

TWO-ELECTRON QUANTUM DOTS WITH PARABOLIC CONFINEMENT (LOW LYING PARA- AND ORTHO-STATES)

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Three low lying energy levels of a 3D two-electron quantum dot (QD) with parabolic confinement are obtained by the variational method. The proposed interpolation formulas for the variation parameters allow one to recover the energy levels in a wide range of the Coulomb interaction constant. The quantum states of the QD are divided into the para- and ortho-states like in the theory of helium atom. The quantum transitions from the ortho-state to the para- state are possible only with account of the spin-orbit interaction. At low temperatures, an ensemble of two-electron QDs contains dots in the ground para-state and in the first excited ortho-state, which is metastable. These QDs have the entangled spin wave functions that are related to the Einstein–Podolsky–Rosen (EPR) states desirable for the quantum information protocol.

para-states. The triplet spin wave functions correspond to the ortho-states. The lowest ortho-state is metastable. The singlet spin wave function of the ground state and one of the triplet spin wave functions associated with the lowest ortho-state are related to EPR states desirable for quantum information protocols [4–7].

The paper is organized as follows. In Section 2, we introduce the variational wave functions and explain the peculiarities of calculation of the variation parameters. Sections 3 and 4 are devoted to the calculation of the variation parameters and the energy levels of the QD. Section 5 discusses the para- and ortho-states of the two-electron quantum dot. The conclusion summarizes the results obtained and discusses the hypothetical many-electron quantum dots manufactured from materials with gigantic dielectric constants.

1. Introduction

The models of quantum wells and quantum dots (QDs) with one electron are widely used in the nanophysics [1, 2]. The modern technology provides a possibility to create QDs with two and more electrons, where the Coulomb interaction between them must be taken into account [3]. Due to the nanoscale localization of electrons, the Coulomb interaction can exceed the average kinetic energy of electrons, which considerably complicates the analytic solution of the Schrödinger equation.

In this paper, we consider three low-lying states of the two-electron spherically symmetric QDs with parabolic confinement. The Coulomb interaction in the typical 10-nm semiconductor QD cannot be treated as small, and the problem is solved with the help of the variational method. The two-electron trial functions are chosen on the bases of one-electron wave functions of the QD with parabolic confinement. We calculated the energies of three first states and carried out the classification of the corresponding spectral terms.

At low temperatures T (much smaller than the distance between the ground and first excited states), the ensemble of QDs consists of dots in the para- and ortho-states. The singlet spin wave functions correspond to the

2. Statement of the Problem

Two interacting electrons in a 3D spherically symmetric quantum dot with the parabolic confinement potential are described by the dimensionless Hamiltonian

$$\hat{H} = -\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 + \frac{1}{2}(r_1^2 + r_2^2) + \frac{\lambda}{|\mathbf{r}_1 - \mathbf{r}_2|}. \quad (1)$$

Here, the dimensionless coordinates of the first and second electrons r_1 and r_2 are measured in units $\sqrt{\hbar/(m^*\omega)}$ (m^* is the effective electron mass, and ω is the frequency of the confinement potential), $\lambda = \frac{1}{\varepsilon}\sqrt{(Ry/\hbar\omega)m^*/m}$ is the constant characterizing the Coulomb interaction between electrons, and ε is the dielectric constant of the quantum dot. Keeping in mind that the Rydberg constant $Ry = me^4/\hbar^2 = 27.2$ eV and setting $\omega \approx 10$ THz, we obtain $\lambda \simeq 20/\varepsilon$. If we assume that $\varepsilon \simeq 10$ and $m^*/m = 0.1$, then $\lambda \simeq 2$. This means that the Schrödinger equation corresponding to Hamiltonian (1) for a semiconductor QD cannot be solved with the help of perturbation theory. It requires variational or numerical methods. In this paper, we use the variational method, which allows us to obtain analytic formulas.

The classification of the states of the two-electron QD is convenient to perform with the help of the quantum numbers for noninteracting electrons. Due to the symmetry of the problem, we use the spherical coordinate system. The one-electron wave functions are known [8]. The energy of the two-electron QD with noninteracting electrons can be written as

$$E_{N_1 N_2} = N_1 + N_2 = 2(n_1 + n_2) + l_1 + l_2 + 3, \quad (2)$$

where $N_i = 2n_i + l_i$ with $n_i = 0, 1, 2, \dots$, are the radial quantum numbers, $l_i = 0, 1, 2, \dots$, are the orbital quantum numbers, and $m_i = 0, \pm 1, \pm 2, \dots \pm l_i$ are magnetic quantum numbers ($i = 1, 2$). The energy levels (2) are described by the symmetrized combinations of products of the one-electron wave functions $\psi_{n_1 l_1 m_1}(r_1, \theta_1, \phi_1) \psi_{n_2 l_2 m_2}(r_2, \theta_2, \phi_2)$. The one-electron wave functions are presented in the standard form $R_{nl}(r) Y_{lm}(\theta, \phi)$.

The ground state of the QD corresponds to a set of quantum numbers $\{n_1 = n_2 = 0, l_1 = l_2 = 0, m_1 = m_2 = 0\}$. We choose the normalized ground-state trial wave function of the two-electron QD in the form

$$\psi_0(\mathbf{r}_1, \mathbf{r}_2) = \left(\frac{\alpha}{\pi}\right)^{3/2} \exp\left\{-\frac{\alpha}{2}(r_1^2 + r_2^2)\right\}, \quad (3)$$

where α is a variational parameter.

The following two sets of quantum numbers correspond to the first excited state: $\{n_1 = n_2 = 0, l_1 = 1, m_1 = 0, \pm 1, l_2 = 0, m_2 = 0\}$ and $\{n_1 = n_2 = 0, l_1 = 0, m_1 = 0, l_2 = 1, m_2 = 0, \pm 1\}$. Below, for the sake of simplicity, we consider only states with $m = 0$.

