Charging time effects and transient current beats in horizontal and vertical quantum dot systems

T. Kwapiński *, R. Taranko

Institute of Physics, M. Curie-Skłodowska University, 20-031 Lublin, Poland

HIGHLIGHTS

• We consider transient effects in different configurations of quantum dots system.
• The charging time of the QDs wire increases linearly with the wire length.
• The system geometry hardly influences the wire charging time for large voltages.
• Transient current beats patterns strongly depend on the wire inter-site couplings.
• The Coulomb interactions reduce the oscillations of the current beats.

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ABSTRACT

The transient electric current and quantum dot (QD) occupation probabilities in a linear wire of $N$ quantum dots coupled with two leads are investigated theoretically for vertical (T-shaped) and horizontal geometries of QDs. The model tight-binding Hamiltonian with inter-dot Coulomb interactions and the equation of motion technique are used in our calculations. The charging time of the initially empty wire is analyzed. It turns out that for both wire configurations the QD charging time grows up linearly for subsequent dots with simultaneously decreasing rate of the charging process, except the $N$-th dot. We have also shown that the transient current beats appearing in response to the sudden change of the bias voltage exhibit different patterns depending on the wire inter-site couplings. In some cases the structure of these beats provides useful information about the system parameters.

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1. Introduction

The studies of the electronic transport in quantum dot systems were commonly focused on the steady-state regime. The stationary properties of the electron current flowing through quantum dots (QDs) displayed in different geometries and coupled with two or more electron reservoirs were investigated in many experimental and theoretical works e.g. [1–14]. More interesting are the transport properties of QDs in the presence of time-dependent external fields (perturbations) or in the case of time-dependent tunnelling couplings between individual QDs. In such systems many interesting effects have been predicted and observed e.g. photon-assisted tunnelling, electron pumping or excited states transport [15–19]. The propagation of sinusoidal or train-like pulses through a quantum wire can also lead to charge or spin pumping [20–22]. Note that the charge distribution along the wire or the current in both stationary and time-dependent cases also depends on the system geometry e.g. [22–24].

A useful way to obtain some information about a QDs system is the detailed study of the transient currents, see for example the pump-and-probe technique used in determination of the spin relaxation time from transient current measurement [25]. These currents appear after abrupt switching on/off the coupling between electrodes and QDs (or between QDs) or after a sudden change of the QDs energy levels. Alternatively, transient effects can be observed when the bias voltage is suddenly stepped e.g. from zero to a finite value. Several studies of QD systems affected by the abruptly changed voltage bias (or values of the QD levels) were reported in the literature. The coherent oscillations and beats of the current were found in a short time scale after a bias voltage was turned on rapidly e.g. [23,26–30]. Depending on the structure of the QD-leads system the current exhibits different time scales. Moreover, different beat patterns of the transient current can be observed. Some useful information about parameters defining the considered system can be extracted from the analysis of such transient oscillations [23].
As the detection of a single electron in QDs systems has become experimentally feasible e.g. [31,32], then in this context, it would be very desirable to investigate the transient electronic occupation of a given QD in different QD systems and transient current appearing in response to instantaneous change of the bias voltage. It is also interesting to study how fast the subsequent QDs begin to be charged in response to the abruptly switched on/off bias voltage or hopping integrals within a QD wire. Such knowledge of the QD occupations, \( n_i(t), i = 1, \ldots, N \), provides useful information about the transport processes (e.g. charge propagation along the wire) and allows us to estimate the time at which a given QD begins to be occupied. Thus in the present paper we explore the transient transport dynamics in two different configurations of \( N \) QDs in order to answer the question whether the system geometry influences the QDs transient charge occupations and currents appearing in the system. The first considered configuration is the T-shaped (vertical) multi-QD system and the second one corresponding to a linear (horizontal) chain between two leads. The transients are generated by abrupt switching on the bias voltage to the system being already in the equilibrium state. These studies allow us to ‘monitor’ the electron signal propagation (in space and time) through the wire in both configurations. In particular, we analyze the parameter we call the charging time of a wire. We define it as the time for which the \( N \)-th QD site begins to be rapidly occupied or explicitly, the time of the first maximum observed for the \( dn_i(t)/dt \) derivative. We expect that QD sites will not be charged instantly but some delay time between neighbouring sites should be observed. Additionally, we analyze the transient beats in these systems. The study of beat patterns allows us to identify the QDs system just from the structure of the transient currents. To calculate the transient current we use the model tight-binding Hamiltonian and the equation of motion technique for the appropriate correlation functions. We assume the energy bandwidths of both leads much larger than any other energies of the system, with the density of states without any energy gaps or peaks, thus the wide band limit approximation [33] applied in our calculations (equivalent to the Markovian limit [34]) should be fully justified. In our study we have taken into consideration also small Coulomb inter-dot electron interactions. Note that in this paper we concentrate mainly on the initial stage of the dot charging process which, as will be shown for short chains of QDs, almost does not depend on the Coulomb interactions for the case of initially empty dots. Then the results obtained for longer chains without Coulomb interactions should also be valid.

