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Polaron motion in complex oxides and high-temperature superconductivity

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Abstract. The novel mechanism of polaron pairing in complex oxides and the possibility of *high-temperature superconductivity as a result* are reported. The peculiarity of complex oxides is taken into account by consideration of a medium with two optical phonon branches satisfying the adiabatic condition of the polaron theory and having different dispersions. The system of non-linear motion equations for the coupled fields of carriers and polarization is solved. It is shown that two carriers localized because of their interaction with one phonon branch form a bipolaron owing to the interaction with the real phonons of another branch under the resonance condition.

Such a novel bipolaron does not need a high static dielectric constant (SDC) for its formation, distinct from other bipolaron models. The novel bipolaron is energetically favourable compared with other bipolarons, when SDC is not high. By taking into account the peculiarity of bosons having a low maximum velocity, the expression for their condensation temperature is modified. As a result, the high-temperature Bose condensation of the novel bipolarons is shown to be possible at lower concentrations, even if their effective mass is very large.

1. Introduction

Most complex oxides have a 'soft' lattice which strongly interacts with the charge carriers. In such a system, charge carriers are likely to be present in the autolocalized (polaron) state (AS). This is the basis for the large number of bipolaronic theories of high-temperature superconductivity. There are also reports on the experimental observation of polarons or bipolarons in superconducting cuprates [1]. However, previously the fact that polarons in complex oxides have substantially different properties from those of the ordinary polaron according to Pecar's theory has not been taken into account. Indeed, Pecar's [2] polaron theory was constructed for alkali halide crystals, which have only one branch of phonons interacting with the charge carriers. In complex oxides, of many phonon branches, there are usually several satisfying the adiabatic condition of the polaron theory [2]. To investigate the effect of this on the carrier states in complex oxides we shall consider in the present paper the peculiar properties of polarons in a medium with two such phonon branches.

It will be shown that the peculiarities of the polaron motion in such a medium can lead to the formation of a novel bipolaron which is the bound state of a pair of polarons and real phonons under the resonance condition (this pairing mechanism has been proposed in [3]). For such bipolaron formation, high values of the

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static dielectric constant (SDC) ϵ_0 are not necessary as is required in other models of bipolarons (one-centre [4] and two-centre [5] models). If the SDC is not high ($\epsilon_\infty/\epsilon_0 > 0.2$, where ϵ_∞ is the high-frequency dielectric permittivity (DP)), our novel bipolaron is energetically favourable compared with the bipolarons mentioned above. The system of novel bipolarons is shown to be characterized by an unusual expression for the Bose condensation temperature so that the carrier concentration sufficient for condensation at a temperature of about 120 K is not high, even if the effective mass of bipolarons is very large. This allows us to overcome the typical difficulty of bipolaronic theories of high-temperature superconductivity.

As has been shown in [6, 7], polaron motion can be correctly investigated only when the dispersion of the phonon branch is taken into account, because the polaron velocity is restricted to the minimum phase velocity of phonons. The most interesting effects turn out to take place when the two phonon branches under consideration have different dispersions.

2. The effects of polaron motion in a medium with two active phonon branches

2.1. *The 'two-coat' polaron model*

Let us consider an AS of the charge carrier moving uniformly in a straight line with velocity v in a medium with two branches of longitudinal phonons. Their dispersion law is assumed to follow $\Omega_i^2(k) = \Omega_i^2 + u_i^2 k^2$, $i = 1, 2$, where u_i is the minimum phase velocity of the ith-branch phonons. The Hamiltonian for such a system can be written, using the mathematical formalism of [7], in the form

$$H = \int \mathrm{d}^3 r \left[\left[\varphi^* \left(E_0 - \frac{\hbar^2}{2m^*}\nabla_r^2 \right) \varphi + \sum_{i=1,2} \left\{ \frac{2\pi}{c_i \Omega_i^2} \left[\Omega_i^2 P_i^2 + \left(\frac{\partial P_i}{\partial t} \right)^2 - u_i^2 \boldsymbol{P}_i \cdot \nabla_r{}^2 \boldsymbol{P}_i \right] + e\boldsymbol{P}_i \cdot \int \frac{|\varphi(r', t)|^2}{|r - r'|} \mathrm{d}^3 r' \right\} \right] \right] \tag{1}$$

