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Negative differential conductance in metallic double quantum dot structures

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Abstract

We show that negative differential conductance (NDC) can be observed in metallic quantum dot structures. For a simple model at zero temperature we have derived an analytical expression for the current–voltage characteristics and a condition for observing NDC. For devices with gates at finite temperatures, using the Monte Carlo method we have suggested diagrams describing a correlation between the gate capacitance or temperature and the inter-dot coupling in producing (or removing) NDC.

1. Introduction

Double quantum dot structures have recently attracted a great amount of attention [1–5]. In these structures not only the charging effect, but also the inter-dot coupling and the asymmetry between two junctions coupling dots to leads can play an important role. The current–voltage (I–V) characteristics are very sensitive to the device parameters and a negative differential conductance (NDC) or even a multiple Coulomb gap may appear at low temperatures.

NDC has been suggested in a number of quantum dot structures [6–11]. It was observed early in single semiconductor quantum dot structures and has been regarded as a result of the existence of excited states [6]. Nakashima and Uozumi [7] have demonstrated NDC in a linear array of metallic islands due to a competition between the forward rate of injecting charges into the array which increases with the bias and the tunnelling rate across some junction (a 'bottleneck') which may be reduced with increasing bias. Shin *et al* [8] have calculated I–V characteristics in a ring-shaped array of metallic dots and shown that the interaction between electrons in two branches of the ring can bring about stationary electron configurations which produce NDC at low temperatures (and multiple Coulomb gap at zero temperature). Heij *et al* [9] have measured a device where an electron box is attached to a single electron transistor as a gate, and reported on NDC for a range of conditions. For double dot structures the NDC

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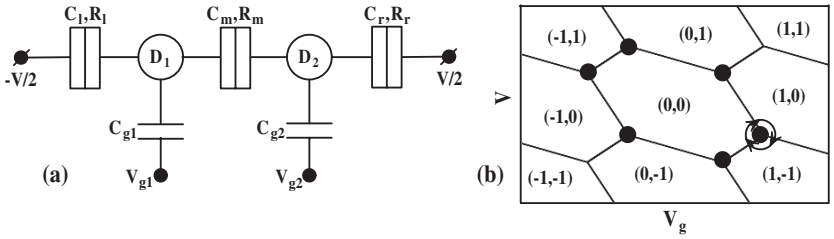

Figure 1. (a) The current diagram of the model (for the simple case studied in section 2 the gates are removed). (b) The schematic diagram used to illustrate how equations (9) and (10) can be derived: the first Coulomb staircase corresponds to electron transfers around one of six triple points (solid circles); in the condition (6) only one of these points (shown in figure) should be carried.

has been analysed by Evans *et al* [10] and by Wang *et al* [11]. The structure studied in [10] is somewhat similar to that of [7] in the sense that electrons have to pass through both dots, while in the structure studied in [11] the two dots are not equivalent: one dot is connected to both external leads, but the other is connected to only one. Very recently [12], we have simulated the I–V characteristics in the double dot device measured by Junno *et al* [13], taking into account the cross-coupling between dots and gates and the finite temperature and random offset charge effects. We have shown that an NDC of different phases, including a second or multiple Coulomb gap, can be manipulated at low temperatures when the coupling capacitances are set with appropriate values. It is however essentially suppressed by increasing the temperature and/or introducing the offset charge, and is very sensitive to the device parameters.

The aims of this paper are (1) to derive an analytical expression for the I–V characteristics and a condition for observing NDC in a simple model of metallic double dot structures (section 2) and (2) to simulate NDC in a structure like that measured in [13] with a focus on mutual correlations between the most characteristic parameters (section 3). The I–V characteristics and the NDC condition have been derived by solving the master equation for the first Coulomb staircase in some range of parameters in the simple model where all the effects associated with the gates, the finite temperature and the offset charge are neglected. For more realistic device models with gate couplings at finite temperatures the I–V characteristics can be simulated and therefore the NDC behaviour can be analysed in detail using the Monte Carlo method. The simulation data, on the one hand, supports very well the master equation solution, and on the other hand, suggests the diagrams showing the correlations between the gate coupling or temperature and the inter-dot coupling in producing (or removing) NDC.

