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Investigation of Magnetic Field Effects on Energy Gap for Nanoscale InAs/GaAs Semiconductor Ring Structures

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Abstact – **We investigate the electron and hole energy states for ellipsoidal and rectangular torus-shaped InAs/GaAs semiconductor quantum rings in an external magnetic field. Our realistic three-dimensional (3D) model construction is based on: (i) the effective mass Hamiltonian in non-parabolic approximation for electrons, (ii) the effective mass Hamiltonian in parabolic approximation for holes, (iii) the position- and energy-dependent quasi-particle effective mass approximation for electrons, (iv) the finite hard wall confinement potential, and (v) the Ben Daniel-Duke boundary conditions. To solve this 3D nonlinear problem, we apply the nonlinear iterative method to obtain self-consistent solutions. Due to the penetration of the applied magnetic field into torus region, we have found a non-periodical oscillation of the energy band gap versus magnetic fields between the lowest electron and hole states. The oscillation is shape- and size-dependent. The result is useful to describe magneto-optical properties of the nano-scale quantum rings.**

I. INTRODUCTION

Due to the unique electronic and optical properties, the semiconductor nanostructures have been of great interests and attractive for quantum computing, photonic device, and lasers applications [1-11]. Both of the micro- and meso-scopic metallic semiconductor rings have attracted much attention and the development of nanoscopic semiconductor rings bridges significantly the gap between nanoscale quantum dots and semiconductor rings. For semiconductor nanoscale rings, the trapping a single magnetic flux and unusual excitation properties for such non-simply connected nanostructures have vary rich physical characteristics. The self-assembled InAs/GaAs nanoscale quantum ring fabricated by solid-source molecular-beam epitaxy has become a well-established technique for high-quality fabrications. The fabrication progresses provide us an alternative to construct nanoscale systems with a wide range of geometries including various nanoscale InAs/GaAs semiconductor rings [1-5]. The ring height of these rings can be in the regime of 2 – 5 nm, and the inner radius is in the range of 5 – 30 nm. The outer radius varies from 10 – 70 nm.

There are many theoretical works has been reported for studying the electronic structure of the InAs/GaAs nano-rings. However, most of these theoretical quantum ring models only assume electrons moving in a 1D or 2D region confined by a parabolic potential [1-3]. These proposed 1D/2D models do not take some important phenomena into consideration, such as (i) effects of the inner or outer radius of the nano-ring, (ii) the finite hard wall confinement potential, and (iii) the effect of non-parabolic band approximation for the electron effective mass. With our derived 3D model, we study electron and hole energy states for a realistic 3D model of InAs/GaAs quantum rings comprehensively. We investigate and compare the electron and hole energy states for ellipsoidal and rectangular torus-shaped InAs/GaAs semiconductor quantum rings under an applied external magnetic field. Without any fitting parameters, we have for the first time found that the dependence of nano-rings' energy band gap with respect to an external magnetic field shows a non-periodical oscillation.

In this study, the theoretical model formulation includes: (i) the effective mass Hamiltonian in non-parabolic approximation for electrons, (ii) the effective mass Hamiltonian in parabolic approximation for holes, (iii) the position and energy dependent quasi-particle effective mass approximation for electrons, (iv) the finite hard wall confinement potential, and (v) the Ben Daniel-Duke boundary conditions. To solve this 3D nonlinear problem, we apply the nonlinear iterative method to obtain self-consistent solutions [6-9]. The computer simulation technique for nanostructures simulation has been proposed by us in our recent works. 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 nanoscale quantum rings.

II. A 3D QUANTUM RING MODEL

As shown in Fig. 1, two different rings, ellipsoidal and rectangular torus-shaped quantum rings, are investigated in this work. From the fabrication point of view, the ellipsoidal torus-shaped quantum ring is more realistic than the rectangular torus-shaped one [2,11]. We

compare their energy state transitions under an applied magnetic field. To model the electronic states, we consider quantum rings with the hard-wall confinement potential that is induced by a discontinuity of conduction band edge of the system components [6-9]. In an applied magnetic field $\boldsymbol{B}$ the effective mass Hamiltonian for electrons ($i = e$) and for holes ($i = h$) is given in the form

$$\hat{H}_i = \Pi_{\mathbf{r}} \frac{1}{2m_i(E,\mathbf{r})} \Pi_{\mathbf{r}} + V_i(\mathbf{r}) + \frac{1}{2} g_i(E,\mathbf{r}) \mu_B \sigma , \quad (1)$$

