Electron Transition between Weakly Coupled Concentric Quantum Rings

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ABSTRACT

We investigate the electron wavefunction localization in double concentric quantum rings when a perpendicular magentic field is applied. In weakly coupled double quantum ring (DCQR), it is possible the situation, when the single electron energy levels associated with different rings may crossed. To avoid degenarasy, the anticrossing of these levels has a place. We show that in this DCQR the electron spatial transition between the rings can occurr due to the electron level anti-crossing. The anti-crossing of the levels with different radial quantum numbers provides the conditions when the electron tunneling between rings becomes possible. To study electronic structure of the semiconductor DCQR, the single sub-band effective mass approach was used. Results of numerical simulation for the electron transition are presented for DCQRs of different geometry.

Keywords: quantum rings, single electron levels, anti-crossing of levels, electron localization

1 INTRODUCTION

Quantum rings (QR) manifest specific electron behavior in the magnetic field [1]. Double concentric rings [2,3] are relativelly new quantum objects which have potential to have aplications in nano science and nano-technology. In the present paper, we visualize interesting features occurring in DCQRs composed of GaAs in an $Al_{0.70}Ga_{0.30}As$ substrate and particularly the single electron transfer from one ring to another under influence of a transverse magnetic field B. Therefore, we concentrate here, in contrast with the previous related papers, to the electron transition between the electron levels with different radial quantum number n. We will see that in the DCQR that have been placed in a magnetic field, the electron spatial transition between the rings can be occurred due to electron levels anti-crossing. Also we study geometry dependence of energy gap between the anti-crossed levels. The present work is close, in essence, to Ref. [4] where the effect of a magnetic field on the energy levels of electron and holes for cylindrical shaped DCQR was determined for fixed size and for radial quantum number n =1,2, with orbital quantum number $|l|$ changing from 1 to 4.

2 MODEL

Thus, we come to the single electron scheme, and using the single subband approach, what is justified due to the relatively large band gap of GaAs, the problem can be expressed by the following Schrodinger equation

$$\left(\hat{H}_{kp} + V_c(\mathbf{r})\right)\Psi(\mathbf{r}) = E\Psi(\mathbf{r}). \qquad (1)$$

Here $\hat{H}_{kp}$ is the single band kp-Hamiltonian operator $\hat{H}_{kp} = -\nabla \dfrac{\hbar^2}{2m^*}\nabla$, $m^*(\mathbf{r})$ is the electron effective mass, and $V_c(\mathbf{r})$ is the band gap potential, $V_c(\mathbf{r}) = 0$ inside the QR and is equal to E_c outside the QR, where E_c is defined by the conduction band offset for the bulk. The Ben-Daniel-Duke boundary conditions are used on interface of the material of QR and substrate. Introducing a constant magnetic field in the z direction ($\mathbf{B} = B\hat{z}$) the Schrödinger equation in cylindrical coordinates can be written in following form:

$$-\frac{\hbar^2}{2}\left(\frac{\partial}{\partial\rho}\left(\frac{1}{m^*}\frac{\partial\Phi_{n,l}}{\partial\rho}\right) + \frac{1}{m^*\rho}\frac{\partial\Phi_{n,l}}{\partial\rho} - \frac{l^2}{m^*\rho^2}\Phi_{n,l}\right) +$$

$$+\frac{\hbar l\omega_c}{2}\Phi_{n,l} + \frac{m^*\omega_c^2\rho^2}{8}\Phi_{n,l} + [V_c(\rho,z) - E]\Phi_{n,l} -$$

$$-\frac{\hbar^2}{2m^*}\frac{\partial^2\Phi_{n,l}}{\partial z^2} = 0. \qquad (2)$$

