Effect of screening of the electron-phonon interaction on the temperature of Bose-Einstein condensation of intersite bipolarons

B.Yavidov\textsuperscript{1,a}, A.Kurmantayev\textsuperscript{2}, D.Alimov\textsuperscript{2}, B.Kurbanbekov\textsuperscript{2}, and Sh.Ramonkulov\textsuperscript{2}

\textsuperscript{1} Institute of Nuclear Physics, 100214 Ulughbek, Tashkent, Uzbekistan
\textsuperscript{2} Ahmed Yasawi Kazakh-Turkish International University, 161200 Turkestan, Kazakhstan

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Abstract. Here we consider an interacting electron-phonon system within the framework of extended Holstein-Hubbard model at strong enough electron-phonon interaction limit in which (bi)polarons are the essential quasiparticles of the system. It is assumed that the electron-phonon interaction is screened and its potential has Yukawa-type analytical form. An effect of screening of the electron-phonon interaction on the temperature of Bose-Einstein condensation of the intersite bipolarons is studied for the first time. It is revealed that the temperature of Bose-Einstein condensation of intersite bipolarons is higher in the system with the more screened electron-phonon interaction.

PACS. 71.38.Mx – Bipolarons, 74.20.Mn – Nonconventional mechanisms (spin fluctuations, polarons and bipolarons, resonating valence bond model, anyon mechanism, marginal Fermi liquid, Luttinger liquid, etc.), 03.75.Lm – Tunneling, Josephson effect, Bose-Einstein condensates in periodic potentials, solitons, vortices, and topological excitations

1 Introduction

An electron-phonon interaction (EPI) in solids plays an important role and in many cases determines their thermodynamic, electronic, optical and other properties. The contribution coming from EPI to the properties of solids is more pronounced in the case when the coupling constant of EPI is much larger than those of the other interactions. The latter may be an interaction between the same charge carriers or an interaction between carrier and non-phonon degree of freedom of the lattice. In solids, the polaron concept has been widely used since the seminal paper of Landau [1]. The formation of a polaron quasiparticle in solids is mainly owing to the presence of EPI. Though there are other possibilities for the formation of a polaron via the other types of interaction. Here we focus our attention only on EPI. Those polarons which are formed by EPI are studied within the major frameworks: (i) Fröhlich model [2], (ii) molecular-crystal Holstein model (HM) [3] and etc. In the first model a polaron forms due to an interaction of an electron with the longitudinal optical vibrations of a polar ionic crystalline. The crystal is assumed to be a continuum. This means that one neglects the detailed structure of the lattice. In the second case polaron formation is due to coupling of a charge carrier to an intramolecular vibration of a lattice. The Holstein model is commonly studied in a discrete lattice. In the past both models have been extensively studied (see for example review papers [4],[5] and books [7],[8],[9]). A many polaron system in a discrete lattice is often studied within the framework of Holstein-Hubbard model [10],[11],[12], extended Holstein-Hubbard model [13] or Fröhlich-Coulomb model [14],[15],[16]. The models with extended interactions enable one to take into account both the long-range feature of EPI and the correlation of electrons at neighboring sites. At sufficiently strong EPI a many polaron system is unstable with respect to the formation of a bipolaron which is a bound state of two polarons. The conditions of the formation of a bipolaron quasiparticle in solids were studied extensively in the last decades for the purpose of pure academic interest [10],[11],[12],[13],[14],[15],[16],[17],[18],[19],[20],[21],[22],[23],[24] and for an interpretation of different phenomena, in particular in the context of cuprates [14],[15],[25],[26],[27],[28],[29],[30] and alkali-doped-fullerides [31].

A bipolaron is a boson. Therefore a bipolaron gas can, under certain conditions, undergo Bose-Einstein condensation and thus would give rise to bipolaronic superfluidity phenomenon (superconductivity). Superconductivity of a charged ideal Bose-gas and superfluidity of an ideal Bose-gas were first studied in Ref.[32] and Ref.[33], respectively. Bipolaronic superconductivity is one of the mechanisms among others proposed for the interpretation of high-$T_c$...
Fig. 1. In a one dimensional lattice of the extended Holstein model an electron hops on the lower chain and interacts with vibrations of the ions of an upper infinite chain via a density-displacement type force $f_{m,\alpha}(n)$. The distances between the chains (b) and between the ions of the same chain (a) are assumed equal to 1.

phenomena in the cuprates. As the problem of high-$T_c$ phenomena in the cuprates to date still remains open an investigation of the properties of a bipolaron gas may supply additional information about its relevance to the problem of high-$T_c$ superconductivity of the cuprates.

