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Condensons and bicondensons in one-dimensional systems

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Abstract. The paper is devoted to simulation of continual strong coupling condensons and bicondensons states in one-dimensional systems by using the Gaussian basis with exponentially correlated multipliers. To determine the accuracy of variational calculations, it has been shown that using the variational function consisting of a sum of 5 Gaussians reproduces the exact value of energy and wave function of the one-dimensional condenson with the accuracy of 7 and 5 significant digits, correspondingly. Analytical expressions for the effective functional of the one-dimensional bicondenson have been obtained. Variational calculations of singlet condenson ground state energy were carried out with simultaneous accounting of single-center correlations and correlations caused by a direct dependence of the bicondenson wave function on the distance between electrons. The graphical dependence of the bicondenson energy on the Coulomb repulsion parameter V_C has been represented. The region of existence of bicondenson was determined as a function of electron-electron repulsion parameter $V_C \le V_C^* \approx 5.4$. The one-center bicondenson model has been considered, and distribution of the two-electron probability density (squared wave function of bicondenson) in the region $2 \le V_C$ has two maxima, the distance between which for $V_C = 2$ is $R_m = 1.8567$. This distribution of the probability density is associated with the low dimensionality of the system under consideration.

Keywords: polaron, 1D-bipolaron, condenson, bicondenson, low-dimensional systems, electron-phonon interaction.

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1. Introduction

The electron-phonon interaction of paramagnetic centers in low-dimensional systems has a number of qualitative features in comparison with three-dimensional (3D) systems. In a 3D system, condenson [1] can be formed only after the potential barrier has been overcome. However, even if it happens, 3D condenson is a deep self-consistent state of a small radius. The continuum theory cannot be used to describe such object. Condenson states of large radius can be realized in strong magnetic fields, since the crystal becomes similar to the one-dimensional (1D) system [2]. The possibility of a barrier-free transition of a band electron to an autolocalized state in a 1D system was considered by Holstein [3]. The Euler equation corresponding to large-radius polaron in the 1D systems has an exact solution [3]. In relation with the fact that 1D polaron can be formed in a molecular chain as a result of electron-phonon interaction with acoustic phonons, it is often possible to find the term “1D acoustic polaron”. In this paper, we will use the term condenson introduced for similar self-trapped states in Ref. [1].

The functional of Holstein polaron does not differ from the functional of large-radius exciton considered by Rashba in the 1D system [4]. The exact solution of the Euler equation corresponding to electron excitations of exciton type was given in Rashba’s work [4], which was published several years earlier than the Holstein work [3]. Holstein draws attention to the fact that the method proposed in his work for large-radius 1D polaron can be extended to 3D systems. In this case, Holstein’s theory coincides with the results of Pekar polaron theory [5]. Apparently, the work of Deigen and Pekar [1] devoted to the theory of condenson and work of Rashba [4] were not known to Holstein. However, one can verify that the functional of 3D-condenson obtained in Ref. [1] and functional of 1D Holstein polaron are identical.

The aim of this paper is to obtain the energy of 1D continual bicondenson with simultaneous consideration of various types of correlation effects. Variational calculations will be carried out using a Gaussian basis with exponentially correlated factors for the one-center condenson configuration.

2. The functional of one-dimensional condenson

For condenson states, the transition from a 3D to the 1D system reduces to a formal procedure of reducing the dimensionality of the system without changing the general form of the Deigen–Pekar condenson functional obtained in [1]:

$$I[\Psi]=\frac{\hbar^2}{2\tilde{\mu}}\int\left|\nabla\Psi\right|^2 d\boldsymbol{\tau}-\tilde{E}_b\int\left|\Psi\right|^4 d\boldsymbol{\tau}\,, \qquad (1)$$

where μ is the effective mass of the band electron, $\nabla=\mathbf{i}\frac{\partial}{\partial x}+\mathbf{j}\frac{\partial}{\partial y}+\mathbf{k}\frac{\partial}{\partial z}$, $\mathbf{i},\mathbf{j},\mathbf{k}$ are unit vectors in the directions of the coordinate axes X, Y, Z, respectively, $\tilde{E}_b$ is the constant characterizing interaction of electron with deformation of the crystal lattice caused by acoustic phonons in the 3D system, $d\boldsymbol{\tau}$ is an element of volume in 3D space.

