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Energy of interaction between polarons and spatial configuration of bipolaron in two-dimensional systems

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Abstract. The work is aimed at studying the influence of correlation effects on the interaction energy of two-dimensional (2D) polarons. The two-center configuration of 2D bipolaron corresponds to a shallow secondary minimum, which occurs when only the correlations associated with the permutation symmetry of the system are taken into account. The correlations associated with the direct dependence of the electron wave function on the distance between electrons lead to stabilization of the one-center configuration, and the secondary minimum corresponding to the two-center configuration disappears. Variational calculations were performed using a multiparameter Gaussian functions with correlation multipliers. The ground state energy of bipolaron is $E_2 = -0.542169\ E_h^*$ for $\eta = \varepsilon_\infty/\varepsilon_0 = 0$, where ε_∞ and ε_0 are the high-frequency and static dielectric constants of the crystal, respectively, E_h^* is the effective Hartree energy. The binding energy of bipolaron was calculated with respect to the double energy of 2D polaron obtained for wave function, consisting of 5 Gaussian exponents. The ground state energy of 2D polaron is $E_1 = -0.202366\ E_h^*$ for $\eta = 0$. The critical value of the ionicity parameter η corresponds to $\eta_c \approx 0.2$. At $\eta > \eta_c$, 2D bipolaron breaks up into two 2D polarons.

Keywords: 2D-polaron, 2D-bipolaron, low-dimensional systems, electron-phonon interaction.

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1. Introduction

Interest in bipolaron (BP) problem increased after the discovery of the high temperature superconductivity (HTSC) in the cuprate metal oxide compounds (MOC) [1]. Vinetsky and Pashitsky predicted the possibility of HTSC due to Bose condensation of BP gas long before the discovery of the HTSC phenomenon [2]. In the same work, the gap nature of superconductivity (SC) and HTSC associated with Bose condensation of large radius BPs was proved. A significant amount of work devoted to studying BP mechanisms of SC was performed both for small-radius BPs [3, 4] and large-radius BPs [5–8].

As known, a decrease in the system dimension leads to a significant increase in the binding energy of low-dimensional atoms [9, 10] and molecules [11, 12], as well as localized and self-localized states in condensed systems, such as shallow impurity centers and their complexes, D– centers, polarons, and BPs [13–16].

Examples of two-dimensional systems are crystal structures that have translational symmetry in only two directions. In the direction perpendicular to the plane of the crystal, the effective mass of the charge carriers is so large that the movement in this direction can be neglected. Two-dimensional crystals can be located on the surface of bulk crystals or at the surface of liquid solutions. An example of a two-dimensional crystal is the well-known graphene [17, 18]. Conductive layers in cuprate MOC, in which HTSC was observed, can be considered as two-dimensional systems. An example is the La_2CuO_4 system, in which electrons are localized in the CuO_2 layers. Two-dimensional and one-dimensional crystals have a band structure and can be both metals and semiconductors or dielectrics. So, pure graphene is a two-dimensional crystal with a zero band gap. In this case, the law of electron energy dispersion in the conduction band has a linear dependence on the wave vector

[17]. At the same time, there are modifications of graphene with an anomalously wide band gap [18]. Thus, by changing the doping value or the properties of the substrate on which the crystal was grown, it is possible to change both the band gap and the dispersion law of current carriers in 2D systems.

In our work, we consider the model of a 2D crystal with a simple conduction band and a quadratic dispersion law of electron energy. It is assumed that interaction with optical phonons leads to formation of large (bi)polaron with energy levels located near the conduction band bottom.

In the problems, related with the calculations of the energy spectrum of localized and autolocalized states in condensed matter, variational methods are used. The development of methods for minimizing multiparameter energy functionals is a central part of the variational calculations. The variational calculations in the work were performed by random search methods [19] and the Hook–Jeeves method [20]. The variational functional was obtained in a simplified integral-analytical form. As a base system, we used Gaussian orbitals with correlation multipliers.

2. The interaction energy of continuous 2D polarons and the configuration of BP in 2D systems

The binding energy of BP is defined as the difference between the doubled energy of polaron and the energy of BP:

$$\Delta E = 2E_1 - E_2, \tag{1}$$

where E_1 is the energy of polaron, E_2 – energy of BP.

A bound state corresponds to a positive binding energy.

