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Effective tuning of electron charge and spin distribution in a dot-ring nanostructure at the ZnO interface

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A B S T R A C T

Electronic states and the Aharonov-Bohm effect in ZnO quantum dot-ring nanostructures containing few interacting electrons reveal several unique features. We have shown here that in contrast to the dot-rings made of conventional semiconductors, such as InAs or GaAs, the dot-rings in ZnO heterojunctions demonstrate several unique characteristics due to the unusual properties of quantum dots and rings in ZnO. In particular the energy spectra of the ZnO dot-ring and the Aharnov-Bohm oscillations are strongly dependant on the electron number in the dot or in the ring. Therefore even small changes of the confinement potential, sizes of the dot-ring or the magnetic field can drastically change the energy spectra and the behavior of Aharonov-Bohm oscillations in the system. Due to this interesting phenomena it is possible to effectively control with high accuracy the electron charge and spin distribution inside the dot-ring structure. This controlling can be achieved either by changing the magnetic field or the confinement potentials.

Semiconductor quantum dots (QDs) and quantum rings (QRs), nanostructures with remarkable similarity to atomic systems, have been extensively investigated for many years given their potential as building blocks for novel devices, such as nanoemitters, efficient solar cells, terahertz detectors etc. [1–5]. These type of nanostructures are so attractive due to the ability to tune their optoelectronic properties by carefully designing their size, composition, strain and shape. In this context, QRs with their doubly-connected structure attracts special attention. Its unique topological structure provides a rich variety of fascinating physical phenomena in this system. Observation of the Aharonov-Bohm (AB) oscillations [6] and the persistent current [7] in small semiconductor QRs, and recent experimental realization of QRs with only a few electrons [8,9] have made QRs an attractive topic of experimental and theoretical studies for various quantum effects in these quasi-one-dimensional systems [10].

Recently an increasing demand can be observed for the realization of complex quantum confined systems, such as laterally coupled QDs, QRs and quantum dot-ring (QDR) complexes [11–13]. These complex structures are very attractive for both practical applications and fundamental studies, including geometrical quantum phase [14], spin-spin interactions [15] and quantum state couplings [16]. Due to the unique topology of the QDR structures the theoretical investigation of their properties has received much attention in recent years. For example in Ref. [17] a few-electron system confined in a QDR in the presence of an external magnetic field have been investigated. It has been shown that the distribution of electrons between the dot and the ring can be influenced by the relative strength of the dot-ring confinement and the magnetic field. As a result transitions of electrons between the two parts of the system can be observed. These transitions are accompanied by changes in the periodicity of the AB oscillations. It has been recently shown [18–20] that spin relaxation, optical absorption and many other measurable properties of a QDRs, can be significantly changed by modifying the confinement potentials. This demonstrates the high controllability and flexibility of QDR systems. Theoretical studies of the dc current through a QDR in the Coulomb blockade regime have revealed that it can efficiently work as a single-electron transistor or a current rectifier [21]. In our recent works the electronic and optical properties of QDRs with hydrogenic donor impurity were investigated in external electric and magnetic fields [22–24].

In the past few years, very exciting developments have taken place with the creation of high-mobility 2DEG in heterostructures involving insulating complex oxides. Particularly the fractional quantum Hall effect in MgZnO/ZnO heterostructures grown by molecular-beam epitaxy, has been observed, in which the electron mobility exceeds 180000 $cm^2\ V^{-1}s^{-1}$ [25]. Also technological advance in all oxide electronics has been demonstrated, which provides opportunities to explore strongly correlated phenomena in quantum transport of dilute carriers. Also it has been shown that electrons are strongly correlated in such systems [26]. Many surprising results were found in the fractional quantum Hall states [27] discovered in the MgZnO/ZnO heterojunction [28,29], in particular, in tilted magnetic fields [28,30,31].

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ZnO also is a perfect material for creation of various semiconductor nanostructures. Preparation of various nanostructures such as nanorings, nanobelts, nanowires etc, using a solid-vapor phase thermal sublimation technique, have been reported in Ref. [32]. Preparation of self-assembled ZnO quantum dots with tunable optical properties have been reported in Ref. [33]. It has been stressed there that electron correlation effects are strong in these systems due to the increased electron effective mass and reduced dielectric constant of ZnO. In our earlier reports, electronic, optical and magnetic properties of ZnO QDs and QRs were investigated [34,35]. We have shown that for both systems the electron-electron interaction effects are much stronger then in traditional semiconductor quantum systems, such as InAs or GaAs. On the other hand the AB effect in a ZnO QR strongly depends on the electron number [35]. In fact, for two electrons in the ZnO ring, the AB oscillations become aperiodic, while for three electrons the AB oscillations completely disappear. Therefore, unlike in conventional quantum ring topology, here the AB effect (and the resulting persistent current) can be controlled by varying the electron number. Taking into account these surprising and interesting results, here we report on our studies of the electronic states and the AB effect in a ZnO QDR containing few electrons. We have shown that in such systems it is possible to control with high accuracy the electron charge and spin inside the dot or the ring at the single- electron level.