The wave function of the first excited state is given by the symmetrized combination

$$\begin{cases} \psi_1^{s,a}(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{\sqrt{2}} \{ \psi_{010}(\mathbf{r}_1) \psi_{000}(\mathbf{r}_2) \pm \psi_{010}(\mathbf{r}_2) \psi_{000}(\mathbf{r}_1) \}, \\ \psi_{010}(r_1) \psi_{000}(r_2) = N_0 \exp\left\{-\frac{1}{2}(\beta r_1^2 + \alpha r_2^2)\right\} r_1 \cos \theta_1. \end{cases} \quad (4)$$

Here, s and a stand for the symmetric and antisymmetric combinations, respectively, $N_0 = \frac{\sqrt{2}\alpha^{3/4}\beta^{5/4}}{\pi^{3/2}}$ is the normalization constant, and β is one more variational parameter. It appears because the electrons are in different states.

The following five sets of quantum numbers correspond to the second excited state of the QD: $\{n_1 = n_2 = 0, l_1 = l_2 = 1\}$; $\{n_1 = 1, n_2 = 0, l_1 = l_2 = 0\}$; $\{n_1 = 0, n_2 = 1, l_1 = l_2 = 0\}$; $\{n_1 = 0, n_2 = 0, l_1 = 2, l_2 = 0\}$; $\{n_1 = 0, n_2 = 0, l_1 = 0, l_2 = 2\}$. The trial wave function corresponding to the first set is

$$\psi_2^{(1)}(\mathbf{r}_1, \mathbf{r}_2) = \frac{2\beta^{5/2}}{\pi^{3/2}} e^{-\frac{\beta}{2}(r_1^2 + r_2^2)} r_1 \cos \theta_1 r_2 \cos \theta_2 \quad (5)$$

with the same variational parameter β as in (4). Four more trial wave functions corresponding to the second, third, fourth, and fifth sets of the quantum numbers are

$$\begin{cases} \psi_2^{(2)s,a}(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{\sqrt{2}} \{ \psi_{100}(\mathbf{r}_1) \psi_{000}(\mathbf{r}_2) \pm \psi_{100}(\mathbf{r}_2) \psi_{000}(\mathbf{r}_1) \}, \\ \psi_{100}(\mathbf{r}_1) \psi_{000}(\mathbf{r}_2) = N_1 \left(\frac{3}{\alpha + \gamma} - r_1^2 \right) e^{-\frac{1}{2}(\gamma r_1^2 + \alpha r_2^2)}, \end{cases} \quad (6)$$

and

$$\begin{cases} \psi_2^{(3)s,a}(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{\sqrt{2}} \{ \psi_{020}(\mathbf{r}_1) \psi_{000}(\mathbf{r}_2) \pm \psi_{020}(\mathbf{r}_2) \psi_{000}(\mathbf{r}_1) \}, \\ \psi_{020}(\mathbf{r}_1) \psi_{000}(\mathbf{r}_2) = N_2 e^{-\frac{1}{2}(\eta r_1^2 + \alpha r_2^2)} r_1^2 (3 \cos^2 \theta_1 - 1), \end{cases} \quad (7)$$

$N_1 = \left[\frac{4\alpha^{3/2}\gamma^{7/2}(\alpha+\gamma)^2}{3\pi^3(5\alpha^2-2\alpha\gamma+5\gamma^2)} \right]^{1/2}$ and $N_2 = \left[\frac{\alpha^{3/2}\eta^{7/2}}{3\pi^3} \right]^{1/2}$ are the normalization constants.

The variational parameters α and β will be obtained after the calculation of the ground and second excited state energies with the help of the wave functions (3) and (5), respectively. The variational parameters γ and η will be obtained after calculating the average of Hamiltonian (1) with the help of the wave functions

$$\psi_3^{(1)}(\mathbf{r}_1, \mathbf{r}_2) = N_3^{(1)} \prod_{i=1}^2 \left(\frac{3}{\alpha + \gamma} - r_i^2 \right) e^{-\frac{\gamma}{2}r_i^2}, \quad (8)$$

$$\psi_3^{(2)}(\mathbf{r}_1, \mathbf{r}_2) = N_3^{(2)} \prod_{i=1}^2 e^{-\frac{\eta}{2}r_i^2} (3 \cos^2 \theta_i - 1), \quad (9)$$

where $N_3^{(1)} = \frac{4\gamma^{7/2}(\alpha+\gamma)^2}{3\pi^{3/2}(5\alpha^2-2\alpha\gamma+5\gamma^2)}$ and $N_3^{(2)} = \frac{\eta^{7/2}}{3\pi^{3/2}}$ are the normalization constants.

One can easily check that all these functions are mutually orthogonal. It is necessary to note that $\psi_3^{(1)}(\mathbf{r}_1, \mathbf{r}_2)$ contains two variational parameters α and γ . The average energy calculated on this function, $E_3^{(1)}(\alpha, \gamma)$, depends on these parameters as well. We take α from the calculations of the ground-state energy and minimize $E_3^{(1)}(\alpha, \gamma)$ only with respect to γ .

For noninteracting electrons ($\lambda = 0, \gamma = \eta = 1$), the wave functions (8) and (9) are related to the fourth excited state of the QD. With account of the Coulomb interaction ($\lambda \neq 0$), they describe different energies. In this paper, we use the trial functions with one variational parameter. Such an approach definitely gives good results for the ground state of the QD. For the higher states, the quantitative reliability of this approach decreases. One can also argue that the style of the trial

functions can be changed with increase of the interaction parameter λ . The limiting λ , after which the style of the wave function is changed considerably can be specified only by the numerical solution of the Schrödinger equation. It would be relevant to refer to paper [9], where the ground-state energy of a 2D electron QD have been obtained with the help of one-, two-, and three-parameter variation functions and compared with the exact numerical solution. It happened to be that, for $\lambda < 2$, all these energies practically coincide. We use the same Gaussian type of trial wave functions that allows us to hope that our results are reliable for the ground state and satisfactory for the first low-lying levels for $\lambda \simeq 2$.

