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2004 J. Phys.: Condens. Matter 16 L85

(http://iopscience.iop.org/0953-8984/16/8/L03)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS: CONDENSED MATTER

J. Phys.: Condens. Matter **16** (2004) L85–L91 PII: S0953-8984(04)75413-2

LETTER TO THE EDITOR

Asymmetric negative differential conductance in double quantum dots

J Fransson[1,2] **and O Eriksson**[2]

[1] Department of Materials Science and Engineering, Royal Institute of Technology (KTH), SE-100 44 Stockholm, Sweden
[2] Physics Department, Uppsala University, SE-751 21 Uppsala, Sweden

E-mail: Jonas.Fransson@fysik.uu.se

Received 30 January 2004
Published 13 February 2004
Online at stacks.iop.org/JPhysCM/16/L85 (DOI: 10.1088/0953-8984/16/8/L03)

Abstract

An explanation for the recently observed asymmetric negative differential conductance (NDC) in a double-quantum-dot system attached to metallic external contacts is proposed. The NDC was observed only for one half of the bias voltage range $(-V, V)$. The theory, which is based on a diagrammatic technique for non-equilibrium many-body operator Green functions, suggests that scattering between the states in the double quantum dot suppresses the total current dynamically as the bias voltage is increased. The effect is present in systems where the double-quantum-dot states are asymmetrically coupled to the left- and right-hand contacts, and we predict that a symmetric coupling will suppress the negative differential conductance completely.

Recent experiments on double quantum dots (DQDs) coupled to metallic contacts show, unexpectedly, asymmetric negative differential conductance (NDC) behaviour in the current–voltage (J–V) characteristics [1]. The J–V characteristics was asymmetric in the sense that the NDC appeared only in one half of the bias voltage range $(-V, V)$. Features of NDC normally occur in semiconductor double- and multi-barrier structures [2, 3] and can then be referred to as band-edge effects [4, 5]. Transport experiments on DQDs fabricated from semiconductor hetero-structures have displayed sharp resonant peaks [6] which are related to the fact that the energy distance between the levels in the two QDs approaches zero, which creates a resonant state in the DQD [7]. Alignments of the levels in the two QDs, however, create symmetric J–V characteristics having sharp resonant peaks with large peak-to-valley ratios, in contrast to the observations in [1]. Thus, when the interacting region, e.g. DQD, is coupled to metallic contacts, having a conduction band width of the order of electronvolts, such explanations cannot be applied. Normally, one expects that the current should increase with increasing bias voltage, possibly with plateaux due to the zero-dimensional confined levels. The NDC was suggested to be an effect of resonant tunnelling between the discrete levels in each dot

