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Research Article

Hydrogenic-Donor Impurity Binding Energy Dependence of the Electric Field in GaAs/$Al_xGa_{1-x}As$ Quantum Rings

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Using a variational method with two-parameter trial wave function and the effective mass approximation, the binding energy of a donor impurity in GaAs/$Al_xGa_{1-x}As$ cylindrical quantum ring (QR) subjected to an external field is calculated. It is shown that the donor impurity binding energy is highly dependent on the QR structure parameters (radial thickness and height), impurity position, and external electric field. The binding energy increases inchmeal as the QR parameters (radial thickness and height) decrease until a maximum value for a central impurity and then begins to drop quickly. The applied electric field can significantly modify the spread of electronic wave function in the QR and shift electronic wave function from the donor position and then leads to binding energy changes. In addition, results for the binding energies of a hydrogenic donor impurity as functions of the impurity position and applied electric field are also presented.

1. Introduction

With rapid advances of modern nanofabrication technology, it has become possible to fabricate novel quantum nanostructures. Many experimental [1–6] and theoretical [7–28] works have triggered strong interest to the study of these semiconductor nanostructures due to their potential applications in electric and optoelectronic devices. The GaAs/$Al_xGa_{1-x}As$ quantum ring (QR) is a special confined structure. The system is assumed to be the symmetric annulations of GaAs material surrounded by $Al_xGa_{1-x}As$ material, which exhibit fascinating behavior and interesting electronic and optical properties. The signal QR and double quantum ring (DQR) systems have been grown experimentally by the use of the droplet epitaxial technique and molecular beam epitaxial technique [4–6]. Many works related to the theoretical investigation of the electron structures, the excitonic property, and the optical properties of semiconductor quantum ring have been studied by different groups [7–12]. Li and Xia [7, 8] studied the electronic states of InAs/GaAs QR (GaAs/$Al_xGa_{1-x}As$ DQR) in the frame of effective mass envelop function theory. The papers show that the electron energy levels are sensitively dependent on the radial thickness, the height of the QR (DQR), and the applied magnetic field. Except for the energy levels of the carriers, other effects can be obtained in the ring, such as the Aharonov-Bohm oscillation induced by the magnetic field [9, 10] and the Stark effect related to the electric field [11, 12]. For instance Barticevic et al. [9] studied the electronic and optical properties of quantum rings under magnetic fields. Farias et al. [10] calculated the energy spectrum of semiconductor quantum rings taking into account the external magnetic field applied perpendicularly to the structure in the finite confinement potential. On the other hand, the influence of lateral-radial electric field on the electronic and optical properties of a QR in the regime of strong quantization was also studied [11]. Harutyunyan [12] has also investigated the effects of lateral strong electric field on (1D) excitonic states and excitonic electroabsorption spectrum.

Impurity states have played an important role in the semiconductor revolution. Recently, many theoretical works have been carried out on shallow donors impurity states in QRs employing the matrix diagonalization method [13], the analytical and numerical approaches [14, 15], or variational

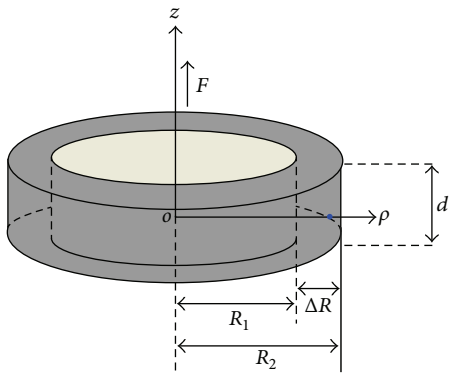


Figure 1: The graph defines the dimensions of the QR heterostructure and shows the radial coordinate ρ and the axial coordinate z. The QR heterostructure: R_1 is the inner radii of the ring, R_2 is the outer radii of the ring, d is the height of the ring, ΔR is the radial thickness of the ring, and the electric field F is applied parallel to the z axis of the QR.

