

Coulomb blockade and negative differential conductance in metallic double-dot devices

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We systematically analyze the stability diagrams and simulate the finite temperature current-voltage characteristics for metallic double-dot devices with cross couplings between dots and gates. The Coulomb blockade is described with respect to each device parameter. The negative differential conductance observed is essentially suppressed by increasing the temperature and/or introducing the offset charge and is very sensitive to the device parameters. © 2004 American Institute of Physics.

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I. INTRODUCTION

Single-electron tunneling devices based on the Coulomb blockade enable the manipulation of per-electron currents. Because of high charge sensitivity, low-power dissipation, and high packing density, these structures are proposed for future generations of computational technology and are therefore being extensively investigated both experimentally and theoretically.

Recently, Junno *et al.*¹ have reported interesting data of differential-conductance measurements for a gold double-dot device. The gold dot is so small that the charging energy is as high as 80 meV, and the Coulomb blockade can be well recognized even at a liquid-nitrogen temperature. The honeycomb stability diagram, typical for the pump devices as designed by Pothier *et al.*,² has been clearly observed at a liquid-helium temperature. The specificity of the device measured is that there exists an essential cross coupling between a dot and the gate belonging to the other dot [cf., the capacitances C_{12} and C_{21} in Fig. 1], which results in a diagonal stretching of the honeycomb cell. An asymmetry of the two junctions, coupling dots to leads, i.e., a difference between capacitances C_s and C_d in Fig. 1, is also believed to make the cells skewed and to yield a distinct Coulomb staircase in the current-voltage (I - V) curves. The charging diagrams have been also measured for silicon germanium double-quantum dots³ but with a focus on the role of electrostatic gates.

The aim of this work is (i) to describe systematically the zero-temperature stability diagrams for the device measured in Ref. 1 and (ii) to simulate the I - V characteristics in the same device, taking into account the finite temperature and the offset charge effects. The results obtained, while describing the experimental data quite well, show a rich variety of features on both the stability diagrams and the I - V curves in dependence on the device parameters. In particular, we find that a negative differential conductance (NDC) of different phases, including a second or a multiple Coulomb gap, can

be manipulated at low temperatures when the coupling capacitances are set with the appropriate values.

II. STABILITY DIAGRAMS

The current diagram of the device under study can be schematically drawn as in Fig. 1, where each of the three junctions (between the source and the dot D_1 , between the drain and the dot D_2 , or between the two dots) is represented by a resistor (R_s , R_d , or R_m) and a capacitor (C_s , C_d , or C_m) connected in parallel. Within the framework of the Orthodox theory,⁴ the stability diagram of a double-dot system without cross couplings (i.e., $C_{12}=C_{21}=0$ in Fig. 1) is well understood (see, for example, van der Wiel *et al.*,⁵ and Ferry and Goodnick⁶). For the device with cross couplings measured in Ref. 1, the charging diagrams can be constructed in the same way as Ref. 5, considering the linear-transport regime, i.e., the case when the external voltage is applied to the device $V_b = V_s - V_d \approx 0$. Assuming that V_d is grounded and $V_s \approx 0$, the total electrostatic energy of the double-dot structure can be written in the form

$$\begin{aligned} \mathcal{E}(n_1, n_2) = & \frac{E_1}{2e^2}(Q_1 - n_1e)^2 + \frac{E_2}{2e^2}(Q_2 - n_2e)^2 \\ & + \frac{E_0}{e^2}(Q_1 - n_1e)(Q_2 - n_2e) - \frac{1}{2}(C_{11}V_{g1}^2 \\ & + C_{12}V_{g2}^2 + C_{21}V_{g1}^2 + C_{22}V_{g2}^2). \end{aligned} \quad (1)$$

Here, e is the elementary charge, $n_1(n_2)$ is the number of

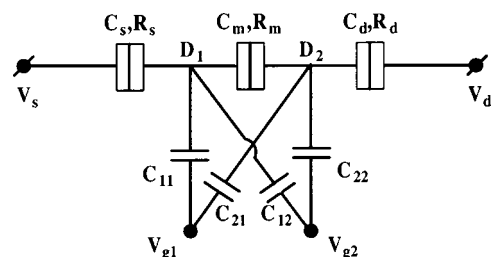


FIG. 1. Current diagram of the device.

