Analysis of negative differential conductance in a two-island Coulomb blockade system by a polytope approximation in phase space

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A two-island single-electron tunneling system is presented that exhibits negative differential conductance (NDC) based on Coulomb blockade. The NDC mechanism is explained by introducing a simple analysis method, the polytope approximation. A condition for NDC to occur is analyzed fully by using the polytope approximation. © *2002 American Institute of Physics.*
[DOI: 10.1063/1.1500786]

I. INTRODUCTION

Single-electron (SE) effects based on the Coulomb blockade (CB) of charge allows the manipulation of current on a per-electron basis. This has stimulated research into the possibility of using such effects to represent one bit of information by a small number of electrons and is hoped to lead eventually to a new generation of digital logic technology. The authors in Refs. 1 and 2 propose interesting devices based on negative differential conductance (NDC).

This article consists of two strands; the first demonstrates, through numerical simulation, a simple two-island SE device that exhibits NDC. NDC is usually associated with quantum levels but, due to SE effects, NDC need does not require energy quantization.

In the second strand, a simple analysis tool, called the *polytope approximation*, is proposed that neatly describes the reason for NDC and is used to derive a condition for NDC to occur. The polytope approximation is used to predict NDC valley positions and currents, both of which compare favorably with simulations.

Previously, Nakashima and Uozumi have demonstrated NDC in a linear array of seven[3] and a nine[4] islands in the context of a zig-zag conduction path through a granular system between two electrodes. The results were explained in terms of the competition between the forward rates of injection of charge into the array with increasing bias and the reduction of the tunneling rate across a junction that is against the electric field set up by the source–drain bias and so this rate reduces with increasing bias.

Shin *et al.*[5,6] demonstrate a different form of NDC in closed rings of islands (the simplest being four islands). In this system, stable configurations of electrons can exist on the islands that form a "crystallike" structure and only when the bias has increased sufficiently to "melt" the crystal can current flow until a different stable configuration occurs. At $T=0$ K, this leads to multiple zero-current regions as the source–drain bias increases, while at finite temperatures, it exhibits finite current and NDC.

Heij *et al.*[7] take a simpler approach and attach a SE box to the gate of a SE transistor (SET) and demonstrate that the system will exhibit NDC for a range of conditions. The electrons in the box act as an additional gate bias to the SET and by biasing the SET and box in the appropriate range, the phase of the SET oscillation can be modified to produce NDC when an extra electron tunnels into/out of the box. A similar system is analyzed by Shin *et al.*[8] in the context of coupled SETs though the possibility of it generating NDC is not discussed.

SE devices show an extreme sensitivity to stray (uncontrolled) charge in the surrounding environment (the *offset-charge problem*), but we will assume that a suitable fabrication process lets us control this. Under these circumstances, NDC devices may be a useful component of future SE logic systems.

II. TWO-ISLAND COULOMB BLOCKADE SYSTEM

The circuit that will be analyzed is shown in Fig. 1 and is similar to Heij[7] *et al.*'s system in that it has two islands, but, like Nakashima and Uozumi's[3,4] device, is arranged linearly such that electrons have to pass through *both* islands. We assume that islands are metallic and that their tunnel resistances and capacitances are independent of bias.

Despite its apparent simplicity, the system exhibits a variety of complex behaviors as the capacitances and the tunnel resistances are varied. However, this article only examines a simple case where all the tunnel resistances are set to 10^6 Ω. The system exhibits NDC over a wide range of circuit parameters.

This circuit is the most general *linear* two-island circuit. Capacitances in parallel to the tunnel junctions can be merged together; capacitances to external gates are merged into the island-to-drain capacitance and the offset charge on the island changed appropriately.
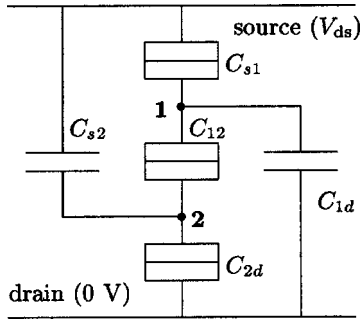
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FIG. 1. Two-island CB system.

