An approach for studying the influence of uniaxial strain (pressure) on the temperature of the Bose-Einstein condensation of intersite bipolarons: possible implementation for RBa$_2$Cu$_3$O$_{7-\delta}$ cuprates

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Abstract

A universal approach is proposed to study the influence of strain (pressure) on the temperature of Bose-Einstein condensation of intersite bipolarons within the extended Holstein model. It is shown that uniaxial strain (pressure) derivatives of the temperature of such a Bose-Einstein condensation strongly depend on the arrangement of ions in the lattice. In particular, they may be positive or negative. A connection between the theoretically obtained results, along with the experimental data, on the influence of uniaxial pressure (strain) on $T_c$ of RBa$_2$Cu$_3$O$_{7-\delta}$ family cuprates is discussed.

Key words: bipolaron, strain (pressure), Bose-Einstein condensation, cuprates

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1. Introduction

The extended Holstein model (EHM) was introduced in Ref. [1], primarily for the explanation of smallness of charge carrier’s mass in the cuprates. In the strong coupling regime (or when the electron-phonon interaction is strong), the small value of EHM polaron’s mass compared to that of the usual Holstein model [2], is primarily ensured by the long-range nature of the electron-phonon interaction (interaction via Fröhlich type density-displacement force). In the last decade, different properties of the EHM were studied by several authors (see review article [3]). In Ref. [4], Kornilovitch studied the ground state energy, effective mass and polaron spectrum with the help of the continuous-time Quantum Monte Carlo algorithm. An anisotropy of the polaron’s mass due to electron-phonon interaction, ground-state dispersion, and density of states of the EHM polaron were studied in Refs. [5, 6]. Fehske, Loos and Wellein [7] investigated the electron-lattice correlations, single-particle spectral function and optical conductivity of a polaron within the EHM in the strong and weak coupling regimes by means of the Lanczos diagonalization method. Other properties of the EHM, such as the ground state spectral weight, the average kinetic energy and the mean number of phonons were studied in Refs. [8–10] by means of the variational and Quantum Monte Carlo simulation approaches. The work of Ref. [11] extended the EHM to the adiabatic limit. The influence of the different types of polarized vibrations, and the arrangement of the ions on the mass of polaron, have been studied in Refs. [12–14]. The EHM with screened electron-phonon interactions was discussed in Refs. [5, 15–19]. The influence of both local and nonlocal electron-phonon interactions on the full polaronic effect within
the EHM was studied in Ref. [20], finding that these interactions can compensate for each other, resulting in the suppression of polaronic effects. The EHM was used to study a polaron formation in semiconducting polymers, finding the polaron’s energy, its size, and lattice deformation as a function of the conjugation length [21].

Quite recently, one of us (B.Ya.Ya.) extended an application of the EHM to La-based cuprate films under pressure (strained films) [22]. Namely, in that work, a unified approach for studying the influence of pressure (stress or strain) on the temperature of Bose-Einstein condensation of intersite bipolarons was proposed. Uniaxial strain derivatives of Bose-Einstein condensation temperature ($T_{BEC}$) of intersite bipolarons were calculated. Having accepted the bipolaronic scenario as a ground for high-$T_c$ superconductivity of cuprates, the experimental results on the influence of lattice mismatch to the critical temperature ($T_c$) of La-based high-$T_c$ films were explained. In particular, the results of two experiments [23, 24] were explained within the framework of the EHM and the bipolaronic theory of superconductivity. The main features of the model proposed in Ref. [22] are: (i) compressive pressure (strain) in the $ab$–plane of cuprates enhances $T_{BEC}$ and (ii) compressive pressure (strain) along $c$–axis of cuprates reduces $T_{BEC}$. Such variations of the $T_c$ of cuprates with respect to applied pressure (strain) are often observed [25]. The proposed model allows one to interrelate strains in each axis with each other and to study their cumulative effect on $T_{BEC}$.

