Computer Simulation of Magnetization for Vertically Coupled Nanoscale Quantum Rings

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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

$$\hat{H} = \Pi_{\mathbf{r}} \frac{1}{2m(E,\mathbf{r})} \Pi_{\mathbf{r}} + V(\mathbf{r}) + \frac{1}{2} g(E,\mathbf{r}) \mu_B \mathbf{B}\sigma \qquad (1)$$

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 ($\mathbf{B} = \mathrm{curl}A$), σ is the vector of the Pauli matrixes, and $m(E,r)$ and $g(E,r)$ are the energy- and position-dependent electron effective mass and Landé factor. The hard-wall confinement potential is given as: $V(r) = 0$ in the inner region of the rings and $V(r) = V_0$ in the environmental crystal matrix. The Ben Daniel-Duke boundary conditions for the electron wave functions $\Psi(r)$ are:

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

where 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.

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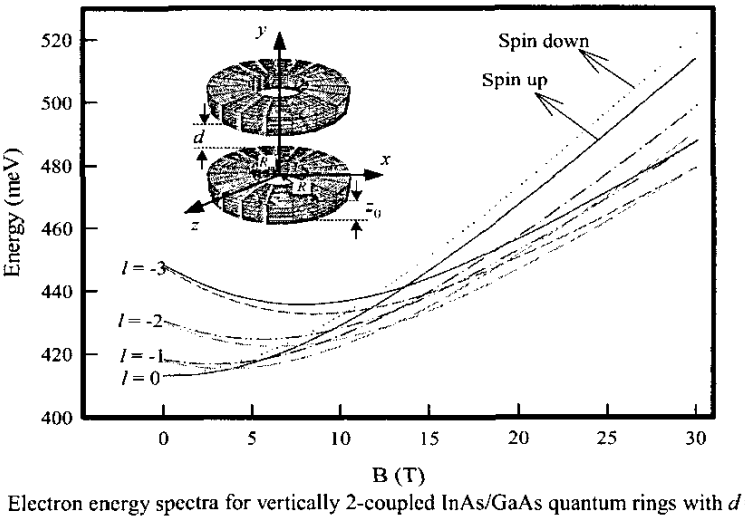

Figure 1: Electron energy spectra for vertically 2-coupled InAs/GaAs quantum rings with $d = 0.8$ nm.

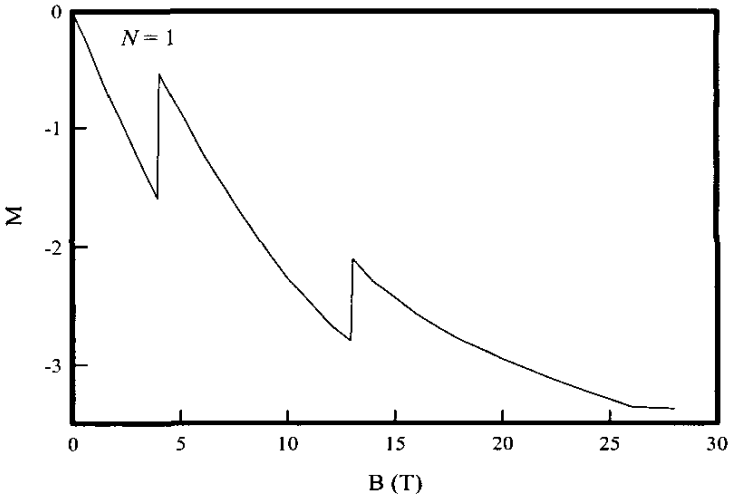

Figure 2: The computed magnetization for the same system showing in Fig. 1 where $N = 1$.