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Effects of on-center impurity on energy levels of low-lying states in concentric double quantum rings

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ABSTRACT

In this paper, the electronic eigenstates and energy spectra of single and two-interacting electrons confined in a concentric double quantum rings with a perpendicular magnetic field in the presence of on-center donor and acceptor impurities are calculated using the exact diagonalization method. For a single electron case, the binding energy of on-center donor and acceptor impurities are also calculated. The effects of centrifugal, confinement and diamagnetic potentials on the binding energy are investigated. It is found that the binding energy decreases by increasing the centrifugal or confinement potential. Also, it is shown that the binding energy increases by increasing the magnetic field. The effects of on-center impurity on the energy spectrum and angular momentum transition of the lowest states are investigated for the both single and two-interacting electrons. It is found that the on-center donor impurity increases the fractional Aharonov-Bohm oscillation period while the acceptor impurity acts inversely and decreases the fractional Aharonov-Bohm oscillation period.

Keywords: *Semiconductor nanostructures; Quantum confinement; Impurity; Aharonov-Bohm effect; Quantum rings.*

INTRODUCTION

The first attention focused on quantum structures with ring shape probably date back to Kekule's famous proposal corresponding to the structure of benzene molecule [1]. Quantum rings are small conducting or semi conducting devices with few electrons. The size of quantum rings is the order of phase-coherence length of the electrons. In this system, the interesting interference phenomena such as Aharonov-Bohm effect [2–5] and persistent current [6–14] can be seen while the electrons move around whole ring without inelastic scattering and maintain a definite phase of their wave functions.

In the past few years, the doping of both donor and acceptor impurities was a routine process in fabricating microstructure semiconductor devices which makes them most useful for constructing electronic devices. For nanostructure semiconductor systems such as quantum dots and rings, investigating the effects of donor and acceptor impurities on the electronic properties of these systems are essential due to their potential application in practical electronic and spintronic devices. The confined donors or acceptors in quantum dots have been investigated vastly [15–21]. For example, Xie has investigated the effects of the on-center donor and acceptor impurities on energy spectra of low-lying states of two-interacting electrons confined in a quantum dot with parabolic confinement potential under an arbitrary strength of magnetic field by using exact numerical diagonalization method [21]. Thus far, there are few studies on hydrogenic donor and acceptor impurities in quantum rings [22–28]. The magnetic field dependence of the low-lying spectra of a single electron in the presence of the inhomogeneous magnetic field and the on-center donor and acceptor impurities has been calculated using numerical diagonalization by Lee *et al.* [24]. The limitation of their research is that they have not considered few-electron case. Using a variational approach within the effective mass and adiabatic approximations, Wang and Zhang have studied the ground state binding energy of a hydrogenic impurity positioned in a self-assembled GaAs/$Ga_{1-x}Al_xAs$ quantum [25]. They have calculated the binding energy as a function of the size (outer radius, height) of the quantum ring, the Al concentration, and the donor impurity position. Li *et al.* have studied the electron states of an on-center impurity in an elliptic quantum ring in the presence of magnetic field applied perpendicularly to the ring plane [28]. The effects of geometrical ring shape on the Aharonov-Bohm oscillation and binding energy have been investigated by using exact diagonalization method. Recently, the double connected quantum rings with different configurations have been studied vastly [29-41]. These complex nanostructures can be considered as artificial molecules. This is because of this fact that when two quantum rings are coupled each other, the inter-ring coupling causes the localized carriers in the individual rings hybridize forming molecular-like states. One type of the double-connected geometry of the quantum rings which has interested researchers during the last recent years is the concentric double quantum rings (DQRs). Concentric DQRs structures have been fabricated by using droplet epitaxial growth [30-31] and atomic force microscope tip oxidation [42-43] techniques. In a number of theoretical works, concentric DQRs have been investigated [29-34, 37, 39-41]. The behavior of Aharonov-Bohm oscillations in the concentric DQRs with a Coulomb impurity has been investigated by Cheng et *al*. [37]. They have considered an electron in a two-dimensional concentric DQR with a magnetic flux threaded through the rings. The concentric DQR structure has been approximated by the hard-wall confinement potential for internal and external boundaries and a tunable constant barrier in the middle. It was found that the appearance of the Aharonov-Bohm oscillations in total energy depends on the position and strength of the screened potential. However, to the best of our knowledge, all previous studies on the electronic structure and binding energy of a hydrogenic donor or acceptor impurity in semiconductor nanostructures have not considered the coupled concentric DQRs with a parabolic confinement potential in the presence of the electron-electron interaction and a magnetic field applied perpendicularly to the plane of the concentric DQRs. In this paper, the effects of on-center donor and acceptor impurities on Aharanov-Bohm oscillation in energy spectra of a single and two electrons confined in a concentric DQR are studied. The effects of the magnetic field, centrifugal and confinement potentials on the binding energies of the donor and acceptor impurities are also investigated. This paper is organized as follows: In Sec. II, we present the theoretical model. In Sec. III, the results of a numerical study for a single electron and two-interacting electrons confined in the presence of the on-center donor and acceptor impurity are presented and discussed. Section IV contains the summary and conclusions.