Here, we continue to study the influence of strain induced by external pressure or lattice mismatch on $T_{BEC}$ for different lattices. Special attention will be given to the possibility of qualitative explanation of such
phenomena as sign difference of the strain (pressure) derivatives of $T_c$ of RBa$_2$Cu$_3$O$_{7-\delta}$ cuprates ($R$ stands for Yb, Y, Dy or Gd) along the $a-$ and $b-$axes. RBa$_2$Cu$_3$O$_{7-\delta}$ compounds stand apart from other cuprates (with the CuO$_2$ planes only) because of the presence of Cu-O chains along the $b$-axis in the crystal structure. Strong anisotropy of crystal structure gives rise to the anisotropy of electronic, thermodynamic, transport and other properties of the RBa$_2$Cu$_3$O$_{7-\delta}$ family of materials. In particular, uniaxial strain derivatives of the critical temperature, $T_c$, along crystallographic axes $a$ and $b$ have opposite sign: $\partial T_c/\partial \varepsilon_a < 0$ and $\partial T_c/\partial \varepsilon_b > 0$. The value of the uniaxial strain derivative of the critical temperature of cuprates along $c-$ axis, $\partial T_c/\partial \varepsilon_c$, lies in a wide range, but all values are negative. There are several works that theoretically explain uniaxial the strain (pressure) derivatives of the critical temperature of RBa$_2$Cu$_3$O$_{7-\delta}$ cuprates [26–31]. Though the theoretical models (see above works) proposed so far were able to somehow explain the uniaxial pressure (strain) derivatives of $T_c$ of RBa$_2$Cu$_3$O$_{7-\delta}$ compounds and reproduce some aspects of the well-known experiments [32, 33], they miss the important issue relevant to all cuprates. The issue is the presence of strong electron-phonon interaction in the cuprates [34, 35] and the polaronic nature of charge carriers [36, 37]. An another point is that those models are applicable to only one cuprate compound, for example to the RBa$_2$Cu$_3$O$_{7-\delta}$ family, and do not discuss the same problems in La- and Bi-based cuprates. In this sense those models lack universality. Therefore, at present, development of a model that explains the uniaxial strain (pressure) derivatives of $T_c$ from the universal point of view and takes into account strong electron-phonon interaction in the cuprates is one of the most important research tasks in the
way of our understanding the microscopic origin of high-$T_c$ phenomena.

Our model, proposed in [22], does not suffer from the above-mentioned imperfections. Below we show that the EHM and Bose-Einstein condensation scenario of intersite bipolarons, if one accepts the latter to be responsible for high-$T_c$ superconductivity of cuprates, are able to qualitatively explain the sign difference of $\partial T_c/\partial \varepsilon_a < 0$ and $\partial T_c/\partial \varepsilon_b > 0$.

2. The Model Hamiltonian and lattices

We write the Hamiltonian of the system of electrons and phonons [1, 38] as

$$ H = H_e + H_{ph} + H_V + H_{e-ph}, \quad (1) $$

where

$$ H_e = \sum_{n \neq n'} T(n - n') c_{n}^{\dagger} c_{n'} $$

(2)

describes the hopping of electrons between adjacent sites,

$$ H_{ph} = \sum_{q, \alpha} \hbar \omega_{q\alpha}(d_{q\alpha}^{\dagger} d_{q\alpha} + 1/2), \quad (3) $$

is the Hamiltonian of the phonon system,

$$ H_V = \sum_{n \neq n'} V_C(n - n') c_{n}^{\dagger} c_{n} c_{n'}^{\dagger} c_{n'}, \quad (4) $$

is the Hamiltonian of interacting particles at sites $n$ and $n'$ via Coulomb forces, and

$$ H_{e-ph} = \sum_{nm\alpha} f_{m\alpha}(n)c_{n}^{\dagger} c_{n} \xi_{m\alpha} \quad (5) $$

is the Hamiltonian of electron-phonon interaction. Here $T(n - n')$ is the transfer integral of electron from site $n$ to site $n'$, $c_{n}^{\dagger} (c_{n})$ is the creation
(annihilation) operator of an electron at site \( n \), \( d_{q\alpha}^\dagger(n) \) is the creation (annihilation) operator of a phonon with \( \alpha (\alpha = x, y, z) \) polarization and wave vector \( q \). \( \omega_{q\alpha} \) is the phonon’s frequency, \( V_C(n - n') \) is the Coulomb potential energy of two electrons located at sites \( n \) and \( n' \), \( f_{m\alpha}(n) \) is the ”density-displacement” type coupling force of an electron at site \( n \) with the apical ion at site \( m \) (Fig.1), and \( \xi_{m\alpha} \) is the normal coordinate of ion’s vibration on site \( m \) which is expressed through phonon creation and destruction operators as