As an example of a system that demonstrates NDC, we set $C_{s1} = C_{12} = C_{d2} = 0.1$ aF, $C_{s2} = 6$ aF, and $C_{d1} = 1$ aF; the offset charge on islands 1 and 2 are denoted by q_1 and q_2 which are assumed to be in units of e. The results are generated using a Master equation simulator ignoring cotunneling.[9] Later, a condition for NDC will be derived.

In this situation, V_{ds} acts as a gate on the second island—producing oscillations in its transfer characteristics, and hence NDC. Eventually, the bias over the second transistor is sufficient high that the gate looses control.

The current as a function of V_{ds} and of q_1 is shown in Fig. 2. q_2 has been set as -0.5 and, qualitatively, the only change in the characteristics as q_2 varies is that the phase of the oscillation changes. Clear NDC can be seen for a small range of the values of q_1; this demonstrates the extreme sensitivity of the characteristic on the offset charge. A change of only a small fraction of an electron charge can change the NDC current by many orders of magnitude or move the system to a non-NDC region.

Figure 7 shows the I_{ds}–V_{ds} characteristics at temperatures between 8.2 to 1.2 K in 1 K steps. The NDC regions exhibit peak-to-valley ratios of up to 10^{10} at 4.2 K. The peak heights for higher biases tend to be only weakly dependent on temperature while the valley currents are much more strongly dependent. This view is shown even more clearly for the different offset charge configuration $(-0.4, -0.5)$ which is shown in Fig. 8. Higher temperatures broaden the peaks, gradually washing them out.
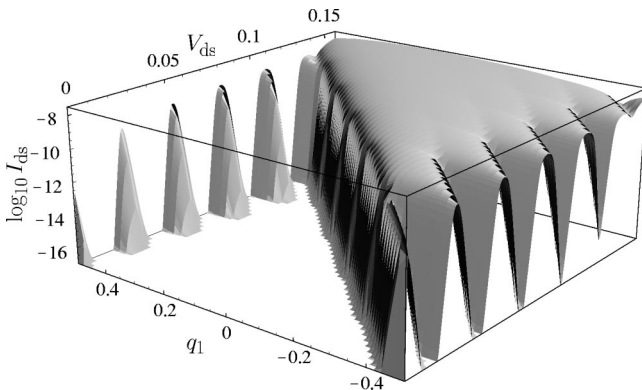

FIG. 2. $\log_{10} I(q_1, V_{ds})$ with $q_2 = -0.5$—clearly there are values of q_1 where a small change produces a drastic change in the current and the existence of NDC.

Comparing Figs. 7 and 8, it is clear that the offset charge change of only $\Delta q_1 = 0.15$ (remembering that the characteristics are periodic in q_1 and q_2) has produced peaks that are a couple of orders of magnitude higher, while also degrading the quality of the peaks.

As a consequence, any logic device relying on the order of magnitude of the current would have to control q_1 to $\ll 0.15$, while the phase of the peaks is controlled by q_2 and a change of 0.5 produces a phase shift of π.

III. ANALYSIS BASED ON THE POLYTOPE APPROXIMATION

In this section, $\tilde{q}$, the phase space for the system, is introduced. A simple non-NDC example is used to motivate an approximation to the full Master equation solution to the current. Using this *polytope*[10] approximation, the explanation of NDC is simply described. The condition for NDC to occur is then derived from this interpretation and the system is related to the device of Nakashima *et al.*[3,4]