2. I–V curves and the NDC condition in a simple model

In general, to study the electron dynamics in Coulomb blockade structures one often uses two methods: the master equation and Monte Carlo simulation. The master equation is regarded as exact, but it could not be solved exactly even in relatively simple structures, whereas Monte Carlo simulation is relatively simple and easily realized even in complex structures. However, as the aim of this section, we like to show an exactly analytical condition for NDC, so we have to solve the master equation. For this end we must restrict ourselves to considering the simple structure drawn schematically in figure 1(a) (without gates). Assuming that the temperature is zero and neglecting the random environment (offset charge) effect, the master equation can then be solved exactly for the first Coulomb staircase range of bias.

Within the framework of the Orthodox theory [14] the state of the system under study is entirely determined by the number of excess electrons in two dots, n_1 and n_2. Supposing that

$p(n_1, n_2)$ is the probability of the state (n_1, n_2), the master equation reads

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}p(n_1,n_2) &= \Gamma_l^+ p(n_1-1,n_2) + \Gamma_l^- p\,(n_1+1,n_2)\\ &\quad + \Gamma_m^+ p\,(n_1+1,n_2-1) + \Gamma_m^- p\,(n_1-1,n_2+1)\\ &\quad + \Gamma_r^+ p\,(n_1,n_2+1) + \Gamma_r^- p\,(n_1,n_2-1)\\ &\quad - [\Gamma_l^+ + \Gamma_l^- + \Gamma_m^+ + \Gamma_m^- + \Gamma_r^+ + \Gamma_r^-]p(n_1,n_2) \qquad (1)\end{aligned}$$

where $\Gamma_\nu^{+(-)}$ is the tunnelling rate across the junction ν ($\nu = l, r, m$) to the right (+) or left (−) at the state determined by the argument of the associated probability p. Equation (1) should be solved in the condition

$$\sum_{(n_1,n_2)} p(n_1,n_2) = 1. \qquad (2)$$

The stationary current is defined as

$$I = e\sum_{(n_1,n_2)} [\Gamma_\nu^+(n_1,n_2) - \Gamma_\nu^-(n_1,n_2)]p(n_1,n_2), \qquad (3)$$

where e is the elementary charge, ν is any of the junctions l, r, or m in figure 1(a). For both equations (1) and (3) one has to know the tunnelling rates $\Gamma_\nu^{+(-)}$ ($\nu = l, r$ and m). At zero temperature the tunnelling rate across a junction is defined as [14]

$$\Gamma = \begin{cases} 0, & \Delta F \geqslant 0,\\ |\Delta F|/e^2R_\mathrm{t}, & \Delta F < 0,\end{cases} \qquad (4)$$

where ΔF is the change in the free energy F of the system after the tunnelling event has occurred, and R_t is the junction tunnelling resistance. For the simple model under study (figure 1(a), without gates) the free energy F has the form

$$\begin{aligned}F &= (en_1 - C_lV/2)^2/2C_l^* + (en_2 + C_rV/2)^2/2C_r^* + (en_1 - C_lV/2)(en_2 + C_rV/2)/C_m^*\\ &\quad + eV(n_l - n_r)/2 - (C_l + C_r)V^2/8. \qquad (5)\end{aligned}$$

Here C_l, C_m and C_r are junction capacitances as shown in figure 1(a), V is the external bias ($V_l = -V/2,\ V_r = V/2$), n_l (n_r) is the number of electrons that has entered the device from the left (right) lead [15], $C_l^* = \Sigma_C/(C_r + C_m)$, $C_r^* = \Sigma_C/(C_l + C_m)$, and $C_m^* = \Sigma_C/C_m$ with $\Sigma_C \equiv C_lC_m + C_mC_r + C_rC_l$.

