Charge transport through a semiconductor quantum dot-ring nanostructure

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Abstract
Transport properties of a gated nanostructure depend crucially on the coupling of its states to the states of electrodes. In the case of a single quantum dot the coupling, for a given quantum state, is constant or can be slightly modified by additional gating. In this paper we consider a concentric dot–ring nanostructure (DRN) and show that its transport properties can be drastically modified due to the unique geometry. We calculate the dc current through a DRN in the Coulomb blockade regime and show that it can efficiently work as a single-electron transistor (SET) or a current rectifier. In both cases the transport characteristics strongly depend on the details of the confinement potential. The calculations are carried out for low and high bias regime, the latter being especially interesting in the context of current rectification due to fast relaxation processes.

Keywords: quantum dot, quantum ring, transport

1. Introduction

In order to meet growing demand for small-scale, low-power consuming devices one has to downscale transistors and logic circuits and to work with a small number of carriers. The natural limit for lowering carrier density is single charge electronics, where phenomena such as electric current flow can be controlled with single-electron precision [1, 2]. Contrary to modern mass production electronics, single- and few-electron devices exhibit purely quantum mechanical effects such as resonant tunneling [1–5] or quantum entanglement [6–8]. Apart from direct applications in nanoelectronics they are also perfect tools for probing fundamental problems in single- and many-body physics. During the last decade a lot of research has been devoted to studying the electronic properties of quantum dots (QDs) [5, 9–14]. For sufficiently low temperatures the discreteness of the energy spectrum of these systems can be clearly visible in transport experiments as Coulomb peaks [1, 4, 15, 16] that demonstrate successive charging and discharging of the QD by single electrons. The Coulomb blockade phenomenon, where the charging energy forbids an electron to jump to the QD, is the basis for most of the applications of QDs [17–19]. Quantum dots arranged into double, triple or more complex systems [20–28] exhibit an abundance of quantum states which manifest themselves, e.g. in Pauli spin blockade [29, 30] current or heat rectification [13] effects.

Another class of interesting quantum systems are quantum rings (QRs) [31–35]. Due to their difference from QDs geometry the phenomena observed in QRs are very sensitive to phase coherence of the electronic wave function. These are, e.g. the Aharonov–Bohm effect demonstrating modification of the electron wave function by a vector potential [36] or persistent currents, i.e. ground state currents that flow in QR even without an external magnetic field [37–39].

In this paper we focus on a complex nanostructure that combines the two above-mentioned, topologically different components: a quantum dot and a quantum ring. The constituents are
aligned concentrically (QD is surrounded by QR) so that the system conserves the circular symmetry. The dot–ring nanostructure (DRN) has already been fabricated by pulsed droplet epitaxy \[40, 41\] with full control of the growth process. It can also be made by using an atomic force microscope to locally oxidize the surface of a sample \[12\] or by lithography.

It has been recently shown \[42, 43\] that many measurable properties of a DRN, such as spin relaxation or optical absorption, can be widely changed by a modification of the confinement potential of the DRN demonstrating its very high controllability and flexibility. These characteristics are mostly determined by the relative distribution of the wave functions in a DRN that, in turn, can be changed by external gates or fields. The purpose of this study is to demonstrate that the conducting properties of a DRN are also very sensitive to the details of confinement. Unlike field effect transistors, single-electron devices are based on an intrinsically quantum phenomenon, namely the tunnel effect. In this case, transport properties are mostly determined by the tunneling rates $\Gamma$’s, which depend on the overlap of the DRN states with the states of the electrodes. These parameters, in turn, depend crucially on the localization of the electron wave function: states localized in QD (QR) are weakly (strongly) coupled to the electrodes. Thus, $\Gamma$’s may strongly depend on the quantum state and have to be determined for each state individually. This property demonstrates one of the advantages of the DRN over QDs, where the possible changes in the couplings are orders of magnitude smaller.

We discuss charge transport through a DRN in the Coulomb blockade regime near the $N = 0 \rightarrow 1$ transition, i.e. when only one electron at a time can tunnel through a DRN between the source (S) and drain (D) electrodes. Throughout this paper we assume the magnetic field $B = 0$ and therefore neglect the electron spin. We show that one can tune the device parameters so that it can work as: (i) single-electron transistor (SET) \[4, 44\] and (ii) electrical current rectifier. The paper is organized as follows: in section 2 we present a general theoretical background that will be needed to study the transport properties of DRNs. In section 3 we demonstrate how by changing the parameters of the confinement potential we can control single-electron tunneling. In section 4 we demonstrate that a DRN can be used as a current rectifier. The results are summarized in section 5.

2. Basic formulas and mechanisms

We consider a quasi-two-dimensional circularly symmetric dot–ring nanostructure. The DRN, placed in the $xy$ plane, is defined by a specific confinement potential, that we will discuss below. We assume that the confinement in the $z$ (growth) direction is much stronger than the lateral confinement and consequently, the $xy$-plane motion and the vertical one can be decoupled. Then, we can write the electron wave function as a product

$$\psi(r) = \psi_f(r)\psi_z(z),$$

where the vector $r$ lies in the $xy$-plane. Additionally, we assume that the electron is always in the lowest energy state of a quantum well in the $z$ direction and that the potential of the well in the $z$ direction is infinite. With these assumptions $\psi_z(z)$ is given by

$$\psi_z(z) = \sqrt{\frac{2}{d}} \cos\left(\frac{\pi z}{d}\right),$$

where $d$ is the height of the structure.

In order to discuss the in-plane confinement potential that forms the DRN we introduce the following notation $|r| = |(x, y)| = r$. Then the DRN is defined by a potential $V(r)$ and occupied by a single electron. The DRN is composed of a QD surrounded by a QR and separated from the ring by a potential barrier $V_d(r)$. A cross section and a top view of a DRN with an explanation of the symbols used throughout the text are presented in figure 1.

