THE SPIN-ORBIT INTERACTIONS OF ELECTRONS IN QUANTUM DOT

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The alternative method is suggested for taking into account the influence of each layer to explain the mechanism of blocking electrons in a quantum dot . The inclusion of the multilayer structure of nanocrystal leads to additional interactions between electrons in quantum dot and this potential is analytically derived. When the relation of distance of electrons is sufficiently small, the additional potential becomes parabolic. The dependence of frequency of the parabolic potential on the difference of dielectric permeability of layers is determined. We assume that the spin-orbital interactions of electrons in quantum dot are defined in an analogous way as a quarks in the nonrelativistic potential model of hadrons. Starting from this suggestion the spin-orbital interactions of electrons in quantum dot are defined. The dependence of the coupling constant of spin-orbital interactions on the image charge and effective size of quantum dot is studied.

1 Introduction

It is experimentally established that if a small number of atoms of germany is implanted on the crystal surface of silicon or arsenide of gallium , after a while these atoms gather in some structures with the size of some tens *nm.* Structures of such a type are the so-called quantum dots [1]. They are local three-dimensional "traps" for electron. At the present time, for application of nanosystems such as quantum dots and a quantum wire [2] in modern semiconductor microelectronics, the control of electron movement in such structures is main problem of nanotechnology. The movement of electrons in nanostructures is controlled by acting on the electron electric charge with the help of an external electric field or on the electron spin with the help of an external magnetic field. When control of movement electrons in nanostructures is carried out due to spin-orbital interaction, such a low-size system is called “spintronics”. For the first time quantum dots have been found [3] in the layered structure on the border of two connections GaAs and GaAlAs. Taking into account the influence of each layer to explain the formation mechanism of blocking electrons in quantum dots is one of the main tasks of modern investigation. However, the consideration of all paired Coulomb interactions of electrons in quantum dots both between themselves and with atoms in a layer, and the determination of the solution of the corresponding Schrodinger equation(SE) from a mathematical point of view to find the solution many-body SE is possibility, but from a practical point of view it is very difficult. Therefore, to find the solution to such a task approximate methods are frequently applied. One of such methods is introduction of an effective parabolic confinement potential for blocking electrons in quantum dots (for details see [4]). However, on the distances from tens up to hundreds *nm,* only Coulomb forces operate between atoms and molecules. The Coulomb potential differs from the parabolic confinement. Thus, our main purpose is to find conditions when the Coulomb potential turn into parabolic potential. This condition gives a possibility to explain the blocking mechanism of electrons in quantum dots. On the other hand, in spintronics [5] the interaction between electrons is defined by spin-orbital interaction of electrons. There arises a question under what conditions of interaction between electrons in nanostructures, in particular, in quantum dots only spin-orbital interaction [6] is defined or under what conditions intensity of spin-orbital interaction becomes dominating above Coulomb interaction between electrons in quantum dots. The given work is devoted to studying these questions within the framework of oscillator representation(OR) method [7].

To answer this question we proceed from the following assumptions: first, in the description of the formation mechanism of quantum dots the essential role is played by quantum-mechanical effects; second, it is necessary to take into account the influence of each layer. On dielectric properties each layer and each quantum dot is homogeneous. However the system as a whole is nonuniform and a condition of continuity of tangential derivative potentials should be satisfied. These assumptions result in introducing an effective positive image charge is which associated with external

factors. This reception is well known in electrostatics in studying of properties dielectrics [8]. Thus, we assume that for explaining the blocking mechanism of electrons in quantum dots(QD) an essential role is played by the image charge that is caused by the difference of dielectric permeability layers such as vacuum and semiconductor, or the semiconductor and dielectric (in detail see [9]). Proceeding from these assumptions the effective potential of confinement is defined.

The work is organized as follows: the second section is devoted to definition of a kind of interaction Hamiltonian with account for the properties of each layer and also some details of the method of two-center adiabatic approximation are stated. In the third section, an energy internal system is calculated in the framework of oscillator representation method. In the fourth section, the behaviour of an additional potential of interaction is analysed. In the fifth section, the constant spin-orbital interaction and its dependence on various parameters of structure which in turn depends on concrete nanocrystal connections is analytically determined. In the sixth section, received basic results are discussed.

2 The interaction Hamiltonian with account the properties each layer

One of actual problems for the investigation main characteristics of nanocrystalical structure is necessary to take into account of the properties each layer. In particulary for the determination of formation mechanism of two electron QD in which arise on border of two connections GaAs and GaAlAs is essential to taking into account influence of each layers the structure. The influence of each layers structure for the formation mechanism of two electron QD can be realized by the image charge in which caused by difference dielectric permeability layers [8, 9]. The interactions between electrons and image charge to be realized by the paired Coulomb interaction. Let us the permeability of first and second layers noted ε_1 and ε_2, respectively. Then the image charge defined as [9]:

$$Z_3 = \frac{(\varepsilon_1 - \varepsilon_2)}{\varepsilon_1 + \varepsilon_2} Q \tag{2.1}$$

where Q is the some positive constants connected with the electrostatic property of the layers. From (2.1) we see that, if medium is uniform then the image charge equal to zero. On the other hand the experimental results shown that the QD arise only on the border every of layers and not arised in the uniform structure. The introductions of image charge give possibility explained the mechanism of blocking electrons in QD and this effect also called dielectrical confainment of electrons in QD [10]. Thus our problem lead to the investigations of formation mechanism three-body Coulomb systems.