where $\Pi_r = -i\hbar \nabla_r + eA(r)$ stands for the electron momentum vector, ∇_r is the spatial gradient, $A(r)$ is the vector potential ($\boldsymbol{B} = \mathrm{curl}\boldsymbol{A}$), σ is the vector of the Pauli matrixes, and $m_i(E,r)$ and $g_i(E,r)$ are the electron (hole) effective mass and Landé factor, respectively. The expressions of $m_i(E,r)$ and $g_i(E,r)$ are [6-9]

$$\frac{1}{m_i(E,\mathbf{r})} = \frac{2P^2}{3\hbar^2}\left[\frac{2}{E - E_g(\mathbf{r}) - V(\mathbf{r})} + \frac{1}{E - E_g(\mathbf{r}) - V_i(\mathbf{r}) + \Delta(\mathbf{r})}\right], \quad (2)$$

and Landé factor

$$g_i(E,\mathbf{r}) = 2\left\{1 - \frac{m_0}{m_i(E,\mathbf{r})} \frac{\Delta(\mathbf{r})}{3(E + E_g(\mathbf{r})) + 2\Delta(\mathbf{r})}\right\}. \quad (3)$$

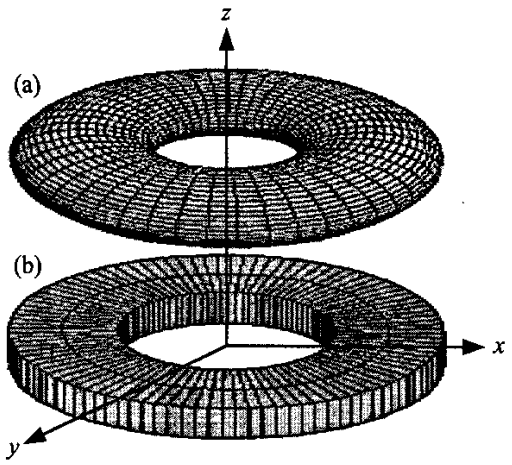

Figure 1: (a) Ellipsoidal torus-shaped quantum ring. (b) Rectangular torus-shaped quantum ring.

The hard-wall confinement potential inside the ring region (*material 1*) and environmental crystal matrix (*material 2*) can be presented as: $V_i(\mathbf{r}) = 0$ for all $\mathbf{r}$ in *material 1* and $V_i(\mathbf{r}) = V_{i0}$ for all $\mathbf{r}$ in *material 2*. $V(\mathbf{r})$ is the confinement potential, $E_g(\mathbf{r})$ and $\Delta(\mathbf{r})$ are the position dependent band gap and spin-orbit splitting in the valence band, P is the momentum matrix element, m_0 and e are the free electron elementary mass and charge. The Ben Daniel-Duke boundary conditions for the electron wave functions $\Psi(\mathbf{r})$ are given by [6-9]

$$\Psi_{i1}(\mathbf{r}_s) = \Psi_{i2}(\mathbf{r}_s) \text{ and } \left(\frac{\hbar^2}{2m_i(E,\mathbf{r})}\nabla_{\mathbf{r}}\right)_n \Psi_i(\mathbf{r}_s) = cont., \quad (4)$$

where $\mathbf{r}_s$ is the interface between the *material 1* and *material 2* of the nanoscale rings.

III. SIMULATION METHODOLOGY

For an applied magnetic field, to compute electron and hole energy states as well as the energy gap with respect to the distinct two quantum rings self consistently, we apply the nonlinear iterative method [6-9] to calculate the self-consistent solution. This simulation technique for nanostructures simulation such as quantum dot and quantum ring was proposed in our recent works [6-9].

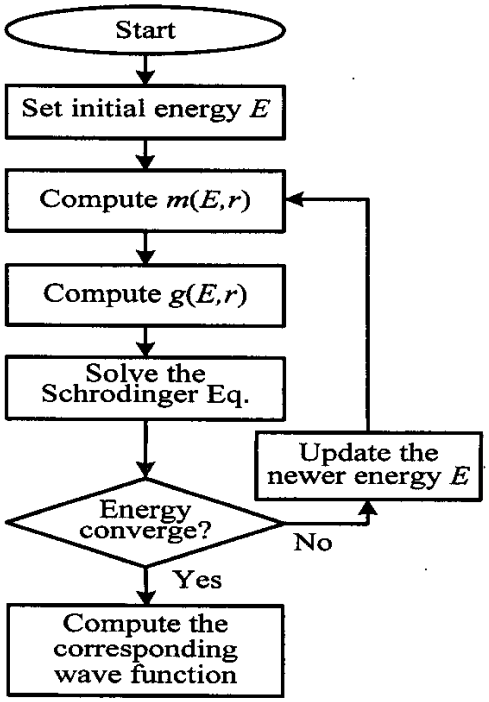

Figure 2: Nonlinear iterative method for quantum ring energy states self-consistent calculation.