![Figure 1. The cross section and the top view of the potential forming the DRN with the marked bottom of the QD potential ($V_QD$), the bottom of the QR potential ($V_{QR}$), the top of the barrier potential ($V_0$), and the value of the potential outside the DRN ($V_0$). We assume the bottom of the quantum ring part as a reference value ($V_{QR} = 0$). This figure shows a DRN with the bottom of the QD below the bottom of the QR ($V_{QD} < 0$), but also the opposite situation ($V_{QD} > 0$) is possible.](image)

In particular, we assume in our model calculations the radius of the DRN $r_0 = 70$ nm. The depth of the quantum well forming the DRN is $V_t = 90$ meV and the zero potential energy is set at the level of $V_{QR}$, i.e. the potential well offset is equal to $V_{QD}$. The calculations are performed for InGaAs systems (with the effective electron mass $m^* = 0.067 m_e$). The results are presented for $V_0 = 20$ meV and for the sample thickness $d = 5$ nm, if not stated otherwise.

We solve numerically the Schrödinger equation assuming the Gaussian form of $V(r)$ \[42\]. The energy spectrum consists of a set of discrete states $E_n$ due to radial motion with radial quantum numbers $n = 0, 1, 2, \ldots$, and rotational motion with angular momentum quantum numbers $l = 0, \pm 1, \pm 2, \ldots$. The energy spectrum as a function of $V_{QD}$ is shown in figure 2. The states situated in QD exhibit an increase in the energy
with increasing $V_{QD}$, whereas those situated in QR have the energy (nearly) constant. The single-particle wave function in the $xy$-plane, i.e. the DRN plane, is of the form

$$
\psi_k(r) \equiv \Psi_{nl}(r, \phi) = R_{nl}(r) \exp(i\phi),
$$

with the radial part $R_{nl}(r)$.

As already mentioned, the main advantage of the DRN is the controllability of the shape and the distribution of the electron wave functions. For instance, if the minimum of the potential of the QR part $V_{QD}$ is much deeper than the potential of the QR, the electrons are located mainly in the QD and the effective size of the ground state (G) wave function is small. On the other hand, if the ring’s potential $V_{QR}$ is much deeper, electrons occupy mostly states in the QR part and the G wave function is much broader. What is more, by fine-tuning the confinement potential we can control positions of individual states. This way we are able to have, e.g. the ground state located in the QD, whereas the first excited state (E) in is the QR and so on. The distributions of the wave functions of the two lowest energy states for three different values of $V_{QD}$ are presented in figure 3. One can see there the case where both the G and E wave functions are in the QD for $V_{QD} = -4$ meV (figure 3(a)), the E wave function is in the QR, whereas the G wave function is still in the QD for $V_{QD} = 1$ meV (figure 3(b)), and finally, for $V_{QD} = 5$ meV both the G and E wave functions are in the QR (figure 3(c)).

The DRN is coupled via tunnel barriers to the S and D electrodes. We assume that one or a few ($n_0$) single-electron states are in the bias window

$$
\mu_S > \epsilon_i > \mu_D, \quad i = 0, \ldots, n_0 - 1,
$$

where $\mu_S$ and $\mu_D$ are the respective chemical potentials, $i$ represents a set of quantum numbers $(n, l)$ and we start the numbering of the energy levels from $i = 0$ ($n = 0$, $l = 0$) (the ground state). Charge transport through a DRN depends crucially on the coupling strength of its states to the electrodes, which is dependent on the wave function overlap that enters the electron tunneling matrix element. Because we are able to control the shape and distribution of the DRN wave functions, we can control the overlap, which, in turn, allows us to control the transport properties.

The tunneling rates $\Gamma$’s are calculated microscopically for each state independently. We follow Bardeen’s approach [45], where

$$
\Gamma(\epsilon) = 2\pi \sum_k |q_k|^2 \delta(\epsilon - \epsilon_k).
$$

Within the framework of this method two separate sets of states are considered: one solves the Schrödinger equation for the DRN and one for the electrode. It is implicitly assumed that the wave functions of the two subsystems are orthogonal. Enforcing this assumption the Bardeen tunneling matrix element in two dimensions is given by

$$
t_{k} = \frac{\hbar}{2m^*} \int_{-\infty}^{\infty} dy \left[ \psi^*_k(r) \frac{\partial \psi_{nl}(r)}{\partial x} - \psi_{nl}(r) \frac{\partial \psi^*_k(r)}{\partial x} \right],
$$

where $\psi_k(r)$ are wave functions in the electrode and $\psi_{nl}(r)$ are wave functions in the DRN. The electrodes are modelled as half-planes with wave functions given in the appendix A. The integral is calculated along the line $x = x_0$ (see figure 4). The explicit form of $t_k$ is also given in the appendix A.

### 2.1. Phonon relaxation in a DRN

When more than one state is included in the transport process one has to take into account mechanisms that allow transitions between the states, i.e. relaxation to the lower energy states. One of the most important and unavoidable mechanisms of scattering in solid state systems is the interaction with lattice phonons. For low-dimensional semiconducting systems such as QDs and QRs the dominant process is the electron–acoustic phonon interaction. This is because the energy distance between the electronic states is small compared to the optical phonon energy [33, 46, 47].

In this section we calculate phonon emission relaxation rates due to interaction of an electron with piezoelectric (PZ) and deformational (DF) phonons. The electron–phonon scattering rate due to transition from the initial state $\psi_i(r)$ to the final state $\psi_f(r)$ with the emission of an acoustic phonon can be calculated using Fermi’s golden rule ($w_{i\rightarrow f} \equiv \tau^{-1}_{i\rightarrow f}$).

$$
w_{i\rightarrow f} = \frac{2\pi}{\hbar} \sum_{q, \lambda} \left| \langle \psi_f | W_{\lambda}(q) | \psi_i \rangle \right|^2 \delta(E_f - E_i - \hbar\omega_q),
$$

where $q$ is the phonon wave vector, $E_f$ ($E_i$) is the energy of the final (initial) electron state, $\hbar\omega_q$ is the energy of a phonon, and $\lambda$ is the polarization index. The interaction operator $W_{\lambda}(q)$ is given by

$$
W_{\lambda}(q) = \Lambda_{\lambda}(q) e^{-i q \cdot \phi},
$$
is the total scattering matrix element \[33\] /uni2223/

\[0\] /uni210F/uni03B0/uni2223/

\[2\] /uni03C0\]

\[\cdot \] where \(\theta\) is the angle between the DRN and the electrodes.