In principle, using equations (4) and (5) one can solve equation (1) and then calculate the current (3). In practice, however, one cannot solve equation (1) exactly with all possible values of n_1 and n_2, but has to accept some cut-off on the value of these numbers. To find an exact expression for the current (3) and then an exact NDC condition we will restrict our consideration to only the first Coulomb staircase, corresponding to the bias range $V_{s1} \leqslant V \leqslant V_{s2}$, where $V_{s2} = e/2C_r$ and V_{s1} is the maximum from $e/2C_l$ and $e|C_l - C_m|/2C_r(C_l + C_m)$ (assuming $C_l \geqslant C_r$). In this case the states of the system are restricted to only some honeycomb cells in the stability diagram with the possible values of n_1 and n_2 as illustrated in figure 1(b). The first Coulomb staircase corresponds to electron transfers around one of six triple points associated with the state (0, 0). Noting that at low temperature and at $V \geqslant V_{s1}$, practically, only the tunnelling transitions along the direction of electric field (from source to drain via QDs for electrons) are allowed, we will here concentrate our attention only on electron transfers between states (0, 0), (1, 0) and (1, −1) around one trip point as drawn by the circle with arrows in figure 1(b). Now, from expressions of the change in free energy ΔF associated to different electron transfers (see the appendix) we learn that the problem becomes easily solved exactly if we adopt the following conditions:

$$\begin{aligned}&C_r \leqslant C_l \leqslant 3C_r,\\ &C_m \leqslant C_r\,(3C_r - C_l)\,/\,(C_l - C_r)\,.\end{aligned} \qquad (6)$$

In these conditions all the probabilities $p(n_1, n_2)$ are equal to zero except those for three states $(0, 0)$, $(1, 0)$ and $(1, -1)$, which for short will be denoted by a, b, and c, respectively:

$$\begin{aligned} p_a &\equiv p(0,0) = \Gamma_{ab}^{-1}\Sigma_\Gamma, \\ p_b &\equiv p(1,0) = \Gamma_{bc}^{-1}\Sigma_\Gamma, \\ p_c &\equiv p(1,-1) = \Gamma_{ca}^{-1}\Sigma_\Gamma, \end{aligned} \tag{7}$$

with $\Sigma_\Gamma \equiv (\Gamma_{ab}^{-1} + \Gamma_{bc}^{-1} + \Gamma_{ca}^{-1})^{-1}$. Here Γ_{xy} is the tunnelling rate from state x to state y $(x, y = a, b, c)$:

$$\begin{aligned} \Gamma_{ab} &= (eR_l)^{-1}[C_l(C_r + C_m)/\Sigma_C](V - e/2C_l), \\ \Gamma_{bc} &= (eR_r)^{-1}[C_r(C_l + C_m)/\Sigma_C](V - e(C_l - C_m)/2C_r(C_l + C_m)), \\ \Gamma_{ca} &= (eR_m)^{-1}[C_lC_r/\Sigma_C](e/2C_l + e/2C_r - V) \end{aligned} \tag{8}$$

(Σ_C was defined in equation (5)).

Now, the current has the simple form

$$I = e\Sigma_\Gamma. \tag{9}$$

Thus, in the conditions (6) we obtain an analytical expression for the tunnelling current in the first Coulomb staircase region, where Σ_Γ is determined by the tunnelling rates between states $(0, 0)$, $(1, 0)$ and $(1, -1)$ as defined in equation (8).