where m^* and E_0 are the effective mass and minimum energy of the free carrier, $c_1 = 1/\epsilon_1 - 1/\epsilon_0$, $c_2 = 1/\epsilon_\infty - 1/\epsilon_1$, ϵ_1 is the intermediate DP determined as $\epsilon_1 = \epsilon_\infty(\Omega_2/\Omega_{2\mathrm{TO}})^2$ if $\Omega_1 < \Omega_2$, and $\boldsymbol{P}_1$ and $\boldsymbol{P}_2$ are the dipole moments due to branch 1 and branch 2, respectively. The term $\boldsymbol{P}_i \cdot \boldsymbol{P}_j$ is absent in H because the vibrations belonging to different branches are independent in the harmonic approximation. The Hamiltonian (1) yields the following equations for the carrier wavefunction $\varphi(r, t)$ (which is supposed to be real) and the polarization charge distributions $\rho_i = -\mathrm{div}\, \boldsymbol{P}_i$, $i = 1, 2$, in a stationary state:

$$\left(\mathrm{i}h\frac{\partial}{\partial t} - E_0 + \frac{\hbar^2}{2m^*}\nabla_r^2 - e\int \frac{\rho_1(r', t) + p_2(r', t)}{|r - r'|} \mathrm{d}^3 r' \right) \varphi = 0 \tag{2}$$

$$(\partial^2/\partial t^2 + \Omega_i^2 - u_i^2 \nabla_r^2)\rho_i(r, t) = -c_i \Omega_i^2 \varphi^2(r, t) \qquad i = 1 \tag{3}$$

$$i = 2. \tag{4}$$

All characteristic effects in such a model can be easily revealed in the particular case $c_1 \ll c_2$. This allows us to consider the polarization $\boldsymbol{P}_1$ as a small perturbation

and to solve the system of the motion equations (2)–(4) by the method of sequential approximations. For a zero approximation $\rho_1^{(0)} = 0$, $\varphi^{(0)}$ and $\rho_2^{(0)}$ are determined from (2) and (4) as in [7]. In the first approximation, $\rho_1^{(1)}(\boldsymbol{r}, t)$ is obtained, substituting $\varphi^{(0)}$ into (3), and the first-order wavefunction $\varphi^{(1)}$ is the function minimizing the following functional:

$$J = -\int \mathrm{d}^3\boldsymbol{r}\,\varphi^{(1)}(\boldsymbol{r})\left(\frac{\hbar^2}{2m^*}\nabla_{\boldsymbol{r}}^2 + \frac{e^2}{2}\int \frac{G_1(\boldsymbol{r}_1-\boldsymbol{r}_2)\varphi^{(0)^2}(\boldsymbol{r}_2)c_1\Omega_1^2}{|\boldsymbol{r}-\boldsymbol{r}_1|} + \frac{G_2(\boldsymbol{r}_1-\boldsymbol{r}_2)\varphi^{(1)^2}(\boldsymbol{r}_2)c_2\Omega_2^2}{|\boldsymbol{r}-\boldsymbol{r}_1|}\,\mathrm{d}^3\boldsymbol{r}_1\,\mathrm{d}^3\boldsymbol{r}_2\right)\varphi^{(1)}(\boldsymbol{r}). \tag{5}$$

In (5) ρ_i are expressed, using the Green function in (3) and (4) obtained in [6, 7]:

$$\rho_i(\boldsymbol{r}, t) = -ec_i\Omega_i^2\int G_i(\boldsymbol{r}-\boldsymbol{r}', t)\varphi^{(0)^2}(\boldsymbol{r}', t)\,\mathrm{d}^3\boldsymbol{r}' \tag{6}$$

$$G_i(\boldsymbol{r}, t)_{i=1,2} = \begin{cases} \dfrac{\exp\{-\Omega_i[(z-vt)^2/\beta_{1i}^2 + r^2]^{1/2}/u_i\}}{4\pi u_i^2\beta_{1i}[(z-vt)^2/\beta_{1i}^2 + r^2]^{1/2}} & v < u_i,\ \beta_{1i}^2 = 1 - \dfrac{v^2}{u_i^2} \\ \dfrac{\cos\{\Omega_i[(z-vt)^2/\beta_{2i}^2 - r^2]^{1/2}/u_i\}}{2\pi u_i^2\beta_{2i}[(z-vt)^2/\beta_{2i}^2 - r^2]^{1/2}} & v > u_i,\ z-vt \leqslant 0,\ r < \dfrac{|z-vt|}{\beta_{2i}} \\ 0 & v > u_i, \begin{cases} z-vt \leqslant 0,\ r > \dfrac{|z-vt|}{\beta_{2i}} \\ z-vt > 0,\ \beta_{2i}^2 = \dfrac{v^2}{u_i^2} - 1 \end{cases} \end{cases} \tag{7}$$

in cylindrical coordinates with the z axis directed along the polaron velocity $\boldsymbol{v}$. It would be convenient to call the polarization charge distributions ρ_i, $i = 1, 2$, the polarization 'coats' of the carrier. It is clear from (6) and (7) that $v = u_i$ is the critical velocity for the polarization 'coat' number i because, in the vicinity of $v = u_i$, $G_i(\boldsymbol{r}, t)$, and hence $\rho_i(\boldsymbol{r}, t)$, changes dramatically. Therefore in the medium under consideration, there are three parts of the velocity axis, namely $v < u_1$, $u_1 < v < u_2$ and $v < u_2$ (if $u_1 < u_2$), corresponding to different states of the carrier.