\[
\xi_{m\alpha} = \sum_q \left( \sqrt{\frac{\hbar}{2NM\omega_{q\alpha}}} e^{i q m} d_{q\alpha}^\dagger + h.c. \right).
\]

Here \( N \) is the number of sites and \( M \) is the ion’s mass. We work with dispersionless phonons and take into account only the \( c \)-polarized vibrations of ions, as charge carriers in the CuO\(_2\) plane of the cuprates strongly interact with \( c-\) polarized vibrations of apical ions \(^{39}\). The lattice of Figure 1A was introduced by Alexandrov and Kornilovitch in Ref. \(^1\) in order to mimic the interaction of a hole on the CuO\(_2\) plane with the vibrations of apical ions in the cuprates (Figure 1B is considered in Ref. \(^{40}\)). Such one dimensional lattices have similarity with some ions arrangements in the real structure of RBa\(_2\)Cu\(_3\)O\(_{7-\delta}\) cuprates. Indeed in the both lattices the upper chain (open circles) represents apical ions of oxygen at position O(4). The lower chain of Fig.1A consists of copper Cu(1) ions of Cu(1)-O(1) chain or copper Cu(2) ions of CuO\(_2\) plane. Fig.1B resembles arrangement of oxygen O(2) ions of CuO\(_2\) plane and O(4) oxygen ions.

The occurrence of an anisotropy of charge carrier’s mass in RBa\(_2\)Cu\(_3\)O\(_{7-\delta}\) compounds we model here by the orientational dependence of the ”density-displacement” type electron-phonon interaction on the relative positions of
Figure 1: An electron hops on a lower chain of ions (squares) and interacts with the $c$-polarized vibrations of ions (open circles) of an upper chain, via a density-displacement type of force $f_m(n)$. The distances between the chains ($|c|$) and between the ions ($|a|$ or $|b|$) of the same chain are assumed equal to 1.

It has been shown that within the model of Eq. (1) intersite bipolarons tunnel in the first order of polaron tunneling and mass of the intersite bipolaron has the same order as polaron’s mass $[38]$. For the sake of simplicity
we suppose here that intersite bipolarons form an ideal gas of charge carriers and mass of bipolaron is \( m_{bp} = 2m_p \) (this point does not lead to loss of generality). Then the temperature of Bose-Einstein condensation of the intersite bipolarons is defined as

\[
T_{BEC} = \frac{3.31 \hbar^2 n^{2/3}}{2k_B m^*} e^{-g^2}.
\]  

(7)

Here \( k_B \) is Boltzmann constant and \( n \) is density of intersite bipolarons. For the ideal gas of charge carriers one can neglect interparticle Coulomb interaction, i.e. the term \( H_V \) (Eq. (4)). In this case one can estimate polaron’s mass within EHM. In the strong electron-phonon coupling limit and nonadiabatic regime, use of the standard procedure such as Lang-Firsov transformation \([41]\) eliminates electron-phonon interaction term \( H_{e-ph} \) (Eq. (5)). Subsequent perturbation expansion of the transformed Hamiltonian with respect to the parameter \( \lambda^{-1} = 2T(a)/E_p \) (\( E_p \)-polaron shift) and estimation of the polaron’s renormalized mass yields \( m_p/m^* = \exp[g^2] \) \([1]\) (see also \([1]\)), where

\[
g^2 = \frac{1}{2M\hbar^2} \sum_m [f_m^2(n) - f_m(n)f_m(n+a)].
\]  

