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EFFECT OF SCREENING OF THE ELECTRON-PHONON INTERACTION ON THE TEMPERATURE OF BOSE-EINSTEIN CONDENSATION OF INTERSITE BIPOLARONS

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.

Keywords: electron-phonon interaction, (bi)polarons, screening.

Кілт сөздер: электрон-фононды әсерлесу, (би)поляронда, экрандау.

Ключевые слова: электрон-фононное взаимодействие, (би)поляроны, экранирование.

Many polaron system in discrete lattices is often studied within the framework of extended Holstein-Hubbard model [1] or Frohlich-Coulomb model [2]. The models enable us to take into account both long-range feature of electron-phonon interaction (EPI) and correlation of electrons at neighbouring sites. At sufficiently strong EPI many polaron system is unstable with respect to the formation of bipolaron which is bound state of two polarons. Bipolaron is a boson. Therefore bipolaron gas (or liquid) can under certain conditions undergo Bose-Einstein condensation and thus would give rise to bipolaronic superfluidity phenomenon (superconductivity). Bipolaronic superconductivity is one of the mechanisms among others proposed for the interpretation of high-T_c phenomena in the cuprates. As the problem of high-T_c phe-nomena in the cuprates to date remains still open an investigation of the properties of bipolaron gas may supply additional information about its relevance to the problem of high-T_c superconductivity of the cuprates. The properties of an bipolaron gas is influenced by the number of factors. For the intersite bipolaron gas these factors are: crystal structure, type of EPI, screening of EPI, charge carriers'

concentration and et al.. Here we study only an effect of screening of EPI on the temperature of Bose-Einstein condensation of intersite bipolarons. The issue is of considerable academic interest for a broad community of (bi)polaron physicist as such a task has not been addressed so far. In doing this we work with extended Holstein-Hubbard model and adopt analytical formula for the screened EPI introduced recently in Refs [3, 4].

$$f_{\vec{m}}\left(\vec{n}\right) = k\left(1+\frac{\sqrt{\left|\vec{n}-\vec{m}\right|^2+1}}{R}\right)\left(\left|\vec{n}-\vec{m}\right|^2+1\right)^{-\frac{3}{2}} Exp\left[-\frac{\sqrt{\left|\vec{n}-\vec{m}\right|^2+1}}{R}\right]. \quad (1)$$

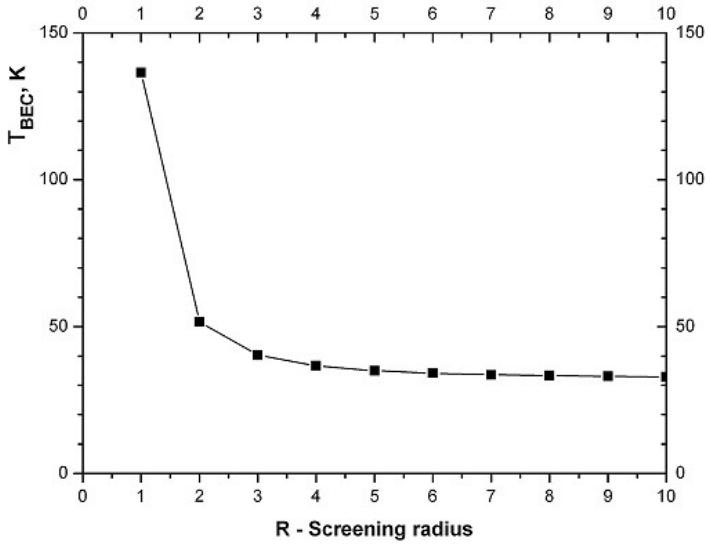
Here $f_{\vec{m}}(\vec{n})$ is the "density-displacement" type coupling force of an electron at site $\vec{n}$ with the apical ion at site $\vec{m}$, R is screening radius of EPI. It has been shown that intersite bipolaron tunnel in the first order of polaron tunneling and its mass has the same order as polaron mass [2]. For the sake of simplicity we suppose that intersite bipolarons form an ideal gas of charged carriers and mass of bipolaron is $m_{bp} = 2m_p$ (this point does not lead to loose of generality). For the ideal gas of charge carriers one can one can estimate polaron's mass within the extended Holstein model (EHM) as $m_p = m^{\bullet}\exp\left[g^2\right]$ [5], where $m^{\bullet}$ is charge carrier's band mass,

$$g^2 = \left(\frac{1}{2M\hbar\omega^3}\right)\sum_{\vec{m}}\left[f^2(\vec{m}) - f(\vec{m})f(\vec{m}+\vec{a})\right], \quad (2)$$