The transition rate in Orthodox Theory[11] for a *hole* tunneling through a tunnel resistance R_{kl} from island k to island ℓ is,

$$\Gamma_{kl} = \frac{1}{e^2 R_{kl}} \frac{-\Delta E_{kl}}{1 - \exp(\Delta E_{kl}/kT)}, \tag{1}$$

where the change in free energy ΔE_{kl} can be expressed as,

$$\Delta E_{kl} = \frac{e^2}{2} \boldsymbol{\epsilon}_{kl}^T \mathsf{C}^{-1} \boldsymbol{\epsilon}_{kl} + e^2 \boldsymbol{\epsilon}_{kl}^T \mathsf{C}^{-1} \tilde{q} - e V_k \xi_k + e V_\ell \xi_\ell \tag{2}$$

and each island i is represented by the ith element of the vectors. C is the (symmetric) capacitance matrix and C_{ij} is the *negative* sum of the capacitances joining islands i and j while C_{ii} is the *positive* sum of all the capacitances connected to island i. $(\boldsymbol{\epsilon}_{kl})_i = -\delta_{ik} + \delta_{i\ell}$ and δ_{ij} is zero if j is a bias. ξ_i is unity if i represents a bias, otherwise is zero. The operator ^{T} is the transpose of the vector.

The dynamics of the system are Markovian and for a fixed V_{ds} the state of the system is *fully* characterized by $(\tilde{q})_i = q_i + \Sigma C_{i'i} V_{i'}/e$, where $q_i = n_i + q_i^0/e$, the number of holes on island i is n_i, the fractional offset charge induced on the island is q_i^0, and the sum i' runs over the capacitances/tunnel resistances connecting i to bias/gate i' at potential $V_{i'}$.

For the two-island system with the drain grounded, then,

$$\mathsf{C} = \begin{pmatrix} C_{1\Sigma} & -C_{12} \\ -C_{12} & C_{2\Sigma} \end{pmatrix}, \quad \tilde{q} = \begin{pmatrix} q_1 + C_{s1} V_{ds}/e \\ q_2 + C_{s2} V_{ds}/e \end{pmatrix},$$

where $C_{1\Sigma} = C_{s1} + C_{12} + C_{d1}$, etc. Clearly the point describing the system $(\tilde{q})$ moves at a velocity of $(C_{s1}, C_{s2})^T/e$ from a start point $(q_1, q_2)^T$.

The set of $\boldsymbol{\epsilon}_{k\ell}$ needed to move a hole from the source (s) to the drain (d) are $s \to 1$: $\boldsymbol{\epsilon}_{s1} = (1,0)^T$, $1 \to 2$: $\boldsymbol{\epsilon}_{12} = (-1,1)^T$, $2 \to d$: $\boldsymbol{\epsilon}_{2d} = (0,-1)^T$. If a transition $k \to \ell$ is taken then $\tilde{q} \to \tilde{q} + \boldsymbol{\epsilon}_{k\ell}$ and so a lattice of states is formed in $\tilde{q}$ space. The current may then be calculated by a Master equation connecting these lattice states using the formulas (1) and (2). A sequence of current-producing transitions make the system hop round a loop in the lattice.
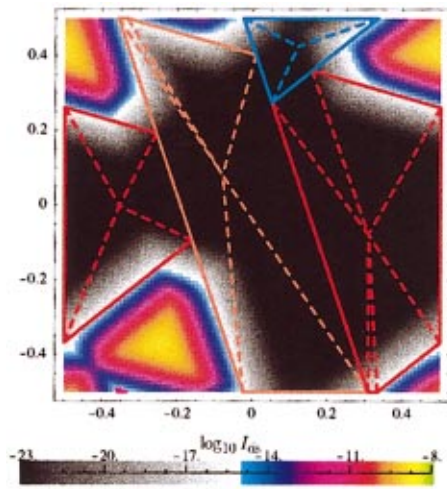
FIG. 3. (Color) Structure: $C_{s1}=C_{12}=C_{d2}=1$ aF, $C_{d1}=1.5$ aF and $V_{ds}=0.01$ V. The $\log_{10}$ of the current is plotted using the scale shown as a function of $\tilde{q}$. Note the periodicity of the characteristic and that surfaces of constant current are reasonably well described by straight line sections. The solid boundaries are those of the polytope approximation, the internal parts of the polytope are indicated by dashed lines.

