Voltage-limitation-free analytical single-electron transistor model incorporating the effects of spin-degenerate discrete energy states

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A physically based analytical single-electron transistor (SET) model is proposed. This model virtually shows no voltage limitation in the scope of the orthodox theory, which makes it particularly suitable for hybrid simulation where the SET is biased by a current source. The model is verified against Monte Carlo simulation with excellent agreement and compared to existing models. It is found that our model is valid and accurate whatever the drain voltage and faster than reported models on the whole. A way to integrate into the model the effects of spin-degenerate quantum energy level discreteness, in the case of a silicon-based SET, is also introduced and observed quantum mechanical effects, such as negative differential conductance, are discussed. © 2008 American Institute of Physics. [DOI: 10.1063/1.2838491]

I. INTRODUCTION

Among all postcomplementary metal–oxide–semiconductor very-large-scale integration candidates, single-electron transistors (SETs) have attracted much attention due to their ultralow power consumption and highly functional features. As well as logic-circuit applications,1–5 hybrid devices combining SETs with metal–oxide–semiconductor field-effect transistor (MOSFET) and/or nanoelectromechanical systems (NEMS) have been recently investigated.6–10 However, simulation of hybrid circuits featuring SETs in a SPICE-like environment (Simulation Program with Integrated Circuit Emphasis) is fairly difficult because of the electrical characteristics of SET that result from the Coulomb blockade phenomenon and accurate, but time-consuming Monte Carlo simulations,11,12 are not adapted to design realistic circuits featuring a large number of components. Therefore, accurate SET analytical models are required to allow fast co-simulations with MOSFETs and NEMS models.

Until now, several physically based analytical models have been reported, but they all have a working voltage limitation.13–16 As mentioned by Mahapatra et al.,16 although the Coulomb blockade only occurs for drain-to-source voltage $|V_{DS}|$ lower than $e/C_S$ (where $C_S$ is the total island capacitance with respect to the ground), models valid for $V_{DS}$ higher than $e/C_S$ are needed once the SET is biased by a current source or a MOSFET.

In this work, we propose a physically based analytical SET model, derived on the basis of the “orthodox theory” of single charge tunneling and the master equation method,17,18 which virtually shows no voltage limitation in the scope of this theory. Further, it is able to adapt by itself its complexity to the operating voltage, so that the calculation time is always kept to the shortest possible. It describes accurately SET characteristics for a wide range of temperatures ($T < e^2/(10k_BT)$), can take the background charge effect into account and is valid for single-gate as well as multigate devices. We also show how the discreteness of the quantum energy levels in the case of a silicon-based SET operating at room temperature modifies the approach. Only two analytical models taking into account the quantum-level spacing have been reported until now.19,20 However, as it will be discussed later, the number of states taken into account in these models is limited or a priori fixed. Our approach enables us to introduce in the model experimentally observed quantum effects, such as negative differential conductance (NDC) or a break in the Coulomb oscillations periodicity.

II. DEVELOPMENT OF THE MODEL

A. Assumptions

In the following, we consider a metallic SET with the conventions described in Fig. 1. We suppose that the relations 1 and 2 are fulfilled, so that the Coulomb blockade can be observed:

$$R_{DS} \gg R_0 = \frac{h}{e^2} \approx 25.8 \ \text{k} \Omega,$$

$$E_C = \frac{e^2}{C} \gg k_BT.$$  

The model is developed within the scope of the orthodox theory of single-electron tunneling,17 which, despite its limi-
that proved to accurately describe systems with metallic conductors and at least qualitatively most semiconductor structures results.18
This theory is based on the following assumptions:

1. quantization of electronic energy inside the island is ignored, the electron energy spectrum is continuous;
2. the time taken by the electron tunneling through the barrier is assumed to be negligible; and
3. “co-tunneling” is ignored.

When there is no tension applied to the SET, the island has a total charge equal to zero if there is no background charge.

The general case is assumed: The background charges induce an image charge $q_0$ in the island, which is added to the classical quantity $ne$ (where $n$ is an integer). If the states are discrete, the master equation can be written as

$$\frac{\partial p_i(t)}{\partial t} = \sum_{j \neq i} \left[ \Gamma_{ij} p_j(t) - \Gamma_{ji} p_i(t) \right],$$

where $\Gamma_{ij}$ denotes the transition rate from state $j$ to state $i$ and $p_i(t)$ is the time dependent occupation probability of state $i$.