2.2. The carrier states in the 'two-coat' model

When $v < u_1$, the AS obtained as the first-order solution to equations (2)–(4) has a smaller radius, a larger binding energy and a larger effective mass than the zero-order approximation does. Indeed, the latter is the AS with one polarization 'coat' consisting of phonons of branch 2 only, whereas in the former case an additional polarization charge appears caused by branch 1. This conclusion can be verified by the calculation of the complete polaron charge; it turns out to be e/ϵ_0. We shall call such a polaron a heavy polaron (HP). The binding energy E_{HP} and radius R_{HP} of

the HP can be evaluated using the ordinary formulae of the polaron theory [2] with the inverted effective DP $c = 1/\epsilon_\infty - 1/\epsilon_0 = c_1 + c_2$.

When $v > u_1$, the Green function $G_1(r,t)$ (7) oscillates with the period $u_1\beta_{2i}/\Omega_1$ along the z axis. It is much less than the radius of the carrier localization region, so that integration in (6) yields $\rho_1 \simeq 0$. Hence, the first-order solution to (2)–(4) does not differ from the zero-order approximation. Thus, it is clear that for the polaron moving with $v > u_1$, the carrier localization is maintained only by the second phonon branch. This polaron has a smaller binding energy and a smaller effective mass than the HP does; so we shall call it the light polaron (LP). Its characteristics E_{LP}, m^*_{LP} and R_{LP} are determined by ordinary polaron theory for the medium with one phonon branch [2, 7].

When $v > u_2$, the Green function $G_2(r,t)$ also becomes oscillating, so that the polarization charge distributions necessary to keep the carrier in the AS cannot be obtained from (6). Thus, the maximum polaron velocity in the model under consideration is $v = u_2$.

2.3. LP braking by the coherent phonon radiation

Since we are interested in the carrier AS in the velocity interval $u_1 < v < u_2$, in further analysis we shall suppose that $u_1 \ll u_2$ and call the corresponding phonon branches the low-velocity (LV) and high-velocity (HV) branches. The form of $\rho_1(r,t)$ at $v \gg u_1$ (which is oscillating quasi-harmonically) leads to the following conclusion made for the first time in [6]. When the LP moves with a velocity exceeding the minimum phase velocity of the LV branch, it excites not virtual but real phonons of this branch as the result of an effect, which is similar to Cherenkov's effect. If $v \gg u_1$, the radiation of different parts of the electron density distribution is coherent, so that a wave of real coherent phonons is formed in the acoustic cone $r < |z - vt|/\beta_{2i}$ behind the LP. Hence, the mechanism of braking by coherent radiation actually occurs for LPs at velocities $u_1 \ll v < u_2$ and the stationary straight-line motion of LPs is possible only if an electric field is present. Nevertheless, it turns out that LP stationary motion is possible without an external field, if it is motion with a circular orbit.

3. The effects of the resonance of LP motion with the vibrations of the medium

3.1. The bound state of one LP and real phonons

Let us find the solutions to the motion equations (2)–(4) corresponding to LP motion on a circular orbit of radius $R_0 \gg R_{LP}$ with frequency ω. The velocity $v = \omega R_0$ of the motion is assumed to satisfy the inequality $u_1 \ll v < u_2$. The features of our model allow us to make the following simplifying suppositions. Since $v \gg u_1$, the third term in the left-hand side of (3) is negligible. It can also be shown that the result changes slightly when (4) is replaced by the simpler Pecar expression $\rho_2(r,t) = -c_2|\varphi(r,t)|^2$ for the polarization charge distribution in polarons because the LP may be considered as an ordinary polaron, occurring owing to the carrier interaction with the HV phonons. We shall denote equations obtained after such a simplification as (3′) and (4′).

