
LATTICE DYNAMICS
AND PHASE TRANSITIONS

Electron Correlations and Instability of a Two-Center Bipolaron

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Abstract—The energy of a large bipolaron is calculated for various spacings between the centers of the polarization potential wells of the two polarons with allowance made for electron correlations (i.e., the explicit dependence of the wave function of the system on the distance between the electrons) and for permutation symmetry of the two-electron wave function. The lowest singlet and triplet 2^3S states of the bipolaron are considered. The singlet polaron is shown to be stable over the range of ionic-bond parameter values $\eta \leq \eta_m \approx 0.143$ ($\eta = \epsilon_\infty/\epsilon_0$, where ϵ_∞ and ϵ_0 are the high-frequency and static dielectric constants, respectively). There is a single energy minimum, which corresponds to the single-center bipolaron configuration (similar to a helium atom). The binding energy of the bipolaron for $\eta \rightarrow 0$ is $J_{Bp} = -0.136512e^4m^*/\hbar^2\epsilon_\infty^2$ (e and m^* are the charge and effective mass of a band electron), or 25.% of the double polaron energy. The triplet bipolaron state (similar to an orthohelium atom) is energetically unfavorable in the system at hand. The single-center configuration of the triplet bipolaron corresponds to a sharp maximum in the distance dependence of the total energy $J_{Bp}(R)$; therefore, a transition of the bipolaron to the orthostate (e.g., due to exchange scattering) will lead to decay of the bound two-particle state. The exchange interaction between polarons is antiferromagnetic (AFM) in character. If the conditions for the Wigner crystallization of a polaron gas are met, the AFM exchange interaction between polarons can lead to AFM ordering in the system of polarons. © 2003 MAIK “Nauka/Interperiodica”.

INTRODUCTION

Interest in polarons was rekindled after the discovery of high-temperature superconductivity (HTSC). Some vexatious computational errors made in early papers on the subject of bipolarons (see review [1]) were corrected in [2]. The minimum found in [2] for the energy of the single-center bipolaron (or the Pekar bipolaron [3]) is significantly lower than the energy minimum of the two-center bipolaron first considered in [4]. Later, the results of [2] were reproduced in [5] using both Pekar and Gaussian functions. In spatial configuration, the single-center bipolaron is similar to a helium atom and the two-center bipolaron, to a hydrogen molecule.

Since the energy of the ground state of the single-center bipolaron was found to be significantly lower than that of the two-center bipolaron, investigation of the molecular configuration of the bipolaron has virtually ceased. We may only cite the papers by Mukhomorov (see, e.g., [6, 7] and references therein), in which the study into the two-center configuration was continued despite the fact that the energy minimum found in [2] was considerably lower than that obtained in [6, 7]. However, the energy of the two-electron system as a function of the distance between the centers of the polarization potential wells of two polarons has not yet been investigated with allowance for electron correlations (here and henceforth, electron correlations are

taken to mean an explicit dependence of the wave function (WF) of the two-electron system on the distance between the electrons).

When the dependence of the energy of a system of two polarons on the distance between the centers of the two polarization wells is calculated using the variational method, preference should be given to the deepest minimum. In solving this problem, success will be achieved if, by taking into account electron correlations, we reproduce (or improve) the results of variational calculations performed to date for any distance between the centers of the polarization wells. Only in that case can one answer the question of whether the atomic or molecular bipolaron configuration is favorable.

Recently, interest in the subject of polarons and bipolarons has also been inspired by studies on the properties of these particles in anisotropic crystals, low-dimensional structures, and systems with quantum wells [8–13]. The proper choice of the bipolaron configuration and the electron correlation effect are also of importance in such systems.

2. BASIC EQUATIONS

The Hamiltonian of the system consisting of two electrons and a phonon field is taken in the form

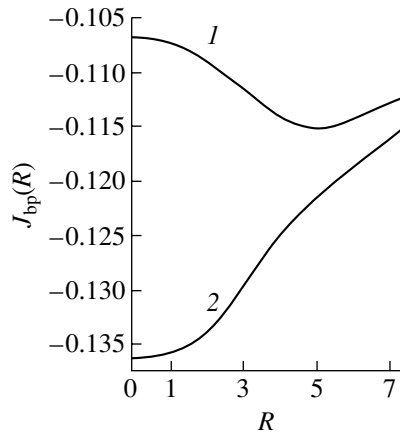


Fig. 1. Dependence of the bipolaron energy on the distance between the centers of the polarization wells (1) without and (2) with regard for electron correlations calculated for $n = 5$ in Eq. (4).

