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Electronic transmission through a coupled quantum dot and ring

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Abstract

We investigate the transmission of electrons through a quantum ring coupled to a quantum dot by applying a finite difference approach augmented by exterior complex scaling for the solution of the corresponding time-independent Schrödinger equation. It is shown that the transmission in the presence of an additional ring- or dot-bound electron is energetically suppressed compared with the transmission for a pure quantum dot–ring system, being reminiscent of the so-called Coulomb blockade effect in quantum dots. The different behaviour for varying parameters as well as in the presence of an attractive impurity in the dot is discussed in some detail.

1. Introduction

Semiconductor nanostructures such as quantum dots, wells and wires are promising candidates for nanoelectronic devices operating on the basis of quantum physical laws. The experimental techniques for preparing these structures, such as molecular-beam epitaxy or chemical vapour deposition followed by etching or lithographic patterning of gates, offer a high degree of control and reproducibility. The dimensionality of the nanostructures plays a particularly important role due to its impact on the density of states. Specifically, for quantum dots their shape and number of electrons can be controlled experimentally (see [1–3] for a review on the electronic structure of quantum dots).

Combining several of the above-mentioned nanostructures allows simultaneously a large degree of variability and control. This holds in particular for the combination of quantum dots and rings (QDR) (see [4–7] and references therein). It was shown in [8] that the distribution of electrons between the dot and the ring can be influenced by the relative strength of the dot and ring confinement as well as the gate voltage. An applied external magnetic field can induce transitions of electrons between the two parts of the system. In view of this flexibility of a

combined quantum dot and ring system one can expect that the transport through an open QDR, i.e. through a QDR with attached leads, will also be of interest (for related studies see [9–11]). A remarkable detailed study of the transport properties of an open QDR was performed in a recent paper by Gudmundsson *et al* [12] where a large series of fascinating dependences of the conductivity on the magnetic field strength was found. Quantum effects in open mesoscopic rings have been studied by Orellana *et al* [11]. A quantum ring (QR) coupled to a reservoir was investigated by Büttiker [13]. A topic related to transport through an open QDR is the influence of single impurities on the conductance of a quasi-one-dimensional channel that was explored in [14–17]. A corresponding experimental study can be found in [18]. For applications of general mathematical methods for scattering in quantum channels and curved wires we refer the reader to [19] and [20], respectively.

For most open QDR the question arises whether single electron transport through a coupled QDR could be controlled by the presence of an additional charge, i.e. a bound electron, in the ring and/or dot. This is precisely the problem to be investigated in the present work.

In detail we proceed as follows. In section 2 we specify our model of an open QDR consisting of potentials for the dot, the ring and the leads (augmented by a constant background potential). Section 3 contains a brief description of our computational approach. Section 4 addresses the spectral properties and bound quantum states of the QDR. The central section 5 contains a discussion of the results on the transmission function $T(E)$ including (i) single-electron transmission through the QDR, (ii) transmission in the case where there is an additional bound electron in the QDR, being in a dot or ring bound state, (iii) a discussion of the transmission behaviour in the case where there is an additional attractive impurity in the central quantum dot. Section 6 contains the summary and conclusions.

2. Modelling the open quantum dot–quantum ring system

We consider the two-dimensional motion of electrons in a potential field $V(x, y)$. Stationary states of a single electron can be obtained by solving the Schrödinger eigenvalue problem

$$\left[-\frac{1}{2}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)+V(x,y)\right]\Psi(x,y)=E\Psi(x,y). \tag{1}$$

When there are no leads attached to the QDR the potential $V(x, y)$ possesses a rotational symmetry, i.e. L_z is conserved, yielding the magnetic quantum number m. It is then most natural to solve the corresponding Schrödinger equation in polar coordinates

$$\left[-\frac{1}{2}\left(\frac{\partial^2}{\partial r^2}+\frac{1}{r}\frac{\partial}{\partial r}-\frac{m^2}{r^2}\right)+V(r)\right]\psi(r)=E\psi(r) \tag{2}$$

where $r=\sqrt{x^2+y^2}$. Here and in the following we use effective atomic units (e.a.u.). For a bulk semiconductor with dielectric constant ε and effective mass m of the electron we have for the energy $E_{\mathrm{eff}}=e^4\hbar^{-2}m^*\varepsilon^{-2}$ and for the length $a_{\mathrm{eff}}=\hbar^2\varepsilon e^{-2}m^{*-1}$. For GaAs with $\varepsilon=12.9$ and $m^*=0.067$ these units are $a_{\mathrm{eff}}=10.2$ nm, $E_{\mathrm{eff}}=11$ meV.

