Polarons and bipolarons in two-dimensional systems

Kashirina N.I.[1], Kashyrina Ya.O.[2], Korol O.A.[3], Roik O.S.[2]

[1]V. Lashkaryov Institute of Semiconductor Physics, NAS of Ukraine , kashirina1506@gmail.com ;

[2]Taras Shevchenko National University of Kyiv; [3]State University of Telecommunications

INTRODUCTION 1

The energy of two-dimensional (2D) bipolaron was obtained by the Buimistrov-Pekar method. Variational calculations were carried out taking into account the direct dependence of the wave function (WF) of the system on the interelectron distance. The variational functions have been chosen in the form of a sum of Gaussian functions with correction multipliers. The region of existence of a 2D bipolaron (BP) is determined as a function of the crystal parameters. It is shown that only a single-center configuration is stable. The minimum corresponding to the two-center configuration is a side extremum, that disappears, when the direct dependence of the wave function of the system on the distance between electrons are taken into account. The study of the fulfillment of the virial theorem (VT) for (bi)polaron functional is carried out. The variational calculations are compared with the calculations performed by other authors using the Buimistrov-Pekar method [1].

Currently, 2D (bi)polaron are studied in connection with the possibility of applying of the (bi)polaron theory to graphene [2-5]. Both gapless graphene models [2, 3] and traditional 2D systems with a wide bandgap and a quadratic dispersion law of a band electron are considered [4,5].

BASIC RELATIOS 2

We consider two electrons in the phonon field of a 2D crystal. The energy E_b of the ground state of the considered system has the form:

$$E_b = \langle \Phi_{12} | H_b | \Phi_{12} \rangle \qquad (1)$$

$$H_b = -\frac{1}{2}(\Delta_1 + \Delta_2) + \frac{1}{\varepsilon_\infty r_{12}} + H_{2e-f} + H_f \qquad (2)$$

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

$$H_f = \sum_{\mathbf{k}} \hbar\omega_{\mathbf{k}} a_{\mathbf{k}}^+ a_{\mathbf{k}} \qquad V_{\mathbf{k}} = \sqrt{\frac{2\pi\alpha}{Sk}}$$

$$\alpha = \frac{1}{\hbar\omega}\frac{e_0^2}{2\varepsilon_\infty}(1-\eta)\cdot\left(\frac{2m^*\omega}{\hbar}\right)^{1/2}, \quad \eta = \varepsilon_\infty/\varepsilon_0,$$

$$\Phi_{12} = \Psi_{12}\exp(-S_1 - S_2), \quad S_1 = \sum_k f_k(a_k^+ - a_k)$$

$$S_2 = \sum_{k,j} g_k(\mathbf{r}_1, \mathbf{r}_2)\exp(-i\mathbf{k}\mathbf{r}_i)a_k^+ + H.c.$$

$$g_k = \varphi_k\left(\exp(-i\mathbf{k}\mathbf{r}_1) + \exp(-i\mathbf{k}\mathbf{r}_2)\right)$$

The electron WF is determined by:

$$\Psi_{12} \equiv \Psi_{12}(r_1, r_2, r_{12}).$$

TWO-CENTER BIPOLARON 3

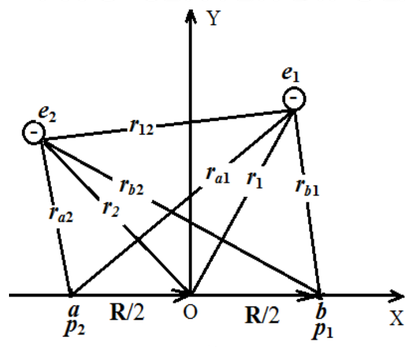

Fig. 1. Two center coordinates system.

$$\Psi_{12} = \sum_{i=1}^{N}(1+P_{12})C_i exp\left(-a_{1i}r_{a1}^2 - 2a_{2i}(\mathbf{r}_{a1}\cdot\mathbf{r}_{b2}) - a_{3i}r_{b2}^2\right), (3)$$

where C_i, a_{1i}, a_{2i}, a_{3i} are variation parameters .

