Optica Applicata, Vol. XXXIX, No. 4, 2009

Transient effects in electron transport through quantum dots

MAŁGORZATA WIERTEL*, PIOTR PARAFINIUK, RYSZARD TARANKO

Institute of Physics, Maria Curie-Skłodowska University,
pl. M. Curie-Skłodowskiej 1, 20-031 Lublin, Poland

*Corresponding author: malgorzata.wiertel@poczta.umcs.lublin.pl

We investigate the transient electron transport through the quantum dot and double quantum dot systems coupled with the time-dependent barriers to infinitely large reservoirs of noninteracting electrons. Time-dependent currents and quantum dot occupancies are calculated using both nonequilibrium Green's functions formalism and the equation of motion method for appropriate correlation functions. We show that the sequence of ultrafast modulation of the tunneling amplitudes between the electron reservoirs and the quantum dots can induce quite different electron occupation of the quantum dot in comparison with the static case. We also find that the oscillations of the transient current following the sudden coupling of the electron reservoirs with the double quantum dot system have the same frequency as Rabi's oscillations of the double dot state vector.

Keywords: quantum dot, double quantum dot, transient current.

1. Introduction

The electron transport through quantum dots (QD) has mostly been studied in the case of constant values of the parameters describing this nanoscopic system. However, in the context of the emerging field of quantum computing and spintronics or experimental advances in the studies of QDs subject to ultrafast voltage pulses, it would be very desirable to perform the time-dependent calculations of the currents and QD occupancies in some quantum dot systems. An important question arises of how fast the QD system can respond to time-dependent perturbations (*cf.* [1, 2]). The answer to this question can be crucial for practical implementation of QD systems in a variety of electronic devices. Several studies of the QD system response to the suddenly changed voltage bias or position of the QD level were reported and some interesting properties of the electron transport were described, *e.g.* [3–7]. For example, the quantum coherent oscillations (ringing) and beats of the electric current and the spin current were found in a transient time scale after a bias voltage was turned on rapidly [3].

In this work, we focus on the transient dynamics of the current and the charge state of a DQD system. The DQD with one excess electron localized on it can play an important role in the quantum computation. Therefore, in the context of quantum computing, it would be very desirable to obtain some information about the state vector of the DQD analyzing, for example, the transient current which appears in response to the suddenly turned on coupling of the DQD with the external reservoirs of electrons. In addition, we also consider the response of the QD occupation probability to a sequence of high-speed pulses which modulate the QD coupling with the external electron reservoirs.

In the next section, we present a model and describe the formalism used to calculate the current and QDs occupation probabilities. The last section includes the results of numerical calculations and a short discussion with a summary.

2. Theoretical approach

We consider two systems: the first one is a single QD coupled with two electron reservoirs and it is described by the Hamiltonian:

$$H^{(1)} = \sum_{i\,=\,k,\,q} \varepsilon_i a_i^+ a_i + \varepsilon_1 a_1^+ a_1 + \sum_{i\,=\,k,\,q} (V_i a_1^+ a_i + \text{h.c.}) \tag{1}$$

and the second system is a DQD (in a linear configuration) placed between two electron reservoirs:

$$H^{(2)} = \sum_{i\,=\,k,\,q} \varepsilon_i a_i^+ a_i + \sum_{j\,=\,1,\,2} \varepsilon_j a_j^+ a_j + \sum_k (V_k a_1^+ a_k + \text{h.c.}) + \\ + \sum_q (V_q a_2^+ a_q + \text{h.c.}) + (V_{12} a_1^+ a_2 + \text{h.c.}) \tag{2}$$

Here, a_k and a_q (a_k^+, a_q^+) are the annihilation (creation) operators of an electron in the "left" and "right" electron reservoirs. Similarly, the operators a_1, a_2 (a_1^+, a_2^+) correspond to the electron localized on the corresponding QDs. In addition, V_k and V_q are the tunneling amplitudes between the QDs and the electron reservoirs, V_{12} corresponds to the electron tunneling between QDs and ε_k, ε_q, ε_1 and ε_2 describe the electron energies in the "left", "right" electron reservoirs and in QDs, respectively.

In the following, we calculate the QD occupancies $n_i(t)$ and the current $J_L(t)$ flowing between the left electron reservoir and the near QD. We use two different techniques to calculate these quantities. The first one is the time-dependent nonequilibrium Green's function (NEGF) formalism and the second one is the equation of motion method for some correlation functions (EQM). The NEGF formalism, in the commonly used form [8], is especially useful for the case of one QD, initially empty, coupled with two electrodes. On the other hand, the EQM method can be simply modified to include more complex systems of coupled QDs or finite bandwidth of electron reservoirs.