2.1.Hamiltonian and the energy functional of polaron

The Hamiltonian of polaron in a 2D system is defined by the expression:

$$H_1 = -\frac{\hbar^2}{2m^*}\Delta_1 + H_{ph} + H_{1e-ph}\,, \tag{2}$$

where m^* is the effective mass of band electron, Δ_1 – 2D Laplace operators of electron with the coordinate r_1; H_{ph} – Hamiltonian of the phonon field:

$$H_{ph} = \sum_{\boldsymbol{k}} \hbar\omega_{\boldsymbol{k}} a_{\boldsymbol{k}}^+ a_{\boldsymbol{k}}\,, \tag{3}$$

where ω_k and k are the frequency and wave vector of optical phonons; a_k^+ and a_k are operators of creation and annihilation of phonons with the wave vector k; in what follows, we consider optical phonons without dispersion $\omega_k = \omega$; H_{1e-ph} is the Hamiltonian of electron-phonon interaction:

$$H_{1e-ph} = \sum_{\boldsymbol{k}} V_{\boldsymbol{k}} \left\{ \exp\left(-i\boldsymbol{k}\boldsymbol{r}_1\right) a_{\boldsymbol{k}}^+ + H.c. \right\}, \tag{4}$$

where (in the dimensionless units $m^* = 1$, $\hbar = 1$, $\omega = 1$) $V_k = \sqrt{\frac{2\pi\alpha}{Sk}}$ – parameter of the electron-phonon interaction, $\alpha = \frac{1}{\sqrt{2}}\frac{e^2}{\tilde{\varepsilon}}$ – dimensionless constant of the electron-phonon coupling, $\tilde{\varepsilon}$ – effective dielectric constant defined by the expression $\tilde{\varepsilon}^{-1} = \varepsilon_\infty^{-1} - \varepsilon_0^{-1}$, ε_∞ and ε_0 are high-frequency and a static dielectric constant, respectively; S is a crystal area.

We choose the polaron wave function (WF) as:

$$\Psi_p(r) = exp\left[\sum_k f_k a_k^+ - f_k^* a_k\right] |0\rangle \Psi_1(r), \tag{5}$$

where f_k is a variational function, $|0\rangle$ – WF of photon vacuum and $\Psi_1(r)$ – electron WF.

Electron WF is chosen in the form:

$$\Psi_1(r_1) = \sum_{i=1}^{N} C_i exp(-a_i r_1^2), \tag{6}$$

where C_i, a_i are variational parameters.

Further, we set $\hbar = 1$, $m^* = 1$, $e^{*2} = e_2/\varepsilon_\infty = 1$. The effective atomic unit of energy is defined by the value $E_h^* = \hbar^2/m^*a^{*2}$ (effective Hartree energy), the effective atomic unit of length $a^* = \varepsilon_\infty\hbar^2/m^*e^2$ (effective Bohr radius) is introduced.

In the adiabatic approximation the energy functional of polaron in a 2D crystal is defined by the expression:

$$J_1 = \frac{T_1 + J_{1ph}/N_1}{N_1} = E_{1kin} + E_{1pot}\,, \tag{7}$$

where $E_{1kin} = T_1/N_1$ is the average value of kinetic energy, $E_{1pot} = J_{1ph}/N_1^2$ – average energy due to the total contribution of the phonon field and electron-phonon interaction, N_1 – normalization integral:

$$N_1 = \int \Psi^2\left(\boldsymbol{r}_1\right) d\sigma_1\,, \tag{8}$$

$d\sigma_1 = dx_1dy_1$ – area element in the 2D system;

$$T_1 = -\frac{1}{2}\int \Psi\left(\boldsymbol{r}_1\right)\Delta_1\Psi\left(\boldsymbol{r}_1\right) d\sigma_1\,, \tag{9}$$

$$J_{1ph} = -\frac{1-\eta}{2}\iint \Psi^2\left(\boldsymbol{r}_1\right)\frac{1}{r_{12}}\Psi^2\left(\boldsymbol{r}_2\right) d\sigma_{12}, \tag{10}$$

here, $\eta = \varepsilon_\infty/\varepsilon_0$ determines the degree of crystal ionicity, $d\sigma_{12} = d\sigma_1 d\sigma_2$.

The polaron energy is found by minimizing the polaron energy functional (7):

$$E_1 = \min_{\{C,a\}} J_1\,, \tag{11}$$

where $\{C,a\} = \{C_1, C_2, \ldots C_N, a_1, a_2, \ldots a_N\}$.