For far-time dc characteristics, the initial lattice point that the system starts at is irrelevant as it will diffuse through the lattice and so the current is periodic in $\tilde{q}$ with the lattice spacing (unity). The polytope approximation assumes that this diffusion process takes the system to a set of loops involving a single state and that the transition rate out of this state dominates the current flow produced by any of the loops going through it. The dynamics of SE systems act such that if a particular transition $\epsilon_{k\ell}$ from a state $\tilde{q}$ is taken then the transition rate for it being taken again from the new state $(\tilde{q}+\epsilon_{k\ell})$ is less ($\Gamma_{k\ell}[\tilde{q}]>\Gamma_{k\ell}[\tilde{q}+\epsilon_{k\ell}]$). Hence, the dynamics do indeed tend to confine the system to a small part of phase space.

A region of sub-I_{th} current is constructed geometrically by calculating the region $\mathcal{Q}$ where all transition rates are less than I_{th}/e. Each point in $\tilde{q}$ space may now be classified as sub-I_{th} if one (or more) of the points of the lattice that it is part of lies within $\mathcal{Q}$. In this way, a set of regions of sub-I_{th} current is constructed and a lattice formed by translations of $\mathcal{Q}$. As the system is periodic, only a single n cube of the space need be considered and this will be taken to be that centered at the origin and shall be denoted as $\mathcal{Q}_0$.

Figure 3 shows $\log_{10}[I_{ds}(\tilde{q})]$ for a more capacitively homogeneous system. Surfaces of constant current are reasonably well approximated by polytopes, though there are *neck* points where the overall current is lower; the necks appear where two or more polytopes are in close proximity. The polytopes for 1 fA current are drawn; the original polytopes overlapped so a set of nonoverlapping polytopes were generated that covered the same area, these are drawn with solid boundaries and their interiors are marked by the dashed lines.

The polytope approximation, despite being so simple, tends to be conservative in which regions of phase space it assigns as sub-I_{th}, in that in all of the examples that the authors have studied, the true sub-I_{th} region is a superset of

the region that the polytope approximation provides. Strongly inhomogeneous tunnel resistances tend to lead to extra polytopelike regions that need further corrections to describe them. It is more difficult to test the validity of the polytope approximation in higher dimensions (more than two islands) but the terminology used in this paper is that for the general n-dimensional system in anticipation for such an extension.

A consequence of the polytope approximation is that, for a particular V_{ds}, the volume of $\mathcal{Q}_0$ (in dimensionless units) is at least the probability that a device with a random offset charge configuration (uniformly distributed in the range -0.5 to 0.5) will have a threshold voltage below V_{ds}.[12,13]

IV. GEOMETRICAL EXPLANATION FOR NEGATIVE DIFFERENTIAL CONDUCTANCE IN THE TWO-ISLAND SYSTEM

The phase space diagram of the two-island system for various values of V_{ds} is shown in Fig. 4. Each line of three diagrams are evenly spaced in V_{ds}, there is a large jump in V_{ds} from one row to the other.

The polytope for this system is long and thin in the q_2 direction and wraps round many times. The polytopes drawn on the diagrams are for $I_{th}=1$ fA, the shading is indicative of the $\log_{10}(I_{ds})$ and the range of each diagram is from -0.5 to $+0.5$ in both directions. The system point starts at $(0.4, -0.5)$ and moves along the thick green line. Thus, in the top left-hand side diagram, the system is in a sub-I_{th} region, the next in an above-I_{th} region and the next again in a sub-I_{th} region—thus, the system has gone through one current peak. We note that the trajectory of the system has wrapped round due to the periodic dependence on $\tilde{q}$.

The system travels very quickly in the q_2 direction, lapping the polytope many times while at the same time, the left-hand side edge of the polytope gradually moves to the right-hand side. The bottom set of diagrams show that polytope decreases in size until eventually it will disappear.

The non-NDC part of Fig. 2 can also be explained. Take for example the center point $(0, 0)$. As V_{ds} increases, then it moves quickly in the q_2 direction, lapping many times, however, as the polytope at that point is all sub-I_{th}, then, the current is sub-I_{th} until suddenly the left-hand side boundary of the polytope runs past it and it has a significant current.

