Correlated parallel electron transport in double- and triple-island single-electron transistors

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Abstract. The single-electron transistor is a key element in future realizations of atomic-scale digital and quantum electronic circuits. Recent advances in the research of single-atom electronic devices drives one to study single-electron transistors with a complex island structure. The quasi-stationary electron transport in the case of a single-island single-electron transistor is theoretically described by the orthodox theory by means of detailed balance equations. However, the description of a single-electron transistor with an island composed of several charge centers requires a nonlinear multidimensional graph of kinetic equations for states and transitions, for which simple recurrent solutions are not applicable. An extensible method is proposed for calculating the electron transport for a single-electron transistor with a double and a triple island. It was shown that the electron transport depends on the coupling between neighbouring centers, which can be electrostatic or tunneling. For the double-island transistor, the key symmetry configurations were simulated. For the triple-island transistor, we calculated and explained the split stability diagrams, which are in good accordance with experimental data.

1. Introduction
The present-day nanotechnology progress makes possible fabrication of electronic devices which have single atoms \cite{1–3} or molecules \cite{4,5} embedded in planar nanostructures as key functional elements. These single elements in combination with control and tunneling electrodes can be used as charge centers (CC) to build atomic-scale single-electron devices \cite{6,7} or spin and charge quantum bits. With a suitable space allocation, these CCs may be coupled electostatically or via weak electron tunneling (in terms of low tunneling transparency $T \ll 1$). The electostatic and tunneling coupling of several atomic-scale CCs is the cause of complicated single-electron transport \cite{6–10} behaviour. This complexity increases with the number of these charge centers.

One example of such a complex system is the planar single-electron transistor (SET) \cite{8,9} with an extremely small island consisting of several arsenic or phosphorus dopants implanted near the surface of crystalline silicon \cite{1,2}. The fabrication of this single-electron transistor, involving the surface implantation of several dopants, is not a deterministic technological process and yields different spacial dopants configurations in every experimental sample. Under favourable circumstances, some spatial configuration can effectively be a single CC configuration – a single-atom transistor. However, in another case, a sequential configuration can be obtained, and the electron transport will be through a chain of dopants \cite{11}. In the case of a parallel dopant distribution in the gap between electrodes of the transistor, the electron tunneling current is...
comprised of tunneling currents through each CC connected in parallel to source and drain electrodes. This case has not been thoroughly studied, but it is of great importance in connection with a fairly frequent experimental implementation [1–3].

In order to explain experimental results, in this article we suggest an original approach to simulation and calculation of the single-electron transport in such transistors and similar structures. Next, using the proposed algorithm, we calculate the CC-CC current for the major asymmetry configurations and current stability diagrams, which allows us to explain the influence of CC-CC electrostatic coupling. We do not take into account the discrete energy spectrum of CCs, because it produces an additional fine structure, which is not of interest here.

2. The split island single-electron transistor model

The single-electron transistor with an island composed of three CCs (atoms, molecules, grains, etc.) is shown schematically in figure 1. It is assumed that electrons can tunnel from and to both source and drain electrodes and in between CCs in some spatial configuration. Also it is implied that the CCs-electrodes and CC-CC mutual capacitances are given, as well as the tunneling conductances.

![Figure 1](image-url)

Figure 1. The system with 3 coupled CCs between two tunneling electrodes and one control gate. The red dashed lines illustrate the CC-CC tunneling “paths”; the blue and green lines denote the source-CC and drain-CC “paths” respectively. The number of excess electrons on the i-th CC is \( n_i \).

The consideration of the electron transport is restricted to the case when electrons tunnel from the source electrode to CCs and from CCs to the drain electrode in parallel. The electrode-CC tunneling events predominate over the CC-CC tunneling events.

For the given electrodes potentials and the environment temperature, the state of the system is determined by the number of excess electrons on each CC, which are denoted as \( n_i = -q_i/|e| \). Thus, the vector \( \vec{n} = (n_1, n_2, n_3) \) describes the charge state of the system between single-electron tunneling events. To determine the possibility of tunneling, one has to calculate the free energy change \( \Delta F \). The \( \Delta F \) is the sum of the electrostatic energy change \( \Delta U \) and the work done by the voltage sources \( \Delta W \). The calculation of \( \Delta U \) is given by a general expression:

\[
\Delta U = \frac{e^2}{2} \left( 2n_1 + \Delta n_1, 2n_2 + \Delta n_2, 2n_3 + \Delta n_3 \right) \cdot (\hat{C}^c)^{-1} \cdot (\Delta n_1, \Delta n_2, \Delta n_3)^T,
\]

where \( \hat{C}^c \) is the CCs electrostatic induction matrix. The work done by the voltage sources is:

\[
\Delta W = V_s(\Delta q_s + \delta_s) + V_d(\Delta q_d + \delta_d) + V_G\Delta q_G,
\]

where \( \Delta q_{s,d,G} \) are the changes of polarized charges of the source, drain and gate electrodes respectively, \( \delta \) denotes the charge tunneled from a corresponding electrode.