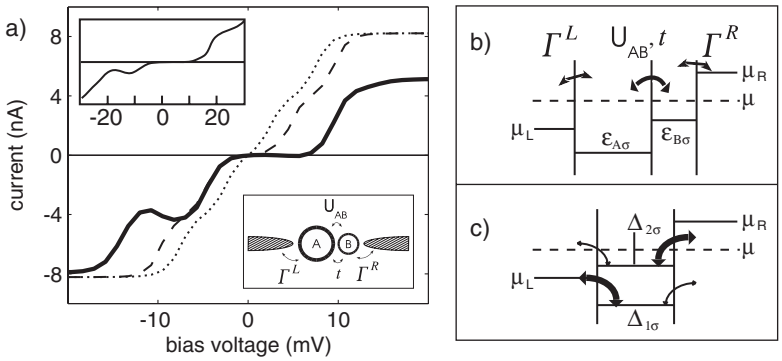

Figure 1. (a) J–V characteristics of the DQD system calculated within the HIA (dotted), with the renormalized transition energies (dashed) and with the theory given by equations (4)–(6) (solid). For the computations we used the left/right coupling strength $\Gamma^{\mathrm{L/R}} = 0.375$ meV and conduction electron band width 2 eV symmetrically around the equilibrium chemical potential $\mu = 0$ at $T = 5$ K. The upper inset shows a typical experimental J–V result on the DQD reported in [1]. The lower inset displays the geometry of the DQD system. (b) Sketch of the energy parameters of the serial DQD coupled to the contacts. The QDs interact via inter-dot Coulomb repulsion U_{AB} and hopping t. In $\mathrm{QD_{A/B}}$ the bare single-particle energy is $\varepsilon_{\mathrm{A}\sigma/\mathrm{B}\sigma}$. Each QD is coupled to a contact with the strength $\Gamma^{\mathrm{L/R}}$. (c) Schematic picture of the energies of the DQD system in the diagonal representation (see the text, where $\mu_{\mathrm{L/R}}$ and $\Delta_{n\sigma}$, $n = 1, 2$, are defined). The arrows illustrate the strengths of the transition probabilities between the one-particle states in the DQD and the contacts.

although the details of the process are not known [1]. Furthermore, the observed asymmetric appearance of the NDC is hitherto an unexplained effect.

There is a vast literature of theoretical studies on transport through DQD in different geometries, e.g. DQD in series [8, 9] and in parallel [9–11]. Most of these studies are devoted to DQDs in the Coulomb blockade regime, where especially phenomena related to Kondo-like physics are under focus. Although being important for the understanding of effects from strong correlations on the transport through the system, to our knowledge, no-one has yet addressed the question of an asymmetric NDC in DQDs coupled to metallic contacts. In this letter, we propose a theoretical many-body model that leads to a significant NDC in the J–V characteristics for a DQD system. In addition, our theory yields an NDC for only negative bias voltages, in agreement with observations [1]. Before we embark on the theoretical modelling, we present the main result of this letter, given in figure 1(a) (solid curve). The plot displays the current, as a function of the bias voltage, through a DQD coupled to external metallic contacts. We suggest that the decreasing current for increasing negative voltages ($-9 \rightarrow -12$ mV) arises due to a dynamical process, causing a strongly decreased probability for tunnelling to one of the one-particle states in the DQD.

We start our theoretical analysis by considering two electrostatically coupled QDs, interacting via an inter-dot Coulomb repulsion U_{AB} and hopping t. The DQD is coupled to external contacts through tunnel barriers where the coupling strength between the left/right (L/R) contact is given by $\Gamma^{\mathrm{L/R}}$ (described in more detail below). The geometry of the system is illustrated in the lower inset of figure 1(a) and the energies of the system are schematically given in figure 1(b). In order to describe the asymmetry of the experimental system in [1], we let $\mathrm{QD_A}$ be larger than $\mathrm{QD_B}$ and, therefore, we impose finite intra-dot Coulomb repulsions $U_{\mathrm{A}} < U_{\mathrm{B}}$ in $\mathrm{QD_A}$ and $\mathrm{QD_B}$, respectively. We also assume that $U_{\mathrm{AB}} < U_{\mathrm{A}}, U_{\mathrm{B}}$. First we consider the situation when the DQD is detached from the contacts. Then, the DQD can be

Table 1. The wavefunctions and energies of the empty and the two spin-degenerate one-particle states. Here $u^{\sigma}_{n1} = (E_{\gamma_{n\sigma}} - \varepsilon_{\mathrm{B}\sigma})/\kappa_{1n}$, $|u^{\sigma}_{n2}|^2 = 1 - |u^{\sigma}_{n1}|^2$, $\kappa_{1n} = \sqrt{(E_{\gamma_{n\sigma}} - \varepsilon_{\mathrm{B}\sigma})^2 + |t|^2}$, $n = 1, 2$, where $\varepsilon_{\mathrm{A}\sigma/\mathrm{B}\sigma}$ is a single-particle level in $\mathrm{QD}_{\mathrm{A/B}}$.