The potential V is defined as

$$V=\begin{cases} V_1:=V_0+V_{\mathrm{dot}}+V_{\mathrm{ring}} & |x|\leqslant R_0 \\ V_2:=V_0+V_{\mathrm{dot}}+V_{\mathrm{ring}}+V_{\mathrm{lead}} & |x|>R_0 \end{cases} \tag{3}$$

where R_0 is the position of the outer minimum of $V_0+V_{\mathrm{dot}}+V_{\mathrm{ring}}$ in the ring. The potential term responsible for the dot is

$$V_{\mathrm{dot}}(r)=-V_{\mathrm{D}}\exp\left(-r^2/d_{\mathrm{D}}^2\right) \tag{4}$$

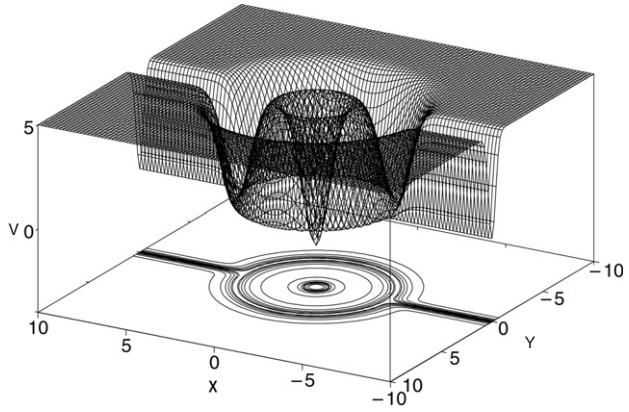

Figure 1. Potential for a dot–ring system with attached leads for $V_D = 7$, $V_R = 5$, $V_0 = 5$, $d_D = d_R = d_L = 1$, $R = 4$, and $Z = 0$. Upper part: three-dimensional potential landscape. Lower part: contour plot. Effective atomic units are used.

and the potential term providing the ring of radius R is

$$V_{\text{ring}}(r) = -V_R \exp\left[-(r - R)^2/d_R^2\right]. \tag{5}$$

V_0 is the background potential. Since we are interested in transport through the open coupled quantum dot and ring system we connect two straight leads smoothly, i.e. without potential barriers, to the quantum ring for $|x| > R_0$. The leads are oriented parallel to the x-axis. This can be achieved by choosing

$$V_{\text{lead}}(x, y) = (V_1(R_0) - V_0) \exp\left(-y^2/d_L^2\right)\left(1 - \exp\left[-\left(|x| - R_0\right)^2/d_R^2\right]\right). \tag{6}$$

The potential V obeys $V_1(R_0) = V_2(R_0)$. The electrons are incoming in the left lead and (partially) transmitted to the right lead. For large values of the y-coordinate only the background potential V_0 remains. The form of the potential (3)–(6) is chosen such that the bottom of the lead is flat. The potential V for $V_D = 7$, $V_R = V_0 = 5$, $d_D = d_R = d_L = 1$, $R = 4$ in the presence of leads is presented in figure 1. In order to reduce the number of parameters to be varied, we choose in the following $V_0 = 5$ and $V_R = 5.05$. Later we will also consider the case when V also contains a potential term due to the interaction of current-carrying charges with an attractive impurity centre located in the centre of the quantum dot $V_C(r) = -Z/r$, $Z = 1$.

3. Computational approach

The smooth form of the potential (3) allows the application of a finite-difference fully numerical method for the solution of the two-dimensional Schrödinger equation (1). Our finite-difference multidimensional approach is described in detail in [22, 23]. In the particular case considered here we solve equation (1) on uniform meshes in Cartesian coordinates (x, y) with typical distances between mesh nodes in the range 0.05–0.1 e.a.u. Typical sizes of the rectangular domain Ω in which the Schrödinger equation is solved are $-10 < y < 10$ and $-L_{x-} < x < L_{x+}$, where $L_{x-} = 100$ and $L_{x+} = 150$. All our calculations are carried out for energies of electrons much lower than V_0, resulting in the wavefunctions decreasing exponentially outside the ring and leads. For these energies and our values of parameters in the potential (3) the boundary conditions $\psi|_{y=\pm 10} = 0$ used in our calculations introduce a negligibly small error in the final result [22]. The presence of potentials possessing different spatial scales in the system

requires us to use rather dense meshes with the typical number of nodes being 2880×160. The strong extension of Ω in the x direction is associated with our need to obtain the transmission coefficient described below. For the situation of two electrons in the system (transmission of an electron through the system with a bound second electron) we employed a fully numerical Hartree–Fock approach that is described in [22, 23]. In fact the motion of the unbound electron takes place in a total potential that is the sum of the potential (3) and the electrostatic potential due to the bound electron. First we calculate the state of the single bound electron subjected to the potential (3). Subsequently its charge distribution is frozen and the resulting potential due to the electron–electron interaction is inserted into the Schrödinger equation for the second electron. The latter also contains, of course, the potential (3). Choosing this approach we neglect effects of the transmitting electron on the wavefunction of the bound electron. Due to the frozen character of the bound electron, processes such as co-tunnelling transfer, in which the incoming electron pushes out the bound electron in the dot, are not taken into account. We remark that the calculations presented in the following focus on the spin-singlet configuration for which no exchange interaction occurs. They show that the dominant effects of the electron–electron interaction depend only on the total charge confined in the system, i.e. the observables considered here show a very weak dependence on the detailed charge distributions of the electrons. This circumstance, along with the small values for the exchange integrals due to the large difference with respect to the spatial distributions of the wavefunctions of the projectile and the confined electrons (especially for confinement in the central dot, but also for the ring-localized states), indicate that one can expect only a minor difference in the results for the spin-singlet and the triplet-spin configurations.