\[
\Lambda_\mu(q) = \sum_{\nu=LA,TA} \Lambda_{\mu\nu}(q)^2.
\]

Because in this paper we focus mainly on transport properties of the DRN, we follow the reference \[33\] and use the angular averaged piezoelectric coupling matrix element for longitudinal and transverse phonon modes. Thus, the total electron–phonon scattering matrix element can be written as \[33, 48\]

\[
\Lambda(q)^2 = \frac{h}{2peV|q|} (D^2|q|^2 + P),
\]

where \(D(P)\) is the deformational (piezoelectric) potential constant, \(p\) is the crystal density, \(c\) is the sound velocity, and \(V\) is the volume. After \[33, 48\] we assume \(D = 2.2 \times 10^{-18}\) J and \(P = 5.4 \times 10^{-20}\) J/m\(^2\). The total relaxation rate from state \(n'l'\) to state \(nl\) at \(T = 0\) can be written as

\[
w_{nl'\rightarrow nl} = \frac{1}{4\pi^2 \hbar^2 c^2 \omega_0 q_0'^2 (D^2 q_0'^2 + P)} \int_0^{2\pi} \int_0^d d\theta d\sin \theta \times \left\{ \int_0^\infty dr \int_0^{2\pi} d\phi' e^{(r-r')2}\cos (\phi' - \phi) \cdot R_{nl'}(r) R_{nl}(r) \right\}^2
\]

\[
\times \frac{2}{d} \int_{d/2}^d \cos^2 \left( \frac{x}{d} \right) e^{-i \omega t \theta} \frac{\sin^2 \theta}{d^2} dz
\]

(11)

where \(q_0 = (E_{nl'} - E_{nl})/hc\) and \(R_{nl}(r)\) is the radial part of the in-plane electron wave function \(\psi_{nl}(r)\). The integral over \(z\) is given by

\[
f(x) = \frac{\sin x}{x^2}
\]

(12)

and the integral over \(\phi'\) can be expressed by the Bessel function. Finally, the relaxation rate can be written as

\[
w_{nl'\rightarrow nl} = \frac{2\pi}{\hbar^2 c^2 \omega_0 q_0'^2 (D^2 q_0'^2 + P)} \int_0^{2\pi} d\theta d\sin \theta F_{nl'\rightarrow nl}(\theta).
\]

(13)

where

\[
F_{nl'\rightarrow nl}(\theta) = f\left( \frac{1}{2} d q_0 \cos \theta \right) \int_0^\infty dr J_{nl'}(q_0 r \sin \theta) \cdot R_{nl'}(r) R_{nl}(r)
\]

(14)

Apart from material constants the factors that affect this rate are the energy gap between states \(n'l'\) and \(nl\), i.e. \(E_{nl'} - E_{nl}\), the mutual distribution of the wave functions given by \(R_{nl}(r)\) and \(R_{nl'}(r)\), and the thickness of the structure \(d\). Function \(F_{nl'\rightarrow nl}(\theta)\) describes how phonons emitted in different directions contribute to the relaxation process. The relaxation through phonons emitted at a given angle \(\theta\) depends on \(d\) through function \(f\) given in equation (12). On the one hand, since its argument is \(\frac{1}{2} d q_0 \cos \theta\) the relaxation is independent of the thickness \(d\) for phonons with wave vectors parallel to the \(xy\) plane (\(\theta = \pi/2\)). On the other hand, there is a strong dependence of the relaxation rate on \(d\) for phonons emitted
in the direction perpendicular to the nanostructure. Figure 5 shows $f^2(x)$. One can see that for $\theta = 0$ a significant contribution to the relaxation comes only from phonons with wavelengths larger than $d$.

Figure 6 shows the square of the function $F$ given by equation (14) for $d = 5$ nm. The value of $q_0$ and the radial parts of the wave functions $R_{nl}(r)$ and $R_{nl}'(r)$ have been calculated for two different values of $V_{QD}$. In the case presented in the left panel ($V_{QD} = -6$ meV) the bottom of the QD potential is much further below the bottom of the QR potential. Therefore, the wave functions are situated mainly in the QD part of the DRN, where the energy level spacing is large (see figure 2). On the other hand, the right panel presents the case of $V_{QD} = 6$ meV, where the bottom of the QD potential is above the bottom of the QR potential. In this situation the wave functions are situated mainly in the QR part of the DRN and, as inferred from figure 2, the level spacing is small. Figure 6 allows one to analyze the directions of the phonons emission in two presented cases. Namely, in the left panel ($V_{QD} = -6$ meV) function $F^2_{nl}(\theta)$ describing the phonon emission is peaked within the range of low values of $\theta$. This indicates that the phonons are emitted mostly perpendicularly to the DRN, which is the direction of the strongest confinement [46]. In the complementary case presented in the right panel ($V_{QD} = 6$ meV), it is not possible to point out a specific direction of emission (it varies with a particular transition $nl' \rightarrow nl$, note the difference in the scales on the horizontal axes).