N_{tot}	State	Energy	
0	$\|0\rangle = \|0\rangle_{\mathrm{A}}\|0\rangle_{\mathrm{B}}$	0	
1	$\|\gamma_{n\sigma}\rangle = u^{\sigma}_{n1}\|\sigma\rangle_{\mathrm{A}}\|0\rangle_{\mathrm{B}}$ $+ u^{\sigma}_{n2}\|0\rangle_{\mathrm{A}}\|\sigma\rangle_{\mathrm{B}}$	$E_{\gamma_{n\sigma}} = \frac{1}{2}\Big(\varepsilon_{\mathrm{A}\sigma} + \varepsilon_{\mathrm{B}\sigma}$ $+ (-1)^n\sqrt{(\varepsilon_{\mathrm{A}\sigma} - \varepsilon_{\mathrm{B}\sigma})^2 + 4\|t\|^2}\Big)$,	$n = 1, 2$

described by the model Hamiltonian

$$\mathcal{H}_{\mathrm{DQD}} = \sum_{\sigma} \varepsilon_{\mathrm{A}\sigma} a^{\dagger}_{\sigma} a_{\sigma} + U_{\mathrm{A}} n_{\mathrm{A}\uparrow} n_{\mathrm{A}\downarrow} + \sum_{\sigma} \varepsilon_{\mathrm{B}\sigma} b^{\dagger}_{\sigma} b_{\sigma} + U_{\mathrm{B}} n_{\mathrm{B}\uparrow} n_{\mathrm{B}\downarrow} + \sum_{\sigma} t\,(a^{\dagger}_{\sigma} b_{\sigma} + \mathrm{H.c.}) + U_{\mathrm{AB}}(n_{\mathrm{A}\uparrow} + n_{\mathrm{A}\downarrow})(n_{\mathrm{B}\uparrow} + n_{\mathrm{B}\downarrow}), \tag{1}$$

where $a^{\dagger}_{\sigma}$ (a_{σ}) creates (annihilates) an electron in QD_{A} at the energy $\varepsilon_{\mathrm{A}\sigma}$, and $b^{\dagger}_{\sigma}$ (b_{σ}) creates (annihilates) an electron in QD_{B} at the energy $\varepsilon_{\mathrm{B}\sigma}$. Further, $n_{\mathrm{A}\sigma} = a^{\dagger}_{\sigma} a_{\sigma}$ ($n_{\mathrm{B}\sigma} = b^{\dagger}_{\sigma} b_{\sigma}$) and σ is the spin ($\uparrow, \downarrow$). From this model one easily finds the empty and the one-, two-, three- and four-particle states [12], where the empty state refers to the state of the DQD with $N - 1$ electrons. For the present purposes it suffices to work with transitions between the empty state $|0\rangle$ and the two one-particle states $|\gamma_{n\sigma}\rangle$, which for clarity are given in table 1. The other states lie out of range of conduction for the parameters used here and can, therefore, be omitted. For simplicity, the model given in equation (1) contains only one level in each QD. We address the question of many levels at the end of this letter.

Now that we know the exact one-particle states of the system, we rewrite equation (1) in diagonal form by introducing the many-body operators $X^{pq} \equiv |p\rangle\langle q|$ [13], describing the transition from the state $|q\rangle$ to $|p\rangle$. Thus, the effective Hamiltonian for the isolated DQD is given by $\mathcal{H}_{\mathrm{DQD}} = \sum_{n\sigma} E_{\gamma_{n\sigma}} X^{\gamma_{n\sigma}\gamma_{n\sigma}}$, where $E_{\gamma_{n\sigma}}$ represents the energies of the many-body states in the DQD. This description of the DQD is convenient when we attach it to the contacts and the full Hamiltonian, including the contacts, is