The functional of 1D condenson has the form:

$$J_1[\Psi]=t\int\limits_{-\infty}^{\infty}\left|\frac{d}{dx}\Psi\right|^2 dx-E_b\int\limits_{-\infty}^{\infty}\left|\Psi\right|^4 dx \qquad (2)$$

where $t=\frac{\hbar^2}{2\mu}$, μ is the effective mass of band electron in the 1D system, E_b – parameter characterizing interaction of electron with elastic deformation in the 1D system.

The nonlinear Schrödinger equation corresponding to the functional of 1D condenson (2) has the form:

$$-t\frac{d^2}{dx^2}\Psi-2E_b\left|\Psi\right|^2\Psi=E_{\mathrm{Sch}}\Psi\,. \qquad (3)$$

Here, E_{Sch} is the energy of Schrödinger term (energy of photodissociation) of condenson.

According to [3, 4], equation (3) has an exact solution:

$$\Psi(x)=\sqrt{E_b/4t}\,\operatorname{sec}h\left[(E_b/2t)(x-x_0)\right], \qquad (4)$$

where x_0 is a constant of integration, indicative of the fact that the centroid of the condenson may be located at an arbitrary point in the specimen.

The ground self-consistent state energy of 1D-condenson or the thermal dissociation energy corresponding to the minimum of the functional (2) has the form:

$$E_{1ex}=-\frac{1}{12}\frac{E_b^2}{t}\,. \qquad (5)$$

In what follows, we shall use dimensionless units assuming $t=1$ and $E_b=1$. The unit of energy according to Eq. (5) is E_b^2/t, the unit of length according to Eq. (4) is t/E_b.

3. The functional of the one-dimensional bicondenson

The functional of 1D bipolaron was previously studied by Emin, Ye and Beckel [6]. The influence of correlation effects on the possibility of formation of a bipolaron stable state was studied in Ref. [6]. Two models of bipolaron were considered: one-center and two-center ones. Correlations stabilizing the single-center model were called in Ref. [6] as “in-out correlations”, correlations stabilizing the two-center model were called as “right-left correlations”. In our work, these correlation effects will be called as the single-center and two-center ones, in accordance with the bipolaron configuration, which becomes stable as a result of taking into account correlations of the corresponding type. In 3D systems, these correlation effects play an important role, but the strongest influence is exerted by correlations associated with account of the direct dependence of the polaron wave function (WF) on the distance between electrons [7, 8]. This kind of correlation effects will be called as interelectronic correlations. These correlations in 1D systems can stabilize both the single-center and two-center configurations of bipolaron. In Ref. [6], the correlations associated with the direct dependence of polaron WF on the electron-electron distance were not taken into account.

In the adiabatic approximation, the effective functional of 1D bicondenson has the form [6, 9]:

$$E_2=2t\int\limits_{-\infty}^{\infty}\int\limits_{-\infty}^{\infty}dx_1dx_2\left|\frac{\partial\Psi_{12}}{\partial x_1}\right|^2-4E_b\int\limits_{-\infty}^{\infty}dx_1\left(\int\limits_{-\infty}^{\infty}dx_2\Psi_{12}^2\right)^2+$$
$$+V_c\int\limits_{-\infty}^{\infty}\int\limits_{-\infty}^{\infty}dx_1dx_2\delta(x_1-x_2)\Psi_{12}^2\,, \qquad (6)$$

where $\Psi_{12}=\Psi_{12}(x_1,x_2)$ is WF of the two-electron system. It is assumed that WF Ψ_{12} is normalized and symmetrized with respect to the electronic coordinates.

4. Obtaining analytical expressions for the condenson and bicondenson functionals

Using the Gaussian basis for modeling the condenson and bicondenson states allows one to calculate exactly all integral expressions that enter into the condenson (1) and bicondenson (6) functionals. The problem of finding the bipolaron ground state energy is reduced to finding the minimum of a multiparameter variational function.

4.1. Condenson

To illustrate the accuracy of Gaussian basis used for modeling condenson and bicondenson states, we present calculations of the condenson ground state energy by using a basis consisting of 5 Gaussians.