The strong coupling energy of BP in a 2D crystal is :

$$E_b = \min\{J_b\}, \quad J_b = \frac{T_b}{N_b} + \frac{V_{ee}}{N_b} + \frac{V_{bf}}{N_b^2}, \qquad (4)$$

where the first, second and third terms in the right side of eq. (4) for J_b , correspond to the kinetic energy, the energy of the Coulomb repulsion and the total contribution of the phonon field and electron-phonon interaction respectively; N_b – is the normalization integral:

$$N_b = \langle \Psi_{12} | \Psi_{12} \rangle$$

STRONG COUPLING

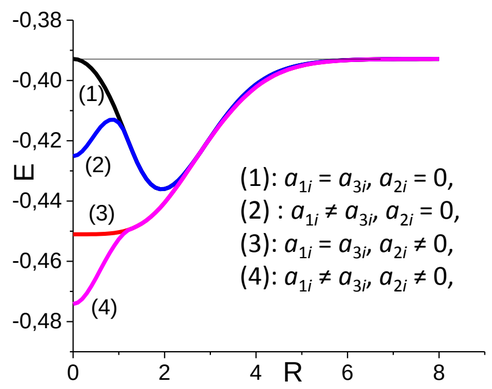

Fig. 2. Energy (in units $E_h^* = \hbar^2/m^*a^{*2}$) of 2D bipolaron on the distance R (in units $a^* = \varepsilon_\infty\hbar^2/m^*e^2$) for different WF (3), N=1, η=0.

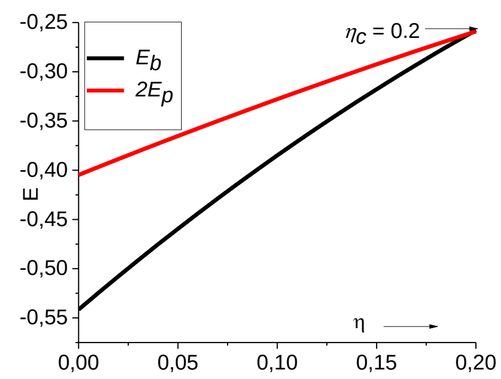

Fig. 3. Dependence of doubled polaron and bipolaron energies on the ionicity parameter η *for* WF (3), *N*=5.

INTERMEDIATE COUPLING

$$E_{bi} = \min\{J_{bi}\}, J_{bi} = \frac{2T_b}{N_b} + \frac{2\alpha V_{12}}{(1-\eta)N_b} + \frac{2\alpha V_{2ph}}{(1-\eta)N_b^2} + \delta J_{bi}, \quad (5)$$

The first three terms in expression (5) correspond to a strong coupling, the last term determines the addition of an intermediate coupling. The eq. (5) is written using Feynman units: $2m^*=1$, $\hbar=1$, $\omega=1$. Then the unit of energy is $\hbar\omega$.

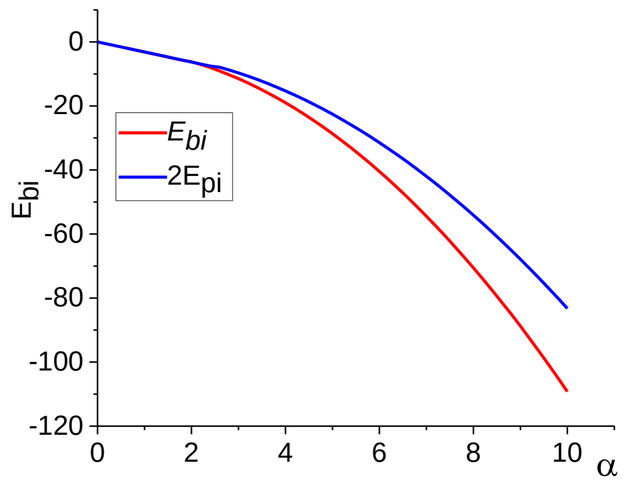

Fig 4. Doubled polaron $2E_{pi}$ and single-center bipolaron $2E_{bi}$ energies (in units $\hbar\omega$) as a parameter α function for η = 0, N=4 in WF (3) .

THE BUIMISTROV-PEKAR METHOD AND THE VIRIAL THEOREM 6

Table 1. Energy and virial relations for 2D bipolaron for η=0. $E_h^* = \hbar^2/m^*a^{*2}$, the electron WF is determined by:

$$\Psi_{12}(r_1, r_2) = N^{-1/2}(1+\gamma\delta^2 r_{12}^2)\exp\left[-\delta^2\left(r_1^2 + r_2^2\right)\right] \qquad (6)$$