$$\mathcal{H} = \sum_{k\sigma \in \mathrm{L,R}} \varepsilon_{k\sigma} c^{\dagger}_{k\sigma} c_{k\sigma} + \sum_{n\sigma} E_{\gamma_{n\sigma}} X^{\gamma_{n\sigma}\gamma_{n\sigma}} + \sum_{n,k\sigma \in \mathrm{L}} [v_{k\sigma} (a_{\sigma})^{0\gamma_{n\sigma}} c^{\dagger}_{k\sigma} X^{0\gamma_{n\sigma}} + \mathrm{H.c.}] + \sum_{n,k\sigma \in \mathrm{R}} [v_{k\sigma} (b_{\sigma})^{0\gamma_{n\sigma}} c^{\dagger}_{k\sigma} X^{0\gamma_{n\sigma}} + \mathrm{H.c.}]. \tag{2}$$

Here $c^{\dagger}_{k\sigma}$ ($c_{k\sigma}$) creates (annihilates) an electron in the left/right-hand contact at the energy $\varepsilon_{k\sigma}$, whereas the last two terms in equation (2) give the tunnelling between the contacts and the DQD. Here $v_{k\sigma} (a_{\sigma'})^{0\gamma_{n\sigma}}$ represents the probability of an electron escaping to the left-hand contact, via the the matrix elements between the empty and the singly occupied states of the DQD, given by $(a_{\sigma'})^{0\gamma_{n\sigma}} \equiv \langle 0|a_{\sigma'}|\gamma_{n\sigma}\rangle = \delta_{\sigma\sigma'} u^{\sigma}_{n1}$, where $u^{\sigma}_{ni}, n, i = 1, 2$ (given in table 1). For an electron escaping to the right-hand contact the corresponding matrix elements are $(b_{\sigma'})^{0\gamma_{n\sigma}} \equiv \langle 0|b_{\sigma'}|\gamma_{n\sigma}\rangle = \delta_{\sigma\sigma'} u^{\sigma}_{n2}$. These results are easily obtained, using the wavefunctions in table 1. Thus, $|(a_{\sigma})^{0\gamma_{1\sigma}}|^2 = |(a_{\sigma})^{0\gamma_{2\sigma}}|^2$ and $|(b_{\sigma})^{0\gamma_{1\sigma}}|^2 = |(b_{\sigma})^{0\gamma_{2\sigma}}|^2$ only if the two quantum dots forming the DQD are of equal size and $\varepsilon_{\mathrm{A}\sigma} = \varepsilon_{\mathrm{B}\sigma}$. For $\varepsilon_{\mathrm{A}\sigma} \neq \varepsilon_{\mathrm{B}\sigma}$ the transition matrix elements become distinct, which influences the resulting current. An example of the transition matrix elements is given in table 2, readily illustrating the degree of asymmetry imposed on the matrix elements of the DQD for different level distributions of the QDs.

Table 2. Equilibrium properties of the DQD given the inter-dot Coulomb repulsion $U_{\rm AB} = 40$ meV and the hopping $t = 0.75$ meV. The single-particle levels $\varepsilon_{{\rm A}\sigma/B\sigma}$ are input parameters.

	(A)	(B)	(C)
$\varepsilon_{{\rm A}\sigma}$ (meV)	−3.5	−2.5	−1.5
$\varepsilon_{{\rm B}\sigma}$ (meV)	−1.5	−2.5	−3.5
$E_{\gamma_{1\sigma}}$ (meV)	−3.75	−3.25	−3.75
$E_{\gamma_{2\sigma}}$ (meV)	−1.25	−1.75	−1.25
$\lvert(a_\sigma)^{0\gamma_{1\sigma}}\rvert^2$	0.9	0.5	0.1
$\lvert(a_\sigma)^{0\gamma_{2\sigma}}\rvert^2$	0.1	0.5	0.9
$\lvert(b_\sigma)^{0\gamma_{1\sigma}}\rvert^2$	0.1	0.5	0.9
$\lvert(b_\sigma)^{0\gamma_{2\sigma}}\rvert^2$	0.9	0.5	0.1

