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High- T_c superconductivity induced by localized donor-impurity vibrations of hole-polarization nature

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Abstract. The proposed development of the hole-polarization concept of high-temperature superconductivity introduces boson modes describing some distortions of unit cells in which the balance of the chemical valencies of the constituent ions is broken so that the copper ions are described by alternating valency. It is important that the modes in question are caused by dynamical charge transfer. They are assumed to be rather high-frequency modes, although there is an inner tendency to their softening. These boson modes lead to the Cooper pairing of holes in the oxygen conduction band. The intermediate character of the relation between the values of the Fermi energy and the energy of the boson mode at hand is the origin of the strong depression of the isotope effect. The contribution of the channel of coherent scattering of holes from hole donors exists in principle but seems to be small practically. The simplest case of lanthanum ceramics is considered. Two possible sets of the values of the parameters, which are in agreement with experiments, are discussed.

1. Introduction

In the last few years the phenomenon of high-temperature superconductivity [1] has undergone great experimental development. After ceramics based on yttrium [2], the new stable systems based on bismuth [3] and thallium [4], which are characterized by higher critical temperatures, have been obtained. There is also evidence in favour of the existence of metastable systems with much higher temperatures of the superconducting phase transition. A large number of theoretical constructions have been proposed to explain this phenomenon [5], the majority of which are devoted to the investigation of non-phonon possibilities [6–9].

The capability of describing the appearance of a superconducting state in different up-to-date types of compound, beginning from the simplest ceramics based on lanthanum, on common grounds is an important requirement on the theory of high-temperature superconductivity. The theory in question must also take into account the essential properties of real materials such as typical structural anisotropy [10], the hole type of conductivity normally intrinsic to these superconductors [11] and the strong depression of the isotope effect [12]. The most intriguing fact in these compounds is the presence of the Cu^{3+} state [13–18], leading to unusual local excitations [16, 19]. We believe that the latter is crucial to all the problems.

As a result of our efforts to couple together all the above peculiarities, the hole polarization concept of a given phenomenon has been formulated [20–23]. Within the

framework of this concept the main electronic properties are due to the process of hole transition from the oxygen valence band to the Cu^{3+} ions and vice versa which happens in unit cells where the balance between the valencies of the constituent ions is broken. In this case both the hole conductivity in the oxygen band and the strong localization of the superconducting hole pairs are natural consequences of the model [23]. The present paper gives the further development of the idea of local hole polarization which is assumed to be the origin of specific boson modes of the vibronic type. These modes are local in space and are described by an energy without any dispersion. They are able to mediate the superconducting coupling.

In the present paper we restrict ourselves to the discussion of lanthanum systems. In the case of the hole-polarization model, without considering any additional degrees of freedom, the channel of interaction via the boson modes at hand is predominant whereas a more accurate analysis shows that the coherent scattering of holes from the static hole donors discussed before [20–23] is depressed by other channels of scattering from the same donors and results only in a small correction to the main effect. It is also worth noting that the corresponding isotope effect is rather small. This peculiar feature of our present result is due to the rather high frequency of the boson modes.

2. Model

In the spirit of the representations in [20–23] we describe our system by the following Hamiltonian:

$$H = \sum_k \omega_k a_{k\sigma}^{\dagger} a_{k\sigma} + \sum_i \eta_i \left((B_0 - A\varphi_i) b_{i\sigma}^{\dagger} b_{i\sigma} + g(b_{i\sigma}^{\dagger} a_{i\sigma} + a_{i\sigma}^{\dagger} b_{i\sigma}) + \frac{P_i^2}{2\mu} + \frac{\lambda\varphi_i^2}{2} \right). \quad (1)$$

Here the sum over the momenta k describes the hole oxygen band with the spectrum ω_k ; $a_{k\sigma}^{\dagger}$ and $a_{k\sigma}$, respectively, are the creation and annihilation operators of a hole in the band; the summation over repeated spin indices σ is assumed. The sum over i runs over all N unit cells of the crystal lattice. The value of $\eta_i = 1$ specifies donor unit cells where there is a deficiency of the cation valency due to either the presence of divalent metal ions or surplus oxygen ions there. In other unit cells, $\eta_i = 0$. In the site representation, $b_{i\sigma}^{\dagger}$ and $b_{i\sigma}$ are the hole operators at donors; $a_{i\sigma}^{\dagger}$ and $a_{i\sigma}$ are the band operators. g is the matrix element of the hole transition from a donor to the band and vice versa. $B_0 - A\varphi_i$ is the energy of a hole at the i th donor, with the deformation response of the i th unit cell being taken into account. Owing to a random distribution of the donor unit cells, it is natural to admit that localization of a hole residing at a donor occurs. In this case the general deformation state of a unit cell at the transition of a hole from the band to a donor and vice versa can be represented as the alternative existence of a unit cell in two potential wells [24, 25], which are, for simplicity, supposed to be parabolic with the same curvature λ . Finally, in equation (1), μ is the reduced mass of ions moving in this process of deformation; P_i denotes the momentum canonically conjugate to the deformation variable φ_i .