As shown in Fig. 2, when the magnetic filed is specified, this solution scheme consists of steps: (i) set initial energy; (ii) compute electron effective mass through Eq. (2); (iii) compute the Landé factor through Eq. (3); (iv) solve the corresponding Schrödinger equation of Eq. (1); and (v) update the newer energy and back to step (ii). The iteration will be terminated when the computed energy is converged to a specified tolerance error. To obtain the complete numerical solution of the Schrödinger equation in step (iv), a finite difference method (the so-called finite box method) with nonuniform mesh technique is applied to discretize the Schrödinger equation with its boundary conditions, where the corresponding algebraic eigenvalue problem is

constructed. The eigenvalue and eigenfunction of the algebraic eigenvalue problem are computed with QR and inverse iteration methods [8,9]. It takes about 10-12 iteration loops to reach final convergent result for all 3D InAs/GaAs quantum ring simulations. Base on the achieved monotone convergence results, our numerical experiences confirm the nonlinear iterative method is an efficient and robust solution methodology for nanoscale quantum ring simulation.

IV. RESULTS AND DISCUSSION

For both ellipsoidal and rectangular torus-shaped rings, we first investigate the electron and hole energy states dependence on an external perpendicular magnetic field $\boldsymbol{B}$. The ring height and ring width is fixed at 2.4 and 24 nm. The ring size used in our simulation is chosen from fabrication results. The ring size variation is in the regime of experimental data. The applied magnetic field induces a transition among energy configurations with the lowest electron (hole) energy state corresponding to the angular momentum $l = 0$ (spin $\sigma = +1/2$), the lowest state of $l = -1$, the lowest state of $l = -2$, and so on.

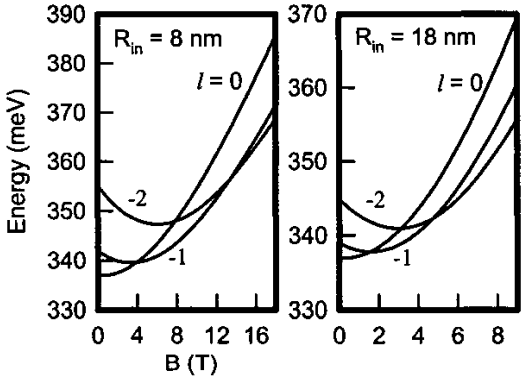

Figure 3: Electron energy versus magnetic field for ellipsoidal torus-shaped InAs/GaAs nano-rings with inner radius equals to 8 (left figure) and 18 (right one) nm, respectively.

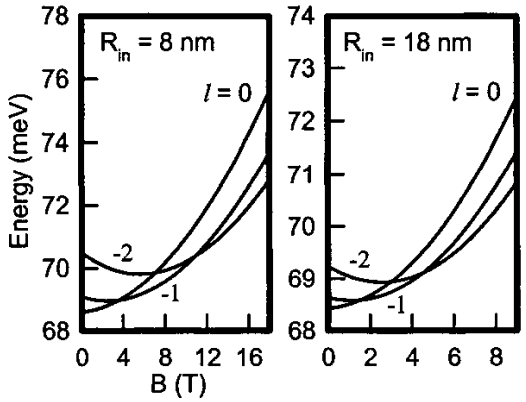

Figure 4: Hole energy versus magnetic field for ellipsoidal torus-shaped InAs/GaAs nano-rings with inner radius equals to 8 (left figure) and 18 (right one) nm, respectively.