Figure 7 shows typical examples of how the relaxation rates are affected by changing the position of the bottom of the QD potential $V_{QD}$ from below to above the bottom of the QR potential ($V_{QR} = 0$). Figure 7(a) shows the relaxation rate from state $(n = 0, l = 1)$ to the ground state $(n = 0, l = 0)$. For large negative value of $V_{QD}$ both the wave functions $\Psi_{01}$ and $\Psi_{10}$ are positioned in the QD, which gives fast relaxation with rates $w$ of the order of GHz. With increasing $V_{QD}$ the excited state moves over to the QR leading to the decrease in the overlap between the wave functions which, in turn, results in the decrease of $w$. For further increased $V_{QD}$ both the ground and the excited states are situated in the QR, the overlap increases, and the relaxation rate increases again. Figure 7(b) presents the relaxation rate from state $(n = 1, l = 0)$ to the ground state. In this case for small $V_{QD}$ the ground state is localized in the QD, while the excited state $(n = 1, l = 0)$ is mostly positioned in the QR. Therefore, the overlap of the corresponding wave functions is small, which in turn results in a slow relaxation. With the increase of $V_{QD}$ the ground state starts to move over to the QR and the overlap with $\Psi_{10}$ starts to rise. One observes this as a sharp increase in the relaxation rate $w_{10 \rightarrow 01}$. However, with a further increase of $V_{QD}$ the ground state remains in the QR, yet the excited state moves over to the QD and changes sign. This altogether causes the decrease in the relaxation rate. Figure 7(c) presents the relaxation rate between states $(n = 1, l = 0)$ and $(n = 0, l = 1)$, a transition that is a part of an indirect relaxation process. What is clearly visible at first glance is the abrupt decrease of $w_{10 \rightarrow 01}$ when the states cross (compare figure 2). In the range of $V_{QD}$ from $-2$ meV to $2$ meV the overlap between $\Psi_{10}$ and $\Psi_{01}$ is strong. Thus, the resulting values of the relaxation rate are high.

As already mentioned, the phonon emission at different angles is strongly dependent on the distribution of the wave functions (see figure 6). This, in turn, affects the dependence of the relaxation rates on the sample thickness $d$. In figure 8 we present the relaxation rate $w_{01 \rightarrow 00}$ as a function of $V_{QD}$. Its dependence on $d$ is pronounced for low values of $V_{QD}$, when the wave functions are situated mainly in the QD region of the DRN. In accordance with what was reported in [33] for QDs, we also observe oscillations of the relaxation rates as a function of the sample thickness $d$ in the range of negative values of $V_{QD}$ (yet in figure 8 we present only a part of the noted oscillations). In the range of low values of $V_{QD}$ the level spacings are of the order of single meVs (figure 2). The corresponding wavelengths of the emitted phonons are of the order of the sample thickness (a couple of nm). This match results in the strong increase in the relaxation rates for such $V_{QD}$. In the complementary range of $V_{QD}$, where the bottom of the QD potential is above the bottom of the QR potential, the level spacings are of order of 0.1 meV. Then, the corresponding wavelengths of the emitted phonons are significantly larger than the sample thickness and we do not observe any strong dependence of $w_{01 \rightarrow 00}$ on the thickness of the structure $d$. Additionally, we would like to stress the strong dependence of the relaxation rates for all other transitions $w_{nl' \rightarrow nl}$ on $d$ (not shown).

3. Single-electron transistor

We are now ready to discuss the transport properties of the DRN. We evaluate the current given the energy spectrum and the subsequent relaxation and tunnel rates. We discuss below the sequential tunneling current in the Coulomb blockade regime near the $N = 0 \leftrightarrow 1$ transition and neglect higher order tunneling events [49]. In the pure quantum dot case a single-electron transistor (SET) is switched to the conducting state when some energy level, shifted by gate voltage, enters the bias window. The current then exhibits the current peak [5]. In case of the DRN the mechanism is different. We keep one or a few states in the bias window and manipulate the distribution of the wave functions to get a proper transistor behavior. The principle of operations is to control the energy states and tunnel couplings by means of gate voltages $V_{QD}$ and $V_{0}$. Many investigations of transport behavior make use of the high tunability of the tunnel barriers by applying voltage pulses [49]. In our approach we utilize instead the high tunability of the
electron states in the DRN while keeping the barrier parameters constant. We assume that the bias window is smaller than the charging energy $E_C$, so that only a single electron at a time can be transmitted through the DRN, $\mu_S - \mu_D < E_C$. In order to determine for what values of the model parameters this condition can be fulfilled we calculate $E_C$ for the DRN. The interaction energy of two particles confined in the potential $V(r)$ was calculated using the configuration interaction approach [50], which is an exact diagonalization method for solving the nonrelativistic Schrödinger equation for a multi-particle system. From the single-particle orbitals $\Psi_{nl}$ we constructed the basis of the Slater determinants $|S_\nu>$. Then, the two-particle Hamiltonian was diagonalized and the exact eigenstates were found, where the $\nu$-th eigenfunction is in the form of the linear combination of the Slater determinants:

**Figure 6.** Square of the function $F_{a'\alpha,\alpha}(\theta)$ given by equation (14) for two different values of $V_{QD}$ for a DRN with $d = 5$ nm.

**Figure 7.** Illustrations of the dependence of different relaxation rates on $V_{QD}$ for $d = 5$ nm. See the text for an explanation.

**Figure 8.** Relaxation rate $w_{\nu_1 \rightarrow \nu_0}$ as a function of $V_{QD}$ for different values of sample thickness.
were calculated by the two-particle Hamiltonian diagonalization. In figure 2 the energy $E_C$ of the lowest two-particle state is shown by the black dotted line as a function of $V_{QD}$. It can be seen there that for the analyzed range of $V_{QD}$, $E_C$ is larger then the five lowest single-particle levels.

The current through the DRN is calculated with the help of the rate equations. Assuming that $n_0$ energy levels lie in the bias window $\mu_S - \mu_D$, the time evolution of the occupation probability $\rho_j$ of a given DRN state $j$ can be expressed by the following formula:

$$\dot{\rho}_j = \frac{1}{\hbar} \sum_{\mu} c_{\mu j} \langle \rho_\mu \rangle.$$  \hspace{1cm} (15)

Coefficients $c_{\mu j}$ were calculated by the two-particle Hamiltonian diagonalization. The vertical line represents the transfer of an electron from the source electrode to state $j$ (from state $j$ to the drain electrode). The solid (dotted) lines represent relaxation from states above state $j$ to state $j$ (from state $j$ to states below state $j$).