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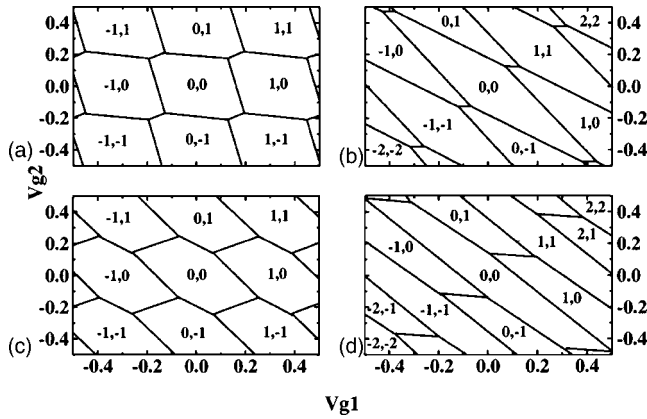


FIG. 2. Stability diagrams of the devices without [(a) and (c): $C_{12}=C_{21}=0$] and with [(b) and (d): $C_{12}=1.6$ aF and $C_{21}=1.8$ aF] cross couplings for two cases: weak interdot coupling [(a) and (b): $C_m=3.0$ aF] and strong interdot coupling [(c) and (d): $C_m=45$ aF]. Everywhere, $C_s=16.9$, $C_d=6.5$ aF, $C_{11}=3.1$ aF, and $C_{22}=2.6$ aF.

excess electrons in the dot $D_1(D_2)$, $E_1(E_2)$ is the charging energy of the dot $D_1(D_2)$: $E_{1(2)} = (e^2/C_{1(2)})(1 - C_m^2/C_1C_2)^{-1}$ with $C_1 = C_s + C_{11} + C_{21} + C_m$ and $C_2 = C_d + C_{12} + C_{22} + C_m$, and E_0 is the coupling energy, counted as the change of the potential on one dot when an electron is added to the other dot: $E_0 = (e^2/C_m)(C_1C_2/C_m^2 - 1)^{-1}$, $Q_1 = C_{11}V_{g1} + C_{12}V_{g2}$, and $Q_2 = C_{21}V_{g1} + C_{22}V_{g2}$.

The stability diagrams can be directly constructed by minimizing the energy [Eq. (1)] with respect to the numbers of the excess electrons n_1 and n_2 . Figure 2 is focused on showing the cross-coupling effect in two typical cases: relatively weak [Figs. 2(a) and 2(b) with $C_m=3$ aF] and strong [Figs. 2(c) and 2(d) with $C_m=45$ aF] interdot couplings. The cross-coupling capacitances C_{12} and C_{21} are specially set to zero in Figs. 2(a) and 2(c), whereas in Figs. 2(b) and 2(d), they have the values of 1.6 and 1.8 aF, respectively. These values of cross-coupling capacitances, as well as the values of other capacitances used for Fig. 2, have been chosen in accordance with Ref. 1. By comparing Fig. 2(a) with 2(b) and 2(c) with 2(d), it is clear that in both cases, the cross coupling strongly stretches the honeycomb cell, making it longer in the diagonal direction and in parallel, which results in a reduction in the separation between the two triple points. The effect is still considerable even in the case of Fig. 2(d), where $C_{12}(1.6)$ and $C_{21}(1.8) \ll C_m(45$ aF). On the other hand, by comparing Fig. 2(a) with 2(c) or Fig. 2(b) with 2(d), one can see that the interdot coupling leads to an inverse effect on the triple-points separation: two points are gradually sepa-

