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Two-electron states and state exchange time control in parabolic quantum dot

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HIGHLIGHTS

- Two-electron states in a spherically symmetric parabolic QD were considered.
- Using uncertainty relations the ground-state energy estimation was made.
- The dependence of ground-state energy on the QD size was studied.
- The state exchange time dependence on the QD size were obtained.

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ABSTRACT

Using the Heisenberg uncertainty relationship and the stationary perturbation theory we consider two-electron states in a spherically symmetric parabolic quantum dot (parabolic helium atom). The dependence of ground-state energy on the QD size is studied. The energy of two-electron system monotonically decreases with QD radius increase. The problem of the state exchange time control in QD is discussed, taking into account the spins of the electrons in the Russell–Saunders approximation. With the increase of the QD radius the state exchange time increases.

1. Introduction

Quantum dots QD or "artificial atoms" [1] have become the subject of researches during the last two decades. The problem of theoretical study of two-electron states in 0-dimensional structures or quantum dots, quantum layers and rings has not only a purely academic but also an applied meaning. The manipulation of the energetic states can be used to create semiconductor nanoelectronic devices of the new generation as well as on researches of fundamental quantum mechanical principles [2–10]. From the theoretical point of view, the problem of the two electrons located in the quantum dots is identical to the problem of the helium atom; however the localization of the electrons here is not due to attracting by Coulomb field of the nucleus, but due to the repulsive confinement potential. The circumstance which significantly distinguishes artificial atoms from real ones is the energy levels manipulation by changing geometrical size and form of the QD.

One of the first articles, devoted to the two-electron states in quantum dots, was the work [11], where the authors viewed the discrete levels of the energy of two electrons depending on QD size and the magnetic field being perpendicularly to the plane of the QD. The two-electron states in QD in magmatic field were considered in the work [12]. Correlation energy of the interaction of the two electrons in the quantum dots was considered in the work [13] using the semiclassical approximation. The authors investigated the energy spectra and wave functions of the two-electron states in the quantum dots using the power series expansion [14]. Applying $1/N$ expansion method, the authors obtained a range of results [15]. The application of various approximate methods in two-electron QD with parabolic confinement potential has been viewed in the work [16]. Basing on Hartree–Fock and Kohn–Sham $1/N$ methods and also numerical solution of the Schrodinger equation, the energy eigenvalues of the two-electron system were obtained. A comparison between the results, based on the indicated methods, has been made. The authors also suggested interpolating formulas for the energy

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eigenvalues. In Ref. [17] a research of the influence of the magnetic field on the spectrum of electrons in QD was carried out. Using the exact numerical schemes of diagonalization, the authors of the work [18] obtained the energy spectrum of two-electrons QD with parabolic confinement potential in the presence of Coulomb impurity, localized in the center of a quantum dot with and without homogeneous magnetic field. The low energy levels of the two-electron quantum dots in the presence of the external homogeneous magnetic field have been calculated by the authors of the work [19], using the variational method based on the construction of trial wave functions. Note that the interest in QD with parabolic confinement potential sharply increased after it has been shown that in quantum systems the generalized Khon theorem may be performed [20]. The effect of symmetry in small-size quantum dots of in the presence of the magnetic field was studied in Ref. [21]. In the work [22], the authors investigated the structural transitions (the symmetry breaking) in the two-electron QD under the influence of the perpendicular magnetic field. The effects, related with the impact of the environment on the two-electron quantum dots, were studied in the work [23].

The characteristic particularity of the two-electron systems is the exchange interaction between the electrons, which is responsible for the exchange between the states in a quantum system [24]. That is a purely quantum effect. It can be shown that two electrons can exchange the states in time, and the exchange time is determined by the exchange integral [25]. In this regard, it is interesting to study the effect of the state exchange in parabolic QD, which contains two electrons. In this paper, the parabolic helium atom is investigated in the framework of the stationary perturbation theory using its analogy with the helium atom. We also estimate the ground-state energy value, using the Heisenberg uncertainty relationship.

In quantum dots with a spherically symmetric parabolic confinement potential $V_{conf}(r)=(\mu\omega^2 r^2)/2$, the value of ω can be estimated using the quantum virial theorem and the Heisenberg uncertainty relation [9]:

$$\omega \sim \frac{\hbar}{\mu R^2}. \tag{1}$$

The Hamiltonian of the system is

$$\hat{H} = \sum_{i=1}^{2} \hat{H}_i + V(\vec{r}_1, \vec{r}_2), \tag{2}$$

where $\hat{H}_i = -\frac{\hbar^2}{2\mu}\vec{\nabla}_i^2 + V_{conf}(r_i)$ is the single-electron Hamiltonian in parabolic QD, and

$V(\vec{r}_1, \vec{r}_2) = \frac{e^2}{\varepsilon\left|\vec{r}_2 - \vec{r}_1\right|}$ is the energy of interaction between the electrons.