The current through the system is calculated by the formula [12, 14]

$$J = -\frac{e}{2h}\,{\rm Im}\sum_{n\sigma}\int\{[\Gamma^{\rm L}|(a_\sigma)^{0\gamma_{n\sigma}}|^2 - \Gamma^{\rm R}|(b_\sigma)^{0\gamma_{n\sigma}}|^2]G^<_{n\sigma}(\omega) + [f_{\rm L}(\omega)\Gamma^{\rm L}|(a_\sigma)^{0\gamma_{n\sigma}}|^2 - f_{\rm R}(\omega)\Gamma^{\rm R}|(b_\sigma)^{0\gamma_{n\sigma}}|^2][G^{\rm r}_{n\sigma}(\omega) - G^{\rm r}_{n\sigma}(\omega)]\}\,{\rm d}\omega, \qquad (3)$$

where $\Gamma^{\rm L/R} = 2\pi\sum_{k\sigma\in{\rm L/R}}|v_{k\sigma}|^2\delta(\omega - \varepsilon_{k\sigma})$, and $f_{\rm L/R}(\omega) = f(\omega - \mu_{\rm L/R})$ is the Fermi function with the chemical potential $\mu_{\rm L/R}$ of the left/right-hand contact. In equation (3) the Fourier transforms of the lesser, retarded and advanced forms of the DQD Green function (GF) $G_{n\sigma}(t,t') \equiv (-{\rm i})\langle{\rm T}X^{0\gamma_{n\sigma}}(t)X^{\gamma_{n\sigma}0}(t')\rangle_U$ appear. The DQD GF is analysed by means of equations of motion and a diagrammatic technique for Hubbard operator GFs [16]. The exact equations of motion for a spin-dependent single-level system have been considered in [15]. With two spin-degenerate levels one obtains analogous equations of motion. The simplest approximation is given by neglecting all correction diagrams, the so-called Hubbard I approximation (HIA) [13]. The first correction dresses the transition energies (symbolized by Δ) in the DQD [15, 16]. In the present case this renormalization yields the following transition energies:

$$\Delta_{n\sigma} = \Delta^0_{n\sigma} + \sum_k |v_{k\bar\sigma}(d_{\bar\sigma})^{0\gamma_{n\bar\sigma}}|^2\frac{f(\varepsilon_{k\bar\sigma}) - f(\Delta_{n\bar\sigma})}{\varepsilon_{k\bar\sigma} - \Delta_{n\bar\sigma}} + \sum_{k\sigma',m\neq n}|v_{k\sigma'}(d_{\sigma'})^{0\gamma_{m\sigma'}}|^2\frac{f(\varepsilon_{k\sigma'}) - f(\Delta_{m\sigma'})}{\varepsilon_{k\sigma'} - \Delta_{m\sigma'}}, \qquad (4)$$

where $n, m = 1, 2$, are eigenstate indices of the DQD, $\bar\sigma$ is the opposite spin of σ, whereas k runs over all states in the leads (both in the right- and left-hand contacts) and $d_\sigma = a_\sigma(b_\sigma)$ for $k \in {\rm L(R)}$. Here, $\Delta^0_{n\sigma} = E_{\gamma_{n\sigma}} - E_0$ is the bare transition energy. Note that the energy $\Delta_{n\sigma}$ for the transition $|0\rangle \to |\gamma_{n\sigma}\rangle$ is renormalized by the other possible transitions in the DQD. The renormalization arises from kinematic effects involving the transitions in the DQD and the coupling to the conduction electrons in the contacts. This is a characteristic feature for systems with complexes of two or more bounded particles interacting with conduction electrons [16, 17].