Let us consider a three-body Coulomb system with particles of masses m_1, m_2, m_3 and charges $-Z_1e$, $-Z_2e$, Z_3e. The Hamiltonian for this system has the form (in the system units $\hbar = c = 1$)

$$H = \frac{1}{2}\sum_{j=1}^{3}\frac{1}{m_j}\vec{P}_j^2 + \frac{Z_1 Z_2 e^2}{|\vec{r}_1 - \vec{r}_2|} - \frac{Z_1 Z_3 e^2}{|\vec{r}_1 - \vec{r}_3|} - \frac{Z_2 Z_3 e^2}{|\vec{r}_2 - \vec{r}_3|} \tag{2.2}$$

Introducing the Jacobi $\{\vec{x}, \vec{y}\}$ and the center of mass $\vec{z}$ coordinates

$$\begin{aligned}
\vec{r}_1 &= \frac{m_2}{m_1 + m_2}\vec{x} + \frac{m_3}{m_1 + m_2 + m_3}\vec{y} + \vec{z} \\
\vec{r}_2 &= -\frac{m_1}{m_1 + m_2}\vec{x} + \frac{m_3}{m_1 + m_2 + m_3}\vec{y} + \vec{z} \\
\vec{r}_3 &= -\frac{m_1 + m_2}{m_1 + m_2 + m_3}\vec{y} + \vec{z}
\end{aligned} \tag{2.3}$$

we transform the Hamiltonian (2.2) to the form

$$H = \frac{1}{2M}\vec{P}_x^2 + \frac{1}{2\mu}\vec{P}_y^2 + \frac{Z_1 Z_2 e^2}{x} - \frac{Z_1 Z_3 e^2}{\left|\vec{x}M/m_1 + \vec{y}\right|} - \frac{Z_2 Z_3 e^2}{\left|\vec{x}M/m_2 - \vec{y}\right|} \tag{2.4}$$

Here, we omit the kinetic energy term of center mass and use the following notations

$$M = \frac{m_1 m_2}{m_1 + m_2}, \quad \mu = \frac{(m_1 + m_2)m_3}{m_1 + m_2 + m_3} \tag{2.5}$$

It is convenient to introduce new dimensionless variables $(\vec{R}, \vec{r})$:

$$\vec{x} = \frac{1}{Me^2}\vec{R}, \qquad \vec{y} = \frac{1}{\sqrt{M\mu e^2}}\vec{r} \tag{2.6}$$

As a result, the SE reads as

$$\left[\frac{1}{2}\vec{P}_r^2 + \frac{1}{2}\vec{P}_R^2 + \frac{Z_1 Z_2}{R} - \frac{Z_1 Z_3 \lambda}{\left|\vec{r} + c_1\vec{R}\right|} - \frac{Z_2 Z_3 \lambda}{\left|\vec{r} - c_2\vec{R}\right|} + \frac{U}{2}\right]\Psi(\vec{R},\vec{r}) = 0 \tag{2.7}$$

where we use the additional notations

$$\lambda = c_1 + c_2, \qquad c_j = \frac{1}{m_j}\sqrt{\frac{m_1 m_2 m_3}{m_1 + m_2 + m_3}}, \quad j = 1, 2 \tag{2.8}$$

The energy of the three-body Coulomb system has the form

$$E = -\frac{e^4}{2}\cdot\frac{m_1 m_2}{m_1 + m_2}\cdot U \tag{2.9}$$

and is determined by the dimensionless parameter *U*.

Our problem is to calculate the energy parameter *U*, and the wave function, from the SE represented in (2.7), in the framework of the OR method [7, 11].

2.1 The adiabatic approximation

In this section we present details of our approach to treat the SE for the three-body Coulomb systems. The main ingredient is the adiabatic approximation for two center developed within the OR, which allows to separate "fast" and "slow" dynamical variables. We remind that the adiabatic approximation was applied by Born and Oppenheimer [12] and later by Born and Fock [13] to find the solution of SE.

We assume that our system is axially symmetric. In the two-center adiabatic approximation [14], the wave function of the three-body Coulomb system can be presented in the form

$$\Psi(\vec{R},\vec{r}) = \chi(\vec{R})\cdot\Phi(R,\vec{r}) \tag{2.10}$$

Here $\Phi(\vec{R},\vec{r})$

$$\Phi(R,\vec{r}) = \frac{e^{im\varphi}}{\sqrt{2\pi}}\cdot\tilde{\Phi}_m(R;\rho,z) \tag{2.11}$$

is the wave function of the intrinsic system, φ is the azimuthally angle and *m* is the magnetic quantum number in the cylindrical system of coordinates. Substituting expressions (2.10), and (2.11) into Eq.(2.7), we obtain after some simplifications

$$\left\{-\frac{1}{2}\left[\frac{\partial^2}{\partial\rho^2} + \frac{1}{\rho}\frac{\partial}{\partial\rho} - \frac{m^2}{\rho^2} + \frac{\partial^2}{\partial z^2}\right] - \frac{Z_1 Z_3 \lambda}{\sqrt{\rho^2 + 2c_1 Rz + c_1^2 R^2}}\right.$$

$$\left. - \frac{Z_2 Z_3 \lambda}{\sqrt{\rho^2 - 2c_2 Rz + c_2^2 R^2}}\right\}\tilde{\Phi}_m(R;\rho,z) \tag{2.12}$$

Here $E_r(R)$ is the eigenvalue of the Hamiltonian of the intrinsic system. In Eq.(2.12) the variable *R*

is considered as an external parameter.

The traditional approach to the eigenvalue problem consists of the use the elongated and oblate spheroidal coordinates [15], while the parameter R defines a focus distance and $E_r(R)$ is called the term. In the two-center approximation the Coulomb three-body problem is separable in the spheroidal coordinates and is analyzed with the aid of the two equations. These ordinary differential equations are solvable in terms of series expansion (the detail see [15, 16]). In present paper we use the OR to determine the $E_r(R)$ term.