It is reasonable to suggest that the typical time of the hole transition between the band and a donor is much less than the characteristic times of the deformation. Thus, it is natural to describe the parabolic potentials, in which the deformation motion takes place, by their statistical weights determining the probabilities of their realization.

Inasmuch as the probability that a hole exists at a donor is experimentally much less than that in the band, the equilibrium point is shifted towards smaller values of φ_i . The appropriate mean value $\langle \varphi \rangle$ is as usual determined by the condition that the mean energy at the site containing a donor is a minimum.

The diagonal hole part of Hamiltonian (1) arises when operators φ_i are replaced by $\langle \varphi \rangle$. The transformation of this part of the Hamiltonian to a diagonal form has been discussed in detail in [21–23], where $B = B_0 - A\langle \varphi \rangle$. In the particular case when B is much larger than the band width of the spectrum ω_k , there is a single hole conduction band, which will be described by the operators $\xi_{k\sigma}^+$ and $\xi_{k\sigma}$, as well as a narrow empty band with a relatively high mean energy, which is not essential for what follows. We also restrict ourselves to the case where $Q = g/B \ll 1$. This is natural inasmuch as the probability that the Cu^{3+} state in a donor unit cell is small experimentally and is determined by Q^2 theoretically. The final Hamiltonian of free holes takes the form

$$H_h = \sum_k f_k \xi_{k\sigma}^+ \xi_{k\sigma}$$

where $f_k = \omega_k - \varepsilon_F$, $\varepsilon_F = cBQ^2$ is the Fermi energy and $c = \langle \eta_i \rangle$ is the concentration of donor unit cells. The total Hamiltonian, which is essential for what follows and to which equation (1) is reduced, can be represented in the form

$$H = H_0 + H_{\text{int}}$$

where

$$H_0 = H_h + H_b$$

$$H_b = \sum_i \Omega_0 \eta_i (d_i^+ d_i + \frac{1}{2})$$

$$H_{\text{int}} = -\frac{Q^2}{N^{1/2}} \sum_{k_1} \sum_{k_2} \xi_{k_1\sigma}^+ \xi_{k_2\sigma} \left[B \eta_{k_2 - k_1} + A \left(\frac{\Omega_0}{2\lambda N} \right)^{1/2} \right. \\ \left. \times \sum_i \eta_i (d_i^+ + d_i) \exp[i(k_2 - k_1) \cdot r_i] \right]. \quad (2)$$

Here d_i^+ and d_i are the local boson operators describing the departure of φ_i from $\langle \varphi \rangle$; $\Omega_0 = \hbar(\lambda/\mu)^{1/2}$, where \hbar is the Planck constant, η_k is the Fourier transform of $\eta_i - c$ and r_i is the radius vector of the i th unit cell. The term containing B in equation (2) corresponds to the interaction introduced in [20–23]. The term containing A describes the interaction of holes with local bosons. Note that the expression of $\langle \varphi \rangle$ in terms of the present hole operators is of the form

$$\langle \varphi \rangle = \frac{AQ^2}{\lambda N} \sum_k \langle \xi_{k\sigma}^+ \xi_{k\sigma} \rangle. \quad (3)$$

3. Boson self-energy

Apart from the normal temperature Green functions $G_{k\sigma}(\tau)$ and $D_i(\tau)$ describing the above holes and bosons, respectively, we as usual introduce the abnormal Green functions $F_{k\uparrow - k\downarrow}(\tau)$ and $F_{-k\downarrow k\uparrow}^+(\tau)$ which are complex conjugates to each other, are non-

zero only in the superconducting phase and describe the Cooper pairing of holes there [26]. In particular,

$$F_{k\uparrow - k\downarrow}(\tau) = -\langle \xi_{k\uparrow}(\tau) \xi_{-k\downarrow} \rangle_{\tau}.$$

The parameter τ changes from $-\beta$ to β , where $T = 1/\beta$ is the temperature measured in energy units; the label τ denotes the ordering of operators [26].