The renormalization of the transition energies is an important ingredient, although alone it does not explain the NDC. This information is contained in the non-equilibrium spectral weights of the transitions. The DQD GF, $G_{n\sigma}$, is constituted by the product $G_{n\sigma}(t,t') = D_{n\sigma}(t,t')P_{n\sigma}(t')$, where the locator, $D_{n\sigma}$, contains information about the pole whereas the end-factor, $P_{n\sigma}(t') \equiv \langle{\rm T}\{X^{0\gamma_{n\sigma}}, X^{\gamma_{n\sigma}0}\}(t')\rangle_U$, gives the spectral weight of the GF. The end-factor is interpreted as the sum of the population numbers of the empty state and $|\gamma_{n\sigma}\rangle$, respectively.

When applying the methods developed in [16], one has to expand *both* the locator and the end-factor. The result of the first-order correction from the expansion of the locator is given in equation (4). However, one also has to perform a first-order expansion in the end-factor. In order to avoid lengthy derivations in this letter, which will be presented elsewhere, we only give the final algebraic expression of the dressed end-factors

$$\mathbb{P}_{n\sigma}(\mathrm{i}\omega) = P_{n\sigma} + \delta P_{nn\bar{\sigma}\sigma}(\mathrm{i}\omega) + \sum_{\sigma',m\neq n} \delta P_{mn\sigma'\sigma}(\mathrm{i}\omega), \tag{5}$$

where

$$\delta P_{mn\sigma'\sigma}(\mathrm{i}\omega) = -\frac{P_{m\sigma'} - P_{n\sigma}}{2\pi} \int \sum_k \frac{|v_{k\sigma'}(d_{\sigma'})^{0\gamma_{m\sigma'}}|^2}{\varepsilon_{k\sigma'} - \omega'} [-2\,\mathrm{Im}\, D^{\mathrm{r}}_{m\sigma'}(\omega')] \times \left(\frac{f(\varepsilon_{k\sigma'}) - [n_{\mathrm{B}}(\Delta_{nm\sigma\sigma'}) + 1]}{\mathrm{i}\omega - \Delta_{nm\sigma\sigma'} - \varepsilon_{k\sigma'}} - \frac{f(\omega') - [n_{\mathrm{B}}(\Delta_{nm\sigma\sigma'}) + 1]}{\mathrm{i}\omega - \Delta_{nm\sigma\sigma'} - \omega'} \right) \mathrm{d}\omega'. \tag{6}$$

In this expression $D^{\mathrm{r}}_{m\sigma'}(\omega')$ is the retarded locator for the transition $|0\rangle \to |\gamma_{m\sigma'}\rangle$ and $n_{\mathrm{B}}(x)$ is the Bose function, whereas $\Delta_{nm\sigma\sigma'} = \Delta_{n\sigma} - \Delta_{m\sigma'}$ is the energy for transitions between the states $|\gamma_{m\sigma'}\rangle$ and $|\gamma_{n\sigma}\rangle$. Clearly, the dressed end-factor is bias voltage and frequency dependent with a finite imaginary part. This function also exhibits attributes concerning scattering processes between the different one-particle states, something which we shall see below is important for the transport properties.

In figure 1(a) we show the main result of this letter, the calculated J–V characteristics, equation (3), for three different approximations (HIA, renormalized transition energies, i.e. equation (4), which are both mean field approximations of the DQD GF in the sense that the spectral weights and imaginary parts of the self-energies are energy independent, and the result based on equations (4)–(6)). The upper inset of figure 1(a) shows the corresponding experimental data and it may be seen that agreement between experiment and theory is good only for the calculation based on equations (4)–(6). For this theory one reproduces in a quantitative way the shape of the J–V curve, including the NDC at $\sim$−10 meV.