approach in [16–20, 22]. The linear and the third-order nonlinear optical absorption spectra of a donor impurity confined by a quantum ring are studied using the matrix diagonalization method within the effective-mass approximation in [13]. An analytical approach to the problem of an impurity positioned in a QR in the presence of crossed magnetic (axial directed) and electric (radial directed) fields is developed in [14]. In the same approach, Monozon et al. [15] also investigated the problem of an impurity in a QR in the presence of a radially directed strong external electric field in detail. On the other hand, a theoretical study of shallow donor states in GaAs-(Ga,Al)As QRs, within the effective mass approximation and using the variational method, is presented in [16, 22]. The explicit dependencies of the binding energy of the impurity electron on the magnetic field strength, the parameters of the QR, and the position of the impurity within the QR are obtained. The effects of a positively charged impurity on the single and many electron energy states in semiconductor QR under applied magnetic field have been put forward in [17]. On the other hand, Barseghyan and coworkers [18, 19] have used the variational method and the effective mass and parabolic band approximations to study the behavior of the binding energy and photoionization cross-section of a hydrogenic-like donor impurity in InAs quantum ring with the Pöschl-Teller confinement potential along the axial direction. In the investigation, the combined effects of hydrostatic pressure and electric and magnetic fields applied in the growth direction have been also taken into account. The hydrogen-like donor binding energy in $GaAs/Ga_{1-x}Al_xAs$ concentric double quantum rings was investigated [20] considering the effects of hydrostatic pressure, temperature, aluminum concentration, and impurity position. We [22, 28] have investigated the hydrogenic impurity binding energy in $GaAs/Al_xGa_{1-x}As$ QR without external influences and the hydrogenic impurity states in GaAs QR in infinite potential barrier by the use of variational approach.

As far as we know, no studies have been made of electric field effect on the binding energy of a donor impurity in a $GaAs/Al_xGa_{1-x}As$ QR by using a variational method with two-parameter trial wave function. In this work, the binding energy of a donor impurity was investigated as functions of the sizes of the QR (radial thickness ΔR and height), the applied electric field, and the impurity position. Calculations are made in the effective mass approximations and finite potential barrier confinement. The paper is organized as follows: in Section 2 we describe the theoretical framework, Section 3 is dedicated to the results and discussion, and finally, our conclusions are given in Section 4.

2. Theoretical Model

Within the frame of the effective mass approximation, the Hamiltonian for a hydrogenic donor impurity in cylindrical $GaAs/Al_xGa_{1-x}As$ QR with an applied electric field parallel to the QR z axis as shown in Figure 1 is given by [13, 21, 22]

$$H = \begin{cases} -\nabla^2 + \eta z - \dfrac{2}{\sqrt{(\rho-\rho_0)^2 + (z-z_0)^2}} + V(\rho,z) \\ \qquad\qquad R_1 \le \rho \le R_2,\ |z| \le \dfrac{d}{2} \\ -\dfrac{m_1^*}{m_2^*}\nabla^2 - \dfrac{2}{\sqrt{(\rho-\rho_0)^2 + (z-z_0)^2}} + V(\rho,z) \\ \qquad\qquad \text{others.} \end{cases} \tag{1}$$

Here, the effective Bohr radius $a^* = \hbar^2\varepsilon_0/m_1^*e^2$ and the effective Rydberg constant $R_y = m_1^*e^4/2\hbar{\varepsilon_0}^2$ in GaAs material are used as the units of length and energy, respectively. One has $\eta = ea^*F/R_y$ which denotes a dimensionless measure of the electric field, where $\rho(\rho_0)$ and $z(z_0)$ are the coordinates of the electron (impurity) in the $GaAs/Al_xGa_{1-x}As$ QR. m_1^* and m_2^* are the electron effective mass in GaAs and $Al_xGa_{1-x}As$ materials, respectively. $V(\rho,z)$ is the electron confinement potential due to the conductor band offset in the $GaAs/Al_xGa_{1-x}As$ QR which is given by [15]

$$V(\rho,z) = \begin{cases} 0 & R_1 \le \rho \le R_2,\ |z| \le \dfrac{d}{2}, \\ V_0 & \text{others.} \end{cases} \tag{2}$$

