Spin-orbit Interaction and Energy States in Nanoscale Semiconductor Quantum Rings

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ABSTRACT

We study the effect of spin-orbit iteration on the electron energy spectra in tree-dimensional (3D) nanoscale semiconductor quantum rings. Ultrasmall InAs quantum ring embedded in GaAs matrix is numerically solved 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. The multishift QR algorithm is implemented in the nonlinear iterative method for solving the corresponding nonlinear eigenvalue problem. It is 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 ring dimension. Meanwhile, it is larger than that of quantum dot and demonstrates an experimentally measurable quantity for relatively small quantum rings.

Keywords : nanoscale semiconductor quantum rings, spin-orbit interaction, mathematical modeling, computer simulation, multishift QR algorithm.

1 INTRODUCTION

Semiconductor quantum nanostructures, such as quantum dots, quantum rings , and quantum molecules in recent years have been of a great interest from experimental and theoretical points of view [1]–[20], [22], [23]. Semiconductor quantum rings have been fabricated and studied recently [13]–[17]. They possess very interesting physical properties including, such as far-infrared spectrum and magnetic effects. Unusual optical and magnetic properties can be controlled by morphological changes during the fabrication of nanostructure and by the number of electrons which are bounded in a quantum ring. Therefore, they are very attractive for potential applications in nanoelectronics and optics. It is known that the electron spin plays an important role in the manipulation of energy states and modify the intrinsic property of structures. Spintronics is currently a fascinating branch in electronics. Study of the spin-dependent energy spectra is an essential element for the development of semiconductor spintronics. In semiconductor spintronic device, the carrier's generation-recombination and transport can be controlled by electron spin polarization and the electron charge. It becomes necessary to study the spin-dependent electron confinement for quantum nanostructures in the development of semiconductor spintronics. It has been known that the spin-orbit interaction impacts the energy and electronic properties for III-V semiconductors [18]–[20]. However, no clear description of the spin-orbit interaction on ultra-small nanoscale quantum rings can be drawn from the literature.

We in this paper investigate the effect of spin-orbit interaction [1]–[5] on the electron energy states in nanoscale semiconductor quantum rings. The effective one-band Hamiltonian approximation with the spin-dependent Ben Daniel-Duke boundary conditions is formulated and solved numerically. Most of calculations of the electron spectra in semiconductor quantum nanostructures were done within different 1D approximations. The confinement potential in the radius direction often was approximated by a parabolic potential and in the height direction was taken to be the infinite outside the quantum ring. We for the first time adopt a realistic hard-wall (of finite height) 3D confinement potential that is induced by real discontinuity of the conduction band at the edge of the quantum ring. To solve the corresponding 3D effective one band Schrödinger equation, the multishift QR algorithm is implemented in the nonlinear iterative method for solving the corresponding nonlinear eigenvalue problem. The QR algorithm for solving the nonsymmetric eigenvalue problem is one of the jewels in the crown of matrix computations. With the multishift QR algorithm [21], it is possible to reduces the cost of simulation time up to $1-2$ orders of magnitude. The nonlinear iterative method was successfully developed by us for the simulation of semiconductor quantum nanostructures [5], [12], [17]. The spin-dependent boundary conditions mainly come from a difference between the spin-orbit interaction parameters in the quantum ring and the semiconductor environment matrix. Due to significant spin-orbit interaction in the nonsimply connected torus topology, experimentally measurable spin splitting can be observed in InAs/GaAs quantum ring. The spin splitting depends on the variations of geometric (dot- and ring-liked) structures. They are dominated by the inner radius, base radius, and height of the quan-

tum ring. Under zero magnetic fields, it is found that quantum ring can produce about 2 meV spin splitting of excited electronic states which is substantially larger than that of quantum dot (˜1 meV).

This article is organized as follows. Section 2 introduces the mathematical model and the simulation technique. Section 3 describes the results illustrating the effect of the spin-orbit interaction on the electron energy spectra for ultra-small InAs/GaAs quantum rings. Section 4 draws conclusions.