In order to make conclusions about the conductivity of our system and/or its potential capability to control single charge transfer it is crucial to know the corresponding flux transmission coefficient T for different geometries. Following the standard definition [21] this value is the ratio of the transmitted to the incoming flux. In order to calculate the transmission coefficient we solve equation (1) by applying special boundary conditions for large absolute values of x. To ensure that the transmitted flux for $x > R_0$ in the outgoing lead does not lead to artificial reflections at the boundary of our grid, i.e. to avoid an artificial incoming wave in the right lead, we apply for $x \gg 0$ an external complex rotation of the coordinate x. This complex rotation is described and investigated in detail in [24]. The complex value of the x coordinate as a function of the real parameter x_r takes on the appearance

$$x(x_\mathrm{r}) = x_\mathrm{r} + \mathrm{i}\,\mathrm{Im}\left[\frac{\mathrm{e}^{\mathrm{i}\Theta}}{2\cos\Theta}\left(\sqrt{(x_\mathrm{r}-b)^2 + Q(x_\mathrm{r})/c^2} - \sqrt{b^2 + Q(0)/c^2} + x_\mathrm{r}\right)\right] \tag{7}$$

where

$$Q(x) = \exp\left[-\left[c(x-b)\right]^2/4\right].$$

Due to the complex rotation the wavefunction converges to zero as $x \to +\infty$. This allows us to establish a boundary condition $\psi = 0$ on $x = L_{x+}$.

On the left boundary of the domain Ω at $x = -L_{x-}$, $L_{x-} > 0$ we can establish an arbitrary non-uniform boundary condition, for example $\psi(x = -L_{x-}) = 1$, which we used in our calculations. The value of the wavefunction on the boundary is arbitrary, because the transmission coefficient depends only on a ratio of values calculated on the basis of the wavefunction (see below). For $E < V_0$ such a wavefunction at $x = -L_{x-}$ is a sum of an incoming and outgoing wave as well as some terms exponentially decreasing with increasing x. If we are not in the immediate neighbourhood of the boundary $x = -L_{x-}$ the wavefunction obtained by imposing the above boundary condition is a sum of an incoming and outgoing (reflected) wave, corresponding to the two possible motions of an incoming and reflected electron along the left lead.

We consider relatively narrow leads with a significant energetic separation of the ground and the first excited states for transverse motion of the electron. For example, for leads with the parameter values $V(R_0) = 5.05$, $V_0 = 5$ and $d_L = 0.5$ the energy of the ground state of the transverse motion is $E_{L0} = 2.384$, and this is the only bound transverse state. In this single-mode regime for the motion of the electron in the leads the absolute value of the wavevector can be expressed as a function of the energy only, and there is a direct proportionality between the spatial probability density of the electron and the corresponding flux. Due to the complex rotation of the x-coordinate the flux F_{out} in the right ($x > R_0$) lead is directed outward.

Outside the region affected by the complex rotation in the right lead the flux F_{out} is proportional to the average electron density D_R in the right lead. There are two fluxes in the left lead: the incoming flux F_{in} and the reflected one F_{ref}. Let us consider an average density D_L of the wavefunction in the left lead D_L. When this density is averaged over a section of the lead much longer than the wavelength of the incident wave it will be (under the conditions specified above) proportional to the sum of F_{in} and F_{ref}. Taking into account that

$$F_{out} = F_{in} - F_{ref}$$

one can easily obtain the formula for the transmission coefficient T

$$T = \frac{F_{out}}{F_{in}} = \frac{2D_R}{D_R + D_L}.$$

4. Spectral properties and bound quantum states

As indicated above, in the absence of the leads, i.e. for the case of a closed quantum dot and ring system, we encounter a rotational symmetry around the axis perpendicular to the (x, y)-plane that passes through the origin and therefore the angular momentum L_z is conserved yielding the magnetic quantum number m. The corresponding potential V_1 depends only on r and the single-electron spectrum can be easily obtained by solving the corresponding one-dimensional Schrödinger equation. This system without leads is similar to the set-up considered in [8] where magnetic field-induced electron charge and spin switching between the laterally coupled quantum dot and ring were investigated.