2.2 The two center adiabatic approximation in the OR

Let us determine the $E_r(r)$ energy spectrum of the intrinsic system in the framework OR. Carrying out substitution of variables

$$\rho = 2\cdot\sqrt{\rho_1\rho_2}\,, \qquad z = (\rho_1 - \rho_2)\,, \tag{2.13}$$

and going over to the parabolic system of coordinates in Eq. (2.12), after relevant calculations, we obtain

$$\begin{aligned}&\left\{-\frac{1}{2}\left[\rho_1\frac{\partial^2}{\partial\rho_1{}^2}+\frac{\partial}{\partial\rho_1}+\rho_2\frac{\partial^2}{\partial\rho_2{}^2}+\frac{\partial}{\partial\rho_2}-\frac{m^2}{4\rho_1}-\frac{m^2}{4\rho_2}\right]\right.\\ &-(\rho_1+\rho_2)E_r-\frac{Z_1Z_{.3}\lambda\cdot(\rho_1+\rho_2)}{\sqrt{(\rho_1+\rho_2)^2+2c_1R(\rho_1+\rho_2)+c_1^2R^2}}\\ &\left.-\frac{Z_2Z_3\lambda\cdot(\rho_1+\rho_2)}{\sqrt{(\rho_1+\rho_2)^2-2c_2R(\rho_1-\rho_2)+c_2^2R^2}}\right\}\tilde{\Phi}_m(r;\rho_1,\rho_2)=0\end{aligned} \tag{2.14}$$

For the determine the $E_r(r)$ energy spectrum of the intrinsic system, now we can apply the oscillator representation method [11], to the SE (2.14).

Before defining the energy spectrum and the wave function of the SE (2.14) using the oscillator representation method [7], it is appropriate to note that this method is based on the ideas and methods of the quantum theory of a scalar field. However, a considerable difference between quantum field theory and quantum mechanics is that in the former case, the quantized fields in the form of a set an infinite number of oscillatory nature in the quantum-field interaction. In quantum mechanics, the behavior of the eigenfunctions for most potentials differs from the Gaussian behavior of the oscillator wave function. For this reason, while applying the methods and ideas of quantum field theory for solving quantum-mechanical problems, the variables in the initial radial SE should be changed so that the wave function would display the Gaussian behavior at large distances, and the transformed equation in a space with a large dimension. It should be noted that a similar idea first was discussed by Fock while solving the problem of the spectrum of the hydrogen atom with the help of transformation to the four-dimensional momentum space [17].

Following Fock [18], we will assume that the asymptotic behavior of the wave function of the intrinsic system is of the Coulomb type. In accordance with what has been said above, we change the variables as follows (see for details [7]):

$$\rho_k = q_k^2 \quad \tilde{\Phi}_m = q_1^{|m|}q_2^{|m|}\Psi_m(q_1^2,q_2^2)\,, \quad \text{k=1,2.} \tag{2.15}$$

For the SE, we obtain from (2.14):

$$\begin{aligned}&\left\{-\frac{1}{2}\sum_{j=1}^{2}\left[\frac{\partial^2}{\partial q_j^2}+\frac{d-1}{q_j}\cdot\frac{\partial}{\partial q_i}\right]-\frac{4Z_1Z_3\lambda(q_1^2+q_2^2)}{\sqrt{(q_1^2+q_2^2)^2+2c_1R(q_1^2-q_2^2)+c_1^2R^2}}\right.\\ &\left.-4E_r(q_1^2+q_2^2)-\frac{4Z_2Z_3\lambda(q_1^2+q_2^2)}{\sqrt{(q_1^2+q_2^2)^2-2c_2R(q_1^2-q_2^2)+c_2^2R^2}}\right\}\Psi_m(q_1^2,q_2^2)=0\end{aligned} \tag{2.16}$$

where d is the dimension of the auxiliary space, which is equal to

$$d = 2 + 2|m| \tag{2.17}$$

As a result of the change of variables, we obtain a modified SE in the d-dimensional auxiliary space R^{d}. It follows from Eqs. (2.16) and (2.17) that the magnetic quantum number m appears in the definition of the dimension d of the space. This approach makes it possible to determine all the characteristics we are interested in, including the spectrum and the wave function, by solving the modified SE for the ground state only in the d-dimensional auxiliary space R^{d}. The wave function $\Psi_m(q_1^2, q_2^2)$ of the ground state in R^{d} is a function of variables q_1^2 and q_2^2 only. For this reason, we identify the operator

$$\frac{\partial^2}{\partial q_{k^2}} + \frac{d-1}{q_k}\frac{\partial}{\partial q_k} = \Delta_{qk}, \qquad k = 1,2 \tag{2.18}$$

with the Laplacian A_{qk} in the auxiliary space R^d, which acts on the wave function of the ground state, which is a function of radius q_k only. Proceeding from the modified SE

$$\mathrm{H}\Psi_m(q_1, q_2) = \varepsilon(\mathrm{E}_r)\Psi_m(q_1, q_2) \tag{2.19}$$

in accordance with Eq.(2.16), we find that the energy spectrum in R^{d} is equal to zero

$$\varepsilon(E_r) = 0 \tag{2.20}$$

We will consider this relation as the condition for determining the energy spectrum E_r of the Hamiltonian (2.12). Following the oscillator representation method, we write the canonical variables in terms of the creation and annihilation operators in the R^{d} space

$$q_j^{(k)} = \frac{a_j^k + a_j^{k+}}{\sqrt{2\omega_k}}; \qquad \mathrm{P}_j^{(k)} = \sqrt{\frac{\omega_k}{2}}\,\frac{a_j^k - a_j^{k+}}{i};$$
$$k = 1,2; \qquad j = 1,\ldots,d, \qquad \left[a_i^k, a_j^{k+}\right] = \delta_{i,j}, \tag{2.21}$$

where ω_k is the oscillator frequency, which is yet unknown. Substituting expressions (2.21) into Eq. (2.16) and ordering in the creation and annihilation operators, we obtain

$$\mathrm{H} = \mathrm{H}_0 + \varepsilon_0(\mathrm{E}_r) + \mathrm{H}_I \tag{2.22}$$