Moreover, from the current expression of equation (9) we can straightforwardly derive the condition for observing NDC:

$$R_m > R_l \frac{C_r^3}{(C_r + C_m)(C_l - C_r)^2} + R_r \frac{C_r^2(C_l + C_m)}{4C_lC_m^2}. \tag{10}$$

The inequality (10), together with inequalities (6), gives the condition for observing NDC in the first Coulomb staircase region in the structure under study. This condition was obtained for the case of asymmetrical structures with $C_l > C_r$ (6). Though in the case considered a difference between C_l and C_r can enhance the NDC, the effect is generally governed by the relative values of tunnelling resistances and by the capacitance C_m. It is here worthy also to mention that the nonlinear I–V characteristics, including NDC, of mesoscopic conductors has been critically studied by Christen and Büttiker [16], using the scattering approach. Our present study is however concerned with the strongly correlated phenomenon of Coulomb blockade.

In figure 2 we present some I–V curves (solid curves) calculated directly from expression (9) in comparison with the Monte Carlo simulation data ($\times$) at the bias voltages corresponding to the first Coulomb staircase. Recalling that expression (9) has been obtained in the condition (6), to calculate the current (9) the parameter values should be chosen appropriately. For the data in this figure as well as in the others below choosing capacitance C_r and the resistance R_r as the basic units, the current and the voltage are measured in units of e/R_rC_r and e/C_r, respectively.

Curve 1 in figure 2 shows regular I–V characteristics without an NDC, when the condition (10) is not satisfied. The Coulomb blockade leads to a Coulomb gap with the width of $1/3$. Following the gap, the first Coulomb staircase ranges to the voltage $V_{s2} = 1/2C_r = 0.5$. Starting from the set of parameters corresponding to curve 1 we can get I–V curves with an NDC by changing the parameters to fulfil the condition (10). There are different ways to achieve this aim, some of which are shown in figure 2: by decreasing R_l (curve 2), by increasing the inter-dot coupling C_m with regard to the condition (6) (curve 3), or by increasing the tunnelling resistance R_m (curve 4). It is clear that, on the one hand, there really is an NDC observed in the I–V curves in all the cases once the condition (10) is fulfilled, and on the other hand, there

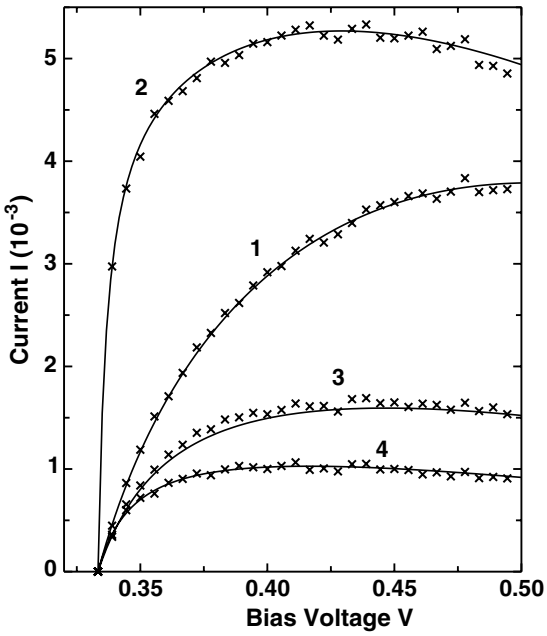

Figure 2. I–V characteristics calculated from equation (9) (solid curves) in comparison with Monte Carlo simulation data ($\times$) for some sets of device parameters: (1) $C_l = 1.5$, $R_l = 1.5$, $C_m = 0.5$, $R_m = 5.0$ (without NDC); (2) $C_l = 1.5$, $R_l = 0.1$, $C_m = 0.5$, $R_m = 5.0$; (3) $C_l = 1.5$, $R_l = 1.5$, $C_m = 3.0$, $R_m = 5.0$; (4) $C_l = 1.5$, $R_l = 1.5$, $C_m = 0.5$, $R_m = 30.0$. In the last three cases the NDC is produced by decreasing R_l (2), by increasing C_m (3) or increasing R_m (4), then the condition (10) is satisfied.

is always a good agreement between analytical curves calculated from equation (9) and Monte Carlo simulation points. Thus, the two results, while agreeing well with each other, show the existence of NDC in the structure under study at least in the first Coulomb staircase at zero temperature.