THEORICAL MODEL

Consider a two-dimensional concentric DQR with a confinement potential as shown in Figure 1.

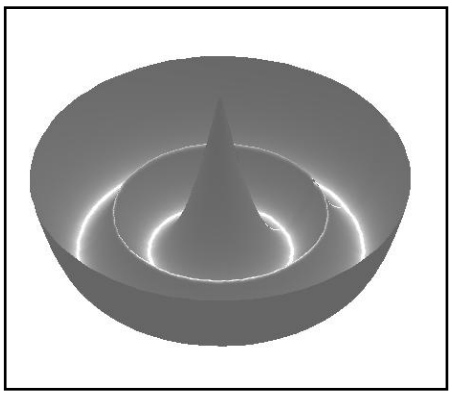

Fig. 1. Schematic view of a parabolic confinement potential for a coupled concentric DQR.

In the presence of an embedded on-center impurity and a magnetic field applied perpendicularly to the DQRs plane (i.e., $\mathbf{B} = B\,e_z$), the Hamiltonian of a single electron can be written as:

$$H_0 = -\frac{\hbar^2}{2m^*}\left(\frac{d^2}{d\rho^2}+\frac{1}{\rho}\frac{d}{d\rho}\right)+\frac{\hbar^2 L^2}{2m^*\rho^2}+\frac{m^*\omega_c^2\rho^2}{8}-\frac{1}{2}\hbar\omega_c L+V(\rho)+V_d(\rho), \quad (1)$$

where $h = 2\pi\hbar$ is the Planck's constant, m^* is the effective mass of electron, ρ is the radial distance of electron, L is the quantum number of angular momentum, $\omega_c = eB/m$ is cyclotron frequency and e is the charge of electron. The second, third and fourth terms in this Hamiltonian are known as the centrifugal, diamagnetic and orbital Zeeman potentials, respectively. The effect of the spin Zeeman potential is neglected in the present study. In Eq. (1),

$$V(\rho) = \frac{1}{2}m^*\min[\omega_1^2(\rho-R_1)^2, \omega_2^2(\rho-R_2)^2] \quad (2)$$

is the lateral confinement potential. Here, ω_1 and ω_2 are the confinement potential strengths for internal and external rings, respectively. Also, R_1 and R_2 are the radius of the internal and external rings, respectively. In addition,

$$V_d(\rho) = \alpha\frac{e^2}{4\pi\varepsilon\varepsilon_o\rho} \quad (3)$$

is the Coulomb interaction between electron and on-center impurity. It is supposed that the on-center impurity is a single ionized donor or acceptor impurity. In Eq. (3), ε is the dielectric constant and ε_o is the permittivity of vacuum and $\alpha = 1$ is assumed for an acceptor impurity while $\alpha = -1$ is selected for a donor impurity.
The two-electron Hamiltonian can be expressed as

$$H = \sum_{i=1}^{2} H_0(\rho_i) + \sum_{i=1}^{2}\sum_{j>i}^{2}\frac{e^2}{4\pi\varepsilon\varepsilon_o|\vec{\rho}_i - \vec{\rho}_j|} \quad (4)$$

where the first term in Eq. (4) is the Hamiltonian of two non-interacting electrons and the second one is the Coulomb interaction between electrons. Also, ρ_i is the position vector of i[th] electron.