We separated angle coordinate

$$\Psi_{n,l}(\rho,z,\varphi) = \Phi_{n,l}(\rho,z)e^{il\varphi}, \qquad (3)$$

where $n = 1,2,3...$ are radial and $l = \pm 0, \pm 1, \pm 2,...$ are orbital quantum numbers. $\omega_c = |e|B/m^*$ is the cyclotron frequency. First magnetic field term in (5) is orbital Zeeman term, the second - so called diamagnetic term. The electron spin Zeeman effect has been ignored here since it is small. We assume that the double concentric quantum rings composed of GaAs in an $Al_{0.70}Ga_{0.30}As$ substrate. The values $m^* = 0.067\,m_0$ and $0.093\,m_0$ were used for the bulk values of the effective masses for the DCQR and substrate respectively. The contribution of strain was ignored in this paper because the lattice mismatch between the rings and the substrate is small. The confinement potential $V_c(\mathbf{r})$ was considered to be zero in the rings and 0.262 eV in the substrate [2].

To indicate the electron localization in the DCQR, we used the electron effective radius $R_{n,l}$ which is defined as root mean square (rms) radius by the relation: $R^2_{n,l} = \int |\Phi^N_{n,l}(\rho,z)|^2 \rho^3 d\rho dz$, where $\Phi^N_{n,l}(\rho,z)$ is the normalized wave function of the electron.

The electron in this weakly coupled DCQR can be localized in inner or outer rings. The parameters which define the state of electron in DCQD are the set of quantum numbers (n,l) and parameter of localization p (position) which can have two values "outer" or "inner". Each state can be described by these three parameters $(n,l),p$. We will see that for DCQR the electron spatial transition between the rings can occurr due to the electron levels anti-crossing that has place in a magnetic field B. The anti-crossing, providing a tunneling, is accompanied by changing the quantum numbers n and p of the $(n,l),p$ set.

3 THE EFFECT

The DCQR is considered to have rotational symmetry about the z-axis with a height of H, the widths D_1 for inner ring and D_2 for outer ring, the rings separation distance S, the inner radius R_1. Rings have semi-ellipsoidal shapes. An example of the DCQR geometry is presented in Fig. 1. Here D_1 keeps at 8 nm while D_2 sets to 18 nm, S =5 nm and H =4 nm, R_1 =5nm. Thus we consider the plane quantum rings with the condition $H \ll D$, what enhances the role of size confinement effect.
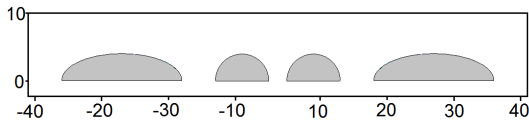

Figure 1. DCQR cross-section. The sizes are given in nm.

Electron transition in the DCQR means the changing of electron localization from outer (inner) to the inner (outer) rings. An example of this transition is presented in Fig. 2-3, where the single electron energies of different quantum states are shown as functions of magnitude B of the magnetic field. The electron transition can be occurred for three values of B: 6 T, 14 T and 18 T. One can assume the initial position (B< 5T) of electron in the (2,-2) state is at outer ring. The localization is changed when the magnetic field reaches the value of 6 T. In this point two energy levels are anti-crossed. The first is with the quantum numbers (2,-2) and the second is (3-2). For B <5 T, the electron of the second state was located in the inner ring. At the B =6 T the electron position change is carried out. If the magnetic field is increasing then the electron takes the energy level with minimal energy. It is

the (2-2) level again. However, the position of the electron is the inner ring. The same effect is occurred at 14 T (and 18 T) of the magnetic field value when the levels (1,-1) and (2,-1) ((1,-2) and (2,-2)) are anti-crossed. In Fig. 3 we show the changing of rms radius of the electron in the magnetic field for the considered above anti-crossings. It is important to note that there is an interval of the magnetic field where the rms radius is smoothly changed from outer ring to inner ring. It is well shown in Fig. 3. One can conclude from Fig. 2 that the electron transition is only possible between levels with different radial quantum numbers.
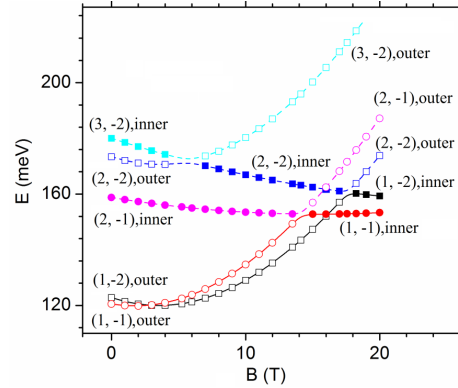