First we consider the boson Green function $D_i(\tau)$. In the present paper we restrict ourselves to the calculation of only the critical temperature of the superconducting phase transition; therefore the contribution of the abnormal Green functions to the value of $D_i(\tau)$ will be ignored in what follows. According to equation (2), the appropriate Dyson equation is then of the form

$$D_i(\tau) = D_i^0(\tau) + \frac{A^2 Q^4 \Omega_0}{2\lambda N^2} \int_0^\beta d\tau_1 d\tau_2 D_i^0(\tau - \tau_1) D_i(\tau_2) \times \sum_{k_1} \sum_{k_2} G_{k_1\sigma}(\tau_1 - \tau_2) G_{k_2\sigma}(\tau_2 - \tau_1). \quad (4)$$

Here $D_i^0(\tau)$ is the Green function of non-interacting bosons, to which $D_i(\tau)$ tends at $H = H_0$. In equation (4) the renormalization of the vertex, which leads to corrections proportional to the small hole-boson interaction constant, is not taken into account. The further introduction of imaginary frequencies in equation (4) is performed in the conventional manner. As a result, we obtain the following solution for equation (4):

$$D_i(\omega_m) = -2\Omega_0/(\omega_m^2 + \Omega_0^2 S_m) \quad (5)$$

where

$$S_m = 1 + \frac{A^2 Q^4 T}{\lambda N^2} \sum_{n=-\infty}^{\infty} \sum_{k_1} \sum_{k_2} G_{k_1\sigma}(\omega_n) G_{k_2\sigma}(\omega_n + \omega_m) \quad (6)$$

$\omega_m = 2\pi Tm$, $\omega_n = \pi T(2n + 1)$, and m and n are integers. To carry out the calculation in equation (6), we restrict ourselves to the leading order in the interaction parameter again. The sum over n is calculated by making use of the appropriate integral in the plane of complex frequencies. As a result, equation (6) takes the form

$$S_m = 1 - \frac{2A^2 Q^4}{\lambda N^2} \sum_{k_1} \sum_{k_2} \frac{\tanh(\beta f_{k_1}/2)(f_{k_1} - f_{k_2})}{(f_{k_1} - f_{k_2})^2 + \omega_m^2}. \quad (7)$$

For further calculations the form of the spectrum ω_k must be defined in detail. For simplicity here and below, we restrict ourselves to a parabolic spectrum with the uniaxial anisotropy:

$$\omega_k = k_{\parallel}^2/2m_{\parallel} + k_{\perp}^2/2m_{\perp}$$

where k_{\parallel} and k_{\perp} are the momentum components along and normal to the plane of anisotropy, respectively, and m_{\parallel} and m_{\perp} are the appropriate effective hole masses. It is also convenient to make use of the formula

$$\lim_{\kappa \rightarrow 0} [1/(x + i\kappa)] = P\{1/x\} - i\pi\delta(x) \quad (8)$$

where $P\{ \}$ denotes that the Cauchy principal value of the appropriate integral must be considered and $\delta(x)$ is the Dirac delta function. In the important particular case when

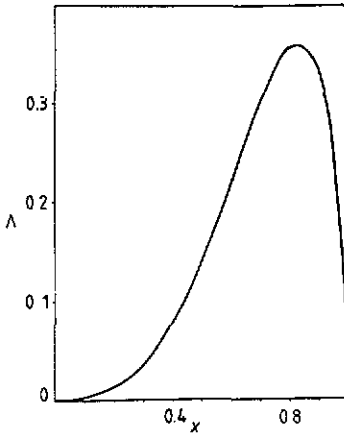


Figure 1. Behaviour of the characteristic function $\Lambda(x)$ describing the renormalization of the boson energy.

$m \rightarrow 0, T \rightarrow 0$, which is predominant in what follows, from equation (7) for the value of S_0 we obtain the following expression:

$$S_0 = 1 - (9A^2Q^4/\lambda h_0^2)\Lambda(h_F/h_0)$$

where

$$h_F = \varepsilon_F^{1/2} \quad h_0 = (3/\gamma)^{1/3} \quad \gamma = vm_{\parallel}(2m_{\perp})^{1/2}/\pi^2\hbar^3$$

$$\Lambda(x) = [(1-x^4)/2] \ln[(1+x)/(1-x)] - x(1-x^2)$$

and v is the volume of the unit cell, which appears on transition to integrals over momenta. The shape of the function $\Lambda(x)$ is shown in figure 1.