2.2.Hamiltonian and the energy functional of BP

The Hamiltonian of a system consisting of two 2D-electrons in the phonon field has the form:

$$H_b = -\frac{1}{2}\left(\Delta_1 + \Delta_2\right) + \frac{1}{r_{12}} + H_{2e-ph} + H_{ph}\,, \tag{12}$$

where Δ_1 and Δ_2 are the 2D Laplace operators of the first and the second electrons; $H_{2e\text{-}ph}$ is the Hamiltonian of electron-phonon interaction:

$$H_{2e-ph} = \sum_{\boldsymbol{k}} V_{\boldsymbol{k}} \left\{ \left[\exp\left(-i\boldsymbol{k}\boldsymbol{r}_1\right) + \exp\left(-i\boldsymbol{k}\boldsymbol{r}_2\right) \right] a_{\boldsymbol{k}}^{+} + H.c. \right\}, \tag{13}$$

r_1 and r_2 are the coordinates of the first and the second electrons in the 2D system.

We place the origin in the middle between points *a* and *b*. The distance between points *a* and *b* is equal to *R*. The vector *R* is directed along the axis OX from *a* to *b*. The two-center coordinate system is shown in Fig. 1.

WF of BP is given by:

$$\Psi_b = exp\left[\sum_k f_k a_k^{+} - f_k^{*} a_k \right] \left|0\right\rangle \Psi_{12}\left(\boldsymbol{r}_1, \boldsymbol{r}_2, R\right) \tag{14}$$

WF $\Psi_{12}(\boldsymbol{r}_1, \boldsymbol{r}_1, R)$ of two-electron system is chosen in the form:

$$\Psi_{12}\left(\boldsymbol{r}_1, \boldsymbol{r}_2, R\right) = \Psi_{12} = \sum_{i=1}^{N} C_i exp\left(-a_{1i} r_{a1}^2 - 2a_{2i}\left(\boldsymbol{r}_{a1} \cdot \boldsymbol{r}_{b2}\right) - a_{3i} r_{b2}^2\right), \tag{15}$$

where the traditional notation for a two-center coordinate system is used: $r_{a1} = r_1 + R/2$; $r_{b2} = r_2 - R/2$; C_i, a_{1i}, a_{2i}, a_{3i} are the variational parameters.

We assume that WF (15) is symmetrized. This procedure can be provided by automatic symmetrization. For this, an even number of terms $N = 2n_0$ is chosen. The terms in Eq. (15) are separated into pairs. Symmetrization is performed for each pair.

Due to the fact that the Hamiltonian of BP (12) does not contain terms that depend on the distance *R* between the centers of the polarization wells for these two polarons, the parameter *R* can be entered only in WF (15). We assume that the centers of the polarization wells of polarons are located at the points *a* and *b*.

The energy functional of BP in the 2D crystal is defined by the expression:

$$J_2 = \frac{T_2 + J_{12} + J_{2ph}/N_2}{N_2} = E_{2kin} + E_{2pot}\,, \tag{16}$$

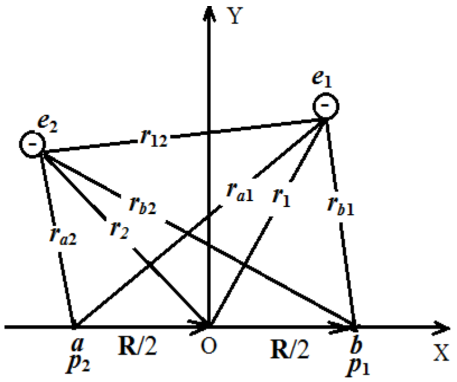

Fig. 1. Two-center coordinate system. The centers of the polarons polarization wells p_1 and p_2 are placed at the points *a* and *b*.

where $E_{2kin} = \dfrac{T_2}{N_2}$ and $E_{2pot} = \dfrac{J_{12} + J_{2ph}/N_2}{N_2}$ are kinetic and potential energy of bipolaron,

$$N_2 = \int \Psi_{12}^2\left(\boldsymbol{r}_1, \boldsymbol{r}_2\right) d\sigma_{12}\,, \tag{17}$$

$$T_2 = -\frac{1}{2}\int \Psi_{12}\left(\boldsymbol{r}_1, \boldsymbol{r}_2\right)\left(\Delta_1 + \Delta_2\right)\Psi_{12}\left(\boldsymbol{r}_1, \boldsymbol{r}_2\right) d\sigma_{12}\,, \tag{18}$$

$$J_{12} = \int \frac{\Psi_{12}^2\left(\boldsymbol{r}_1, \boldsymbol{r}_2\right)}{r_{12}} d\sigma_{12}\,. \tag{19}$$