Indices $i$ and $j$ denote pairs of quantum numbers $(n, l)$ with $i = 0$ describing the ground state $(n = 0; l = 0)$; the states are ordered so that $\epsilon_i > \epsilon_j$ if $i > j$ and

$$d_i = \begin{cases} 1 & \text{if } i \text{ denotes a state with } l = 0, \\ 2 & \text{if } i \text{ denotes a state with } l > 0 \end{cases} \hspace{1cm} (17)$$

is the orbital degeneracy of $i$th state ($E_{nl} = E_{nl-1}$). The processes that enter equation (16) are illustrated in figure 9. The first term on the rhs describes the rate at which electrons tunnel from the S electrode. Due to the Coulomb blockade such a transfer is possible only when none of the DRN states is already occupied, which is ensured by the expression in parentheses. The second term describes relaxation to state $j$ from higher-lying states. The last term describes tunneling to the D electrode and relaxations from state $j$ to lower-lying states. If $j = n_0 (j = 0)$ the second (third) sum in equation (16) should be omitted since there are no states from (to) which relaxation is possible.

As we are interested in the steady-state current we put $\dot{\rho}_i = 0$ in equation (16). Then, introducing $\rho_i \equiv d\rho_i$, the system of equations for $\rho_j$ can be rewritten as

$$\begin{pmatrix} D_0 & U_{0,1} & U_{0,2} & \cdots & U_{0,n_0-1} \\ \Gamma_1 & D_1 & D_2 & \cdots & D_{n_0-1} \\ \Gamma_2 & \Gamma_2 & D_3 & \cdots & D_{n_0-1} \\ \vdots & \vdots & \ddots & \cdots & \vdots \\ \Gamma_{n_0-1} & \Gamma_{n_0-1} & \Gamma_{n_0-1} & \cdots & D_{n_0-1} \end{pmatrix} \begin{pmatrix} \rho_0 \\ \rho_1 \\ \rho_2 \\ \vdots \\ \rho_{n_0-1} \end{pmatrix} = \begin{pmatrix} \Gamma_0^S \\ \Gamma_1^S \\ \Gamma_2^S \\ \vdots \\ \Gamma_{n_0-1}^S \end{pmatrix}, \hspace{1cm} (18)$$

where the diagonal elements $D_i$ are given by:

$$D_i = \Gamma_i^S + \frac{1}{d_0} \Gamma_i^D + \frac{1}{d_0} \sum_{j=0}^{i-1} w_{j\rightarrow i} \rho_j$$  \hspace{1cm} (19)

The elements of the upper triangle are $U_{ij} = \Gamma_i^S - w_{i\rightarrow j}$ for $0 < i < n_0$. In the absence of magnetic field $d_0$ is always equal to 1, but we have left it in the first equation for consistency of notation.

The solutions can be easily found in limiting cases of a very slow relaxation and of a very weak couplings to the electrodes. In the former case, when we put $w_{i\rightarrow j} \rightarrow 0$ for all $i$ and $j$, the solution for a symmetric coupling ($\Gamma_i^S = \Gamma_j^D$) takes on a simple form $\rho_i = 1/(n_0 + 1)$. In the latter case, when we put $\Gamma_i^S, \Gamma_j^D \rightarrow 0$ for all $i$, we get $\rho_0 = 0$ for all $i > 0$, which means that only the ground state participates in the transport. In a general case the system of linear equations (18) can be solved analytically, but with increasing $n_0$ the formulas quickly become very long. With the help of the occupation probabilities $\rho_i$, the steady-state current can be expressed as a sum of currents $I_{\text{in}}$ carried by electrons which tunnel from the S electrode to all the states that lie in the bias window. Since in the steady state the currents through both the barriers are equal, the total current can be also expressed as a sum of currents $I_{\text{out}}$ carried by electrons which tunnel from the DRN to the D electrode. Then, the total current can be written as

$$I = \sum_{i=0}^{n_0-1} I_{\text{in}} = \sum_{i=0}^{n_0-1} I_{\text{out}}, \hspace{1cm} (20)$$

where the currents carried by electrons tunneling to and from individual levels are given by

$$I_{\text{in}} = e \Gamma_i^S (1 - \rho_i), \hspace{0.5cm} I_{\text{out}} = e \Gamma_i^D \rho_i. \hspace{1cm} (21)$$

We assume, following the experiments in [9, 10], $k_B T \approx 0.01$ meV. Thus, in our studies both the energy spacings and the bias window are much larger than the thermal energy and we neglect the temperature smearing out of the energy levels. Then for a forward bias ($\mu_S - \mu_D > 0$) the electrons cannot tunnel only from the S electrode to the DRN and then from the DRN to the D electrode. The tunnel rates in equation (18) depend on the DRN geometry. We assume this so that $\Gamma$ for the most strongly coupled state is equal to 5 GHz, and calculate all the
other couplings accordingly. That way all the tunnel rates are in the range of the experimentally accessible values [51].

We start with the low bias regime where only the ground state lies in the bias window \((v_0 = 1)\). In this case the total current is given by equation (21) with the requirement that \(I_v^0 = I_v^0\).

\[
I = e \frac{\Gamma^S \Gamma^D}{\Gamma^S + \Gamma^D},
\]

(22)

We assume symmetric tunneling barriers to the S and D electrodes \(\Gamma^S = \Gamma^D\) and numerically calculate their values. The mechanism of the SET is as follows: if the bottom of the QD potential is significantly below the bottom of the QR potential, the ground state is localized in the QD near the center of the DRN. Since for a deep enough QD potential the wave function decreases almost exponentially with increasing distance from the QD, its overlap with the electrode’s wave functions is negligible. With an increase of \(V_{QD}\) this state moves to the outer (QR) part of the structure where it has a much larger overlap with the states in the electrodes. This results in a strong increase in the current. We calculate the current as a function of the gate voltage \(V_{QD}\) for three different values of \(V_0\). The results are presented in figure 10. One can see in this figure that the steepness of the \(I(V_{QD})\) characteristics increases significantly with an increase of \(V_0\). If \(V_0\) is small, the ground state wave function gradually moves with increasing \(V_{QD}\) towards the outer part of the DRN. This leads to a slow increase in the current. On the other hand, if \(V_0\) is large, there are two pronounced minima of the confining potential (one in the QD and one in the QR) and with increasing \(V_{QD}\) at some point the ground state wave function ‘jumps’ from the QD to the QR. It results in step-like \(I(V_{QD})\) characteristics. This dependence is clearly seen in the insets in figure 10, where the differential conductance \(dI/dV_{QD}\) is presented for different heights of the barrier \(V_0\) separating the DRN.