2 MATHEMATICAL MODEL AND SIMULATION METHOD

Consider the electrons are confined in three-dimensional quantum dot structures and apply an effective one electronic band Hamiltonian, we have [5], [12], [17], [18]

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

where $\hat{H}_0$ is the system Hamiltonian without spin-orbit interaction and $V_{so}(\mathbf{r})$ indicates the spin-orbit interaction for the conduction band electrons. The expression for $\hat{H}_0$ is as follows:

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

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

$$\frac{1}{m(E,\mathbf{r})} = \frac{P^2}{\hbar^2}[\frac{2}{E+E_g(\mathbf{r})-V(\mathbf{r})} + \frac{1}{E+E_g(\mathbf{r})+\Delta(\mathbf{r})-V(\mathbf{r})}]. \tag{3}$$

In (3), $V(\mathbf{r})$ is the confinement potential, $E_g(\mathbf{r})$ and $\Delta(\mathbf{r})$ stand for the position dependent band gap and the spin-orbit splitting in the valence band, respectively. P in (3) is the momentum matrix element. The spin-orbit interaction for the conduction band electrons $V_{so}(\mathbf{r})$ is given by [2], [5], [12], [17]

$$\hat{V}_{so}(\mathbf{r}) = i\nabla\beta(E,\mathbf{r})\cdot[\widehat{\boldsymbol{\sigma}}\times\nabla], \tag{4}$$

where $\beta(E,\mathbf{r})$ 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. The energy and position dependent $\beta(E,\mathbf{r})$ has the form

$$\beta(E,\mathbf{r}) = \frac{P^2}{2}[\frac{1}{E+E_g(\mathbf{r})-V(\mathbf{r})} - \frac{1}{E+E_g(\mathbf{r})+\Delta(\mathbf{r})-V(\mathbf{r})}]. \tag{5}$$

For those quantum ring systems that have sharp discontinuity on the conduction band interfaces between the quantum ring (material 1) and semiconductor matrix (material 2), the hard-wall confinement potential is

$$V(\mathbf{r}) = \begin{cases} 0, & \mathbf{r}\in \text{material 1} \\ V_0, & \mathbf{r}\in \text{materia l 2}, \end{cases} \tag{6}$$

where V_0 is the structure band offset. Combining the Hamiltonian in equations (1), (2), (4), and taking an integration of this Schrödinger equation with respect to the direction perpendicular to the system interface, the spin dependent Ben Daniel-Duke boundary conditions for the electron wave function $\Psi(\mathbf{r})$ is written as follows:

$$\begin{array}{l} \Psi_{\text{material 1}}(\mathbf{r}_s) = \Psi_{\text{material 2}}(\mathbf{r}_s) \\ \left\{\frac{\hbar^2}{2m(E,\mathbf{r}_s)}\nabla - i\beta(E,\mathbf{r}_s)\left[\widehat{\boldsymbol{\sigma}}\times\nabla\right]\right\}_n \Psi(\mathbf{r}_s) = C_0, \end{array} \tag{7}$$

where C_0 is some constant, $\mathbf{r}_s$ denotes the position of the system interface. We note that the expressions of electron effective mass in (3), spin-orbit coupling parameter in (5), and the equations of Ben Daniel-Duke boundary condition in (7) are all energy and position dependent relationships in this study.

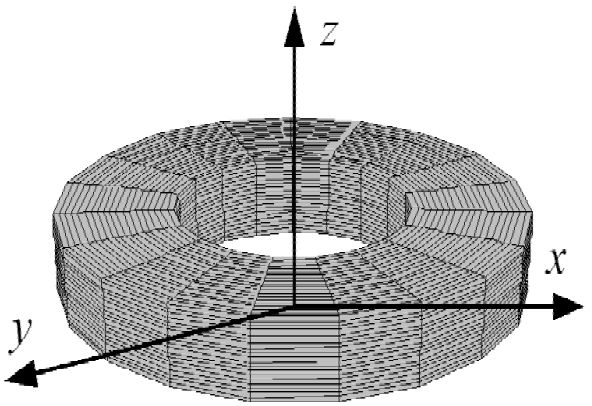

Figure 1: A 3D plot of the nanoscale semiconductor quantum ring.