Here, the aluminum concentration is $x = 0.3$, and the finite barrier height $V_0 = 0.6\,(1.36x + 0.22x^2)$ (eV) [16, 25]. If we assume that the in-plane and on-axis motions of the electron are weakly coupled in calculating the energy of the hydrogenic donor impurity in the $GaAs/Al_xGa_{1-x}As$ QR, the trial wave function may be written [21] as

$$\psi(\rho,\varphi,z) = N\phi(\rho,\varphi)\, f(z) \exp\left[-\lambda(\rho-\rho_0)^2 - \tau(z-z_0)^2\right], \tag{3}$$

where λ, τ are variational parameters. The radial wave function $\phi(\rho,\varphi)$ can be obtained using the ordinary (modified) Bessel functions of order m ($m = 0, 1, 2, \ldots$). Employing the

continuity relation of radial wave function at $\rho = R_1$ and $\rho = R_2$, the radial part of wave function is given by [9]

$$\phi(\rho,\varphi) = \begin{cases} \dfrac{N_0 J_0(\beta R_1) + Y_0(\beta R_1)}{I_0(\alpha R_1)} I_0(\alpha\rho) & \rho < R_1, \\ N_0 J_0(\beta\rho) + Y_0(\beta\rho) & R_1 \le \rho \le R_2, \\ \dfrac{N_0 J_0(\beta R_2) + Y_0(\beta R_2)}{K_0(\alpha R_2)} K_0(\alpha\rho) & \rho > R_2. \end{cases} \tag{4}$$

By the requirement of the continuity of the derivative of the radial wave function at $\rho = R_1$, the constant N_0 is given by

$$N_0 = \frac{-m_2^* \beta Y_1(\beta R_1) I_0(\alpha R_1) - m_1^* \alpha Y_0(\beta R_1) I_1(\alpha R_1)}{m_2^* \beta J_1(\beta R_1) I_0(\alpha R_1) + m_1^* \alpha J_0(\beta R_1) I_1(\alpha R_1)}, \tag{5}$$

using the boundary condition [22]

$$\begin{aligned} &\frac{1}{m_1^*} \frac{\partial \left[N_0 J_0(\beta\rho) + Y_0(\beta\rho)\right]}{\partial\rho}\bigg|_{\rho=R_2} \\ &\quad = \frac{1}{m_2^*} \frac{N_0 J_0(\beta R_2) + Y_0(\beta R_2)}{K_0(\alpha R_2)} \frac{\partial K_0(\alpha\rho)}{\partial\rho}\bigg|_{\rho=R_2}, \end{aligned} \tag{6}$$

where the radial ground state energy $E_{0\rho}$ and the constants (α, β) are determined by (5) and (6), which are given by

$$\alpha = \sqrt{\frac{m_2^*}{m_1^*}\left(V_0 - E_{0\rho}\right)}, \qquad \beta = \sqrt{E_{0\rho}}. \tag{7}$$

In addition, $f(z)$ is the eigenfunction of the electron along the growth direction of the GaAs/Al_xGa_{1-x}As QR [24]:

$$f(z) = \begin{cases} C_1 \exp\left[k_1\left(z + \dfrac{d}{2}\right)\right] & z < \dfrac{-d}{2}, \\ D_1 Ai(\xi) + D_2 Bi(\xi) & |z| \le \dfrac{d}{2}, \\ C_2 \exp\left[-k_2\left(z - \dfrac{d}{2}\right)\right] & z > \dfrac{d}{2}, \end{cases} \tag{8}$$

where $Ai(\xi)$ and $Bi(\xi)$ are the Airy functions. The coefficients C_1 and C_2 are determined by the continuity relation of the wave function $f(z)$ at $z = \pm d/2$:

$$\begin{aligned} C_1 &= D_1 Ai(\xi_1) + D_2 Bi(\xi_1), \\ C_2 &= D_1 Ai(\xi_2) + D_2 Bi(\xi_2), \end{aligned} \tag{9}$$

where

$$\begin{aligned} \xi &= \frac{\eta z - E_{0z}}{\eta^{2/3}}, \\ \xi_1 &= \frac{\eta(-d/2) - E_{0z}}{\eta^{2/3}}, \\ \xi_2 &= \frac{\eta(d/2) - E_{0z}}{\eta^{2/3}}, \\ Ai(Bi)(\xi_1) &= Ai(Bi)\left(\frac{\eta(-d/2) - E_{0z}}{\eta^{2/3}}\right), \\ Ai(Bi)(\xi_2) &= Ai(Bi)\left(\frac{\eta d/2 - E_{0z}}{\eta^{2/3}}\right), \\ Ai'\left(Bi'\right) &= \frac{dAi(\xi)\left[Bi(\xi)\right]}{d\xi}, \\ k_{1,2} &= \sqrt{\frac{m_2^*}{m_1^*}\left(V_{1,2} - E_{0z}\right)}, \quad V_{1,2} = V_0 \mp \eta\frac{d}{2}. \end{aligned} \tag{10}$$

Using the continuity relation of the derivative of the axis wave function at $z = \pm d/2$ [25],

$$\begin{aligned} &\frac{1}{m_1^*} \frac{d\exp\left\{C_1\left[k_1(z + d/2)\right]\right\}}{dz}\bigg|_{z=-d/2} \\ &\quad = \frac{1}{m_2^*} \frac{d\left[D_1 Ai(\xi) + D_2 Bi(\xi)\right]}{dz}\bigg|_{z=-d/2}, \\ &\frac{1}{m_1^*} \frac{d\exp\left\{C_1\left[-k_2(z - d/2)\right]\right\}}{dz}\bigg|_{z=d/2} \\ &\quad = \frac{1}{m_2^*} \frac{d\left[D_1 Ai(\xi) + D_2 Bi(\xi)\right]}{dz}\bigg|_{z=d/2}. \end{aligned} \tag{11}$$

The axial ground energy E_{0z} with the applied electric field with no impurity may be obtained by solving the transcendental equation using the boundary condition [25]

$$\begin{aligned} &m_2^2 \eta^{2/3}\left[Ai'(\xi_2) Bi'(\xi_1) - Ai'(\xi_1) Bi'(\xi_2)\right] \\ &\quad + m_1 m_2 k_1 \eta^{1/3}\left[Ai(\xi_1) Bi'(\xi_2) - Bi(\xi_1) Ai'(\xi_2)\right] \\ &\quad - m_1 m_2 k_2 \eta^{1/3}\left[Ai(\xi_2) Bi'(\xi_1) - Ai'(\xi_1) Bi(\xi_2)\right] \\ &\quad - m_1^2 k_1 k_2\left[Ai(\xi_1) Bi(\xi_2) - Ai(\xi_2) Bi(\xi_1)\right] = 0. \end{aligned} \tag{12}$$

With the adiabatic approximation, the binding energy of a hydrogenic donor impunity E_b is defined as the difference between the ground state energy of the system without impunity and the ground state energy of the system with impurity [20]; that is,

$$E_b = E_{0\rho} + E_{0z} - \min_{\lambda,\tau} \frac{\left\langle \psi \mid \widehat{H} \mid \psi \right\rangle}{\left\langle \psi \mid \psi \right\rangle}. \tag{13}$$

