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Two-electron impurity in the parabolic quantum dot: Uncertainty relation and perturbation approach

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ABSTRACT

Two-electron impurity states in parabolic confinement have been investigated. We have estimated the ground-state energy value, using the Heisenberg uncertainty relation. Using variational methods the ground state energy and wave function of the single-electron impurity problem have been achieved. The dependence of ground-state energy and Coulomb electron–electron interaction energy correction on the QD size is studied. The dependence of the state exchange time on the QD radius has been calculated. It has been shown that the presence of the impurity leads to the appearance of negative values of the energy of the system on the one hand, and to the saturating character of the state exchange time.

1. Introduction

There has been growing interest in the electronic structure and optical properties of the semiconductor quantum dots (QDs) in recent years [1–4] because of the rapid development of fabrication technology. Quantum dots, QDs, or “artificial atoms” [1] have become the subject of researches during the last two decades. These systems are thought to have vast potential for future technological applications, such as possible applications in memory chips [5], as qubits in quantum computation [6–11], quantum cryptography [12], in room-temperature quantum-dot lasers [13], photovoltaic elements based on quantum dots [14,15] and so on.

The problem of theoretical study of two-electron and impurity states in 0-dimensional structures or quantum dots, quantum layers and rings has not only a purely academic but also an applied meaning [16–23]. The manipulation of the energetic states can be used to create semiconductor nanoelectronic devices of the new generation as well as on research of fundamental quantum mechanical principles. Note that there is an interesting relationship between the problem of two-electron states in a parabolic QD and the Thomson helium atom problem. If one considers quantum Thomson model [24] it is possible to show that this problem is similar to the problem of two-electron states in a spherical QD with a parabolic confining potential.

The presence of the impurity centers in QDs can significantly affect their physical characteristics. Therefore, it is of great interest to investigate the nature of the impurity states in QDs, taking into account the limitation of motion of the electron. One of the first problem which has been solved in this field was the problem of the behavior of the hydrogenic donor impurity in a spherical QD with a rectangular confining potential. It was assumed that the impurity is located in the center of the QD [25]. The authors showed that the total energy of the system depending on the radius of the QD can be greater than zero and less as well. This is a direct result of competition between the size quantization and Coulomb quantization of the impurity.

The study of hydrogenic impurity states in semiconductor nanostructures has been initiated in recent years through the pioneering work of Bastard [26]. A number of theoretical investigations of hydrogenic impurity states in low dimensional semiconductors have been published [27,28]. In the paper [22] the binding energy of hydrogenic impurity states in spherical QD has been studied using the variational method. Later, the same author calculated the binding energies of the hydrogenic impurity states in spherical QDs with parabolic confinement by using the perturbation method [29]. Different effects in the two-electron systems are discussed in following Refs. [30–35]. Particularly, the impurity effect in a two-electron quantum dot with parabolic confinement in the framework of diagonalization method has been discussed in [36]. Also, the impurity effects on auto-ionizing two-electron resonances in spherical QD have been studied in [37]. The ground state energies of the hydrogen-like impurity in a

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lens-shaped QD have been calculated using the variational method in [38]. The two-electron bunching in transport through a QD associated with Kondo correlations has been investigated [39]. Entanglement effects of impurity states in the two-electron QD and coupled QD have been studied [40,41].

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. 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 [33]. In this regard, it is interesting to study the effect of the state exchange in parabolic QD which contains an impurity with two electrons.

The current paper where we have discussed two-electron states in parabolic QD is a continuation of the paper [33]. Currently, we are discussing the system with the donor impurity in the center of QD. As it will be shown the presence of the donor impurity can lead to two new effects: the total energy of the two-electron system will decrease monotonically reducing from the positive region to the negative through zero depending on the QD radius, and there is a saturating character of the behavior of the state exchange time with the increase of QD radius.