V. GEOMETRICAL CONDITION FOR NEGATIVE DIFFERENTIAL CONDUCTANCE

We define that a device exhibiting NDC has a current that falls from above I_{th} to below I_{th} as V_{ds} increases i.e., $\ni V:[dI(V)/dV_{ds}<0$ and $I(V)=I_{th}]$. This is a more specific definition of NDC than usually used ($\ni V:dI(V)/dV_{ds}<0$).

A necessary condition for NDC is that the system can head from a point outside the polytope (with $I>I_{th}$) into the polytope (where $I<I_{th}$). Thus, the system must move faster toward a polytope boundary faster than the boundary recedes. This can be done for each face and can be used to construct a region of phase space ($\tilde{q}$) that can hit the face before it completely disappears—thus providing a criterion under which at least one dip of at least I_{th} can occur.
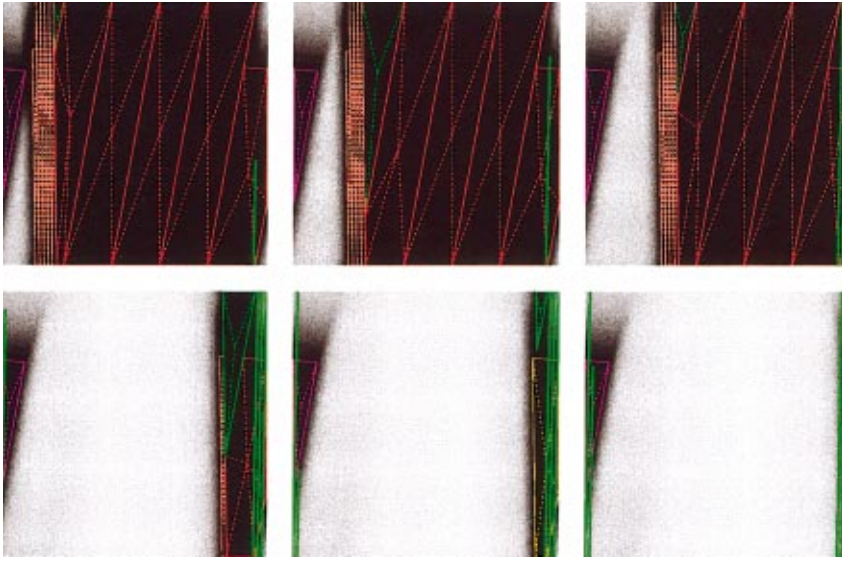
FIG. 4. (Color) Phase space diagrams for an NDC system. The polytopes have solid boundaries and their interiors are marked by dashed lines. V_{ds} in the top row of diagrams are 10.5, 21.0, and 31.5 mV (left- to right-hand side), while V_{ds} for the bottom rows are 105, 115, and 126 mV. The system point starts at $(0.4, -0.5)$ and moves along the thick green line (that is almost vertical). As V_{ds} increases from one diagram to the next, the line moves out of a subthreshold (1 fA) region and back again. The bottom set of diagrams shows the system shortly before the polytope disappears and all points have above threshold current.

The phase-space diagram for a voltage V_{ds} is drawn in Fig. 5, the sub-I_{th} region is the triangle ABC, the shaded triangle is one of the images of ABC due to the periodicity in $\tilde{q}$ space. The transition $s \rightarrow 1$ corresponds to the edge BC and this is the only edge that moves, and its velocity is v_{s1}. The edge AB corresponds to the interisland transition $1 \rightarrow 2$, while CA is the transition $2 \rightarrow d$. The normal to the face AB is n_{12}. The system is described by the point $\tilde{q}$, indicated by the circle, and travels at velocity $v_q = (C_{s1}, C_{s2})^T/e$.