V_{2ph}/N_2^2 is the total contribution of the average values of the phonon field operator and the electron-phonon interaction operator. In the strong coupling approximation, after functional variation of the energy functional with respect to the function f_k in WF (14) and averaging over phonon variables, J_{2ph} is defined by the expression:

$$J_{2ph}\left(R\right) = -\frac{1-\eta}{2} \cdot \iint \Psi_{12}^2 \left(\frac{1}{r_{13}} + \frac{1}{r_{14}} + \frac{1}{r_{23}} + \frac{1}{r_{24}} \right) \Psi_{34}^2 d\sigma_{12} d\sigma_{34} \tag{20}$$

The total potential energy E_{2pot} of BP is defined by the sum of the energy of interelectron repulsion, the energy caused by the electron-phonon interaction and the energy of the phonon field.

The BP energy is defined as a minimum of the energy functional (16):

$$E_2 = \min_{\{C;a\}} J_2\,, \tag{21}$$

where $\{C,a\} = \left\{ \begin{matrix} C_1, C_2 \ldots C_N \\ a_{11}, a_{12}, \ldots a_{1N} \\ a_{21}, a_{22}, \ldots a_{2N} \\ a_{31}, a_{32}, \ldots a_{3N} \end{matrix} \right\}$ is a set of variation parameters.

2.3. Simplified expressions for various contributions to the energy functional of BP

All integral expressions that are part of the BP functional can be reduced to analytical expressions (the kinetic energy), or significantly simplified (components of potential energy) by calculating the integrals in the Cartesian coordinates.

WF (15) can be converted to a more convenient form:

$$\Psi_{12}(\boldsymbol{r}_1,\boldsymbol{r}_2,R)=\sum_{i=1}^{N}\Psi_{12i}(\boldsymbol{r}_1,\boldsymbol{r}_2,R)\,, \tag{22}$$

$$\Psi_{12i}(\boldsymbol{r}_1,\boldsymbol{r}_2,R)=\Psi_{12xi}(x_{a1},x_{b2})\Psi_{12yi}(y_1,y_2) \tag{23}$$

$$\Psi_{12xi}(x_{a1},x_{b2})=C_i exp(-a_{1i}x_{a1}{}^2-2a_{2i}x_{a1}x_{b2}-a_{3i}x_{b2}{}^2), \tag{24}$$

where $x_{a1}=x_1+R/2$; $x_{b2}=x_2-R/2$;

$$\Psi_{12yi}(y_1,y_2)=exp\left(-a_{1i}y_1^2-2a_{2i}y_1y_2-a_{3i}y_2^2\right). \tag{25}$$

WF (24) can be represented in an equivalent form:

$$\begin{gathered}\Psi_{12xi}(x_{a1},x_{b2})=\Psi_{12xi}(x_1,x_2,R)=\\ C_i' exp(-a_{1i}x_1^2-2a_{2i}x_1x_2-a_{3i}x_2^2+2a_{4i}x_1+2a_{5i}x_2),\end{gathered} \tag{26}$$

where

$$C_i'=C_i\exp\left[-0.25\left(a_{1i}-2a_{2i}+a_{3i}\right)R^2\right], \tag{27}$$

$$a_{4i}=-0.5\left(a_{1i}-a_{2i}\right)R\,,\; a_{5i}=0.5\left(a_{3i}-a_{2i}\right)R\,. \tag{28}$$

The normalization integral is defined by the expression:

$$N_2(R)=\sum_{i,j=1}^{N}N_{ij}\,, \tag{29}$$

$$N_{ij}=A_{ij}\exp\left[\left(\mu_{1ij}^2/\zeta_{ij}+\xi_{ij}^2\right)/\alpha_{ij}\right], \tag{30}$$

$$A_{ij}=\frac{\pi^2C_i'C_j'}{\zeta_{ij}}\,, \tag{31}$$

where simplified designations are introduced:

$$\alpha_{ij}=a_{1i}+a_{1j},\ \beta_{ij}=a_{2i}+a_{2j},\ \gamma_{ij}=a_{3i}+a_{3j}, \tag{32}$$

$$\zeta_{ij}=\alpha_{ij}\cdot\gamma_{ij}-\beta_{ij}{}^2,\quad \xi_{ij}=a_{4i}+a_{4j},\ \theta_{ij}=a_{5i}+a_{5j}, \tag{33}$$

where the parameters a_{4i} and a_{5i} are defined by the expression (28);

$$\mu_{1ij}=\theta_{ij}\cdot\alpha_{ij}-\xi_{ij}\cdot\beta_{ij},\ \mu_{2ij}=\xi_{ij}\cdot\gamma_{ij}-\theta_{ij}\cdot\beta_{ij}. \tag{34}$$