The presence of the leads breaks the cylindrical symmetry. Without a Coulomb impurity in the centre of the dot only a few bound states of the ring–dot system remain. When the leads and the ring are of the same width there are two types of bound states with an energy below that of the ground transverse state in the leads: states that are localized in the quantum dot and states that are localized in the ring. The number of dot-localized states depends on its depth and width. On the other hand, there typically exist two ring-localized states that are bound due to the weaker confinement of the electrons in the regions of the junctions of the ring and the lead, which reduces the electronic kinetic and total energy compared with the energy of the states in the leads.

The effect of the weaker confinement acting on the electrons at the junctions is similar to the effect of two fictitious potential wells acting at the junctions of the leads with the ring. As a result the ground and the first excited ring state of this type are similar to the symmetric and antisymmetric states of a double well separated by a barrier. The energetic difference of these states depends on the width of the ring. This difference is very small for thin rings and increases with increasingly broader rings. Two examples of the corresponding states are shown in figure 2. For a narrow ring $d_R = 0.5$ (figures 2(a), (b)) the probability amplitude is strongly localized at the junctions of the ring and leads and the energetic difference of the ground and the first excited state is approximately 5×10^{-6}. For a relatively broad ring $d_R = 2$ (figures 2(d), (e)) the probability amplitude is leaking away from the junction along the bottom of the ring for the

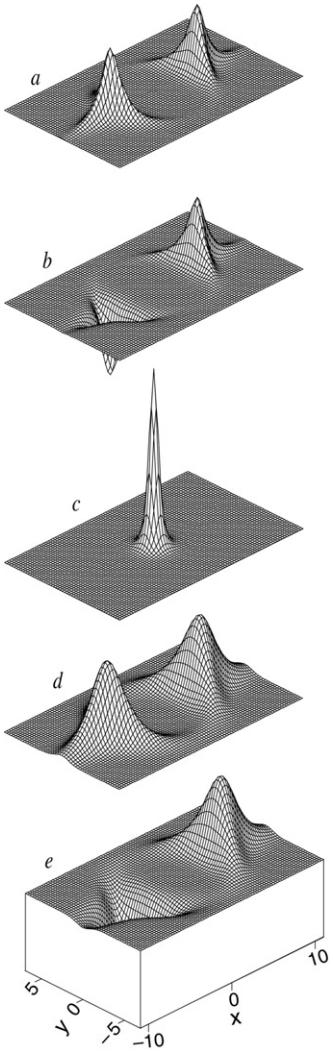

Figure 2. Wavefunctions (in arbitrary units) of ring and dot states for the parameter values $V_R = 5.05$, $V_0 = 5$ and $R = 5$, $-11 \leqslant x \leqslant 11$, $-7 \leqslant y \leqslant 7$. Narrow ring and leads $d_R = d_L = 0.5$ and $V_D = 9.5$: (*a*) ground ring state $E = 2.040\,394$, (*b*) first excited ring state $E = 2.040\,407$, and (*c*) ground dot state $E = 2.058\,702$. Broad ring and leads $d_R = d_L = 2$ and $V_D = 3.1$: (*d*) ground ring state $E = 0.517\,53$ and (*e*) first excited ring state $E = 0.517\,66$. Effective atomic units are used for the coordinates.

ground ring state. The energetic difference of the ground and first excited state is here of the order of 2×10^{-4}. The energetically lowest state localized in the dot depends strongly on V_D and d_D. Its energy E_{D0} can be lower or higher than the energy of the bound ring states. For the states shown in figure 2 the parameters are chosen such that the lowest impurity/dot states lie energetically slightly above the lowest pair of ring states. However, in the case of $E_{D0} > E_{L0}$, where E_{L0} is the lowest energy level for transverse motion in the leads, this dot state becomes quasi-stationary. We remark that tuning the ratio of the widths of the leads and the ring allows us to energetically shift the lead states with respect to the states in the ring.

The energy of the transverse ground state in the leads for the parameter values $V_R = 5.05$, $V_0 = 5$, and $d_L = 0.5$ is $E_{L0} = 2.384$ and there is no bound excited state for the transverse motion in the lead. For the case of broader leads $d_L = 2$ the ground state possesses the energy $E_{L0} = 0.69$ whereas the energy of the first excited state is $E_{L1} = 2.08$ e.a.u.

Let us now consider the case of the additional presence of an attractive impurity at the centre of the dot. This system possesses an infinite number of bound states localized in the ring and increasingly spreading into the leads with increasing degree of excitation. The two energetically lowest states correspond to the above-discussed ring states in the absence of the impurity, i.e. their wavefunctions possess a similar appearance. In figure 3 we present the wavefunctions of the five energetically lowest bound states of the impurity–ring–dot–lead system for a broad ($d_R = 2$) ring. The parameters for this example are chosen such that the lowest impurity/dot state lies below the lowest pair of ring states.