M is ion's mass and ω is its vibration frequency. Then the temperature of Bose-Einstein condensation of the intersite bipolarons defines as

$$T_{BEC} = \left(\frac{3.31\hbar^2 n_{bp}^{\frac{2}{3}}}{2k_B m^*}\right)\exp\left[-g^2\right], \quad (3)$$

where n_{bp} is density of intersite bipolarons. 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. The calculation is performed at $\left(\frac{1}{2M\hbar\omega^3}\right) = 8.51$ in order to get T_{BEC} comparable with T_c (transition temperature to superconducting state) of the cuprates. The data are presented graphically in Figure.



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 $\left(\frac{1}{2M\hbar\omega^3}\right) = 8.51$.

The temperature is measured in Kelvins and screening radius is given inunits of lattice constant a

As one can see from the graphic the value of T_{BEC} is decreased with the screening radius R. The relative change of the value of T_{BEC} is more pronounced at small values of screening radius R. It seems that such a feature is hallmark of EHM as similar behavior have early been observed for mass [3] and optical conductivity of polarons as well [4]. For our case decrease of R from ∞ to the value R=5 increases the T_{BEC} from ≈32 K up to ≈35 K, i.e. increased only by ≈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_{BEC} is considerably large. So the increase of the value of T_{BEC} may reach ≈10 K (increase by ≈28$ %) or even ≈85 K (increase by ≈164 %) in case of decreasing R from 3 to 2 or from 2 to 1 respectively.

An estimation of such a kind is necessary when one study charge carriers dynamics and their binding (formation of bound state of two carriers) at short distances (i.e. within a few lattice units). The revealed here 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 considering this scenario of superconductivity to apply to real systems.

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Резюме

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ЭЛЕКТРОН-ФОНОН ӘСЕРЛЕСУІНІҢ (БИ)ПОЛЯРОНДАРДЫҢ ТҮЙІНДЕРІНДЕГІ БОЗЕ-ЭЙЕНШТЕЙН КОНДЕНСАЦИЯ ТЕМПЕРАТУРАСЫНА ЭКРАНДАУ ЭФФЕКТІСІ

Мақалада Холстейн-Хаббардтың кеңейтілген модель рамкасында электрон фононды әсерлесуші жүйе қарастырылады. Мұнда күшті электрон-фононды әсерлесу шегінде (би)поляронлар жүйенің негізгі квази-бөлшектері болып табылады. Электрон-фононды әсерлесу экрандалған деп қарастырылып және оның потен-циалы Юкава формасына ұқсас аналитикалық формаға ие. Алғаш рет электрон-фононды әсерлесудің экран-далуының екі түйінді биполяронда рдың бозе-эйнштейндік температурасына әсері зерттелді. Екі түйінді биполяронда рдың бозе-эйнштейндік температурасы экрандалған электрон-фононды әсерлесу жүйесінде жоғары болатындығы анықталған.

Кілт сөздер: электрон-фононды әсерлесу, (би)поляронда р, экрандау.

Резюме

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ЭФФЕКТ ЭКРАНИРОВАНИЯ ЭЛЕКТРОН-ФОНОННОГО ВЗАИМОДЕЙСТВИЯ НА ТЕМПЕРАТУРУ БОЗЕ-ЭЙНШТЕЙНОВСКОЙ КОНДЕНСАЦИИ НА МЕЖУЗЕЛ БИПОЛЯРОНОВ

В статье рассматривается взаимодействующая электрон-фононная система в рамках расширенной мо-дели Холстейна-Хаббарда в пределах достаточно сильного электрон-фононного взаимодействия, в котором (би)поляроны являются основными квазичастицами системы. Предполагается, что электрон-фононное взаимодействие экранировано и его потенциал имеет аналитическую форму, подобную форме Юкавы. Впервые изучено влияние экранирования электрон-фононного взаимодействия на температуру бозе-эйнш-тейновской конденсации двухузловых биполяронов. Установлено, что температура бозе-эйнштейновской конденсации двухузловых биполяронов выше в системе с более экранированным электрон-фононным взаи-модействием.

Ключевые слова: электрон-фононное взаимодействие, (би)поляроны, экранирование.

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