In the next sections, we obtain the variational parameters α, β, γ , and η from the minimization of the corresponding energies.

3. Ground State of Two-electron QD

The ground state of a two-electron QD is described by the symmetric wave function (3). Calculating the average of Hamiltonian (1) with this wave function, we obtain

$$E_0(\lambda) = \frac{3}{2} \left(\alpha + \frac{1}{\alpha} \right) + K_0. \tag{10}$$

The first term represents the kinetic and potential energies of the noninteracting electrons in the parabolic potential well. The second term is the Coulomb interaction of electrons in the ground state,

$$K_0 = \int \psi_0^*(\mathbf{r}_1, \mathbf{r}_2) \frac{\lambda}{r_{12}} \psi_0(\mathbf{r}_1, \mathbf{r}_2) dv_1 dv_2. \tag{11}$$

To calculate K_0 , we use the formula

$$\frac{1}{r_{12}} = \frac{1}{r_1} \sum_{l=0}^{\infty} \left(\frac{r_2}{r_1} \right)^l P_l(\cos \theta), \quad r_1 > r_2,$$

$$\frac{1}{r_{12}} = \frac{1}{r_2} \sum_{l=0}^{\infty} \left(\frac{r_1}{r_2} \right)^l P_l(\cos \theta), \quad r_1 < r_2, \tag{12}$$

where $P_l(\cos \theta)$ is the Legendre polynomial, and θ is the angle between \mathbf{r}_1 and \mathbf{r}_2 . According to the addition theorem for spherical harmonics [10, 11], we have

$$P_l(\cos \theta) = P_l(\cos \theta_1) P_l(\cos \theta_2) + 2 \sum_{m=1}^l \frac{(l-m)!}{(l+m)!} \times$$

$$\times P_l^m(\cos \theta_1) P_l^m(\cos \theta_2) \cos m(\phi_1 - \phi_2), \tag{13}$$

where θ_1, ϕ_1 and θ_2, ϕ_2 are the polar angles of the vectors \mathbf{r}_1 and \mathbf{r}_2 , respectively. When the above formulas are substituted into (11) and integrated with respect to ϕ_1, ϕ_2, θ_1 , and θ_2 , we obtain that the second term of (13) vanishes, and the contribution to the integral comes out of $P_0(\cos \theta_1) = P_0(\cos \theta_2) = 1$. Using the wave function (3), we obtain

$$K_0 = \lambda \left(\frac{\alpha}{\pi} \right)^3 (4\pi)^2 \int_0^{\infty} \left[\int_0^{r_1} \frac{1}{r_1} e^{-\alpha(r_1^2+r_2^2)} r_2^2 dr_2 + \int_{r_1}^{\infty} \frac{1}{r_2} e^{-\alpha(r_1^2+r_2^2)} r_2^2 dr_2 \right] r_1^2 dr_1. \tag{14}$$

Performing the integration in (14), we get

$$K_0 = \lambda \sqrt{\frac{2\alpha}{\pi}}. \tag{15}$$

The variational parameter α , which provides the minimum of energy (10), is obtained from the condition $\frac{dE_0(\alpha)}{d\alpha} = 0$. With account of (10) and (15), this gives the equation

$$\alpha^2 + \frac{\lambda}{3} \sqrt{\frac{2}{\pi}} \alpha^{3/2} - 1 = 0. \tag{16}$$

In the case $\lambda = 0$, Eq. (16) has the solution $\alpha = 1$. For $\lambda \ll 1$, (16) can be solved with the help of the expansion in the small parameter $\alpha = 1 + \lambda\alpha_1 + \lambda^2\alpha_2 + \dots$. The result is

$$\alpha = 1 - \frac{\lambda}{3\sqrt{2\pi}} + \frac{\lambda^2}{18\pi}, \quad \lambda \ll 1. \tag{17}$$

Substituting (17) in (10) with account of (15), we obtain the ground-state energy with the same accuracy

$$E_0(\lambda) = 3 + \lambda \sqrt{\frac{2}{\pi}} - \frac{\lambda^2}{12\pi}, \quad \lambda \ll 1. \tag{18}$$

If λ is not small, Eq. (17) can be solved numerically. In Table 1, we present the calculated ground-state energy E_0 and the variational parameter α for different λ .

With the help of Eq. (10) and numerical values of α calculated for various λ , we can propose the following interpolation formulas for the variational parameter:

$$\alpha(\lambda) = \frac{1}{1 + \frac{\lambda}{3\sqrt{2\pi}}}. \tag{19}$$

One can check that the ground-state energy $E_0(\lambda)$ (10) of the two-electron QD with α given by (19) is in excellent agreement with the data of Table 1.

Table 1. Ground-state energy E_0 and the variational parameter α for different λ

λ	0.0	0.5	1.0	1.5	2.0	2.5	3.0	3.5	4.0
α	1.000000	0.937685	0.882828	0.834268	0.791048	0.752380	0.717610	0.686200	0.657690
$E_0(\lambda)$	3.000000	3.392520	3.773010	4.142550	4.502080	4.852450	5.194400	5.528560	5.855200

Table 2. Excited-state energy $E_2^{(1)}$ and the variational parameter α for different λ when two electrons are in the state $n = 0, l = 1, m = 0$

λ	0.0	0.5	1.0	1.5	2.0	2.5	3.0	3.5	4.0
β	1.000000	0.968452	0.938854	0.911050	0.884895	0.860259	0.837023	0.815079	0.794329
$E_2^{(1)}(\lambda)$	5.000000	5.323190	5.641330	5.954640	6.263350	6.567660	6.867780	7.163870	7.456110