We proceed by analysing the cause of the NDC in the result based on equations (4)–(6). From the mean field theories we see in figure 1(a) that the main contribution to the current comes from the direct tunnelling through the DQD via the one-particle states $|\gamma_{n\sigma}\rangle$, $n = 1, 2$, and although the states couple asymmetrically to the left- and right-hand contacts the resulting current is symmetric. This is expected since the transmission coefficient for the DQD, as is given in mean field theory, is equal for electrons entering from the left-hand contact and from the right. However, the mean field results for the DQD GF do not include the transitions $|\gamma_{1\sigma}\rangle\langle\gamma_{2\sigma}|$ and vice versa, since such transitions are not included in the Hamiltonian, equation (2). In contrast, when the approximation based on equations (4)–(6) is included in the calculations, effects from these transitions will be accounted for, as is seen in equation (6). However, contrary to what one might think, the importance of this correction becomes significant for bias voltages around $\Delta_{n\sigma}$, $n = 1, 2$. To see this we simplify the expression in equation (6) by putting $-2\,\mathrm{Im}\, D^{\mathrm{r}}_{m\sigma}(\omega') = 2\pi\delta(\omega' - \Delta_{m\sigma})$ and assume k-independent hybridization matrix elements, $v_{k\sigma}$, and wide and flat conduction bands in the contacts. The contribution to equation (6) from the interactions between particles in the left-hand contact and the DQD then reduces to

$$\delta\mathbb{P}^{\mathrm{r}}_{21\sigma\sigma}(\omega) \sim -\frac{P_{2\sigma} - P_{1\sigma}}{\omega - \Delta_{1\sigma}} \Gamma^{\mathrm{L}} |(a_\sigma)^{0\gamma_{2\sigma}}|^2 \left(\log \left| \frac{\mu_{\mathrm{L}} - \Delta_{2\sigma}}{\omega - \Delta_{12\sigma\sigma} - \mu_{\mathrm{L}}} \right| - \mathrm{i}\, f_{\mathrm{L}}(\omega - \Delta_{12\sigma\sigma})/2 \right).$$

This contribution, of which the imaginary part is peaked around $\Delta_{\gamma_{1\sigma}}$, provides a decreased population, $N_1 = \sum_\sigma N_{1\sigma}$, of the transition $|\gamma_{1\sigma}\rangle\langle\gamma_{1\sigma}|$, as compared to the mean field results. Indeed, the population number approaches zero for negative bias voltages $eV \sim \Delta_{1\sigma}(<0)$, which leads to the transition $|\gamma_{1\sigma}\rangle\langle 0|$ becoming less available for conduction through the

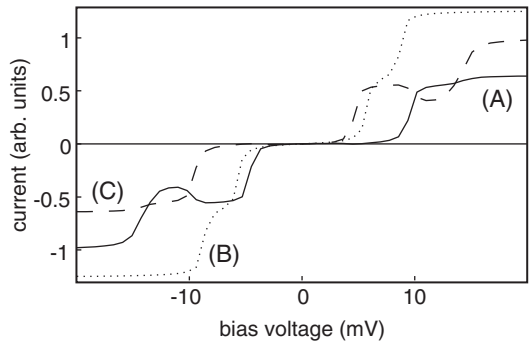

Figure 2. DQD J–V characteristics for case (A) (solid), case (B) (dotted) and case (C) (dashed) listed in table 2.

DQD. For the transition $|\gamma_{2\sigma}\rangle\langle 0|$ this effect also appear for negative bias voltages, but becomes negligible due to the much smaller coupling of this transition to the left-hand contact. For positive bias voltages, the situation is the opposite in the sense that $|\gamma_{1\sigma}\rangle\langle 0|$ couples more weakly to the right-hand contact than $|\gamma_{2\sigma}\rangle\langle 0|$ does. Thus, the effect from the scattering between the two one-particle states becomes stronger for the latter, which results in the absence of the current step for bias voltages around $-\Delta_{\gamma_{2\sigma}}$ (>0).