$$H = \hbar\omega \sum_{\mathbf{k}} a_{\mathbf{k}}^+ a_{\mathbf{k}} + \sum_{\mathbf{k}} V_{\mathbf{k}} (a_{\mathbf{k}} - a_{-\mathbf{k}}^+) (\exp(i\mathbf{k}\mathbf{r}_1) + \exp(i\mathbf{k}\mathbf{r}_2)) - \frac{\hbar^2}{2m^*} \Delta_1 - \frac{\hbar^2}{2m^*} \Delta_2 + \frac{e^2}{\epsilon_{\infty} |\mathbf{r}_1 - \mathbf{r}_2|}, \quad (1)$$

$$V_{\mathbf{k}} = -i \frac{e}{k} \sqrt{\frac{2\pi\hbar\omega}{V\tilde{\epsilon}}}, \quad \frac{1}{\tilde{\epsilon}} = \frac{1}{\epsilon_{\infty}} - \frac{1}{\epsilon_0},$$

Here, V is the volume of the crystal; ω is the frequency of an optical phonon; \mathbf{k} is the wave vector of a phonon; $a_{\mathbf{k}}^+$ and $a_{\mathbf{k}}$ are the creation and annihilation operators, respectively, for a phonon with wave vector \mathbf{k} ; ϵ_{∞} and ϵ_0 are the high-frequency and static dielectric constants, respectively; \mathbf{r}_1 and \mathbf{r}_2 are the position vectors of the electrons; and m^* is the effective mass of an electron.

In Eq. (1), the first term is the Hamiltonian of optical phonons, the second term is the Frölich electron–phonon interaction Hamiltonian for the two-electron system, the third and fourth terms are the kinetic energy of the electrons, and the last term describes the Coulomb repulsion between the electrons.

We perform a canonical transformation of the Hamiltonian (1) $\exp(S_a)H\exp(-S_a)$ with $S_a = \sum_{\mathbf{k}} C_{\mathbf{k}} (a_{\mathbf{k}}^+ - a_{\mathbf{k}})$, vary the Hamiltonian with respect to the parameters $C_{\mathbf{k}}$ (characterizing the shift transformation), and take the average over the phonon variables. As a result, we obtain the following functional for the ground state of the bipolaron:

$$J_{\text{Bp}} = \bar{T} + \bar{V}_{\text{ee}} + \bar{V}_{\text{ef}},$$

$$\bar{T} = -\frac{\hbar^2}{2m^*} \langle \Psi(\mathbf{r}_1, \mathbf{r}_2) | \Delta_1 + \Delta_2 | \Psi(\mathbf{r}_1, \mathbf{r}_2) \rangle, \quad (2)$$

$$\bar{V}_{\text{ee}} = \left\langle \Psi(\mathbf{r}_1, \mathbf{r}_2) \left| \frac{e^2}{\epsilon_{\infty} r_{12}} \right| \Psi(\mathbf{r}_1, \mathbf{r}_2) \right\rangle,$$

$$\bar{V}_{\text{ef}} = -\frac{2e^2}{\tilde{\epsilon}} \int \frac{|\Psi(\mathbf{r}_1, \mathbf{r}_2)|^2 |\Psi(\mathbf{r}_3, \mathbf{r}_4)|^2}{r_{13}} d\tau_{12} d\tau_{34}.$$

In what follows, atomic units with an energy unit $e^4 m^* / \hbar^2 \epsilon_{\infty}^2$ and the effective Bohr radius $a_0^* = \hbar^2 \epsilon_{\infty} / m^* e^2$ as a unit of length are used.

As a trial WF, we take the following linear combination of Gaussian functions:

$$\Psi_S(\mathbf{r}_1, \mathbf{r}_2) = \Phi(\mathbf{r}_1, \mathbf{r}_2) + (-1)^S \Phi(\mathbf{r}_2, \mathbf{r}_1), \quad (3)$$

$$\Phi(\mathbf{r}_1, \mathbf{r}_2)$$

$$= \sum_{i=1}^n C_i \exp(-a_{1i} r_{a1}^2 - 2a_{2i}(\mathbf{r}_1, \mathbf{r}_2) - a_{3i} r_{b2}^2), \quad (4)$$