The value of the renormalized boson energy as a function of the concentration c is discussed below for several typical sets of values of the model parameters. It is important that such renormalization promotes the local character of the boson modes at hand on the energy axis. Their spatial locality also persists as can easily be shown. Note that the account of the distinction of the curvature parameter for the potential, when a hole resides at a copper ion, also promotes both the localization of the discussed boson modes and their separation from the regular phonon spectrum.

4. Damping parameter of hole states

The Dyson equations for the Green functions $G_{k\uparrow}(\tau)$ and $F_{-k\downarrow k\uparrow}^+(\tau)$ can be written in a manner similar to (4). In the representation of imaginary frequencies the joint solution of these equations takes the form

$$G_{k\uparrow}(\omega_n) = \Xi_{kn}^*/(|\Xi_{kn}|^2 + |\Delta_n|^2)$$

$$F_{-k\downarrow k\uparrow}^+(\omega_n) = \Delta_n/(|\Xi_{kn}|^2 + |\Delta_n|^2)$$
(9)

where

$$\Xi_{kn} = i\omega_n - f_k - \frac{B^2Q^4c(1-c)}{N} \sum_{k_1} G_{k_1\uparrow}(\omega_n)$$

$$+ \frac{A^2Q^4\Omega_0cT}{2\lambda N} \sum_{m=-\infty}^{\infty} \sum_{k_1} G_{k_1\uparrow}(\omega_n - \omega_m) D_i(\omega_m)$$
(10)

$$\Delta_n = \frac{B^2 Q^4 c(1-c)}{N} \sum_k F_{-k \downarrow k \uparrow}^+(\omega_n) - \frac{A^2 Q^4 \Omega_0 c T}{2\lambda N} \sum_{m=-\infty}^{\infty} \sum_k F_{-k \downarrow k \uparrow}^+(\omega_n - \omega_m) D_c(\omega_m). \quad (11)$$

To calculate the last two terms in equation (10), it is in order to note that these terms are small corrections, so that the unperturbed values may be used under the summation signs. It is also important that the real parts of these terms give rise to small corrections to the value of ε_F and can be ignored within the accuracy to the leading order. As far as the appropriate imaginary parts are concerned, we restrict ourselves to the case of small n again. Then for the leading correction term we obtain from the third term on the right-hand side of equation (10) the following relationship:

$$\text{Im} \left(\frac{1}{N} \sum_k G_{k \uparrow}(\omega_n) \right) = -\frac{\pi \gamma h_F}{2} \text{sgn}(\omega_n) \quad (12)$$

where equation (8) is taken into account. The sum over n in the last term of equation (10) can be calculated upon considering the appropriate integral on a plane of complex frequencies. On representing the self-energy part of the boson Green function approximately in the form $\Omega^2 = \Omega_0^2 S_0$, in the limit $\beta\Omega \gg 1$ we obtain the relationship

$$\text{Im} \left(T \sum_m \frac{1}{(\Omega^2 + \omega_m^2)(i\omega_n - i\omega_m - f_k)} \right) = -\frac{\pi \text{sgn}(\omega_n)}{\Omega} \exp(-\beta\Omega) [\delta(\Omega + f_k) + \delta(\Omega - f_k)].$$

The subsequent calculation of the integral over momenta can be performed directly. Finally, the value of Ξ_{kn} in the non-superconducting phase in the case of small $|\omega_n|$ and low temperatures is of the form

$$\Xi_{kn} = i[\omega_n + \delta \text{sgn}(\omega_n)] - f_k \quad (13)$$

where

$$\delta = (\pi \gamma Q^4 c/2) \{ B^2(1-c)h_F + [A^2 \Omega_0^3 \exp(-\beta\Omega)/\lambda \Omega] \times [(\Omega + \varepsilon_F)^{1/2} + (\varepsilon_F - \Omega)^{1/2} \theta(\varepsilon_F - \Omega)] \}. \quad (14)$$

$\theta(\varepsilon_F - \Omega)$ is the Heaviside step function.