We now consider the quantum ring as shown in Fig. 1, with the inner radius R_{in}, radius R_0 and the thickness z_0 in the cylindrical coordinate (R,ϕ,z). The origin of the system is at the center of the structure and the z axis is chosen along the rotation axis. Since the system is cylindrically symmetric, the wave function can be represented as

$$\Psi(\mathbf{r}) = \Phi(R,z)\exp(il\phi), \tag{8}$$

where $l = 0, \pm1, \pm2, ...$ is the electron orbital quantum number and the original model remains a two-dimensional problem in (R, z) coordinate. From Eqs. (1)-(6) and (8), we obtain equations

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

$$E\Phi_1(R,z),\ \forall(R,z)\in \text{material 1} \tag{9}$$

$$-\frac{\hbar^2}{2m_2(E)}\left(\frac{\partial^2}{\partial R^2}+\frac{\partial}{R\partial R}+\frac{\partial^2}{\partial z^2}-\frac{l^2}{R^2}\right)\Phi_2(R,z)$$

$$+V_0\Phi_2(R,z)=$$

$$E\Phi_2(R,z),\ \forall(R,z)\in \text{material 2.} \tag{10}$$

For the same reasons that the problem is symmetry along the z axis, the spin-dependent boundary conditions in (7) are given by

$$\Phi_1(R,z)=\Phi_2(R,z), z=f(R) \text{ and} \tag{11}$$

$$\frac{1}{m_1(E)}\{\frac{\partial\Phi_1(R,z)}{\partial R}+\frac{df(R)}{dR}\frac{\partial\Phi_1(R,z)}{\partial R}\}_{z=f(R)}$$

$$-\frac{1}{m_2(E)}\{\frac{\partial\Phi_2(R,z)}{\partial R}+\frac{df(R)}{dR}\frac{\partial\Phi_2(R,z)}{\partial R}\}_{z=f(R)}$$

$$+\frac{2\boldsymbol{\sigma}(\beta_1-\beta_2)}{\hbar^2}\frac{l}{R_0}\Phi_1(R_0,z)=0, \tag{12}$$

where $z=f(R)$ is the generating contour of the quantum ring on $\{R,z\}$ plane, σ refers to the electron spin polarization along the z direction. The electron energy state and wave function in this model have a tightly coupled and complicated relationships with the parameters of quantum ring and the electron angular momentum. The solution of the equations $(9)-(10)$ together with the boundary conditions $(11)-(12)$ is solved with the proposed numerical method.

The energy dependence of the electron effective mass and spin-orbit coupling parameter complicates the analytical solution [5], [12], [17], [22], [23]. The finite volume discretized Schrödinger equation leads to a nonlinear algebraic eigenvalue problem and is solved with the nonlinear iterative method to calculate all bounded energy levels. To solve the corresponding matrix eigenvalue problem efficiently, we use the multishift QR method. Computationally, this method converges monotonically and is highly cost effective in the computer simulation of 3D quantum rings. The nonlinear iterative method is outlined as:

Step 1. Set initial energy E_0;

Step 2. Compute electron effective mass m;

Step 3. Compute spin-orbit coupling parameter β;

Step 4. Solve the Schrödinger equation; and

Step 5. Update the newer computed energy and back to *Step* 2.

The iteration is terminated when the computed energy is convergent to a specified tolerance error. To obtain the complete numerical solution of the Schrödinger equation in *Step* 4, the Schrödinger equation is discretized with the finite volume method. The discretized Schrödinger equation with its boundary conditions leads to a generalized algebraic eigenvalue problem. The eigenvalues of the problem are computed with the multishift QR method. The key idea of the multishift QR method is to introduce carefully chosen perturbations to reveal deflations that are not yet evident on the subdiagonal. In our experience, the proposed nonlinear iterative method converges monotonically. The cost of simulation time can be reduced about 1.5 orders of magnitude.

The energy spectrum of the quantum ring is a set of discrete energy states that is formed and numerated by a set of numbers (n, l, σ), where n is the nth solution of the problem with a fixed l and σ. For the same value of n, the parallel (antiparallel) orbital momentum, and spin, the energy states still have two-fold degenerate (well-known Kramers degeneracy). But nth states with antiparallel orbital momentum and spin are separated from the nth state with parallel orbital momentum and spin. For cylindrical quantum rings, a conventional notation nL_σ for the electron energy states is adopted, where $L=S,P,D,...$ denotes the absolute value of l , and $\sigma=\pm1$ refers to the electron spin directions corresponding to the electron angular momentum direction. For all calculations we choose the lowest energy states ($n=1$).