Variational WF of the condenson ground state can be written in the form:

$$\Phi(x,C,\alpha)=\sum_{i=1}^{n}C_i\exp(-\alpha_i^2x^2), \tag{7}$$

where C_i and α_i are the variational parameters.

The normalization integral corresponding to WF (7) has the form:

$$N_1(C,\alpha)=\int_{-\infty}^{\infty}\Phi(x,C,\alpha)^2\,dx, \tag{8}$$

where C and α are the matrix columns, elements of which are the variational parameters C_i and α_i, the index $i=1, 2, ..., n$ enumerates the rows of corresponding matrices.

Determination of the ground state energy of 1D-condenson E_1 reduces to minimizing the multiparameter function:

$$J_1(C,\alpha)=T_1(C,\alpha)+V_{1ph}(C,\alpha),\ E_1=\min_{C,\alpha}\{J_1(C,\alpha)\}, \tag{9}$$

where the following notation is introduced:

$$T_1(C,\alpha)=\frac{t}{N_1(C,\alpha)}\int_{-\infty}^{\infty}dx\left|\frac{d\Phi(x,C,\alpha)}{dx}\right|^2, \tag{10}$$

$$V_{1ph}(C,\alpha)=-\frac{E_b}{N_1(C,\alpha)^2}\int_{-\infty}^{\infty}dx\left|\Phi(x,C,\alpha)\right|^4, \tag{11}$$

The corresponding analytical expressions obtained by us using WF (7) are:

$$N_1(C,\alpha)=\sqrt{\pi}\sum_{i=1}^{n}\sum_{j=1}^{n}C_iC_j\frac{1}{\sqrt{\alpha_i^2+\alpha_j^2}}, \tag{12}$$

$$T_1(C,\alpha)=t\frac{2\sqrt{\pi}}{N_1}\sum_{i=1}^{n}\sum_{j=1}^{n}C_iC_j\frac{\alpha_i^2\cdot\alpha_j^2}{\left(\alpha_i^2+\alpha_j^2\right)^{3/2}}, \tag{13}$$

$$V_{1ph}(C,\alpha)=-E_b\frac{\sqrt{\pi}}{N_1^2}\times$$
$$\times\sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{k=1}^{n}\sum_{l=1}^{n}C_iC_jC_kC_l\frac{1}{\sqrt{\alpha_i^2+\alpha_j^2+\alpha_k^2+\alpha_l^2}}. \tag{14}$$

4.2. Bicondenson

Trial WF for bicondenson is chosen in the form of a Gaussian basis with exponentially correlated factor:

$$\Psi_{12}\equiv\Psi_{12}(x_1,x_2)=(1+P_{12})\times$$
$$\times\sum_{i}^{n}C_i\exp\left(-a_i^2x_1^2-c_i^2x_2^2\right)\cdot\exp\left(-b_ix_1x_2\right), \tag{15}$$

where C_i, a_i, b_i, c_i are the variational parameters, P_{12} is the permutation operator of the electron coordinates.

To simplify the analytical calculations, we carry out symmetrization with respect to the electron coordinates in WF (15) by using the automatic symmetrization procedure. To do this, we always choose an even number of terms in the sum over n, setting $n=2m$ and group the terms in pairs, assuming, $C_i=C_i$, $a_i=a_i$, $c_i=c_i$ if $i\le m$; and $C_i=C_{i-m}$, $a_i=c_{i-m}$, $c_i=a_{i-m}$ if $i>m$. After this procedure, the factor $(1+P_{12})$ in the expression (7) can be omitted. Further, we assume that WF of bipolaron is symmetrized, so that $\Psi_{12}(x_1,x_2)=\Psi_{21}(x_2,x_1)$.