Going along the NEGF formalism we can give analytical formulas for $n(t)$ and $J_L(t)$ in the case of single QD coupled with the electron reservoirs by the rectangular-pulse modulated tunneling amplitudes $V_{k/q}(t)$:

$$n(t) = \sum_{i = L, R} \Gamma^i \int \frac{\mathrm{d}\varepsilon}{2\pi} f_i(\varepsilon, T) \left| A^{(i)}(\varepsilon, t) \right|^2 \tag{3}$$

$$J_L(t) = -\frac{e}{\hbar}\left[\Gamma^L n(t) + \Gamma^L \int \frac{\mathrm{d}\varepsilon}{\pi} f_i(\varepsilon, T) \mathrm{Im}\left(A^{(L)}(\varepsilon, t)\right)\right] \tag{4}$$

where $A_i(\varepsilon, t)$ can be described in terms of the appropriate retarded Green's function [8] and for $T_{2n-1} < t \le T_{2n}$ takes the form:

$$A^{(\alpha)}(\varepsilon, t) = \sum_{j = 1}^{n} A_j^{(\alpha)n}(\varepsilon, t) \tag{5}$$

$$A_{j<n}^{(\alpha)n}(\varepsilon, t) = -i \int_{T_{2j-1}}^{T_{2j}} \mathrm{d}t_1 \exp\left[i\left(\varepsilon - \varepsilon_1 + i\frac{\Gamma}{2}\right)(t - t_1) - \frac{\Gamma}{2}\sum_{s = 2j}^{2n-1}(-1)^s T_s\right] \tag{6}$$

$$A_n^{(\alpha)n}(\varepsilon, t) = -i \int_{T_{2n-1}}^{t} \mathrm{d}t_1 \exp\left[i\left(\varepsilon - \varepsilon_1 + i\frac{\Gamma}{2}\right)(t - t_1)\right] \tag{7}$$

Here, we assume the tunneling amplitude in the form

$$V_{k/q}(t) = V_{k,q} \sum_{i = 1}^{\infty} \theta(t - T_i)\theta(T_{i+1} - t)$$

where $\theta(t)$ is the Heaviside step function and T_i define the rectangular-pulse form of $V_{k/q}(t)$, T denotes the temperature and $f_i(\varepsilon, T)$ is a Fermi distribution function of the i-th electron reservoir,

$$\Gamma_{k/q} = 2\pi \sum_{k/q} \left| V_{k/q} \right|^2 \delta(\varepsilon - \varepsilon_{k/q})$$

and $\Gamma = \Gamma_k + \Gamma_q$.

The same quantities, $n(t)$ and $J_{L,R}(t)$, can be obtained within the EQM method solving the set of differential equations for appropriate correlation functions. For example, the current $J_L(t)$ takes the following form:

$$J_k(t) = -\frac{2e}{\hbar}\mathrm{Im}\left\{\sum_k V_k(t) e^{i\varepsilon_k t}\langle a_k^+(0) a_1(t)\rangle + i\frac{\Gamma_k}{2}\langle a_1^+(t) a_1(t)\rangle\right\} \tag{8}$$

where $\langle a_k^{+}(0)a_1(t)\rangle$ and $\langle a_1^{+}(t)a_1(t)\rangle \equiv n(t)$ should be found solving the coupled set of differential equations obtained within the Heisenberg equation of motion for some operators.

3. Results and discussion

On the basis of the formulae for the QD occupancies and for the current given in the previous section, we study numerically two different configurations of QDs placed between the electron reservoirs. In the first case, we consider a single QD coupled with two electron reservoirs for which the tunneling amplitudes are rectangular-pulse modulated. In the second case, the DQD (prototype of the qubit in the quantum computations) coupled with the electron reservoirs in different ways is considered. In the calculations, all energies, the current and the time, are given in the units of Γ_L ($\Gamma_L = \Gamma_R = 1$), $(e\Gamma_L)/\hbar$ and $\hbar/\Gamma_L$, respectively.