To solve the system (2), (3′), (4′) we shall express the unknown $\rho_1(r,t)$ in (2) in terms of φ, using (3′) and (6). The specialized Green function for (3′) corresponding to periodic LP motion on a circular orbit is obtained (in cylindrical coordinates with

coordinate origin at the orbit centre and the z axis perpendicular to the orbit plane) as the solution to the following equation:

$$(\partial^2/\partial t^2 + \Omega_1^2)G(\boldsymbol{r}, \boldsymbol{r}', t) = \delta(r - r')\delta(z - z')\delta(\phi - \phi' - \omega t)/r'. \tag{8}$$

The stationary states are obviously characterized by the stationary polarization charge distribution $\rho_1(\boldsymbol{r}, t)$. As has been found in [5], it takes place at the frequencies

$$\omega = 2\Omega_1/(2l + 1) \qquad l = 0, 1, 2, \ldots \tag{9}$$

and the corresponding Green function has the form [5]

$$G_l(\boldsymbol{r}, \boldsymbol{r}', t) = [(2l + 1)/4r'\Omega_1^2] \sin[(2l + 1)(\phi - \phi')/2 - \Omega_1 t]\, \delta(r - r')\delta(z - z'). \tag{10}$$

Now, to solve equation (2) we can apply the direct variational method. The ground-state wavefunction must minimize the following functional:

$$J = -\int \mathrm{d}^3\boldsymbol{r}\, \varphi(\boldsymbol{r}) \left[\frac{\hbar^2}{2m^*} \nabla_{\boldsymbol{r}}^2 + \frac{e^2}{2} \int \mathrm{d}^3\boldsymbol{r}_1 \left(c_1 \int \mathrm{d}^3\boldsymbol{r}_2\, G(r_1, r_2)\varphi^2(r_2) + c_2\varphi^2(r_1) \right) \right] \varphi(\boldsymbol{r}). \tag{11}$$

As the test function we use the Gaussian normalized function

$$\varphi(r, t) = (2/\pi)^{3/4}(\sqrt{\alpha}\beta)^{1/2} \exp\{-\alpha r^2 \sin^2(\phi - \omega t) - \beta[r\cos(\phi - \omega t) - R_0]^2 - \beta z^2\} \tag{12}$$

which allows us to take into account the violation of spherical symmetry of the charge distribution in LPs due to the interaction with the 'LV' polarization charge, with the coordinate origin still at the orbit centre.

The numerical computation according to $l = 0$ has shown that the functional (10) has a minimum in a certain region of the parameters of the medium. The quasi-particle corresponding to this minimum is the bound state of LP and real LV phonons. From (9) for the frequencies of LP stationary motion the conclusion can be derived that the bound state occurs as a result of the resonance with the vibrations of branch 1 in the medium. The motion of the localized charge particle here plays the role of external force (which is periodic but not harmonic). The set of stationary motion frequencies turns out to be characteristic for the parametric resonance. To emphasize this we shall call the quasi-particle a 'parametreson'. Its binding energy exceeds the LP energy E_{LP} by about 0.01 eV. Its radius, which is approximately equal to the orbit radius R_0, is determined therefore by the equilibrium of forces affecting the LP.

The parametreson may be regarded as the excited state of an HP because it includes real LV phonons which are present in an HP as virtual phonons. If the minimum of the functional (11) also exists when $l \neq 0$, other parametresons exist with

a certain binding energy, radius and effective mass for each l-value. The minimum of the functional (11) provides the parametreson stability. The factors which are not taken into account in (1) and (11) cannot lead to the destruction of the parametreson because of their weakness. For instance, phonon relaxation is negligible, since the width of the phonon level is much less than the parametreson binding energy E_P. As the kinetic energy of LV phonons is also much less than E_P, the parametreson is not broken by the radiation of LV phonons.

3.2. Resonance LP pairing

Let us consider in the same model the motion of two LPs on a circular orbit. The Hamiltonian of such a system has the form

$$H = \int d^3r \left[\psi^+(r) \left(E_0 - \frac{\hbar^2}{2m^*} \nabla_r^2 \right) \psi(r) + \sum_{i=1,2} \frac{2\pi}{c_i \Omega_i^2} \left(\frac{\partial P_i}{\partial t} + \Omega_i^2 P_i^2 - v_i^2 P_i \cdot \nabla_r^2 P_i \right) \right.$$
$$+ e(P_1 + P_2) \cdot \nabla_r \int \frac{\psi^+(r')\psi(r')}{|r - r'|} d^3r'$$
$$\left. + \frac{1}{2} \int \frac{\psi^+(r)\psi^+(r')e^2\psi(r')\psi(r)}{\epsilon_\infty |r - r'|} d^3r' \, d^3r \right] \tag{13}$$

