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Dependence of energy gap on magnetic field in semiconductor nano-scale quantum rings

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Abstract

We study the electron and hole energy states for a complete three-dimensional (3D) model of semiconductor nano-scale quantum rings in an external magnetic field. In this study, the model formulation includes: (i) the position dependent effective mass Hamiltonian in non-parabolic approximation for electrons, (ii) the position dependent effective mass Hamiltonian in parabolic approximation for holes, (iii) the finite hard wall confinement potential, and (iv) the Ben Daniel–Duke boundary conditions. To solve this 3D non-linear problem, we apply the non-linear iterative method to obtain self-consistent solutions. We find a non-periodical oscillation of the energy band gap between the lowest electron and hole states as a function of external magnetic fields. The result is useful in describing magneto-optical properties of the nano-scale quantum rings.

Keywords: Computer simulations; Magnetic phenomena (cyclotron resonance, phase transitions, etc.); Quantum effects; Indium arsenide; Gallium arsenide; Heterojunctions

1. Introduction

Recent progress in the fabrication of semiconductor nano-structures makes it possible to fabricate nano-scopic quantum rings [1–3]. Although micro-scopic and meso-scopic metallic semiconductor quantum rings have been of a considerable attention in recent years, the development in fabrication of semiconductor nano-scopic rings significantly bridges the gap between quantum dots and meso-scopic quantum ring structures. The trapping a single magnetic flux and unusual excitation properties for such non-simply connected quantum systems determine the practical interest to nano-scale quantum rings. Various investigations have been performed to study the electronic structure for semiconductor quantum rings; however, most theoretical quantum ring models assume only electrons moving in a 1D or 2D parabolic confinement potential [2,6–8]. These models do not consider some important phenomena, such as (i) effects of the inner or outer radius of the ring, (ii) the finite hard wall confinement potential, and (iii) the effect of non-parabolic band approximation for the electron effective mass.

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In this work we study electron and hole energy states for a realistic 3D model of InAs/GaAs quantum rings under an external magnetic field **B**. Our model formulation includes: (i) the position dependent effective mass Hamiltonian in non-parabolic approximation for electrons, (ii) the position dependent effective mass Hamiltonian in parabolic approximation for holes, (iii) the finite hard wall confinement potential, and (iv) the Ben Daniel–Duke boundary conditions. To solve this 3D non-linear problem, we apply the non-linear iterative method to calculate self-consistent solutions. The non-linear iterative method for electron and hole energy levels calculation of quantum dots and rings has been proposed by us [4,5].

We investigate the electron and hole energy state dependence on an external magnetic field. The field includes a transition between configurations with the lowest electronic (hole) energy state corresponding to the electron angular momentum $l = 0$ and $s = +1$ and with the one corresponding to the electron angular momentum $l = -1$ and $s = +1$. These transitions are related to the persistent current in the ring and the Aharonov–Bohm oscillations. The non-periodic Aharonov–Bohm oscillations obtained by us in 3D nano-rings are in a good agreement with experimental data [2,6] and do not obey well-known rules for the 1D models [6]. Therefore, our calculations observe that there is a non-periodical oscillation of the energy band gap between the lowest electron and hole states as a function of external magnetic fields. The calculation results presented in this work demonstrate the importance of the 3D modeling and simulation in the characteristics and physics of nano-scopic semiconductor quantum rings. The outline of the paper is as follows. Section 2 states the 3D quantum ring model and the solution method. Section 3 is the results and discussion. Section 4 draws the conclusions and suggests the future works.

2. 3D quantum ring model and method of solution

We consider quantum rings with the hard-wall confinement potential [9–11]. In a magnetic field, the effective mass Hamiltonian for electrons ($k = e$) and for holes ($k = h$) is given in the form

$$\widehat{H}_k = \Pi_{\mathbf{r}} \frac{1}{2m_k(E,\mathbf{r})} \Pi_{\mathbf{r}} + V_k(\mathbf{r}) + \frac{1}{2} g_k \times (E,\mathbf{r}) \mu_{\mathrm{B}} \mathbf{B} \sigma, \tag{1}$$