4. First and Second Excited States

The first excited state wave functions (4) contain the already calculated variational parameter α and the still unknown variational parameter β . As was mentioned above, we find it with the help of the wave function (5). The calculation of the average Hamiltonian (1) with the help of the wave function (5) gives the following result:

$$E_2^{(1)}(\lambda) = \frac{5}{2} \left(\beta + \frac{1}{\beta} \right) + K_2^{(1)}. \quad (20)$$

The first term in this equation is the kinetic and potential energies of two noninteracting electrons in the second excited state. The Coulomb interaction of two-electrons $K_2^{(1)}$ is given by the integral

$$K_2^{(1)} = \int \psi_2^{(1)*}(\mathbf{r}_1, \mathbf{r}_2) \frac{\lambda}{r_{12}} \psi_2^{(1)}(\mathbf{r}_1, \mathbf{r}_2) dv_1 dv_2. \quad (21)$$

To calculate this integral, we use (5), (12), (13) and the relation $\cos^2 \theta_{1,2} = \frac{1}{3}[P_0 + 2P_2(\cos \theta_{1,2})]$. The integration with respect to $d\phi_1 d\phi_2$ kills the sum over m in (13), and the integration with respect to $d\theta_1 d\theta_2$ gives a contribution from the Legendre polynomials with $l = 0, l = 2$ only. The final result of the integration in (21) is

$$K_2^{(1)} = \frac{49\lambda\sqrt{\beta}}{30\sqrt{2\pi}}. \quad (22)$$

The variational parameter β is found from the condition $\frac{dE_2^{(1)}(\lambda)}{d\beta} = 0$ with the help of (20) and (22). We obtain the following equation for β :

$$\beta^2 + \frac{49\lambda}{150\sqrt{2\pi}} \beta^{3/2} - 1 = 0. \quad (23)$$

At $\lambda = 0$, Eq. (23) has the solution $\beta = 1$. For $\lambda \ll 1$, it can be solved by the expansion in the small parameter. The result is

$$\beta = 1 - \frac{49\lambda}{300\sqrt{2\pi}} + \left(\frac{49}{300} \right)^2 \frac{\lambda^2}{2\pi}, \quad \lambda \ll 1. \quad (24)$$

With the same accuracy, the energy of the second excited state, which corresponds to the symmetric wave function (5), is

$$E_2^{(1)}(\lambda) = 5 + \frac{49\lambda}{30\sqrt{2\pi}} - \frac{(49)^2 \lambda^2}{(300)^2 8\pi}, \quad \lambda \ll 1. \quad (25)$$

In Table 2, we present the calculated excited state energy $E_2^{(1)}$ and the variational parameter β for various values of λ .

For not small λ , we can propose the following interpolation formula:

$$\beta(\lambda) = \frac{1}{1 + \frac{49\lambda}{300\sqrt{2\pi}}}. \quad (26)$$

One can check that the second excited state energy $E_2^{(1)}(\lambda)$ (20), (22) of the two-electron QD with β given by (26) is in excellent agreement with the data of Table 2.

Now we consider the first excited state of our QD, which corresponds to the state where one electron is in the ground state with $n = 0, l = 0, m = 0$ and the second one is in the first excited state with $n = 0, l = 1, m = 0$ represented by the symmetrized wave function (4). The variation parameters α and β are given by relations (19) and (26), respectively. The calculation of the average Hamiltonian (1) with the help of the wave functions (4), polynomial expansions (12), and (13) gives the following result:

$$E_1^{(s,a)}(\lambda) = \frac{3}{4} \left(\alpha + \frac{1}{\alpha} \right) + \frac{5}{4} \left(\beta + \frac{1}{\beta} \right) + K_1 \pm A_1. \quad (27)$$

$$K_1 = \int |\psi_{010}(\mathbf{r}_1)|^2 \frac{\lambda}{r_{12}} |\psi_{000}(\mathbf{r}_2)|^2 dv_1 dv_2. \quad (28)$$

$$A_1 = \int \psi_{010}(\mathbf{r}_1) \psi_{000}(\mathbf{r}_1) \frac{\lambda}{r_{12}} \psi_{010}(\mathbf{r}_2) \times$$

$$\times \psi_{000}(\mathbf{r}_2) dv_1 dv_2. \tag{29}$$

After the integration, we get the energy of the Coulomb interaction between electrons

$$K_1 = \frac{2\lambda}{3\sqrt{\pi}} \left[\frac{\sqrt{\alpha\beta}(2\alpha + 3\beta)}{(\alpha + \beta)^{3/2}} \right] \tag{30}$$

and the exchange energy

$$A_1 = \frac{\lambda}{3\sqrt{\pi}} \left(\frac{8\alpha^{3/2}\beta^{5/2}}{(\alpha + \beta)^{7/2}} \right). \tag{31}$$

In Table 3, we present the calculated energies $E_1^{(s)}(\lambda)$ and $E_1^{(a)}(\lambda)$, the Coulomb interaction energy K_1 , and the exchange energy A_1 , respectively, for various λ using the calculated values of the variational parameters α and β .

The second excited state of the two-electron QD can also be organized by putting either one electron in the ground state with the energy $3/2$ ($n_1 = 0, l_1 = 0, m_1 = 0$) and another one in the excited state with the energy $7/2$ ($n_2 = 1, l_2 = 0, m_2 = 0$) represented by a wave function (6) or putting one electron in the ground state with the energy $3/2$ ($n_1 = 0, l_1 = 0, m_1 = 0$) and another one in the excited state with the energy $7/2$ ($n_2 = 0, l_2 = 2, m_2 = 0$) described with the wave function (7). For the noninteracting electrons, its energy is 5. The variational parameters γ and η can be determined from the wave functions (8) and (9), respectively.