The triangle ABC gradually shrinks until it disappears to the point A at a voltage V_{ds}^{max}. All points in the triangle AXB will have flowed through AB by this time and so will have experienced at least one section of NDC between V_{ds} and V_{ds}^{max} as they move from a point outside the triangle (where
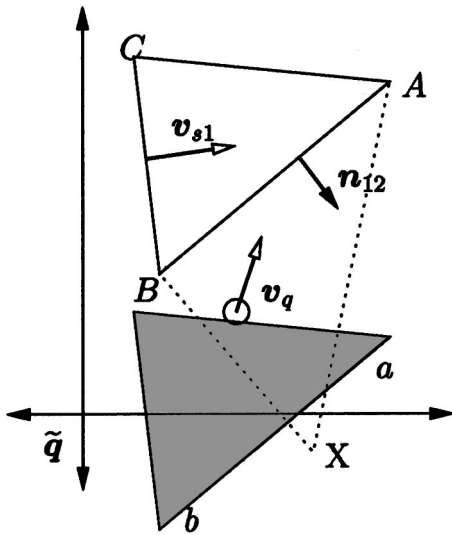

FIG. 5. Phase-space diagram: the interior of the polytope ABC is a region of sub-I_{th} current. BC moves to the right-hand side with increasing V_{ds} at a velocity v_{s1}, the lines that the other edges are part of are not dependent on V_{ds}. The shaded triangle is one of the periodic images of ABC. The outward normal to the edge AB is n_{12}. A particular system, indicated by the circle, moves at a velocity v_q. A system in the region AXB will move through AB before the polytope disappears and thus will exhibit NDC.

$I > I_{th}$) to inside ($I < I_{th}$). Those points that also cross through ab will have two NDC sections with $I > I_{th}$.

The outward pointing normal to the region for a transition $\epsilon_{k\ell}$ is $-\mathsf{C}^{-1}\epsilon_{k\ell}$, and so a necessary condition for the system to be able to go through face AB is that v_q is directed oppositely to the outward normal to AB (n_{12}),

$$v_q \cdot n_{12} < 0$$
$$(C_{s1}, C_{s2}) \begin{pmatrix} C_{2\Sigma} - C_{12} \\ C_{12} - C_{1\Sigma} \end{pmatrix} < 0$$
$$C_{s2}(C_{s1} + C_{d1}) > C_{s1}(C_{s2} + C_{d2})$$
$$\frac{C_{d1}}{C_{s1}} > \frac{C_{d2}}{C_{s2}}. \tag{3}$$

Similarly, the condition for the system to be able to go through BC is,

$$v_q \cdot (-n_{s1}) - |v_{s1}| > 0$$
$$(C_{s1}, C_{s2}) \cdot \begin{pmatrix} C_{2\Sigma} \\ C_{12} \end{pmatrix} - (C_{1\Sigma}C_{2\Sigma} - C_{12}^2) > 0$$
$$C_{s1}C_{2\Sigma} + C_{s2}C_{12} - C_{1\Sigma}C_{2\Sigma} + C_{12}^2 > 0$$
$$-C_{d1}C_{2\Sigma} - C_{12}C_{d2} > 0, \tag{4}$$

which can never be satisfied.

Doing the same for edge CA,

$$v_q \cdot n_{2d} < 0$$
$$(C_{s1}, C_{s2}) \cdot \begin{pmatrix} C_{12} \\ C_{1\Sigma} \end{pmatrix} < 0$$
$$C_{s1}C_{12} + C_{s2}C_{1\Sigma} < 0, \tag{5}$$

which again can never happen (geometrically, this is because the outward normal and the system velocity are both lie in the same quadrant).

Thus, the system can only travel fast enough toward the face AB and to do this it must obey Eq. (3). The physical interpretation of this is that the transition rate corresponding
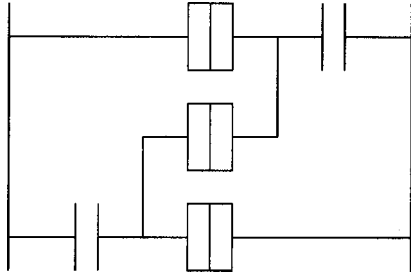
FIG. 6. The circuit remapped to a zig-zag path.