The kinetic energy can be represented in an analytical form by the following expressions:

$$T_2(R)=\sum_{i,j=1}^{N}T_{2ij}\,, \tag{35}$$

$$\begin{aligned}&T_{2ij}=2\left(a_{4i}a_{4j}+a_{5i}a_{5j}\right)N_{ij}-\\ &2\left(a_{1i}a_{1j}+a_{2i}a_{2j}\right)N_\alpha-\\ &\left(a_{1i}a_{2j}+a_{2i}a_{1j}+a_{3i}a_{2j}+a_{2i}a_{3j}\right)N_\beta-\\ &2\left(a_{3i}a_{3j}+a_{2i}a_{2j}\right)N_\gamma-\\ &\left(a_{1i}a_{4j}+a_{4i}a_{1j}+a_{2i}a_{5j}+a_{5i}a_{2j}\right)N_\xi-\\ &\left(a_{3i}a_{5j}+a_{5i}a_{3j}+a_{2i}a_{4j}+a_{4i}a_{2j}\right)N_\theta\end{aligned} \tag{36}$$

$$N_\alpha=-N_{ij}\zeta_{ij}^{-2}\cdot\begin{pmatrix}-2\theta_{ij}\xi_{ij}\beta_{ij}\gamma_{ij}+\theta_{ij}^2\beta_{ij}^2+\\ \xi_{ij}^2\gamma_{ij}^2-\gamma_{ij}\beta_{ij}^2+\gamma_{ij}^2\alpha_{ij}\end{pmatrix},$$

$$N_\beta=2N_{ij}\zeta_{ij}^{-2}\cdot\begin{pmatrix}-\beta_{ij}^3-\xi_{ij}\beta_{ij}^2\theta_{ij}+\xi_{ij}^2\beta_{ij}\gamma_{ij}+\\ \beta_{ij}\gamma_{ij}\alpha_{ij}+\theta_{ij}^2\alpha_{ij}\beta_{ij}-\theta_{ij}\alpha_{ij}\xi_{ij}\gamma_{ij}\end{pmatrix},$$

$$N_\gamma=-N_{ij}\zeta_{ij}^{-2}\begin{pmatrix}\xi_{ij}^2\beta_{ij}^2-2\xi_{ij}\beta_{ij}\theta_{ij}\alpha_{ij}+\\ \theta_{ij}^2\alpha_{ij}^2-\alpha_{ij}\beta_{ij}^2+\gamma_{ij}\alpha_{ij}^2\end{pmatrix},$$

$$N_\xi=2N_{ij}\mu_{2ij}\zeta_{ij}^{-1}\,,\ N_\theta=2N_{ij}\mu_{1ij}\zeta_{ij}^{-1}\,.$$

The average value of the Coulomb repulsion of electrons has the form:

$$J_{12}(R)=\sum_{i,j=1}^{N}J_{12ij}\,, \tag{37}$$

$$J_{12ij}=\frac{N_{ij}}{\sqrt{|q_{12ij}|}}\frac{1}{\sqrt{\pi}}f\left(0.5\frac{|p_{12ij}|}{\sqrt{|q_{12ij}|}}\right), \tag{38}$$

$$q_{12ij}=0.25\left(\alpha_{ij}+2\beta_{ij}+\gamma_{ij}\right)/\zeta_{ij}\,,\; p_{12ij}=\left(\mu_{2ij}-\mu_{1ij}\right)/\zeta_{ij}\,,$$

where parameters μ_{1ij} and μ_{2ij} are defined by the expressions (34);

$$f(b)=\int_0^1 dt\frac{\exp\left(-b^2t^2\right)}{\sqrt{1-t^2}}\,. \tag{39}$$

The average value of the total contribution of the phonon field and electron-phonon interaction has the form:

$$J_{2ph}(R)=(\eta-1)\sum_{i,j.k.l=1}^{N}J_{2ph\,ijkl} \tag{40}$$

$$J_{2ph\,ijkl}=2\frac{N_{ij}\,N_{kl}}{\sqrt{|q_{1ij}+q_{2kl}|}}\frac{1}{\sqrt{\pi}}f\left(0.5\frac{|p_{1ij}+p_{2kl}|}{\sqrt{|q_{1ij}+q_{2kl}|}}\right) \tag{41}$$

where $q_{1ij}=0.25\gamma_{ij}/\zeta_{ij}$, $q_{2ij}=0.25\alpha_{ij}/\zeta_{ij}$, $p_{1ij}=0.25\mu_{2ij}/\zeta_{ij}$, $p_{2ij}=0.25\mu_{1ij}/\zeta_{ij}$.

2.4. Paired interaction potential of 2D polarons

The calculations of the two-polaron system energy for the distance between the centers of polarization wells were performed for WFs of various flexibility. We choose WFs for the $N = 2$ in Eq. (15) in the following cases:

$$a_{1i} = a_{3i},\ a_{2i} = 0, \tag{42}$$

$$a_{1i} \neq a_{3i},\ a_{2i} = 0, \tag{43}$$

$$a_{1i} = a_{3i},\ a_{2i} \neq 0, \tag{44}$$

$$a_{1i} \neq a_{3i},\ a_{2i} \neq 0. \tag{45}$$

Fig. 2 shows the dependences of two polarons energy on the distance between them. As WF flexibility increases, the two-center configuration (curve (*1*)) becomes energetically disadvantageous. The most flexible wave function with parameters (45) corresponds to a single-center configuration (curve (*4*)).

Figs 3 and 4 show the dependence of the energy of BP E_2 on the distance between polarons for the parameters defined by Eqs (42) and (45), respectively, $\eta = 0$. The same figures show the corresponding dependences of the kinetic energy E_{2kin} of BP taken with the opposite sign and half of the potential energy E_{2pot}. At the points corresponding to the minimum of energy functional, the virial theorem is satisfied:

$$E_{2kin} = -E_2, \qquad E_{2pot} = 2E_2, \tag{46}$$

where E_2 is the ground state energy, E_{2kin} – kinetic energy, E_{2pot} – potential energy of BP.

For the two-center configuration shown in Fig. 3, the virial theorem is fulfilled in 3 points: for $R = 0$, $R = R_m$ and $R = \infty$. At the points $R = 0$ and $R = \infty$, correlation effects are absent, and BP decays into two polarons. For one-center configuration (Fig. 4), the virial theorem holds for $R = 0$ and $R = \infty$. The only deep minimum corresponds to $R = 0$. For $R = \infty$, BP breaks up into two polarons.

An increase in the number of terms in WF (15) does not lead to qualitative changes in the behavior of the dependences of the BP energy on the distance between polarons. However, the energy minimum at the point $R = 0$ can be significantly reduced.

The best values of E_2 were obtained by us for WF (15), which is the sum of 5 independent terms, *i.e.* for $N = 2n_0$, $n_0 = 5$. Further increase of N did not affect the value of the energy minimum. The energy value of BP for WF (15) for $n_0 = 5$ and $\eta = 0$ is $E_2 = -0.542169\ E_h^*$.

Polaron WF was chosen as the sum of Gaussian exponents (6). Variational calculations of the polaron energy performed using the variational method with WF (6) and $N = 5$, for $\eta = 0$ gave the following value:

$$E_1 = -0.202366. \tag{47}$$

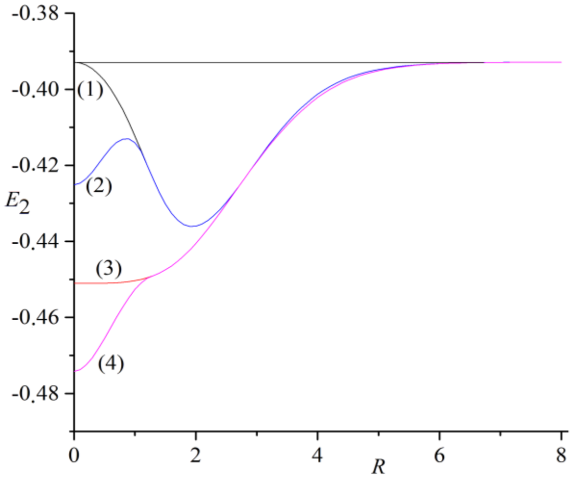

Fig. 2. Dependences of the interaction energy of two 2D polarons on the distance between the centers of the polarization wells for $\eta = 0$. The curves (*1*) to (*4*) correspond to the parameters (42)–(45), respectively. The horizontal curve corresponds to twice the polaron energy calculated in the same approximation. The unit of energy is the effective Hartree energy $E_h^* = \hbar^2/m^* a^{*2}$, the unit of length is the effective Bohr radius $a^* = \varepsilon_\infty \hbar^2/m^* e^2$.

