Spin Dependent Boundary Conditions and Spin Splitting in Cylindrical Quantum Dots

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ABSTRACT

To study a spin dependence of the electron energy states in tree dimensional cylindrical semiconductor dots we consider theoretically the spin-orbit interaction impact on the electron quantum confinement in the dots. We solve the problem for InAs quantum dot embedded into GaAs matrix with the effective one electronic band Hamiltonian, the energy and position dependent electron effective mass approximation, and the spin-dependent Ben Daniel-Duke boundary conditions. It has been found that the spin-dependent boundary conditions lead to a spin-splitting of the electron energy states with non zero angular momentum. The splitting is strongly dependent on the dot size and can gain an experimentally measurable value for relatively small quantum dots.

Keywords : Quantum dots, Spin-orbit interaction, Balanced QR algorithm, Inverse iteration method.

1 INTRODUCTION

The study of semiconductor quantum dots (QD) in recent years has been of a great interest from experimental and theoretical points of view (see [1] and references therein). The semiconductor quantum dots are very attractive for possible applications in micro and nano optoelectronics [2], [3]. Thus, the electron energy level hierarchy in QDs is an object of extensive investigations. The electron spin plays an important role in the design of the dot electron energy levels and can significantly alter the properties of the electron energy states. A new branch of semiconductor electronics (so called spintronics) has produced much interest in the spin-dependent energy structure of semiconductor quantum dots [4], [5]. A study of the spin-dependent energy structure can be an essential part of semiconductor spintronics development.

While it has been found that the spin-orbit interaction can impact essentially the energy state systems and electronic properties of III-V semiconductor quantum structures [6]–[9], the spin-orbit interaction effect in quantum dots is largely unknown. In this work we consider theoretically the spin-orbit interaction impact on the electron quantum confinement in cylindrical semiconductor dots. We solve the problem with the effective one electronic band Hamiltonian, the energy and position dependent electron effective mass approximation and the spin-dependent Ben Daniel-Duke boundary conditions [6]. The spin-dependent boundary conditions come from a difference between the spin-orbit interaction parameters in the dot and the semiconductor matrix. The quantum dot has a quantum disk shape of radius R_0 and of thickness z_0 and we treat the problem in cylindrical coordinates (R, ϕ, z). Most of calculations of the electron spectrum in semiconductor quantum dots are done within one-dimensional approximations and the confinement potential in R-direction often approximated by a parabolic potential and in z-direction is taken to be the infinite out the dot. In contrast to those works we use a realistic hard-wall (of finite height) three-dimensional confinement potential that is induced by real discontinuity of the conduction band at the edge of the dot. To solve three-dimensional Schrödinger equation we use the balanced QR method [10] and inverse iteration algorithm [11]. Our results show that the spin-orbit interaction can significantly modify the electron energy spectrum of InAs semiconductor QDs.

2 SPIN-DEPENDENT BOUNDARY CONDITIONS

We will consider electrons confined in three dimensional quantum structures and use the approximate one band effective Hamiltonian [6]

$$\hat{H} = \hat{H}_0 + \hat{V}_{so}(\mathbf{r}) \tag{1}$$

In equation (1): H_0 is the system Hamiltonian without spin-orbit interaction

$$\hat{H}_0 = -\frac{\hbar^2}{2}\nabla_{\mathbf{r}}\left(\frac{1}{m(E,\mathbf{r})}\right)\nabla_{\mathbf{r}} + V(\mathbf{r}),$$

$\nabla_{\mathbf{r}}$ stands for the spatial gradient, $m(E,\mathbf{r})$ is the energy and position dependent electron effective mass

$$\frac{1}{m(E,\mathbf{r})} = \frac{P^2}{\hbar^2}\left[\frac{2}{E + E_g(\mathbf{r}) - V(\mathbf{r})}\right.$$

$$\left. + \frac{1}{E + E_g(\mathbf{r}) + \Delta(\mathbf{r}) - V(\mathbf{r})}\right],$$