where $S = 0$ for the singlet state (symmetric with respect to the permutation of the coordinates of the electrons) and $S = 1$ for the triplet (antisymmetric) state of the bipolaron and $\mathbf{r}_1(\mathbf{r}_2)$ is the position vector of the first (second) electron, with the origin taken at a point midway between the points a and b (the centers of the polarization wells). The z axis passes from the point a to the point b . The distance between these points is R . The quantities C_i , a_{1i} , a_{2i} , and a_{3i} are variational parameters. Electron correlations are taken into account by the term $\exp[-2a_{2i}(\mathbf{r}_1, \mathbf{r}_2)]$ in Eq. (4). The polaron WF is taken in the form

$$\Psi_p(\mathbf{r}) = \sum_{i=1}^n c_i \exp(-\alpha_i r^2), \quad (5)$$

where c_i and α_i are variational parameters.

3. RESULTS OF COMPUTATIONS

3.1. Singlet Bipolaron

Figure 1 shows the dependence of the energy of the ground (singlet) state of the bipolaron on the distance between the centers of the polarization wells calculated for $\eta = \epsilon_{\infty}/\epsilon_0 = 0$ using wave function (3) with $n = 5$ in Eq. (4) without regard for electron correlations ($a_{1i} = a_{3i}$, $a_{2i} = 0$, $i = 1, \dots, n$) and with allowance for them. It can be seen from Fig. 1 that as the distance between the polarons increases, the effect of electron correlations decreases; the energy functional of the bipolaron approaches the product of the two functionals corresponding to two noninteracting polarons and the bipolaron energy tends to twice the polaron energy calculated within this approximation ($J_p = -0.0542564$). We note that this value of the polaron energy is calculated

by us using a polaron wave function approximation (5) with five exponentials and exactly reproduces the result obtained in [14].

Thus, the minimum corresponding to the two-center bipolaron state in the distance dependence of the energy calculated without regard for electron correlations (curve 1 in Fig. 1) is due to a poor choice of the trial electron wave function. Such minima were considered in [4, 6, 7]. We note that, to our knowledge, Vinetskiĭ and Gitterman [4] were the first to demonstrate (on the basis of microscopic calculations) the possible existence of a bipolaron, which sets off their paper from the later publications devoted to bipolarons, in spite of the fact that the choice of the trial WF in [4] was not the best.

When comparing the results of variational calculations based on different trial WFs, one should compare the absolute values of the minima of the energy functional under study. However, the binding energy is presented, as a rule, in units of the polaron energy calculated within the same approximation. The results obtained in [2] using the Pekar trial WF $\Psi(\mathbf{r}_1, \mathbf{r}_2) = N(1 + \gamma r_{12})(1 + \alpha r_1)(1 + \alpha r_2)\exp(-\alpha(r_1 + r_2))$ were reproduced in [5]. With this trial function, it was found that $\Delta E/2J_p \approx 0.22$ for $\eta = 0$. The binding energy of the bipolaron is defined as $\Delta E = J_{Bp} - 2J_p$, where $J_p = -0.0542564$ is the exact value of the polaron energy calculated in [14] using a numerical method within the strong-coupling approximation. The region of existence of the bipolaron with the Pekar trial WF is $\eta \leq \eta_m = 0.125$. In [2], the absolute values of the ground-state energy of the bipolaron were not presented and the binding energy and the range of existence of the bipolaron ($\Delta E/2J_p \approx 0.25$, $\eta_m \approx 0.14$) were somewhat overestimated, because the binding energy of the bipolaron was calculated using a somewhat overestimated value of the polaron energy, which was found for the trial WF in the form $(1 + \alpha r)\exp(-\alpha r)$. The bipolaron binding energy for $\eta \rightarrow 0$ presented in [15] is also overestimated ($\Delta E/2J_{pol} \approx 0.22$, $J_{pol} = 1/6\pi$), because the calculations were performed for the polaron WF taken in the form of a single Gaussian. If we replace J_{pol} by the exact strong-coupling approximation value of J_p for the two-electron WF $\varphi(r_1, r_2) = N(1 + \gamma r_{12}^2)\exp(-\mu^2(r_1^2 + r_2^2))$ used in [15], we will obtain $\Delta E/2J_p \approx 0.193$.

The absolute value of the ground-state energy found by us using WF (3) with $n = 11$ in Eq. (4) is $J_{bp} = -0.136512$ or, in dimensionless units, $\Delta E/2J_p \approx 0.258$, and $\eta_m \approx 0.143$.