The normalization integral is given by:

$$N=\int_{-\infty}^{\infty}dx_2\int_{-\infty}^{\infty}dx_1\left|\Psi_{12}(x_1,x_2)\right|^2. \tag{16}$$

Determination of the bicondenson ground state energy is reduced to minimizing the multiparameter function:

$$J_2(C,a,b,c)=T(C,a,b,c)+V_C(C,a,b,c)+V_{ph}(C,a,b,c),$$
$$E_2=\min_{C,a,b,c}\{J_2(C,a,b,c)\}, \tag{17}$$

where the notation is introduced:

$$T=-\frac{2t}{N}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\Psi_{12}\frac{\partial^2}{\partial x_1^2}\Psi_{12}\,dx_1dx_2, \tag{18}$$

$$V_C=\frac{V_c}{N}\int_{-\infty}^{\infty}dx_2\int_{-\infty}^{\infty}dx_1\delta(x_1,x_2)\left|\Psi_{12}(x_1,x_2)\right|^2, \tag{19}$$

$$J_{ph}=-4\frac{E_b}{N^2}\int_{-\infty}^{\infty}\left[\int_{-\infty}^{\infty}\Psi_{12}^2dx_2\right]^2dx_1. \tag{20}$$

We also introduce simplifying notation in the expression for squared WF:

$$\Psi_{12}^2=\sum_{i}^{n}\sum_{j}^{n}C_iC_j\exp\left(-\alpha_{ij}^2x_1^2-\chi_{ij}^2x_2^2\right)\cdot\exp\left(-\beta_{ij}x_1x_2\right), \tag{21}$$

where $\alpha_{ij}=\sqrt{a_i^2+a_j^2}$, $\chi_{ij}=\sqrt{c_i^2+c_j^2}$, $\beta_{ij}=b_i+b_j$.

The normalization integral:

$$N \equiv \sum_{i=1}^{n}\sum_{j=1}^{n} N_{ij} = 2\pi \sum_{i=1}^{n}\sum_{j=1}^{n} C_i C_j \frac{1}{\sqrt{\eta_{ij}}}, \tag{22}$$

where:

$$\eta_{ij} = 4\alpha_{ij}^2 \chi_{ij}^2 - \beta_{ij}^2,\ \eta_{ij} > 0. \tag{23}$$

The Coulomb repulsion energy:

$$V_{\mathrm{C}} = V_c \frac{\sqrt{\pi}}{N} \sum_{i=1}^{n}\sum_{j=1}^{n} C_i\, C_i \frac{1}{\sqrt{\kappa_{ij}}}, \tag{24}$$

$$\kappa_{ij} = \alpha_{ij}^2 + \chi_{ij}^2 + \beta_{ij},\ \kappa_{ij} > 0. \tag{25}$$

The full energy of the phonon field and the energy of the electron-phonon interaction:

$$J_{ph} = -4E_b \frac{\pi\sqrt{\pi}}{N^2} \times$$

$$\times \sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{k=1}^{n}\sum_{l=1}^{n} C_i C_j C_k C_l \frac{1}{\alpha_{ij}\alpha_{kl}} \frac{1}{\sqrt{\mu_{ij} + \mu_{kl}}}, \tag{26}$$

$$\mu_{ij} = \chi_{ij}^2 - \frac{\beta_{ij}^2}{4\alpha_{ij}^2}. \tag{27}$$

The kinetic energy determined using Eq. (18) was calculated by differentiation with respect to the parameters of the normalization integral (22).

We introduce the subsidiary function:

$$f_i(x_1, x_2) = C_i \exp\left(-a_i^2 x_1^2 - c_i^2 x_1^2\right) \cdot \exp\left(-b_i x_1 x_2\right). \tag{28}$$

Twice differentiating (28) on the coordinate of the first electron, we multiply the result by f_j:

$$f_j(x_1, x_2) \frac{\partial^2}{\partial x_1^2} f_i(x_1, x_2) = \sum_{k=1}^{4} \tilde{T}_{ki} f_i f_j, \tag{29}$$

where the subsidiary matrix $\tilde{T}_{ki}$ is defined by the expression:

$$\tilde{T}_{ki} = \begin{vmatrix} \tilde{T}_{1i} \\ \tilde{T}_{2i} \\ \tilde{T}_{3i} \\ \tilde{T}_{4i} \end{vmatrix} = \begin{vmatrix} -2a_i^2 \\ 4a_i^4 x_1^2 \\ 4a_i^2 b_i x_1 x_2 \\ b_i^2 x_2^2 \end{vmatrix},\ k = 1, 2, 3, 4. \tag{30}$$

The index k in the expressions (29) and (30) enumerates the rows of the matrix $\tilde{T}_{ki}$.