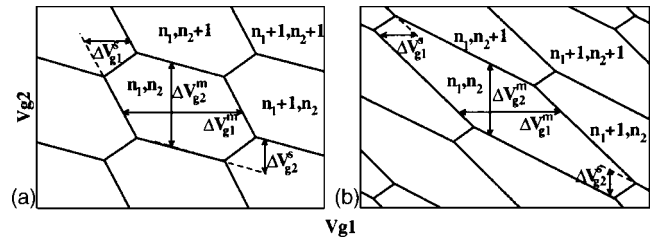


FIG. 4. Diagram cell dimensions of Eqs. (2) and (3) for the devices (a) without cross couplings and (b) with cross couplings [$C_{12}=C_{21}=1.5$ aF]. Everywhere, $C_s=C_d=10.0$ aF, $C_{11}=C_{22}=3.0$ aF, and $C_m=8.0$ aF.

rated with increasing C_m . Quantitatively, the magnitude of these effects is very sensitive to the values of capacitances in the device.

In Fig. 3, we show the stability diagrams for the devices of an asymmetrical [Fig. 3(a)] and symmetrical [Fig. 3(b)] dot-to-lead couplings. The values of all the capacitances used for this figure are respectively the same as those reported in Ref. 1, except the dot-to-lead coupling capacitances C_s and C_d , which have been set in equal in Fig. 3(b): $C_s=C_d=12$ aF [i.e., about the average of experimental values of $C_s=16.9$ and $C_d=6.5$ aF used in Fig. 3(a)]. From a direct comparison of the two diagrams in these figures, we see that an asymmetry of the dot-to-lead couplings brings about a move of triple points in the way that the direction of the shortest line between them forming an angle of about 45° with the V_{g1} axis in the case of the symmetrical device [Fig. 3(b)], becomes almost parallel with this axis [Fig. 3(a)]. The directions of the other sides as well as the size of the honeycomb cells are mostly affected by the interdot and the cross couplings as can be seen in Fig. 2. Note that the diagram in Fig. 3(a) resembles well that presented in Fig. 2 of Ref. 1.

Taking into account the cross couplings C_{12} and C_{21} , the dimensions of a charging diagram cell can be derived in the same way as discussed in Ref. 5

$$\Delta V_{g1}^m = \frac{eC_2}{C_{11}C_2 + C_{21}C_m}, \quad \Delta V_{g2}^m = \frac{eC_1}{C_{22}C_1 + C_{12}C_m} \quad (2)$$

and

$$\Delta V_{g1}^s = \Delta V_{g1}^m(C_m/C_2), \quad \Delta V_{g2}^s = \Delta V_{g2}^m(C_m/C_1). \quad (3)$$

The meaning of the symbols in these expressions is given in Fig. 4. Without the cross couplings ($C_{12}=C_{21}=0$), when the expressions in Eqs. (2) and (3) turn into the Eqs. (8) and (10) of Ref. 5, respectively, the size ΔV_{g1}^m (or ΔV_{g2}^m) depends only on the gate direct coupling C_{11} (or C_{22}). In the presence of

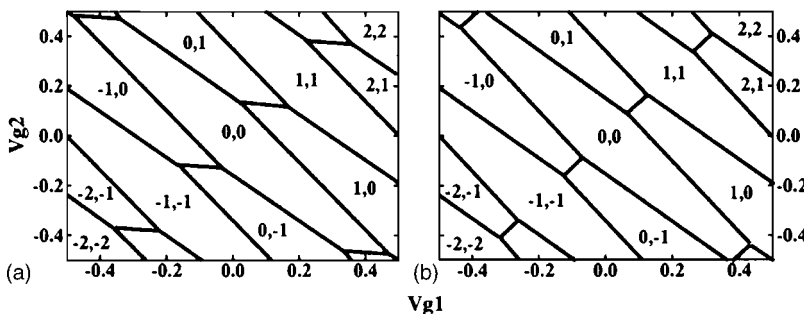


FIG. 3. Stability diagrams of the devices with asymmetrical dot-to-lead couplings (a) [$C_s=16.9$ aF and $C_d=6.5$ aF] and symmetrical dot-to-lead couplings (b) [$C_s=C_d=12$ aF]. Everywhere, $C_m=13.0$ aF, $C_{11}=3.1$ aF, $C_{21}=1.8$ aF, $C_{12}=1.6$ aF, and $C_{22}=2.6$ aF.