Figure 2 shows the dependence of the bipolaron binding energy on the distance between the centers of the polarization wells for various values of η and $n = 5$ in Eq. (4).

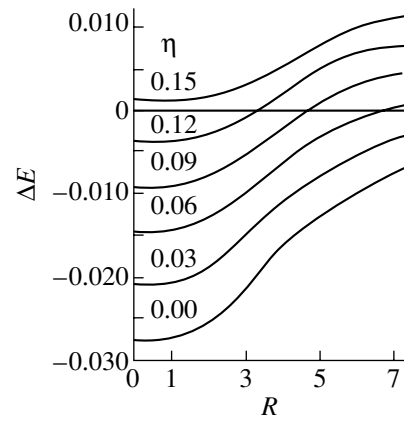


Fig. 2. Dependence of the bipolaron binding energy on the distance between the centers of the polarization wells calculated for various values of the ionic-bond parameter η and $n = 5$ in Eq. (4).

3.2. Triplet Bipolaron

When studying photoconductivity in YBCO, Deving and Salje [16] observed a wide absorption band in the infrared region with a peak near $5.5 \times 10^3 \text{ cm}^{-1}$ and assigned this peak to transitions of bosons from the ground (singlet) state to the excited metastable triplet state. It was also assumed in [16] that, in addition to singlet bipolarons, there exist triplet bipolarons in a certain temperature range and that it is the triplet bipolarons that are responsible for the broadening of the NMR lines of Cu and O in YBCO. The population of the triplet levels was assumed to increase with temperature, so that at $T \approx 200 \text{ K}$, the conductivity was due predominantly to the triplet bipolarons. Later, the change in the shape of the conductivity versus temperature curve predicted in [16] was indeed observed in the vicinity of the temperature indicated above (see review [17] and references therein).

We calculated the energy of the triplet bipolaron (similarly to an orthohelium atom). The lowest numerical value of the energy obtained using WF (3) for $\eta = 0$ for the single-center ($R = 0$) configuration of the triplet bipolaron was $J_{or} = -0.076082$.

As the distance between the centers of the polarization wells increases, the energy corresponding to the triplet bipolaron term decreases monotonically (in perfect analogy with the ${}^3\Sigma_u$ term of the hydrogen molecule). At $R = 0$, a fairly sharp peak is observed on the energy versus distance curve. This peak is indicative of the instability of the triplet $2{}^3S$ state, which can occur, for example, under nonequilibrium conditions where exchange scattering of band electrons by bipolarons takes place. In this case, bipolarons break down into single polarons.

3.3. Interaction between Polarons at Large Distances

Now, we will show that there is antiferromagnetic (AFM) exchange interaction between polarons. Indeed, at sufficiently large distances between polarons, the correlation effects become insignificant and the bipolaron WF can be written as a symmetrized or antisymmetrized product of the polaron WFs for the singlet and triplet states, respectively. In this case, to within the terms quadratic in the overlap integral K , the interaction energy of the two polarons has the form

$$E_{\text{int}} = E_1 - J_{\text{ex}} S_1 S_2, \quad (6)$$

where S_1 and S_2 are the spins of the first and second electrons

$$E_1 = \frac{1}{\epsilon_0} \int \frac{a(1)^2 b(2)^2}{r_{12}} d\tau_{12}, \quad (7)$$

$$J_{\text{ex}} = \frac{1}{\epsilon_\infty} K_1 - \frac{4}{\epsilon} K_2 K,$$

$$K_1 = \int \frac{a(1)b(1)a(2)b(2)}{r_{12}} d\tau_{12}, \quad (8)$$

$$K_2 = \int \frac{a(1)b(1)b(2)^2}{r_{12}} d\tau_{12}, \quad K = \int a(1)b(1) d\tau_1.$$

Here, we introduced the notation common for two-center systems: $a(1)$ and $b(1)$ are the polaron WFs centered at the points a and b , respectively; i.e., $a(1) \equiv \Psi_p(\mathbf{r}_{a1})$ and $b(1) \equiv \Psi_p(\mathbf{r}_{b1})$.

In Eq. (8), the first term corresponds to ferromagnetic Coulomb exchange and the second term describes AFM interaction between the polarons via phonons.