(8)

and \( m^* = \hbar^2/2T(a)a^2 \) is the bare band mass. In order to consider the stress of a lattice and its influence on the (bi)polaron mass, and consequently on the temperature of Bose-Einstein condensation of intersite bipolarons, the analytical expression

\[
f_m(n) = \frac{\kappa c(1 - \varepsilon_c)}{\sqrt{|(n - m)(1 - \varepsilon_i)|^2 + (c(1 - \varepsilon_c))^2}^{3/2}}
\]  

(9)

will be used for the density-displacement type force \((i = a \text{ or } b)\). Here \( \kappa \) is some coefficient, and \( \varepsilon_a, \varepsilon_b \) and \( \varepsilon_c \) are lattice strains along the \( a-, b- \)
Figure 2: The temperature of Bose-Einstein condensation of the intersite bipolarons as a function of strains along the $b$-axis $\varepsilon_b$ (solid line) and along the $c$-axis $\varepsilon_c$ (dashed line) for the lattice of Fig.1A. Here we put $\kappa^2/(2M\hbar\omega^3) = 5.885$ in order to coincide $T_{BEC}$ at $\varepsilon_i = 0$ ($i = b, c$) with the bulk value of $T_c \approx 91$ K of YBCO high-$T_c$ cuprates at optimal doping.

and $c$-axes, respectively. The distance $|\mathbf{n} - \mathbf{m}|$ is measured in units of the lattice constant $|\mathbf{a}| = 1$ (or $|\mathbf{b}| = 1$). The lattice strains are defined as $\varepsilon_a = (a_{unst} - a_{str})/a_{unst}$ ($\varepsilon_b = (b_{unst} - b_{str})/b_{unst}$) and $\varepsilon_c = (c_{unst} - c_{str})/c_{unst}$, where subscripts $unstr$ and $str$ stand for unstrained and strained, respectively. Eq.(9) is a generalization of the force considered in Ref. [1] (see Eq.(9) therein) and allows one to interrelate the temperature of Bose-Einstein condensation of the intersite bipolarons with the lattice strains through the mass of the intersite bipolaron.
Figure 3: The temperature of Bose-Einstein condensation of the intersite bipolarons as a function of strains along $a$-axis $\varepsilon_a$ (solid line) and along $c$-axis $\varepsilon_c$ (dashed line) for the lattice of Fig.1B. Here we put $\kappa^2/(2M\hbar \omega^3) = 9.265$ in order to coincide $T_{BEC}$ at $\varepsilon_i = 0$ ($i = a, c$) with the bulk value of $T_c \approx 91$ K of YBCO high-$T_c$ cuprates at optimal doping.
3. Results and discussion

The expression Eq. (7) expresses \( T_{\text{BEC}} \) through two basic parameters of a system: (i) the density of intersite bipolarons \( n \) and (ii) the exponent \( g^2 \) of the polaron mass enhancement. Eq. (7) allows one to study the dependence of \( T_{\text{BEC}} \) on the model lattices (Fig.1) strains \( \varepsilon_a, \varepsilon_b \) or \( \varepsilon_c \) at constant \( n \). This dependence, of course, originates from polaronic effects. We have calculated the values of \( T_{\text{BEC}} \) as a function of the strains along the \( b \)-axis \( \varepsilon_b \) and \( c \)-axis \( \varepsilon_c \) for the model lattice given in Fig.1A. The results are given in Fig.2. Here we put \( n = 1 \cdot 10^{21} \text{ sm}^{-3} \) and \( \kappa^2/(2M\hbar\omega^3) = 5.885 \) in order to coincide \( T_{\text{BEC}} \) in the absence of the strains with the bulk value of \( T_c \approx 91 \text{ K} \) of YBCO cuprates. The results calculation of \( T_{\text{BEC}} \) for the lattice in Fig.1B are shown in Fig.3. As one can see from Fig.2, compressive strain along \( b \)-axis gives rise to increase the value of \( T_{\text{BEC}} \), while that along \( c \)-axis acts on the contrary. Compressive strain along both the \( a \)– and \( c \)-axes in the model lattice of Fig.1B lowers the value of \( T_{\text{BEC}} \). The uniaxial strain derivatives of \( T_{\text{BEC}} \) for the model lattice given in Fig.1A at \( \kappa^2/(2M\hbar\omega^3) = 5.885 \) are: \( \partial T_{\text{BEC}}/\partial \varepsilon_b \approx +278 \text{ K} \) and \( \partial T_{\text{BEC}}/\partial \varepsilon_c \approx -1210 \text{ K} \). The same uniaxial strain derivatives of \( T_{\text{BEC}} \) for the model lattice given in Fig.1B at \( \kappa^2/(2M\hbar\omega^3) = 9.265 \) are: \( \partial T_{\text{BEC}}/\partial \varepsilon_a \approx -115 \text{ K} \) and \( \partial T_{\text{BEC}}/\partial \varepsilon_c \approx -874 \text{ K} \).