Here, H_0 is the Hamiltonian of two uncoupled oscillators,

$$\mathrm{H}_0 = \omega_1\left(a_j^{+(1)} \cdot a_j^{(1)}\right) + \omega_2\left(a_j^{+(2)} \cdot a_j^{(2)}\right) \tag{2.23}$$

and $\varepsilon_0(E_r)$ is the ground-state energy in the zeroth approximation of the OR [7], which has the form

$$\varepsilon_0(E_r) = \frac{d}{4}\omega_1 + \frac{d}{4}\omega_2 - 2\frac{E_r \cdot d}{\omega_1} - 2\frac{E_r d}{\omega_2} - 4(\omega_1\omega_2)^{d/2} \times$$
$$\times \int_0^\infty\int_0^\infty \frac{d\beta_1 d\beta 2}{\Gamma^2(d/2)}\left\{\frac{Z_1 Z_3 \lambda(\beta_1 \cdot \beta_2)^{d/2-1}(\beta_1 + \beta_2)}{\sqrt{(\beta_1 + \beta_2)^2 - 2c_2 R(\beta_1 - \beta_2) + c_1^2 R^2}} + \right. \tag{2.24}$$
$$\left. + \frac{Z_2 Z_3 \lambda(\beta_1 \cdot \beta_2)^{d/2-1}(\beta_1 + \beta_2)}{\sqrt{(\beta_1 + \beta_2)^2 - 2c_2 R(\beta_1 - \beta_2) + c_2^2 R^2}}\right\}\exp\left(-\omega_1\beta_1 - \omega_2\beta_2\right)$$

The kind of interaction Hamiltonian H_I given in [19]. The contribution of the interaction Hamilto-

nian H_I is considered as a small perturbation [7]. In quantum field theory, after representing the canonical variables in terms of the creation and annihilation operators and representing the interaction Hamiltonian in normal form, we find that the requirement of the absence of second-degree field operators in the interaction Hamiltonian is essentially equivalent to renormalizations of the coupling constant and the wave function [20]. Moreover, such a procedure makes it possible to take into account the main quantum contribution through the renormalization of mass and through the energy of the vacuum. In other words, all quadratic forms are completely included in the Hamiltonian of a free oscillator. This requirement makes it possible to formulate, in accordance with the OR, the conditions [7]:

$$\frac{\partial \varepsilon_0(E)}{\partial \omega_1} = 0, \quad \frac{\partial \varepsilon_0(e)}{\partial \omega_2} = 0 \tag{2.25}$$

for determining the frequencies $\omega 1$ and Ω_2 of the uncoupled oscillators, which determine the main quantum contribution. Taking into account Eq. (2.24), we can use Eqs (2.20) and (2.25) for calculating the energy E_r of the intrinsic system as a function of parameter R.

3 Determination of the dependence on the term $E_r(R)$ from the parameter R

We proceed to the determination of the dependence the term $E_r(R)$ on the parameter R in the zeroth order approximation of OR. Taking into account (2.24) and from the system of equations which are represented in (2.25) and (2.20) we can determine the oscillator frequencies ω_1 and ω_2, and also the energy spectrum of the intrinsic system $E_r(R)$ as a function of the parameter R. In the general case, this system of equations, of course, is not solved analytically. Therefore, first of all we considered the particular cases. Let us consider the case when $R = 0$, then from (2.24) we have

$$\varepsilon_0(E_r) = \frac{d\omega_1}{4} + \frac{d\omega_2}{4} - \frac{2dE_r}{\omega_1} - \frac{2dE_r}{\omega_2} + 4Z_3\lambda(Z_1 + Z_2) \tag{3.1}$$

In this case from (2.26) we get

$$\omega_1 = \omega_2 = \sqrt{-8E_r} \tag{3.2}$$

So the oscillator frequencies are equal $\omega_1 = \omega_2$. Now we consider the other limiting case: $R = \infty$; in this limit, from (2.24) we have

$$\varepsilon_0(E_r) = \frac{d\omega_1}{4} + \frac{d\omega_2}{4} - \frac{2dE_r}{\omega_1} - \frac{2dE_r}{\omega_2} \tag{3.3}$$

Thus, in the limits $R = 0$ and $R = \infty$, the frequencies of the oscillators are equal, and the term of the two-Coulomb center is defined analytically.