Thus, at large distances, the polarons repel each other and the spin-dependent part of the interaction (total exchange) is antiferromagnetic in nature (at $\eta \rightarrow 0$, we have $E_1 \approx 1/\epsilon_0 R$, $J_{\text{ex}} \approx -3K^2/R$). We also note that there is a potential barrier to the formation of the bipolaron state.

4. DISCUSSION

Thus, polarons repel one another at large distances and, therefore, a system of polarons may behave as an electron gas with Coulomb repulsion between particles. If the concentration of polarons is sufficiently low, a transition may occur (as in an electron gas [18]) to the Wigner crystal state, provided that $k_B T < e^2/\epsilon_0 a$ (a is the distance between particles). There are a number of papers devoted to the Wigner crystallization of a polaron gas. For example, it was shown in [19, 20] that a system of polarons (considered within a continuum approximation) can crystallize into a hexagonal lattice with a period which depends on the polaron concentration, as in the Wigner theory. In [21], the stability of the polaronic Wigner crystal was investigated and the pos-

sibility of the insulator–superconductor transition in the process of destruction of a polaron lattice was substantiated theoretically. Without going into details, we will simply note that when the conditions for the Wigner crystallization are met, the AFM exchange interaction between polarons can cause AFM ordering to occur in a system of polarons. Antiferromagnetism in the electronic Wigner crystal was discussed in [22, 23].

The AFM interaction between polarons can also lead to a decrease in the paramagnetic component of the magnetic susceptibility of a polaron gas with increasing polaron concentration, even if bound bipolaron states do not arise.

The instability of the 2^3S term of the bipolaron with respect to its decay into single polarons, shown by us in terms of the Fröhlich Hamiltonian describing the interaction of electrons with optical phonons, does not rule out the possible formation of bound triplet states of the two-electron system [13] or the existence of triplet bipolarons resulting from the interaction of electrons with elementary excitations of other types, e.g., with spin waves. The formation of self-localized electronic states in antiferromagnets with a low Néel temperature (a spin polaron in an AFM crystal) was considered in [24, 25]. In [17], it was supposed that high-temperature superconductivity is due to a triplet bound state of spin polarons, which forms in much the same way as the bipolaron.

Based on the Fröhlich Hamiltonian, we can consider only large polarons and bipolarons. The continuum approximation is applicable if the effective polarization potential in which self-trapped electrons move varies smoothly over distances of the order of the lattice constant b [3]. In [3], the effective polarization radius r_p of an electron was defined as the length over which the self-consistent polarization potential decreases by a factor of 2. For the simplest, hydrogenic, polaron WF, we have $r_p \approx 10\hbar^2 \tilde{\epsilon}/m^* e^2$.

The continuum approximation can be applied if $r_p > b$. In the opposite case of $r_b \leq b$, the spatial dispersion of the dielectric constants ϵ_0 and ϵ_∞ becomes significant; the difference in value between ϵ_0 and ϵ_∞ decreases with decreasing size of the region of polaron localization, and we have $\epsilon_0 \approx \epsilon_\infty \approx 1$. In most ionic crystals, SrTiO₃, and layered cuprates (along an “easy-plane” direction), the value of r_p is approximately 3–5 lattice constants.

The spatial dispersion of the dielectric constants can be included in a qualitative way by using the phenomenological interpolation model by Inkson [26]. In this case, an increase in the electron–phonon coupling is compensated by the dielectric-constant dispersion; as a result, if we take into account only the interaction of electrons with optical phonons, the case of $r_p \leq b$ is not realized in nearly all ionic crystals. It should also be noted that spatial dispersion of the dielectric constants (in the case of polarons and bipolarons of an intermedi-

ate radius) causes the bipolaron binding energy to decrease in absolute value, whereas any anisotropy of the crystal increases the ratio $\Delta E/2J_p$ [8, 9].

Interaction of carriers with acoustic phonons [27] or with short-wavelength optical phonons may lead to the formation of self-trapped states of a small radius. In this case, the continuum model is inadequate. Small-radius bipolarons treated within the strong-coupling approximation and superconductivity caused by their Bose condensation in narrow-band metals were considered in [28]. When considering such states, the binding energy of the bipolaron is generally taken to be a phenomenological parameter. Various aspects of the large-bipolaron theory as applied to the HTSC problem are discussed in [1, 8, 9, 29]. Review [17] is concerned with small-bipolaron states. In [19, 20], a system of large bipolarons in a layered high-temperature superconductor is treated as a Wigner crystal, in which plasma oscillations occur and favor carrier pairing in the conducting layers.

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