$V(\mathbf{r})$ is the confinement potential, $Eg(\mathbf{r})$ and $\Delta(\mathbf{r})$ stand for the position dependent band gap and the spin-orbit splitting in the valence band, and P is the momentum matrix element. The spin-orbit interaction for the conducting band electrons $V_{so}(\mathbf{r})$ is described by [12]

$$\hat{V}_{so}(\mathbf{r}) = i\nabla\beta(E,\mathbf{r})\cdot[\widehat{\boldsymbol{\sigma}}\times\nabla], \tag{2}$$

where

$$\beta(E,\mathbf{r}) = \frac{P^2}{2}\left[\frac{1}{E+E_g(\mathbf{r})-V(\mathbf{r})} - \frac{1}{E+E_g(\mathbf{r})+\Delta(\mathbf{r})-V(\mathbf{r})}\right],$$

is the spin-orbit coupling parameter, and $\widehat{\boldsymbol{\sigma}}=\{\boldsymbol{\sigma}_\mathbf{x},\boldsymbol{\sigma}_\mathbf{y},\boldsymbol{\sigma}_\mathbf{z}\}$ is the vector of the Pauli matrices.

For systems with the sharp discontinuity of the conduction band edges between the QD (material 1) and the semiconductor matrix (material 2) the hard-wall confinement potential can be presented as

$$V(\mathbf{r}) = \begin{cases} 0, & \mathbf{r}\in 1 \\ V_0, & \mathbf{r}\in 2 \end{cases}.$$

From integration of the Schrödinger equation with Hamiltonian (1) along the direction perpendicular to the interface ($\mathbf{r}_n$) we obtain the spin dependent Ben Daniel-Duke boundary conditions for the electron wave function $\Psi(\mathbf{r})$

$$\Psi_1(\mathbf{r}_s) = \Psi_1(\mathbf{r}_s);$$

$$\left\{\frac{\hbar^2}{2m(E,\mathbf{r}_s)}\nabla - i\beta(E,\mathbf{r}_s)\left[\widehat{\boldsymbol{\sigma}}\times\nabla\right]\right\}_n \Psi(\mathbf{r}_s) = const., \tag{3}$$

where $\mathbf{r}_s$ denotes the position of the system interface. The boundary conditions above are obviously dependent on the electron spin and originates from the difference of the spin-orbit interaction parameters in different materials.

When the quantum dot has a disk shape of radius R_0 and of thickness z_0 we can solve the problem with cylindrical coordinates (R,ϕ,z). The origin of the system lies in the center of the disk and the z-axis is chosen along the rotation axis. Because of the cylindrical symmetry the wave function can be represented as

$$\Psi(r) = \Phi(R,z)\exp(il\phi),$$

where $l = 0, \pm1, \pm2, ...$ is the electron orbital quantum number and the problem remains two dimensional in (R, z) coordinates

$$-\frac{\hbar^2}{2m_1(E)}\left(\frac{\partial^2}{\partial R^2} + \frac{\partial}{R\partial R} + \frac{\partial^2}{\partial z^2} - \frac{l^2}{R^2}\right)\Phi_1(R,z) = E\Phi_1(R,z),\ R\le R_0,\ |z|\le\frac{z_0}{2}$$

$$-\frac{\hbar^2}{2m_2(E)}\left(\frac{\partial^2}{\partial R^2} + \frac{\partial}{R\partial R} + \frac{\partial^2}{\partial z^2} - \frac{l^2}{R^2} + V_0\right)\Phi_2(R,z) = E\Phi_2(R,z),\ R> R_0,\ |z|>\frac{z_0}{2} \tag{4}$$

and the spin dependent boundary conditions (3) (for reasons of the problem symmetry along z-axis) become of the form