The simulation program used for the present work is the one described in detail in [12, 17]. The same program was also used to calculate the I–V characteristics and to analyse the NDC behaviour in more realistic structures discussed in the next section.

3. The gate and temperature effects

In this section we analyse the NDC effect in a more realistic structure with two gates as drawn in figure 1(a). Though the Monte Carlo method enables us to simulate I–V curves without any restriction on the value of structure parameters as well as the range of bias voltage (see [12, 17]), we will only study the influence of gates and temperature on the NDC behaviour. With the gates included, the free energy of the system can be obtained from (5) by adding $C_{\mathrm{g1(2)}}$ to $C_{l(r)}$ and $C_{\mathrm{g1(2)}}V_{\mathrm{g1(2)}}$ to $(-/+)C_{l(r)}V/2$, respectively:

$$\begin{aligned} F = {} & (en_1 + C_{\mathrm{g1}}V_{\mathrm{g1}} - C_lV/2)^2/2C_l^{(g)} + (en_2 + C_{\mathrm{g2}}V_{\mathrm{g2}} + C_rV/2)^2/2C_r^{(g)} \\ & + (en_1 + C_{\mathrm{g1}}V_{\mathrm{g1}} - C_lV/2)(en_2 + C_{\mathrm{g2}}V_{\mathrm{g2}} + C_rV/2)/C_m^{(g)} \\ & + (n_l - n_r)eV/2 - (C_l + C_r)V^2/8 - (C_{\mathrm{g1}}V_{\mathrm{g1}}^2 + C_{\mathrm{g2}}V_{\mathrm{g2}}^2)/2, \end{aligned} \tag{11}$$

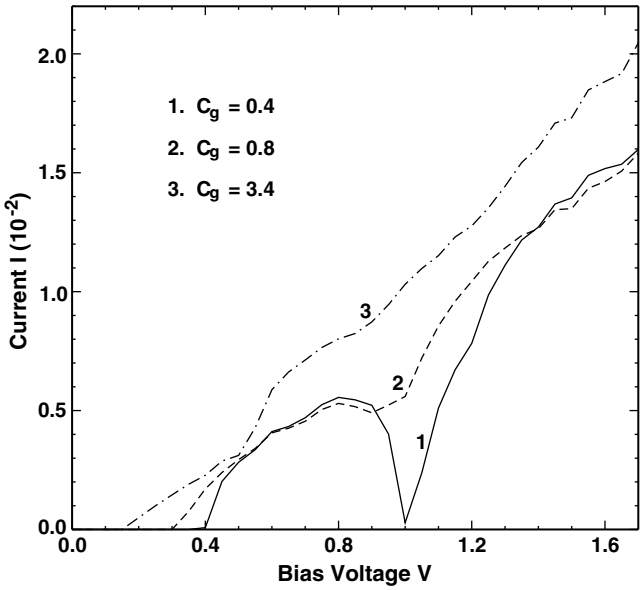

Figure 3. To demonstrate how an NDC can be manipulated by changing, for example, the gate capacitance: $C_g = 0.4$ (curve 1), 0.8 (2), and 3.4 (3); everywhere $C_l = 1$, $R_l = 10$, $C_m = 0.4$, $R_m = 0.5$, $V_g = 0.0$, and $T = 0$.

where $C_l^{(g)} = \Sigma^{(g)}/C_2$, $C_r^{(g)} = \Sigma^{(g)}/C_1$ and $C_m^{(g)} = \Sigma^{(g)}/C_m$ with $C_1 = C_l + C_{g1} + C_m$, $C_2 = C_r + C_{g2} + C_m$ and $\Sigma^{(g)} = C_1C_2 - C_m^2$. The meanings of the other symbols are the same as in expression (5).