where $\Pi_{\mathbf{r}} = -\mathrm{i}\hbar\nabla_{\mathbf{r}} + e\mathbf{A}(\mathbf{r})$ stands for the electron momentum vector, $\nabla_{\mathbf{r}}$ is the spatial gradient, $\mathbf{A}(\mathbf{r})$ is the vector potential ($\mathbf{B} = \mathrm{curl}\ \mathbf{A}$), and σ is the vector of the Pauli matrixes. For electrons, $m_{\mathrm{e}}(E,\mathbf{r})$ and $g_{\mathrm{e}}(E,\mathbf{r})$ are the energy- and position-dependent effective mass and the Landé factor, respectively

$$\frac{1}{m_{\mathrm{e}}(E,\mathbf{r})} = \frac{2P^2}{3\hbar^2}\left(\frac{2}{E + E_{\mathrm{g}}(\mathbf{r}) - V_{\mathrm{e}}(\mathbf{r})} + \frac{1}{E + E_{\mathrm{g}}(\mathbf{r}) - V_{\mathrm{e}}(\mathbf{r}) + \Delta(\mathbf{r})}\right), \tag{2}$$

$$g_{\mathrm{e}}(E,\mathbf{r}) = 2\left\{1 - \frac{m_0}{m_{\mathrm{e}}(E,\mathbf{r})} \frac{\Delta(\mathbf{r})}{3[E + E_{\mathrm{g}}(\mathbf{r})] + 2\Delta(\mathbf{r})}\right\}, \tag{3}$$

where $V_{\mathrm{e}}(\mathbf{r})$ is the confinement potential, $E_{\mathrm{g}}(\mathbf{r})$ and $\Delta(\mathbf{r})$ stand for position-dependent energy band gap and spin–orbit splitting in the valence band, P is the momentum matrix element, m_0 is the free electron mass, and e is the charge. For holes, $m_{\mathrm{h}}(\mathbf{r})$ and $g_{\mathrm{h}}(\mathbf{r})$ are assumed to be only position dependent. For both the electron and hole, the hard-wall confinement potential in the inner region of the ring (**1**) and environmental crystal matrix (**2**) can be presented as: $V_k(\mathbf{r}) = 0$ for all $\mathbf{r} \in \mathbf{1}$ and $V_k(\mathbf{r}) = V_{k0}$ for all $\mathbf{r} \in \mathbf{2}$, respectively. The Ben Daniel–Duke boundary conditions for the electron and hole wave functions $\Psi(\mathbf{r})$ are given by [9–11]

$$\Psi_{k\mathbf{1}}(\mathbf{r}_{\mathrm{s}}) = \Psi_{k\mathbf{2}}(\mathbf{r}_{\mathrm{s}}) \quad \text{and}$$
$$\left(\frac{\hbar^2}{2m_k(E,\mathbf{r}_{\mathrm{s}})}\nabla_{\mathbf{r}}\right)\Big|_{\mathbf{n}} \Psi_k(\mathbf{r}_{\mathrm{s}}) = \text{const.},$$

where $\mathbf{r}_{\mathrm{s}}$ denotes the position of the system interface.

Because the cylindrical symmetry of the system, the wave function for electrons and holes can be represented as $\Psi_k(\mathbf{r}) = \Phi_k(R,z)\exp(\mathrm{i}l\phi)$ where $l = 0, \pm1, \pm2, \ldots$, is the orbital quantum number. This leads to a problem in the (R,z) coordinates, and the Schrödinger equation for electrons ($k = \mathrm{e}$) and holes ($k = \mathrm{h}$) is

$$-\frac{\hbar^2}{2m_{kj}(E)}\left(\frac{\partial^2}{\partial z^2}+\frac{\partial^2}{\partial R^2}+\frac{1}{R}\frac{\partial}{\partial R}-\frac{l^2}{R^2}\right)\Phi_{kj}(R,z)$$
$$+\left[\frac{m_{kj}(E)\Omega_{kj}^2(E)R^2}{8}+s\frac{\mu_B}{2}g_{kj}(E)\mathbf{B}\right.$$
$$\left.+\frac{\hbar\Omega_{kj}(E)}{2}l+V_{k0}\delta_{j\mathbf{2}}\right]\Phi_{kj}(R,z)$$
$$=E\Phi_{kj}(R,z), \tag{4}$$