For a SET structure, a simplified master equation, which connects only the closest states with different island charge, may be written as

$$\frac{\partial p_n}{\partial t} = \Gamma_{n+1,n} p_{n+1} + \Gamma_{n-1,n} p_{n-1} - (\Gamma_{n+1,n} + \Gamma_{n-1,n}) p_n,$$

where $p_n$ is the probability of the charge state $n$ (Fig. 2). As the tunneling process changing the island charge may occur through the drain or through the source tunnel junctions, the two corresponding tunneling rates and the transition rate are connected as follows:

$$\Gamma_{n+1,n} = \Gamma_S^{n+1,n} + \Gamma_D^{n+1,n},$$

$$\Gamma_{n-1,n} = \Gamma_S^{n-1,n} + \Gamma_D^{n-1,n}.$$

From the orthodox theory, the tunneling rate of an electron tunneling through a potential barrier can be expressed as

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

where $\Delta F$ is the total energy variation related to the electron tunneling, $R_i$ is the tunnel resistance of the junction, and $T$ is the temperature. $\Delta F$ should be determined for each transition and each lead ($i$ denotes the source $S$ or drain $D$ lead):

$$\Delta F_{n+1,n} = \epsilon_n - F_{n} = -\Delta F_{n,n+1},$$

where $\epsilon_n$ is the “effective” electrostatic energy of the state $n$, and $F_{n}$ is the effective Fermi energies of the corresponding lead:

$$E_{n} = \frac{e}{C} \left( e/2 + ne + q_0 \right),$$

$$E_S = \frac{e}{C} \left( -C_D V_{DS} - C_S V_{GS} \right),$$

Writing the effective energy of one single-electron state in this way will facilitate the generalization to the silicon-based SET in the following part.

B. Solving the master equation

We will first assume that there is no background charge. This assumption does not call the reasoning into question, but simplifies the approach. We will see later how the background charge modifies results.

We consider here the steady state regime, i.e., the charge states are in equilibrium with the polarizations. Thus, the probabilities $p_n(t)$ do not depend on time, but directly on $V_{DS}$ and $V_{GS}$. The master equation can be written as follows:

$$0 = \Gamma_{n+1,n} p_{n+1} + \Gamma_{n-1,n} p_{n-1} - (\Gamma_{n+1,n} + \Gamma_{n-1,n}) p_n.$$

Probabilities verifying the following conditions are solutions of Eq. (12):

$$\Gamma_{k+1,n} p_{k+1} = \Gamma_{k+1,n} p_{k}. $$

Equation (13) leads to a complementary property for these properties. If $q(t=0)=0$, the probabilities $p_n$ verify:
\begin{align}
    n > 0, \quad p_n &= p_0 \prod_{m=0}^{n-1} \frac{\Gamma_{m+1,m}}{\Gamma_{m,m+1}}, \\
    n < 0, \quad p_n &= p_0 \prod_{m=n+1}^{0} \frac{\Gamma_{m-1,m}}{\Gamma_{m,m-1}}.
\end{align}

To determine \( p_0 \) (and then calculate all the probabilities), we may combine the transition rates equations (5) and (6) and the normalization condition:

\[ \sum_{n=-\infty}^{+\infty} p_n = 1. \]

Once the probabilities \( p_n \) are determined, we may inject them in the following current expression (in the steady state, currents through the source tunnel barrier and through the drain tunnel barrier are equal):

\[ I_{DS}(V_{DS}, V_{GS}) = e \sum_{n=-\infty}^{+\infty} \left[ \Gamma_{n+1,n}^{S} - \Gamma_{n-1,n}^{S} \right]. \]

The general form of the master equation shows that every charge state has influence on the drain-to-source current \( I_{DS} \). However, it is of course not possible to take all values of \( n \) into account and we will now see a way to simplify it without losing accuracy.

**C. Simplification of the drain current expression**

**1. Concept**

The idea is to consider only the states that are essential, depending on the values of \( V_{DS} \), and to take advantage of the periodicity in \( V_{GS} \). Let us consider the \((V_{DS}, V_{GS})\) space. As the current period is \( e/C_G \), we can translate along the \( V_{GS} \) direction every point of the space inside a fixed zone, which has a width of \( e/C_G \), without any loss of accuracy. Now, according to the location of the translated point inside the zone, we decide which set of states \([-N,N]\) are needed to determine the current.