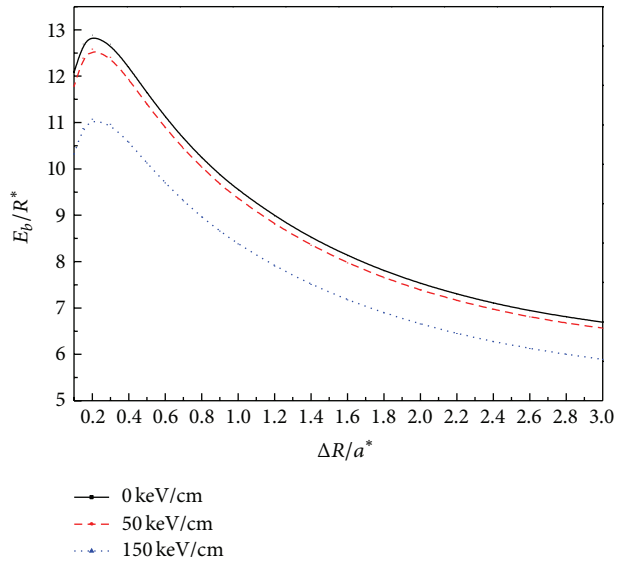


FIGURE 2: Binding energy of a donor impurity in a cylindrical GaAs/Al_xGa_{1-x}As QR as a function of the QR radial thickness (ΔR) for $R_1 = 0.3a^*$, $d = 1.0a^*$, and several values of the applied electric field.

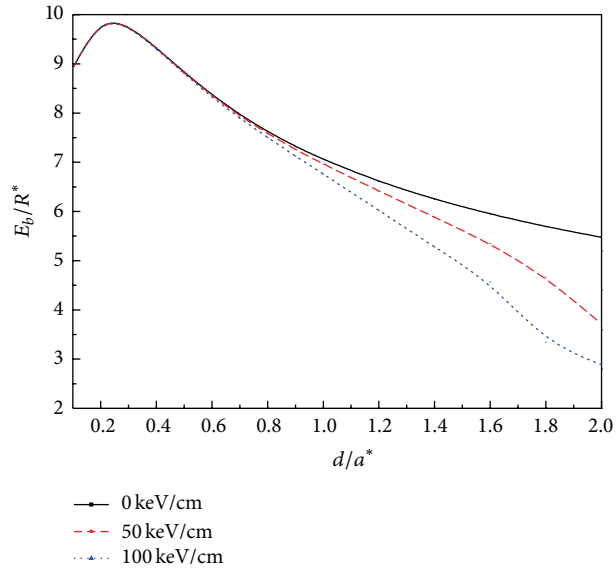
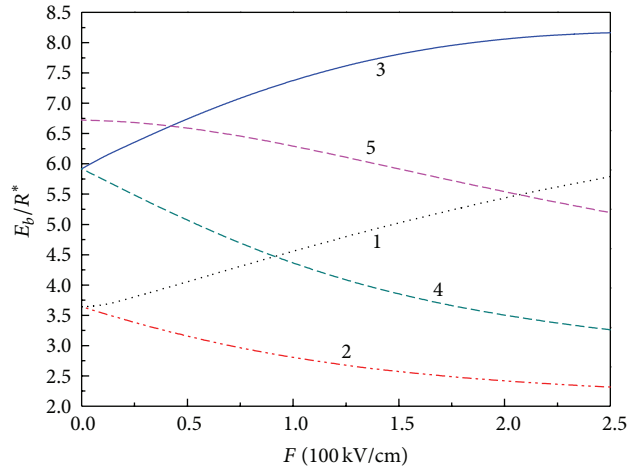


FIGURE 3: Binding energy of a donor impurity in a cylindrical GaAs/Al_xGa_{1-x}As QR as a function of the QR height for $R_1 = 0.5a^*$, $R_2 = 3.0a^*$, and several values of the applied electric field.

3. Results and Discussions

The binding energy of a hydrogenic donor impurity was calculated as a function of the impurity position and the applied electric field and the QR structure parameters (radial thickness and height) in the framework of the effective mass approximation and using a variational method. The parameters were chosen in our calculation as follows [8, 22]: $a^* = 10$ nm, $R_y^* = 5.72$ meV, $x = 0.3$, $m_1^* = 0.067m_0$, and $m_2^* = (0.067 + 0.083)m_0$. The results are illustrated in Figures 2–6.



