T_c and crystal structure distortions of high-temperature superconductors

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Abstract. The influence of orthorhombic distortions of CuO_2 layer on T_c is considered within the framework of kinematic mechanism. The dependence of the interaction constant on orthorhombicity is calculated. It is shown that orthorhombic distortions may result in the increase of T_c by 10% in accordance with experiment.

Keywords. Hubbard model; kinematic mechanism; orthorhombic distortions.

1. Introduction

In the initial researches on high-temperature superconductors (HTSC), the structural phase transition from the tetragonal to the orthorhombic phase was undeservedly given much importance. After the discovery of HTSC-cuprates, based on Bi and Tl which can be tetragonal, the structural transition for reaching high temperatures of superconductor junction T_c has been given less importance.

There are, however, many studies which showed increase of T_c when $\text{YBa}_2\text{Cu}_3\text{O}_{7-y}$ changes from a tetragonal to an orthorhombic phase. This increase of T_c with increase of orthorhombic deformation of plane CuO_2 was observed in isovalent substitution of Y by Al, substitution of Cu by Fe and increasing the oxygen content in CuO chains in $\text{YBa}_2\text{Cu}_3\text{O}_{7-y}$. In order to reveal the inter-relation between the observed changes in T_c and the orthorhombic distortions, Perrin *et al* (1989) studied the oxygen content where an increase of T_c from 75 to 88 K was observed in fluorinating $\text{YBa}_2\text{Cu}_3\text{O}_{6.7}$ at 100% Meissner effect.

2. Hopping integral in HTSC-compounds

In the present work the influence of the orthorhombic distortions of square a - b lattice on T_c is discussed within the framework of the kinematic mechanism of superconduction (Zaitsev and Ivanov 1987; Ivanov and Zaitsev 1989). The classical Hubbard model of a two-dimensional lattice with infinite repulsion of orbital nondegenerate $3d$ -electrons has been selected as the HTSC. This model is roughened by the fact that the tunnelling of $3d(x^2-y^2)$ electrons with the effective transfer integral t between copper cations is realized through oxygen anions with fixed valence-2. Orthorhombic distortions of the lattice with parameters $a = d - \delta \neq b = d + \delta$ result in a difference of transfer integrals $t_a = t + \Delta t$ and $t_b = t - \Delta t$ along directions a and b . The relationship of the value of transfer integral of electrons $t_{a,b}$ and interatomic distance d necessary in future for quantitative estimation can be evaluated by approximating the radial part $3d(x^2 - y^2)$ of the wavefunction of the electron by means of the Gauss' law, so that when it is normalized by the unit:

$$\psi_{x^2-y^2} = (8/\pi)^{1/4} (15/r_B^3) \exp(-r^2/r_B^2), \quad (1)$$

where r_B is the ionic radius of the copper cation. In this approximation:

$$t_{x^2-y^2} = (15/32)\phi_0 \exp(-d^2/2r_B^2), \quad (2)$$

where ϕ_0 is the decrease of the lattice potential with respect to the isolated atoms.

3. DOS in orthorhombic system

The orthorhombic distortions are taken into account in the seeding density of states of non-interacting electrons:

$$\rho_0(z) = \frac{1}{N} \sum_p \delta\{z - 2t[\cos(ap_x) + \cos(bp_y)] + 2t[\cos(bp_y) - \cos(ap_x)]\} \quad (3)$$

expressed through complete elliptic integrals of the first order K and has logarithmic singularity in points $\pm 4\Delta t$:

$$\rho_0(z) = \begin{cases} \frac{2}{\pi^2(4t^2 - z^2/4)^{1/2}} K\left[\left(\frac{4t^2 - \Delta t^2}{4t^2 - z^2/4}\right)^{1/2}\right], & |z| < 4\Delta t \\ \frac{1}{\pi^2(t^2 - \Delta t^2)^{1/2}} K\left[\left(\frac{4t^2 - z^2/4}{4t^2 - 4\Delta t^2}\right)^{1/2}\right], & 4\Delta t < |z| < 4t. \end{cases} \quad (4)$$

In further calculations $\rho_0(z)$ was approximated by the sum of rectangular and logarithmic components:

$$\rho_0(z) = \frac{1 - 2T^*/\pi^2(t_a t_b)^{1/2}}{4(t_a + t_b)} \theta(2t_a + t_b) + \rho_{\log}(z), \quad (5)$$

$$\rho_{\log}(z) = \frac{(-1)}{4\pi^2(t_a t_b)^{1/2}} \left\{ \ln \left| \frac{z - 4\Delta t}{2T^*} \right| \theta(2T^* - |z - 4\Delta t|) + \ln \left| \frac{z + 4\Delta t}{2T^*} \right| \theta(2T^* - |z + 4\Delta t|) \right\}. \quad (6)$$

In (5) and (6) the coefficients were selected from considerations that in the point of logarithmic singularity $K(z) \sim \frac{1}{2} \ln |1-z|$, and the density of states is normalized by the unit, since not more than one electron can be on the node with the infinite Hubbard energy. The width of logarithmic peak T^* was selected equal to t which agrees with the calculated expression for $\rho_0(z)$ through elliptic integrals.