Let us consider a two dimensional quantum dot-ring structure with cylindrical symmetry, based on the 2DEG at the ZnO interface, containing few interacting electrons. The Hamiltonian of our system is

$$\mathcal{H} = \sum_{i}^{N_e} \mathcal{H}_{\mathrm{SP}}^{i} + \frac{1}{2}\sum_{i\neq j}^{N_e} V_{ij}, \tag{1}$$

where N_e is the number of electrons in the QDR, $V_{ij} = e^2/\epsilon|\mathbf{r}_i - \mathbf{r}_j|$ is the Coulomb interaction term, with dielectric constant of the material ϵ. The single-particle Hamiltonian $\mathcal{H}_{\mathrm{SP}}$ in the presence of an external perpendicular magnetic field will have the form

$$\mathcal{H}_{\mathrm{SP}} = \frac{1}{2m}\left(\mathbf{p} - \frac{e}{c}\mathbf{A}\right)^2 + V_{\mathrm{conf}}(r) + \frac{1}{2}g\mu_B B\sigma_z, \tag{2}$$

where $\mathbf{A} = B/2\ (-y, x, 0)$ is the vector potential, and m is the electron effective mass. The last term of (2) is the Zeeman splitting. We choose the confinement potential of the QDR consisting of double parabolas [17,24]. $V_{\mathrm{conf}}(r) = \min\left[\frac{1}{2}m\omega_{\mathrm{d}}^2 r^2,\ \frac{1}{2}m\omega_{\mathrm{r}}^2(r-R)^2\right]$, where ω_{d} and ω_{r} are the parameters describing the strength of the confinement potential and also the sizes of the dot and the ring respectively. The radius of the ring R is defined as the sum of oscillator lengths for the dot and ring related wells and the barrier thickness d between dot and ring according to $R = \sqrt{2\hbar/m\omega_d} + \sqrt{2\hbar/m\omega_r} + d$. In Fig. 1 the QDR confinement potential is presented schematically.

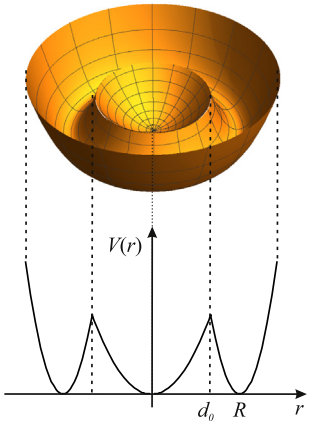

Fig. 1. The schematic picture of QDR confinement potential.

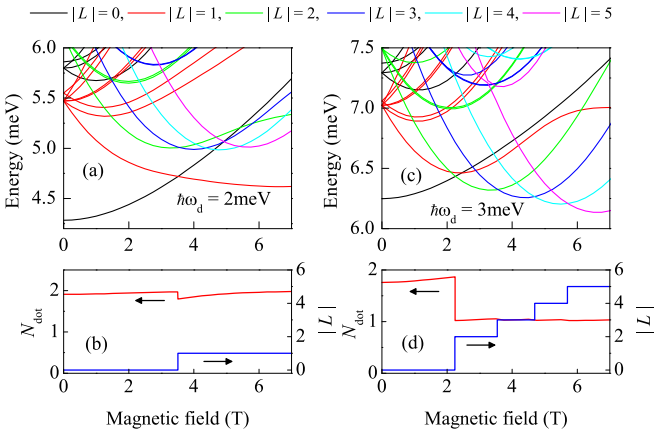

Fig. 2. Magnetic field dependencies of two-electron energy spectra, the corresponding average electron number in the dot (left scales of lower row) and the ground state angular momenta (right scales of lower row) for $\hbar\omega_d = 2$ meV (a), (b) and for $\hbar\omega_d = 3$ meV (c), (d). All results are for $\hbar\omega_r = 8$ meV and $d = 10$ nm.

We have used exact diagonalization technique with the basis of wave functions of the cylindrical QD with larger radius in order to determine the eigenfunctions and the eigenenergies of the single-electron Hamiltonian (2). We have used the exact diagonalization scheme also to calculate the energy spectra and wave functions of few-electron QDR, which is very accurate and widely used by many authors [1]. In this case we diagonalize the matrix of the Hamiltonian (1) in a basis of the Slater determinants constructed from the single-electron basis functions [35]. In our model we have used 132 single- electron basis states. As a result we got 8646 two-electron states and 374660 three-electron basis states which is adequate for determining the first few energy eigenvalues for each value of the total angular momentum of electrons with high accuracy.