Thus, the choice of the calculation zone is crucial for the model simplicity. The chosen motif, as well as an example, are depicted in Figs. 3 and 4. Mathematically, the approach simply consists in calculating the number \( N \) and how much the point is translated along the \( V_{GS} \) direction:

\[ N = \left\lfloor \frac{|V_{DS}|}{2e/C_S} \right\rfloor + 1, \]

\[ V_{GS} = V_{GS} - \frac{e}{C_G} \left\lfloor \frac{V_{GS} - x_1}{e/C_G} \right\rfloor, \]

where \( x_1 = \left\lfloor V_{DS}(C_S - 2C_D) - e \right\rfloor / 2C_G \) and \( \lfloor \cdot \rfloor \) is the floor function.

Then, we calculate the probabilities \( p_n \) for \( n \in [-N,N] \), and inject them in

**FIG. 3.** (Color online) Representation of the stability zones related to the charge states \( n \) in the \((V_{DS}, V_{GS})\) space. Each diamond-shaped thick dotted line delimits the set of stability zones related to the charge states \( n = -N, \ldots, N \). The area inside of the two oblique solid lines is the calculation zone, where every point of the space can be translated. Equations of these straight lines in the Cartesian coordinate system are \( y = [2C_G/(C_S - 2C_D)] x \pm [e/(C_S - 2C_D)] \). The combination of the two values determines the horizontal limits for \( N \).

\[ I_{DS}(V_{DS}, V_{GS}) = \sum_{n=-N}^{N} p_n [\Gamma_{n+1,n}^{S}(V_{DS}, V_{GS}) - \Gamma_{n-1,n}^{S}(V_{DS}, V_{GS})]. \]

For example, if \( |V_{DS}| < 2e/C_S \), the calculated \( N \) is then 1 and the current expression is

\[ I_{DS} = e p_0 [\Gamma_{1,0}^{S} - \Gamma_{-1,0}^{S} + X \Gamma_{0,-1}^{S} - Y \Gamma_{0,1}^{S}], \]

with \( p_0 = 1/(1+X+Y) \), \( X = (\Gamma_{1,0}^{S} + \Gamma_{1,-1}^{D})/((\Gamma_{0,-1}^{S} + \Gamma_{1,0}^{D})/\Gamma_{0,1}) \), and

**2. Optimal model**

Until now, the division along the \( V_{DS} \) direction was \([-2Ne/C_S, 2Ne/C_S]\), forcing the division along the \( V_{GS} \) di-

**FIG. 4.** (Color online) Example of translation of the working point from outside to inside the calculation zone. First, the drain voltage value \( V_{GS} \) determines the value of \( N \) (here \( N=2 \)). Then, the point is translated of integer times of \( e/C_G \) along the \( V_{GS} \) direction, until it is inside the calculation zone, which is fixed, and the gate voltage value used in the calculation is determined as \( V_{GS} \).
The summation in the current expression has also to be redefined as follows:

\[ I_{DS}(V_{DS}, V_{GS}, q_0) = I_{DS}(V_{DS}, V_{GS} - q_0/C_G) \]  

(26)

This method has the advantage of avoiding to redefine the calculation zone in the \((V_{DS}, V_{GS})\) space.

### III. MODEL VERIFICATION AND COMPARISON WITH EXISTING MODELS

#### A. Model verification

Our model has been verified against simulations from the hybrid simulator CAMSET (a circuit analysis program including a model of single electron tunneling). Different SET device characteristics have been simulated and compared with excellent agreement with CAMSET simulation as demonstrated in Figs. 7 and 8.

Figure 9 shows several drain currents \(I_{DS}\) obtained at different temperature levels (from 10 to 300 K), with \(V_{GS} = 0\) V and without background charge. The Coulomb blockade gradually disappears when the temperature increases. It can be noted that our model is once again in excellent accordance with CAMSET simulation. We also verified it for several capacitances values, and the same performances were ob-

![Representation of the final space partition: the number of states taking into account increases by one with each \(V_{DS}\) step of \(e/C_G\).](image)

**FIG. 6.** Representation of the final space partition: the number of states taking into account increases by one with each \(V_{DS}\) step of \(e/C_G\).
served. In fact, the pertinent quantity to estimate a SET model is \(k_BT/E_C\). Our model has been validated until \(k_BT/E_C=0.1\).