The paper is organized as follows. In Section 2 the model Hamiltonian and the theoretical method are described. In Section 3 we analyze numerical results for the charging time of a wire (assuming different wire-leads configurations and Coulomb interaction effects) as well as the transient beats in different system geometries. Section 4 is a short summary.

2. Model and theoretical approach

We consider a linear QDs chain in two different configurations (vertical and horizontal) coupled with two (\( L \) and \( R \) – left and right) electron reservoirs shown schematically in Fig. 1.

![Fig. 1. Schematic diagrams of (a) vertical (T-shape) and (b) horizontal configurations of the system consisting of \( N \) QDs coupled with the left (L) and right (R) leads.](image-url)

Each \( i \)-th QD is described by a single electron energy level \( \varepsilon_i(t) \) (\( i = 1, \ldots, N \)), which can vary with time (it is assumed that other QD levels do not modify the electron transport as they lie beyond the voltage window). The nearest-neighbour QDs are coupled to each other by the inter-dot tunnelling amplitudes \( V_k \) and the first QD (for the T-shape configuration) or the first and last QDs (for the horizontal geometry) are coupled with the leads by tunnelling amplitudes \( V_{\alpha \text{L}} (\alpha = L, R) \) labelled by a wave vector \( k \). Possible electron energies in both leads are characterized by \( \varepsilon_{\alpha \text{L}}(t) \) which in general depend on time. The Coulomb interactions between electrons localized in neighboring dots are denoted by \( U \) and because we consider only linear geometries of the QDs then the next-neighbor Coulomb interactions are neglected in our calculations. The total Hamiltonian, \( H = H_{\text{QD}} + H_{\text{L}} + H_{\text{int}} \), can be written in terms of the creation, annihilation and number operators for electrons localized on \( i \)-th QD and in \( \alpha \)-th lead, \( c_i^+, c_i, n_i \), respectively. Here \( H_{\text{QD}} \) describes electrons in the QDs chain, \( H_{\text{L}} \) refers to electrons in the left and right reservoirs and \( H_{\text{int}} \) corresponds to the lead-QDs interactions:

\[
H_{\text{QD}} = \sum_{i=1}^{N} \sum_{\alpha = L, R} \varepsilon_i(t) n_i + \sum_{i=1}^{N} V_{L,i} c_i^+ c_{i+1} + h.c. + \sum_{i=1}^{N-1} U n_i n_{i+1},
\]

\[
H_{\text{L}} = \sum_{\alpha = L, R} \sum_{\alpha = L, R} \varepsilon_{\alpha \text{L}}(t) n_{\alpha \text{L}},
\]

\[
H_{\text{int}} = \sum_{k} (V_{L,k} c_{kL}^+ c_{kR} + V_{R,k} c_{kR}^+ c_{kL}) + h.c.,
\]

for the T-shaped geometry and

\[
H_{\text{int}} = \sum_{k} (V_{L,k} c_{kL}^+ c_{kL} + V_{R,k} c_{kR}^+ c_{kR}) + h.c.,
\]

for the horizontal configuration of QDs. To calculate the time dependence of the QDs occupation probabilities, \( n_i(t) = (c_i^+ c_i) \), and the transient current appearing in the system due to the abrupt change of the system parameters we use the equation of motion method for the appropriate correlation (Green’s) functions. The current flowing from the \( \alpha \)-th lead, \( j_{\alpha \text{L}}(t) \), can be calculated from the evolution of the \( \alpha \)-lead occupation operator number \( n_{\alpha \text{L}} = \sum_n n_{n \text{L}} \) i.e.