Let us determine the term of the two-Coulomb center as a function of the parameter R in the intervals of the values for the parameter: $0 < R < \infty$. Now we introduced new parameters

$$\omega_+ = \frac{\omega_1 + \omega_2}{2}, \quad \omega_- = \frac{\omega_1 - \omega_2}{2} \tag{3.4}$$

and these new parameters also depend on the parameter R. According to (3.2), at $R = 0$ and $R = \infty$, the parameter ω_- is equal to zero, since the electron wave function becomes spherically symmetric. Thus, the parameter ω_- is connected with the dipole moment interactions. From (2.24) for the ground state ($m = 0$) energy of the modified SE, we obtain:

$$\varepsilon_0(E_r) = \omega_+ - \frac{8E_r\omega_+}{\omega_+^2 - \omega_-^2} - 4(\omega_+^2 - \omega_-^2)\int_0^\infty\int_0^\infty d\beta_1 d\beta_2 \exp\{-\omega_+(\beta_1+\beta_2) - \omega_-(\beta_1-\beta_2)\}\times$$
$$\times\left[\frac{Z_1Z_3\lambda(\beta_1+\beta_2)}{\sqrt{(\beta_1+\beta_2)^2 + 2c_1R(\beta_1-\beta_2) + c_1^2R^2}} + \frac{Z_2Z_3\lambda(\beta_1+\beta_2)}{\sqrt{(\beta_1+\beta_2)^2 - 2c_2R(\beta_1-\beta_2) + c_2^2R^2}}\right] \tag{3.5}$$

For further calculation we introduced the following new variables

$$\beta_1 = \frac{s+t}{\sqrt{2}}; \quad \beta_2 = \frac{t-s}{\sqrt{2}}; \quad s = xt;$$

$$\omega = \omega_+; \quad \gamma = \frac{\omega_-}{\omega_+}; \quad b_j = c_j R; \quad \text{j=1,2.} \tag{3.6}$$

and after some simplification from (3.5) we have

$$\varepsilon_0(E_r) = \omega - \frac{8E_r}{\omega} * \frac{1}{1-\gamma^2} - 2\omega^2(1-\gamma^2)\times$$

$$\times \int_0^\infty dt t^2 \int_0^\infty dx * \{Z_1 b_1^2 e^{-b_1 t\omega(1+x\gamma)} + Z_2 b_2^2 e^{-b_2 t\omega(1-x\gamma)}\} \frac{Z_3\lambda}{\sqrt{1+2xt+t^2}} \tag{3.7}$$

According to (2.20), (2.24) and (2.26), the term of two-Coulomb center is defined in the following way:

$$E_r^{(0)}(R) = \frac{\omega^2}{2} - \omega_0\omega(2\frac{1-e^{-\omega R}}{\omega R} - e^{-\omega R}) \tag{3.8}$$

4 The interaction potentials of electrons in QD

The solution of SE defines the property and behaviour of electrons in QD. Taking into account (2.10), and (2.12) and after averaging of the wave function of the intrinsic systems $\Phi(\vec{R},\vec{r})$ from (2.7) we obtain for the SE with taking into account the influence of the layers

$$\left\{\frac{1}{2}\vec{P}_R^2 + V_{tot}(R) + \frac{U}{2}\right\}\chi(\vec{R}) = 0 \tag{4.1}$$

where $V_{tot}(R)$ is the total potential of electrons in QD and in the ordinary units[4] is represented as

$$V_{tot} = \frac{\hbar}{a^*\sqrt{m_e^*}} * \frac{1}{R} + E_r(R) + \frac{1}{2}(\frac{1}{\omega} * \frac{\partial\omega}{\partial R})^2 \tag{4.2}$$

and m^* is the effective mass of electrons, and a^* is the effective Bohr radius. The first term in Eq. (4.2) is the Coulomb potential and $E_r(R)$ is the potential creating electrostatical field of image charge. The third term in Eq.(4.2) is connected with the relative motion of electrons in QD and the contribution of this term as compared to $E_r^{(0)}(R)$ is less than an order [11] and the further calculation it should be neglected. All parameters of the total potentials which are represented in (4.2) are determined and the potential consists of two parts: the Coulomb potential and the confinement potential. Let us consider the limit $R << 1$; from (3.8) we get

$$E_r^{(0)}(R) = \frac{\omega_0^2}{2}(-1 + \frac{1}{3}\omega_0^2 R^2 + O(R^4)) \tag{4.3}$$

where

$$\omega_0 = \frac{4hZ_3}{a^*\sqrt{m_e^*}} \equiv \frac{4Z_3\sqrt{m_e^*}}{\hbar} * \frac{e^2}{4\pi\varepsilon\varepsilon_0}$$

Thus, in the limit $R<<1$ the additional potential which is created by the image charge is parabolic. Now the total potential, represented in (4.2), can be rewritten in the form

$$V = V_V(R) + V_S(R) \tag{4.4}$$

where V_V is the vector or the one-photon exchange potential

$$V_V = \frac{\hbar}{a^* \sqrt{m_e^*}} * \frac{1}{R} \tag{4.5}$$

and V_S is the potential confinement which blocks electrons in QD

$$V_S = \frac{\omega^2}{2} - \omega_0 \omega (2 \frac{1 - e^{-\omega R}}{\omega R} - e^{-\omega R}) \tag{4.6}$$

So the blocked electrons in QD are influenced by Coulomb force connected with the electric charge and confinement potential which is caused by the difference of dielectric permeability layers.

5 Spin-orbital interactions of electrons in QD

In (4.4) we analytical by defined the interaction potential of two electrons in QD. This potential consists of two parts: first, the V_V vector potential connected with the one-photon exchange and second, the V_S blocking potential. However, for determination of the interaction potential of two electrons in QD we cannot take into account spin interactions of electrons. Let us determine the potential of electrons in QD with spin-orbital interactions. First of all, we should like to note some difference between electrons in QD and electrons in ordinary atoms. In usual atoms a bound state is realized via the central Coulomb force and for electrons in QD the attraction central force is absent. Therefore, we must determine the spin-orbit interaction of electrons in which a bound state is realized via the blocking parabolic potential and the repulsed vector potential. On the other hand, fermions with interaction potentials of a similar nature are common by known in particle physics, namely the nonrelativistic quark model, and the spin-orbital potentials are defined as (for details see [21])

$$H_{SL} = \frac{1}{2m_1 \cdot m_2} \cdot \frac{1}{x} \cdot [3 \cdot \frac{d}{dx} V_V(x) - \frac{d}{dx} V_S(x)] \cdot (\vec{L} \cdot \vec{S}) \tag{5.1}$$

