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## Electronic structure and relativistic terms of one-electron spherical quantum dot

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### ABSTRACT

We calculated the energy eigenvalues and eigenfunctions of the ground and excited states of a hydrogenic impurity located at the center of a spherical quantum dot using the Quantum Genetic Algorithm (QGA) and Hartree–Fock Roothaan (HFR) method. In addition, we carried out the relativistic effects such as the relativistic correction to the kinetic energy, spin–orbit and Darwin terms by using the perturbation method. The electronic charge density for the Darwin term is computed from the Hiller, Sucher and Feinberg formulation instead of the traditional delta function operator. The results show that impurity, dot radius and confining potential have a great influence on the relativistic effects. In addition, as the absolute value of confining potential increases, the peak values of relativistic corrections increase and move toward lower dot radii.

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### 1. Introduction

Theoretical study related to relativistic terms on low-dimensional structures is a relatively new field of research. An excellent match between theory and experiment requires rather precise estimates of the calculation of relativistic effects to the ground and excited energy states of semiconductor nanostructures. Therefore, the relativistic effects which are sometimes called subtle effects are important for many properties of nanostructures. Quantum Dots (QDs) whose charge carriers (electrons and holes) are confined in three-dimensions are often referred to as artificial atoms because their electronic states are quantized and their shell structures are similar to those of atoms [1]. Thanks to modern technology, it has now become possible to produce QDs by using various techniques such as etching or molecular epitaxy etc. [2]. QDs are widely used to model a variety of problems in physics and chemistry [1,3]. Due to their small size, these structures display an interesting behavior and play an important role in microelectronic and optoelectronic devices. Therefore, a number of authors have devoted themselves to study the electronic structure of QDs [4–14].

It should be noted that the role of the electron spin and the corresponding effects significantly change the physical properties of the semiconductor nanostructures, especially in QDs [15]. Thus,

calculating of the spin-related effects is attractive and important not only from the fundamental scientific point of view, but also because of their effects on the electronic and other properties of QD [16,17]. Recently, some authors have studied the spin effects in low-dimensional structures [16–27]. Gharati and Khordad [18] calculated the effects of magnetic field and spin orbit interaction on energy levels of quasi-one dimensional quantum wire. They also carried out the Lande-g factor in quantum wire under an applied magnetic field and the Rashba effect. Glazov and Kulakovskii [21] studied theoretically the spin–orbit effects in disk-shaped QDs. Hassanabadi et al. [22] performed a detailed investigation of the nonlinear optical properties of a QD in the presence of the Rashba spin–orbit interaction. In single InAs/GaAs QDs grown by metal–organic chemical vapor deposition, a systematic change of the exciton fine structure splitting with quantum dot size was observed experimentally by Seguin et al. [25]. Yang et al. [26] studied theoretically the relativistic effects such as the relativistic correction to the kinetic energy, spin–orbit interaction and Darwin term for a hydrogenic impurity located at the center of a spherical QD by using a simpler exact solution for the finite potential well. Huang et al. [27] calculated the relativistic effects as a function of atomic number  $Z$  for a hydrogen like ions located at the center of a spherical cavity by using the B-spline method. Up to now, there are a few theoretical studies on the relativistic effects in QDs. The impurity effects associated with the spin–orbit interaction and Darwin term were not considered theoretically in the above mentioned works. In addition, in calculation of Darwin term, the contribution coming from  $\ell \neq 0$  states was not taken into account in several studies related to the

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nanostructures. A detailed theoretical study on the relativistic effects is still lacking in QDs. Therefore, studies in this field are still important for both theoretical research and practical applications.

In our previous study [28], we calculated the energies of the ground and excited states and the wavefunctions of a spherical QD with infinite confining potential well and also carried out the relativistic terms. In the present study, we have extended our previous study to a spherical QD with finite confining potential well. We also investigated the relativistic terms such as the relativistic correction to the kinetic energy, which is sometimes called the mass-velocity term, the spin-orbit interaction and Darwin terms. The Darwin term has been calculated from a global operator defined by Hiller, Sucher and Feinberg as opposed to the local delta function operator.

## 2. Theory and definitions

The nonrelativistic Hamiltonian of a hydrogenic impurity located at the center of a spherical cavity can be written as follows:

$$H_0 = -\frac{\hbar^2 \nabla^2}{2m} - \frac{k e^2}{\epsilon r} + V_C(r), \quad (1)$$

where  $k$ ,  $m$  and  $\epsilon$  are electric constant, the mass of free electron and dielectric constant of medium, respectively. The term  $V_C(r)$  is the spherical confining potential:  $V_C(r) = V_0$  for  $r < R$  and  $V_C(r) = 0$  for  $r \geq R$ .

The energy eigenvalues of the nonrelativistic Hamiltonian may be further improved by including the relativistic effects such as the mass-velocity, spin-orbit interaction and Darwin term. These effects can be calculated perturbatively because they are relatively small when they are compared with the magnitude of unperturbed Hamiltonian, but they may be important.

In relativistic calculations, the Hamiltonian can be written as

$$H = H_0 + H', \quad (2)$$

where  $H_0$  is the unperturbed Hamiltonian,  $H'$  is the relativistic perturbation Hamiltonian and it is given by

$$H' = H_K + H_{SO} + H_D \quad (3)$$

The relativistic terms have been defined in the literature in a number of different ways. The first term  $H_K$  on the right of Eq. (3) is the relativistic correction to the classical kinetic energy because it rises from the relativistic variation of mass with velocity, and it is given as follows [26]:

$$H_K = \frac{-p^4}{8m^3 c^2}, \quad (4)$$

in which  $c$  is the speed of light in vacuum and  $P$  is linear momentum operator of electron.