\[
j_{\alpha \text{L}}(t) = 2 \text{Im} \sum_k \varepsilon_k (c_k^+ c_k)(t) b_{\alpha \text{L}}(t),
\]

where the operators are given in the Heisenberg representation, the bracket (...) denotes the quantum-statistical average and the units \( e = \hbar = 1 \) were used. Solving the equation of motion for \( c_{\alpha \text{L}}(t) \) and inserting its solution i.e.

\[
c_{\alpha \text{L}}(t) = c_{\alpha \text{L}}(0) \exp \left( - \frac{1}{2} \int_0^t \varepsilon_{\alpha \text{L}}(t') \, dt' \right)\]

\[-i \int_0^t V_{\alpha \text{L}}(t) \exp \left( - i \int_{t_0}^t \varepsilon_{\alpha \text{L}}(t_2) \, dt_2 \right) c(t_1) \, dt_1 \]

into Eq. (5) one obtains e.g. for the T-shaped configuration:

\[
j_{\alpha \text{L}}(t) = 2 \text{Im} \left( \sum_k \tilde{V}_{\alpha \text{L}}(t) (c_k^+ c_k)(0) - i \int_0^t K_{\alpha \text{L}}(t, t_1) (c_k^+ c_k)(t_1) \right).
\]

where \( \tilde{V}_{\alpha \text{L}}(t) = V_{\alpha \text{L}}(t) \exp(\int_0^t \varepsilon_{\alpha \text{L}}(t') \, dt') \), \( \varepsilon_{\alpha \text{L}}(t) = \varepsilon_{\alpha \text{L}} + \Delta_{\alpha \text{L}}(t) \) and \( K_{\alpha \text{L}}(t, t_1) = \sum_k \tilde{V}_{\alpha \text{L}}(t) \tilde{V}_{\alpha \text{L}}(t_1) \). The function \( u_{\alpha \text{L}}(t) \) is responsible for the initial switching effects in the system i.e. \( u_{\alpha \text{L}}(t) = 0 \) for \( t \leq 0 \) and \( u_{\alpha \text{L}}(t) = 1 \) for \( t > 0 \). Similarly, writing the equation of motion for
\( \langle \dot{c}_j^+ (t) \rangle \) and using Eq. (6) one obtains the following set of differential equations for the QDs occupation probabilities, \( \eta_j(t) \), \( j = 1, \ldots \): 

\[
\frac{d}{dt} \eta_j(t) = 2 \sum_{k = L R} \left\{ \delta \eta_j \left( \sum_{k = L R} \Delta \eta_j(t) \right) \right\} 
- i \sum_{\alpha = \delta} \int_0^t dt \Delta \eta_j(t) \langle c_{j+1}^+ (t) c_j^+ (t) c_{j+1}^\alpha (t) c_j^\alpha (t) \rangle 
+ \left( 1 - \delta \eta_j \right) V_{j+1} \langle c_j^+ (t) c_{j+1}^\alpha (t) c_{j+1}^\alpha (t) c_j^\alpha (t) \rangle 
- \left( 1 - \delta \eta_j \right) V_{j-1} \langle c_j^+ (t) c_{j-1}^\alpha (t) c_{j-1}^\alpha (t) c_j^\alpha (t) \rangle , 
\]