The unknown variational parameter γ will be used below along with the already known parameter α for constructing the second excited state variational wave function of the two-electron QD. The calculation of the average Hamiltonian (1) with the help of the wave function (8) gives

$$E_3^{(1)}(\gamma) = \frac{1}{2(5\alpha^2 - 2\alpha\gamma + 5\gamma^2)} \left[\gamma\delta + \frac{\sigma}{\gamma} \right] + K_3^{(1)}, \tag{32}$$

where $\delta = 11\alpha^2 + 10\alpha\gamma + 35\gamma^2$ and $\sigma = 35\alpha^2 + 10\alpha\gamma + 11\gamma^2$. The first term in this equation is the kinetic and potential energies of two noninteracting electrons in the fourth excited state. The Coulomb interaction of two electrons $K_3^{(1)}$ is given by the integral

$$K_3^{(1)} = \int \psi_3^{(1)*}(\mathbf{r}_1, \mathbf{r}_2) \frac{\lambda}{r_{12}} \psi_3^{(1)}(\mathbf{r}_1, \mathbf{r}_2) dv_1 dv_2, \tag{33}$$

where $\psi_3^{(1)}(\mathbf{r}_1, \mathbf{r}_2)$ is given by (8). To calculate this integral, we use (12), (13), and (33). The final result is

$$K_3^{(1)} =$$

$$= \lambda \frac{\sqrt{\gamma}(755\alpha^4 - 868\alpha^3\gamma + 2178\alpha^2\gamma^2 - 1540\alpha\gamma^3 + 1571\gamma^4)}{24\sqrt{2\pi}(5\alpha^2 - 2\alpha\gamma + 5\gamma^2)^2}. \tag{34}$$

The variational parameter γ is found from the condition $\frac{dE_3^{(1)}(\alpha, \gamma)}{d\gamma} = 0$ with the help of (32) and (34). In Table 4, we present the calculated $E_3^{(1)}(\alpha, \gamma)$ and the variational parameters α and γ for various λ .

For arbitrary λ , we can propose the following interpolation formulas for $\gamma(\lambda)$ and $E_3^{(1)}(\lambda)$:

$$\gamma(\lambda) = 1 - 0.0531\lambda - 0.00053\lambda^2 + 0.0003\lambda^3, \tag{35}$$

$$E_3^{(1)}(\lambda) = 7 + 0.54183\lambda - 0.003\lambda^2 + 0.0003\lambda^3. \tag{36}$$

Similarly, the variational parameter η can also be used along with the already known parameter α for constructing the second excited state variational wave function of the two-electron QD. The calculation of the average Hamiltonian (1) with the help of the wave function (9) gives the following result:

$$E_3^{(2)}(\eta) = \frac{7}{2} \left(\eta + \frac{1}{\eta} \right) + K_3^{(2)}. \tag{37}$$

The first term in this equation is the kinetic and potential energies of two noninteracting electrons in the considered excited state. The Coulomb interaction of two electrons $K_3^{(2)}$ is given by the integral

$$K_3^{(2)} = \int \psi_3^{(2)*}(\mathbf{r}_1, \mathbf{r}_2) \frac{\lambda}{r_{12}} \psi_3^{(2)}(\mathbf{r}_1, \mathbf{r}_2) dv_1 dv_2, \tag{38}$$

where $\psi_3^{(2)}(\mathbf{r}_1, \mathbf{r}_2)$ is given by Eq. (9). With the help of (12), (13), and (38), we obtain

$$K_3^{(2)} = \lambda \frac{229\sqrt{\eta}}{56\sqrt{2\pi}}. \tag{39}$$

Table 3. The first excited state energies $E_1^{(s)}(\lambda)$, $E_1^{(a)}(\lambda)$, the Coulomb interaction energy K_1 , and the exchange energy A_1 for various λ using the values of the variational parameters α and β

λ	K_1	A_1	$E_1^{(s)}(\lambda)$	$E_1^{(a)}(\lambda)$
0.5	0.325556	0.065933	4.395890	4.264020
1.0	0.638172	0.130632	4.785450	4.524180
1.5	0.938980	0.193972	5.168500	4.780560
2.0	1.229020	0.255888	5.545020	5.033240
2.5	1.509210	0.316361	5.915070	5.282350
3.0	1.780390	0.375399	6.278800	5.528000
3.5	2.043290	0.433034	6.636390	5.770320
4.0	2.298560	0.489309	6.988060	6.009440

Table 4. Excited state energy $E_3^{(1)}(\alpha, \gamma)$ and the variational parameters α and γ for various values of λ when two-electrons are in the state $n = 1, l = 0$, and $m = 0$

λ	0.0	0.5	1.0	1.5	2.0	2.5	3.0	3.5	4.0
α	1.000000	0.937685	0.882828	0.834268	0.791048	0.752380	0.0.717610	0.0.68620	0.657690
γ	1.000000	0.973576	0.946810	0.920161	0.893979	0.868512	0.843921	0.820301	0.797699
$E_3^{(1)}(\lambda)$	7.000000	7.27072	7.53936	7.80682	8.07361	8.33996	8.60598	8.87159	9.13675

Table 5. Excited state energy $E_3^{(2)}(\lambda)$ and the variational parameter η for various λ when two-electrons are in the state $n = 0, l = 2, m = 0$

λ	0.0	0.5	1.0	1.5	2.0	2.5	3.0	3.5	4.0
η	1.000000	0.944965	0.895775	0.851622	0.811823	0.775802	0.743072	0.713220	0.685895
$E_3^{(2)}(\lambda)$	7.000000	7.804150	8.586480	9.348730	10.09250	10.81910	11.52980	12.22570	12.90780

The variational parameter η is found, by using (37) and (39) from the condition $\frac{dE_3^{(2)}(\eta)}{d\eta} = 0$. This gives the following equation for η :

$$\eta^2 + \lambda \frac{229}{392\sqrt{2\pi}} \eta^{3/2} - 1 = 0. \quad (40)$$

In Table 5, we present the calculated excited state energy $E_3^{(2)}(\lambda)$ and the variational parameter η for various λ .

