Computer Simulation of Magnetization for Vertically Coupled Nanoscale Quantum Rings

Yiming Li
Department of Computational Nanoelectronics, National Nano Device Laboratories
Microelectronics and Information Systems Research Center, National Chiao Tung University
Corresponding address: P.O. BOX 25-178, 1001 Ta-Hsueh Rd., Hsinchu 300, Taiwan
Tel: +886-930-330766 Fax: +886-3-5726639 Email: ymli@faculty.nctu.edu.tw

In this paper we computationally investigate the energy spectra and magnetization for a system consisting of vertically coupled nanoscale semiconductor quantum rings (VCNSQRs) under an external magnetic field **B**. We use the three-dimensional (3D) effective one-band Hamiltonian, the energy- and position-dependent quasi-particle effective mass approximation, and the Ben Daniel-Duke boundary conditions. For a system consisting of vertically 2-coupled nanoscale InAs/GaAs quantum rings, our 3D simulation finds that its magnetization (M) is non-periodical oscillating function of **B** due to penetration of **B** into the torus and vertically coupled regions. It depends not only on the ring's radius (e.g., base, inner, and outer radius) but also the inter-distance (d) of stacked layers. Jumping period of M is non-periodical and the jumping magnitude is gradually weakened when **B** is increased. Numerical results provide interesting information for exploring the energy shell structure of vertically coupled nanoscale semiconductor quantum rings. We believe that the study is useful for optoelectronics, spintronics, and quantum Q-bit applications using these structures.

Semiconductor nanostructures have recently been of great interest and have generated huge quantities of theoretical and experimental data [1-3]. Progress of fabrication technology provides us a diverse way to construct nanoscale systems with a wide range of geometries including VCNSQRs [2]. In a system of VCNSQRs, the electron moves in a 3D torus confinement region and tunnels among stacked layers which complicates the electronic structure of the system. In this paper, we preliminary calculate the energy spectra and magnetization for a system of VCNSQRs under an external **B**. The aforementioned 3D model is solved with the nonlinear iterative method. Quite different from the Aharonov-Bohm periodic unsaturated oscillation in mesoscopic quantum rings. We find penetration of **B** into regions of torus and coupled layers leads to a non-periodically oscillating M and it saturates when **B** increases. As shown in the inset of Fig. 1, we consider a system of vertically 2-coupled nanoscale semiconductor quantum rings with the hard-wall confinement potential induced by a discontinuity of conduction band edge of the system [3]. With a given **B**, the electron Hamiltonian is

$$\hat{H} = \boldsymbol{\Pi}_{\mathbf{r}} \frac{1}{2m(E,\mathbf{r})} \boldsymbol{\Pi}_{\mathbf{r}} + V(\mathbf{r}) + \frac{1}{2} g(E,\mathbf{r}) \mu_B \mathbf{B}\boldsymbol{\sigma} \tag{1}$$

where $\Pi\boldsymbol{r} = -i\hbar\nabla\boldsymbol{r} + eA(\boldsymbol{r})$ stands for the electron momentum vector, $\nabla\boldsymbol{r}$ is the spatial gradient, $A(\boldsymbol{r})$ is the vector potential ($\mathbf{B}$ = curlA), $\boldsymbol{\sigma}$ is the vector of the Pauli matrixes, and $m(E,\boldsymbol{r})$ and $g(E,\boldsymbol{r})$ are the energy- and position-dependent electron effective mass and Landé factor. The hard-wall confinement potential is given as: $V(\boldsymbol{r}) = 0$ in the inner region of the rings and $V(\boldsymbol{r}) = V_0$ in the environmental crystal matrix. The Ben Daniel-Duke boundary conditions for the electron wave functions $\Psi(\boldsymbol{r})$ are:

$$\Psi_1(\mathbf{r}_s) = \Psi_2(\mathbf{r}_s) \text{ and } \left(\frac{\hbar^2}{2m(E,\mathbf{r})}\nabla_{\mathbf{r}}\right)_n \Psi(\mathbf{r}_s) = const., \tag{2}$$

where $\boldsymbol{r}_s$ is the position of system interface. The one-electron $M = -\partial E^N_{tot} / \partial B$, where E^N_{tot} is the summation of all states [3]. The system's M with one electron is normalized to the effective Bohr magneton in InAs. We use the nonlinear iterative method to compute energy states and magnetization for the vertically 2-coupled nanoscale InAs/GaAs quantum rings. This method is accurate and robust in nanostructure simulation [3]. For z_0 = 2 nm, R_{in} = 10 nm, $R - R_{in}$ = 20 nm, and d = 0.8 nm, Fig. 1 shows the computed energy versus **B** for $l = 0 \sim -3$. Transition of energy is non-periodical among states. Contrary to Aharonov-Bohm periodical phenomenon in mesoscopic quantum rings and 1D modeling for nanoscale quantum rings [1], shown in Fig. 2, we find the magnetization of the studied system of vertically 2-coupled nanoscale InAs/GaAs quantum rings has a non-periodical oscillation. Each non-periodical jump relates to the crossing of single-electron states and changes in the ground states. The magnitude of jump relies on the system's dimension. It saturates when **B** increases. Both the ring's radius and inter-distance are important roles in controlling M's oscillations and saturation. We note that the penetration of **B** into the torus and vertically coupled regions leads to non-periodical oscillation in both the magnetization and magnetic susceptibility.