where ψ is the particle-field operator. Other notation in (13) is analogous to that in (1). It is convenient here to use for the electron part of the system the self-consistent field (SCF) approximation and to characterize the two carriers under consideration by the single-particle wavefunctions $\varphi_1(r, t)$ and $\varphi_2(r, t)$. They are orthogonal to each other because they do not overlap. Supplementing them to obtain the complete set, we can expand the particle-field operator in terms of single-particle functions. Substituting this expansion in the motion equation for ψ, then acting on both parts of it by the operator of the creation of the first or the second particle and, finally, averaging them over the state under consideration, we obtain the following system of equations for the single-particle wavefunctions φ_1 and φ_2:

$$\left[-ih \frac{\partial}{\partial t} + E_0 - \frac{\hbar^2}{2m^*} \nabla_r^2 - e \left(\int \frac{\rho_1(r', t) + \rho_2(r', t)}{|r - r'|} d^3r + V_j(r, t) \right) \right]$$
$$\times \varphi_i(r, t) = 0. \tag{14}$$

Here the potential V_j of the SCF of another carrier has the form

$$V_j(r, t) = \frac{e}{\epsilon_\infty} \int \frac{\varphi_j^2(r, t)}{|r - r'|} d^3r' \qquad i = 1, 2 \qquad i \neq j. \tag{15}$$

Owing to the symmetry of the problem, single-particle wavefunctions satisfy the condition $\varphi_1(r, \phi - \omega t, z) = \varphi_2(r, \phi - \omega t + \pi, z)$. After taking this condition into consideration, the system of equations (14) becomes a pair of independent identical

equations. This equation with the two following equations for the polarization charge distributions

$$[(1/\Omega_1^2)(\partial^2/\partial t^2) + 1]\rho_1(\boldsymbol{r}, t) = -ec_1[\varphi_1^2(\boldsymbol{r}, t) + \varphi_2^2(\boldsymbol{r}, t)] \tag{16}$$

$$\rho_2(\boldsymbol{r}, t) = -ec_2[\varphi_1^2(\boldsymbol{r}, t) + \varphi_2^2(\boldsymbol{r}, t)] \tag{17}$$

form a system which should be solved as in section 3.1.

The specialized Green function for (16) satisfies the following equation:

$$[(1/\Omega_1^2)(\partial^2/\partial t^2) + 1]G(\boldsymbol{r}, \boldsymbol{r}', t) = \delta(r - r')\delta(z - z')[\delta(\phi - \phi' - \omega t) + \delta(\phi + \pi - \phi' - \omega t)]/r'. \tag{18}$$

Myasnikov and Popov [6] have shown that equation (18) has stationary solutions in the form

$$G_n(\boldsymbol{r}, \boldsymbol{r}', t) = [(2n + 1)/2r'\Omega_1^2]\sin[(2n + 1)(\phi - \phi') - \Omega_1 t]\delta(z - z')\delta(r - r') \tag{19}$$

at the frequencies

$$\omega = \omega_n = \Omega_1/(2n + 1) \qquad n = 0, 1, 2, \ldots . \tag{20}$$

The solution to (16) is expressed in terms of $G_n(\boldsymbol{r}, t)$ in accordance with (6). Here we shall confine ourselves to consideration of the case $n = 0$. Similarly to the analysis carried out in section 3.1, the single-particle wavefunction corresponding to the bound state must minimize the following functional:

$$J = -\int \mathrm{d}^3\boldsymbol{r}\, \varphi_1(\boldsymbol{r}) \left[\frac{\hbar^2}{2m^*}\nabla_r^2 + \frac{e^2}{2}\int \frac{\mathrm{d}^3\boldsymbol{r}'}{|\boldsymbol{r} - \boldsymbol{r}'|} \times \left(c_2\varphi_1^2(\boldsymbol{r}') - \frac{\varphi_2^2(\boldsymbol{r}')}{\epsilon_\infty} + c_1\int G_0(\boldsymbol{r}', \boldsymbol{r}_1)\varphi_1^2(\boldsymbol{r}_1)\,\mathrm{d}^3\boldsymbol{r}_1\right)\right]\varphi_1(\boldsymbol{r}). \tag{21}$$

We have minimized functional (21) numerically, using the test function (12) for several sets of parameters of the medium. For instance, for the parameters

$$\Omega_1 = 34\ \mathrm{cm}^{-1} \qquad \Omega_2 = 360\ \mathrm{cm}^{-1}$$
$$\epsilon_\infty = 2.2 \qquad \epsilon_1 = 7.2 \qquad \epsilon_0 = 10 \tag{22}$$
$$m^* = m_e$$

the function (12) minimizes (21) when $\alpha = 0.012$ Å and $\beta = 0.014$ Å. The quasi-particle corresponding to the minimum of the functional can be called the Bose parametreson (BP). Applying this to (22), its binding energy with respect to the energy of two LPs is about 0.026 eV. The BP radius R_{BP}, which is considered to