Taking into account that in Eq. (29)

$$f_i f_j = C_i C_j \exp\left(-\alpha_{ij}^2 x_1^2 - \chi_{ij}^2 x_2^2\right) \cdot \exp\left(-\beta_{ij} x_1 x_2\right). \tag{31}$$

Integration with respect to the coordinates of electrons in (18) can be reduced to differentiating with respect to the parameters of the normalization integral. Calculating the necessary expressions, we get:

$$T = 2\frac{1}{N} \sum_{k=1}^{4} K_k, \tag{32}$$

where the subsidiary matrix K is given by:

$$K = \begin{vmatrix} K_1 \\ K_2 \\ K_3 \\ K_4 \end{vmatrix} = \begin{vmatrix} 2\sum_{i=1}^{n}\sum_{j=1}^{n} a_i^2 N_{ij} \\ 2\sum_{i=1}^{n}\sum_{j=1}^{n} \frac{a_i^4}{\alpha_{ij}} N_{\alpha ij} \\ 4\sum_{i=1}^{n}\sum_{j=1}^{n} a_i^2 b_i N_{\beta ij} \\ \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} \frac{b_i^2}{\chi_{ij}} N_{\chi ij} \end{vmatrix}, \tag{33}$$

in its turn:

$$N_{ij} = 2\pi \frac{C_i C_j}{\sqrt{\eta_{ij}}}, \tag{34}$$

$$N_{\alpha ij} \equiv \frac{d}{d\alpha_{ij}} N_{ij} = -8\pi \frac{C_i C_j \alpha_{ij} \chi_{ij}^2}{\eta_{ij}\sqrt{\eta_{ij}}}, \tag{35}$$

$$N_{\chi_{ij}} \equiv \frac{d}{d\chi_{ij}} N_{ij} = -8\pi \frac{C_i C_j \alpha_{ij}^2 \chi_{ij}}{\eta_{ij}\sqrt{\eta_{ij}}}, \tag{36}$$

$$N_{\beta_{ij}} \equiv \frac{d}{d\beta_{ij}} N_{ij} = 2\pi \frac{C_i C_j \beta_{ij}}{\eta_{ij}\sqrt{\eta_{ij}}}. \tag{37}$$

5. Results of minimizing the condenson and bicondenson functionals

5.1. Condenson energy

To illustrate the accuracy of the energy and WF calculations with using the Gaussian basis, we present the results of minimizing the condenson functional and compare the results obtained with the exact values of WF and condenson energy, which are determined by the equations (4) and (5), respectively.

We supplement this WF (7) with the variational parameter γ, which we will consider as a scale transformation parameter:

$$\Phi'(x, C, \alpha, \gamma) = \sum_{i=1}^{n} C_i \exp\left(-\alpha_i^2 \gamma^2 x^2\right). \tag{38}$$

For $\gamma = 1$, WF (38) and (7) coincide, *i.e.*, $\Phi'(x, C, \alpha, 1) = \Phi(x, C, \alpha)$. The normalization integral corresponding to WF (38) has the form:

$$N_1(C, \alpha, \gamma) = \int_{-\infty}^{\infty} \Phi'(x, C, \alpha, \gamma)^2 dx = \gamma^{-1} \int_{-\infty}^{\infty} \Phi(x, C, \alpha)^2 dx \,. \quad (39)$$

By taking into account Eq. (39), normalized WF of condenson can be written in the form:

$$\tilde{\Phi}(x, C, \alpha, \gamma) = N_1^{-1/2} \sum_{i=1}^{n} C_i \exp\left(-\alpha_i^2 \gamma^2 x^2\right). \quad (40)$$

We can perform an analytic variation of polaron functional (2) on the scale transformation parameter γ:

$$\gamma = -\frac{V_{1ph}(C, \alpha)}{2T_1(C, \alpha)}, \quad (41.a)$$

where V_{1ph} and T_1 are determined by Eqs. (12)-(14).