Figure 2. Single electron energies of DCQR as function of magnetic field. Open (solid) symbols mean that the electron is located in outer (inner) ring. Here D_1 =8 nm, D_2 =18 nm, H = 4 nm, and S =5 nm (see Fig.1).
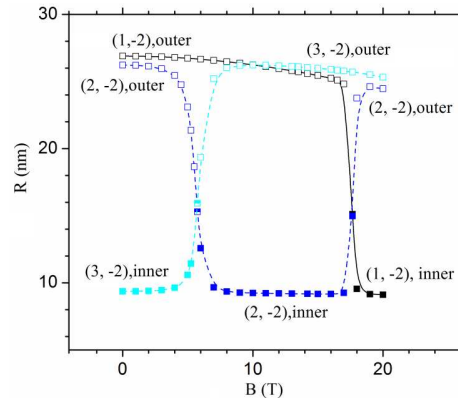

Figure 3. Rms radius of electron in DCQR as function of magnetic field for $l = -2$. Open (solid) symbols mean that the electron is located in outer (inner) ring.

4 EXPERIMENTALLY FABRICATED RING

In this section we consider the DCQR geometry motivated by the fabricated DCQR in Ref. [2]. The cross section of the DCQR is presented in Fig. 4a. Structure of the single electron levels with $l \le 18$ is shown in Fig. 4b for $B = 0$. One can see the double sub-bands with $n = 1,2$, $n = 3,4$ and $n = 5,6$. The electron is well localized in outer ring for $n = 1$, $l = 1,...$, and in inner ring for $n = 2$, $l = 1,...,3$.
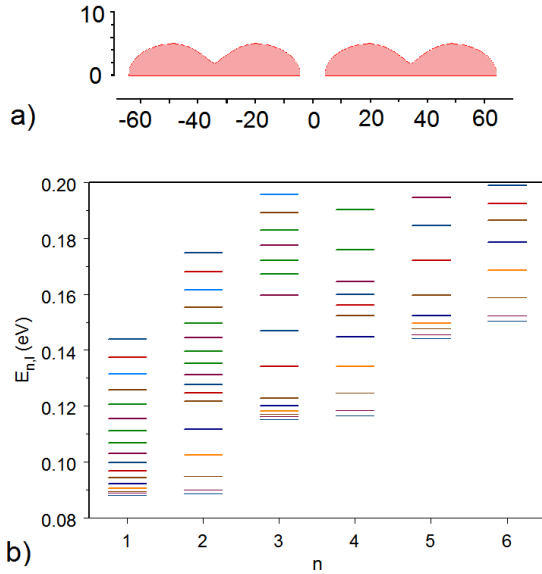
Figure 4. a) Cross section of the DCQR. The sizes are given in nm. b) Single electron energies in DCQR $E_{n,l}$, $n = 1,...,6$, $l = 1,...,18$.