coincide with the orbit radius, is determined from the centripetal force acting on each LP. It should be noted that the parameters of the medium in a wide range fulfil the inequality $R_{BP} \gg R_{LP}$ and the applicability condition of the continual approximation $R_{LP} > a$ (a is the lattice constant). The minimum phase velocities of the phonons must satisfy the inequality $u_1 \ll v_0 < u_2$, where $v_0 = \omega R_{BP}$ is the LP velocity in the BP. For the parameters (22), one can obtain $v_0 \simeq 10^6$ cm s^{-1}, so that BP formation is possible only if the HV phonon branch has a high dispersion. It should also be noted that the BP size is characterized by significant anisotropy. Indeed, the BP size is determined by R_{BP} in the orbit plane and in the direction perpendicular to it by R_{LP}. This anisotropy will lead to a coherence length anisotropy which is typical for superconducting cuprates.

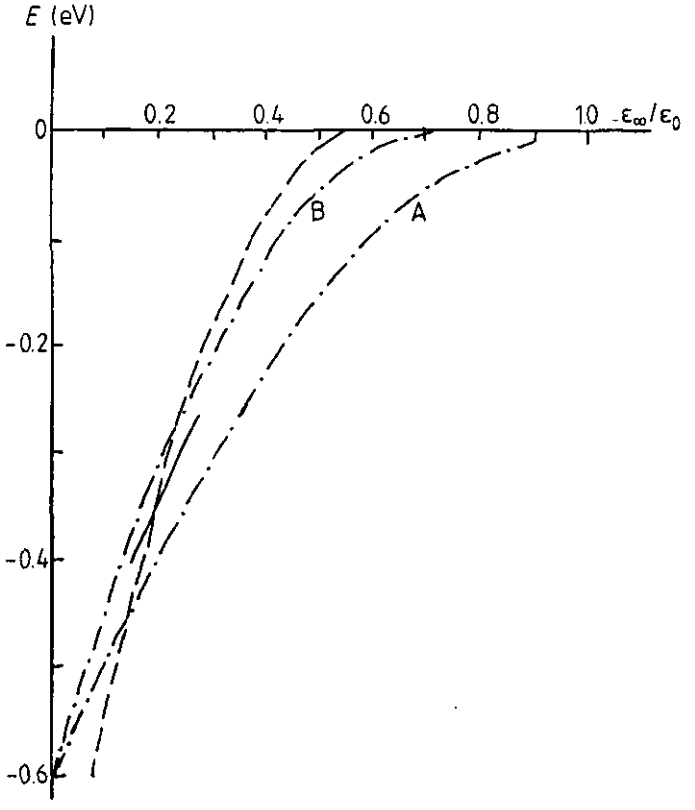

Figure 1. The energies of states of two carriers in a medium with two phonon branches which can participate in carrier localization (in the case of $\epsilon_\infty = 2.2$, $\epsilon_1/\epsilon_0 = 0.72$): ——, BPs; — · —, curve A, HPs; — · —, curve B, LPs; – – –, Suprun–Moijes bipolarons. (The energies are with respect to the level of two free carriers.)

Figure 1 (full curve) presents the BP energy E_{BP} (obtained with respect to the energy of two free carriers) versus $\epsilon_\infty/\epsilon_0$. The chain curves A and B in figure 1 display the energies of two HPs and two LPs, respectively. The broken curve demonstrates the energy of the Suprun–Moijes [4] bipolaron which is a one-centre bipolaron of the Pecar type with correlation of the carrier motion. Figure 1 corresponds to the parameters (22) apart from those which are variable in the figure. As is clear from figure 1, in the region $\epsilon_\infty/\epsilon_0 > 0.2$ the BP state is energetically favourable in com-

parison with a one-centre bipolaron and two LPs. Although the double-HP energy level is lower than the other energy levels, the HP concentrations in the system are shown below to be restricted to small values negligible in comparison with the carrier concentrations in high-temperature superconductors.

The effective mass m^*_{BP} of the BP is determined mostly by the mass of real LV phonons contained in the BP. Until the solution to equation (3) with $u_1 \neq 0$ is found, m^*_{BP} can be estimated as a product of the average number $n_{ph} = E_{own}/\hbar\Omega_1$ of LV phonons in the BP and the mass $m^*_{ph} = \hbar\Omega_1/u_1^2$ of one LV phonon (for quadratic dispersion and small values of the wavevector). The BP mass obtained by such a method is expressed as $m^*_{BP} = E_{own}/u_1^2$, where E_{own} is the energy of LV polarization.