cross couplings, these sizes $\Delta V_{g1,2}^m$ [Eq. (2)] become like $\Delta V_{g1,2}^s$ [Eq. (3)], mutually depending on all coupling capacitances in the structure. Figure 4 is also aimed to demonstrate how the cross coupling affects the dimensions of a cell for a symmetrical device ($C_s=C_d=10$ aF) with a moderate interdot coupling ($C_m=8$ aF). A direct comparison of the two diagrams in Figs. 4(a) and 4(b) shows that for the device concerned, an inclusion of cross couplings [Fig. 4(b)] yields a reduction in all the cell dimensions by about 15%.

Note that Fig. 2 can be used for the same purpose for devices with relatively weak and strong interdot couplings when one compares the corresponding diagram cells in the two figures of the same line [(a) with (b) and (c) with (d)]. Moreover, by comparing the corresponding diagram cells in the two figures of the same column [(a) with (c) and (b) with (d)], Fig. 2 also describes the effect of the interdot coupling C_m on the honeycomb cell dimensions. Without cross couplings [Figs. 2(a) and 2(c)], the interdot coupling lengthens the sizes $\Delta V_{g1,2}^s$ leaving the two other sizes $\Delta V_{g1,2}^m$ unchanged. In the presence of cross couplings [Figs. 2(b) and 2(d)], the interdot coupling affects all the cell dimensions but in different ways: $\Delta V_{g1,2}^s$ increases with increasing C_m , whereas $\Delta V_{g1,2}^m$ decreases. Quantitatively, all the effects mentioned can be easily evaluated analytically using the expressions in Eqs. (2) and (3).

III. MONTE CARLO SIMULATION

In order to calculate the I - V curves in the device drawn in Fig. 1, taking into account both the temperature and the offset charge effects, the dynamics of the electron transfer through junctions was simulated using the standard Monte Carlo method. For the sake of simplicity, the tunnelling resistances of all the three junctions of the device are assumed to be equal: $R_s=R_d=R_m\equiv R_t$. Then, the tunnelling rate for any junction in the structure can be uniquely defined as

$$\Gamma = (e^2 R_t)^{-1} \Delta F / (1 - \exp(-\Delta F/k_B T)), \quad (4)$$

where ΔF is the change in the free energy F of the system after the tunnelling event has occurred. For the given V_s and V_d ($V_b=V_s-V_d$ does not need to be small), the free energy F can be obtained from the energy $\mathcal{E}$ in Eq. (1) by (i) replacing everywhere $Q_{1(2)}$ by $Q_{1(2)}+C_{s(d)}V_{s(d)}+q_{1(2)}$, where q_1 (q_2) is a (random) offset charge in the quantum dot D_1 (D_2): $q_{1,2} \in [-Z_{1,2}Z_{1,2}]$ with the magnitudes $Z_{1,2}<e$ (Ref. 7) and (ii) adding the term $(-V_s Q_l - V_d Q_r)$, where Q_l (Q_r) is the charge at the left (right) lead (see Ref. 8 and 9 for detailed reference). Focusing the attention on the interdot and cross-coupling effects, all the simulation samples are taken symmetrical with $C_s=C_d\equiv C_0$ except the particular device for Fig. 6 specified as follows. Choosing C_0 and e as the basic units, the temperature, the voltage, and the current will then be measured in the units of $e^2/k_B C_0$, e/C_0 , and $e/R_t C_0$, respectively. The method as well as all the details of calculating procedure have been thoroughly discussed in Ref. 9.