5. Transmission through a quantum ring–dot system with leads

Let us consider the case of the open ring–dot system without an impurity. In figure 4 we present the dependence of the transmission coefficient for a single electron. This picture is obtained for a narrow ring and narrow leads $d_R = d_L = 0.5$, the remaining parameters being $V_D = 9.5$, $d_D = 0.5$, and $R = 5$.

Transmission occurs only above the energy E_{L0} of the ground state of the transverse motion in the leads and shows an oscillatory behaviour with increasing energy. This can be interpreted as the result of the interference of electronic waves in the ring–dot structure: for the maxima of the transmission, all possessing a value close to unity, an integer number of electronic wavelengths match into the ring. Indeed the energetic separation of the maxima of the transmission increases linearly within the energetic order of the maximum. This is reminiscent of the situation of an infinitely narrow closed ring for which the spectrum scales as $\propto \frac{m^2}{R^2}$ where m is the magnetic quantum number and R is the radius of the ring and where the energetic separation of neighbouring states obeys $\propto \frac{2m+1}{R^2}$. One therefore can associate the oscillating structure of $T(E)$, more precisely the positions of the maxima, with resonances in the open finite size ring–dot system.

A second example is provided in figure 5 for broader leads and ring $d_L = d_R = 2$, the other parameters being $V_D = 3.1$, $d_D = 1$ and $R = 5$. The system possesses two bound electronic states in the ring with nearby energies $E_{R0} = 0.517\,525$ and $E_{R1} = 0.517\,656$ e.a.u. The values of the parameters V_D and d_D for the system are too small to allow for a bound dot-located state below E_{L0}. Figure 5 shows two transmission curves as a function of the energy: $T_1(E)$ (full curve) represents the single-electron transmission whereas $T_2(E)$ (broken curve) represents the transmission of an electron through the dot–ring system with a second bound electron. The single-electron transmission curve is quite similar to the one shown in figure 4 whose properties have been discussed above. Obviously a major discrepancy between the two transmission curves $T_1(E)$, $T_2(E)$ is the different energies for the onset of non-zero transmission which is 0.7 e.a.u. for $T_1(E)$ and, apart from the very narrow resonance at 0.868 e.a.u., it is 0.9 e.a.u. for $T_2(E)$. This means that we encounter a Coulomb blockade effect, i.e. the bound ring electron blocks the transmission of the second electron to be transported across the ring–dot device. This blockade is to a good approximation independent of the ring state occupied by the bound electron. The transmissions $T(E)$ belonging to the case of the bound electron being in the ground and the first excited state are indistinguishable on the scale of figure 5.

In figure 6 we show the real part of the wavefunction and the corresponding electronic probability density in the dot–ring system and the neighbouring part of the leads for the case

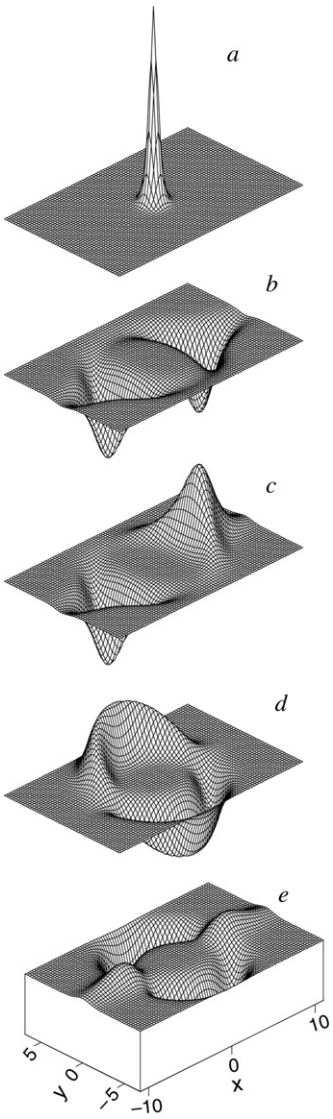

Figure 3. Wavefunctions (in arbitrary units) of the eigenstates of a system with leads and a centred impurity. $V_R = 5.05$, $V_0 = 5$, and $R = 5$. Broad ring and leads $d_R = d_L = 2$ and $V_D = 8$: (*a*) ground dot state $E = -3.218\,75$, (*b*) ground ring state $E = 0.336\,13$, (*c*) first excited ring state $E = 0.336\,36$, (*d*) second excited ring state $E = 0.508\,88$, (*e*) third excited ring state $E = 0.521\,73$. Effective atomic units are used for the coordinates.

of single-electron transmission, i.e. for no bound electron in the ring. The parameters are the same as in figure 5 and the energy is $E = 1.1$, i.e. it is somewhat below the maximum of $T_1(E)$ at $E = 1.13$ in figure 5. The oscillations of the density (figure 6(b)) in the left lead originate from an interference of the incoming and reflected waves. No oscillations of the density are encountered in the right lead, where only an outgoing wave is present. For energies corresponding to $T = 1$ these oscillations are not encountered both in the left or in the right lead.