Thus, we have shown that in a medium of complex-oxide type, apart from two polaron states, novel (parametreson) stationary states of the charge carriers and polarization can exist. In these states, the carriers localized because of the interaction with phonons of one (HV) branch move in resonance with the vibrations of another (LV) branch. To draw a conclusion about the possibility of BP high-temperature superconductivity it is required to ascertain the equilibrium concentrations of all the quasi-particles described above.

4. Thermodynamical equilibrium in the system of carriers in our model of the medium

4.1. The velocity distribution of polarons

Since polarons exist only in a limited velocity interval, it is important to consider the question about velocity (or momentum) distribution of autolocalized fermions. Let us show that the effect of the fermion origin of carriers on the velocity distribution of polarons is negligible, as was assumed in [2], if their concentration does not exceed a certain critical value. Indeed, the AS is a wave packet with certain dispersion of the carrier coordinate and momentum with respect to their average values. Localization of carriers in different regions of coordinate and momentum space provides orthogonality of such single-particle states. Let us consider filling these states for the simple model of AS. In this model the probability density of finding the carrier is constant inside a cube of side $2\Delta q_0$ in the coordinate space and sphere of radius Δp_0 in the momentum space and is equal to zero outside them. Such a model accurately corresponds to the real polaron from the viewpoint of the phase-space volume per one state, if the coordinate dispersion Δq and momentum dispersion Δp in both states coincide. For instance, if the carrier wavefunction has the form [2] $\varphi(r) \sim (1 + \alpha r)\exp(-\alpha r)$, $\Delta q = 2.4/\alpha$ and $\Delta r = 0.655\alpha$, and one can easily obtain $\Delta q_0 = \Delta q$ and $\Delta p_0 = \Delta p/0.775$.

In accordance with the principle of minimum energy, the states with zero momentum are filled in the ground state in the first place, so that the critical concentration $n_{cr} = 2/(8\Delta q_0^3)$ is distinguished clearly. Until this concentration is reached, the maximum carrier momentum is Δp_0 (the temperature $T = 0$ K) and it does not depend upon carrier concentration. Therefore, when the carrier concentration is less than n_{cr} (and even a little over n_{cr}), the fermion origin of autolocalized carriers can be neglected (especially as they experience Coulomb repulsion). We shall consider here polarons at such concentrations, applying Boltzmann statistics to them.

4.2. The equilibrium concentrations of the quasi-particles

The equilibrium (at certain temperature) concentrations of carrier bound states are determined by their binding energy, effective mass and range of momenta accessible to them. In sum they give the total carrier concentration in the system:

$$n = \frac{1}{\pi^2\hbar^3}\left\{\int_{m^* u_2}^{\infty} \frac{p^2\,dp}{\exp[(p^2/2m^* - \mu)/T] + 1} + \int_0^{p_1} \exp\left(-\frac{p^2/2m^*_{HP} + E_{HP} - \mu}{T}\right) p^2\,dp + \int_{p_2}^{p_3} \exp\left(-\frac{p^2/2m^*_{LP} + E_{LP} - \mu}{T}\right) p^2\,dp + \int_0^{p_4} p^2\,dp \left[\exp\left(\frac{2(p^2/4m^*_{BP} + E_{BP}/2 - \mu)}{T}\right) - 1\right]^{-1}\right\} \tag{23}$$

where μ is the chemical potential of 'free' carriers. The terms on the right-hand side of (23) correspond to the concentrations of 'free' carriers, HPs, LPs and BPs, respectively. The parametresons described in section 3.1 (which can be called Fermi parametresons) are absent in (23) because, for the parameters of the medium considered here, the LP orbital velocity in the Fermi parametreson is higher than the LP maximum velocity u_2. The main special feature of (23) is determined by the AS property which exists only in a limited velocity interval. For HPs and LPs they are $v < u_1$ and $u_1 < v < u_2$, respectively, so that the notation in (23) can be expressed as follows: $p_1 = m^*_{HP}u_1$, $p_2 = m^*_{LP}u_1$ and $p_3 = m^*_{LP}u_2$. The BP velocity is also limited. It cannot exceed either the maximum group velocity u_2 of LV phonons (because the BP includes real LV phonons) or the difference Δv between the maximum LP velocity u_2 and its velocity v_0 in the BP: $\Delta v = u_2 - v_0$. Thus, the upper limit of the BP momentum is $p_4 = m^*_{BP}v_k$, where v_k is the smaller of the two velocities u_2 and Δv.