On the other hand, simulating the problem at finite temperature, instead of (4), one has to deal with the following tunnelling rate [14]:

$$\Gamma = (e^2R_t)^{-1}\Delta F/(\exp(\Delta F/k_BT) - 1). \tag{12}$$

Using the expressions (11) and (12) one can simulate the electron transfer across the structure and calculate the I–V curve for different gate parameters and at various temperatures.

First, focusing attention on the gate effects we assume that the temperature is zero and two gates are identical with $C_{g1} = C_{g2} \equiv C_g$ and $V_{g1} = V_{g2} \equiv V_g$. Appearing in the energy (11) only in the terms of induced charges C_gV_g, the gate voltage V_g, as is well-known, leads mainly to an oscillation of the conductance spectroscopy (see, for example, figure 5(b) in [12]). On the other hand, the gate capacitance and the inter-dot one are added together in all the denominators of the first three (important) terms in the energy F (11). We can then in some approximation guess that in affecting the form of the I–V curves (and therefore, the NDC behaviour) these two capacitances should merely act as a single variable $(C_m + C_g)$.

For a given value of V_g, we have simulated the I–V characteristics and searched for NDC at different 'points' $(C_m + C_g)$, keeping all other parameters fixed. Figure 3 shows I–V curves for some values of C_g. It is clear that a change of C_g alone can bring about an NDC or bring it down. The simulation shows that for a given value of V_g the NDC can be observed only when C_m and/or C_g is small enough. So, by changing C_m and/or C_g gradually we were able to fix the upper bounding points of the NDC region at which any increase of C_m and/or C_g will at once cause the NDC to disappear. The check has been done for $V_g = 0$, -0.5 and -1.5. Interestingly, for a given value of V_g, as can be seen in figure 4, all these simulation points are within the error bars fitted well to a straight line, which divides the $(C_g - C_m)$-space into two

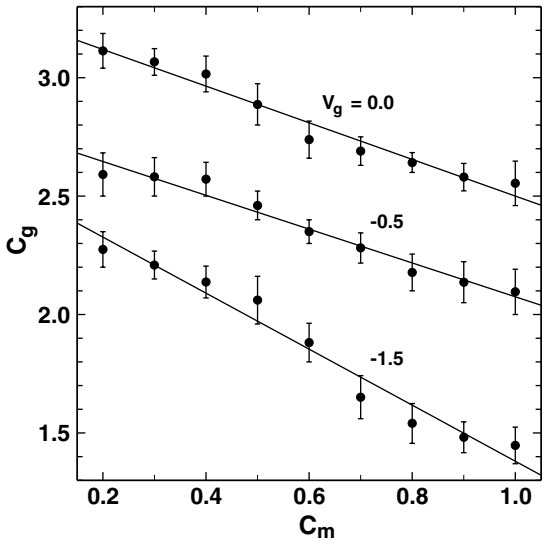

Figure 4. $(C_g - C_m)$-diagrams for some gate voltages V_g (from top): 0, −0.5, and −1.5. For each V_g the simulation data (solid circles) are fitted to a (solid) straight line. For a given value of V_g, the line divides the $(C_g - C_m)$-space into two parts; the NDC can be observed only in the lower one.