2. The estimation of the parabolic helium atom ground state energy by the uncertainty relationship method

The energy value of the system is

$$E(\vec{r}_1, \vec{r}_2) = \frac{p_1^2}{2\mu} + \frac{p_2^2}{2\mu} + \frac{\mu\omega^2 r_1^2}{2} + \frac{\mu\omega^2 r_2^2}{2} + \frac{e^2}{\varepsilon\left|\vec{r}_2 - \vec{r}_1\right|}. \tag{3}$$

Note that the permutation of the particles does not change the energy. So, minimization conditions by $r_1$and r_2: $\partial E/\partial r_1=0$ and $\partial E/\partial r_2=0$ give the same value r_{min}. Let us assume that the electrons are located diametrically. Suppose that $p_1=p_2=p$ and $r_1=r_2=r$. Then for the energy estimation we can use the Heisenberg uncertainty principle for position and momentum:

$$E(r) \sim \frac{\hbar^2}{\mu r^2} + \mu\omega^2 r^2 + \frac{e^2}{2\varepsilon r}. \tag{4}$$

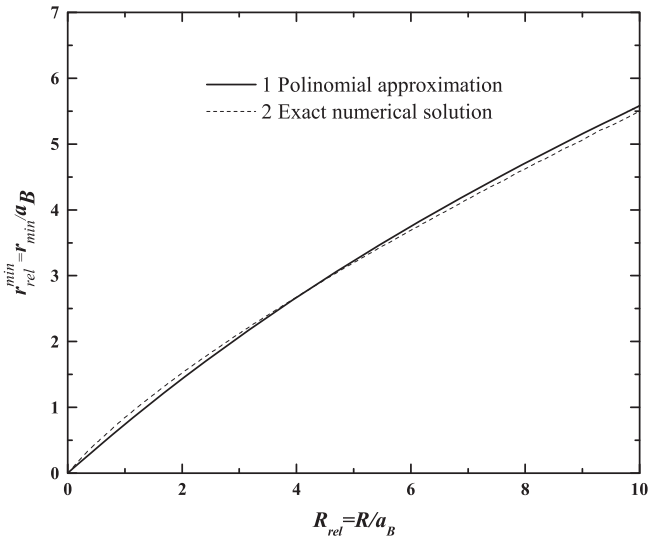

Fig. 1. The dependence of the ground state radius on QD radius. 1 – Polynomial approximation and 2 – exact numerical solution.

Writing down the condition for minimization the energy of the system

$$\frac{dE(r)}{dr} = 0, \tag{5}$$

we come to the equation

$$\mu\omega^2 r^4 - \frac{e^2}{4\varepsilon} r - \frac{\hbar^2}{\mu} = 0. \tag{6}$$

Multiplying Eq. (4) by $\mu/\hbar^2$, taking into account Eq. (5) and making the following designations:

$$r_{rel} = \frac{r}{a_B}; \quad R_{rel} = \frac{R}{a_B}, \tag{7}$$

where $a_B=(\hbar^2\varepsilon)/(\mu e^2)$,
we obtain

$$\frac{r_{rel}^4}{R_{rel}^4} - r_{rel} - 1 = 0. \tag{8}$$

The numerical solution of Eq. (8) leads to the following dependence $r_{rel}(R_{rel})$ (Fig. 1).

Fig. 1 shows the dependence r_{rel} of the QD radius. Here are numerical solutions of Eq. (8). The curve 1 is polynomial approximation of the exact numerical solution (curve 2). As seen from Fig.1 with the increase of the QD radius r_{rel} value increases. This was expected because with the increase of the QD radius the distance between the colliding electrons increases and the characteristic radius of ground state increases.

On the base of this result we can calculate the energy dependence on R_{rel} by substituting $r_{rel}(R_{rel})$ in Eq. (4). Finally, we obtain:

$$E_{min} = \frac{\hbar^2}{\mu a_B^2}\left(\frac{1}{r_{rel}^2} + \frac{r_{rel}^2}{R_{rel}^4}\right) + \frac{e^2}{2a_B}\frac{1}{r_{rel}}. \tag{9}$$

The quantities $\hbar^2/\mu a_B^2$ and $e^2/2a_B$ have the dimension of energy, and equal, respectively, $2R^*$and R^*,where $R^*=\hbar^2/2\mu a_B^2$ is the effective Rydberg energy. We obtain to the following dependence (Fig. 2). Fig. 2 shows that the energy of our system, calculated using the uncertainty relationship method, monotonically decreases with QD radius increase, because the interaction between the electrons increases and also the size quantization becomes weaker. As the result the curve of the $E(R_{rel})$ monotonically decreases.