The wave functions of the rest states are distributed between inner and outer rings. To illustrate this distribution, the electron energies in the DCQR and rms radius R for the states $n = 1,...,6$, $l = 0$ are shown in Fig. 5. The electron is strongly localized in outer (inner) ring when $n = 1$ ($n = 2$); 10 nm<R< 30 nm for inner ring and 45 nm<R< 60 nm, for outer.
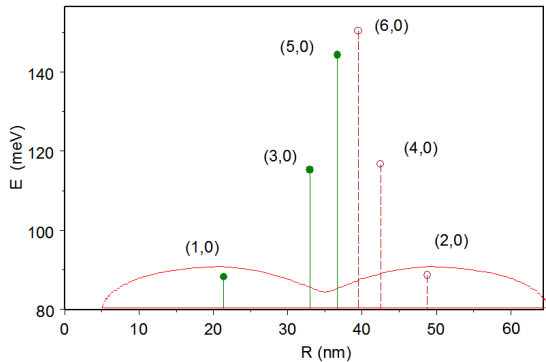

Figure 5. Single electron energies in DCQR and electron rms radius R for the states $n = 1,...,6$, $l = 0$. Contour of the DCQR cross section is shown to note corresponding electron location in DCQR.

Electron states of the sub-bands $n = 1,2$ with different orbital momentum l are also well separated by the rings. The electron of the ground state (1,0) is located in inner ring (see Fig. 5). The states with $|l| \neq 0$ are the states of the sub-band $n = 1$ and are lower members of the doublet $n = 1,2$. The electron of these states is located in outer ring. We illustrate this fact in Fig. 6 where the excitation energy of several low-lying levels is shown along with electron

position in DCQR. We can explain the situation, shown in Fig. 6, by competition of two terms of the Hamiltonian of Eq. (2). The first term includes first derivative of wave function over ρ in kinetic energy; the second is the centrifugal term. For $|l| = 0$, when the centrifugal force is absent, the most probably localization of the electron is inner ring. For $|l| \neq 0$ the electron must be localized in outer ring. Summarizing, one can say that for B=0 the well separated states are only the states $(1,l), p$ and $(2,l), p$. Thus, used notation is proper only for these states (see Fig.5). Other states $(n > 2, l)$ of this DCQR are strongly coupled states.
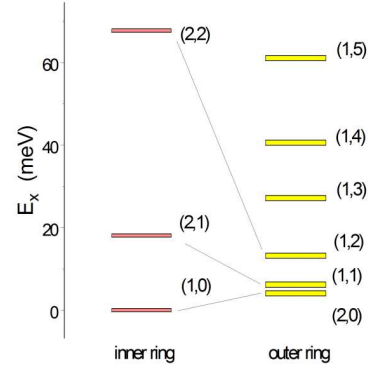

Figure 6. Excitation energy E_x and position of single electron in DCQR for the states $n = 1,2$, $l = 0,1,2,...5$. The quantum number each state is shown. Fine lines connect the upper and lower members of the doublets $(1,l) \cdot (2,l)$, $l = 0,1,2$.

Note that in Ref. [4] the $(2,l), p$ and $(1,l), p$ are alternatively denoted as the L and H states, respectively. Crossing of electron levels in the magnetic field B are presented in Fig. 7. Two crossings can be accompanied by the electron transfer from one ring to another. The first is at 1 T, another one is at 1.35 T. However at the first value of B there is no electron transfer. Effective radius of electron is not changed. This situation is like when we have crossing levels of two independent rings. There is no tunneling. The radial quantum numbers are the same. Another situation is at 1.35 T. There is the crossing of the states with different n, the states (1,-1) and (2,-1) of independent single rings have to cross at 1.35 T. In the DCQR this crossing becomes anti-crossing with possibility for electron tunneling between rings. These anti-crossed states are members of the double sub-band which is resulting in double QR system when single QR spectrum is splited [5]. In Fig. 8 we show how the effective radius is changed due to the tunneling at anti-crossing. Transformation of the profile of the electron wave function with B is given in Fig. 9. In the case of planar QRs ($H << R$) the relationship between the energy and the magnetic flux Φ can approximately be described by the following relation
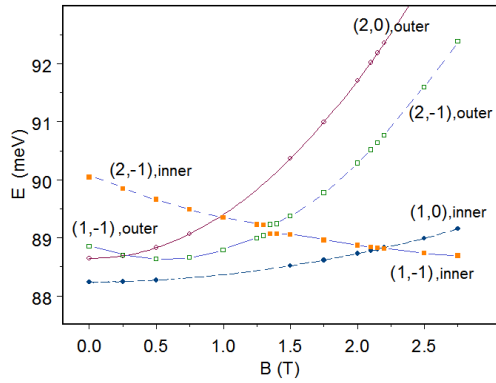
Figure 7. Single electron energies of DCQR as a function of magnetic field magnitude B. Open (solid) symbols mean that the electron is located in outer (inner) ring. The quantum numbers of the states are shown.
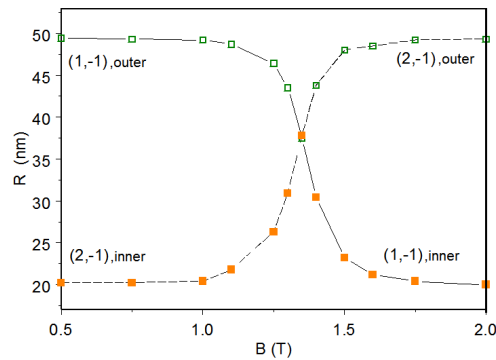