Here V_V is the vector potential connected with the one-gluon exchange and V_S is the growing potential which provides confinement of quarks, x is the distance between quarks, and m_1, m_2 is the mass of quarks. The behaviour and the blocking mechanism of electrons in QD have a similar nature with confinement of quarks in hadrons. Therefore, we assume that the spin-orbital interaction of electrons in QD and quarks in meson is analogous. Then, according to (5.1), the spin-orbit interaction Hamiltonian for electrons in QD can be rewritten in the form

$$H_{LS} = \frac{1}{2m_e^* \cdot \hbar^2} \cdot \frac{1}{R} \cdot [3 \cdot \frac{d}{dR} V_V(R) - \frac{d}{dR} V_S(R)] \cdot (\vec{L} \cdot \vec{S}) \tag{5.2}$$

where $V_V(R)$ is the vector potential and $V_S(R)$ is the blocking potential electrons in QD, and this potentials are presented in (4.5) and (4.6), respectively. In (5.2) L is the operator of orbital momentum determined in a standard way

$$\hbar \vec{L} = [\vec{R} \times \vec{P}_R] = -i\hbar [\vec{R} \times \vec{\nabla}_R]; \;\; \vec{L} = -i[\vec{R} \times \vec{\nabla}_R] \tag{5.3}$$

and S is the spin operator satisfying the following identity

$$(\vec{L} \cdot \vec{S}) = i(\vec{R} \cdot [\vec{S} \times \vec{\nabla}_R]) \tag{5.4}$$

Then the total potential of electrons in QD with the spin-orbital interaction has the form

$$V_{tot}(R) = V_V(R) + V_S(R) + H_{SL}(R) \tag{5.5}$$

Let us determine the condition of domination of the spin-orbital interaction of electrons in QD. The electrons in QD have two forms of interaction: the vector potential $V_V(R)$ is the repulsed Coulomb

potential and $V_S(R)$ is the blocking potential. The results of experimental investigation of nanostructure shows that, the QD is a more or less stable object. This indicates that the repulsed and the blocked forces are balanced. Then we assume that there exists such a distance $R = R_0$ at which the repulsed and the blocking potential annul themselves. So this distance is determined from the equation

$$V_V(R_0) + V_S(R_0) = 0 \tag{5.6}$$

From this equation the parameter R_0 is determined as a function of effective mass electrons and of the image charge Z_3. On the other hand, the parameter R_0 can be considered as an effective size of QD. Taking into account (5.6) and after some standard simplifications from (5.2) we get for the Hamiltonian of the spin-orbital interaction:

$$H_{SL} = \frac{1}{m_e^* \cdot \hbar^2}\left(\frac{\omega^2}{4R_0} - \frac{2}{R_0^2} \cdot \frac{\hbar}{a^* \sqrt{m_e^*}}\right) \cdot \frac{1}{R_0} \cdot i(\vec{R} \cdot [\vec{S} \times \vec{\nabla}_R]) \Big|_{R=R_0} \tag{5.7}$$

where ω is the oscillator frequency. Now the dimensionless variables (η, τ) are introduced

$$\omega = \omega_0 \eta\,,\ R_0 = \frac{\tau}{\omega_0} \tag{5.8}$$

and these variables are substituted in (5.7); after some simplifications the spin-orbital interaction Hamiltonian is rewritten in the following way:

$$H_{SL} = \frac{1}{m_e^* \cdot \hbar^2} \cdot \frac{\omega_0^4}{4\tau^3 Z_3} \cdot (\tau\eta^2 Z_3 - 2) \cdot i(\vec{R} \cdot [\vec{S} \times \vec{\nabla}_R]) \Big|_{R=R_0} \tag{5.9}$$

Taking into account (5.8) and (5.6) we have two systems of equations for the dimensionless variables τ, η:

$$\begin{cases} \dfrac{1}{8Z_3} \cdot \dfrac{1}{\tau} + \dfrac{\eta^2}{4} - \dfrac{1 - e^{-\eta\tau}}{\tau} + \dfrac{\eta}{2} e^{-\eta\tau} = 0 \\ \eta - (1 + \eta\tau) e^{-\eta\tau} = 0 \end{cases} \tag{5.10}$$

From this systems of equations the variables τ, η are determined as functions of the image charge Z_3. Using the representations for the spin operator $(\vec{S} = 1/2 \cdot \vec{\sigma})$ and for the momentum operator $(\vec{P}_R = -i\vec{\nabla}_R)$ and taking into account (2.6), from (5.9) we get for the spin-orbital Hamiltonian

$$H_{SL} = K_{SO}(\sigma_x P_y - \sigma_y P_x)\,, \tag{5.11}$$

where σ is the Pauli matrix, and K_{SO} is the spin-orbit coupling constant

$$K_{SO} = \frac{1}{2} m_e \alpha_{em}^2 \cdot \tau_e \cdot \frac{1}{\varepsilon} \cdot \frac{1}{R_b^2} (2 - \tau\eta^2 Z_3) \cdot \left(\frac{m_e}{m_e^*}\right)^2, \tag{5.12}$$

here α_{em} is the coupling constant electromagnetic interaction and 0, $5 m_e \alpha_{em}^2$ = 13, 605698 eV is the Rydberg energy; $r_e = e^2/4\pi\varepsilon_o m_e$ = 2, 81794·10^{-15}[m] is the classical radius of electron, and R_b is the distance between electrons in QD in which the repulsed and the blocked forces annul themselves; in the units of Bohr radius this distance is rewritten as follows:

$$R_b = \frac{R_0}{a_b} = \tau \frac{\varepsilon}{4Z_3} \left(\frac{m_e}{m_e^*}\right)^2. \tag{5.13}$$