5. Superconducting transition temperature

The substitution of solution (9) into equation (11) gives rise to the matching condition on the parameters Δ_n . On taking account of equations (5) and (13) in the case of where $S_m = S_0$, the condition at the onset of superconductivity is represented in the form

$$\Delta_n = \frac{B^2 Q^4 c(1-c)}{N} \sum_k \frac{\Delta_n}{(|\omega_n| + \delta)^2 + f_k^2} + \frac{A^2 Q^4 \Omega_0^2 c T}{\lambda N} \times \sum_m \sum_k \frac{\Delta_{n-m}}{(\Omega^2 + \omega_m^2)[(|\omega_{n-m}| + \delta)^2 + f_k^2]} \quad (15)$$

Here the first term on the right-hand side corresponds to the channel of scattering from hole donors and was discussed in [20–23] where, however, the contribution of δ was ignored. As shown below, the latter contribution is critical. It prevents in an independent way the possibility that superconducting instability arises because of this channel. Indeed, the term in question is proportional to Δ_n , with the coefficient of proportionality obtained as in equation (12); it can be combined with the left-hand side of equation (15). As a result, the equation for the superconducting transition temperature takes the form

$$\frac{A^2 Q^4 \Omega_0^2 c T}{\lambda N} \sum_k \sum_m \frac{1 + \delta_0/(|\omega_{n-m}| + \delta_1)}{(\Omega^2 + \omega_m^2)[(|\omega_{n-m}| + \delta)^2 + f_k^2]} = 1. \quad (16)$$

The calculation of the sum over m in equation (16) can be carried out in the same manner as previously by consideration of the appropriate integral on a complex frequency plane. However, there is a complication connected with the fact that the integrand is not a continuous function; therefore, two complex half-planes are to be considered. In each half-plane the integration is performed independently herein. As a result, in the case of $0 < \omega_n \ll \Omega$ and $\delta \ll \Omega$ for the sum over m multiplied by T we derive

$$\begin{aligned} & \frac{1}{2\Omega} P\left\{\frac{1}{f_k^2 - \Omega^2}\right\} + \frac{1}{2\pi} \int_0^\infty d\omega \tanh\left(\frac{\beta\omega}{2}\right) P\left\{\frac{1}{\Omega^2 - \omega^2}\right\} \\ & \times \text{Im} \left[\frac{1}{\omega + i\delta_1} \left(\frac{1}{f_k - \omega - i\delta} - \frac{1}{f_k + \omega + i\delta} \right) \right] \end{aligned} \quad (17)$$

where δ_0 and δ_1 correspond to the first and second terms on the right-hand side of equation (14), respectively. It seems to be convenient to perform the further summation over k in (16) under the integral sign in equation (17), where integration over momenta is assumed. In this case the integrals over momenta and ω may be calculated with the help of equation (8) independently. Thus to the leading order the result does not depend on the values of δ_0 and δ_1 . Hence, for the model of the superconducting pairing at random centres, the Anderson [27] theorem is justified, i.e. the effects of scattering from these random centres do not affect the superconductivity to the leading order of the interaction parameter. On the other hand, the channel discussed in [20–23] gives the principal contribution to equation (16), although its effect is negligibly small in the adopted weak-coupling approximation. It is important here that the interactions in both the channels are assumed to be of the same order of magnitude. The case of strong coupling requires special consideration.

As a result of all the indicated transformations, in the limit $\beta\Omega \gg 1$, equation (16) can be represented in the following form:

$$\frac{A^2 Q^4 \Omega_0^2 c \gamma}{4\lambda} \int_{-\varepsilon_F}^{h_0^2 - \varepsilon_F} \left[\frac{1}{f} \tanh\left(\frac{\beta f}{2}\right) - \frac{1}{\Omega} \right] \frac{(f + \varepsilon_F)^{1/2} df}{\Omega^2 - f^2} = 1$$

where the Cauchy principal value of the integral at hand is assumed. The expression of BCS type for the critical temperature following therefrom takes the form

$$T_c = (8 \exp C \varepsilon_F / \pi) [(h_0 - h_F)/(h_0 + h_F)]^{1/2} [(\alpha - 1)/(\alpha + 1)]^{\alpha/2} W \exp(-R) \quad (18)$$

where

$$W = \begin{cases} \exp\{\gamma[\tan^{-1}(h_0/h_F\gamma) - \tan^{-1}(1/\gamma)]\} \\ [(1 - \gamma)(h_0 + h_F\gamma)/(1 + \gamma)(h_0 - h_F\gamma)]^{\gamma/2} \end{cases} \quad \text{at} \begin{cases} \varepsilon_F < \Omega \\ \varepsilon_F > \Omega. \end{cases}$$