$$\Phi_1(R_0,z) = \Phi_2(R_0,z),\ |z|\le\frac{z_0}{2};$$

$$\Phi_1(R,\pm\frac{z_0}{2}) = \Phi_2(R,\pm\frac{z_0}{2}),\ R\le R_0;$$

$$\frac{1}{m_1}\frac{\partial\Phi_1(R,z)}{\partial R}\bigg|_{R_0} - \frac{1}{m_2}\frac{\partial\Phi_2(R,z)}{\partial R}\bigg|_{R_0} + \frac{2\boldsymbol{\sigma}(\beta_1-\beta_2)}{\hbar^2}\frac{l}{R_0}\Phi_1(R_0,z) = 0,\ |z|\le\frac{z_0}{2};$$

$$\frac{1}{m_1}\frac{\partial\Phi_1(R,z)}{\partial z}\bigg|_{\pm\frac{z_0}{2}} - \frac{1}{m_2}\frac{\partial\Phi_2(R,z)}{\partial z}\bigg|_{\pm\frac{z_0}{2}} = 0,\ R\le R_0, \tag{5}$$

where σ refers to the electron spin polarization along z-axis.

The electron energy states are complicated functions of the dot parameters, the electron angular momentum, and spin. We can obtain the solution only by means of a numerical solving of the Schrödinger equation (4) and the boundary conditions (5).

3 NUMERICAL METHODS

There are many numerical methods have been developed for a numerical solution of the one-dimensional Schrödinger equation and applications in atomic physics, nuclear physics, and semiconductor microstructures (see [13] and references therein). In this work, the energy states and wave functions of the confined electrons are found by the finite difference, balanced QR, and inverse iteration methods. Due to the energy dependence of the effective electron mass and spin-orbit coupling parameters our calculation should consists of iteration loops to reach a "self-consistent" energy solution. A feedback nonlinear iteration scheme is presented here to find the "self-consistent" numerical solution: (i) Set energy $E = 0$. (ii) Compute effective mass m and electron spin-orbit coupling parameter β. (iii) Solve Schrödinger equation for energy E. (iv) Back to (ii). The iteration is terminated when a specified stopping criterion on energy is reached. To obtain a complete numerical solution of the three-dimensional Schrödinger equation in (iii), a finite difference method with nonuniform mesh technique is firstly applied to discretize the Schrödinger equation (4). The discretized Schrödinger equation with spin dependent boundary conditions (5) leads to an eigenvalue problem

$$A\mathbf{X} = \lambda\mathbf{X}, \tag{6}$$

where A is the matrix rising from discretized Schrödinger equation and boundary conditions, $\mathbf{X}$ and λ are the corresponding eigenvectors (wave functions) and the eigenvalues (energy levels) of the matrix A. To motivate our consideration of the system (6) we consider the Schrödinger equation (4) in a rectangular domain $\mathbf{\Omega}= (0, R_T) \times (0, z_T)$, where R_T and z_T are the artificial boundaries. The artificial boundary conditions are applied far enough so that it does not significantly affect the results. Let $h = R_T/M$, $k = z_T/N$ and let $R_i = ih$, $z_j = jk$, where M and N are the total number of intervals along the R and z directions, respectively. Consider the set of points (R_i, z_j) in $\mathbf{\Omega}$, we define $x_{i,j} = \Phi(R_i, z_j)$, then the standard central difference approximation for the differential, spin dependent boundary conditions in (4) and (5), and artificial boundary conditions leads to a finite-difference system in the form

$$\frac{1}{hk}(a_{i,j}x_{i,j} - (b_{i,j}x_{i-1,j} + c_{i,j}x_{i+1,j}) \\ -(d_{i,j}x_{i1,j-1} + e_{i,j}x_{i,j+1})) = \lambda x_{i,j}. \qquad (7)$$

