left(C_{n_x+1,n_yN_z} + C_{n_x-1,n_yN_z}\right) -\\ &- W_y\left(C_{n_xn_y+1,N_z} + C_{n_xn_y-1,N_z}\right) - W_z(1-\Phi)C_{n_xn_yN_z-1}\Big]\Big\},\end{aligned} \tag{10}$$

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

$$\begin{aligned}H_{\mathrm{V}} = \textstyle\sum_{n_x,n_y}\sum_{n_z=0}^{N_z-1} \Big\{&C^{+}_{n_xn_y0}\Big[\Lambda C_{n_xn_y0} - W_x\left(C_{n_x+1,n_y0} + C_{n_x-1,n_y0}\right) -\\ &- W_y\left(C_{n_xn_y+1,0} + C_{n_xn_y-1,0}\right) - W_z(1-\Phi)C_{n_xn_y1}\Big] +\\ &+C^{+}_{n_xn_yN_z}\Big[\Lambda C_{n_xn_yN_z} - W_x\left(C_{n_x+1,n_yN_z} + C_{n_x-1,n_yN_z}\right) -\\ &- W_y\left(C_{n_xn_y+1,N_z} + C_{n_xn_y-1,N_z}\right) - W_z(1-\Phi)C_{n_xn_yN_z-1}\Big]\Big\}.\end{aligned} \tag{11}$$

3. SINGLE-PARTICLE STATES OF THE SYSTEM

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

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

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:

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

On the basis of 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:

$$A_{n_x,n_y,n_z} = A_{n_z}e^{i(n_xa_xk_x + n_ya_yk_y)} \tag{14}$$

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

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

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

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

where $Q\equiv Q_{k_xk_y}=W_x\sin^2\left(\frac{a_xk_x}{2}\right)+W_y\sin^2\left(\frac{a_yk_y}{2}\right)$. We shall perform further analysis in the continual approximation in order to avoid the complications arising during the determination of the coefficient A_n from the system of difference equations (15). Introduction 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):

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

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

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

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

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:

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

By the assumption:

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

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

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

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). For satisfying this requirement we must take the known condition of the finiteness for the solutions for Hermite-Weber equation: $\kappa=2\mu+1; \mu=0,1,2,...$ On the basis of this, we find:

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

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):

$$2\mu\ge b^{-1}\sqrt{2/\Phi}-1. \quad (22)$$

It means that the minimum 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:

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

and

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

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 essentially define the normal behavior of the system.
– From 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:

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

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:

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

(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: $\sum_{n_x n_y n_z} \longrightarrow \tau \bar{a}_z^{-1} \sum_{n_x n_y} \int_{-\infty}^{\infty} d\zeta$).

2) From the operators $C_{n_x n_y}(\zeta)$ we go over to new operators $C_{k_x k_y \mu}$ using the canonical transformations:

$$C_{n_x n_y}(\zeta) = \sum_{k_x k_y \mu} A_{n_x n_y}^{k_x k_y}(\mu, \zeta) C_{k_x k_y \mu}. \quad (26)$$

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

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

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

$$H = \frac{\tau}{\bar{a}_z} \sum_{k_x k_y \mu} \sum_{q_x q_y \nu} C_{q_x q_y \nu}^{+} C_{k_x k_y \mu} \sum_{n_x n_y} \int_{-\infty}^{\infty} d\zeta \left[A_{n_x n_y}^{q_x q_y}(\nu; \zeta)\right]^* \Big\{\Lambda A_{n_x n_y}^{k_x k_y}(\mu; \zeta) -$$
$$-2W_x \left[A_{n_x+1, n_y}^{k_x k_y}(\mu; \zeta) + A_{n_x-1, n_y}^{k_x k_y}(\mu; \zeta)\right] - 2W_y \left[A_{n_x n_y+1}^{k_x k_y}(\mu; \zeta) + A_{n_x n_y-1}^{k_x k_y}(\mu; \zeta)\right] -$$
$$- 2W_z \left(1 + \frac{4\Phi\tau^2}{L^2}\zeta^2\right) \left[2A_{n_x n_y}^{k_x k_y}(\mu; \zeta) + \frac{\bar{a}_z^2}{\tau^2} \frac{d^2 A_{n_x n_y}^{k_x k_y}(\mu; \zeta)}{d\zeta^2}\right]\Big\}. \quad (28)$$

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

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

Using this and the orthonormalization condition from (12), we diagonalize the expression (28) for 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 Hamiltonian of the phonon subsystem derived earlier [5–7], it enables the continuation of the investigation of 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 perovskites behavior. It is primarily related to the proved 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 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:

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

where $g_\pm^2(\mu)=23^{-h}\hbar^2a^{-2}f^2(\mu)\left[1\pm\sqrt{1-2f^{-2}(\mu)}\right]$; $f^2(\mu)=b^2(2\mu+1)^2\Phi$. For the phase velocity we get:

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

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 more expressive minimum than the state with the energy E_2. For the second derivative we get:

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

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

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

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

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

Then the wave function (12) has the form:

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

where $|A^{k_xk_y}_{n_xn_y}(\mu;\zeta)|_{1;2}=N_{1;2}e^{i(n_xa_xk_x+n_ya_yk_y)}A_\mu(\zeta)$ 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:

$$P_{1;2}(\mu;\zeta) = \left(\frac{\tau_{1;2}}{\bar{a}_z}\right)^2 |A_{n_x n_y}^{k_x k_y}(\mu;\zeta)|_{1;2}^2 = N_x^{-2} N_y^{-2} A_\mu^2(\zeta) \tag{36}$$

wherefrom:

$$P_1(\mu;\zeta) = P_2(\mu;\zeta) \equiv P_\mu(\zeta) \tag{37}$$

On the basis of the last expression, we can see that both states appear with equal probabilities!

The entropy of the system under consideration is:

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

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:

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

(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 behaviour 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 on the basis of 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 in the conventional superconductors, but BCS model was not able to explain high critical temperature. For that reason and on the basis of 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 it is necessary that the energy (heat) is bigger than the energy gap.

The analysis of the electron spectrum in these symmetrically deformed structures (with respect to 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 value of energy is related to more populated states and contains the term depending on the sputtering. This term decreases with increasing the film thickness. The higher value of energy 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 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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8. REFERENCES

[1] J. G. Bednorz and K. A. Müller: *Perovskite-Type Oxides* – the New Approach to High-T_c Superconductivity; *Nobel Lecture,* Stockholm, December 8, (1987)

[2] P. H. Hor, et.al, Superconductivity above 90 K in the square-planar compound system $ABa_2Cu_3O_{6+x}$ with $A=Y$,La,Nd,Sm,Eu,Gd,Ho,Er and Lu, *Phys.Rev.Lett.* 58, 1891 (1987)

[3] A. A. Abrikosov: Theory of High−Tc Superconducting Cuprates Based on Experimental Evidence, *http://www.lanl.gov./find/cond.mat.* No: 9912394 (1999)

[4] N. M. Plakida: High-Temperature Superconductors, *Springer-Verlag*, Berlin 1995

[5] B. S.Tošić, J. P. Šetrajčić, R. P. Djajić and D. Lj. Mirjanić; Phonons in Broken-Symmetry Structures, *Phys.Rev.* B 36, 9094 (1987)

[6] J. P. Šetrajčić, R. P. Djajić, D. Lj. Mirjanić and B. S. Tošić; Phonon Spectra in Superconducting Ceramics, *Phys. Scr.* 42, 732 (1990)

[7] J. P. Šetrajčić, V. M. Zorić, N. V. Delić, D. Lj. Mirjanić and S. K. Jaćimovski, Phonon Participation in Thermodynamics and Superconductive Properties of Thin Ceramic Films, Chapter 15, pp. 317-348, In „Thermodynamics", Ed. M. Tadashi, ISBN: 978-953-307-544-0, *InTech*, Vienna (Austria) 2011; Available from:

[8] http://www.intechopen.com/articles/show/title/phonon-participation-in-thermodynamics-and-superconductive-properties-of-thin-ceramic-films

[9] J. P. Šetrajčić, S. M. Vučenović and S. K. Jaćimovski, Possible States of Charge Carriers in Thin Multilayered Superconductive Ceramics, *Zaštita Materijala* **57**/2, 239-243 (2016)

[10] S. M. Vučenović, J. P. Šetrajčić and D. I. Ilić, Superconductivity of Lanthanum Hydride To 250 K, *Proceedings 12th ContMat* (ISBN 978-99976-42-30-1), 91-103 (2020).

[11] Ch. Kittel, Introduction to Solid State Physics, *Wiley*, New York 2004

[12] P. Hoffmann, Solid State Physics, *Wiley*, New York 2015

[13] S. M. Girvin and K. Yang, Modern Condensed Matter Physics, *Cambridge Univ. Press*, Cambridge 2019

[14] R. Simon; High-*T*c Thin Film and Electronic Devices, *Physics Today* 44, 64 (1991)

[15] D. R. Harshman and A. P. Mills, *Phys.Rev. B* 45, 10684 (1992)

[16] W. E. Pickett *Rev. Mod. Phys.* 61, 433 (1989)