In Fig. 5, we show some examples of the current I vs bias V_b [Fig. 5(a)] and the current I vs gate voltage V_g [Fig. 5(b)] for devices of different C_m : $C_m=0, 1$, and $10 C_0$ (zero, moderate, and strong interdot coupling). In reality, Fig. 5(b)

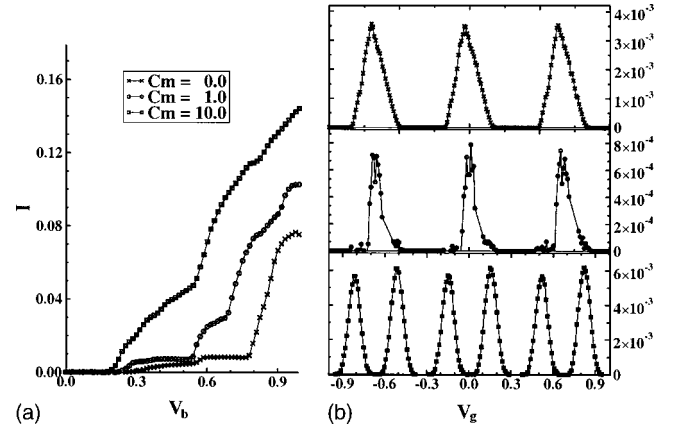


FIG. 5. Current I vs bias V_b (a) and current I vs gate voltage $V_{g1}=V_{g2}=V_g$ (b) for devices with different C_m (from top): 0, 1, and $10 C_0$ [$C_s=1.0 C_0$, $C_d=1.0 C_0$, $C_{11}=0.8 C_0$, $C_{21}=0.7 C_0$, $C_{12}=0.7 C_0$, and $C_{22}=0.8 C_0$].

describes how the Coulomb-blockade conductance spectroscopy of the device varies as C_m increases. It is well known that a system of two isolated, identical QDs has an oscillation structure of the conductance spectroscopy in the Coulomb-blockade regime as demonstrated by the upper curve in Fig. 5(b) for the case of $C_m=0$ (Ref. 10). As the interdot coupling is included, the conductance peaks start to split at the top (the middle curve for $C_m=C_0$), and the two subpeaks should gradually separate with increasing C_m . When the interdot coupling is strong enough [the curve at the bottom of Fig. 5(b) for $C_m=10 C_0$], the spectroscopy has the form like that for a single-dot device, but the peak-to-peak distance is two times shorter. The observed peak split is well documented as a manifestation of the Coulomb blockade in double-dot structures and directly relates to the separation of the two triple points discussed in Fig. 2.

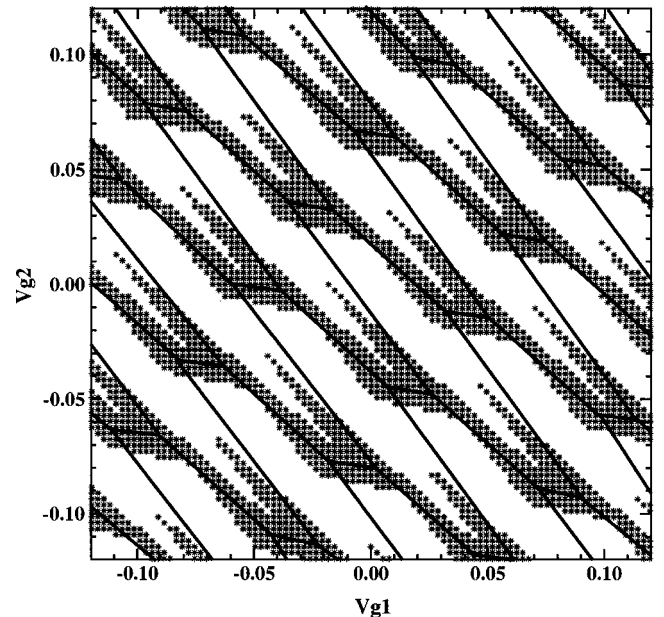


FIG. 6. Monte Carlo simulation conductance fits to the charging diagram from Fig. 3(a) for the device with the same capacitances as those in Ref. 1: $C_s=16.9$ aF, $C_d=6.5$ aF, $C_{11}=3.1$ aF, $C_{22}=2.6$ aF, $C_{12}=1.6$ aF, $C_{21}=3.1$ aF, and $C_m=13.0$ aF. Bright regions correspond to the low-conductance regime ($T=3.72$ K).