In the above system the coefficients $a_{i,j}$, $b_{i,j}$, $c_{i,j}$, $d_{i,j}$, and $e_{i,j}$ are associated with the differential operator, coefficient functions, and boundary coefficients. The λ to be determined is the corresponding eigenvalues of the system (7). Typical choice of these coefficients for all points (R_i, z_j) can be found, such as in [14]. The system (7) may be cast in the form of a matrix equation as shown in equation (6). The matrix A in (6) is a block tridiagonal matrix with diagonal submatrices $\widetilde{A}_0, \ldots, \widetilde{A}_N$, and off-diagonal submatrices $-\widetilde{D}_1, \ldots, -\widetilde{D}_N$ and $-\widetilde{E}_1, \ldots, -\widetilde{E}_N$, respectively, and $\mathbf{X} = (X_1, \ldots, X_N)^T$. The submatrices $\widetilde{A}_j$ is given

$$\widetilde{A}_j = \begin{bmatrix} a_{0j} & -c_{0j} & & & 0 \\ -b_{ij} & a_{1j} & & -c_{1j} & \\ & \ddots & \ddots & & \ddots \\ & -b_{M-1,j} & & a_{M-1,j} & -c_{m-1,j} \\ 0 & & & -b_{Mj} & a_{Mj} \end{bmatrix}$$

and $\widetilde{D}_j = diag(d_{0j}, \ldots, d_{Mj})$, $\widetilde{E}_j = diag(e_{0j}, \ldots, e_{Mj})$, where $j = 0, 1, \ldots, N$.

A number of numerical linear algebra methods, such as QR and Davison methods [10], [15]–[17] have been proposed to solve a class of nonsymmetric matrix. In this work we used a balanced QR method to find the eigenvalues of the problem. The matrix A, in general, is a nonsymmetric and large sparse matrix, the eigenvalues of such matrix can be very sensitive to small changes in the matrix elements. In order to reduce the sensitivity of eigenvalues, we perform a balancing algorithm [10] to matrix A. Then the next strategy for finding the eigenvalue of the balanced matrix A is transferring it into a simpler form, Hessenberg form, with a sequence of Householder transformations. An upper Hessenberg matrix has zeros everywhere below the diagonal except for the first subdiagonal row. The eigenvalues of the Hessenberg matrix are directly computed with QR method [10], [17]. When the eigenvalues are found, we solve the corresponding eigenvectors with the inverse iteration method [11]. The fundamental idea of this method is to solve the linear system

$$(A - \zeta I)y = b,$$

where b is a trial vector and ζ is one of the computed eigenvalues of matrix A. The solution y will be the candidate eigenvector corresponding to ζ.

The energy spectrum of the dot consists of a set of discrete levels numerated by the set of numbers $\{n, l, \sigma\}$, n is nth solution of the problem with fixed l and σ. States having the same value of n and parallel (antiparallel) orbital momentum and spin remain two-fold degenerate (the known Kramers degeneracy). But n states with antiparallel orbital momentum and spin are separated from the nth states with parallel orbital momentum and spin.

For cylindrical QDs we can use a conventional notation for the electron energy states: nL_σ, where $L = S, P, D, ...$ denotes the absolute value of l , and $\sigma = \pm 1$ refers to the electron spin directions in respect to the electron angular momentum direction. For all calculations we choose the lowest energy state ($n = 1$).

4 CALCULATION RESULT DISCUSSION AND CONCLUSIONS

In calculation of the electron energy spectra for InAs cylindrical QDs in GaAs matrix we choose the semiconductor band structure parameters for InAs: energy gap is $E_{1g} = 0.42$ eV, spin-orbit splitting is $\Delta_1 = 0.48$ eV, the value of the nonparabolicity parameter is $E_{1p} = 3m_0P_1^2/\hbar^2 = 22.2$ eV, m_0 is the free electron effective mass. For GaAs we choose: $E_{2g} = 1.52$ eV, $\Delta_2 = 0.34$ eV, $E_{2p} = 24.2$ eV. The band offset is taken as $V_0 = 0.7$ eV.