Then from (5.12) for the effective spin-orbital coupling constant we have

$$K_{SO} = 0.06134\left(\frac{m_e}{m_e^*}\right)^2 \frac{Z_3^2}{\varepsilon^3\tau^2}(2-\tau\eta^2 Z_3) \quad [10^{-11}\ eV{\cdot}m] \tag{5.14}$$

From (5.13) and (5.14) we see that the effective size of QD, or the parameter R_b, and the spin-orbital coupling constant K_{SO} of electrons in QD are determined as functions of the image charge and the effective mass of electrons. According to (2.1), the image charge depends on the difference of dielectric permeability of layers, so the variables R_b and K_{SO} also depend on this difference. The numerical values of these parameters, of course, should depend on a concrete structure of the nanocrystal. Therefore, for investigation of the dependence spin-orbital coupling constant on the dielectric permeability of layers and also on the electronic density of the system the consideration of a concrete nanostructure is necessary.

6 Results and Discussion

We assume that the image charge is positive. This assumption gives a possibility to explain the mechanism of blocking electrons in QD. From (2.2) we see that the image charge depends on the difference of dielectric permeability of layers. On the other hand, we know that the existence of nanostructures of different of dielectric permeability of layers influences the electrical and optical properties of the system. Such nanostructures are: semiconductor nanocrystal [22] and quantum wire [23] arising in the dielectric matrix and also porous silicon [24] and others. In Eq.(5.14) the spin-orbital coupling constant is analyticaliy determined and this gives the possibility to investigate the dependence of this constant on the image charge and other properties of the system. From (5.14) we see that the constant K_{SO} quadratically depends on the effective mass electrons. The effective mass of electrons in the nanostructures, of course, depends on the composition of the structure. The results of experimental investigations [25] show that the effective mass of electrons depends on the density of electrons and the linear size of QD. Thus, the constant K_{SO} depends on the effective mass of electrons and the linear size of QD.

Let us consider the two-electron QD which arises on the border of two connections GaAs and GaAlAs. The dielectric permeability of QD arises on the border of these connections depending on the QD size and changes the limits (the detail see [10, 26]): $\varepsilon_{GaAs} = 6{,}1 \div 13$; in this case, the effective mass of electrons equals $m^*_e = 0,067 m_e$.

Figure 1 illustrates the dependence of the spin-orbital coupling constant *KSO* on the image charge for the given values of ε. From Fig.1 we can see that with growing Z_3 the coupling constant K_{SO} also increases. At small values of ε dielectric permeability of the QD the increase in the coupling constant K_{SO} is drastic.

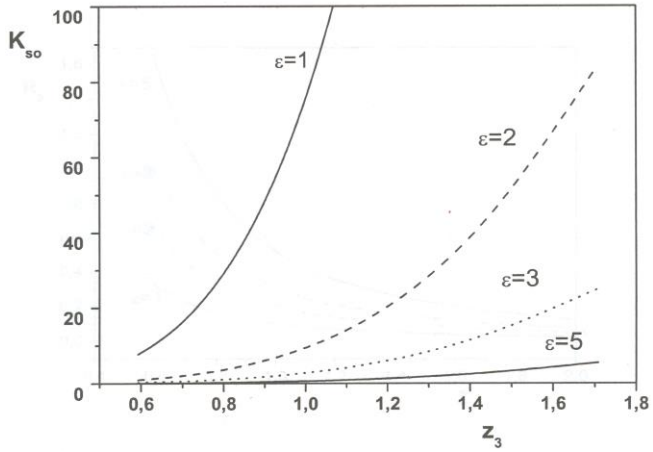

Figure 1

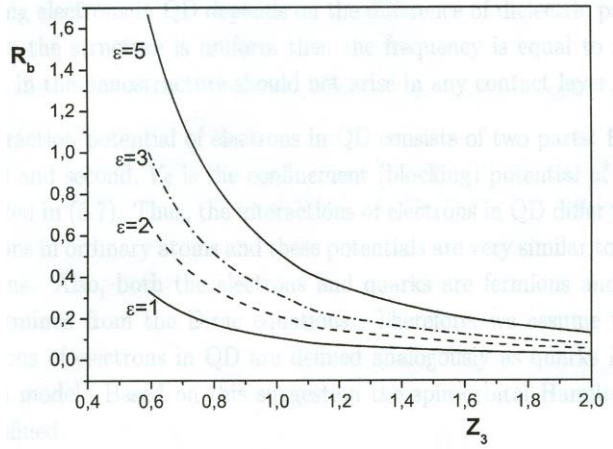

Figure 2

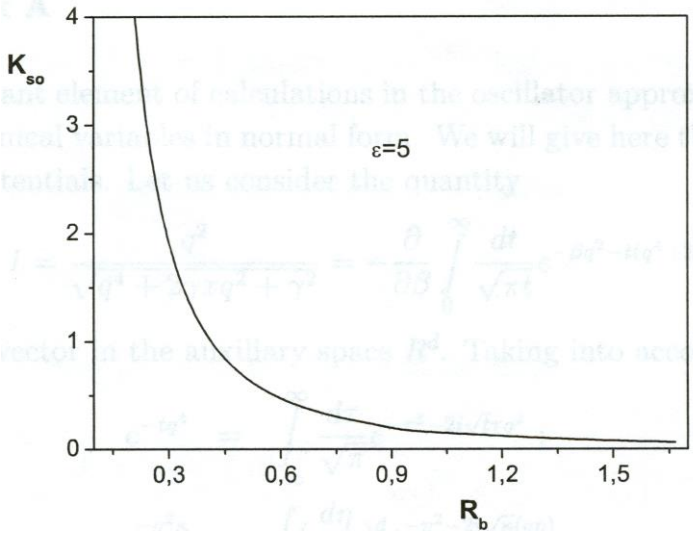

Figure 3

Figure 2 represents the R_b dependence of the effective size of QD on the image charge Z_3 for the given values of ε. Prom Fig.2 we can see that with growing Z_3 the size R_b decreases. This means that the blocking electrons in QD are realized due to Z_3.