Effects of the background charge and of a second gate on SET characteristics are shown in Fig. 10. If the background charge \(q_0/e\) is a fractional number, \(I_{DS}-V_{GS}\) characteristics are shifted on the \(V_{GS}\) axis by an amount \(q_0/C_G\). Similarly, the second gate also shifts the \(I_{DS}-V_{GS}\) characteristics on the \(V_{GS}\) axis and hence can be used to compensate the background charge effect.

### B. Comparison with existing models

Several SET analytical models, each of them based on the orthodox theory, have been reported until now. Among the most recent ones, one can notably name the models proposed by the following.

1. Uchida et al.\(^{13}\) valid for \(|V_{DS}| \leq e/C_S\). This model, applicable to resistively symmetric devices only, was later extended to asymmetric devices by Inokawa et al.\(^{14}\) but does not account for the background charge effect.

2. Le Royer\(^{15}\) valid for \(|V_{DS}| < 2e/C_S\).

3. Mahapatra et al.\(^{16}\) valid for \(|V_{DS}| \leq 3e/C_S\). Actually, this model is fairly fast because it considers only one direction flow in order to minimize the number of exponential terms. On the other hand, the accuracy is worsened at low drain voltage and at high temperatures.

![Graph](Image)

FIG. 8. (Color online) \(I_{DS}-V_{GS}\) verification of our model for symmetric device with \(C_G=0.2\ a\ F,\ C_D=C_S=0.15\ a\ F,\) and \(R_D=R_S=1\ \Omega\), at \(T=173\ K\). Here symbols represent Monte Carlo simulation (CAMSET) (Ref. 12) and the solid line represents our model.

Although a limitation to \(|V_{DS}| < e/C_S\ (N=\frac{1}{2})\) is enough for digital circuits application, as mentioned by Mahapatra et al.,\(^{16}\) the use of constant current-biased SET or the association with MOS devices may impose \(|V_{DS}| > e/C_S\ (N=1\ or\ \frac{3}{2})\). However, the extension to \(|V_{DS}| > e/C_S\ makes the model more complex and hence more time consuming for low drain voltages. Be that as it may, usual extensions remain limited in the \(V_{DS}\) direction.

Another worthy SET model proposed by Lentschnig et al.\(^{21}\) can handle arbitrarily high bias voltages. However, as well as the convenient use of the current periodicity, our model differs from this one at least in its flexibility, which avoids the \(a\ priori\) choice of the relevant number of states and simultaneously enables to fasten the simulation for low operating voltages in case of need.

Our model is indeed able to adapt its complexity by itself in accordance with the operating voltage: the more \(V_{DS}\) increases, the more states it takes into account, but choosing only the strictly essential ones so that the calculation time is always kept to the shortest possible. In order to compare with conventional models, we implemented three different models with the basic theory explained previously, but without the ability of self-increasing their complexity, i.e., they take into account a fixed number of states: (1) a \(|V_{DS}| < e/C_S\)-limited model (which takes the states 0 and −1 into account), (2) a \(|V_{DS}| < 2e/C_S\)-limited model (which takes the states 1, 0, and −1 into account) and (3) a \(|V_{DS}| < 3e/C_S\)-limited model (which takes the states 1, 0, −1, and −2 into account).

As it is demonstrated in Fig. 11, whereas all the limited models inescapably show a limitation when increasing \(V_{DS}\), our model remains in excellent agreement with CAMSET simulation, whatever \(V_{DS}\). If these conditions are extreme in a way (Coulomb oscillations progressively disappear when increasing \(V_{DS}\)), the current biased SET is a basic structure used in most hybrid circuit architectures, which forces the Coulomb oscillations to occur at drain voltages higher than \(e/C_S\).\(^{6,7}\) Figure 12 shows that our model remains able to predict, with excellent accuracy, the behavior of such a structure whatever the bias, whereas a simple model cannot. For low bias, the advantage of our model over the complicated ones is that the calculation time is reduced to its minimum with the same accuracy.
Please note that whereas the implemented models (2) and (3) basically represent the models in Refs. 15 and 16, model (1) differs in some way from the model in Ref. 14, as this model makes the summation of \( n \) components of the current in the relevant gate voltage range, instead of shifting the calculation window. It compensates the inaccuracy caused by the insufficient number of charge states and suppresses the broken line anomaly. However, the accuracy is still not perfect as soon as \( |V_{ds}| > e/C_2 \) and the convenient periodicity feature of our model is lost.