In order to determine the average electron numbers in the dot or in the ring we have also studied the electron densities for few-electron states in the QDR $\rho(\mathbf{r}) = \int d\mathbf{r}_2 d\mathbf{r}_3 \ldots |\Psi_i(\mathbf{r}, \mathbf{r}_2, \mathbf{r}_3, \ldots)|^2$, where $\Psi_i(\mathbf{r}, \mathbf{r}_2, \mathbf{r}_3, \ldots)$ is the wave function of the few-electron state i. For the average electron number in the dot region of QDR we get $N_{\mathrm{dot}} = \int_0^{d_0}\int_0^{2\pi}\rho(\mathbf{r})rdrd\varphi$, where $d_0 = \omega_r R/(\omega_{\mathrm{d}} + \omega_{\mathrm{r}})$ is the radius of the border between the dot and the ring.

Our investigations were carried out for the ZnO QDR with parameters $m = 0.24\ m_0$, $g = 4.3$, $\epsilon = 8.5$ [36]. In Fig. 2(a) The magnetic field dependence of the first few energy levels are presented for two-

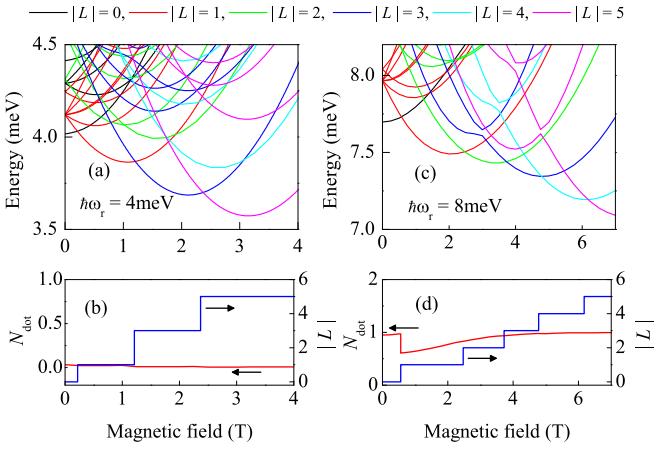

Fig. 3. Magnetic field dependencies of two-electron energy spectra, corresponding average electron number in the dot (left scale of lower row) and ground state angular momenta (right scales of lower row) for $\hbar\omega_r = 4$ meV (a), (b) and for $\hbar\omega_r = 8$ meV (c), (d). All results are for $\hbar\omega_d = 4$ meV and $d = 10$ nm.

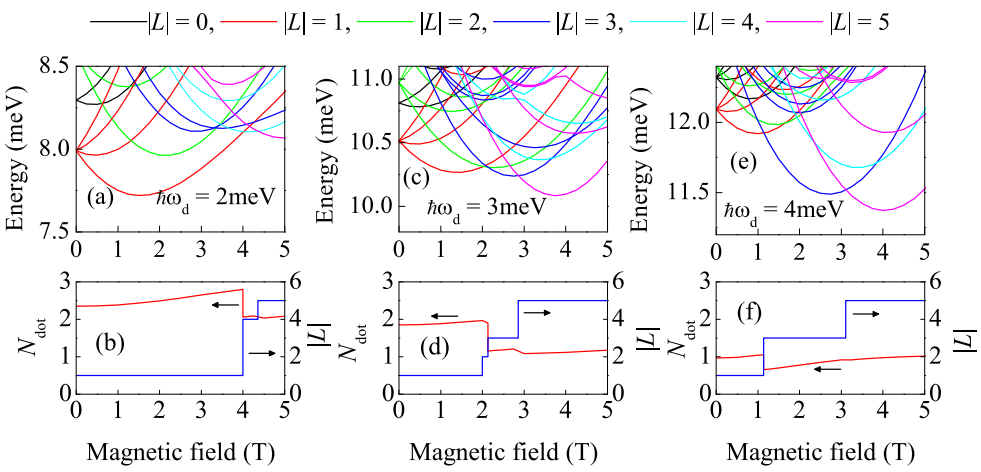

Fig. 4. Magnetic field dependencies of three-electron energy spectra, corresponding average electron number in the dot (left scales of lower row) and ground state angular momenta (right scales of lower row) for $\hbar\omega_d = 2$ meV (a), (b), for $\hbar\omega_d = 3$ meV (c), (d) and for $\hbar\omega_d = 4$ meV (e), (f). All results are for $\hbar\omega_r = 8$ meV and $d = 10$ nm.