FIG. 7. $(0.4, -0.5)$: $\log_{10} I_{ds}(V_{ds})$ characteristics at temperatures 8.2 K (top) to 1.2 K (bottom) in 1 K steps. Marked by vertical lines are the predicted positions of minimum currents and also are shown the predicted currents by the nonoscillating lines.

to the interisland transition $(1 \rightarrow 2)$ *decreases* with *increasing* V_{ds}. The condition (3) implies that Fig. 1 can be redrawn more suggestively as Fig. 6 which now is reminiscent of Nakashima and Uozumi's[3,4] configuration—indeed, this is the simplest zig-zag pattern possible. Island one couples more strongly to the drain and island two to the source, this means that the potential drop across the central tunnel resistance is in an energetically unfavorable direction for holes to tunnel from island one to island two *en route* from source to drain.

The condition (3) is a *necessary* condition under the polytope approximation even in the case when the polytopes from adjacent lattice points overlap because the resultant above-I_{th} region is bounded by line segments that have the same normals and velocities as the polytopes making it up $\{\boldsymbol{n}_{s1}, \boldsymbol{n}_{12}, \boldsymbol{n}_{2d}\}$. As a consequence, the condition required is identical.

Relaxing the definition for NDC to the most general case $(\ni V : dI(V)/dV_{ds} < 0)$ still delivers the same condition as it is independent of the choice of I_{th}.

As an aside, the parameters can be chosen such that the system point moves parallel to the edge AB of the polytope and thus the current remains constant while this is the dominant edge. Trivially, the condition to produce this constant current step is obtained by setting the inequality of Eq. (3) to equality.

The polytope method implies that the prediction of the minimum current is an easily accessible quantity. In general, it is difficult to write analytic formulae for these currents due to the periodicity of the space. However, in our specific example, then the minimum current should be when the transition rate for processes $\boldsymbol{\epsilon}_{2d}$ and $\boldsymbol{\epsilon}_{12}$ are identical.

If both tunnel resistances are identical then, this is equivalent to saying their transition energies are identical:

$$\boldsymbol{\epsilon}_{2d}^T \mathsf{C}^{-1} \tilde{\boldsymbol{q}} + \tfrac{1}{2} \boldsymbol{\epsilon}_{2d}^T \mathsf{C}^{-1} \boldsymbol{\epsilon}_{2d} = \boldsymbol{\epsilon}_{12}^T \mathsf{C}^{-1} \tilde{\boldsymbol{q}} + \tfrac{1}{2} \boldsymbol{\epsilon}_{12}^T \mathsf{C}^{-1} \boldsymbol{\epsilon}_{12}$$

$$(\boldsymbol{\epsilon}_{2d}^T - \boldsymbol{\epsilon}_{12}^T) \mathsf{C}^{-1} \tilde{\boldsymbol{q}} = -\tfrac{1}{2} [\boldsymbol{\epsilon}_{2d}^T \mathsf{C}^{-1} \boldsymbol{\epsilon}_{2d} + \boldsymbol{\epsilon}_{12}^T \mathsf{C}^{-1} \boldsymbol{\epsilon}_{12}]$$

$$\frac{e^2}{|\mathsf{C}|} \begin{pmatrix} 2C_{12} - C_{2\Sigma} \\ -C_{12} + 2C_{1\Sigma} \end{pmatrix} \cdot \tilde{\boldsymbol{q}} = \frac{e^2(C_{2\Sigma} - C_{12})}{2|\mathsf{C}|} \qquad (6)$$

$$\begin{pmatrix} 2C_{12} - C_{2\Sigma} \\ -C_{12} + 2C_{1\Sigma} \end{pmatrix} \cdot \tilde{\boldsymbol{q}} = \frac{C_{2\Sigma} - C_{12}}{2},$$

this line intersects the system velocity point $\tilde{\boldsymbol{q}} = (q_1, q_2) + (C_{s1}, C_{s2}) V_{ds}/e$ when,