In a DQD system, such as the one considered in [1], it is far from obvious that the level distribution of the two QDs, cf figure 1(b), is such that the conducting level in $\mathrm{QD_A}$ lies below the corresponding level in $\mathrm{QD_B}$, i.e. $\varepsilon_{\mathrm{A}\sigma} < \varepsilon_{\mathrm{B}\sigma}$. If one considers the same principal quantum number this is in general true, if $\mathrm{QD_A}$ is larger than $\mathrm{QD_B}$. The conducting states in the two QDs, however, may be of non-equal principal quantum number, say $|n_{\mathrm{A}} = N + 1\rangle_{\mathrm{A}}$ and $|n_{\mathrm{B}} = N\rangle_{\mathrm{B}}$. Then, the corresponding energies may be shifted such that $\varepsilon_{\mathrm{A}\sigma}^{(N+1)} > \varepsilon_{\mathrm{B}\sigma}^{(N)}$, which is the configuration listed in table 2 (C). From our theoretical model we predict that in this case the NDC will occur for positive bias voltages. As a matter of fact we predict that a number of interesting features will occur as a function of the level distribution inside the DQD, i.e. when the relative positions of $\varepsilon_{\mathrm{A}\sigma}$ and $\varepsilon_{\mathrm{B}\sigma}$ are modified. This is illustrated in figure 2 where we display J–V characteristics for three cases of $\varepsilon_{\mathrm{A}\sigma}$ and $\varepsilon_{\mathrm{B}\sigma}$ (they are also listed in table 2). In the figure it may be seen that J–V characteristics without an NDC, with an NDC for negative bias and with an NDC for positive bias can be obtained, depending on the relative position of $\varepsilon_{\mathrm{A}\sigma}$ and $\varepsilon_{\mathrm{B}\sigma}$. The position of $\varepsilon_{\mathrm{A}\sigma}$ (or $\varepsilon_{\mathrm{B}\sigma}$) can be varied by applying a gate voltage only on $\mathrm{QD_A}$ (or $\mathrm{QD_B}$). In this way it is possible to tune the energy levels of the DQD. An experimental study of our prediction in figure 2 would be very intriguing.

Although the currently proposed model successfully describes the experiment in [1] in a quantitative way, one must bear in mind that several approximations have been introduced. We have for instance ignored the shape of the DQD in the experiment and replaced it with an effective model Hamiltonian. The geometrical confinement of the DQD is in the experiment composed of two single-walled nano-tubes. However, the spatial constraints in these nano-tubes will give rise to level quantization, which is of main importance for the conductance, and this is captured by our model. One may argue that more than one level in each QD should be included for the calculations. The level spacing in each QD, however, is in the order of half the maximum value of the bias voltage applied to the system. Moreover, the discussed effect appears for all transitions that add or remove one electron to/from the DQD and, hence, for the present purposes it is not required to include more levels in the QDs. Also, we have made use of a perturbational treatment of the coupling between the states in the contacts and the

states in the DQD. This approximation is motivated by the smallness of the coupling strength between the DQD and the contacts, compared to the energetics inside the DQD [18]. Also, the high degree of accuracy of the diagrammatic expansion of the DQD transition energy shifts and spectral weights motivates a perturbational treatment.

In conclusion, we suggest a theoretical explanation for the recently observed NDC in a DQD coupled to external metallic contacts [1]. Because of the large band width in normal metals, that is in the order of electronvolts, the standard explanation of band-edge effects, that is relevant for semiconductor systems, cannot be applied in this context. Instead we show that the observation of an NDC in mesoscopic systems attached to metallic contacts is related to scattering between different states in the interacting region. In order to understand this theoretically one has to perform highly accurate calculations, involving loop corrections to the end-factors of the DQD GF. In particular, for asymmetric systems the resulting current becomes strongly asymmetric, with respect to the bias voltage, showing an NDC for one half of the voltage range.

We acknowledge valuable discussions with Professor I Sandalov. Support from the Göran Gustafsson foundation, the Foundation for Strategic Research (SSF) and the Swedish National Science Foundation (VR) is acknowledged.

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