NUMERICAL STUDY AND DISCUSSION

In this section, the Hamiltonian of a single electron and two-interacting electrons are diagonalized by using exact diagonalization method. For numerical calculation, the rings radii (i.e. R_1=50 nm and R_2=100 nm) and widths (i.e., d_1=d_2=47.75 nm) are used corresponding to the fabricated structures by tip oxidation technique [42]. Confinement strengths of internal and external rings can be found using $\omega_1 = \frac{2\hbar}{m^* l_1^{\,2}}$, $\omega_2 = \frac{2\hbar}{m^* l_2^{\,2}}$ where l_1 and l_2 are the half-width of the internal and external rings, respectively [32]. This yields $\hbar\omega_1 = \hbar\omega_2 = 4meV$. For electron effective mass and dielectric constant, the parameters of GaAs are chosen, (i. e., $m^* = 0.067\,m_o$, where m_o is the free electron mass and $\varepsilon = 12.4$).

A single electron

In this subsection, the effects of on-center impurities (i.e., donor and acceptor) on the energy spectra and probability densities of a single electron are investigated. In order to calculate the eigenstates and energy spectra of Hamiltonian in Eq. (1), the finite difference method and exact diagonalization technique are used [32]. The electron localization in the DQRs in the presence and absence of on-center impurity by using

probability density calculation of a single electron for L=0 and B=0 is shown in Figure 2.

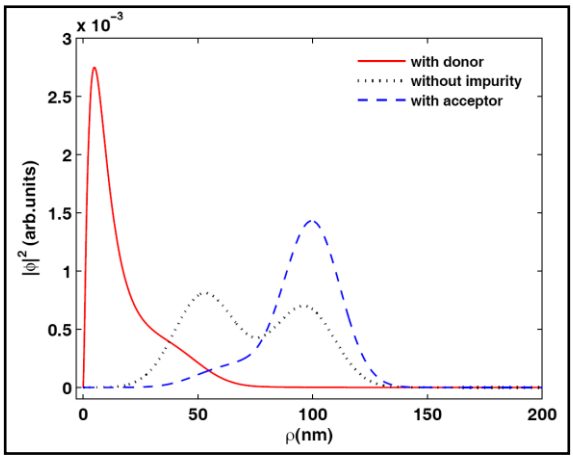

Fig. 2. The electron probability density of the lowest state for L=0 and B=0 in a DQR with on-center donor (solid curve), acceptor (dashed curve) and without impurity (dotted curve).

The solid and dashed curves represent the probability density of an electron in presence of the donor and acceptor, respectively. The probability density of an electron in absence of impurity (dotted curve) is also shown in this figure for comparison. It is clear that the attractive (repulsive) potential of the on-center donor (acceptor) causes the localization of electron near the donor (acceptor) which minimizes the potential energy. Figures 3a and 3b show respectively the energy levels of a single electron corresponding to the different quantum numbers of angular momentum up to 6 which are plotted by different colors in the presence of the donor and acceptor impurities. The energy levels in the absence of impurity (dashed curves) are also shown for comparison.

It can be seen that the acceptor impurity increases the energy of levels while the donor impurity decreases it significantly. Also, it is found that the ground state transition of angular momentum has a different behavior in the presence of impurity rather than its absence. In general, the ground state transition of angular momentum is induced by increasing the magnetic field that minimizes the potential energy of electron. Figure 4 shows the ground state transition of angular momentum in a DQR in the presence of donor impurity (solid line), acceptor impurity (dashed line) and in the absence of impurity (dotted line). It can be observed that the acceptor impurity increases the ground state transition of angular momentum while in the presence of the donor there are not any transitions for ground state energy. This is because of this fact that in the presence of the attractive potential of the on-center donor, the electron is localized in the small radius then the minimum value of the electron potential energy (i.e., sum of the centrifugal potential, orbital Zeeman term and diamagnetic potential) for this interval of the magnetic field strength corresponds to L=0 angular momentum.