The properties of a bipolaron gas are influenced by a number of factors. For the intersite bipolaron \[44\] gas these factors are: crystal structure, type of EPI, screening of EPI, charge carriers’ concentration, etc. Here we study only an effect of screening of EPI on the temperature of Bose-Einstein condensation of intersite bipolarons. On the one hand the issue is of considerable academic interest for a broad community of (bi)polaron and Bose-Einstein condensation physicists as such a task has not been addressed so far. On the other hand the study is interesting from a practical point of view as the obtained results can be used in a wide range of phenomena \[35\], in particular in the cuprates \[33\] and metal-ammonia solutions \[37\].

In doing this we work with extended Holstein-Hubbard model and adopt the analytical formula for the screened EPI introduced recently in Refs. \[38,39\].

2 The model

We consider an electron performing hopping motion on a lower chain consisting of static sites, but interacting with all ions of an upper chain via a long-range density-displacement type force, as shown in Fig.1. The motion of an electron is always one-dimensional and the upper chain’s ions vibrate perpendicular to the chains. Such a situation was studied in Ref. \[10\] for polarons and in Ref. \[10\] for bipolarons. Dynamics of an electron (or hole) in such a model lattice mimics the situation in the cuprates in which charge carriers belonging to CuO$_2$ - plane and performing hopping motion along $a$- or $b$- axes coupled with the apical ions. In the model lattice one can show that small polarons have a small mass (as it was shown for the first time by Alexandrov and Kornilovitch \[40\]) and it is also helpful for the explanation of dependence of $T_c$ (the critical temperature of superconductivity) of cuprates on the uniaxial strain (pressure) along $a$, $b$- and $c$-crystallographic axis \[11,42\]. Here the model lattice will be implemented for the study of the dependence of Bose-Einstein condensation temperature of the ideal gas of intersite bipolarons on the screening of EPI.

We write the Hamiltonian of the system of electrons and phonons \[14,40\] as

$$H = H_e + H_{ph} + H_V + H_{e-ph},$$

(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,

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

(3)

is the Hamiltonian of the phonon system,

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

(4)

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

$$H_{e-ph} = \sum_{n,m,\alpha} f_{m,\alpha}(n)c_n^\dagger c_m \xi_{m,\alpha}$$

(5)

is the Hamiltonian of the electron-phonon interaction. Here $t(n-n')$ is the transfer integral of an electron from site $n$ to site $n'$, $c_n^\dagger (c_n)$ is the creation (annihilation) operator of an electron at site $n$, $d_{q\alpha}$ ($d_{q\alpha}^\dagger$) is the creation (annihilation) operator of a phonon with $\alpha = x, y, z$ polarisation 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

$$\xi_{m,\alpha} = \sum_{q} \left( \frac{\hbar}{2NM\omega_{q\alpha}} \right)^{1/2} d_{q\alpha}^\dagger + h.c. \right).$$

(6)

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 $c$-polarised (perpendicular to the chains) vibrations of ions, as charge carriers in the CuO$_2$ plane of the cuprates strongly interact with $c$-polarised vibrations of apical ions with corresponding energy of the apical phonons 75 meV \[43\]. This apical phonon mode significantly contributes to polaron energy, 1.5 eV in La$_2$CuO$_4$
and 1.7 eV in YBa2Cu3O6, and these values of polaron binding energy suggest that EPI in the cuprates are very strong [44]. Another evidence of the fundamental role of EPI in the cuprates comes from the recent pump-probe optical spectroscopy data [45].

Early McQueeney and et al. reported that coupling of charge carriers to the 75 meV mode increases with increasing doping [46]. Theoretical treatment of doping dependence of EPI has also shown that EPI remains significant at whole doping regimes and charge carriers are in the non-adiabatic or near-adiabatic regimes depending on doping level [47]. Therefore our study will be restricted to two (non-adiabatic and adiabatic) limits of strong EPI regime.