In conclusion, we have presented a 3D model and applied the computational technique to study energy spectra and magnetization of a system of VCNSQRs. For the system of vertically 2-coupled

A full journal publication of this work will be published in the Journal of Computational Electronics.

nanoscale InAs/GaAs quantum rings, we found M has a non-periodical and saturated jump when **B** increases. Ring's radius and the inter-distance among stacked layers also dominate the dependency of M with respect to **B**.

This work is supported in part by Taiwan NSC under contracts No. NSC-92-2112-M-429-001 and NSC-93-2752-E-009-002- PAE and the grant of Ministry of Economic Affairs, Taiwan under contract No. 92-EC-17-A-07-S1-0011.

[1] D. Grandaos and J. M. García, *Appl. Phys. Lett*. **82** (2003) 2401; Y. N. Chen and D. S. Chuu, *Solid State Commun*. **130** (2004) 491; D. Granados *et al*., *J. Crystal Growth* **251** (2003) 213; R. Blossey, *et al*., *Phys. Rev. E* **65** (2002) 021603; J. Planelles, *et al*., *Phys. Rev. B* **65** (2002) 033306; A. Fuhrer *et al*., *Nature* **413** (2001) 822; Y. Aharonov and D. Bohm, *Phys. Rev.* **115** (1959) 485; K Tanaka, *Annals of Phys*. **268** (1998) 31.
[2] K. H. Ahn and P. Fulde, *Phys. Rev. B* **62** (2000) R4813; F. Suárez *et al*., *Nanotech*. **15** (2004) S126.
[3] Y. Li *et al*., *Comput. Phys. Commun*. **141** (2001) 66; Y. Li *et al*., *Comput. Phys. Commun*. **147** (2002) 209; Y. Li *et al*., *Jpn. J. Appl. Phys.* **42** (2003) 2404; Y. Li, *J. Comput. Elec.* **2** (2003) 49.

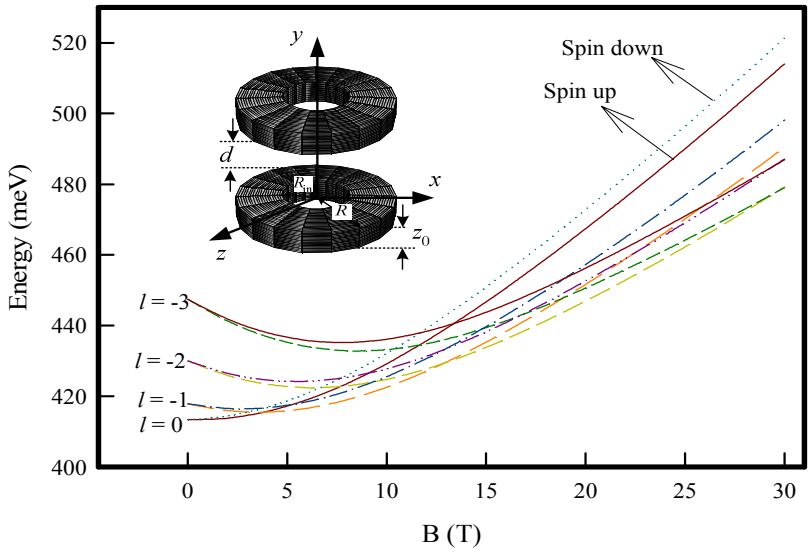

Figure 1: Electron energy spectra for vertically 2-coupled InAs/GaAs quantum rings with $d = 0.8$ nm.

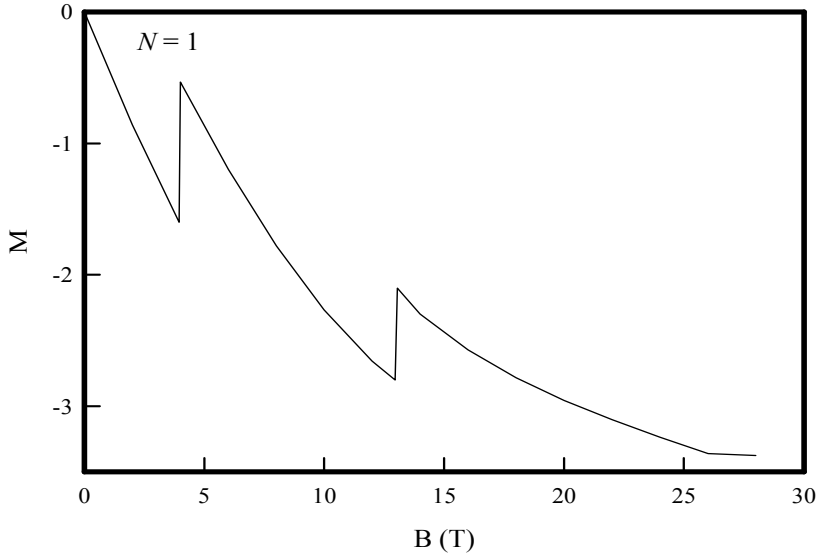

Figure 2: The computed magnetization for the same system showing in Fig. 1 where $N = 1$.