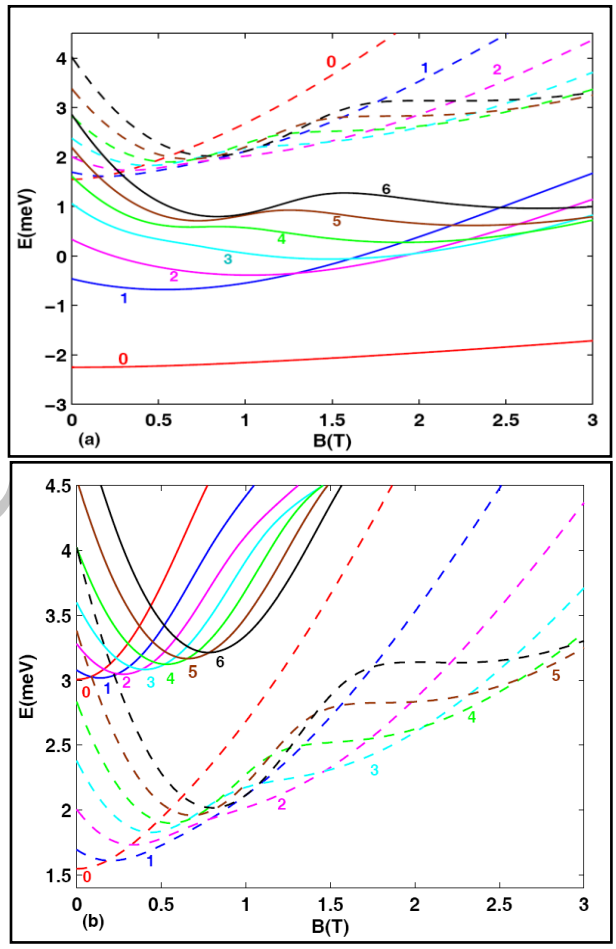

Fig. 3. The single-electron energy spectrum of a DQR with (a) donor impurity and (b) acceptor impurity. The energy levels corresponding to the different quantum numbers of angular momentum are plotted by different colors as a function of magnetic field. The energy levels of the DQR in the absence of impurity are shown by dashed curves for comparison.

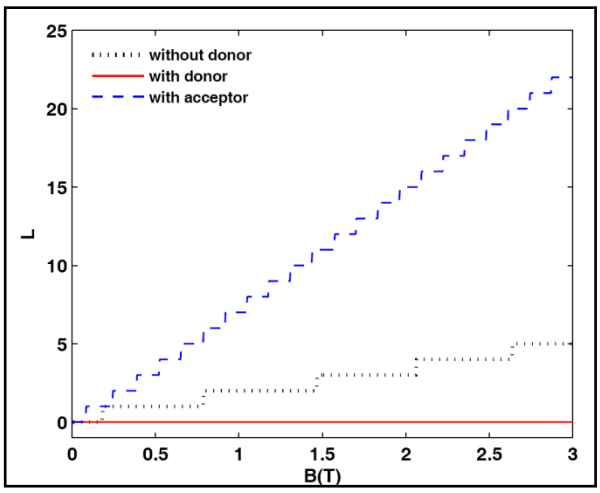

Fig. 4. The ground state transition of angular momentum as a function of magnetic field in a DQR in the presence of donor (solid line), acceptor (dashed line) and in the absence of impurity (dotted line).

For a better understanding of the on-center impurity effect on the energy levels of the concentric DQR, the binding energy of the donor and acceptor impurities is calculated. The effects of centrifugal, diamagnetic and confinement potentials on the binding energy are investigated. The binding energy (Eb) of the impunity is defined as the difference between the energy of the system without impurity and the energy of the system with impurity, i.e., Eb_{nL}= E_{nL}(without impurity)-E_{nL}(with impurity), where n and L are the radial and angular quantum numbers, respectively. Figures 5a and 6b respectively show the binding energies of on-center donor and acceptor impurities corresponding to the different quantum numbers of angular momentum up to 6 which are plotted as a function of magnetic field with different colors. It can be seen that the centrifugal potential decreases the binding energy and the magnetic field increases it. This is due to the magnetic field localizes electrons in the internal ring but the centrifugal potential localizes them in the external ring [32].

To see the effect of confinement potential on the binding energy, the binding energies of donor and acceptor impurities for L=0 and B=0 are calculated as a function of the confinement strength and shown in Figures 6a and 6b, respectively. It is found that the binding energy decreases when the confinement strength increases and finally reaches to a constant value for higher confinement strengths. This is due to that for the high confinement strength the confinement potential is very large relative to the Coulomb interaction between electron and donor or acceptor impurity. Then the effect of on-center impurity on energy levels is negligible. Also, it can be seen that the binding energy of donor impurity decreases more rapidly than the acceptor impurity because the electron in a DQR with on-center donor is localized closer to the DQR center than acceptor case. So, the electron-donor interaction becomes weaken more rapidly by increasing the confinement strength.