Figure 8. Rms radius of an electron in DCQR as a function of magnetic field for the states $(1,-1)$ and $(2,-1)$. Open (solid) symbols mean that the electron is located in outer (inner) ring. The solid (dashed) line is associated with lower (upper) state of the doublet $n = 1, 2$.
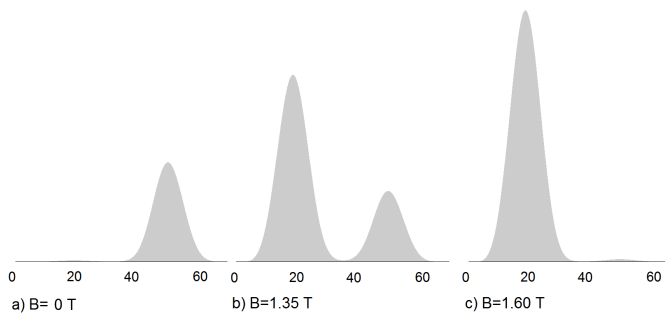

Figure 9. Profiles of the normalized square wave function of electron in the states a) $(1,-1)$,outer; b) $(1,-1)$ or $(2,-1)$ and c) $(1,-1)$,inner for different magnetic field magnitude B. a) is the "initial" state (B =0) with R =49.5 nm, b) is the state of electron transfer (B =1.35 T) with R =37.5 nm, c) is the "final" state (B =1.6 T) with R =22.0 nm. The radial coordinate ρ is shown in nm (see Fig. 6 for the DCQR cross section).

for the ideal quantum ring of radius R in a perpendicular magnetic field B: $E_p(l) = \hbar^2 / (2m * R_p^2)(l + \Phi / \Phi_0)^2$, where $\Phi = \pi R^2 B$, $\Phi_0 = h / e$, p means inner or outer ring, $\Phi_0 = 4135.7$ Tnm^2. It is clear that this relation leads to the periodic oscillations of the energy with the Aharonov-Bohm period $\Delta B = \Phi_0 / \pi / R^2$. Using rms radius as R, one can obtain for the inner ring $\Delta B / 2$ =1.73 T, for the outer ring - $\Delta B / 2$ =0.274 T. The R s are 19.5 nm and 49 nm, respectively. The obtained values for $\Delta B / 2$ are corresponding to the level crossing (Fig. 7) about 2.2T and 0.25 T, respectively. Our rough estimatation $\Delta B / 2$ qualitatively represents the situation in the Fig. 7.

5 CONCLUSION

Concluding, we say that the fate of the single electron in DCQRs is governed by the structure of the energy levels with their crossing and anti-crossing and changing with magnetic field. The above described behavior is the result of the nontrivial excitation characteristic of the DCQRs. Effect of the trapping of electron in inner QR of DCQR may be interesting from the point of view of quantum computing.

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