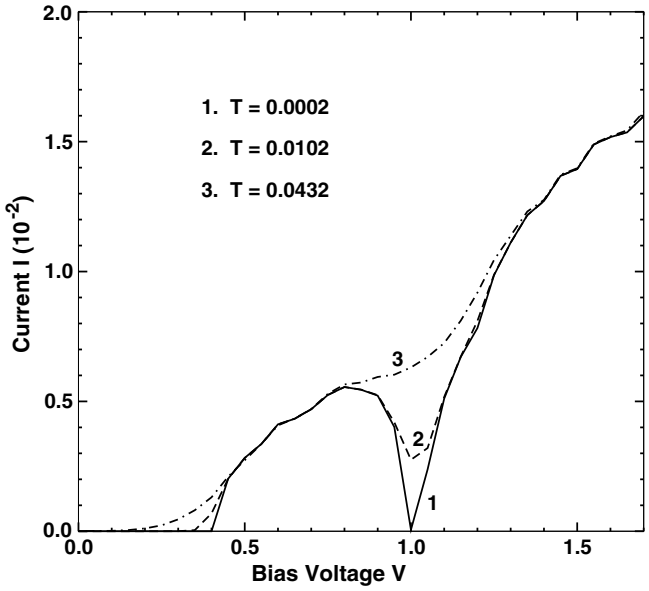

Figure 5. To demonstrate how the temperature can remove NDC: $T = 0.0002$ (curve 1), 0.0102 (2), and 0.0432 (3); everywhere $C_l = 1$, $R_l = 10$, $C_m = 0.4$, $R_m = 0.5$, $C_g = 0.4$, and $V_g = 0.0$.

parts: in the upper part the NDC is absent, whereas in the lower part it can be observed. This supports the idea mentioned above that the NDC behaviour depends on C_m and C_g mostly in the form of a single capacitance $(C_m + C_g)$. The error bar showing a uncertainty in defining the boundary between two phases is very sensitive to the form of the I–V curve. The slope

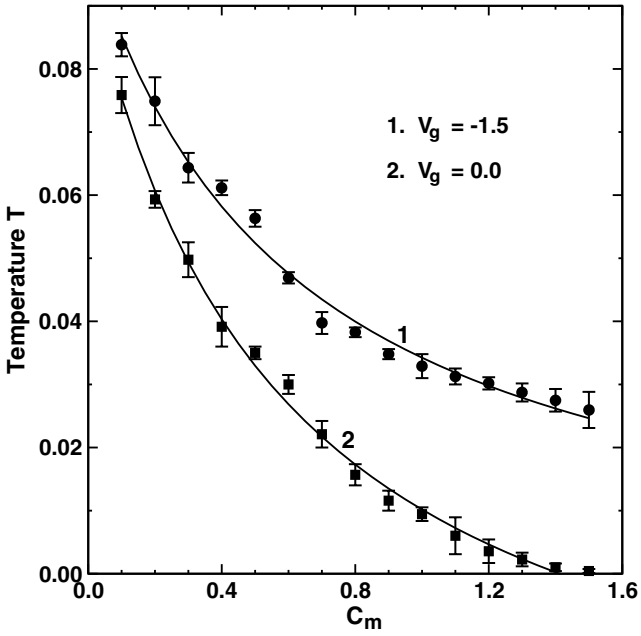

Figure 6. $(T–C_m)$-diagrams for two values of V_g (from top): -1.5 and 0. For each V_g the simulation data (solid circles) are fitted with a function of the form $T = (a + bC_m)/(c + dC_m)$ (solid curve). For a given value of V_g, the NDC can be observed only in the lower space part from the fitted line.

of the fitted (solid) straight line depends mutually on other device parameters. Note again that for the data in figures 3 and 4 the temperature was set to zero.

The temperature, as is widely known, can remove the NDC. Figure 5 shows, for example, how the temperature removes the NDC and simultaneously smears the Coulomb gap for the set of device parameters mentioned in the figure caption. The phenomenon observed is very general; however, quantitatively, the picture depends on the device parameters. For a given set of device parameters, by changing T gradually we can fix the limiting temperature T_c for observing NDC. Focusing our attention on the correlation between T_c and the inter-dot coupling C_m, the obtained simulation data are shown in figure 6 for two cases, $V_g = -1.5$ and 0. For a given value of V_g, the simulation points divide the $(T - C_m)$-space into two parts in the sense similar to figure 4: NDC can be observed only in the lower part. The fitted (solid) curves have been judged in the following way.