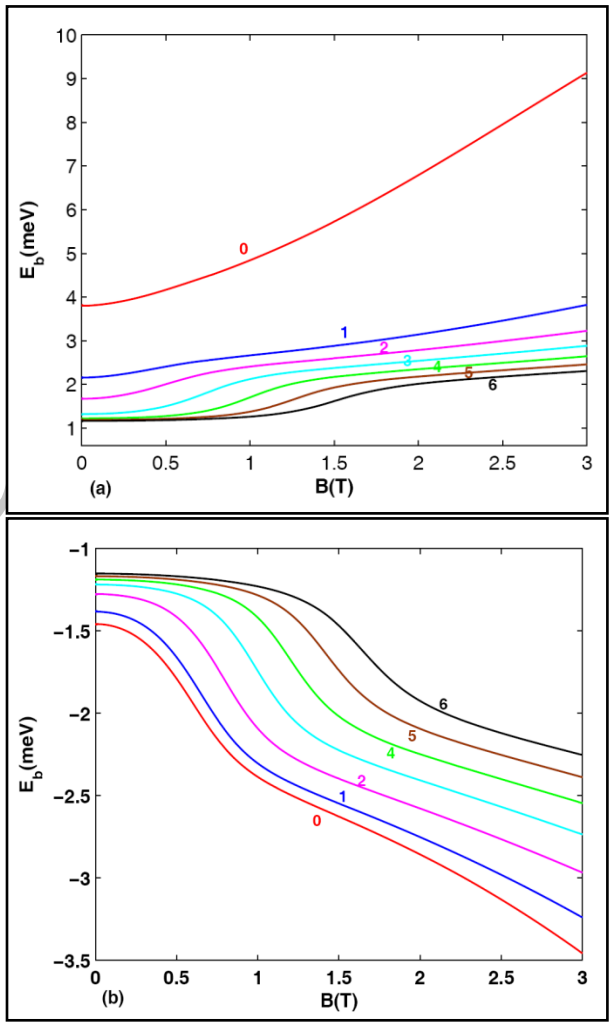

Fig. 5. The binding energy of (a) donor impurity and (b) acceptor impurity as a function of the magnetic field for different quantum numbers of angular momentum.

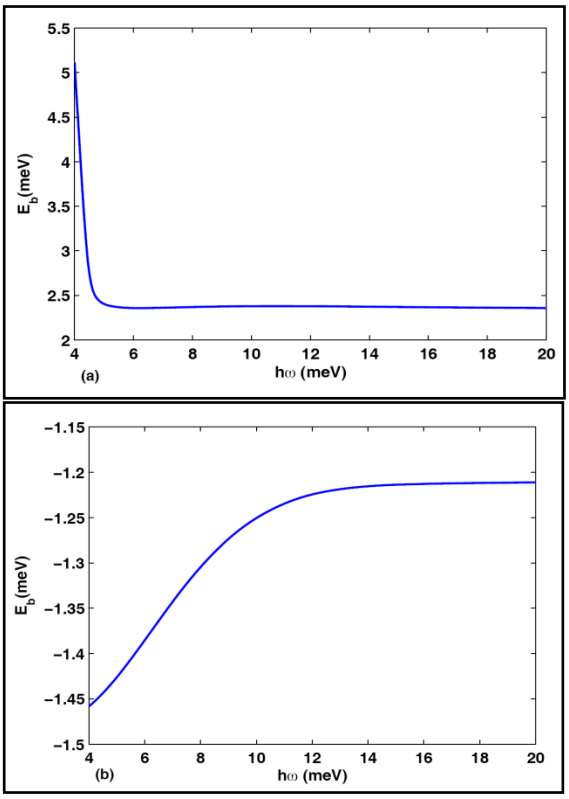

Fig. 6. The binding energy of an on-center impurity as a function of the confinement strength for (a) donor impurity and (b) acceptor impurity.