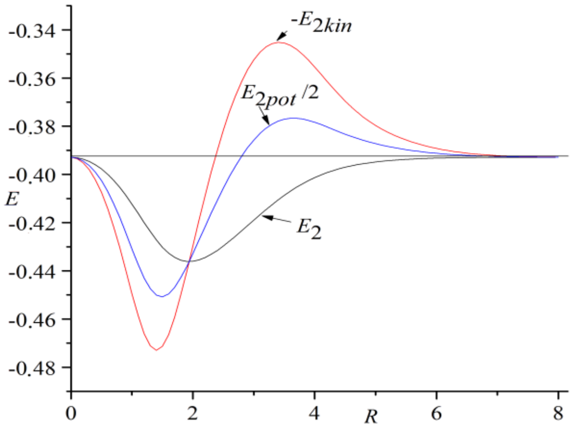

Fig. 3. Dependence of 2D BP energy on the distance between polarons for the case $a_{1i} = a_{3i}$, $a_{2i} = 0$. E_2 is the energy of BP, E_{2kin} – kinetic energy, E_{2pot} – potential energy representing the sum of the Coulomb repulsion energy, the electron-phonon interaction energy and phonon contribution energy. The unit of energy is the effective Hartree energy $E_h^* = \hbar^2/m^* a^{*2}$, the unit of length – effective Bohr radius $a^* = \varepsilon_\infty \hbar^2/m^* e^2$.

Conversion of 2D polaron energy for an arbitrary η should be performed according to the formula:

$$E_1 = -0.202366(1-\eta)^2 \,. \tag{48}$$

Fig. 5 shows the dependence of the BP energy E_2 and the double polaron energy E_1 on the ionicity parameter η. For $\eta = \eta_c \approx 0.2$ the BP binding energy $\Delta E_2 = 2E_1 - E_2$ becomes zero.

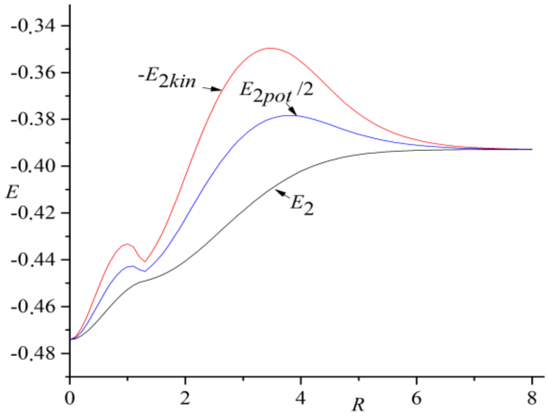

Fig. 4. Dependences of the energy E_2 for interaction between two 2D polarons on the distance between the centers of the polarization wells for the case $a_{1i} \neq a_{3i}$, $a_{2i} \neq 0$. E_{2kin} is the kinetic energy, E_{2pot} – potential energy. The unit of energy is the effective Hartree energy $E_h^* = \hbar^2/m^* a^{*2}$, the unit of length is the effective Bohr radius $a^* = \varepsilon_\infty \hbar^2/m^* e^2$.

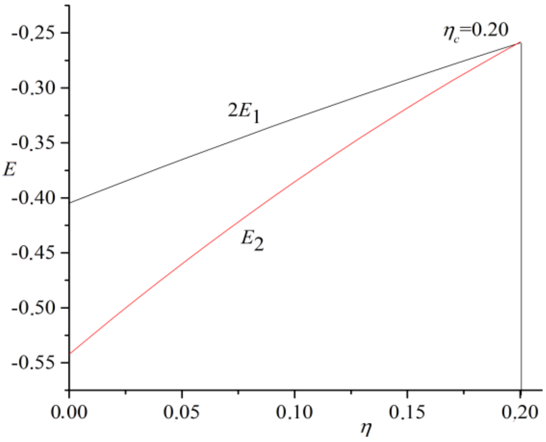

Fig. 5. Dependences of the BP energy E_2 and the double polaron energy $2E_1$ on the parameter of ionicity η. The unit of energy is the effective Hartree energy $E_h^* = \hbar^2/m^* a^{*2}$.