The most important feature we want to see in Fig. 5(a) is the existence of a Coulomb gap. As in Ref. 9, certainly, one can evaluate the width of the gap (Coulomb-blockade threshold) and examine its dependence on various parameters of the device simulated. Here, we are however interested in the other characteristics of the effect. At a given low bias V_b (much lower than the Coulomb-blockade threshold for the case of zero-gate voltages V_{g1} and V_{g2}), we can calculate the conductance for various values of V_{g1} and V_{g2} and then construct the conductance diagrams at a finite temperature. The result obtained specifically for the device with the same coupling capacitances as those reported in Ref. 1 at $T=3.72$ K is presented in Fig. 6. The temperature narrows the Coulomb gap (see also Fig. 2 in Ref. 9), smearing its boundary. Such a smear corresponds to the dark regions in the figure, whereas the bright regions correspond to the low-conductance (blockade) regime. The honeycomb net is the corresponding (zero-temperature) stability diagram shown in Fig. 3(a) for the same set of parameters. Clearly, the Monte Carlo (finite temperature) result fits the stability diagram well, and moreover, the obtained conductance diagram in Fig. 6 is in good agreement with the experimental data shown in Fig. 2 of Ref. 1.

Returning to the Fig. 5(a), we highlight the staircase structure, accompanying the NDC, obtained in the I - V curves for devices of small C_m . The NDC has been suggested in various nanosystems.^{11–17} It was observed early in single-semiconductor quantum-dot structures and has been regarded as a result of an existence of excited states.¹¹ Nakashima and Uozumi¹² have demonstrated the NDC in a linear array of metallic islands as a result of a competition between the forward rate of injecting charges into the array, which increases with the bias and the tunnelling rate across some junction, which may be reduced with increasing bias. Shin *et al.*¹³ have calculated the I - V characteristics in a ring-shaped array of dots and have shown that the interactions between electrons in two branches of the ring can bring about stationary electron configurations, which produce NDC at low temperatures (and multiple Coulomb gaps at zero temperature). Heij *et al.*¹⁴ have measured the device, where an electron box is attached to a single-electron transistor as a gate, and reported on the NDC for a range of conditions. Recently, for double-dot structures, the NDC has been analysed by Evans and Mizuta¹⁵ and by Wang *et al.*¹⁶ The structure studied in Ref. 15 is somewhat similar to that in Ref. 12 in the sense that electrons have to pass through both dots, whereas in the structure studied in Ref. 16, the two dots are not equivalent; one dot is connected to both external leads, but the other is connected to only one. Several NDC mechanisms have been suggested for different structures. However, due to a mutual correlation of device parameters, the conditions for the NDC cannot be always formulated exactly. Even as the conditions can be written out for relatively simple models,¹⁵ they are often too complicated for a practical purpose. Despite such a variety of phenomena, it is generally accepted that the NDC is gradually removed by increasing the temperature^{11–16} or introducing the offset charge.^{13,15} The interdot coupling also plays an important role; it stimulates the NDC in the structures studied in Refs. 14 and 16.

Our device of study is much more complicated than the

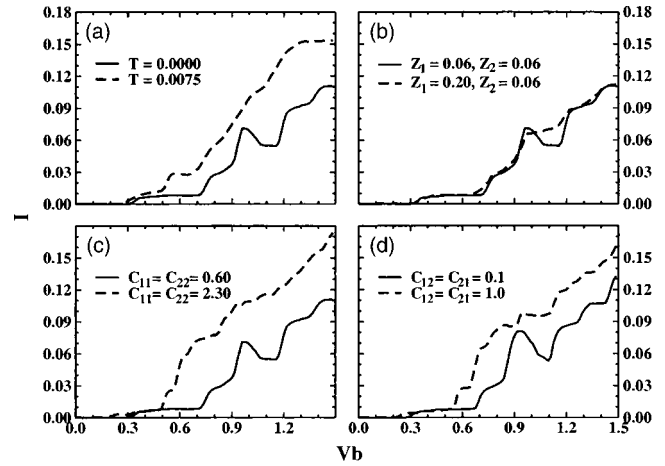


FIG. 7. NDC in dependence on (a) temperature, (b) offset charge, (c) gate (direct) couplings, and (d) cross couplings ($C_s=1.0 C_0$, $C_d=1.0 C_0$, $C_m=0.8 C_0$).