where $j=\mathbf{1},\mathbf{2}$, $\Omega_{kj}(E)=e\mathbf{B}/m_{kj}(E)$, and $s=\pm1$ refers to the orientation of the electron spin along z-axis. The Ben Daniel–Duke boundary conditions can be written as

$$\Phi_{k\mathbf{1}}(R,z)=\Phi_{k\mathbf{2}}(R,z),\quad z=f(R),$$
$$\frac{1}{m_{k\mathbf{1}}(E)}\left(\frac{\partial\Phi_{k\mathbf{1}}(R,z)}{\partial R}+\frac{\mathrm{d}f(R)}{\mathrm{d}R}\frac{\partial\Phi_{k\mathbf{1}}(R,z)}{\partial z}\right)_{z=f(R)}$$
$$=\frac{1}{m_{k\mathbf{2}}(E)}\left(\frac{\partial\Phi_{k\mathbf{2}}(R,z)}{\partial R}\right.$$
$$\left.+\frac{\mathrm{d}f(R)}{\mathrm{d}R}\frac{\partial\Phi_{k\mathbf{2}}(R,z)}{\partial z}\right)_{z=f(R)}, \tag{5}$$

where $z=f(R)$ presents the generating contour of the ring on $\{R,z\}$ plane. To compute electron and hole energy states in a quantum ring with an ellipsoidal cross-section (the inserted figure in Fig. 1), we apply the non-linear iterative method to calculate the self-consistent solution. We briefly state the solution scheme and details can be found in [4,5].

For a given magnetic field, our calculation consists of iteration loops to reach a "self-consistent" energy solution: (1) set initial energy; (2) compute the effective mass; (3) compute the Landé factor; (4) and solve the Schrödinger equation and return to step (2). The iterations will be terminated when the maximum norm error of the computed energy is less than a specified error bound. In our calculation experience, the proposed computational method converges monotonically, and a strict convergence criteria on energies (the maximum norm error is less than 10^{-12} eV) can be reached by only 12–15 feedback non-linear iterative loops.

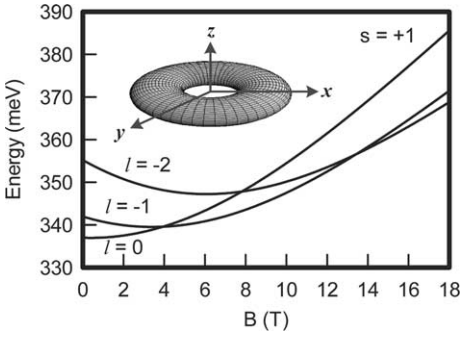

Fig. 1. A plot of electron energy states for the ellipsoidal InAs/GaAs nano-rings with the inner radius $R_{in}=8$ nm.

With the computed electron and hole energy levels, we investigate the magnetic field dependence of the system energy band gap. The energy band gap $\Delta E(\mathbf{B})$ is defined as: $\Delta E(\mathbf{B})=\Delta E_{ge}(\mathbf{B})+\Delta E_{gh}(\mathbf{B})+\Delta E_{gR}(\mathbf{B})$, where E_{ge} and E_{gh} are the ground state energies for electrons and holes, and E_{gR} is the energy gap in the quantum ring, respectively.

3. Results and discussion

We simulate the InAs/GaAs ring when the material parameters for InAs inside the rings are $E_{1g}=0.42$ eV, $\Delta_1=0.38$ eV, and $m_1(0)=0.024m_0$. The parameters for GaAs outside of the rings are $E_{2g}=1.52$ eV, $\Delta_2=0.34$ eV, $m_2(V_0)=0.067m_0$, and $V_0=0.77$ eV [10]. The energy states are numerated by a set of quantum numbers $\{n,l,s\}$, where $n=0,1,2,\ldots$ is the main quantum number. Fig. 1 shows the electron energy spectrum versus $\mathbf{B}$ for the ellipsoidal quantum ring with the inner radii $R_{in}=8$ nm [2], height $h=2.4$ nm, and width $\Delta R=R_{out}-R_{in}=24$ nm (R_{out} is the outer radius) [2,3]. For the clarity, we plot only $E_{0,l,+1}(\mathbf{B})$ states. We note that the energy difference between two sets $\{0,l,s\}$ and $\{1,l,s\}$ of energy states is controlled by the cross section area of the ring. The energy difference for this ring is $E_{1,0,s}-E_{0,0,s}\simeq 0.298$ eV. Using the same calculation method, we obtained hole energy states for rings of the same shape and size. The hole effective mass was taken as $m_{1h}=0.4m_0$ and $m_{2h}=0.5m_0$ [10], respectively. The hole band offset is taken as $V_{h0}=0.33$ eV [10]. Fig. 2 shows the energy dependence versus $\mathbf{B}$ for holes.