For arbitrary λ , we can propose the following interpolation formula for the values in Table 5:

$$\eta = \frac{1}{1 + \lambda \frac{229}{784\sqrt{2\pi}}}. \quad (41)$$

We now consider the second excited state of the QD, which corresponds to the state where one electron is in the ground state with $n_1 = 0, l_1 = 0, m_1 = 0$, and the second one is in the excited state with $n_2 = 1, l_2 = 0, m_2 = 0$ described with the symmetrized wave function (6). The calculation of the average Hamiltonian (1) with the help of the wave functions (6) and the Legendre polynomial expansions (12) and (13) gives

$$E_2^{(2)s,a}(\lambda) = \frac{1}{4} \left\{ 3\alpha + \frac{3}{\alpha} + \frac{1}{5\alpha^2 + 2\alpha\gamma + 5\gamma^2} \times \right.$$

Table 6. Excited state energies $E_2^{(2)s}(\lambda)$, $E_2^{(2)a}(\lambda)$, the Coulomb interaction energy $K_2^{(2)}$, and the exchange energy $A_2^{(2)}$ for various λ using the calculated values of the variational parameters α and γ

λ	$K_2^{(2)}$	$A_2^{(2)}$	$E_2^{(2)s}(\lambda)$	$E_2^{(2)a}(\lambda)$
0.5	0.312949	0.050543	5.386690	5.285600
1.0	0.6192590	0.101808	5.768720	5.565110
1.5	0.918043	0.153069	6.145180	5.839040
2.0	1.208880	0.203850	6.559940	6.152240
2.5	1.491690	0.253847	6.932310	6.424610
3.0	1.766580	0.302884	7.297660	6.691890
3.5	2.033840	0.350866	7.656270	6.95454
4.0	2.293790	0.397759	8.008480	7.212960

$$\times \left[\gamma(11\alpha^2 + 10\alpha\gamma + 35\gamma^2) + \frac{11\gamma^2 + 10\alpha\gamma + 35\alpha^2}{\gamma} \right] \} + K_2^{(2)} \pm A_2^{(2)}, \quad (42)$$

$$K_2^{(2)} = \int |\psi_{100}(\mathbf{r}_1)|^2 \frac{\lambda}{r_{12}} |\psi_{000}(\mathbf{r}_2)|^2 dv_1 dv_2, \quad (43)$$

$$A_2^{(2)} = \int \psi_{100}(\mathbf{r}_1) \psi_{000}(\mathbf{r}_1) \frac{\lambda}{r_{12}} \psi_{100}(\mathbf{r}_2) \times \psi_{000}(\mathbf{r}_2) dv_1 dv_2. \quad (44)$$

After the integration, we get the energy of the Coulomb interaction between electrons

$$K_2^{(2)} = \lambda \frac{2\sqrt{\alpha\gamma}(8\alpha^2 - 4\alpha\gamma + 15\gamma^2)}{3\sqrt{\pi}\sqrt{\alpha + \gamma}(5\alpha^2 - 2\alpha\gamma + 5\gamma^2)} \quad (45)$$

and the exchange energy

$$A_2^{(2)} = \lambda \frac{8\alpha^{3/2}\gamma^{7/2}}{\sqrt{\pi}(\alpha + \gamma)^{5/2}(5\alpha^2 - 2\alpha\gamma + 5\gamma^2)}. \quad (46)$$

In Table 6, we present the calculated energies $E_2^{(2)s}(\lambda)$, $E_2^{(2)a}(\lambda)$, the Coulomb interaction energy $K_2^{(2)}$, and the exchange energy $A_2^{(2)}$, respectively, for various values of λ , using the values of the variational parameters α and γ .

Finally, we consider the second excited state of the QD, which correspond to the state where one electron is in the ground state with $n_1 = 0, l_1 = 0, m_1 = 0$ and the second one is in the excited state with $n_2 = 0, l_2 = 2, m_2 = 0$. The wave functions of this state is given by (7). The variation parameters α and η are given by relations (19) and (41), respectively. The calculation of

the average Hamiltonian (1) with the help of the wave functions (7) and expansions (12) and (13) gives

$$E_2^{(3)s,a}(\lambda) = \frac{3}{4} \left(\alpha + \frac{1}{\alpha} \right) + \frac{7}{4} \left(\eta + \frac{1}{\eta} \right) + K_2^3 \pm A_2^3, \quad (47)$$

$$K_2^{(3)} = \int |\psi_{020}(\mathbf{r}_1)|^2 \frac{\lambda}{r_{12}} |\psi_{000}(r_2)|^2 dv_1 dv_2, \quad (48)$$

$$A_2^{(3)} = \int \psi_{020}(\mathbf{r}_1) \psi_{000}(\mathbf{r}_1) \frac{\lambda}{r_{12}} \psi_{020}(\mathbf{r}_2) \times \psi_{000}(\mathbf{r}_2) dv_1 dv_2. \quad (49)$$

After the integration, we get the energy of the Coulomb interaction between electrons

$$K_2^{(3)} = \lambda \frac{2\alpha^{3/2} \sqrt{\eta} (15(\alpha + \eta)^2 - 7\alpha(\alpha + \eta) - 3\alpha\eta)}{15\sqrt{\pi} \alpha (\alpha + \eta)^{5/2}} \quad (50)$$

and the exchange energy

$$A_2^{(3)} = \lambda \frac{2\alpha^{3/2} \eta^{7/2}}{5\sqrt{\pi} (\alpha + \eta)^{9/2}}. \quad (51)$$

In Table 7, we present the calculated energies $E_2^{(3)s}(\lambda)$ for the para-state with the total spin equal to zero and $E_2^{(3)a}(\lambda)$ for the ortho-state with the total spin equal to 1, the Coulomb interaction energy $K_2^{(3)}$, and the exchange energy $A_2^{(3)}$, respectively, for various λ , using the calculated values of the variational parameters α and η .