3. Discussion of the obtained results

For comparison, we give the energy values calculated in [15] for single-center 2D BP by using other WFs:

$$\varphi(\mathbf{r}_1,\mathbf{r}_2) = A\exp\left(-\delta^2\left(r_1^2+r_2^2\right)\right)\left(1+\gamma\delta^2 r_{12}^2\right),\ \gamma > 0, \tag{49}$$

$$\varphi(\mathbf{r}_1,\mathbf{r}_2) = A\exp\left(-\delta^2\left(r_1^2+r_2^2\right)\right)\left(1-b\exp\left(\gamma\delta^2 r_{12}^2\right)\right),$$

$$\gamma > 0,\ b < 1, \tag{50}$$

where A is the normalization factor; α, γ, δ and b are the variation parameters.

The BP energy obtained using WFs (50) and (51) for $\eta = 0$ was $-0.49087\,E_h^*$ and $-0.50658\,E_h^*$, respectively, which is higher than our results.

The dependences of the 2D polarons interaction energy, taking into account all types of electronic correlations, on the distance between polarons were obtained by us for the first time. 2D BP forms a bound state in the configuration corresponding to a single-center BP (helium atom configuration). The two-center configuration of BP in 2D crystals can be realized only for the case of a system consisting of two impurity centers. This system can be considered as a hydrogen molecule placed into the phonon field. The paper does not provide examples of numerical calculation of energies of such system. However, the analytical expressions for the kinetic energy, electron repulsion energy through the Coulomb interaction and the electron attraction energy due to electron-phonon interaction and the phonon field do not change for an exchange-coupled pair of shallow impurities interacting with optical phonons.

In 2D systems, the spatial configuration of bipolaron is similar to the configuration of the two-dimensional helium atom. The one-center configuration of bipolaron is also realized in three-dimensional (3D) crystals [21, 22]. The two-center configuration in 3D crystals, as well as in 2D systems, corresponds to a shallow minimum, which disappears when sufficiently flexible WF is chosen. The decisive factor in this case is consideration of interelectronic correlations associated with the direct dependence of polaron WF on the distance between electrons. At the same time, in one-dimensional crystals, both one-center and two-center configurations of bipolaron can coexist [23, 24].

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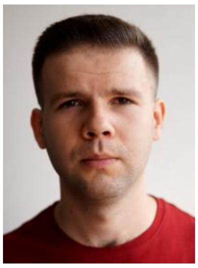

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Енергія взаємодії поляронів та просторова конфігурація біполярону в двовимірних системах

Н.І. Каширіна, Я.О. Каширіна, О.А. Король, О.С. Роїк

Анотація. Метою роботи є вивчення впливу кореляційних ефектів на енергію взаємодії двовимірних (2D) поляронів. Двоцентрова конфігурація 2D-біполярону відповідає мілкому побічному мінімуму, який виникає тоді, коли враховуються лише кореляції, пов'язані з перестановочною симетрією системи. Кореляції, зумовлені прямою залежністю хвильової функції електронів від відстані між електронами, приводять до стабілізації одноцентрової конфігурації, а побічний мінімум, який відповідає двоцентровій конфігурації, зникає. Варіаційні розрахунки проводилися із застосуванням багатопараметричних гауссових функцій з кореляційними множниками. Енергія основного стану біполярону становить $E_2 = -0.542169\, E_h^*$ для $\eta = \varepsilon_\infty/\varepsilon_0 = 0$, де ε_∞ і ε_0 – високочастотна і статична діелектрична проникність кристала відповідно; E_h^* – ефективна енергія Хартрі. Енергія зв'язку біполярону була розрахована по відношенню до подвоєної енергії 2D полярону, отриманої для хвильової функції, що складається з 5 гауссових експонент. Енергія основного стану 2D полярону становить $E_1 = -0.202366\, E_h^*$ при $\eta = 0$. Критичне значення параметра іонності η відповідає $\eta_c \approx 0,2$. При $\eta > \eta_c$ 2D біполярон розпадається на два 2D полярони.

Ключові слова: 2D-полярон, 2D-біполярон, низьковимірні системи, електрон-фононна взаємодія.