Fig. 3 shows the electron energy states of the ellipsoidal torus-shaped ring with ring inner radius equals to 8 and 18 nm, respectively. We found the non-periodical transition of energy states depends on the inner radius. For the ring with larger inner radius, the crossing point of the transition occurs at lower magnetic fields. Fig. 4 presents the similar results for holes with difference inner radius. In our simulation, the parameters are summarized here. For InAs, the energy gap E_{1g} is 0.42 eV, Δ_1 is 0.38 eV, $m_1(0) = 0.024m_0$. For GaAs, we set $E_{2g} = 1.52$ eV, $\Delta_2 = 0.34$ eV, and $m_2(0) = 0.067m_0$. The band offset parameter is taken as $V_0 = 0.77$ eV.

To investigate the shape effects for the non-periodical oscillation of the nano-ring, we further simulate the rectangular torus-shaped rings with inner radius 8 and 18 nm, respectively. Figs. 5 and 6 show the simulated electron and hole energy for inner radius equals to 8 and 18 nm, respectively. Comparing with the results of ellipsoidal torus-shaped ring, we found the electron energy states are strongly controlled by inner radius. For ring with $R_{in} = 8$ nm, the rectangular torus-shaped ring requires larger magnetic field to modify the electron lowest energy transition.

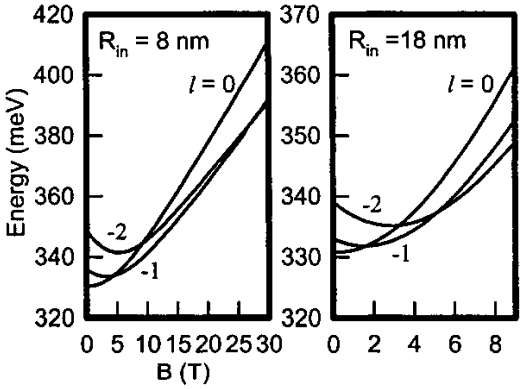

Figure 5: Electron energy versus magnetic field for rectangular torus-shaped InAs/GaAs nano-rings with inner radius equals to 8 (left figure) and 18 (right one) nm, respectively.

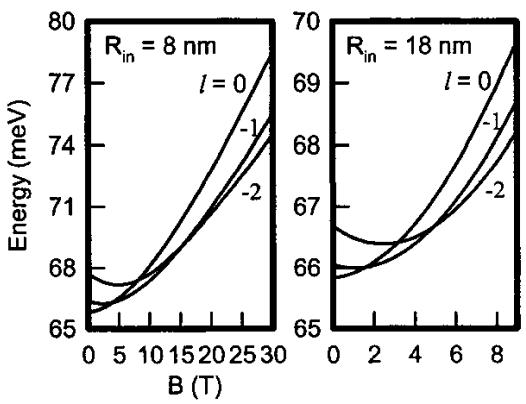

Figure 6: Hole energy versus magnetic field for rectangular torus-shaped InAs/GaAs nano-rings with inner radius equals to 8 (left figure) and 18 (right one) nm, respectively.

For these nanoscale rings under an applied magnetic flux, we found the crossing point occurs between l = 0 and l = -1 states and between l = -1 and l = -2 states clearly. The non-periodical oscillation of electron and hole energy does not obey the well-known rule ($\Phi_c/\Phi_0 = n$, where $\Phi_c = \pi(R_{width} + R_{in})^2 B$ is a typical applied magnetic flux, and n is an integer number) for various 1D models. For example, as shown in Fig. 3, the first fracture $\Phi_c \sim 0.65\Phi_0$ is larger than $\Phi_0/2$, where Φ_0 is the quantum of magnetic flux (The commonly quoted value $\Phi_0/2$ follows 1D approaches [10]). Our result has good agreement with experimental measured data [10]. Fig. 7 is the contour plots of wave functions distribution for different shape rings with R_{in} = 8 nm at B = 0 T.

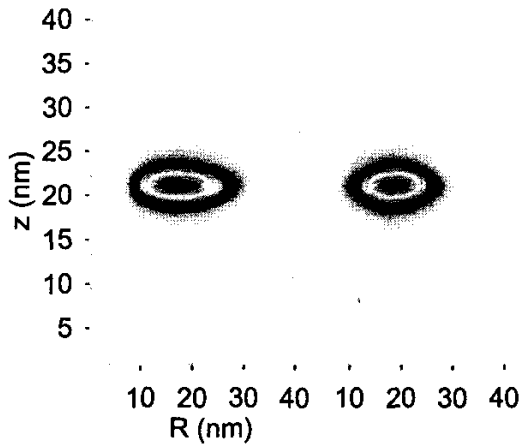

Figure 7: Contour plots of wave functions for rectangular (left figure) and ellipsoidal (right one) torus-shaped rings with R_{in} = 8 nm at B = 0 T.