2. The estimation of the ground state energy using the uncertainty relation method

In quantum dots with a spherically symmetric parabolic confinement potential $V_{conf}\left(r\right) = \mu\omega^2 r^2/2$, the value of ω can be estimated using the quantum virial theorem and the Heisenberg uncertainty relation [31]:

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

where R is the QD's radius. The Hamiltonian of the system (Fig. 1) is

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

where $\hat{H}_i = -\hbar^2/2\mu\vec{\nabla}^2 + \mu\omega^2 r^2/2 - \mathrm{Ze}^2/\varepsilon r$ is the single-electron Hamiltonian in parabolic QD with the impurity in the center, where μ – effective mass, Ze – charge of the impurity, ε – dielectric

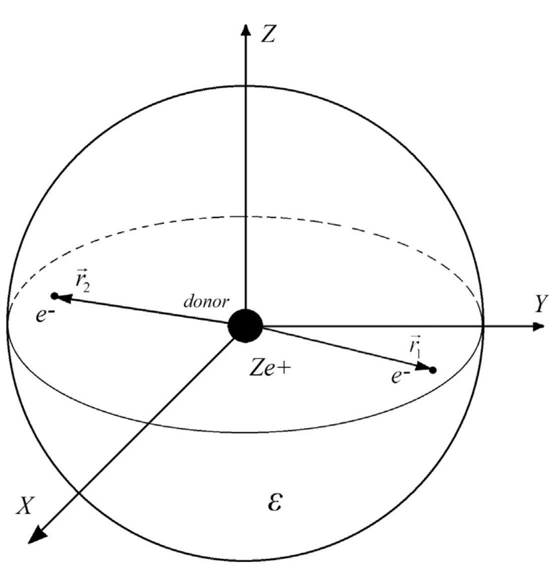

Fig. 1. Schematic diagram of the considered system.

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

The energy value of the system can be written as

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

Notice that the permutation of the particles does not change the energy. So, minimization conditions by r_1 and r_2: $\partial E/\partial r_1 = 0$, $\partial E/\partial r_2 = 0$ give the same value $r_{\min}$. Let us assume that the electrons are located diametrically [33], and $p_1 = p_2 = p$, $r_1 = r_2 = r$. Then we can use the Heisenberg uncertainty principle for position and momentum for the energy estimation:

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

Minimization condition of the energy of the system has the form:

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

Introducing dimensionless quantities $r_{rel} = r/a_B^*$; $R_{rel} = R/a_B^*$, where $a_B^* = \hbar^2\varepsilon/\mu e^2$ is the effective Bohr radius, we come to the equation

$$\frac{r_{rel}^4}{R_{rel}^4} + (Z - \frac{1}{4})r_{rel} - 1 = 0. \tag{6}$$

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

$$E_{min} = \frac{\hbar^2}{\mu a_B^{*2}}(\frac{1}{r_{rel}^2} + \frac{r_{rel}^2}{R_{rel}^4}) - \frac{e^2}{a_B^*}(Z - \frac{1}{4})\frac{1}{r_{rel}}. \tag{7}$$

The quantities $\hbar^2/\mu a_B^{*2}$ and $e^2/2a_B^*$ have the dimension of energy and equal to respectively $2Ry$ and Ry where $Ry = \hbar^2/2\mu a_B^{*2}$ is the effective Rydberg energy. We obtain the following dependence (Fig. 2).

Fig. 2 shows that the energy of our system, calculated using the uncertainty relation method, monotonically decreases reducing from the positive region to the negative through zero, with QD radius increase. With the decrease of QD radius, the positive repulsion energy of confinement becomes larger than the negative attraction Coulomb energy of the impurity. Due to this fact total energy of the system becomes positive. With the increase of QD radius, energy of size quantization decreases and total energy of

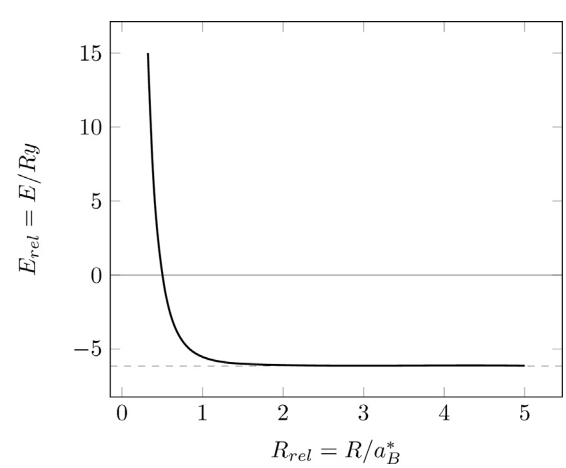

Fig. 2. The dependence of the ground state energy (Rydberg energy units) on the QD radius (with Z=2).