The low bias limit, however, not always can be reached. In many cases the evolution of the DRN’s spectrum shows several level crossings when \(V_{QD}\) is changed. In such cases the bias \(\mu_s = \mu_0\) cannot be adjusted to include only the ground state for all values of \(V_{QD}\) for which the transistor effect occurs. We see in figure 2 that depending on \(V_{QD}\) two or three (or even more) states have to be accounted for. It is known that transport in the Coulomb blockade regime can be suppressed by the occupation of excited states [52]. Therefore, we analyze below how the system should be designed to get a good transistor behavior in the high bias regime. The dc currents are calculated as steady state solutions to the rate equations (equations (18)–(21)) for the occupation probabilities for all relevant states considering all the processes transferring electrons, namely the tunnel rates \(\Gamma^{-}\)’s and subsequent relaxation rates \(\Gamma^{+}\)’s. It turns out that the major factor that determines the current is the relations between the tunnel and relaxation rates. When the coupling to the electrodes is small compared to the corresponding relaxation rates, most of electrons that travel through the DRN will relax to the ground state before leaving the DRN by tunneling to the drain electrode. Then, the total current is determined mostly by the transport only through the ground state even if some of the excited states are in the bias window. In this case the system behaves like low bias limit described above. This situation is illustrated in figure 11.

What we have also noted from our numerical calculations is that if the relaxation rates \(\Gamma^{+}\)’s are comparable to the coupling constants \(\Gamma^{-}\)’s, then only a minor influence of higher excited states appears. They do not change the switching characteristics but increase the current amplitude.

As follows from the calculations in section 2.1 the relaxation rates are of the order of a few GHz in the broad range of \(V_{QD}\). Therefore, one can easily obtain smaller \(\Gamma^{-}\)’s or ones comparable to the corresponding relaxation rates and consequently get the desired transistor behavior, as shown in the inset in figure 11(b).
Current rectification plays an important role in electron transport and is fundamental for the development of novel basic elements in nanoelectronics. Attempts have been made to build downscaled rectifiers. A Coulomb blockade rectifier on a triple dot system \cite{26, 53} has been recently introduced. The rectification properties of a quantum wire coupled asymmetrically to a quantum dot have also been studied \cite{54}. We propose here a rectifier built on a DRN which utilizes a different distribution of the ground and excited states wave functions.

To show the idea we discuss, at first a case where the two lowest states are in the bias window and we present the analytical solutions for the currents.

The confinement potential of the DRN is tuned so that the first excited state (E) has a significantly larger overlap with the leads than the ground state (G). Thus, the same holds true for the corresponding tunneling rates, i.e. $\Gamma_G \ll \Gamma_E$. To get current rectification we have to break the left-right symmetry, therefore we assume an asymmetric coupling to the source and drain electrodes, i.e. the drain electrode is much closer to the DRN than the source one. This results in the following relations between the tunneling rates:

$$\Gamma_j^S \ll \Gamma_j^E (j = G, E),$$

where $\Gamma_j^S$ is assumed to be so small that the current between the ground state and the source electrode is negligible ($\Gamma_G^S \ll 100$ kHz \cite{5}). One can tune the distances between the DRN and electrodes to ensure the above relation. Moreover, it follows from equations in the appendix A that the ratio of the tunneling rates to the ground and excited states is independent of this distance, so that

$$\frac{\Gamma_j^S}{\Gamma_j^E} = \frac{\Gamma_j^G}{\Gamma_j^E}.$$

which is in line with the assumptions made, e.g. in \cite{10, 51} in the interpretation of their experiments.

The proposed mechanism of the rectification is the following: for forward bias ($V_D - V_S > 0$, see figure 12(a)) the current from the source electrode flows to the DRN through the excited state and then either further flows to the drain electrode through the excited state or the electron relaxes and leaves the DRN through the ground state. This is the forward direction of the rectifier. On the other hand, for reverse bias ($V_D - V_S < 0$, see figure 12(b)) an electron can enter either the ground or the excited state. If the electron enters the ground state, it cannot leave the DRN because of the negligible coupling to the source electrode (we assume the temperature to be low enough to prevent from exciting the electron to the next energy level and from tunneling back to the drain electrode). If the electron enters the excited state, it will relax to the ground state due to fast relaxation (section 2). Then, in either case the electron gets stuck in the ground state, thus

\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{figure11.png}
\caption{The total current along with contributions that flow through particular DRN’s levels for $\Gamma = 500$ MHz, $V_0 = 10$ meV (a) and $V_0 = 30$ meV (b). In both panels the meaning of the lines is the same. The inset in the right panel shows the total current in non-logarithmic scale.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{figure12.png}
\caption{The scheme of a rectifier with two energy levels in the bias window for forward (a) and reverse (b) bias. The red dotted line represents the tunneling rate $\Gamma_j^G$ between the source electrode and the ground state that is assumed to be extremely small. The solid zig-zag line represents the relaxation $\omega$ from the excited state.}
\end{figure}

\begin{table}[h]
\centering
\begin{tabular}{cccc}
$V_{QD}$ & $\Gamma_j^G/\Gamma_j^E$ & $I_1$ & $I_R$ & $|I_1/I_R|$ \\
\hline
1 meV & 100 & 9 pA & 0.09 pA & 100 Figure 3(b) \\
0 meV & 200 & 4 pA & 0.012 pA & 320 \\
\end{tabular}
\caption{Examples of model parameters and resulting currents.}
\end{table}
blocking the current through the excited state by means of the Coulomb blockade. This is the reverse direction of the rectifier.