electron QDR with $\hbar\omega_d = 2$ meV, $\hbar\omega_r = 8$ meV, $d = 10$ nm for various values of the total angular momenta L. In Fig. 2(b) corresponding ground state average electron number in the dot (left scale, red line) and the ground state angular momentum (right scale, blue line) are presented. From these figures it is clear that for all values of the magnetic field, both electrons are localized in the dot region and the ground state behaves like in a two-electron single QD [34]. For weak values of the magnetic field the ground state is a singlet state with angular momentum $L = 0$ and total spin $S = 0$. With the increase of the magnetic field, at $B \approx 3.5$ T, a singlet-triplet transition of the ground state is observed to the state $L = -1$, $S = -1$. Similar results are presented also in Fig. 2(c) and (d) but for $\hbar\omega_d = 3$ meV. In this case again for weak values of the magnetic field both electrons are located in the dot region, but starting from $B \approx 2.2$ T one of the electrons moves to the ring region (Fig. 2(d) red line) and the ground state changes to the triplet state $L = -2$, $S = -1$. Starting from 2.2 T the behavior of the energy spectra in Fig. 2(c) changes drastically and the regular periodic AB oscillations of the ground state can be observed with periodic change of the total angular momentum by $\Delta L = 1$. This result is qualitatively similar to the case of one-electron ZnO QR, observed in our previous work [35], but in contrast to that now all AB oscillations occur between the triplet states.

Fig. 3 is the same as Fig. 2 but for a fixed value of $\hbar\omega_d = 4$ meV and for two values of the ring confinement parameter $\hbar\omega_r = 4$ meV (Fig. 3(a) and (b)) and $\hbar\omega_r = 8$ meV (Fig. 3(c) and (d)). For $\hbar\omega_r = 4$ meV both electrons are localized in the ring (Fig. 3(b)) and the energy spectra is similar to the one of the two-electron ZnO QR previously observed in Ref. [35]. In this case irregular AB oscillations are observed and the singlet-triplet crossings disappear from the ground state, which is typical for ZnO QRs. With the increase of magnetic field all obserrossings of the ground states occur only between triplet states with odd number of total momentum. With the increase of $\hbar\omega_r$ one of the electrons moves to the dot region (Fig. 3(d)) while the other remains in the ring. In this case the magnetic field almost does not change the average electron number in the dot, and therefore we observe almost regular AB oscillations similar to ZnO QR with one electron (Fig. 3(c)).

The energy spectra and average electron numbers in the dot region are presented in Fig. 4 against the magnetic field for a QDR containing three electrons for fixed value of $\hbar\omega_r = 8$ meV and for various values of $\hbar\omega_d$. For $\hbar\omega_d = 2$ meV (Fig. 4(a) and (b)) and for weak magnetic fields all three electrons are mostly located in the dot region, the ground state is $L = -1$, $S = -1/2$ and AB oscillations are not observed. But at $B \approx 4$ T one of the electrons moves to the ring region and the ground state changes to $L = -4$, $S = -3/2$. Starting from $B \approx 4$ T the usual AB effect appears.

For $\hbar\omega_d = 3$ meV (Fig. 4(c) and (d)) without the magnetic field, only two electrons are located in the dot and one in the ring region. With an increase of the magnetic field we can observe a charge switching between the dot and the ring of the QDR. At $B \approx 2.1$ T the electron number in the dot changes to 1 and the irregular AB effect is observed with odd angular momenta $|L| = 3, 5\ldots$.

Finally, for $\hbar\omega_d = 4$ meV (Fig. 4(e) and (f)) and for all observed range of the magnetic field, only one electron is located in the dot region and the other two stays in the ring. Therefore, in Fig. 4(e) the irregular AB oscillations are observed for the ground state, similar to the case of two-electron ZnO QR, as we found earlier [35].

To summarize: we have studied the electronic states and the Aharonov-Bohm effect in ZnO quantum dot-ring nanostructures containing few electrons. We have shown that in contrast to QDRs of conventional semiconductors, such as InAs or GaAs, QDRs in ZnO heterojunctions demonstrate several unique characteristics. In particular the energy spectra of the ZnO QDR and the Aharnov-Bohm oscillations are strongly dependant on the electron number in the dot or in the ring. Therefore even small changes of the confinement potential, sizes of the dot-ring or magnetic field can drastically change the energy spectra and the behavior of Aharonov-Bohm oscillations in the system. Due to this interesting phenomena it is possible to effectively control with high accuracy the electron charge and spin distribution inside the dot-ring structure. These unique properties will certainly have important implications for possible applications in spintronic devices and quantum information technologies.

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