In Figure 1, we present the results for the QD occupancies under different time--dependent accomplishment of the coupling $V_k(t)$ and $V_q(t)$ between the QD and the electron reservoirs. The QD electron levels are chosen to be well above or below the Fermi energy, so for the constant couplings V_k and V_q the QD occupancies take a relatively small and large values, respectively, as expected. However, if we assume that during τ_1 (τ_2) time interval $V_k(t)$ and $V_q(t)$ take non-zero (zero) values, and subsequently, we repeat endlessly such sequence of $V_k(t)$ and $V_q(t)$ values, then we observe that the asymptotic values of $n(t)$ strongly differ from those obtained for

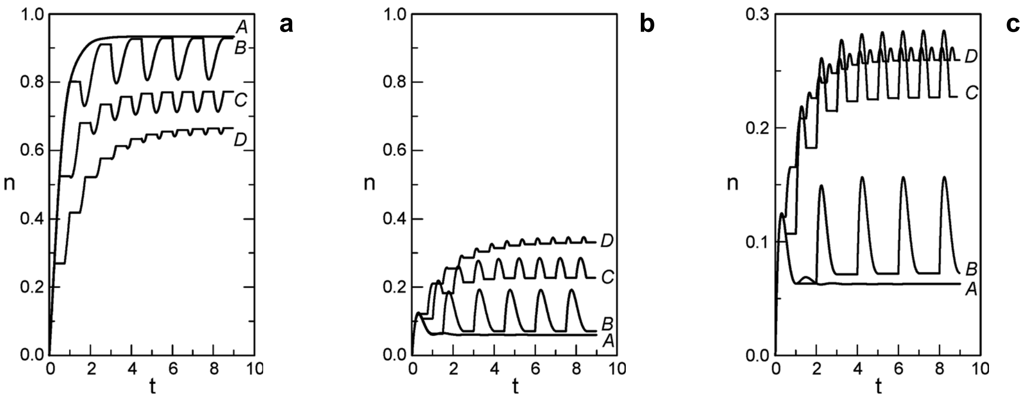

Fig. 1. Time dependent QD occupancy n vs. time t for the QD coupled with two electron reservoirs by the rectangular-pulsed tunneling coupling. In panels **a** and **b**, the curves B, C and D correspond to a sequence of pulses of the form $(\tau_1, \tau_2) = (1, 0.5)$, $(0.5, 0.5)$ and $(0.25, 0.5)$, respectively. Here, (τ_1, τ_2) denotes that during the time interval τ_1 (τ_2) the QD was connected (disconnected) with the electron reservoirs. In panel **c** the curves B, C and D correspond to $(\tau_1, \tau_2) = (1, 1)$, $(0.5, 0.5)$ and $(0.25, 0.25)$, respectively. The curves A describe the case of an unmodulated coupling of the QD with the electron reservoirs. Other parameters: $\varepsilon_1 = -5$ (5) for panel **a** (panels **b**, **c**), $\Gamma_k = \Gamma_q = 1$, and the bias voltage equals zero.

the constant couplings V_k and V_q. This difference is greater for sequences (τ_1, τ_2) with shorter τ_1 time interval. Therefore, we find that the time-dependent coupling of a special form can induce a strongly nonequilibrium occupancy of the QD. In Fig. 1**a**, we show another example of such behavior.

In Figure 2, we show the QD occupancies and currents in the system of two QDs coupled by a constant tunneling amplitude with two (one) electron reservoirs, panels **a**, **b** (**c**, **d**). The coupling between QDs is switched on at $t = 5$. The most interesting behavior is observed short time after the moment of switching on V_{12}. We observe the time oscillations of the transient current with the frequency equal to the oscillation frequency of the QD occupancies in an isolated DQD (qubit). This observation can have important practical consequences as it points out to a possibility of detecting the charge oscillations in the DQD through the measurement of the transient currents. In order to give more transparent example of such possibility, we consider an isolated DQD which is brought into contact with electron reservoirs at some subsequent moments of time. In this manner, the appearing transient current should contain some information about the evolution of the DQD state vector, and especially, the information about the state vector at the moment of switching on the coupling. As the DQD state vector periodically changes with Rabi's frequency, the transient current at subsequent moments of switching on the couplings V_k and V_q should also