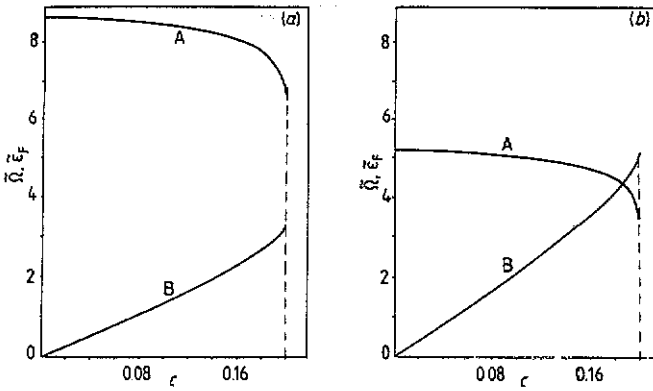


Figure 2. Dependences of $\tilde{\Omega} = 100\Omega$ (eV) (curves A) and $\tilde{\varepsilon}_F = 100\varepsilon_F$ (eV) (curves B) on the concentration c for the parameters in (a) set 1 and (b) set 2: ---, $c = c_c$ which restricts the region of solutions.

The following notation is introduced here:

$$R = 2\lambda S_0/cA^2 Q^4 \gamma h_F \quad \alpha = [(\Omega + \varepsilon_F)/\varepsilon_F]^{1/2}$$

$$\gamma = |(\Omega - \varepsilon_F)/\varepsilon_F|^{1/2}$$

\mathcal{C} is Euler's constant. For the limiting cases of the dependence (18) we have

$$T_c = \begin{cases} 0.6138\varepsilon_F \exp[(\pi/2)(\Omega/\varepsilon_F)^{1/2} - R] \\ 1.3041\Omega[(h_0 - h_F)/h_0 - h_F]^{1/2} \exp(-R) \\ 1.1339\Omega \exp(-R) \end{cases} \quad \text{at } \begin{cases} \varepsilon_F \ll \Omega \\ \varepsilon_F = \Omega \\ \varepsilon_F \gg \Omega. \end{cases}$$

6. Discussion

Equation (18) contains apart from the initial model parameters the set of quantities which are to be determined in the self-consistent manner as far as their concentration dependences are concerned. The case of low temperatures compared with the typical hole and boson energies is of importance. So the zero-temperature limit is instructive in what follows. For further estimates we adopt the following values of the parameters: $A^2/\lambda = 2 \times 10^4$ eV and, at the concentration $c = 0.2$, according to [13], $Q = 0.1$, $T_c = 36.2$ K and $\gamma h_F = 1$ eV $^{-1}$. We may, for example, consider the two sets of solutions corresponding to $B_0 = 20.6$ eV, $\Omega_0 = 1000$ K (set 1) and $B_0 = 31.9$ eV, $\Omega_0 = 600$ K (set 2), which are in agreement with the above experimental data at $c = 0.2$.

According to (3), the predominant dependence of B on c is specified by the equation

$$B(1 + 2A^2 g^5 c^{3/2} / \lambda h_0^3 B^{9/2}) = B_0.$$

The particular feature of this equation is the absence of the solution when the concentration is more than the critical value of $c = 0.20024$, which is almost the same for both the above sets of data. The dependences of Ω and ε_F on c , which are connected with the behaviour of $B(c)$, are plotted in figure 2. Despite some quantitative distinction between the ratios ε_F/Ω for the two sets of data at the concentration $c = 0.2$, the comparable order of magnitude of the parameters ε_F and Ω still gives evidence of the

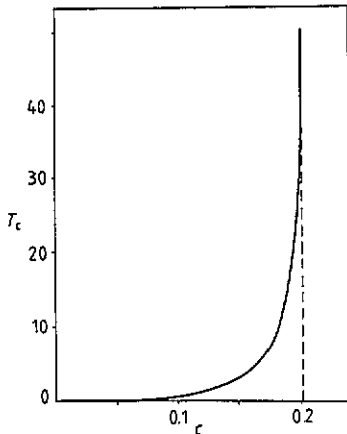


Figure 3. $T_c(K)$ versus the concentration c , which is the same for both sets of parameters: ---, $c = c_c$.