5. Para- and Ortho-States of Two-electron QD

The total wave functions of the two-electron QD including spin variables must be antisymmetric under the permutation of electrons. In Section 2, we introduced the variation coordinate wave functions of the QD. The ground-state wave function (3) is symmetric under the interchange of the electron coordinates and requires the antisymmetric spin function

$$S_{\text{ent}}^{(a)} = \frac{1}{\sqrt{2}} (|\uparrow_1 \downarrow_2\rangle - |\downarrow_1 \uparrow_2\rangle). \quad (52)$$

It is the entangled singlet state, and (a) indicates ‘‘antisymmetric’’. Therefore, the total ground-state wave function is $\Psi_0(1, 2) = \psi_0(\mathbf{r}_1, \mathbf{r}_2) S_{\text{ent}}^{(a)}$ (1, and 2 denote the space and spin variables of the first and second electrons, respectively). In agreement with the theory of

helium atom, we call it the para-state of a two-electron QD [12].

All symmetric combinations of the coordinate wave functions (4), (6), (7), including function (5), require the antisymmetric spin functions (52). Those are the singlet states with spin zero relating to the para-states of the QD.

The antisymmetric combinations of the coordinate wave functions (4), (6), and (7) require the symmetric spin wave functions that organize the following triplet:

$$S_1 = |\uparrow_1\rangle |\uparrow_2\rangle, S_2 = |\downarrow_1\rangle |\downarrow_2\rangle, \quad (53)$$

$$S_{\text{ent}}^{(s)} = \frac{1}{\sqrt{2}} (|\uparrow_1 \downarrow_2\rangle + |\downarrow_1 \uparrow_2\rangle). \quad (54)$$

The spin functions S_1 and S_2 correspond to the spin projections ± 1 , respectively. The spin function (54) is the symmetric entangled state corresponding to the spin projection 0. The states (4), (6), and (7) are related to the ortho-states.

The system of energy levels of the two-electron QD splits into two classes – singlet (para-) and triplet (ortho-), accordingly to the symmetry of the spin functions like that in a helium atom. The transitions between the para- and ortho-states are possible only with account of the spin-orbit interaction. The probability of such transitions is very small. This allows us to claim that there are two ‘‘modifications’’ of two-electron QDs: para- and ortho-dots. In agreement with the spectroscopic nomenclature, we can introduce the following spectral terms. Para states: the ground state $^1S_0(\psi_0(3))$, first excited state $^1P_1(\psi_1^{(s)}(4))$, second excited states: $^1D_2(\psi_2^{(1)}(5))$; $^1S_0(\psi_2^{(2)s}(6))$; $^1D_2(\psi_2^{(2)s}(7))$. Ortho-states: the lowest state $^3P_2(\psi_1^{(a)}(4))$ (metastable), second excited states: $^3S_1(\psi_2^{(2)a}(6))$; $^3D_3(\psi_2^{(2)a}(7))$. These spectral terms do not coincide with the ones of a helium

Table 7. Excited state energies $E_2^{(3)s}(\lambda)$, $E_2^{(3)a}(\lambda)$, the Coulomb interaction energy $K_2^{(3)}$, and the exchange energy $A_2^{(3)}$ for various λ , using the calculated values of the variational parameters α and η

λ	$K_2^{(3)}$	$A_2^{(3)}$	$E_2^{(3)s}(\lambda)$	$E_2^{(3)a}(\lambda)$
0.5	0.277420	0.004876	5.291330	5.281580
1.0	0.540505	0.009542	5.582930	5.563850
1.5	0.790099	0.014017	5.874050	5.846010
2.0	1.028090	0.018318	6.164100	6.127470
2.5	1.255710	0.022461	6.452670	6.407750
3.0	1.474540	0.026457	6.738170	6.686500
3.5	1.684360	0.030211	7.024110	6.963470
4.0	1.887170	0.034063	7.306580	7.238450

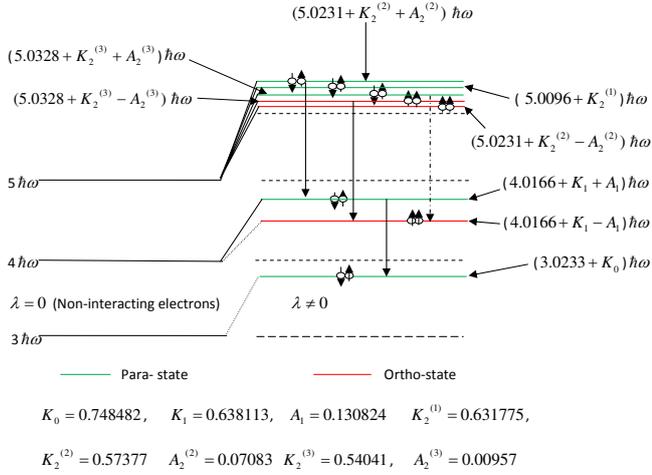


Fig. 1. Energy levels of para- and ortho-states of QD with $\lambda = 1$ (para- and ortho-states are denoted by green and red lines, respectively)

atom, because, in our case, the radial and orbital quantum numbers n and l are independent. The energy levels of the two-electron QD are schematically depicted in Fig. 1.

The most interesting characteristic of the energy levels of the two-electron QD is that they are very close to linear functions of the parameter λ , as is seen from Fig. 2. The familiar behavior was found for the ground-state energy of a 2D two-electron QD in [10].

The calculated energies E_0 , $E_1^{(s)}$, $E_1^{(a)}$, $E_2^{(2)s}$, and $E_2^{(2)a}$ as functions of λ are shown in Fig. 2.