α	2	3	6	8	10	20
$-E_b$	0.7853	0.5963	0.5156	0.5042	0.4989	0.4918
$-F'$	0.3926	0.4860	0.4893	0.4895	0.4895	0.4895
E_{kin}	0.3926	0.4860	0.4893	0.4895	0.4895	0.4895
$-E'_f/2$	0.1963	0.4309	0.4762	0.4821	0.4848	0.4883
$-E'_{el}/3$	0.3926	0.4860	0.4893	0.4895	0.4895	0.4895
$-E'_{int}/4$	0.3926	0.4860	0.48935	0.4895	0.4895	0.4895
α	30	50	100	200	300	
$-E_b$	0.4905	0.4899	0.4896	0.4895	0.4895	0.4895
$-F'$	0.4895	0.4895	0.4895	0.4895	0.4895	0.4895
E_{kin}	0.4895	0.4895	0.4895	0.4895	0.4895	0.4895
$-E'_f/2$	0.4890	0.489	0.4895	0.4895	0.4895	0.4895
$-E'_{el}/3$	0.4895	0.4895	0.4895	0.4895	0.4895	0.4895
$-E'_{int}/4$	0.4895	0.4895	0.4895	0.4895	0.4895	0.4895

Various contributions to the bipolaron energy functional are defined by the expressions:

$$E_{bi} = E_{bi}^s + \delta E_{bi} = E_{kin}^s + \delta E_{kin} + E_{ee} + E_{\text{int}}^s + \delta E_{\text{int}} + E_f^s + \delta E_f$$

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The additions to the energy from the terms of the intermediate bond are determined as follows:

$$\delta E_{kin} = \sum_k V_k^2 k^2 \frac{P_{12}(k)^2}{\left[P_{12}(k)+k^2\right]^2}, \quad \delta E_{\text{int}} = -\sum_k 2V_k^2 \frac{P_{12}(k)^2}{P_{12}(k)+k^2},$$

$$\delta E_f = \sum_k V_k^2 \frac{P_{12}(k)^3}{\left[P_{12}(k)+k^2\right]^2}, \qquad P_{12} = 2 + 2W_{12k} - W_k^2,$$

$$W_k = \int d^2r_1 d^2r_2 \left[\exp(i\mathbf{k}\mathbf{r}_1) + \exp(i\mathbf{k}\mathbf{r}_2)\right]|\Psi_{12}|^2,$$

$$W_{12k} = \int d^2r_1 d^2r_2 \exp\left(i\mathbf{k}(\mathbf{r}_1 - \mathbf{r}_2)\right)|\Psi_{12}|^2.$$

We introduce additional notation:

$$F' = E_{kin} + \frac{1}{2}E'_{\text{int}}, \quad E'_{\text{int}} = E_{\text{int}} + 2E_{ee}, \quad E'_{el} = E_{kin} + E'_{\text{int}},$$

$$E_{\text{int}} = \langle \Phi_{12} | H_{2e-f} | \Phi_{12} \rangle, \quad E_{ee} = \langle \Phi_0 | \frac{e^2}{\varepsilon_\infty |\mathbf{r}_1 - \mathbf{r}_2|} | \Phi_0 \rangle.$$

Table 1 illustrates that for an arbitrary coupling VT has the form $1:3:4$, in the strong-coupling limit the VT holds as

$$1:2:3:4:$$

$$E_{kin} = -F', E'_f = -2F', -E'_{el} = -3F', -E'_{\text{int}} = -4F',$$

where $E'_f \equiv E_f - E_{ee}$.

The prime at the notation denotes expressions that contain the electron-electron Coulomb repulsion.

Table 2 shows the dependence of the BP energy and the parameters that minimize the BP functional.

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Table 2. The bipolaron energy (in units of ħω) and variation parameters of WF (6) for different values of α. Feynman units are used, 2m = 1, ħ = 1, ω = 1.

α	δ	γ	$-E_b$
2	$2.87219\cdot10^{-3}$	0.17308	6.283184
3	2.065201	0.702054	10.734444
6	4.585443	0.707788	37.129680
8	6.190659	0.708639	64.539776
10	7.781783	0.708942	99.78560
20	15.67773	0.70934	393.5168
30	23.547991	0.709413	883.0746
50	78.56928	0.709470	2448.255
100	157.14982	0.709470	9791.620
200	157.14982	0.709470	39166.48
300	235.72786	0.709470	88122.240

CONCLUSIONS

For the region of existence of a 2D bipolaron, the two-center configuration of a 2D BP is unstable. The only minimum corresponds to a one-center bipolaron. The addition of an intermediate coupling δE_{bi} only slightly lowers the energy of the BP in comparison with the strong-coupling limit. In the region α < 1.8, the addition δE_{bi} becomes dominant. This phenomenon can be characterized as a transition from a localized to a delocalized state of 2D (bi)polaron. The exchange energy of two 2D polarons is antiferromagnetic in nature.

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