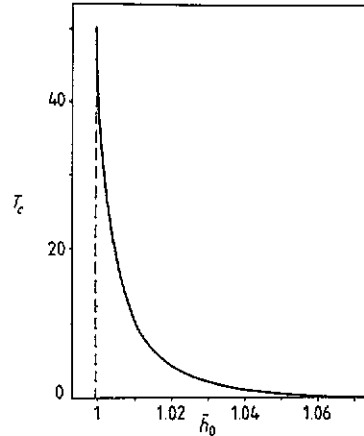


Figure 4. Dependence of the critical temperature T_c on the parameter $\hat{h}_0 = h_0/h_{00}$ at the concentration $c = 0.2$: ---, $\hat{h}_0 = 0.999$ which is the boundary of the region of solutions.

depression of the isotope effect [25]. It is also seen that the boson modes become softer upon increasing c . At the same time the local character of the boson modes in question excludes the appearance of any anomaly in the density of states, which could result in an additional enhancement of the critical temperature. The dependence of T_c on c is shown in figure 3, where within the scale of the picture it is the same for both sets of parameters considered. Hence, the obtained result is insensitive to the choice of values of the energy parameters within the adopted procedure of fitting them to the experimental data. The rather narrow concentration range where the values of T_c are high enough is also a peculiar feature, which is in agreement with experiments [28]. It is worth noting that the weak-coupling condition on which equation (18) is based is fulfilled in all the concentration range, although this condition becomes less strong near the limiting values of T_c . Making use of the momentum representation gives the averaged effect of the local bosons divided by shorter distances than the coherent length.

Inasmuch as the values of Ω and ε_F are of the same order of magnitude here, some comment is appropriate at this stage of the discussion. Low values of ε_F are typical of modern high- T_c superconductors [11]. Hence, the effect of the Coulomb interaction is a common problem for all the theories of superconductivity here. In our case the non-trivial character of manifestation of the Coulomb interaction can be expected. Like the local specificity of boson modes, it is associated with the supposed localization of the hole charge that is natural for polarizing unit cells distributed at random in the crystal lattice. However, this problem requires special investigation. The present mechanism can be treated as some type of model [6] with negative- U centres.

The character of the dependence of T_c on the cut-off momentum h_0 is shown in figure 4 and seems to be rather instructive. Here we see that the curves for both sets of solutions coincide almost on the plane of reduced coordinates as well. The critical temperature attains its limiting value of $\max T_c = 50$ K at $h_0/h_{00} = 0.999$, where h_{00} is the value of h_0 corresponding to the case of $c = 0.2$ for each set of data. It is interesting that the value of $\max T_c$ agrees with the maximal values obtained experimentally for lanthanum

ceramics under pressure [29, 30]. Some useful inference can be derived from the obtained dependence of T_c on h_0 . Indeed, the effect of the trivial contraction of a substance must apparently lead to a broadening of the hole conduction band due to increasing overlap integrals and hence to an increase in h_0 . On the basis of the opposite experimental tendency [10], we may maintain that conformal distortions appear in the case of longitudinal contraction of the oxygen layer as an element of the crystal structure, as will be discussed separately.

It is important that another type of temperature behaviour is admitted by the above solution as well. This takes place if some fixed value of Q is maintained [31]. Then, upon increasing c , the boson energy drops to zero, at which value the system becomes unstable. The appropriate behaviour of T_c versus c is described by a curve with a maximum, which is also experimentally confirmed [28]. In this case the corresponding curve with a maximum is typical for the dependence of T_c on h_0 too.

7. Conclusion

So we see that the hole polarization of unit cells in which the balance of chemical valencies is broken is capable of affecting the system in different ways. First, a hole conductivity arises in the oxygen band. The hole transitions from donors to the band and vice versa result in a dynamical charge redistribution with the appropriate polarization effect leading to local boson modes with a rather high frequency although the latter has the tendency to soften. These boson modes can be responsible for the superconducting pairing of holes. Even in the simplest case of the lanthanum systems mentioned above, the high critical temperatures can be achieved for natural values of the parameters. The depression of the isotope effect compared with the conventional case of the pure electron-phonon interaction is a peculiar feature of the obtained results.

In order to extend the present mechanism of superconductivity to more complicated metal oxide compounds, the representations developed in [32, 33] would be useful, where the idea that competition of copper ions as sites of hole polarization provides the random distribution and the local character of the excitations in question.

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