The second term  $H_{SO}$  in Eq. (3) is the spin-orbit interaction due to the fact that the moving electron's spin changes the energy levels. The electron spin makes it act like a little electromagnet. As known from classical electrodynamics, a moving magnet interacts with the electric field of the nucleus and it changes the energy levels. The understanding and control of fine structure splitting in QDs is a relevant issue for quantum information applications [23,29]. The spin-orbit Hamiltonian is given by [26]

$$H_{SO} = \left( \frac{kZe^2}{\epsilon} \right) \frac{1}{2m^2 c^2 r^3} \mathbf{S} \cdot \mathbf{L} \quad (5)$$

where  $\mathbf{L}$  and  $\mathbf{S}$  are the operators of orbital and spin angular momentum of electron. Since the unperturbed state function,  $\phi$ , is also an eigenfunction of  $L^2$ ,  $S^2$  and  $J^2$ , we have

$\mathbf{S} \cdot \mathbf{L} |\phi\rangle = 1/2[j(j+1) - l(l+1) - 3/4]\hbar^2 |\phi\rangle$ , where  $j$  is the total angular momentum quantum number of electron.

The last term  $H_D$  in right of Eq. (3) is Darwin term. It may be thought of arising from a relativistically induced electric moment of the electron, and this term is given by [26]

$$H_D = \left( \frac{kZe^2}{\epsilon} \right) \frac{\pi \hbar^2}{2m^2 c^2} \delta(\vec{r}), \quad (6)$$

where the term  $\delta(\vec{r})$  is the delta function operator.

The electronic charge density,  $\rho$ , is usually evaluated from an expectation value of the traditional delta function operator,  $\delta(\vec{r})$ , at the origin of the coordinate system,  $\rho^\delta(0) = \langle \phi | \delta(\vec{r}) | \phi \rangle$ . The expectation value of a delta function operator has non zero only for  $s$  type orbitals, and so the expectation value of the delta function operator vanishes for the states with  $\ell \neq 0$ . In calculations made with the delta function, even if the appropriate wavefunctions are selected, these calculations may have significant errors at origin. Hiller, Sucher and Feinberg (HSF) have shown that the delta function operator,  $\rho^\delta$ , can be replaced by a global operator,  $\rho^{HSF}$ , and they have obtained the electronic charge density at origin from the global operator for a multi-electron system as follows [30]:

$$\rho^{HSF}(0) = \begin{cases} \frac{1}{2\pi} \langle \phi | \sum_i \frac{\partial V}{\partial r_i} - \frac{L_i^2}{r_i^3} | \phi \rangle, & \text{for a state with } \ell \neq 0 \\ \frac{1}{2\pi} \langle \phi | \sum_i \frac{\partial V}{\partial r_i} | \phi \rangle, & \text{for a state with } \ell = 0. \end{cases} \quad (7)$$

here, the term  $V$  indicates the total potential energy operator (impurity attraction plus confining potential) in Eq. (1) and  $L_i^2$  is the angular momentum operator for the  $i$ th electron. The HSF formulation has been tested in several electronic charge and spin density studies for atomic systems and the expectation values of  $\rho^{HSF}(0)$  showed smaller errors by an order of magnitude or more than those from the traditional delta function calculation of  $\rho^\delta(0)$  [31]. For the nonrelativistic Hamiltonian, the eigenvalue equation is given by

$$H_0 \phi_{n\ell m_\ell} = E_{n\ell} \phi_{n\ell m_\ell} \quad (8)$$

in which  $n$ ,  $\ell$ ,  $m_\ell$  are quantum numbers of one-electron wavefunction  $\phi$ . In the HFR approach [32,33], the wave function is normalized and it can be written as linear combination of basis sets [32],  $\chi_k$ ,

$$\begin{aligned} \phi_i &= \Theta(R-r) \phi_i^{r < R} + \{1 - \Theta(R-r)\} \phi_i^{r > R} \\ &= \Theta(R-r) \sum_{k=1}^{v^{r < R}} c_{ik}^{r < R} \chi_k(\zeta_{ik}^{r < R}, \vec{r}) + \{1 - \Theta(R-r)\} \sum_{k=1}^{v^{r > R}} c_{ik}^{r > R} \chi_k(\zeta_{ik}^{r > R}, \vec{r}), \end{aligned} \quad (9)$$

where  $i$  denotes the quantum numbers of atomic orbitals,  $\Theta(x)$  is the Heviside step function,  $v^{r < R}$  ( $v^{r > R}$ ) is the size of the basis set used for the inner (outer) part of the wave function,  $c_{ik}^{r < R}$  ( $c_{ik}^{r > R}$ ) is the expansion coefficients and  $\zeta_{ik}^{r < R}$  ( $\zeta_{ik}^{r > R}$ ) is the screening parameters for  $k$ th basis function which is Slater Type Orbital (STO) [34].

In order to calculate spin-orbit term, the coupled wavefunction  $\phi_{n\ell j m_j}$  is constructed from linear combination of the spin wavefunction,  $\phi_{n\ell m_\ell m_s}$ , as follows:

$$\phi_{n\ell j m_j} = \sum_{m_\ell m_s} \langle \ell s m_\ell m_s | j m_j \rangle \phi_{n\ell m_\ell m_s}, \quad (10)$$

where  $j$  is the total angular momentum quantum number,  $\langle \ell s m_\ell m_s | j m_j \rangle$  is Clebsch-Gordon coefficient and  $\phi_{n\ell m_\ell m_s}$  is the zero-order wavefunction of nonrelativistic state, and it is given  $\phi_{n\ell m_\ell m_s} = \phi_{n\ell m_\ell} \sigma_{m_s}$ , where  $\sigma_{m_s}$  is spin function.

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