double-dot structures studied in Refs. 13–16. Restricting to a qualitative description, we present in Fig. 5(a) and Figs. 7 and 8 some typical NDC behaviours and their dependence on various device parameters. Note that the NDC is always accompanied by a staircase; the I - V curves with the NDC show complex forms (in comparison with smooth curves in Ref. 9). In contrast to the structures considered in Refs. 14 and 16, Fig. 5(a) demonstrated that for the device under the present study, the NDC may be weakened by increasing the interdot coupling C_m . This gives an argument to suggest that, physically, the NDC observed in our double-dot device has a root similar to that for linear arrays of many islands discussed in Ref. 12. Importantly, though the NDC or even the second Coulomb gap as shown in Fig. 8 can be always realized for some particular sets of coupling capacitances, it is very easily removed by (i) increasing the temperature [Fig. 7(a)], (ii) increasing the magnitude of the offset charges [Fig. 7(b)], and (iii) changing the gate (direct) coupling [Fig. 7(c)] or the cross coupling [Fig. 7(d)]. For the first two factors, our simulations generally show that the NDC can be maintained only at very low temperatures (about $\leq 0.0015 e^2/k_B C_0$) and in devices with a small offset-charge magnitude (of 0.15 or

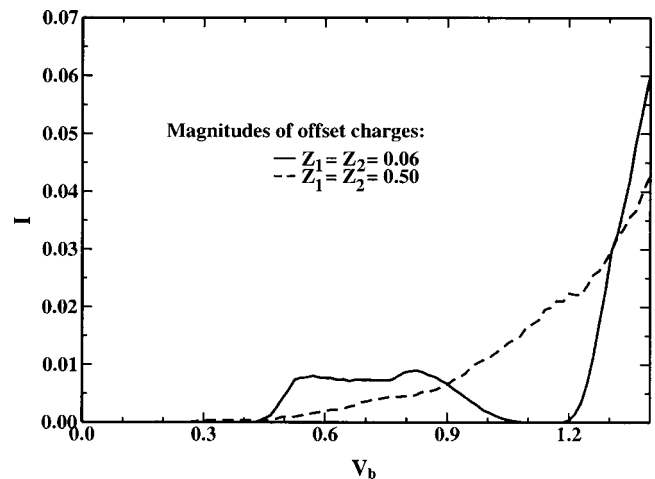


FIG. 8. Example of a second Coulomb gap and its destruction by an offset charge.

less, consistent with Ref. 14). Figure 8 gives one more example about the offset-charge effect, which can remove even a second Coulomb gap, making the I - V curves almost monotonic. The last two factors of gate couplings show a more complicated effect; they may enhance or suppress the NDC, depending on the values of the other device parameters. Since the NDC has many potential applications,^{14,17} it may be necessary to learn the role of each device parameter. This can be done simply by using the present Monte Carlo simulation, which allows us to deal with both the finite temperature and the environment (random offset charge) effects. One can include into the simulation, even the other couplings, such as the dot self-capacitance considered by Berven and Wybourne,¹⁸ which may affect both the stability diagram and the I - V curves, depending on its value in relation to the other capacitances associated with the dot.

IV. CONCLUSION

We have reported a systematic analysis of the stability diagrams, depending on each of the coupling capacitances for the metallic double-dot device measured in Ref. 1. Besides the interdot coupling, the cross couplings are shown to affect essentially both the size and the shape of the diagram cells. We have also shown shortly the Monte Carlo simulation results, which on the one hand, profoundly demonstrate the Coulomb blockade in good agreement with the experimental data, and on the other hand, give the I - V characteristics, taking into account the finite temperature and random-offset-charge effects. From a rich variety of I - V curve behaviours, depending on a mutual correlation between the device parameters, the NDC and even the multiple Coulomb gap can be actually realized. They are however easily removed by the temperature and/or the offset charge and are very sensitive to the device parameters.

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