The obtained results clearly demonstrate a strong dependence of \( T_{\text{BEC}} \) on the arrangement of ions in the lattice. This has a crucial effect on the value of \( T_{\text{BEC}} \). The sign of \( \partial T_{\text{BEC}}/\partial \varepsilon \) is different for \( a \)- and \( b \)-axes, which is caused by mutual arrangements of ions. In particular, for the lattices in Fig.1A and Fig.1B one finds \( \partial T_{\text{BEC}}/\partial \varepsilon_b \approx +278 \text{ K} \) and \( \partial T_{\text{BEC}}/\partial \varepsilon_a \approx -115 \text{ K} \), respectively. The uniaxial strain derivatives, \( \partial T_{\text{BEC}}/\partial \varepsilon_c \), of the two lat-
tices are both negative. These results clearly show that the two model lattices in some ways qualitatively characterize the situations in RBa$_2$Cu$_3$O$_{7-\delta}$ compounds under pressure (strain). Thus compressive pressure (or strain) along the $b$-axis ($a$-axis) increases (lowers) the value of $T_{\text{BEC}}$ in analogy with increase (decrease) of $T_c$ of RBa$_2$Cu$_3$O$_{7-\delta}$ compounds under compressive pressure (or strain) in the same direction. The effect of compressive pressure (strain) along the $c$-axis is similar to that of along the $a$-axis. In terms of quantity, one should be aware that our findings obtained relative to the lattices in Fig.1, and not to real cuprates. Considering more real model structures similar to the real structure of YBCO cuprates, one may obtain better value of $\partial T_{\text{BEC}}/\partial \varepsilon_i$, close to the $\partial T_c/\partial \varepsilon_i$ of YBCO. On the other hand, the values of the uniaxial pressure (strain) derivative of $T_c$ along crystallographic axes $i = a, b, c$, measured, in different experiments, are spread over a wide range, and in some cases contradicts to each other. Welp et al. were the first to present direct measurements of $\partial T_c/\partial p_i$ for the untwinned YBa$_2$Cu$_3$O$_{7-\delta}$ single crystal [33]. Their results are: $\partial T_c/\partial p_a = -2.0 \pm 0.2$ K/GPa, $\partial T_c/\partial p_b = +1.9 \pm 0.2$ K/GPa and $\partial T_c/\partial p_c = -0.3 \pm 0.1$ K/GPa. Bud’ko et al. obtained uniaxial pressure (strain) derivatives of the critical temperature of RBa$_2$Cu$_3$O$_{7-\delta}$ cuprate from the hydrostatic pressure dependence, measured on the films of different crystalline orientations [42]. According to Ref. [42], $\partial T_c/\partial p_a = -3.06 \pm 0.35$ K/GPa ($\partial T_c/\partial \varepsilon_a \approx -362 \pm 50$ K), $\partial T_c/\partial p_b = +0.38 \pm 0.18$ K/GPa ($\partial T_c/\partial \varepsilon_b \approx +301 \pm 30$ K) and $\partial T_c/\partial p_c = +3.45 \pm 0.43$ K/GPa ($\partial T_c/\partial \varepsilon_c = +239 \pm 24$ K). Pickett, in his paper [29], quoting to the experimental results of Refs. [32, 33], gives unexpected data: $\partial T_c/\partial \varepsilon_a \approx +212$ K, $\partial T_c/\partial \varepsilon_b \approx -244$ K and $\partial T_c/\partial \varepsilon_c = -8$ K. One can see
that our results are close to the $\partial T_c/\partial \varepsilon_i$ of Ref. [42].