At strong coupling regime \( \lambda = E_p/D \gg 1 \) (\( D^- \) and \( E_p^- \) are the half-bandwidth and polaron shift energies, respectively) and non-adiabatic limit \( t/\hbar\omega < 1 \) one can use an analytical method based on the extended (or non-local) Lang-Firsov transformation and subsequently perturbation theory with respect to the parameter \( 1/\lambda \) [48]. It has been shown that within the model [11] an intersite bipolaron "can tunnel from one cell to another via a direct single polaron tunneling from one apex oxygen to its apex neighbor" [48] and its mass has the same order as polaron's mass [41]. For the sake of simplicity we suppose that intersite bipolarons form an ideal gas of charged carriers and that the mass of the bipolaron is \( m_{bp} = 2m_p \) (this point does not lead to loose of generality). Then the temperature of Bose-Einstein condensation of an ideal gas of the intersite bipolarons is defined as (for details of derivation see [49])

\[
T_{BEC} = \frac{3.31\hbar^2 n_{bp}^{2/3}}{2k_B m_p}. \tag{7}
\]

Here \( k_B \) is the Boltzmann constant and \( n_{bp} \) is density of intersite bipolarons. For the ideal gas of charge carriers one can neglect interparticle Coulomb interaction, i.e. the term \( Hv \) (Eq. (4)). In this case one can estimate polaron's mass within the extended Holstein model (EHM) as [40]:

\[
m_{\text{non-ad-pol}} = m^* e^2
\]

where \( m^* \) is the electron's band mass and

\[
g_{\text{non-ad}}^2 = \frac{1}{2M\hbar^3} \sum m [f_{m}(0) - f_{m}(0)f_{m}(1)]. \tag{9}
\]

For the determination of the mass of a small polaron at strong coupling regime \( \lambda \gg 1 \) and adiabatic limit \( t/\hbar\omega > 1 \) we adopt a more general form of screened interparticle interaction, i.e. the term \( Hv \) (Eq. (4)). The same is done for the adiabatic regime \( \Delta = \Delta \exp(-g_{ad}^2) \),

\[
\Delta = \frac{\hbar\omega}{\pi} \sqrt{\frac{E_p}{2\hbar\omega \kappa^{3/2}}} \left[ 1 - \sqrt{1 - \left(\frac{E_p}{2\hbar\omega \kappa^{1/2}}\right)^{-1}} \right], \tag{10}
\]

\[
g_{ad}^2 = \frac{E_p}{2\hbar\omega \kappa^{1/2}} \left[ 1 - \sqrt{1 - \left(\frac{E_p}{2\hbar\omega \kappa^{1/2}}\right)^{-1}} \right], \tag{11}
\]

and

\[
E_p = \frac{1}{2M\omega^2} \sum m f_{m}^2(0). \tag{12}
\]

Here \( \kappa = \omega\sqrt{\kappa} \) is the renormalised phonon frequency, \( \kappa = (1 - 1/\lambda^2) \) and \( \lambda = E_p/(2t) \).

As one can see from equation (7) at \( n_{bp} = const \) the temperature of Bose-Einstein condensation of intersite bipolarons is mainly determined by the form of EPI force \( f_m(n) \) which is in general screened. For the screened EPI potential we adopt a more general form of screened interaction potential which is Yukawa-type potential [38,39]:

\[
U_m(n) = \frac{\kappa}{(n - m)^2 + b^2} \times \exp \left[ -\frac{\sqrt{(n - m)^2 + b^2}}{R} \right],
\]

where \( \kappa \) is some coefficient and \( R \) is the screening radius measured in units of \( a \). Such a potential was used in order to explain the small value of charge carrier's mass and infrared absorption in the cuprates [39]. Here we use the Yukawa-type EPI potential to study the influence of screening of EPI on the temperature Bose-Einstein condensation of intersite bipolarons.

From the potential Eq. (13) one obtains an analytical expression for the screened force of EPI corresponding to the interaction of an electron on site \( m \) with the ion's vibration on site \( n \):

\[
f_m(n) = \frac{kb}{(n - m)^2 + b^2} \left[ 1 + \sqrt{\frac{(n - m)^2 + b^2}{R}} \right] \exp \left[ -\frac{\sqrt{(n - m)^2 + b^2}}{R} \right]. \tag{14}
\]

The formulas (7)-(14) are main analytical results according to which, in the next section, we discuss the dependence of \( T_{BEC} \) on the screening radius \( R \).