(8)

and for \( \langle \dot{c}_j^\alpha (t) c_k^\beta (t) \rangle \):

\[
\frac{d}{dt} \langle \dot{c}_j^\alpha (t) c_k^\beta (t) \rangle = \langle \dot{c}_j^\alpha (t) c_k^\beta (t) \rangle 
+ \delta \eta_j \left( \sum_{\alpha = \delta} \sum_{\beta = \delta} \langle c_{j+1}^\alpha (t) c_j^\beta (t) c_{j+1}^\alpha (t) c_j^\beta (t) \rangle \right) 
+ \left( 1 - \delta \eta_j \right) V_{j+1} \langle c_j^\alpha (t) c_{j+1}^\alpha (t) c_{j+1}^\beta (t) c_j^\beta (t) \rangle 
+ \left( 1 - \delta \eta_j \right) V_{j-1} \langle c_j^\alpha (t) c_{j-1}^\alpha (t) c_{j-1}^\beta (t) c_j^\beta (t) \rangle . 
\]

(9)

The information about the \( \alpha \)-th lead electron states is contained in the memory kernel

\[
\kappa_{ia}(t, t_1) = V_{ia}^2 u_a(t) u_a(t_1) \exp \left( - i \int_{t_1}^t \Delta \kappa_{ia}(t') dt' \right) 
\times \int_{t_1}^\infty dED_a(E) \exp(-IE(t - t_1)),
\]

(10)

where \( D_a(E) \) is the \( \alpha \)-th lead density of states, \( V_{ia} = V_a \) and \( \Delta \kappa_{ia}(t) = \Delta \kappa_{ia}(t) \) are independent of \( k \). The memory kernel e.g. for the square density of states takes the form of the damping oscillatory function \( \sin(w(t-t_1))/\sin(w(t-t_1)) \) and with increasing bandwidth \( w \) the integrals of the non-local terms appearing in Eqs. (7)–(9) can be approximated by

\[
-i \frac{\Gamma_a(t)}{2} \langle \eta_1(t) \rangle, 
-i \frac{\Gamma_b(t) + \Gamma c(t)}{2} \langle \eta_1(t) \rangle 
\text{ and } 
-i \frac{\Gamma_{ia}(t)}{2} \langle \dot{c}_j^\alpha (t) \rangle,
\]

respectively. Here \( \Gamma_{ia}(t) = 2 \pi u_a^2(t) \sum_{k} |V_{ia}|^2 \delta (e - e_k^a) = u_a^2(t) \Gamma_{ia} \). This Markovian limit arises under the condition that the leads density of states varies slowly over sufficiently broad energy range around the QD level energy, or in other words, when the energy bandwidths of both leads are much larger in comparison with other characteristic energies of the considered system [34]. In this case the corresponding non-local in time equations for the current, QD occupations or other required correlation functions (see Eqs. (7)–(9)) can be replaced by local in time equations. More rigorous treatment of the transient properties of the open quantum systems based on the density matrix formalism beyond the Markov and WBL approximations can be found e.g. in Refs. [35–42,44] see also [18,43]. In the following we will consider the case in which the leads energy bandwidths are the largest energies in the system so the WBL is sufficiently good approximation and Eqs. (7)–(9) become local in time. However, the above set of differential equations is not closed and the higher-order correlation functions are generated. The functions of two types appear in the calculations: the first type is the averages of some number of the QD electron operators taken at a given time \( t \) e.g. \( \langle c_{j+1}^\alpha(t) c_j^\alpha(t) \rangle, \langle \eta_1(t) \rangle, \ldots \), and they form a closed set of differential equations. For the system consisting of e.g. \( N = 2, 3 \) and 4 QDs, the corresponding set of coupled equations contains 4, 13 or 41 different correlation functions of this type, respectively. Functions of the second type are the averages of some number of QD electron operators taken at a given time \( t \) and leads electron operators taken at the initial time \( t = 0 \): \( \langle \dot{c}_j^\alpha (t) \rangle \). These functions do not form a closed set of equations and some approximations are needed in the calculations. In the following we decouple the higher-order functions according to the rule

\[
\langle f(a_j^\alpha (t), a_i(t)) \rangle = \langle f(a_j^\alpha (t), a_i(t)) \rangle \langle \eta_1(t) \rangle, \langle \eta_2(t) \rangle \langle \eta_3(t) \rangle, \ldots , 
\]