Now let’s imagine that one has a hypothetic a quasi-two-dimensional anisotropic lattice in which the interaction of charge carriers (holes or electrons) with out-of-plane ions is strong, and that when external pressure is applied along the $a$- ($b$-) axis this interaction occurs in the analogous way to that as in the one-dimensional lattice of Fig.1B (Fig.1A). Then, the quasi-two-dimensional anisotropic lattice has all features of YBCO cuprates with respect to the influence of uniaxial strain (pressure) on $T_c$. Indeed, solving the system of equations

$$\sum_j C_{ij} \frac{\partial T_{BEC}}{\partial p_j} = \frac{\partial T_{BEC}}{\partial \varepsilon_i},$$

with the set of elastic constants of the YBCO cuprate (all in GPa) $C_{aa} = 231$, $C_{ab} = 132$, $C_{ac} = 71$, $C_{bb} = 268$, $C_{bc} = 95$ and $C_{cc} = 186$ taken from Ref. [43], one finds $\partial T_{BEC}/\partial p_a = -0.65$, $\partial T_{BEC}/\partial p_b = +3.58$ and $\partial T_{BEC}/\partial p_c = -6.27$ (all in K/GPa). Use of other set of elastic parameters (all in GPa) $C_{aa} = 283$, $C_{ab} = 148$, $C_{ac} = 83.1$, $C_{bb} = 304$, $C_{bc} = 109$ and $C_{cc} = 236$ taken from Ref. [44], yields $\partial T_{BEC}/\partial p_a = -0.54$, $\partial T_{BEC}/\partial p_b = +2.91$ and $\partial T_{BEC}/\partial p_c = -4.86$ (all in K/GPa). These findings indicate that the Bose-Einstein condensation scenario of the ideal Bose-gas of intersite bipolarons is, in principle, able to qualitatively explain the uniaxial strain (pressure) experiments, regarding the effect of the strain (pressure) on $T_c$ of YBCO cuprates. Quantitative discrepancies of our results and experimental data may be the result of several factors: (i) the simplicity of the model lattices under consideration. In reality one should consider more complex structures than in Fig.1; (ii) the choice of the analytical formula for the density-displacement
type electron-lattice force; (iii) the assumption that intersite bipolarons form an ideal Bose-gas: in reality, due to other factors, there may be deviation from the ideal case, leading to the formation of a nonideal Bose-gas or Bose-liquid; (iv) superconductivity of the YBCO cuprate may be due not only to electron-phonon interaction, but may also have contributions from other interactions as well. These factors suggest that we should undertake more comprehensive research on the studied problem.

The proposed model serves as a universal tool for studying strain (pressure) induced effects in the cuprates. Its common features are relevant to all cuprates. In contrast with some theoretical approaches (see for example [28]) the model allows one to interpret the influence of pressure (strain) on $T_{\text{BEC}}$ ($T_c$) along each axe, independently of the others. Meanwhile, the model is able to account for interference of strains between axes via the Poisson relation $\nu = \varepsilon_a/\varepsilon_c$ or $\nu = \varepsilon_b/\varepsilon_c$. This may be also useful in theoretical studies of cuprate films grown on different substrates.

4. Conclusion

In conclusion, we have studied the effect of uniaxial strain (pressure) on the temperature of Bose-Einstein condensation of intersite bipolarons within the framework of the Extended Holstein model. Uniaxial strain derivatives of $T_{\text{BEC}}$ are determined for different lattices. It is found that $\partial T_{\text{BEC}}/\partial \varepsilon_i$ depends strongly on the arrangement of ions in the lattice. In particular, it may be positive or negative. The results for the lattices under study (Fig.1) in some way mimic the influence of uniaxial strain (pressure) on the critical temperature, $T_c$, of YBCO cuprates. The calculated values of the pressure
derivatives of $T_{BEC}$ for the hypothetic lattice qualitatively agree with the observed values of $\partial T_c / \partial p_i$ ($i = a, b, c$) for YBCO cuprates.

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