IV. EFFECTS OF DISCRETE ENERGY STATES

A. Beyond the orthodox theory

In nonsuperconducting systems, two major effects are not accounted for by the orthodox theory. The first one is the coherent quantum process consisting of several simultaneous tunneling events, known as co-tunneling (see Ref. 22 for a review). This phenomenon is the cause of an extra current within the Coulomb blockade range proportional to \( R_D^2/R_D R_C \). However, in the case of silicon dioxide barriers, which is our case of interest, this parasitic effect is negligible as their tunnel resistance range is from \( 10^8 \) to \( 10^{14} \) \( \Omega \).

The second one is due to the discreteness of the quantum energy levels. The operation of SET at room temperature requires indeed an extremely small feature size. For the Coulomb blockade to be observed, the total island capacitance has to verify:

\[
E_C = \frac{e^2}{C_2} \gg k_BT.
\]

This condition involves capacitances around \( 10^{-19} \) F. As the total island capacitance is roughly \( \varepsilon l \) (where \( \varepsilon \) is the permittivity of the material surrounding the island and \( l \) the feature size of the island), it implies that \( l \) must be smaller than 5 nm. However, for these dimensions, the quantum confinement energy cannot be neglected compared to the other energies (\( E_C \) and \( k_BT \)). This means that the energy levels in the dot are quantized and the quantum level spacing \( \Delta \varepsilon_n \) will determine the transport characteristics: one gets off the scope of the orthodox theory.

Actually, in metallic SET, if we consider an island with a 1 nm diameter (around 30 atoms), the quantum-level spacing is around 150 meV and the charging energy around 200 meV.\(^{23} \) In the case of silicon-based SET, the quantum level spacing becomes comparable to the charging energy (\( \sim 200 \) meV) for larger sizes (around 5 nm).\(^{23} \)

In the following, we therefore intend to extend our model mainly in the case of a silicon-based SET able to operate at room temperature, as it was experimentally demonstrated in Refs. 24 and 25.

B. Development of the model

As it was first shown by Averin and Korotkov,\(^{26} \) it is still possible to describe this case by using the same master equations as in the orthodox theory, on condition to use a different tunneling rate expression:

\[
\Gamma = \frac{1}{1 + \exp[\Delta F/k_BT]},
\]

where \( \Gamma_0 \) is the seed tunneling rate.

However, the summation of the master equations has to be extended over two indexes as for a given number of electrons, several distributions are possible, making the solution all the more complex.

In order to keep the complexity reasonable, we chose to consider that for a given ground state \( n \), three transitions are allowed: the ground states \( n-1 \) and \( n+1 \), and the excited state \( (n+1)^\prime \), which is energetically the most favored [Fig. 13(a)]. Neglecting the transition \( n' \leftrightarrow n+1 \) may seem a little
bit tricky, but it drastically simplifies the model, simultaneously keeping the accuracy acceptable, as will be discussed later.

As before, we sum up the tunneling rates through the drain and through the source junctions to obtain the transition rate from one state to another state. However, because of the spin degeneracy, we need to add a coefficient before the tunneling rate:

1. from lower state $|i\rangle$ to upper state $|j\rangle$:
\[
\Gamma_{j,i} = (2 - m_{j,i}) \Gamma_j^{S} + (2 - m_{i,j}) \Gamma_i^{D};
\]
(29)
2. from upper state $|j\rangle$ to lower state $|i\rangle$:
\[
\Gamma_{i,j} = m_{i,j} \Gamma_j^{S} + m_{j,i} \Gamma_i^{D},
\]
(30)

where $m_{ij}$ is the initial number of electrons in the level where the transition from state $|i\rangle$ to state $|j\rangle$ occurs (either 0, 1, or 2). Note that it is possible to neglect the spin degeneracy in this model [see Fig. 13(b)]. In this case, one just needs to suppress the coefficient before the tunneling rate (i.e., consider $m_{ij}=1$).