To describe the proposed rectifier effect in a quantitative way we calculate the currents using the steady state solutions of the rate equations for the occupation probabilities (equations (18)–(21)). Taking into account only the two lowest states we obtain the current $I_F$ for the forward bias and the reverse current $I_R$ for the reverse bias:

$$I_F = e\Gamma_F \frac{d_1(\Gamma_E^0 + w)}{\Gamma_E^0 + d_1w(1 + \frac{\Gamma_S}{\Gamma_E^0})},$$

$$I_R = -e\Gamma_R \frac{w + \Gamma_S}{w},$$

where $w$ is the relaxation rate for the first excited state and $d_1$ is its degeneracy. These formulas allow us to find the conditions under which DRN behaves as a rectifier, i.e. for which

$$\left| \frac{I_F}{I_R} \right| \gg 1. \tag{27}$$

Since $\Gamma_F \ll w$ we get

$$\left| \frac{I_F}{I_R} \right| = \frac{\Gamma_F}{\Gamma_R} \frac{d_1(\Gamma_E^0 + w)}{\Gamma_E^0 + d_1w(1 + \frac{\Gamma_S}{\Gamma_E^0})}. \tag{28}$$

One can see that the ratio of the forward and reverse currents depends crucially on the ratio between the couplings of the ground and excited states to the $S$ electrode and this is a parameter that can easily be tuned in a DRN.

We calculate the tunneling rates $\Gamma_E^S$, $\Gamma_E^G$ and $\Gamma_S^D$, $\Gamma_G^D$ and the relaxation rates $w$ as a function of $V_{QD}$ under the assumption that the geometry of the DRN is that the maximal value of $\Gamma_E^0$ is $5 \text{ GHz}$.

Choosing $V_{QD} = -4 \text{ meV}$ (only two states in the bias window) for $\Gamma_E^0/\Gamma_E^S = 100$ we get from equations (25), (26) and (28) $I_F = 60 \text{ fA}$, $I_R = 0.9 \text{ fA}$, which gives $|I_F/I_R| = 64$.

In this reference situation we get very small currents because both the $G$ and $E$ states are placed in the inner part of the DRN (see figure 3(a)). To get a stronger current $I_F$ we have to choose larger $V_{QD}$, for which some excited states are placed in the outer part of the DRN resulting in the larger ratio of the respective tunneling rates $\Gamma_E^S/\Gamma_E^G$. For $V_{QD} > -2 \text{ meV}$ we have to consider three states in the bias window, as can be inferred from figure 2. In table 1 we present two examples of our numerical results.

The wave functions in these two cases differ only qualitatively and therefore only the case of $V_{QD} = 1 \text{ meV}$ is presented in figure 3(b). The above example illustrates that it is possible to design a DRN that allows one to get a substantial forward current and a high degree of rectification. The Coulomb blockade due to the electron being stuck in the ground state will prevent transport through any of the excited states in the reverse direction. On the other hand, they will all participate in the transport in the forward direction, which increases the total current. Because $\Gamma_G^S$ is not exactly equal to zero, we get some leakage current in the reverse direction but still substantial rectifying behavior occurs.

The crucial requirement for the rectifier is the strong difference between the coupling to the ground state and to the excited states. This is the point where the advantage of the DRN over a QD is clearly visible. We performed, for comparison, calculations for QD with $R = 70 \text{ nm}$, $\Gamma_E/\Gamma_E^S = 100$ and got in the most favorable case: $I_F = 9 \text{ pA}$, $I_R = 1.6 \text{ pA}$, $|I_F/I_R| = 5.7$. One cannot obtain here a high degree of rectification because it is impossible to change the relative distribution of the ground and excited state wave functions in a QD. As a result, one cannot decrease the current $I_R$ without the simultaneous decreasing of $I_F$. In QDs the ratio $\Gamma_E/\Gamma_G$ is usually below 10, whereas in the DRN the confining potential can
be tuned to give $\Gamma_E/\Gamma_0$ up to $10^3$ (see figure 13). We see that the tunnel coupling to the reservoirs in the DRN is tunable over a much wider range than in QD. This, in turn, results in larger values of currents and more efficient rectification.

5. Summary

The fundamental requirement for future, low power consumption electronics is to control and manipulate single charges or spins. Quantum dots are the most popular and developed few-electron systems due to the relative ease of fabrication and manipulation. On the other hand, the simple geometry of QDs allows the modification of their electronic properties only to some extent, which encourages scientists to explore more complex systems like double or triple QDs. In this paper we performed systematic studies of electronic properties of a concentric dot–ring nanostructure and showed that, thanks to its non-trivial geometry, the structure offers unique possibilities to manipulate the electron wave functions. In particular, we have shown that by simple electrostatic gating one can move over the electron between the outer ring and the inner dot changing orbital relaxation by orders of magnitude and switching the character of a DRN from insulating to conducting. The presented so-called wave function engineering technique allows the design of the properties of a system from the lowest quantum mechanical level. This is exactly how modern nanotechnology works and is the way to reach the limits of device miniaturization and to make the next step in the development of quantum computers.