(11)

where \( f(a_j^\alpha, a_i) \) are the appropriate functions appearing in the subsequent steps of the equation of motion procedure. This approximation (decoupling into two parts which depend separately on the QD and lead electron operators defined at different time arguments) can be compared with the truncation scheme of the Hubbard I approximation employed in the equilibrium Green’s function approach to the Hubbard model (see also a similar approach in the calculations of the time-dependent properties of electrons pumping through a QD [45]). Within such a decoupling procedure the corresponding set of coupled equations for the functions of the second type consists of 8, 28 and 93 equations (for every \( kl \) and \( kR \) vectors) for the system of \( N = 2, 3 \) and 4 QDs, respectively. The number of vectors taken in the calculations of the corresponding summations over these vectors (see Eq. (8)) usually extends from 200 for small source–drain voltages to over 2000 for larger voltages. Note that Eqs. (8) and (9) refer to the T-shape geometry of the QD chain between two leads but similar equations can also be obtained for the horizontal configuration of coupled QDs. In the next section both system configurations will be discussed.

3. Numerical results and discussion

In our calculations all energies are given in \( \Gamma_l = \Gamma_h = \Gamma \) units, the current and time are expressed in \( eF/h \) and \( h/\Gamma \) units respectively (we set \( e = \hbar = k_B = 1 \)). The chemical potentials of both leads taken at vanishing bias voltage are the reference energy point, \( \mu_0 = 0 \). As an illustration of the transient effects appearing in the horizontal and vertical QD systems we consider two different situations resulting in appearing transients in the system. Firstly, the transients arise after all couplings between leads and QDs are abruptly turned on at \( t = 0 \) (at vanishing or finite bias voltage). In that case the transient current and QDs occupations appear and after some delay time the asymptotic, steady-state values of the QDs occupations and current are achieved. This process is analyzed in Section 3.1. Secondly, in Section 3.2 we consider also the beating of the transient current appearing in the system which was initially in the equilibrium state (at vanishing voltages) and then the bias voltage was suddenly applied.

3.1. Charging time of a QDs wire

In order to study the charging time processes in a QD wire we assume that electrons occupy the QD states flowing only from the left electrode (the right lead is empty) and take the QDs energy levels equal to the left electrode Fermi energy. In the first step we investigate the role of the Coulomb interaction in the system, \( U \), which can modify the QDs charging process in comparison with the case of vanishing \( U \). Fig. 2 depicts the QDs occupation probabilities as a function of time for the T-shaped QDs structure.

We consider the initially separated system with empty QDs \( \eta_i(0) = 0, i = 1, 2, 3 \), and next the leads-QDs couplings and inter-QDs tunnelling are abruptly included at \( t = 0^+ \). This procedure initiates the charging process of all QDs. After some time the system approaches the stationary state (all QDs are filled up to 0.5 for \( U = 0 \), upper panel, or approximately
up to 0.4 for $U=2$, bottom panel) and again, at $t=15$ the leads Fermi energies are abruptly changed up to $\mu_1=\mu_2=20$. It leads to new stationary state of the system with nearly filled QDs. We observe a characteristic behaviour of the initial QDs charging process, namely, the first QD $(i=1)$ starts to be occupied rapidly but the third QD (the last one in the considered structure, $i=3$) after some delay time $\approx 3$ is most occupied in comparison with other dots. This scenario is repeated again after the potential drops at $t=15$ but only in the case of vanishing Coulomb interactions (upper panel) despite of different initial conditions. Note that for partially occupied QDs in the presence of the Coulomb interactions (see Fig. 2 at $t=15$, bottom panel) the response of the system on the abrupt change of the leads chemical potentials is somewhat different in comparison with that for small $t$. As one can see all $n_i(t)$ curves oscillate in time for $t>15$ and almost do not cross each other. For our later considerations it is very important that the QDs charging process (beginning from the moment when all dots are unfilled) is nearly the same for $U=0$ as well as for $U \neq 0$. It is obvious that it is a consequence of small amount of charge localized on dots and therefore negligible influence of the Coulomb interactions on the electron passage between dots. Thus the first charge impulse which achieves the subsequent dots is almost independent of the Coulomb interactions. Therefore, in the following we neglect the Coulomb interactions in the studies of longer wires with the initially empty QDs.