### 3 Results and discussion

We have calculated the values of the temperature of Bose-Einstein condensation \( T_{BEC} \) of the intersite bipolarons on different values of the screening radius \( R \) for two regimes: non-adiabatic (\( t/\hbar\omega \ll 1 \)) and adiabatic (\( t/\hbar\omega \gg 1 \)). The results are visualised in Fig.2 and Fig.3 for non-adiabatic and adiabatic regimes, respectively. In non-adiabatic regime the calculation is performed at \( k^2/2M\hbar^2 = 8.51 \) in order to get \( T_{BEC} \) comparable with \( T_c \) (transition temperature to superconducting state) of the cuprates (Fig.2). The same is done for the adiabatic regime (\( t/\hbar\omega \gg 1 \)) at \( k^2/2M\hbar^2 = 0.188 \) (Fig.3A). In the latter case the calculations are performed with the \( \hbar\omega = 75 \) meV and \( t = 0.2 \) eV [51], in order to ensure the fulfillment of the condition of adiabaticity (\( t/\hbar\omega \gg 1 \)).

As one can see from the graphics the value of \( T_{BEC} \) decreases with the screening radius \( R \), regardless of adiabaticity parameter \( t/\hbar\omega \). In both regimes the relative change
and screening radius is given in units of lattice constant.

The dependence of the temperature of Bose-Einstein condensation of an ideal gas of the intersite bipolarons on the screening radius \( R \) of EPI at nonadiabatic regime and \( k^2/2M\hbar\omega^3 = 8.51 \). The temperature is measured in Kelvin and screening radius is given in units of lattice constant \( a \).

![Diagram](image)

**Fig. 2.** The dependence of the temperature of Bose-Einstein condensation of an ideal gas of the intersite bipolarons on the screening radius \( R \) of EPI at nonadiabatic regime and \( k^2/2M\hbar\omega^3 = 8.51 \). The temperature is measured in Kelvin and screening radius is given in units of lattice constant \( a \).

of the value of \( T_{\text{BEC}} \) is more pronounced at the small values of screening radius \( R \). It seems that such a feature is hallmark of EHM as similar behaviour has previously been observed for mass and optical conductivity of polarons as well [99]. In the non-adiabatic regime a decrease of \( R \) from \( \infty \) to the value \( R = 5 \) increases the \( T_{\text{BEC}} \) from \( \approx 32 \text{ K} \) up to \( \approx 35 \text{ K} \), i.e. increased only by \( \approx 9 \% \). While at regimes of strong screening of EPI, i.e. when screening radius is comparable to the lattice constant, the increase of the value of \( T_{\text{BEC}} \) is considerably large. So the increase of the value of \( T_{\text{BEC}} \) may reach \( \approx 10 \text{ K} \) (increase by \( \approx 28 \% \)) or even \( \approx 85 \text{ K} \) (increase by \( \approx 164 \% \)) in the case of decreasing \( R \) from 3 to 2 or from 2 to 1 respectively. A similar dependence of \( T_{\text{BEC}} \) on screening radius \( R \) is observed in the adiabatic limit too (Fig.3). An estimation of such a kind is necessary when one studies charge carrier dynamics and their binding (formation of a bound state of two carriers) at short distances (i.e. within a few lattice units). It should be noted that the value of \( T_{\text{BEC}} \) in our model strongly depends on the model parameters \( k^2/2M\hbar\omega^3 \) in non-adiabatic regime and \( k^2/2M\omega^2 \) in adiabatic regime. These parameters in turn depend on the structure of cuprate through \( k, M \) and \( \omega \) and can take values in a wide range. In order to illustrate this dependence, in Fig.3B we plot \( T_{\text{BEC}} \) versus \( R \) in the adiabatic regime for an another value of \( k^2/2M\omega^2 = 0.148 \). As it is seen from the plot, \( T_{\text{BEC}} \) can reach almost 195 K at values of \( R \) comparable to the lattice constant.

It is also instructive to investigate the dependence of \( T_{\text{BEC}} \) on charge carrier’s (in our case polaron’s) concentration. In doing this one distinguishes two regimes of screening of EPI. The first regime is weak and moderate screening of EPI in which \( R \gg 1 \) and \( T_{\text{BEC}} \) is nearly independent of \( R \). The second regime is strong screening of EPI, i.e. \( R \) is comparable to the lattice constant, \( R \approx a \). For the latter case, to simplify the consideration, one can use a crude approximation to scale \( T_{\text{BEC}} \) as \( \sim R^{-1} \) (in both regimes of adiabaticity). It is appropriate to recall that the screening radius itself depends on a number of parameters among which is carriers’ concentration. In the metallic regime of solids the screening radius can be estimated within the Thomas-Fermi model as \( R_{TF} = (E_F/2\pi\epsilon^2n_0)^{1/2} \), where \( E_F \) - Fermi energy, \( n_0 \) - charge carrier’s concentration. While in the semiconducting regime one estimates the screening radius within the Debye model as \( R_D = (\varepsilon_0kBT/4\pi\epsilon^2n_0)^{1/2} \), where \( \varepsilon_0 \) and \( T \) are dielectric permittivity and absolute temperature of a solid, respectively. As one can see in both models \( R \) scales as \( \sim n_p^{-1/2} \). Here we replace \( n_0 \) with \( n_p \) - polarons’ concentration. Summarising, one writes (for a general case)

\[
T_{\text{BEC}} \sim n_p^{2/3}n_p^{1/2}.
\]