Each tunneling rate can be expressed as ($t$ denotes the source $S$ or drain $D$ lead):
\[
\Gamma_{j,i} = \gamma_{j,i} \frac{1}{1 + \exp[\Delta F_{j,i} / k_B T]}.
\]
(31)
The energy variation $\Delta F_{j,i}$ can be expressed as before:
\[
\Delta F_{j,i} = \epsilon_{j,i} - E_F - \Delta E_{j,i}.
\]
(32)
The effective Fermi energy $E_F$ remains the same for each lead. However, $\epsilon_{j,i}$ becomes
\[
\epsilon_{j,i} = \frac{e}{C_S} (e/2 + n_i e + q_0) + \epsilon_{j,i}^K,
\]
(33)
where $n_i$ is the number of electrons in the island in state $|i\rangle$ and $\epsilon_{j,i}^K$ is the energy relative to Fermi level of the level where the transition occurs, reflecting the addition energy due to level quantization. Thus, $\epsilon_{j,i}$ is the energy needed to add an electron to state $|i\rangle$ to obtain state $|j\rangle$. It is also possible to include in this term the interaction between the two electrons when the second electron is added.

$\gamma_{j,i}$ includes the modeling of junction $t$ transparency $T$, which depends on the kinetic energy $E_F$ of the incoming electron and on the voltage $V_t$ applied to the junction:
\[
\gamma_{i} = \gamma_{0,i}(T(E_F,V_t)),
\]
(34)
where $\gamma_{0,i}$ is the bare tunneling rate of the junction.

As for the transparency, we may, for example, use the parabolic barrier model, which is easily described by a barrier height $\phi_0$ and thickness $t$, like the Wentzel–Kramers–Brillouin approximation, but which has the advantage of also applying to thin and low barriers:
\[
T(E,V) = \frac{1}{1 + \exp[\gamma_0(\phi_V - E)]},
\]
(35)
Calculations of $\gamma=(\sqrt{2 \pi} / h)\sqrt{(m/\phi_0)}$ and $\phi_V=\phi_0(1-eV/4\phi_0)^2$, where $m$ and $h$ are, respectively, the electron mass and the Planck’s constant, can be found in Ref. 27.

Under the $(V_{DS},V_{GS})$, bias, the voltages $V_t$ applied to the source and to the drain junctions are, respectively:
\[
V_S = \frac{C_D V_{DS} + C_G V_{GS} + n_i e + q_0}{C_S},
\]
(36)
\[
V_D = \frac{(C_S + C_G) V_{DS} - C_G V_{GS} - n_i e - q_0}{C_S},
\]
(37)

As for the energy $E_t$ of the incoming electron, we use the Fermi energy of the corresponding lead.

Considering the steady state, the master equation for state $n$ and state $n'$ may respectively be written as
\[
\frac{\partial p_n}{\partial t} = \Gamma_{n,n+1} p_{n+1} + \Gamma_{n,(n+1)'} p_{(n+1)'} + \Gamma_{n,n-1} p_{n-1} - \left( \Gamma_{n+1,n} + \Gamma_{(n+1)',(n)} + \Gamma_{n-1,n} \right) p_n = 0
\]
(38)
and
\[
\frac{\partial p_{n'}}{\partial t} = \Gamma_{n',n-1} p_{n-1} - \Gamma_{n-1,n'} p_n = 0.
\]
(39)

Therefore, Eqs. (14) and (15) are still valid and we may write for probabilities $p_{n'}$:
\[
p_{n'} = p_{n-1} \frac{\Gamma_{n',n-1}}{\Gamma_{n-1,n'}}.
\]
(40)

The normalization condition is now:
\[
\sum_{n=-N}^{+N} p_n + p_{n'} = 1.
\]
(41)

And we finally obtain the drain current expression:
\[
I_{DS} = e \sum_{n=-N}^{N} p_n (\Gamma_{n+1,n} + \Gamma_{(n+1)'} + \Gamma_{n-1,n} - \Gamma_{n-1,n'-1})
\]
(42)