In Fig. 3 we analyze, assuming $U=0$, the case when an initially uncharged long wire is suddenly coupled to the leads and electrons start to occupy QD sites, so after some time (we call it a wire charging time) the last QD begins to be occupied. Note that the QD sites are not charged simultaneously but some delay time is observed between charging of the subsequent sites. This effect is clearly visible in the upper panels where the QD occupations are shown as functions of time. Here we consider both horizontal (right panels) and vertical (left panels) configurations for the wire length $N=10$ and show the time dependent occupations of all wire sites, $i=1, \ldots 10$. As expected, for both cases the first QD site, $i=1$, starts to be occupied suddenly after the system is coupled with electrodes. Next sites are charged with some delay time so the last QD in the wire stays the longest time unoccupied (the last QD occupations, thick curves, start to increase relatively late in comparison with other QDs). However, until all occupancies achieve their equilibrium values, electrons occupy faster the last QD and, in consequence, QDs occupations are characterized by a kind of a time plateau (their occupancies do not change in some time intervals). Interestingly, the QD sites which are closer to the source electrode are occupied only partially (in the first stage of the electron transport) and they ‘wait’ until the last QD achieves its almost equilibrium occupancy. Note that the asymptotic occupation (for $t=\infty$, not shown here) of the last QD for the vertical configuration ($\sim 0.24$) is larger than the occupation of the corresponding site in the horizontal geometry ($\sim 0.2$) – thick curves in the upper panels. Such a result is a consequence of electron tunnelling from the $N$-th QD directly to the right electrode in the horizontal geometry which decreases the occupation of this dot.

As we are mainly interested in the determination of the first charging impulse observed in the subsequent QDs, then we analyze the time-derivatives of the QDs occupations (Fig. 3, bottom panels). These curves, except the one corresponding to the last dot, possess the form of peaks of decreasing heights and approximately equal half-widths. The peak heights fall down monotonically which denotes that the charging process of the subsequent dots is slower and slower but the charging process of the last dot ($N$-th dot), in both configurations, is characterized by faster charge accumulation compared to the neighboring dots. This especially large value of $dn_{i_0}/dt$ can be understood as a result of weak coupling between the last QD and the right electrode (in the horizontal geometry) or absence of this coupling in the vertical configuration. For the smaller and smaller $\Gamma_L$ parameter the sequence of $dn_{i_0}(t)/dt$ curves obtained for the horizontal configuration is similar to this one for the vertical geometry (not shown here). It is also interesting that there is one crucial difference in the behaviour of the last but one dot in the vertical and horizontal configurations. Namely, for $i=N-1=9$ in the vertical geometry the charging rate is much smaller in comparison with other dots. Thus the heights of $dn_{i}/dt$ peaks of the last and last but one QDs distinguish between both wire configurations and provide some information about the strength of the wire-lead couplings. Moreover, as one can see, the heights of $dn_{i}/dt$ peaks are larger for the horizontal geometry which means that the QD sites are more occupied than in the vertical configuration. It results from the fact that all electrons which leave the left lead are transferred through all wire sites in the horizontal geometry and mainly through the first wire site in the vertical case. Note, however, that the wire charging time (time-position of the first maximum of $dn_{N}/dt$) is almost the same for both considered configurations.