3 RESULTS AND DISCUSSION

In the calculation of the electron energy spectra for InAs/GaAs quantum ring we choose the semiconductor band structure parameters for InAs as follows. The energy gap is $E_{1g}=0.42$ eV and the spin-orbit splitting $\Delta_1=0.48$ eV. The value of the nonparabolicity parameter $E_{1p}=3m_0P_1^2/\hbar^2=22.2$ eV, where m_0 is the free electron effective mass. For GaAs, $E_{2g}=1.52$ eV, $\Delta_2=0.34$ eV, and $E_{2p}=24.2$ eV. The band offset is taken as $V_0=0.77$ eV. The spin splitting effect is obviously zero for the lowest energy state $1S_{\pm1}$. The dependence of the $1P$ energy level splitting

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

on the ring size is shown in Fig. 2. Our calculation demonstrates significant spin splitting for ultrasmall semiconductor quantum rings. The splitting is strongly dependent on the ring radius and decreases

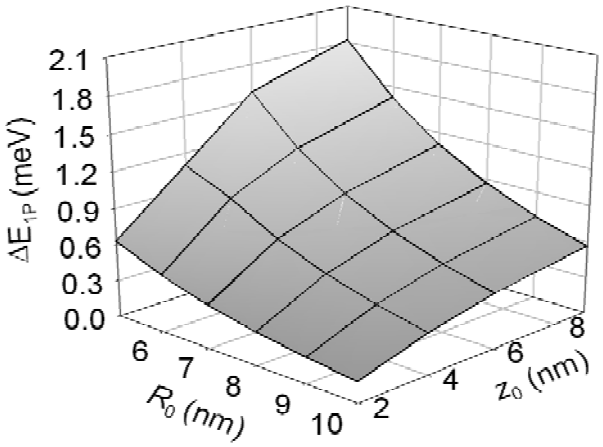

Figure 2: Spin splitting of $|l| = 1$ states for InAs/GaAs quantum rings with different base radii and heights, where the inner radius is chosen as 2 nm.

when the radius increases. At the same time for quantum rings with relatively small thickness the spin splitting is small. This is a direct result of electron wave function tunneling into the barrier along z-direction and energy dependence of the electron effective mass and spin-orbit coupling parameters. To clarify the result we have compared the "weight" of electron wave function inside and outside the quantum ring [5], [12], [17]. For the quantum ring with small thickness the electron "spreads" out of the quantum ring, the energy level properties are controlled by band parameters of GaAs matrix. Under 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. It makes the spliting effect lager for lager z_0.

Table 1: The $1P$ energy level splitting vs. R_{in}

R_{in} (nm)	2	4	6	8	10
ΔE_{1P}	0.81	0.72	0.66	0.58	0.47

The energy splitting for the state $1P$ depending on the ring size is defined as ΔE_{1P} and is shown in Fig. 2, where the ring's inner radius is 10 nm [13]–[17]. Our approach demonstrates a significant spin splitting (˜2 meV) for ultrasmall quantum ring. It is larger than that of quantum dot (˜1 meV) which was reported in our works [5], [12], [17]. For the small InAs/GaAs quantum ring ($z_0 = 2$ nm and $R = 6$ nm), spin splitting of $|l| = 1$ states with different inner radii R_{in} is summarized in Tab. 1. It reports the variation of ΔE_{1P}, it increases when the inner radius decreases.

4 CONCLUSIONS

The spin-orbit interaction play an important role in the formation of electron energy states in nanoscale quantum nanostructures and lead to a significant modification of the electron energy spectrum under zero magnetic field. We have studied the effect of the spin-orbit interaction on the electron energy states for ultrasmall semiconductor quantum rings. We found the spin-orbit interaction can significantly modify the electron energy spectrum of InAs/GaAs semiconductor quantum rings. Under zero magnetic fields, ultrasmall InAs/GaAs quantum ring produces 2 meV spin splitting of excited electronic states which is substantially larger than that of quantum dot (˜1 meV).

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