With allowance of Eq. (41.a), the ground state functional and polaron energy can be written as:

$$J_1(C, \alpha) = -\frac{V_{1ph}(C, \alpha)^2}{4T_1(C, \alpha)}, \quad E_1 = \min_{C, \alpha}\{J(C, \alpha)\}. \quad (41.b)$$

As a result of numerical variation of the multiparameter function (41.b), we obtain the following variational parameters:

$$C = \begin{pmatrix} 1 \\ 0.246500115887 \\ 1.760314005061 \\ 1.591572741714 \\ 0.409524000885 \end{pmatrix}, \qquad \alpha = \begin{pmatrix} 0.476081694490 \\ 0.673158005810 \\ 0.336979279877 \\ 0.222715592810 \\ 0.140692537706 \end{pmatrix},$$
$$\gamma = 0.9999668842 \,. \quad (42)$$

The condenson energy corresponding to the variational parameters (42) is:

$$E_1 = -0.0833333312 \,. \quad (43)$$

According to Eq. (5), the exact value of the polaron energy in the energy units chosen by us is determined by the expression:

$$E_{1ex} = \frac{1}{12} = 0.08(3) \,. \quad (44)$$

Since we varied the polaron functional with using a scale transformation with a parameter γ determined by Eq. (40), the virial theorem is fulfilled identically:

$$E_1 = -E_{1kin} = E_{1ph}/2 \,, \quad (45)$$

Table. Dependence of exact WF for condenson $\Psi(x)$ (4) and variational WF $\tilde{\Phi}(x)$ (40) on the coordinate x for $n = 5$ and parameters (42).

x	$\Psi(x)$	$\tilde{\Phi}(x), n = 5$
0.0	0.500000000	0.499996383
0.5	0.484771815	0.484780995
1.0	0.443409442	0.443423506
1.5	0.386194837	0.386189960
2.0	0.324027137	0.324016915
2.5	0.264771064	0.264772559
3.0	0.212548017	0.212550325
3.5	0.168680242	0.168670421
4.0	0.132901114	0.132884136
4.5	0.104241209	0.104229412
5.0	0.081535616	0.081534995

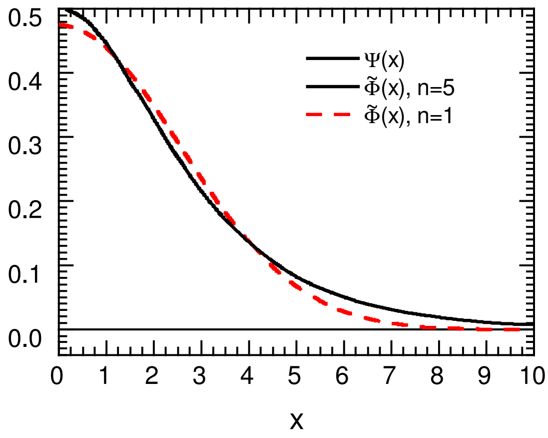

Fig. 1. Exact condenson WF $\Psi(x)$ determined using Eq. (4) and WF $\tilde{\Phi}(x)$ determined using Eq. (40) for $n = 1$ and $n = 5$. WF $\Psi(x)$ and $\tilde{\Phi}(x)$ determined by the expression (40) for $n = 5$ fully coincide in the graphical representation.

where E_{1kin} and E_{1ph} are the average values of the kinetic and potential energy of condenson at the minimum.

Table compares exact WF (4) and normalized variational WF (40) with the parameters determined by the expression (42).

Fig. 1 shows exact WF $\Psi(x)$ (4) and variational WF $\tilde{\Phi}(x)$ (40) for $n = 1$ and $n = 5$. WF $\Psi(x)$ and $\tilde{\Phi}(x)$ determined by the expression (40) for $n = 5$ fully coincide in the graphical representation. Thus, to simulate WF of bipolaron states with high accuracy, it is sufficient to use the five terms in WF (15).

5.2. The energy of singlet bicondenson

Minimization of the bicondenson functional (6) was carried out using WF (15) for $n = 5$. Analytic expressions for the kinetic energy, energy of the Coulomb interaction of electrons and total energy of the phonon field and the electron-phonon interaction are presented in Section 4.2.