From the expression of the tunnelling rate (12), the only expression that contains T, we learn that the temperature effect should be discussed in relation to the change in free energy ΔF. Considering C_m as the only variable, while all other parameters are fixed, from equation (11) one can see that ΔF depends on C_m mostly in the form of $(a + bC_m)/(c + dC_m)$, where a, b, c and d are constants depending on other device parameters. This enables us to guess that the simulation points in figure 6 could be fitted with a function of the form $T = (a+bC_m)/(c+dC_m)$. Within the range of C_m under study, as can be seen in figure 6, the fit is really nice for both cases of different V_g. For a larger value of C_m (see the condition (6)), however, the NDC can no longer be maintained even at zero temperature. We note again that the inter-dot coupling is the most characteristic parameter in double dot structures. That is why it has attracted most of our attention. Similarly, one can study the influence of other device parameters on the NDC

behaviour. In particular, we have shown before that NDC is very sensitive to the presence of off-set charges. It can be maintained only if the magnitude of the off-set charges is as small as $\leqslant 0.15e$ [12].

4. Conclusion

We have studied the NDC phenomenon in metallic double dot structures. In a simple model, limited to the first Coulomb staircase, at zero temperature we have been able to derive an analytical expression for the I–V characteristics and a condition for NDC, which are in good agreement with Monte Carlo simulation data. In more realistic models with gates at finite temperature the effect is very complicated, depending on a mutual correlation between device parameters. Our Monte Carlo simulation data show that the NDC is maintained only in devices with gate (C_g) and inter-dot (C_m) capacitances small enough at low temperatures T and with a small off-set charge magnitude. The correlation between the most important parameters, C_g, T and C_m, in producing NDC can be described by simple functions which form the NDC phase diagrams in ($C_g - C_m$)- and ($T - C_m$)-space, and therefore which are convenient for practical purposes. Due to a potential application [9, 18] it may be necessary to analyse the NDC with respect to the other device parameters. This can be directly done using this Monte Carlo program. The program can also be extended easily for various quantum dot structures within the framework of the Orthodox theory.

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Appendix

Defining $\Delta F_\nu^{+(-)}$ as the change in the free energy F (5) associated with an electron tunnelling across the junction ν ($\nu = l, m, r$) to the right (left) at the state (n_1, n_2), we have

$$\begin{aligned}
\Delta F_l^+ &= F(n_l - 1, n_1 + 1, n_2, n_r) - F(n_l, n_1, n_2, n_r) \\
&= e^2(2n_1 + 1)/2C_l^* + n_2e^2/C_m^* - eV(1 + C_l/C_l^* - C_r/C_m^*)/2, \\
\Delta F_l^- &= e^2(1 - 2n_1)/2C_l^* - n_2e^2/C_m^* + eV(1 + C_l/C_l^* - C_r/C_m^*)/2, \\
\Delta F_m^+ &= e^2(1 - 2n_1)/2C_l^* + e^2(n_1 - n_2 - 1)/C_m^* + e^2(1 + 2n_2)/2C_r^* \\
&\quad + eV(C_l/C_l^* + C_r/C_r^* - C_l/C_m^* - C_r/C_m^*)/2, \\
\Delta F_m^- &= e^2(1 + 2n_1)/2C_l^* + e^2(n_2 - n_1 - 1)/C_m^* + e^2(1 - 2n_2)/2C_r^* \\
&\quad - eV(C_l/C_l^* + C_r/C_r^* - C_l/C_m^* - C_r/C_m^*)/2, \\
\Delta F_r^+ &= e^2(1 - 2n_2)/2C_r^* - n_1e^2/C_m^* - eV(1 - C_l/C_m^* + C_r/C_r^*)/2, \\
\Delta F_r^- &= e^2(1 + 2n_2)/2C_r^* + n_1e^2/C_m^* + eV(1 - C_l/C_m^* + C_r/C_r^*)/2.
\end{aligned}$$

In the condition (6) the difference in free energy $\Delta F \geqslant 0$ (i.e. corresponding electron transfer is impossible) for all transitions from states $(0, 0)$, $(1, 0)$, and $(1, -1)$ except those between them.

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