We shall show that, when this peculiarity of parametreson states is taken into account in (23), one comes to the conclusion that Bose condensation at a temperature of about 120 K is possible in the system of BPs at not very high concentrations, even if the BP effective mass is very large. As is clear from (23), the condition of BP Bose condensation has the form $\mu = E_{BP}/2$. For the medium (22) at such a μ and a temperature $T \simeq 0.01$ eV, the concentration of carriers in all states, except BP, is negligible compared with their number in the BP state. (Their maximum, the HP concentration n_{HP}, is about 2×10^{19} cm^{-3}, so that the condition $n_{HP} < n_c \approx 6 \times 10^{20}$ cm^{-3} is satisfied.) Therefore the carrier concentration necessary for BP Bose condensation at a temperature T_0 (which would be the temperature of the superconducting transition in this case) can be expressed as

$$n_{BC} = (2/\pi^2\hbar^3)m^{*2}_{BP}v_kT_0 = (2/\pi^2\hbar^3)E^2_{own}v_kT_0/u_1^4 \tag{24}$$

if the inequality $m^*_{BP}v_k^2/2 < 0.5T_0$ is fulfilled.

Since the calculation was performed at $u_1 = 0$, the E_{own} dependence on u_1 is unknown and either of the following two variants can take place. If $E^2_{own} \simeq u_1^l$,

$l > 3$, then the smaller concentration n_{BC} will be realized at $u_1 \to 0$. If $l \leqslant 2$, the minimum n_{BC} will correspond to high (but, of course, satisfying the condition $u_1 \ll v < u_2$) values of u_1. In the latter case, $v_k = \Delta v$.

It is clear from (24) that, changing this new parameter v_k of the theory which is determined by the oscillator strengths and dispersions of the two phonon branches, at constant temperature one can change the n_{BC}-value. It should be noted that the described peculiarity in the expression for the quasi-particle concentration versus chemical potential of 'free' carriers and temperature takes place not only for a BP but for any quasi-particle which includes phonons or other quasi-particles with a low-velocity limit. (For the Suprun–Moijes bipolaron, for instance, the upper velocity limit is u_1.) Thus, the described property of the BP state enables us to overcome a typical difficulty of the bipolaron superconductivity theories—the necessity of high bipolaron concentrations because of their large effective mass.

5. Conclusion

The present consideration of the charge-carrier states in a medium with two phonon branches capable of participating in carrier autolocalization (which reflects the peculiarity of the complex oxides) allows us to draw the following conclusions. If the dispersions of these two branches (characterized by the phonon minimum phase velocities u_1 and u_2) are different ($u_1 < u_2$), the LV branch cannot take part in the autolocalization of the charge carrier moving with $v > u_1$ which is autolocalized owing to the interaction with HV phonons ($u_2 > v$). This leads to the existence of two polaron types in such a medium in different velocity ranges. Nevertheless, the presence of the LV branch results in radiation of real coherent LV phonons by the LP moving with velocity v, if $u_1 \ll v < u_2$. Apart from the LP translation braking by coherent phonon radiation, this effect can lead to the formation of a novel stationary state of a pair of LP and real LV phonons, i.e. a BP.

If the inequality $\epsilon_\infty/\epsilon_0 > 0.2$ is satisfied, this BP state is energetically favourable compared with bipolarons that occur owing to the carrier interaction with only virtual phonons. As shown in section 4, if the concentration of the carriers is about 10^{20}–10^{21} cm^{-3}, almost all of them are in the BP state. Because of the restriction of the BP velocity, Bose condensation at a temperature $T_0 \simeq 0.01$ eV can take place in the system of BPs at a much smaller concentration than the ordinary formula for ideal bosons of the same effective mass yields. (Moreover, such a situation is realized for any bosons including quasi-particles with a comparatively low maximum velocity.) Thus, we conclude that, in a medium such as a complex oxide, high-temperature superconductivity by means of BPs can take place at carrier concentrations close to that in high-temperature superconductors.

Since the BP effective mass and, consequently, n_{BC} (24) do not depend on the phonon frequencies in the open form and since E_{own} depends slightly on them, the superconductivity isotopic effect must be weak in our model, as occurs in superconducting complex oxides. The anisotropy of the coherence lengths, the pair size and the binding energy obtained in our model correspond well to the experimental data on complex oxides. So the model proposed here turns out to describe the effects experimentally observed in superconducting cuprates. To verify the correspondence of the model considered here to the superconducting oxides it would be useful to check the presence in them of at least two phonon branches participating in the carrier autolocalization and to examine their dispersion. (The calculation in [8] shows

that the condition of high dispersion of one active phonon branch can be satisfied in complex oxides at least in the region of small wavevectors which is important in this problem.) Finally, as is shown in [9], another characteristic feature of the 'two-coat' model is the unusual behaviour of low-temperature carrier mobility. This may also be used to verify the applicability of this model to the explanation of superconductivity in complex oxides.

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