Fig. 2 shows the dependence of the bicondenson ground-state energy on the parameter of Coulomb

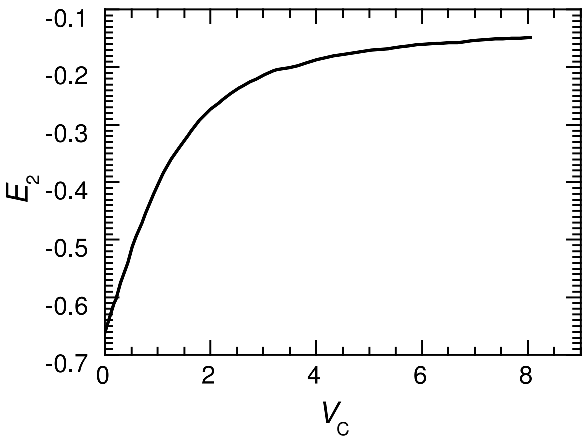

Fig. 2. Dependence of the bicondenson energy E_2 on the parameter of electron-electron repulsion V_C.

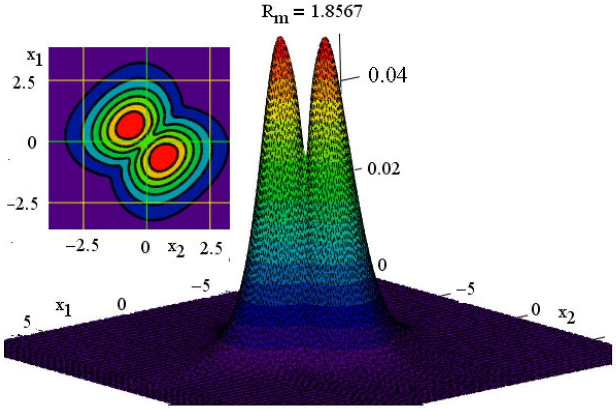

Fig. 3. Distribution of the probability density $\rho(x_1, x_2) = \Psi_{12}^2 / N$ of two-electron WF (15) with the parameters (46) for $V_C = 2$.

repulsion. Approximately from the value $V_C^* = 4.8$, bipolaron becomes unstable and breaks up into two polarons. In the limit $V_C = 0$, the energy of bipolaron reproduces the polaron energy (5) increased by the factor of 8. The obtained with using WF (15) for $n = 5$ energy was $E_2 = -0.66666367$ in comparison with the exact value $8E_p = -0.(6)$.

Let us pay attention to the fact that in the case when we are dealing with an optical 1D bipolaron, the region $V_C < 2$ corresponds to nonphysical parameters, since in our notation $V_C = 2$ corresponds to an extremely strong coupling, when the ionicity parameter $\eta = \varepsilon_\infty / \varepsilon_0 \to 0$. In the same limit, uncorrelated bipolaron in both 3D and 1D systems breaks up into two noninteracting polarons. In the case when condenson or the polaro-condenson are considered, the entire range of the parameter $0 \le V_C$, shown in Fig. 2, should be taken into account.

As an example, we present the results of the variational calculations obtained by us for a parameter $V_C = 2$ that is the boundary of the existence of an uncorrelated condenson. The variational parameters of WF (15), which minimize the functional (17), can be represented in the form of matrix columns:

$$C = \begin{pmatrix} 1.000000000 \\ 1.119493330 \\ -0.857246055 \\ 0.857486871 \\ -0.205051508 \end{pmatrix}, \quad a = \begin{pmatrix} 0.455606116 \\ 0.430352661 \\ 0.923448862 \\ 0.600500332 \\ 4.708425389 \end{pmatrix}$$

$$b = \begin{pmatrix} 0.145293331 \\ -0.027742887 \\ -1.616171898 \\ 0.039265060 \\ -44.504011125 \end{pmatrix}, \quad c = \begin{pmatrix} 0.329734583 \\ 0.213400345 \\ 1.037035245 \\ 0.222991699 \\ 4.760304925 \end{pmatrix}, \qquad (46)$$

$$E_2 = -0.275406293, \quad T_2 = 0.275402680,$$
$$V_{2pot}/2 = -0.2754045, \quad V_C = 2, \qquad (47),$$

where the potential energy of bicondenson $V_{pot} = V_C + V_{ph}$.