(1) $z_0 = -d/2$
(2) $z_0 = d/2$
(3) $z_0 = -d/4$
(4) $z_0 = d/4$
(5) $z_0 = 0$

FIGURE 4: Binding energy of a donor impurity in a cylindrical GaAs/Al_xGa_{1-x}As QR as a function of the applied electric field for $R_1 = 0.5a^*$, $R_2 = 3.5a^*$, $d = 1.0a^*$, and five different positions of the donor impurity.

Figure 2 presents the binding energy of a donor impurity as a function of the radial thickness (ΔR) of the QR with the parameters ($R_1 = 0.3a^*$, $d = 1.0a^*$, $\rho_0 = (R_1 + R_2)/2$, $z_0 = 0.0a^*$) and different values of the applied electric field ($F = 0$, 50, 150 kV/cm). The figure shows that the binding energy of a donor impurity increases with decreasing the radial thickness (ΔR) in all cases, reaches a maximum value, and then decreases sharply. It can be understood that with the strengthening of the size quantization (with the decrease of radial thickness of the QR), the electron cloud moves towards the impurity, the expectation values of the electron-impurity distance increase, and the leakage of electron wave function into surrounded finite barrier region becomes stronger especially for smaller QR radius thickness, thus resulting in a decrease of the binding energy. Figure 2 also displays that the larger the applied electric field is, the smaller the binding energy of a donor impurity placed at the center of the QR is. It is well known that the wave function can be shifted from the impurity ion by the electric field, thus leading to a lower binding energy for a large electric field. This can be explained by the fact that the probability of the electron leaking into barrier region increases greatly and the coulomb confinement action between the electron and the impurity diminishes gradually. It is exciting that the results of the QR are in quite good agreement with those of the quantum dot [27].

Figure 3 displays the binding energy of a donor impurity as a function of the QR height with the parameters ($R_1 = 0.5a^*$, $R_2 = 3.0a^*$, $\rho_0 = (R_1 + R_2)/2$, $z_0 = 0.0a^*$) and different values of the applied electric field ($F = 0$, 50, 100 kV/cm). The figure shows that the binding energy increases, as the height of the QR is reduced, reaches a maximum value, and then drops slowly for a given value

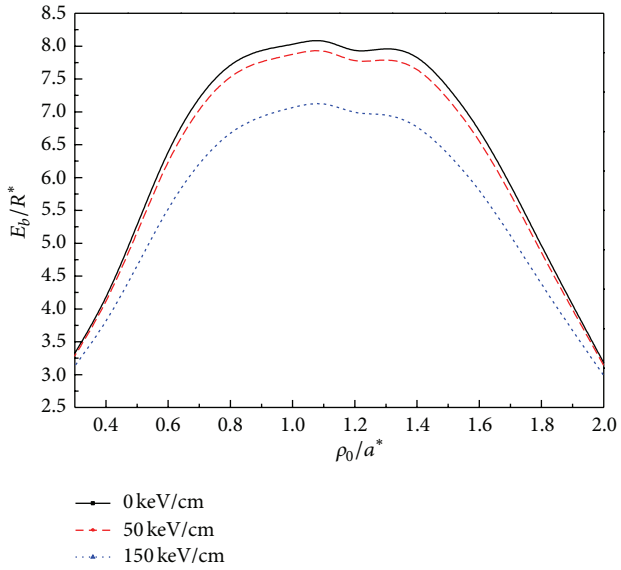


FIGURE 5: Binding energy of a donor impurity in a cylindrical GaAs/Al_xGa_{1-x}As QR as a function of the impurity radial position ρ_0 for $R_1 = 0.3a^*$, $R_2 = 2.0a^*$, $d = 1.0a^*$, and several values of the applied electric field.