To study the charging effect in more detail in Fig. 4 we show the first peak of the time derivative of the last QD occupancy for different wire lengths, $N$, and for two values of the hopping integrals between QDs (upper panel for $V_{ij}=0.5$ and $N=2, 3, 4, 5$ and bottom panel for $V_{ij}=1$ and $N=2, 3, 4, 5, 10, 15, 20, 30$). All $dn_{N}/dt$ curves are characterized by local maxima and minima but the first maxima are crucial as their positions on the time scale define the QD charging time. Note that for weak QD couplings all peaks are rather wide (large half-width) contrary to the regime of stronger hopping integrals (bottom panel), where relatively narrow and high $dn_{N}/dt$ peaks are observed. In the last case the charging of the subsequent dots propagates faster along the QD wire (see e.g. time positions of $dn_{N}(t)/dt$ peaks for $N=5$). Note that the wire charging time is proportional to the wire length. One can find that the charging time of the last QD, $T_N$, increases linearly with $N$. $T_N=\Gamma_N=2+\kappa_0(N-2)$, where $\kappa_0$ depends on the number of dot couplings ($V_{ij}=V$) and for two wires with different $V_{ij}$ (i.e. $V_{ij}=V_1, V_2, V_3$), $\kappa_0$ satisfies the relation $\kappa_0/V_1=\kappa_0/V_2, \kappa_0$. It appears also that approximately up to $N=10$ the linear approximation of the first maxima values of $dn_{N}(t)/dt$ versus time is valid (see the broken straight line) but for greater $N$ one can observe that the
corresponding rates converge to some constant value on a significantly longer timescale. It is worth noting that in the horizontal geometry the behavior of \(dn_i/dt\) versus time is very similar to that one observed in the vertical configuration of QDs. It means that the time-dynamics depends mainly on the parameters describing the QD wire and not on the wire configuration between the source and drain electrodes. Note that the knowledge of the charge rate and the charging time for different wires can be useful in nanoelectronics where charging/discharging processes often take place. In these systems it is possible to control in time and space the propagation of the electron charge through the wire by changing the couplings between wire sites.

### 3.2. Transient beats in different QDs configurations

In this section we analyze the transient current which appears in the system due to the abrupt change of the leads chemical potentials. For sufficiently large changes of \(\mu_{L,R}\) (in comparison with \(\Gamma\)) the beats pattern in the transient current can be observed. As will be shown the behaviour of beats is strongly related to specific system parameters thus the knowledge of beats allows us to determine the system structure. In particular, we investigate the influence of the system geometry (vertical and horizontal setups) on the transient current.

In Fig. 5 the transient current flowing from the left lead is analyzed for the vertical configuration of QDs for vanishing (left panel) and nonzero (right panel) Coulomb interactions. The system is prepared in the equilibrium state \((\mu_L = \mu_R = 0)\) and at \(t=15\) a sudden change of the chemical potentials took place (up to \(\mu_L = -\mu_R = 50\) and the QDs energy levels remain unchanged). The upper, middle and bottom curves correspond to different inter-dot couplings as is indicated in the figure. We observe that \(U\) does not destroy the overall form of the current beats although the amplitude of \(i_\text{f}\) oscillations is reduced and beats are less visible. As small Coulomb interactions do not change significantly the structure of beats then in explanation of such different behaviour of corresponding beats for different values of \(V_H\) we concentrate on the case \(U=0\). It is known that the transient current appearing in response to the sudden jump of the bias voltage oscillates with the frequency \(|e_d - \mu|/\hbar\), where \(e_d - \mu\) is the difference between the QD energy level and the electrode chemical potential just after the voltage jump [26]. The system of three QDs discussed here is equivalent to the molecule with three energy levels: \(e_0\), \(e_0 \pm \sqrt{V_{12}^2 + V_{23}^2}\). The current flowing through this system is a superposition of three currents flowing through these three molecular levels. This superposition of the currents reveals fast oscillations with the frequency \(\omega = V_H / \omega_0\) with superimposed beats. The high frequency of oscillations is independent of the inter-dot tunnelling amplitude \(V_H\) but the structure and the beats frequency strongly depends on \(V_H\). It is interesting that for \(V_{12} \ll V_{23}\) there is no transient current beating which is in opposition to the case \(V_{12} \gg V_{23}\) for which beats are very well visible (the upper and bottom curves in Fig. 5). This fact can be helpful in experimental estimation of the \(V_{12}/V_{23}\) ratio. Note, however, that here we have considered only different coupling strengths \((V_{12}, V_{23}) = (1, 4)\) and \((4, 1)\) between QDs, so the position of the molecular states did not change at all. Thus what is the reason that
leads take the values: \((\frac{1}{\sqrt{3}} V_{LR}^{1}, \frac{4}{\sqrt{3}} V_{LR}^{1}, \frac{1}{\sqrt{3}} V_{LR}^{1})\) and \((\frac{3}{\sqrt{17}} V_{LR}^{1}, \frac{4}{\sqrt{34}} V_{LR}^{1}, \frac{8}{\sqrt{17}} V_{LR}^{1})\), respectively. Thus although the energy positions of \(E_i\) are the same, their effective couplings to the leads depend on the ratio of the inter-dot tunnelling couplings. For that reason we observe different behaviour of the current oscillations for \(\xi = 4\) and \(\xi = 1/4\) (upper and bottom curves in Fig. 5).