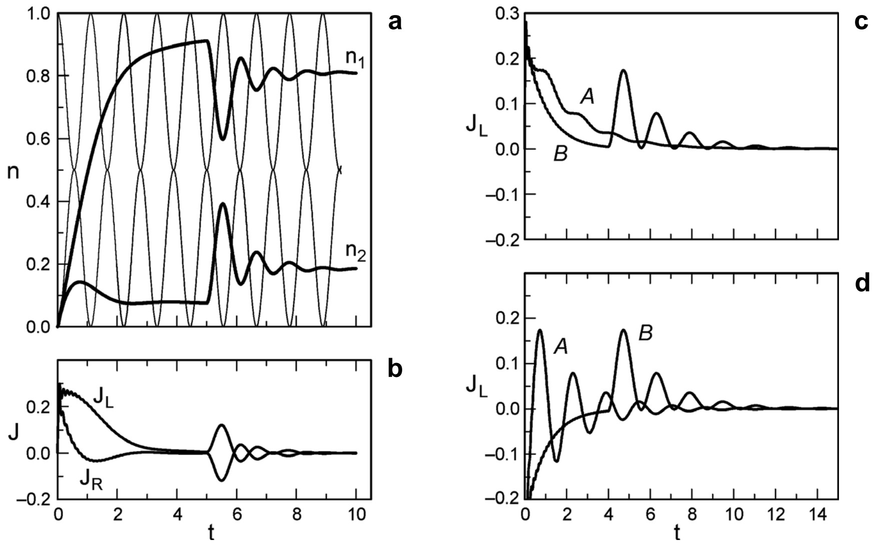

Fig. 2. The QDs occupancies (panel **a**) and transient currents J_L and J_R (panel **b**) vs. time for the case where the coupling between QDs was switched on at $t = 5$. The QD was coupled with the electron reservoirs at $t = 0$. Other parameters: $\varepsilon_1 = -\varepsilon_2 = -2$, $V_{12} = 2$, $\Gamma_k = \Gamma_q = 1$, $n_1(0) = n_2(0) = 0$ and the bias voltage equals zero. In panel **a**, the oscillations of QD occupancies for isolated DQD are also displayed (thin curves). In panel **c** (**d**), the curve *A* show the transient current J_L vs. time t for the DQD coupled with one electron reservoir obtained for the initial DQD occupancies $n_1(0) = n_2(0) = 0$ ($n_1(0) = 1$, $n_2(0) = 0$). The curve *B* correspond to the case of switching on the tunneling amplitude V_{12} at $t = 4$. Other parameters: $\varepsilon_1 = \varepsilon_2 = 0$, $\Gamma_k = 1$, and the bias voltage equals zero.

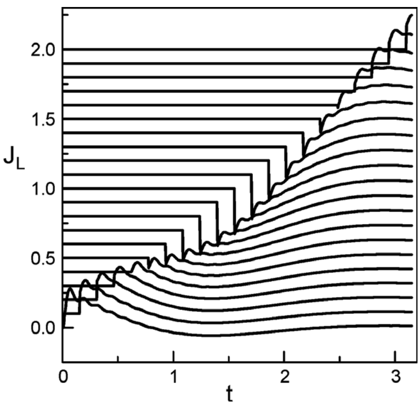

Fig. 3. The transient current J_L vs. time t for different values of the delay time of switching of the coupling between the left electron reservoir and the near QD of the DQD system. The ordinates of the curves are successively offset by 0.1 of the time unit for better visualization. The QDs energy levels $\varepsilon_1 = \varepsilon_2 = 0$, $V_{12} = 0.5$, $\Gamma_k = \Gamma_q = 1$, $n_1(0) = 0$, $n_2(0) = 1$, and the bias voltage equals zero. The lowest curve corresponds to the case where the DQD was coupled with the electron reservoirs at $t = 0$.

periodically (with Rabi's frequencies) change with time. In Figure 3, we show such transient currents which appear in the system of two QDs connected in a line configuration between the source and the drain at zero bias voltage. The moment of switching on the coupling between the DQD and the electron reservoirs is moved with time beginning at $t = 0$ to $t = T_R$, where T_R is the period of the DQD occupation oscillations. At $t = 0$, we localize the electron in the DQD on the QD near the right electrode. Therefore, we expect that when the coupling with the left and right electrodes is switched on at $t = 0$, the J_L current takes positive values at the beginning. On the contrary, at $t = T_R/2$ the current J_L should be negative, as at this moment the excess electron of the DQD is localized on the QD near the left electrode. Exactly such behavior of J_L can be observed in Fig. 3.

Summing up, we presented theoretical treatment of transient effects in the DQD system placed between the electron reservoirs with zero bias voltage. We identified the transient oscillations of the current flowing between one electrode and the near QD with the QD occupancy oscillations. We found the dependence of the transient currents on the time moment of switching on the coupling between the electrodes and the DQD. This dependence illustrates, to some extent, the oscillation of the DQD state vector and this information may be valuable in quantum information processing and quantum computation.

Acknowledgements – The work of R.T. has been partially supported by the Polish State Committee for Scientific Research (KBN) Grant no. N N202 1878 33 and the work of P.P. was partially supported by the Polish Ministry of Science and Higher Education (MNiSzW) Grant no. N N202 109036.

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Received June 19, 2009