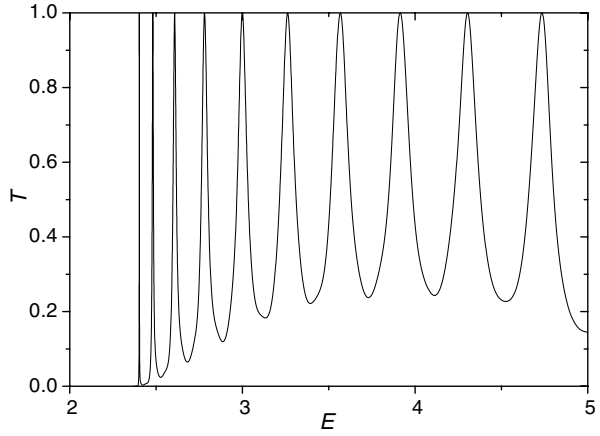

Figure 4. Transmission coefficient $T(E)$ as a function of energy for an electron in the potential (3) for $V_D = 9.5$, $V_R = 5.05$, $V_0 = 5$, $d_D = d_R = d_L = 0.5$, and $R = 5$. Effective atomic units are used.

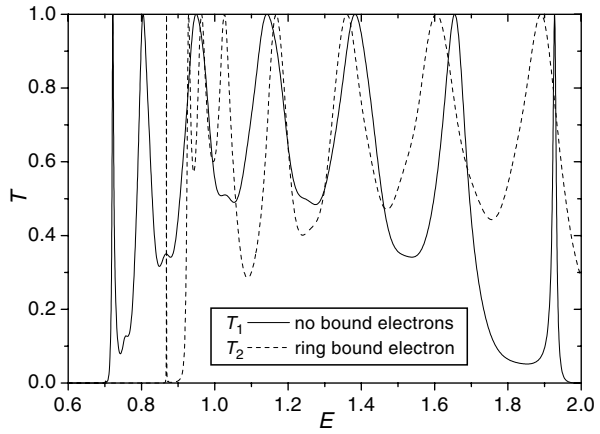

Figure 5. Transmission coefficient $T(E)$ as a function of energy for $V_D = 3.1$, $V_R = 5.05$, $V_0 = 5$, $d_D = 1$, $d_R = d_L = 2$, and $R = 5$. Solid line (T_1): single electron. Dashed line (T_2): a second electron is bound in the ring ($E = 0.517\,525$). Effective atomic units are used.

Owing to a broad potential barrier between the ring and the dot the parameter V_D as well as the value of the energy E_{D0} of the electron in a dot-localized state do not significantly affect the transmission coefficient for a single electron. The energies of the dot-localized states for different values of V_D (the values of the remaining parameters being the same as the ones given above) are $E_{D0} = 0.4402$, $1.177\,98$, $1.894\,78$, 2.5844 for $V_D = 8, 7, 6, 5$, respectively. For all these parameter values the transmission coefficient coincides with the one presented in figure 5, as can be seen by comparing figures 5 and 7. The behaviour of the transmission $T_2(E)$ for a two-electron system with a bound electron in the central dot (see figure 7) is qualitatively similar to the transmission $T_3(E)$ for an electron being bound in the ring. The two curves are shifted with respect to each other and possess somewhat different values for their minima. The energetic positions of the onset of the transmission agree very well ($E \approx 0.92$).

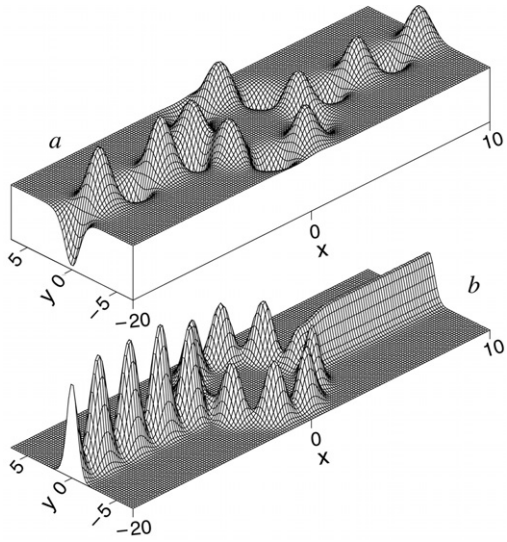

Figure 6. (*a*) Real part of the wave function and (*b*) electronic density including the region of the QDR as well as the neighbouring leads (see figure 5) for a single electron $E = 1.1$. Effective atomic units are used.