In this paper we present the results for a DRN build as an InGaAs structure. However, the idea of a nanosystem where the wave functions can be moved over to different spatially separated parts can be applied also to other physical systems, for example graphene nanostructures [55–58]. We also neglect the spin effects. Yet, exploiting them we would allow one to use a DRN in nanospintronics. The effect of spin on the Coulomb blockade has been studied in single QDs [5, 52, 59, 60] and in double QDs [29, 61, 62]. A spin blockade in an SET in a QD [45] the tunneling matrix according to Bardeen’s approach [45] the tunneling matrix element is given by

$$t_k = \frac{\hbar}{2m^*} \int_0^\infty d\omega \left[ \psi^*_k(r) \nabla \psi_{nl}(r) - \psi_{nl}(r) \nabla \psi^*_k(r) \right], \quad (A.1)$$

what in two dimensions can be written as

$$t_k = \frac{\hbar}{2m^*} \int_{-\infty}^{\infty} dy \left[ \psi^*_k(r) \frac{\partial \psi_{nl}(r)}{\partial x} - \psi_{nl}(r) \frac{\partial \psi^*_k(r)}{\partial x} \right] \bigg|_{x=x_0}, \quad (A.2)$$

where $\psi_{nl}(r)$ is the DRN’s wave function and $\psi_k(r)$ is the electrode’s wave function. The electrodes are modelled as half-planes and their wave functions and eigenenergies are given by

$$\psi_k(r) = \frac{\sqrt{2}}{L} e^{ik_y y} \sin \left( \frac{\theta}{2} \right) e^{i(x-x_0)}, \quad (A.3)$$

$$\epsilon_k = \frac{\hbar^2 k_x^2}{2m^*} + U - \frac{\hbar^2 \kappa^2}{2m^*}, \quad (A.4)$$

where

$$\kappa = \frac{1}{\hbar} \sqrt{2m^* \left( U - \frac{\hbar^2 k_x^2}{2m^*} \right)}, \quad (A.5)$$

$$\sin \theta = \frac{2ck_x}{k^2 + k_x^2}. \quad (A.6)$$

The wave function of the DRN can be written as

$$\Psi_{nl} = R_{nl}(r) e^{i\phi} = R_{nl}(\sqrt{x^2 + y^2}) e^{i\arctan \frac{y}{x}}. \quad (A.7)$$

The derivatives in equation (A.2) are given by

$$\frac{\partial \psi_{nl}(r)}{\partial x} = \left[ \frac{dR_{nl}(r)}{dr} \frac{x}{\sqrt{x^2 + y^2}} + R_{nl}(r) \frac{y}{x^2 + y^2} \right] \exp \left( i \arctan \frac{y}{x} \right), \quad (A.8)$$

and

$$\frac{\partial \psi_k(r)}{\partial x} = \kappa \frac{\sqrt{2}}{L} e^{ik_y y} \sin \left( \frac{\theta}{2} \right) e^{i(x-x_0)}, \quad (A.9)$$

For each $k$ in equation (A.1) one has to calculate $\kappa$ and $\theta$ (equations (A.5) and (A.6)), insert equations (A.3), (A.7)–(A.9) into (A.2) and (numerically) calculate the integral. It is convenient to express $\theta$ in polar coordinates where it takes the following form

$$\theta = \sqrt{2} \frac{\hbar \chi_0}{2m^* L} \sin \left( \frac{\theta}{2} \right) e^{i(x_0-x_0)} \int_{-\pi/2}^{\pi/2} d\phi \frac{e^{ik_{x_0} \tan \phi + i\phi}}{\cos^2 \phi}
\times \left[ R_{nl}(x_0) \cos \phi + R_{nl}(x_0) \cos \phi \left( i \frac{\sin 2\phi}{2x_0} - \kappa \right) \right]. \quad (A.10)$$

Appendix A. Derivation of the tunneling matrix element

According to Bardeen’s approach the tunneling matrix element is given by

$$t_k = \frac{\hbar}{2m^*} \int_0^\infty d\omega \left[ \psi^*_k(r) \nabla \psi_{nl}(r) - \psi_{nl}(r) \nabla \psi^*_k(r) \right], \quad (A.1)$$

where $\psi_{nl}(r)$ is the DRN’s wave function and $\psi_k(r)$ is the electrode’s wave function. The electrodes are modelled as half-planes and their wave functions and eigenenergies are given by

$$\psi_k(r) = \frac{\sqrt{2}}{L} e^{ik_y y} \sin \left( \frac{\theta}{2} \right) e^{i(x-x_0)}, \quad (A.3)$$

$$\epsilon_k = \frac{\hbar^2 k_x^2}{2m^*} + U - \frac{\hbar^2 \kappa^2}{2m^*}, \quad (A.4)$$

where

$$\kappa = \frac{1}{\hbar} \sqrt{2m^* \left( U - \frac{\hbar^2 k_x^2}{2m^*} \right)}, \quad (A.5)$$

$$\sin \theta = \frac{2ck_x}{k^2 + k_x^2}. \quad (A.6)$$

The wave function of the DRN can be written as

$$\Psi_{nl} = R_{nl}(r) e^{i\phi} = R_{nl}(\sqrt{x^2 + y^2}) e^{i\arctan \frac{y}{x}}. \quad (A.7)$$

The derivatives in equation (A.2) are given by

$$\frac{\partial \psi_{nl}(r)}{\partial x} = \left[ \frac{dR_{nl}(r)}{dr} \frac{x}{\sqrt{x^2 + y^2}} + R_{nl}(r) \frac{y}{x^2 + y^2} \right] \exp \left( i \arctan \frac{y}{x} \right), \quad (A.8)$$

and

$$\frac{\partial \psi_k(r)}{\partial x} = \kappa \frac{\sqrt{2}}{L} e^{ik_y y} \sin \left( \frac{\theta}{2} \right) e^{i(x-x_0)}, \quad (A.9)$$

For each $k$ in equation (A.1) one has to calculate $\kappa$ and $\theta$ (equations (A.5) and (A.6)), insert equations (A.3), (A.7)–(A.9) into (A.2) and (numerically) calculate the integral. It is convenient to express $\theta$ in polar coordinates where it takes the following form

$$\theta = \sqrt{2} \frac{\hbar \chi_0}{2m^* L} \sin \left( \frac{\theta}{2} \right) e^{i(x_0-x_0)} \int_{-\pi/2}^{\pi/2} d\phi \frac{e^{ik_{x_0} \tan \phi + i\phi}}{\cos^2 \phi}
\times \left[ R_{nl}(x_0) \cos \phi + R_{nl}(x_0) \cos \phi \left( i \frac{\sin 2\phi}{2x_0} - \kappa \right) \right]. \quad (A.10)$$

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