(15)

Taking into account that the total number of charge carriers in the system is conserved \( n_p + n_{bp} = N = \text{const} \) one rewrites the Eq. (15) as

\[
T_{\text{BEC}} \sim (1-x)^{2/3}x^{1/2},
\]

(16)

where \( x = n_p/N \). In Fig4 the latter relation between \( T_{\text{BEC}} \) and \( x \) is presented graphically. The relation (16) separates \( (x,T_{\text{BEC}}) \) plane into two regions. An area below of the line (16) represents Bose-Einstein condensate of an ideal gas of intersite bipolarons. In the area above the line Bose-Einstein condensation of intersite bipolarons is impossible. Thus Fig4 is a phase diagram of an ideal gas of intersite bipolarons. The form of the area of Bose-Einstein condensate of intersite bipolarons as seen from Fig4 is slightly asymmetric and shifted to the low values of \( x \). It is trivial that there is no Bose-Einstein condensate...
at $x = 0$ (no polarons and consequently no bipolarons) and $x = 1$ (all charge carriers are polarons). At some point determined by the condition $\partial T_{\text{BEC}}/\partial x = 0$ the temperature of Bose-Einstein condensation of intersite bipolarons reaches a maximum. The point is $x = 3/7$. It is worthwhile to notice that this phase diagram is obtained under crude approximations and represents a particular case of screening regime of EPI and its effect on $T_{\text{BEC}}$ of intersite bipolarons. However, the model in which polarons and bipolarons can coexist, and EPI plays an important role, seems to be a plausible model for explaining qualitatively (i) high values of $T_c$ ($= T_{\text{BEC}}$) and (ii) "bell-shaped" form of the dependence of $T_c$ ($= T_{\text{BEC}}$) versus charge carrier's concentration, which in our case is polarons, $n_p$. Previously, a system in which large polarons and large bipolarons coexist, was studied in the context of high-$T_c$ superconductivity and typical behaviour of $T_c$ versus $x$ found in the cuprates was reproduced in Ref. [23]. Such a system of polaron-bipolaron mixture, and Bose-Einstein condensation of bipolarons in such a system deserves a more detailed consideration as polarons in this mixture stabilise the isolated nonstable large bipolaron states [29]. This is the very case that is considered in this paper. Though we study here an ideal gas of intersite bipolarons, our calculation of $T_{\text{BEC}}$ indirectly takes into account screening of the Coulomb interaction, which is responsible for the doping dependence of the bipolaron binding energy and its effective mass [11,52]. In this work such an account is done by expressing $T_{\text{BEC}}$ through the screening radius $R$ via the mass of a bipolaron $m_{bp} = 2m_p$.

As a rule, when screening is increased, the effects of EPI become weaker, and consequently the probability of the formation of bipolarons decreases as well. Therefore one must bear in mind that our study is valid only to the case when bipolaron formation is possible. For a comprehensive study of the problem with all aspects one should take into account nonideality of Bose-gas or other factors in the system. Study of Bose-Einstein condensation of nonideal Bose-gas may be useful in Fermi-Bose-liquid scenarios of superconductivity as well [33,51,55]. Consideration of the more general cases is in progress.

### 4 Conclusion

In conclusion, we have studied the effect of screening of EPI on the temperature Bose-Einstein condensation of an ideal gas of intersite bipolarons. It is shown that the effect is more pronounced at the values of screening radius comparable with the lattice constant. The screening of EPI gives rise the increase of the temperature of Bose-Einstein condensation of the intersite bipolarons. The here-revealed feature of an ideal gas of intersite bipolarons i.e. dependence of its Bose-Einstein condensation temperature on screening radius should be taken into account when applying this scenario of superconductivity to real systems.

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**Fig. 4.** Phase diagram of the ideal gas of intersite bipolarons at strong EPI screening regime on $(x,T_{\text{BEC}})$ plane.
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