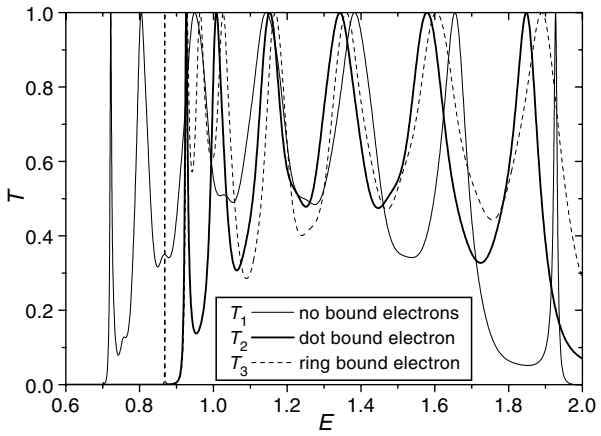

Figure 7. Transmission coefficient $T(E)$ as a function of energy for $V_D = 8$, $V_R = 5.05$, $V_0 = 5$, $d_D = 1$, $d_R = d_L = 2$ and $R = 5$. Solid line (T_1): single electron. Bold line (T_2): a second electron is bound in the dot ($E_c = 0.4402$). Dashed line (T_3): the second electron is bound in the ring (ring ground state $E = 0.517\,52$). Effective atomic units are used.

Let us now consider the situation of the presence of an additional impurity, i.e. of a point charge in the central dot. The corresponding transmission coefficients are presented in figure 8. If there are no electrons bound to the impurity, i.e. for the case of single-electron transmission ($T_1(E)$ in figure 8), we observe a series of resonances for energies close to the onset of the transmission. This behaviour is a consequence of the long-range character of the Coulomb attraction which affects the potential in the leads. The Coulomb attraction shifts the energy threshold for the onset of the transmission to its minimal possible value, i.e. to the ground transverse energy of the electron in the leads.

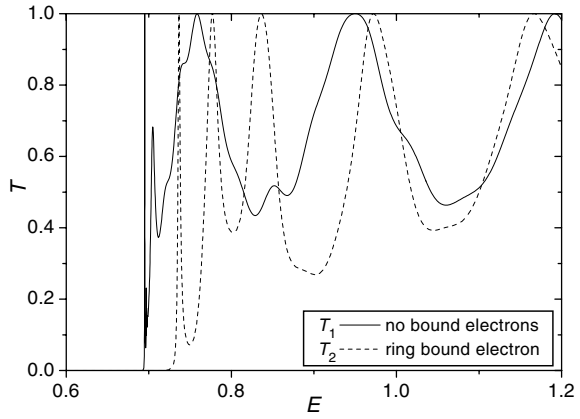

Figure 8. Transmission coefficient $T(E)$ as a function of energy in the presence of a centred impurity for $V_D = 3.1$, $V_R = 5.05$, $V_0 = 5$, $d_D = 1$, $d_R = d_L = 2$ and $R = 5$. Solid line (T_1): single electron. Dashed line (T_2): a second electron is bound in the ground ring state ($E_c = 0.336\,13$). Effective atomic units are used.

Let us assume there is a (second) electron in the ring that is bound and feels the Coulomb interaction with the impurity in the dot (see $T_2(E)$ in figure 8). Then the Coulomb attraction due to the impurity is screened by the electron in the ring and the incoming electrons do not encounter a long-range interaction in the leads. As a result the transmission $T(E)$ becomes much simpler again, and indeed it is quite similar to the one presented in figures 5 and 7. However, the effect of Coulomb blockade is much less pronounced: the potential due to the central charge weakens the effect of the repulsion of the incoming electron due to the electron bound to the ring (the net charge of the impurity and ring-bound electron is zero). The transmissions $T(E)$ belonging to the cases of the bound electron being in the ground and the first excited states are indistinguishable on the scale of figure 8. On the other hand, the threshold energy for the onset of transmission in the case of the ring-bound electron is higher than the corresponding threshold energy for a dot-bound electron (see figure 9). The latter can be explained by the fact that, opposite to the three-dimensional case, a two-dimensional system of a positive point charge $Z = 1$ and an electron bound to it repels a second electron when it is far from the centre of the system [25, 26]. This repulsion increases with the dispersion of the probability distribution of the bound electron.

Finally, we investigate the case of two bound electrons (figure 9). Binding of two electrons in the absence of the impurity, one being in the central dot and the other one in the ring, is not possible because the repulsive potential due to the dot electron does not allow for bound ring states. On the other hand, binding of two electrons in the dot requires high values of V_D. In contrast to this two electrons can easily be bound in the dot in the presence of the impurity. For the parameter values $V_D = 8$, $d_D = 1$, $d_R = d_L = 2$ and $R = 5$ corresponding to figure 9 two electrons with antiparallel spins are bound in the dot with the single electron energy $E = -0.6696$ (the interaction of these two electrons is taken into account in the Hartree–Fock approximation). We see that the corresponding energy threshold for transmission of electrons approximately coincides with the threshold in case of no impurity and one bound electron (see figure 7). Thus, we can conclude that the decisive factor responsible for the value of the energy threshold for transmission is the sum of the charges in the system. For neutral systems in the presence of the impurity minor variations of the threshold energy can be a result of different spatial distributions of bound electrons.