Two electrons

To solve the two-electron Schrodinger equation corresponding to the Hamiltonian in Eq. (4), we construct the basis sets of two-electron system by using the single-electron eigenstates and diagonalize the mentioned Hamiltonian in these basis states. Figure 7 shows the energy levels of the two-interacting electrons corresponding to the different quantum numbers of total angular momentum as a function of the magnetic field for a concentric DQR with (a) on-center donor, (b) on-center acceptor, respectively. The two-electron energy spectrum in the absence of impurity is shown in Figures 7c for comparison. In these figures, the solid curves indicate the spin-singlet state and the dashed ones represent the spin-triplet states. In the presence of the on-center donor, there is only one transition for the angular momentum of the ground state in this range of the magnetic field that takes place from L=0 to L=1. In other words, the donor impurity increases the fractional Aharanov-Bohm oscillation period. In addition, it is clear that the spin-singlet and triplet states of the small total orbital angular momentum are separated from each other but for the large quantum numbers of angular momentum the degenerate spin-singlet and triplet states can be observed. This is because of the large value of the angular momentum where two-interacting electrons are localized far away from each other so the electron-electron interaction becomes so weak which causes degenerating of the energy of the symmetric and antisymmetric spatial wave functions.

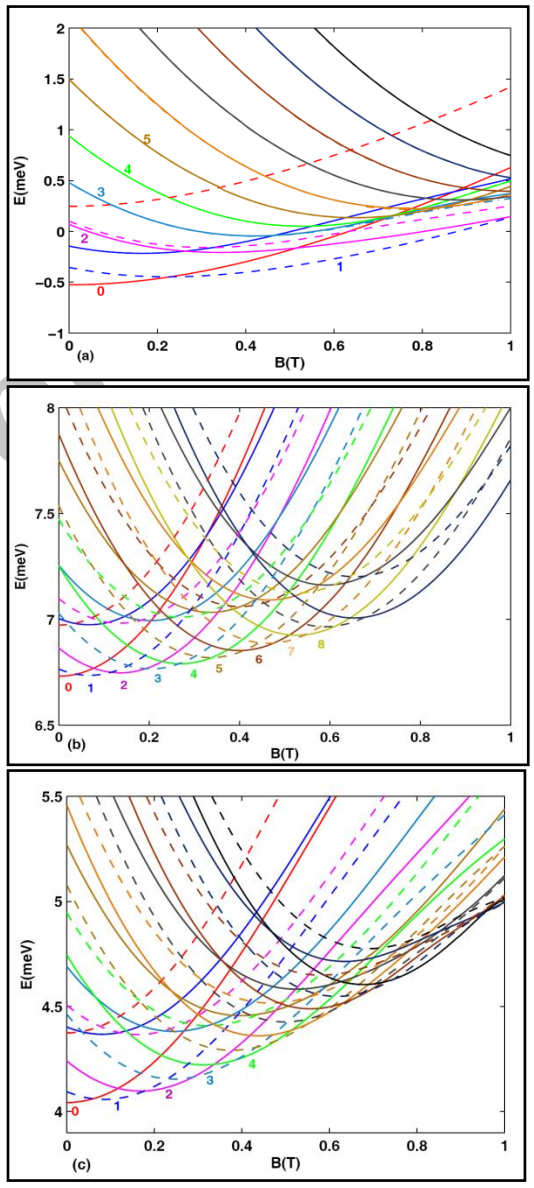

Fig. 7. The two-electron energy spectrum of a DQR with (a) donor impurity, (b) acceptor impurity. The two-electron energy spectrum of a DQR in the absence of impurity is shown in Fig. 7 (c) for comparison.

For the concentric DQR with on-center acceptor, unlike previous case, electrons have transitions to higher orbital quantum numbers for the lower magnetic fields. This is because when the magnetic field increases, the electrons are pushed toward acceptor impurity which leads the repulsive interaction energy to increase. Then the electrons move to the higher orbital to decrease repulsive energy. From this subsection, it can be deduced that the acceptor impurity decreases the period of Fractional Aharanov-Bohm oscillation while the donor impurity acts inversely and increases the Fractional Aharanov-Bohm oscillation period.

CONCLUSION

In this paper, the effects of on-center donor and acceptor impurities on the Aharonov-Bohm oscillations of energy spectra are investigated for single and two-interacting electrons by using exact diagonalization method. It is found that the on-center donor increases the Aharonov-Bohm oscillation period while the acceptor impurity acts inversely and decreases it. In addition, the effects of magnetic field, centrifugal and confinement potentials on the binding energies of on-center donor and acceptor impurities are studied. The results show that the binding energy increases by increasing the magnetic field while it decreases by increasing the centrifugal and confinement potentials. These results are useful for deeper understanding of the effects of on-center donor on concentric DQRs which are fabricated by tip oxidation technique.

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