Note that the summation over $n$ applies for, and only for, the considered $n'$ (in this case $n'\in[-N+1,N]$). For example, if $N=1$, the states taken into account are $n=-1$, 0, 1, and the current expression is
\[
I_{DS} = e p_0 (\Gamma_{0,1} + \Gamma_{1,0} - \Gamma_{0,-1} - \Gamma_{0,1}) - \Gamma_{0,0} Y_{0,0}^{G_S} - \Gamma_{0,0} Y_{0,1}^{G_S} + \Gamma_{0,1} Y_{0,0}^{G_D}
\]
(43)
with $p_0=1/(1+X+Y+Xp+Yp)$, $X=(\Gamma_{0,1} + \Gamma_{1,0} + \Gamma_{0,-1})/(\Gamma_{0,-1} + \Gamma_{0,1})$, $Y=(\Gamma_{0,-1} + \Gamma_{1,0})/(\Gamma_{0,-1} + \Gamma_{0,1})$, $Xp=[(\Gamma_{0,1} + \Gamma_{0,-1})/\Gamma_{0,-1}]X$, and $Yp=(\Gamma_{0,1} + \Gamma_{1,0})/\Gamma_{0,1}$. Please also note that depending on the initial state and thanks to a simple change in the summation, it would be possible to consider that the lowest nonfully occupied quantum level corresponding to $n=0$ is not empty, but singly occupied.

As the Coulomb diamonds do not necessarily have the same size anymore, the Coulomb oscillations may not be periodic and the use of the partition introduced in Sec. II is limited to very special cases. Nevertheless, the model can still handle an arbitrary number of electrons thanks to its simple recursion formula, which avoids solving the time-
consuming master equation. One just needs to decide where to start and where to stop the summation accordingly to the simulation voltage window.

C. Comparison with existing models

Only two analytical models that take into account the energy levels discreteness have been reported until now:

(1) Miyaji et al.\textsuperscript{19}; whereas in our case all the states are linked together, this model considers for a given ground state \( n \) the transitions to the ground state \( n+1 \) and to the first excited state \( (n+1)^{\prime} \) only, which makes it limited to \( V_{DS} \ll \epsilon/C_S \). Further, it does not deal with the spin degeneracy.

(2) Bonet et al.\textsuperscript{20}; this model is based on the full solution of the master equation for a fixed number of spin-degenerate levels accessible to a fixed number of electrons. Therefore, the corresponding analytical expressions become complicated as soon as more than one level is accessible to more than one electron.

In order to compare with our model, we implemented these two models assuming the states and transitions depicted in Fig. 14. Note that for a more meaningful comparison, we slightly adapted the original formulas available in the references to make them include, or not, the parabolic barrier model.

To simply illustrate the model operation, we used in this section the average quantum level spacing \( \Delta \epsilon \) \textsuperscript{18}:

\[
\Delta \epsilon = \frac{\hbar^2 \pi^2}{2m^* l^2},
\]

where \( \hbar \) is the reduced Planck’s constant, \( m^* \) the electron effective mass and \( l \) the island feature size, and we simulated the characteristics of a silicon-based SET having a 5 nm large island operating at room temperature. We also neglected the interaction between electrons on the same level. Effects of nonconstant quantum level spacing and variations in the interaction on the drain voltage dependency of the current have already and respectively been discussed in Refs. 19 and 20.

We first considered that the transparency \( T \) of each junction was equal to 1. As you can see in Fig. 15, results given by the models given in Refs. 19 and 20 are classic and very similar. As the number of electrons allowed to enter the island is limited to one, the current stops increasing and remains constant as soon as the first step is NDC eventually occurs. Around \( V_{DS}=0.5 \) V, the ground state in the dot indeed goes below the conduction band edge of the source, which cuts the corresponding current channel. The current then decreases as \( V_{DS} \) increases, until the next level is available for the current to flow, here around \( V_{DS}=0.85 \) V. Thus, our model enables to observe the NDC, whereas the junction transparency is kept constant. This effect has already been observed in Ref. 19 but it was obtained thanks to the parabolic barrier model, as it will be discussed in the following.

Figures 16–18 were obtained after implementation of the parabolic barrier model. As it is shown in Fig. 16, the expected NDC is observable for all of the three models. In the case of the models in Refs. 19 and 20, as it was seen before,
the number of allowed electrons is limited and the current stop increasing from a certain voltage. This, combined to the fact that the parabolic barrier model tends toward zero, makes one NDC mathematically inescapable. Actually, the attenuation introduced by the parabolic model is so strong that even the current simulated with our model vanished in the considered drain voltage range.