Figure 3 shows the dependence of the spin-orbital coupling constant K_{SO} *on* R_b the effective size of QD for the given values of ε. From Fig.3 we can see that with growing R_b the coupling constant K_{SO} decreases.

The effective coupling constant of the spin-orbital interaction for the structure *InGaAs* with effective mass of electron $m^* = 0.042m_e$ was experimentally obtained in Ref. [27]: $K_{SO} = 1{,}5\cdot10^{-11}$ $[eV\cdot m]$. From (6.14) at the values of the parameters ε = 3 and Z_3 = 0,68 we have $K_{SO} = 1{,}5\cdot10^{-11}[eVm]$. Unfortunately, in our analytical results, for coupling constant K_{SO} represented in (6.14) depends some parameters such as the *s* dielectric permeability of the QD, effective mass m^* of electrons and the difference of dielectric permeability of layers. At the present time these parameters for every QD cannot be defined experimentally. However, just these parameters can be determined experimentally for the given nanostructure.

On the basis of the obtained results we can conclude:

- The account of the multilayer structure of nanocrystal leads to additional interactions between electrons in QD and the explicit form of this potential is represented in (5.7). On the other hand, to describe the properties of QD one can successfully use the phe-nomenological potentials, in particular, the parabolic confinement [4] and in this case, the frequency of the oscillator is a free external parameter. If we assume that the relative distance of electrons or the effective size of QD are sufficiently small then from (5.7) we obtain the parabolic potential. In our case, the frequency of the oscillator or the intensity of blocking electrons in QD depends on the difference of dielectric permeability of layers, and when the structure is uniform then the frequency is equal to zero. So "traps" for electrons in the nanostructure should not arise in any contact layer.
- The interaction potential of electrons in QD consists of two parts: first, *VV* is the vector potential and second, *VS* is the confinement (blocking) potential of electrons in QD and represented in (5.7). Thus, the interactions of electrons in QD differ from the interactions of electrons in ordinary atoms and these potentials are very similar to the potential quarks in hadrons. Also, both the electrons and quarks are fermions and the wave functions are determined from the Dirac equations. Therefore, we assume that the spin-orbital interactions of electrons in QD are defined analogously as quarks in the nonrelativistic potential model. Based on this suggestion the spin-orbital Hamiltonian of electrons in QD is defined.
- The results of experimental investigations of the QD show that the QD is a stable equilibrium state. This means that the forces of the Coulomb repulsion and blocking of electrons in QD are

balanced. Therefore, we assume that there should exist such a distance at which these forces are cancelled. In this case, only spin-orbital interactions acts between electrons in QD. This suggestions was used to study the dependence of the coupling constant of spin-orbital interactions on the image charge and the effective size of QD

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КВАНТТЫҚ НҮКТЕДЕГІ ЭЛЕКТРОНДАРДЫҢ СПИН-ОРБИТАЛЫҚ ӘСЕРЛЕСУІ

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Электрондарды кванттық нүктеде ноқталаудың нанокристаллдың әрбір қабатының әсерін ескеретін баламалы әдісі ұсынылған. Нанокристаллдың көпқабатты құрылымын ескеру электрондар арасындағы қосымша әсерлесуге алып келеді. Осы әсерлесудің сипаты анықталған. Электрондардың өзара қашықтығы мардымсыз аз болғанда ол парабола түрінде екен. Осы парабола жиілігінің қабаттардың диэлектрлік өтімділігінен тәуелділігі зерттелген. Кванттық нүктедегі электрондардың спин-орбиталық әсерлесуі адронның релятивті емес потенциалдық моделіндегі кварктардың әсерлесуіне ұқсас деп жорамалданған. Осы жорамал негізінде электрондардың кванттық нүктедегі спин-орбиталық әсерлесуі анықталған. Спин-орбиталық әсерлесудің байланыс тұрақтысының бейнелеу заряды мен кванттық нүктенің тиімді өлшемінен тәуелділігі зерттелген.

СПИН-ОРБИТАЛЬНОЕ ВЗАИМОДЕЙСТВИЕ ЭЛЕКТРОНОВ В КВАНТОВОЙ ТОЧКЕ

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Для объяснения удержания электронов в квантовой точке предложен альтернативный метод, учитывающий влияние каждого из слоев нанокристалла. Учет многослойной структуры нанокристалла приведет к дополнительным взаимодействиям между электронами. Найден вид этого взаимодействия. Когда относительное расстояние между электронами достаточно маленькое, оно имеет параболический вид. Изучена зависимость частоты такого параболического потенциала от диэлектрической проницаемости слоев. Предположено, что спин-орбитальное взаимодействие электронов в квантовой точке аналогично взаимодействию кварков в нерелятивистской потенциальной модели адронов. В таком предположении определено спин-орбитальное взаимодействие электронов в квантовой точке. Изучена зависимость константы связи спин-орбитального взаимодействия от заряда изображения и эффективного размера квантовой точки.