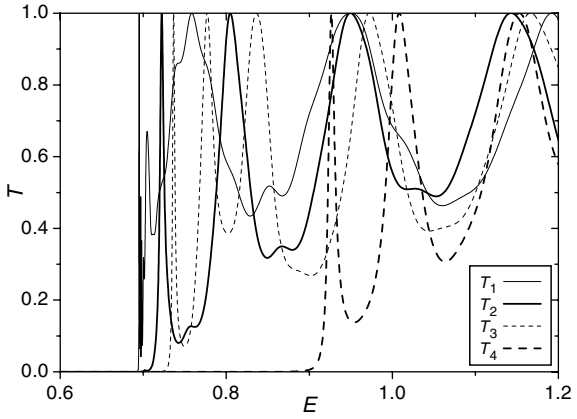

Figure 9. Transmission coefficient $T(E)$ as a function of energy in the presence of a centred impurity for $V_D = 8$, $V_R = 5.05$, $V_0 = 5$, $d_D = 1$, $d_R = d_L = 2$ and $R = 5$. Solid line (T_1): single electron. Solid bold line (T_2): an electron in the central dot. Dashed line (T_3): a second electron is bound in the ground ring state ($E_c = 0.336\,13$). Dashed bold line (T_4): two electrons bound in the central dot. Effective atomic units are used.

6. Summary and conclusions

We have investigated charge transmission through a coupled quantum dot and ring system. Our interest was not only to study single-electron transmission but also to explore the transmission in cases where there is an additional electron bound to the quantum dot–ring.

The modelling of the open QDR, i.e. with attached leads, contains independent potentials for the dot, the ring and the leads that are matched together smoothly. Changing the parameters of the combined potential allows for a substantial variability of its appearance and of the resulting properties such as the number of bound electronic states and their characteristics. Our computational approach to solving the corresponding two-dimensional Schrödinger equation is a finite-difference fully numerical method. For the case of two electrons (an incoming and a bound one) the electronic interaction has been treated via the Hartree–Fock method. Special boundary conditions have been employed, such as external complex rotation of the corresponding coordinates, in order to avoid artificial reflections at the boundary of the grid. Our study of the flux transmission focuses on the single-mode regime for the transverse motion of the electrons in the leads.

The open QDR typically possesses a few bound states that can be localized either in the dot or in the ring. For leads and ring of equal width the ring states are bound due to the weaker confinement of the electrons in the regions of the junctions of the ring and the lead. Indeed, the energetically lowest two ring states are reminiscent of the symmetric and antisymmetric states of a double well separated by a barrier. Tuning the ratio of the widths of the leads and the ring allows the lead states to be energetically shifted with respect to the states in the ring. For the case of an additional presence of an impurity in the central dot the open QDR possesses an infinite number of bound states localized in the ring. Some of them show a limited leaking into the leads.

The transmission T_1 of an electron through the QDR without bound electrons shows the well-known oscillatory behaviour as a function of the energy, which is due to the resonances, i.e. standing electronic waves, in the ring. The transmission T_2 in the case where there is a second bound electron in the ring differs significantly from T_1. A major discrepancy of the

two transmission curves is the different threshold energy for the onset of a finite transmission. As a result we obtain a Coulomb blockade effect, i.e. the bound ring electron blocks the transmission of the incoming electron. This blockade is to some extent independent of the ring state occupied by the bound electron. In the presence of a dot-bound electron it turns out that the transmission of lead electrons is largely independent of the parameters, i.e. the shape of the dot. The corresponding transmission $T_3(E)$ is qualitatively, but not quantitatively, similar to $T_2(E)$ for the case of a ring-bound electron.

Combining the open QDR with a centred attractive impurity leads, in the case of no additional electrons in the QDR, to a strong change in the transmission behaviour, in particular close the threshold of a finite transmission, which is due to the long-range character of the Coulomb interaction: The Coulomb attraction shifts the threshold of the transmission to its minimal possible value, i.e. to the energy of the ground transverse state of an electron in the lead. When there is a ring electron bound to the impurity, the long-range Coulomb interaction of the impurity is screened by the electron in the ring and the transmitting electrons do not encounter a long-range interaction in the leads. However, the effect of Coulomb blockade is much less pronounced in the presence of a positive Coulomb impurity. We have also studied electron transmission for a system with two electrons being bound to an attractive impurity in the dot. It turns out that the dominating factor responsible for the position of the transmission threshold is the sum of the charges in the system. Minor variations of the threshold energy are possible in electrostatically neutral systems due to the different localization of the bound electrons.

Having shown the existence of a Coulomb blockade effect in our coupled quantum dot and ring system one might think of using our device in order to control, i.e. trigger or block, single charge transfer. To verify this possibility the question would have to be answered about how to control the presence of single charges on the quantum dot–ring system which goes beyond the scope of the present investigation.

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