In the last studies we compare the beats of the transient currents appearing in the vertical and horizontal geometries of the QD wire. In Fig. 6 we present the transient currents for \(N = 2\) for horizontal (solid curves) and vertical (broken curves)
geometries. We consider weak (upper panel) and strong (bottom panel) couplings strengths between dots. One notices that after sudden change of the chemical potentials (at $t=0$) the transient current oscillations are visible for both configurations. However, there are some important differences between them. The time dependence of amplitudes is different for horizontal and vertical configurations for small values of the inter-dot tunnelling coupling (upper panel). The asymptotic current values are also different but the periods of beats which are visible on the current curves are almost the same for both geometries. On the other hand, for larger values of $V_{12}$ the picture of the transient currents is very similar for both configurations. Now, the asymmetric currents and overall structure of oscillations are nearly the same. One can ask, why the transient currents for small inter-dot couplings are different in both geometries but for greater couplings they are similar. The answer is related with the different time-dependence of the QD occupations. Namely, in the case of the horizontal geometry the QD occupancies do not oscillate in time and are equal to 0.5 (for parameters chosen here) almost independent of the bias jump. However, for the vertical geometry the QD occupancies change in time after the bias jump. The corresponding charge oscillations are sufficiently large for small inter-dot coupling but for greater couplings they are rather small and the QDs occupancies are nearly constant (equal to 0.5).

4. Conclusions

In summary, the transient currents in a QD linear wire between two electrodes have been investigated theoretically for the vertical (T-shaped) and horizontal configurations. The equation of motion technique for appropriate correlation functions was used to obtain the currents flowing in the system as well as the QDs electron occupancies. For short wires the Coulomb interactions between the neighboring QDs were considered and the higher-order correlation functions were decoupled similarly as in the Hubbard I approximation. We have studied two kinds of the transient effects: (i) which appear just after switching on the couplings between QDs and (ii) after a sudden jump of the bias voltage applied to the system being already in the equilibrium state.

It was shown that for initially empty QDs the Coulomb interactions hardly influence the transient current and time-dependent occupancies of the QDs. For initially uncharged wire coupled with two leads we have calculated the charging time which characterizes the electron transfer through the whole wire. We have found that the charging time increases linearly with the wire length, $N$. It was shown that for large source–drain voltages the system geometry (vertical or horizontal) hardly influences the charging time of the wire and the wire QDs occupations always increase in time until the system achieves its equilibrium state. As a main feature of the QD wire we have found that for a given wire length the charging rate of subsequent dots, $i=1,\ldots,N$, decreases monotonically with $i$, but for longer wires this decreasing is much slower.

For both wire configurations we have also investigated the current beats which appeared as a response to the sudden voltage drop. The periods of beats are similar for the vertical and horizontal configurations, however, there are some important differences between them. Namely, for small values of the inter-dot tunnelling coupling the amplitudes of the current oscillations as well as the asymptotic current values are different for both geometries. It was also found that the asymmetry in the wire inter-site couplings is reflected in the transient current curves and the transient beats are the unique feature of a given distribution of these couplings along the wire. In the presence of the Coulomb interactions the transient current oscillations are reduced which leads to less visible current beats in the vertical and horizontal QD systems.

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References