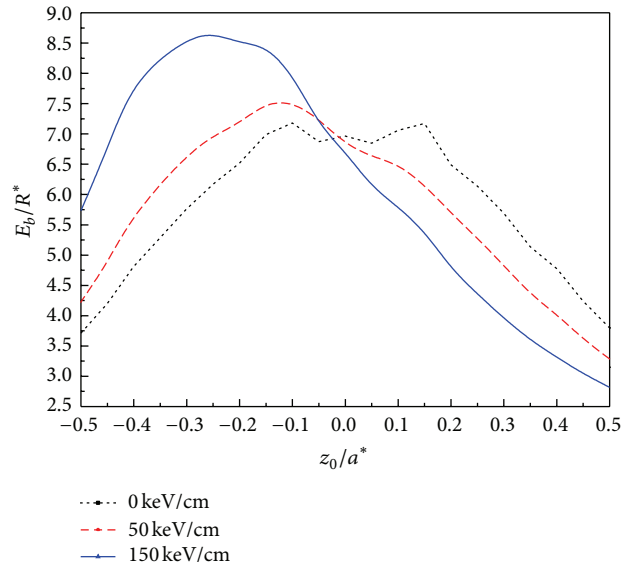


FIGURE 6: Binding energy of a donor impurity in a cylindrical GaAs/Al_xGa_{1-x}As QR as a function of the axial impurity position for $R_1 = 0.4a^*$, $R_2 = 3.0a^*$, $d = 1.0a^*$, and several values of the applied electric field.

of the electric field. As expected, it is because the electron wave function is compressed with decreasing the height of the QR, leading to enhancement of the binding energy [22, 28]. However, below a certain value of the height (d), the binding energy starts decreasing until it reaches the bulk value due to leakage of the wave function into the barrier region. It follows that the external electric field has prominent effect on donor binding energy for $d > 6$ nm and has a little effect on donor binding energy for $d \leq 6$ nm, which is due to the geometrical or spatial localization, which overcomes the effect of the electric field. As it should be expected, the effect of the electric field is more pronounced for the larger value of the QR height. For the height of the QR $d \leq 2$ nm, the binding energy drops correspondingly. It is because the probability of the electron leaking into barrier region increases greatly and the coulomb confinement action between the electron and the impurity diminishes gradually.

In Figure 4, the binding energy of a donor impurity in a GaAs/Al_xGa_{1-x}As QR is presented as a function of the applied electric field for a donor impurity implanted at five values of impurity position $z = -d/2$ (curve 1), $z = d/2$ (curve 2), $z = -d/4$ (curve 3), $z = d/4$ (curve 4), and $z = 0$ (curve 5) for the parameters ($R_1 = 0.5a^*$, $R_2 = 3.5a^*$, $d = 1.0a^*$), respectively. It can be clearly seen that the electric field tends to concentrate the electron on one of the sides of the QR. Therefore, the electric field effect may either increase or reduce the binding energy of a donor impurity. The results obtained for the binding energy dependency of external electric field effect are in good agreement with those reported by Duque and coworker [26] concerning density plot of the electron probability cloud for the ground state in the QR. For curve 1 and curve 3, it can be seen that the binding energy of a donor impurity increases monotonically with the increment of the electric field. It is because the probability of the electron wave function confined around the impurity ion increases greatly and the Coulomb interaction between the electron and the impurity ion becomes larger with the increase of the applied electric field; the behavior is caused by strengthening the electron confinement because of the stark effect. Curve 2, curve 4, and curve 5 show that the binding energy drops gradually as the electric field becomes large. It is because of the shifting effect of the electric field on the probability densities of the electron wave function, and the increment of the electric field weakens the Coulomb interaction between the electron and the impurity.