In relation with the fact that the scale transformation was not used, the virial relations

$$E_2 = -T_2 = V_{pot}/2 \qquad (49)$$

are satisfied only approximately. Variation of the functional (17) in the analytic form on the scale transformation parameter leads to the identical fulfillment of the virial theorem, but very insignificantly lowers the total energy of the system.

The variational function (15) corresponds to the one-center bipolaron configuration. This is due to the fact that there is no parameter corresponding to the distance between the centers of the polarization wells of condensons in WF (15). A spherically symmetric function corresponds to bipolaron of a similar configuration in 3D system [10]. In 1D-system, coordinates of first and second electrons can be arranged along the axes X and Y. The two-electron probability density state will be located in the upper half-space along the axis Z. Fig. 3 shows the two-electron probability density distribution of WF (15) with parameters (46) minimizing the bicondenson functional (17). In the upper left corner in Fig. 3, the lines of equal probability density of condenson are shown. The corresponding 3D image is shown in the same figure. Direction, along which the polarons are located, corresponds to the diagonal on which the maxima of the probability density of the WF bicondenson states are located. As shown in Fig. 3, the probability density of 1D-condenson has two maxima. This result is not obvious in advance, since in a 3D-system it is distinctive feature of the two-center bicondenson configuration.

The distance R_m between the maxima Ψ_{12}^2 depends on the parameter of Coulomb repulsion V_C. For $V_C = 2$ and parameters (46) $R_m = 1.8567$. With growth of Coulomb repulsion V_C, the distance R_m is growing. In the range $0 \le V_C < 2$, the maxima merge into one for $V_C = 0$.

6. Discussion

The results obtained in this paper allow us to suggest that in 1D systems the principal difference between the two-center and one-center configurations related to the spatial distribution of the probability density of the two-electron state is not manifested in the region $V_C \geq 2$. In both cases, the two-electron density matrix $\rho(x_1, x_2) = \Psi_{12}^2 / N$ has 2 maxima, the distance between which R_m increases with the increase of the electron-electron repulsion parameter. When $V_C \to 0$, distance R_m decreases to zero. The latter corresponds to the complete absence of interelectron correlations. This statement agrees with the conclusions obtained earlier in Refs. [11, 12]. Calculations of the bicondenson energy associated with taking into account the direct dependence of WF on the interelectron distance for the two-center model will be carried out in another paper. The formal qualitative difference between the two-center and the one-center model in the Gaussian basis is the presence of linear in the electronic coordinates terms in the exponents of basis functions [8].

Linear chains consisting of weakly bound sites can serve as an example of actual objects, where the methods considered in the present paper can be applied. These can be organic molecules consisting of identical chromoform groups, as well as polymers consisting of identical atoms, molecules, or molecular groups, the number of which in the polymer chain can be measured by millions. The continuum theory suggests that the molecular or atomic chain is sufficiently long to neglect edge effects. Calculations associated with the transfer of charge and energy in DNA are actively carried out in the framework of discrete model of 1D Holstein–Hubbard polaron [11]. In the continuum limit, similar models pass to the case of condenson and bicondenson considered by us. From the experiments related with studying the conductivity of DNA, it is known that DNA can possess the properties of dielectrics, semiconductors, and metals [13]. There is also a report that in DNA it was possible to get a transition to the superconducting state [14] at $T_C \approx 3K$. The theory of superconductivity and the possibility of transition to a high-temperature superconducting state on the basis of a bipolaron mechanism in 1D systems, including DNA, is presented in [15].

7. Conclusion

Simulation of condenson and single-center bicondenson states in the 1D system using the Gaussian basis with exponentially correlated factors has been performed. The energy of the ground state of 1D-bicondenson has been obtained as a function of system parameters. The region of bipolaron stability with respect to the Coulomb repulsion parameter V_C has been determined: $V_C \leq V_C^* \approx 5.4$. The variation calculations were carried out in the frameworks of one-center model, and distribution of the probability density $\rho_{12} = \Psi_{12}^2 / N$ of states in the region $V_C \geq 2$ has two maxima, which is a distinctive feature of the two-center configuration of polaron in 3D systems.

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