The spin splitting effect is obviously zero for the lowest energy state $1S_{\pm 1}$. The dependence of the $1P$ energy level splitting

$$\Delta E_{1P} = E_{1P_{+1}} - E_{1P_{-1}}$$

on the dot size is shown in Fig. 1. The theory demonstrates valuable spin splitting for small QDs. The splitting is strongly dependent on the dot radius and decreases when the radius increases. In the same time for dots of small height the spin splitting is small. This is a result of electron wave function tunneling into the barrier along z-direction and energy dependence of the

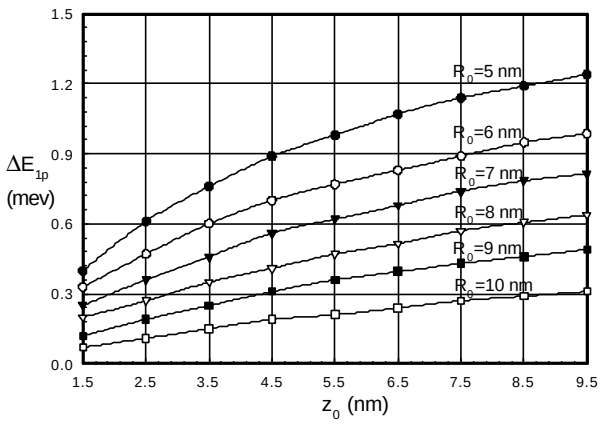

Figure 1: $1P$ energy level spin-splitting versus the dot size.

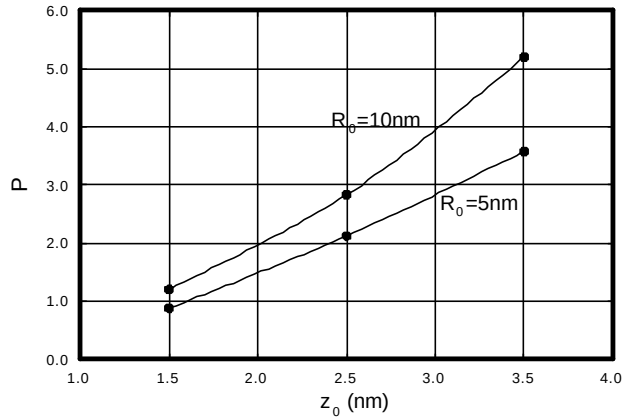

Figure 2: The ratio P versus the dot size for $\{n = 1, l = 1, \sigma = -1\}$ energy state.

electron effective mass and spin-orbit coupling parameters. To clarify the result we compare the electron wave function relative weight inside and outside the dot. In Fig. 2 we present the ratio

$$P = \frac{\int_{r\in 1} d\mathbf{r}^3 |\Phi(R,z)|^2}{\int_{r\in 2} d\mathbf{r}^3 |\Phi(R,z)|^2}$$

versus the dot size. For the QD of small height the electron "spreads" out of the dot ($P \sim 1$) the energy level properties are controlled by band parameters of GaAs matrix. In this situation an effective difference of spin-orbit coupling parameters is smaller then $\beta_1(E = 0) - \beta_2(E = 0)$. When z_0 increases the difference also increases and then becomes z-independent. That makes the spliting effect lager for lager z_0.

In short conclusion we have studied theoretically the impact of the spin-orbit interaction on the electron energy states in small semiconductor cylindrical quantum dots. Our calculations are based on the simple effective one electronic band Hamiltonian and spin dependent boundary conditions. To solve the problem we employ the balanced QR method and inverse iteration algorithm. Our results show that the method and algorithm give us opportunity to solve this tree-dimensional problem. We found the spin-orbit interaction can significantly modify the electron energy spectrum of InAs semiconductor QDs build-in into GaAs matrix. The splitting is strongly dependent on the dot size and can gain an experimentally measurable value for relatively small quantum dots.

Finally, we would like to point out that our model of calculations can be used as the starting point in estimations of the spin-orbit interaction effects in semiconductor QDs. To make proper quantitative calculations one should solve the Schrödinger equation with use of the self-consistent potential within the multiband approach.

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