Figure 5 presents the binding energy of a donor impurity in a GaAs/Al_xGa_{1-x}As QR as a function of the radial impurity position ρ_0 with the parameters ($R_1 = 0.3a^*$, $R_2 = 2.0a^*$, $d = 1.0a^*$, $z_0 = 0.0a^*$) and different values of the applied electric field ($F = 0$, 50, 150 kV/cm). In Figure 5, The curves show that the binding energy firstly increases and then decreases as the radial displacement ρ_0 of the impurity moves from the internal boundary R_1 of the QR to the external boundary R_2. Taking curve 1, for example, the maximum value of the binding energy is located at the point $[(R_1 + R_2)/2, 0]$. The reason is that the electron probability distribution is symmetrical around the axis of the QR ($\rho_0 = (R_1 + R_2)/2$) and the electron wave function is distributed mainly around the axis of the QR. Therefore, the Coulomb interaction between the electron and the impurity becomes the largest, when the impurity is positioned at the middle point of the radial cross-section of the QR. At the same time, the curves also demonstrate that the binding energy of a donor impurity reduces correspondingly with increasing the electric field. As we can expect, the probability of the electron wave function removed from the central along the z-direction increases greatly, which leads to the reduction of the Coulomb interaction between the electron and the impurity

with the increment of the electric field. The same effect has also been observed for quantum well wires [27].

In Figure 6, the binding energy of a donor impurity is investigated as a function of the impurity position z_0 in z-direction with the parameters ($R_1 = 0.4a^*$, $R_2 = 3.0a^*$, $d = 1.0a^*$, $\rho_0 = (R_1 + R_2)/2$) and different values of the external electric field ($F = 0$, 50, 150 kV/cm). It is also seen from Figure 6 that the dot curve for zero applied electric field is absolutely asymmetry, and the binding energy changes irregularly with the impurity axial position $-1.5\,\text{nm} \leq z_0 \leq 1.5\,\text{nm}$. The binding energy increases gradually when the impurity is moved from the plane $z = \pm d/2$ (5 nm) to the symmetry plane $z = \pm 1.5$ nm along the growth direction of the QR. It is because the topology structure of the QR modifies the spread of the electron wave function in the QR; therefore, the maximum value of the binding energy is not located at the point $[(R_1 + R_2)/2, 0]$. The narrower the QR radial thickness is, the more sensitive the irregular change of the maximum binding energy due to the QR special structure is. Our result accords with [16]. From the dash curve and the solid curve, one can see that the binding energy exhibits a maximum with moving the impurity from the plane $z = -d/2$ to the plane $z = d/2$ of the QR. In addition, the curves also show that the stronger the applied electric field is, the larger the peak value of the impurity binding energy is with the same parameters (d, ΔR, and ρ_0). Moreover, the position of the peak value of the binding energy is also shifted to negative z direction. It is because the electronic wave function is obviously modified and the higher concentration of the electron wave function is squeezed strongly around the impurity. In addition, the stronger the applied electronic field is, the bigger the localization effect of the electron wave function is, so that the peak value of the binding energy increases accordingly. Therefore, the distributing of the electron wave function is not central symmetrical about the QR in presence of an electric field.

4. Conclusions

The binding energy of a hydrogenic donor impurity subjected to an external electric field in a GaAs/Al_xGa_{1-x}As QR with the framework of the effective mass approximation was calculated by using the variational approach. We found that the impurity binding energy depends strongly on ring geometry, applied electric field strength, and impurity position in the finite confinement potential. The binding energy increases firstly, reaches a maximum value, and then drops slowly as the radial thickness and/or the height of the QR decrease. Meanwhile, the binding energy exhibits a maximum as the radial displacement of the impurity moves from the internal boundary R_1 of the QR to the external boundary R_2. In addition, the position of the peak value of the binding energy is also shifted towards negative z direction. The electronic wave function distribution is also obviously modified by the applied electric field. Moreover, the stronger the applied electric field is, the larger the peak value of the impurity binding energy is with the same spatial confinement as the impurity position moves along the symmetry axis of the QR from the bottom of the QR to the top. These theoretical results obtained in this paper are useful for the design of some photoelectric devices constructed based on GaAs/Al_xGa_{1-x}As QR structures.

Acknowledgments

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