Figure 17 shows the current as a function of the gate voltage at room temperature. Because the models in Refs. 19 and 20 are limited to $N=0$ or 1, only one peak is observable, whereas oscillations are properly reproduced with our model. Please also note that the amplitude of the oscillations increases with the gate voltage.

Finally, Fig. 18 shows the Coulomb oscillations at different temperature levels as simulated by our model. This temperature dependency is qualitatively in good agreement with experimental results reported in Ref. 24. The height and width broadening of the current peaks with increasing temperature indicate that only one level contributes significantly to one current peak and is an other illustration of the mechanical quantum effects. Further, if you closely look at the oscillations, you can see that the interval between the peaks is not strictly constant. This effect is in this case due to the spin degeneracy and is even more accented if the interaction between electrons is considered or if the level spacing is not constant.

D. Effects of the states approximation

The model in Ref. 20 solves the full master equation for a number of levels available for tunneling and of electrons. This makes the solution very accurate but too complicated and of a limited usefulness for an analytical model unless doing appropriate approximations. Moreover, the model is not adaptive: once the solution for a given number of states is calculated, the model needs to solve the full master equation again as soon as one wants to add a new state.

We deliberately decided to neglect some states and transitions not only to make the model easier but also to make it self-adaptive. Whenever a new state is needed, the model calculates the corresponding probabilities and transition rates thanks to its simple recursion formula.

In order to evaluate the effects of this approximation, we implemented the full master equation solution for two levels accessible to up to two electrons following the method described in Ref. 20, and we compared it to our model deliberately limited to the states $n=0$, 1, and 2. Corresponding states and transitions considered in each model are depicted in Fig. 19.

As is shown in Fig. 20, both models show good agreement at low drain voltage, but our model underestimates the current because of the lack of considered states that can contribute to the current flow when the drain voltage is increased. However, if for the same given number of electrons, our model is not as accurate as the corresponding full solution of the master equation, it still gives a better idea of the current evolution than a nonadaptive model. For reference, we also plotted in Fig. 20 the results given by the model in Ref. 20 when only one level is accessible to one electron. Our model parameters are $C_G=0.1$ aF, $C_D=C_S=0.5$ aF, and $\gamma_0=\gamma_{de}=10^{-11}$. It is able to increase by itself the calculated current because of the lack of considered states that can contribute to the current flow when the drain voltage is increased. However, if for the same given number of electrons, our model is not as accurate as the corresponding full solution of the master equation, it still gives a better idea of the current evolution than a nonadaptive model. For reference, we also plotted in Fig. 20 the results given by the model in Ref. 20 when only one level is accessible to one electron, as discussed in the previous part: the calculated current is quite different from the same model when two levels are accessible to two electrons. Our model catches the essential current component, simultaneously providing flexibility and adaptiveness.

FIG. 18. (Color online) $I_{DS}$ versus $V_{GS}$ characteristics of a silicon-based SET having a 5 nm large island operating at $V_{DS}=10$ mV and at different temperature levels as simulated by our model, including the parabolic barrier. Here model parameters are $C_G=0.1$ aF, $C_D=C_S=0.5$ aF, $\gamma_0=\gamma_{de}=10^{-11}$, $\phi_{ib}=\phi_{ib}=200$ meV, and $t_F=t_D=1.5$ nm.

FIG. 19. (Color online) States and transitions considered when up to two electrons are allowed to enter the island: (a) in our model and (b) in the model in Ref. 20 (for two levels available for tunneling).

FIG. 20. (Color online) $I_{DS}$ versus $V_{GS}$ characteristics of a silicon-based SET having a 5 nm large island operating at $T=298$ K, as simulated by (parabolic model not included): (1) our model and (2) the model in Ref. 20 (for two levels accessible to up to two electrons). For reference, symbols represent results given by the model in Ref. 20 when one level is accessible to one electron. Here models parameters are $C_G=0.1$ aF, $C_D=C_S=0.5$ aF, and $\gamma_0=\gamma_{de}=10^{-11}$.
degenerate quantum energy levels into account has also been introduced and it enabled the observation of several mechanical quantum effects.

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