The calculated result of the energy gap between the lowest electron and hole states for the InAs/GaAs ring is shown in Fig. 3. We find a non-periodical oscillation of the energy band gap between the lowest electron and hole states as a function of external **B**. The oscillation of $\Delta E(\mathbf{B})$ does not obey the well-known rule for 1D models: $\Phi_c/\Phi_0 = n$, $\Phi_c = \pi(R_{in} + \Delta R)^2\mathbf{B}$ is a typical applied magnetic flux and n is an integer number, and Φ_0 is the quantum of magnetic flux. In addition, the first fracture $\Phi_c \sim 0.65\Phi_0$ is substantially larger than the commonly quoted value $\Phi_0/2$ that follows the 1D and 2D approaches [6]. For large inner radii $R_{in} = 18$ and 28 nm (when $h = 2.4$ nm and $R_{out} = R_{in} + 24$ nm), we have the same non-periodical oscillation phenomena in the energy gap (see Fig. 4). The non-periodical oscillation behavior of the energy gap is a direct sequence of our correct 3D description. It doesn't appear in the traditional 1D approach. This phenomenon should be seen in the magnetic-photo-luminescence spectra of nano-rings.

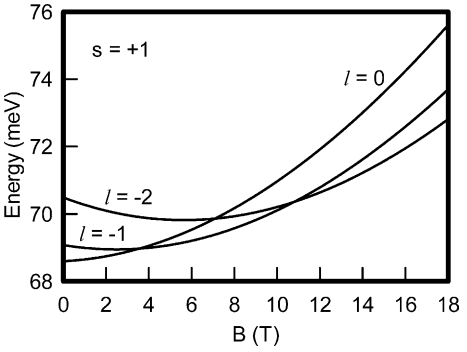

Fig. 2. A plot of hole energy states for ellipsoidal InAs nano-rings with the inner radius $R_{in} = 8$ nm.

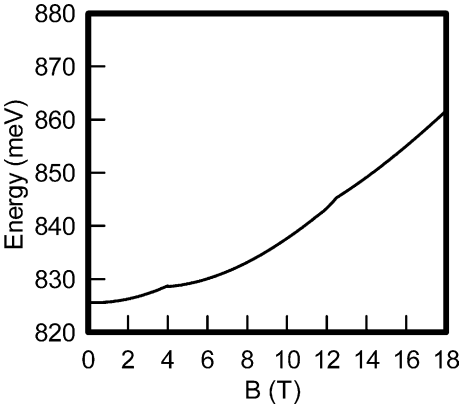

Fig. 3. The energy gap for the ellipsoidal InAs/GaAs nano-rings with the inner radius $R_{in} = 8$ nm.

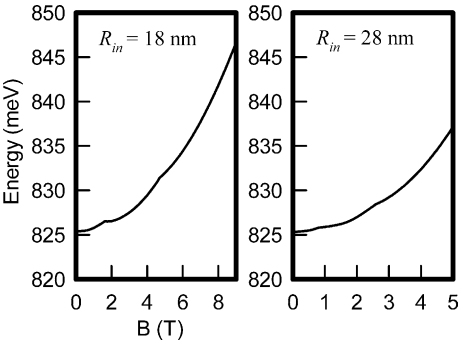

Fig. 4. The energy gap for the ellipsoidal InAs/GaAs nano-rings with different inner radii $R_{in} = 18$ nm (left figure) and $R_{in} = 28$ nm (right one).

4. Conclusions

In a short conclusion, we have investigated the electron and hole energy states for a 3D model of semiconductor nano-scale quantum rings in an external magnetic field. We found a non-periodical oscillation of the energy band gap between the lowest electron and hole states as a function of external magnetic fields. The result is useful in describing magneto-optical properties of the nano-scale quantum rings.

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