$$V_{ds} = e$$

$$\cdot \frac{(C_{2\Sigma} - C_{12})/2 - [q_1(2C_{12} - C_{2\Sigma}) + q_2(-C_{12} + 2C_{1\Sigma})]}{C_{s1}(2C_{12} - C_{2\Sigma}) + C_{s2}(-C_{12} + 2C_{1\Sigma})},$$

$$(7)$$

and so the coefficient of q_2 is the period of the oscillations,

$$\Delta V_{ds} = e \cdot \frac{-C_{12} + 2C_{1\Sigma}}{C_{s1}(2C_{12} - C_{2\Sigma}) + C_{s2}(-C_{12} + 2C_{1\Sigma})}$$

$$= \frac{e}{C_{s2}} \cdot \frac{1}{1 - \dfrac{C_{s1}}{C_{s2}} \cdot \dfrac{C_{2\Sigma} - 2C_{12}}{2C_{1\Sigma} - C_{12}}},$$

for our example system this gives 0.0279 V which is within error margins of the numerical simulation. The second factor in this term increases the period by $\approx 4.5\%$ compared to e/C_{s2}.

The V_{ds} positions of the valleys can also be found from Eq. (7) though care is needed to cope with the periodicity of the space. These are shown by the vertical red lines in Figs. 7 and 8. From their intersection points, the current can also be estimated and these are draw using black lines on the figures.

The agreement of valley positions is excellent, however, the current predictions are too high by about a factor two for Fig. 7 and, for some cases in Fig. 8, by over an order of magnitude. This poor agreement is due to the breakdown of the assumptions of the polytope approximation. In these cases, there are at least two loops of states and the lowest transition rate step may not be the limiting factor of the loop as reverse transition rates (holes hopping backwards) may limit the current.

VI. CONCLUSIONS

This article has introduced the polytope approximation as a tool to analyze the behavior of SE systems. It has been used to demonstrate that a two-island SET system with no quantum energy levels can exhibit NDC due to CB. Furthermore, from a purely geometric point of view, a condition for
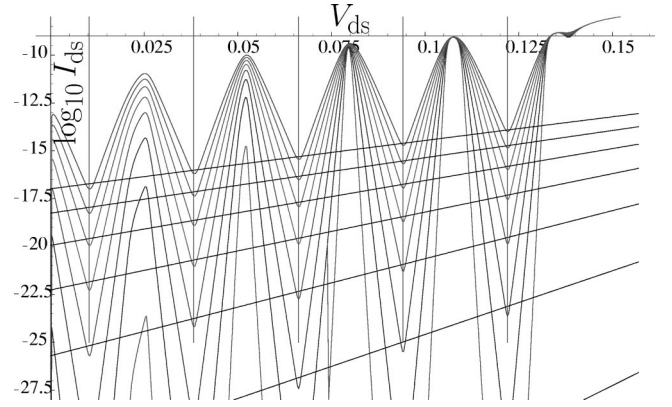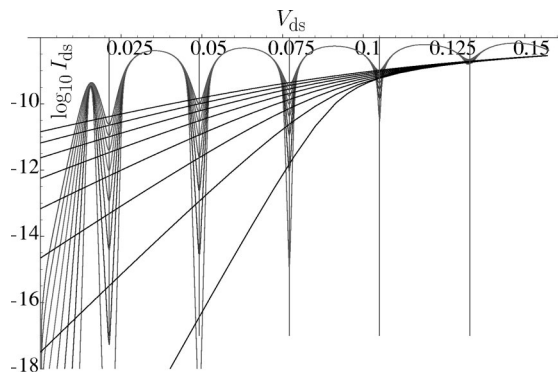
FIG. 8. $(-0.45, -0.5)$: $\log_{10} I_{ds}(V_{ds})$ characteristics at temperatures 8.2 K (top) to 1.2 K (bottom) in 1 K steps. Marked by vertical lines are the predicted positions of minimum currents and also are shown the predicted currents by the nonoscillating lines.

NDC has been derived by showing that the system must move through phase space at sufficient velocity that it can pass through one of the faces of the polytope. This leads to an algebraic condition for NDC.

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