4. T_c dependence from orthorhombicity of CuO_2 layer

In the ordinary way, temperature T is determined by the condition of origin of the singularity in two-particle crest of dispersion of electrons at zero total momentum, spin and frequency. In the diagram technique for Hubbard operators (Zaitsev 1976) for T_c , the following equation is obtained (Zaitsev and Ivanov 1987):

$$I = \int \rho_0(z) \frac{z \text{th}(\xi(z)/2T_0)}{\xi(z)} dz \quad (7)$$

where $\xi(z) = (I + X)z/2 - \mu$, μ is the chemical potential and x the doping parameter.

In the case of orthorhombic distortions of the square lattice for $\rho_0(z)$ in the form (5), equation (7) assumes the following form:

$$1 - \frac{1 - 2t/\pi^2(t_a t_b)^{1/2}}{4(t_a + t_b)} \left[-\frac{8\mu}{(1+x)^2} + \frac{4\mu}{(1+x)^2} \ln \left| \frac{(1+x)^2 4t^2 - \mu^2}{4T_c^2} \right| \right] \\ = \int \rho_{\log}(z) \frac{z}{\xi(z)} \operatorname{th} \frac{\xi(z)}{2T_c} dz \quad (8)$$

Equation (8) determines the dependence of T_c on the value of orthorhombic distortions. As seen on the right side, the increase of T_c is maximum in the case of coincidence of the pole of the expression under the integral sign with the logarithmic singularity of the density of states, i.e.

$$\mu/(1+x) = 2\Delta t. \quad (9)$$

The analogous condition determines the greatest increase of T_c in the case of Van Hove singularities in the electron density of states for different versions of the electron-phonon mechanism of superconductivity. But, as a rule, only logarithmic density of electron states is considered, which results in substitution of interaction constant in the expression for T_c by $\sqrt{\lambda}$: $T_c \sim \exp(-1/\lambda) \rightarrow T_c \sim \exp(-1/\sqrt{\lambda})$. In this case, because of the presence of the rectangular part in (5), one cannot restrict oneself during calculations only by term $\ln^2(t/T_c)$ in (8), which leads to substitution $\lambda \rightarrow \sqrt{\lambda}$, but the quadratic equation relative to $\ln(t/T_c)$ should be solved.

Having solved equation (8), it is possible to find an explicit expression for T_c , but the complexity of the analytical expressions makes it impossible to compare the interaction constants in tetragonal and orthorhombic phases. Therefore, the calculated constant values λ are graphically presented in figure 1. Plotted on the lower abscissa axis in the

Figure 1. Interaction constants in tetragonal and orthorhombic phases.

figure is the degree of fill of x of the lower Hubbard subzone for which appropriate values λ are calculated; plotted on the upper abscissa axis is $(b - a)/(b + a)$ which was determined with the help of (2) so that at a given x the condition (9) was met. The expression for T_c was brought into the form $T_c = t \exp(-1/\lambda)$, in this case λ turned to be strongly dependent on x . Therefore, values are calculated for the average interval $0 \times 1/3$. Values characteristic of $\text{YBa}_2\text{Cu}_3\text{O}_{7-y}$: $r_B = \text{\AA}$, $(b + a)/2 = 3.75 \text{\AA}$ were taken in the calculations.

It is clear that for T_c in the orthorhombic phase to exceed the maximum value T_c in the tetragonal phase, the $b - a$ difference should be not less than $0.01 \text{\AA}$. Normally, the experimental values of orthorhombic distortions do not exceed $(b - a) \sim 0.07 \text{\AA}$, though a number of authors consider that greater values of $(b - a)$ up to $0.16 \text{\AA}$ are possible.

Note that the T_c value obtained is considerably less in the absence of the rectangular component of the density of states (5).

5. Conclusion

The present results indicate a marked increase of T_c calculated within the framework of the kinematic mechanism, as a consequence of orthorhombic deformations CuO_2 of the plane in laminated HTSC-cuprates. Normally, the shortage of oxygen and the value of orthorhombic distortions in HTSC, type $\text{YBa}_2\text{Cu}_3\text{O}_{7-y}$, are interconnected in a definite manner, so it is unlikely that conditions (9) will be met experimentally on one specimen for several values of x . On the contrary, in experiments (Perrin *et al* 1989) in which the oxygen content was noted, an increase of T_c is possible as the Fermi level approaches the logarithmic singularity in the considered density of the electron states (5).

Two peaks on curve $T_c(x)$ were found for $\text{La}_{2-x}\text{Ba}_2\text{CuO}_4$ (Suzuki and Fujita 1989) (similar results for $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ were obtained by V I Simonov, Inst. of Crystallography of the USSR Academy of Sciences). These peaks can be explained by the presence of two phases—tetragonal and orthorhombic with different positions of the maxima of concentration dependence $T_c(x)$ assuming that maximum T_c in the orthorhombic phase is shifted towards lesser concentrations of holes.

Let us emphasize once again that if in orthorhombic deformations the oxygen content changes, then because of strong concentration dependence of $T_c(x)$ the change of T_c can be greater due to change of x than change of T conditioned by orthorhombic distortions.

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