Let us focus on the lowest energy levels of the QD. For $\lambda \leq 1$, the distance between the ground and first excited states $\hbar\omega$ with the typical $\omega = 10^{13}$ is of the order of $T = 100$ K. At $T \ll \hbar\omega$, the transition from the ortho-state 3P_2 to the ground para-state 1S_0 has a very small probability and the ortho-state can be treated as a metastable one. The ensemble of the two-electron QDs at $T \ll 100$ K contains “para-dots” and “ortho-dots”. They possess the entangled spin functions $S_{\text{ent}}^{(a,s)} = \frac{1}{\sqrt{2}}(|\uparrow_1\downarrow_2\rangle \mp |\downarrow_1\uparrow_2\rangle)$ for a long enough time.

From Fig. 2, one can see that the energy levels of the ground- and the lowest ortho-states getting closer with increment in λ . According to Section 2, $\lambda < 2$ for the typical QDs, which allows us to hope for that the presented variational calculations are reliable.

As was stated above, the ensemble of two electron QDs contains, according to our theory, para- and ortho-dots. We considered the parabolic potential with the infinite confinement. The more realistic situation corresponds to

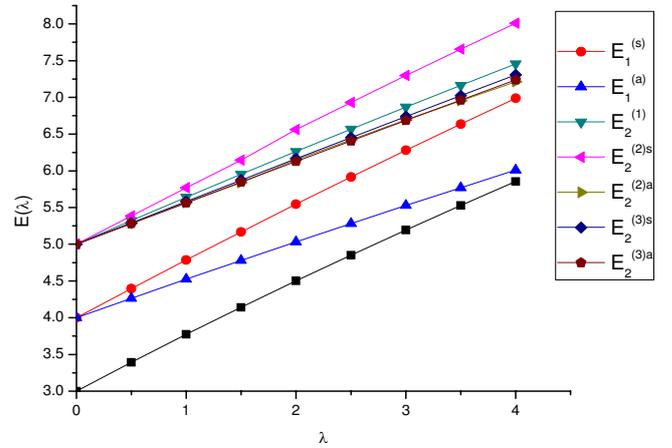


Fig. 2. Energy of para- and ortho-states of a QD versus λ

a finite height U_0 of the potential barrier. If $\hbar\omega \ll U_0$, then the low-lying energy levels of the two-electron QDs calculated above will be slightly affected due to a finite barrier height. It is clear that, at very low temperatures, the ionization potential of the para-dot is given by $I_{\text{para}} = U_0 - E_0(\lambda)$. At the same time, the ionization potential of the ortho-dot is given by $I_{\text{ortho}} = U_0 - E_1^a(\lambda)$. The values of $E_0(\lambda)$ and $E_1^a(\lambda)$ are given in Table 1 and Table 3 (see also Fig. 2). The ionization potential of the para-dot is larger than that of the ortho-dot. Their difference is $\Delta I = E_1^a(\lambda) - E_0(\lambda)$. For example, using a typical value $\lambda = 2$, we get $\Delta I = 5.3$ THz.

These considerations remain true for any shape of the confining potential of QDs. The measurements of the ionization potential of the QDs can confirm the existence of two-electron QDs with para- and ortho-states.

6. Conclusion

We have calculated three first energy levels of the two-electron QD with the parabolic confinement by using the variational functions. The analysis of our numerical calculations allowed us to propose the interpolation formulas for the variational parameters that recover the energy levels for the typical parameters of the QDs.

There are two classes of electron states in the two-electron QDs: para-states with the total spin equal to zero and ortho-states with the total spin equal to 1. The lowest energy level of the ortho-state is metastable. We claim that the experimental realization of the quantum transition of the two-electron QDs will give para- and ortho-QDs. The lowest energy state of the QD has the symmetric coordinate wave function and the antisymmetric singlet spin wave function 1S_0 and is related to

the para-state. All para-states have the total spin equal to zero and should not manifest a multiple structure. These QDs must be related to the para-QDs. The ortho-QDs have energy levels that form close triplets with the total spin equal to 1. The lowest energy state of the ortho-dot 3P_2 is metastable. The only transition from this state is ${}^3P_2 \rightarrow {}^1S_0$ with a change of the spin direction of one electron. At low temperatures $T \ll \hbar\omega$, such a transition has a low probability and we deal with two types of the entangled spin states with $S = 0$ and $S = 1$.

The para- and ortho-QDs have different ionization potentials. The measurement of these potentials can confirm the existence of two-electron QDs.

It would be interesting to mention about the hypothetical QDs manufactured from the materials with gigantic dielectric constant $\epsilon \sim 10^3$ [13]. The Coulomb interaction in this case is practically negligible. The energy levels and the wave functions of a such many-electron system are well known, which considerably simplifies the description of the physical properties of such QDs.

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ДВОЕЛЕКТРОННІ КВАНТОВІ ТОЧКИ
З ПАРАБОЛІЧНИМ КОНФАЙНМЕНТОМ
(НИЗЬКО РОЗТАШОВАНІ ПАРА- ТА ОРТО-СТАНИ)

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Резюме

Варіаційним методом розраховано три перших енергетичних рівня двоелектронної квантової точки (КТ) з параболічним потенціалом. Запропоновані інтерполяційні формули для варіаційних параметрів дозволяють розраховувати енергетичні рівні в широкому діапазоні константи кулонової взаємодії між електронами. Стани КТ можна поділити на пара- та орто-стани подібно до атомів гелію. Квантові переходи між пара- та орто-станами можливі лише з урахуванням спін-орбітальної взаємодії. При низьких температурах ансамбль КТ складається з точок в основному пара-стані та першому збудженому орто-стані, який є метастабільним. Ці КТ мають заплутані спінові хвильові функції, що відносяться до ЕПР (Ейнштейн–Подольський–Розен) станів та становлять інтерес для квантового інформаційного протоколу.