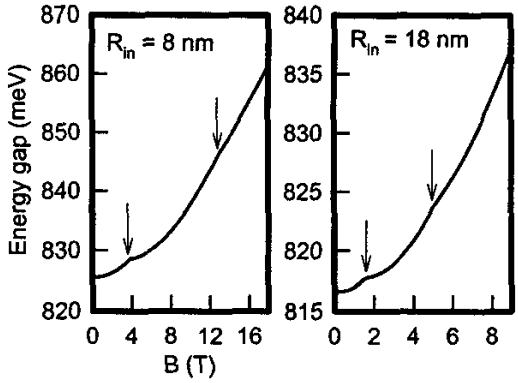

Figure 8: The energy gap vs. magnetic field for the ellipsoidal torus-shaped InAs/GaAs nano-ring.

We have calculated and analyzed the electron and hole energy states transitions for two ring shapes with R_{in} = 8 and 18 nm. With these computed data, we perform the energy band gap calculation. Our calculation is based on the formula $\Delta E(B) = E_{ge}(B) + E_{gh}(B) + E_{gR}$, where the energy band gap E_{ge} and E_{gh} are the ground state energies for electrons and holes, and E_{gR} is the energy gap of the ring, respectively. The calculated results for InAs/GaAs rings with R_{in} = 8 and 18 nm are shown in Figs. 8 and 9. The $\Delta E(B)$ oscillation is non-periodical and $\Phi_c > \Phi_0/2$.

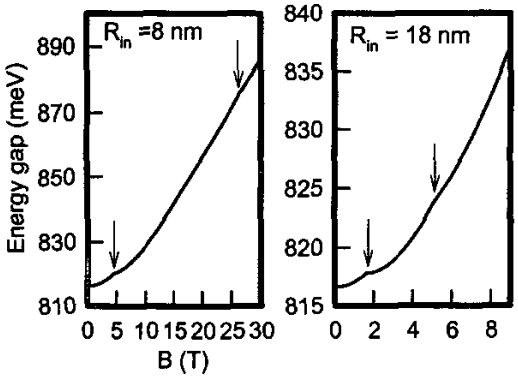

Figure 9: Energy gap versus magnetic field for the rectangular torus-shaped InAs/GaAs nano-ring.

V. CONCLUSION

A three-dimensional quantum ring model and a unified computational technique have been applied to study the energy band gap transition of InAs/GaAs rings. With the developed simulator, we have found the non-periodical oscillation of the energy band gap for a 3D semiconductor nanoscale quantum ring in an external magnetic field, and the oscillation of electron and hole energy is non-periodical and does not obey the conventional 1D rule. We note here that all calculations were without using any fitting parameters to calibrate the results. The modeling, numerical method, and study presented here clarify principal dependencies of energy states on magnetic field, ring shape, and size. It is useful to describe magneto-optical properties of the nano-scale quantum rings. The InAs/GaAs semiconductor nanoscale rings provide abundant applications in quantum computing, photonic device, and lasers applications.

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REFERENCES

[1] V. Halonen, et. al., Europhys. Lett., 33, p.337 (1996).
[2] A. Lorke, et al., Phys. Rev. Lett., 84, p.2223 (2000).
[3] H. Pettersson, et al., Physica E 6, p.510 (2000).
[4] Tsai C.-H., et al., IEEE Photo. Tech. Letters 10, p.751 (1998)
[5] A. Bruno-Alfonso, et al., Phys. Rev. B, 61, p.15887 (2000).
[6] Y. Li, et al., in: Tech. Proc. 5th Int. Conf. Modelling and Simulation of Microsystems (MSM 2002), p.540 (2002).
[7] Y. Li, et al., in: Simulation of Semiconductor Processes and Devices 2001 (SISPAD 01), D. Tsoukalas and C. Tsamis (Ed.), Springer, p.324 (2001).
[8] Y. Li, et al., Comput. Phys. Commun., 141, p.66 (2001).
[9] Y. Li, et al., Int. J. Modern Phys. C, 13(4), p.453 (2002).
[10] A. Emperador, et al., Phys. Rev. B, 62, p.4573 (2000).
[11] R. Blossey and A. Lorke, Phys. Rev. E, 65, p.021603 (2002).