The tunneling conductance \( G \) depends on the density of states, the tunneling barrier profile and the distance between those CCs or electrodes from and to which an electron tunnels. One can define conductance as a function of initial \( \vec{n} \) and final \( \vec{n}' \) states: \( G = G(\vec{n}', \vec{n}) \). In this article, we imply that electrons tunnel one at a time, hence \( \sum_i |n_i' - n_i| = 1 \) in the case of electrode-CC
tunneling, $\sum_i |n_i' - n_i| = 2$ in CC-CC tunneling, and they do not tunnel from electrode to electrode, i.e. $\vec{n}' \neq \vec{n}$. For pairs of $\vec{n}$, which do not satisfy these conditions we set $G(\vec{n}', \vec{n}) = 0$.

The orthodox theory of single-electron tunneling states that, under certain conditions, the electron transport can be calculated using the master equation for the charge state probability distribution function $\sigma(\vec{n})$, which is the probability for a system to be in $\vec{n}$ state [6]. The tunneling rate $\Gamma(\vec{n}', \vec{n})$ from $\vec{n}$ state to $\vec{n}'$ in a low impedance environment is given by [10]:

$$\Gamma(\vec{n}', \vec{n}) = \frac{G(\vec{n}', \vec{n}) \Delta F(\vec{n}', \vec{n})}{e^2 \left[ \exp(\Delta F/k_B T) - 1 \right]}.$$  \hfill (3)

Usually the characteristic time between tunneling events is much smaller than the time resolution of measuring instruments, therefore the stationary system of linear equations can be used to calculate the charge state probability distribution. Including the normalization criteria, the system is:

$$\begin{align*}
\sum_{\vec{n}'} \Gamma(\vec{n}', \vec{n}) \sigma(\vec{n}') - \Gamma(\vec{n}, \vec{n}') \sigma(\vec{n}) &= 0 \\
\sum \sigma(\vec{n}) &= 1
\end{align*}.$$  \hfill (4)

3. The algorithm of linear equations solution

For the double-island system the charge state space can be represented by a two dimensional diagram, which is partly shown in figure 2. If one assumes that the detailed balance solution of equation 4 is true, i.e. $\Gamma(\vec{n}', \vec{n}) \sigma(\vec{n}') = \Gamma(\vec{n}, \vec{n}') \sigma(\vec{n})$, then this assumption directly leads to $\Gamma(\vec{n}', \vec{n}) \Gamma(\vec{n}'', \vec{n}') = \Gamma(\vec{n}'', \vec{n}) \Gamma(\vec{n}, \vec{n}'')$ relation for any loop, which is generally not true.

Figure 2. The charge state diagram for the double-island system. Only $\vec{n}$ state neighbours are shown. The dotted lines denote possible transitions. The emphasized $\vec{n}, \vec{n}'$ pair can not be solved without $\vec{n}''$ state involved (no detailed balance).

Partial graphs can be applied for systems described by the master equation without a detailed balance. This method, first used by Kirchhoff in 1847 [12], strongly depends on the number of states involved and the topological structure of the graph. The main idea of this approach is to create directional partial graphs (without loops) towards a given state, and then the probability of that state is determined by the rate products along the branches of these graphs.
If one thinks of a SET with several islands as of a combination of single-electron transistors connected in parallel, the amount of states grows with \( N \) as \( O(MN) \), where \( M \) is the number of states involved in tunneling in a one island system at some bias voltage. Moreover, the number of tunneling paths for any given state \( \vec{n} \) is exactly \( 2N + N(N-1) \), where the first term is given by island-electrode tunneling and the second term is due to island-island tunneling. As a result, the \( \Gamma \) matrix from equation 4 has \( O(MN^2) \) matrix elements. However, among these elements, only the \( O(N^2/MN) \) fraction is non-negative. To overcome the complexity of the system under consideration, we set our goal to minimize the matrix itself, neglecting the states that do not significantly contribute to the overall tunneling current. To do so, we use a combination of the above method of directed graphs and the gradient descent with randomization. One can see the illustration in figure 3. Calculation algorithm can be performed using the following steps:

(i) We start from the initial guess point in the parametric space, given by: \( n_i^0 = \left[ \frac{1}{2} + \frac{C_i V_G}{e} \right] \), where \( C_i \) is the \( i \)-th island-gate capacitance. With absence of extreme asymmetries between the CCs and the source/drain electrodes in terms of their capacitances and conductances, the state given by the guess point is the most probable state. When significant asymmetry arises, some corrections need to be made to \( n_i^0 \), however, considering the following search algorithm, the result will not change.

(ii) From the starting point, we “explore” the parametric space of states, creating a graph without loops. At first we choose some random direction \((\vec{n}^0 = (2, 1) \rightarrow \vec{n}^1 = (2, 2) \) in figure 3) and calculate \( p_0 = \Gamma(\vec{n}^1, \vec{n}^0) \). Next, we choose any direction except \( \vec{n}^1 \rightarrow \vec{n}^0 \), but now we calculate \( p_1 = \Gamma(\vec{n}^2, \vec{n}^1)p_0 \). This procedure continues recursively until, for example, \( p_3 < \varepsilon \) for any direction (the end of the black branch). Parameter \( \varepsilon \) is the predefined accuracy.

(iii) Next, we move one step back and repeat the search, only now we start the calculation from \( p_1 \) (blue branch begins). Just as the black branch at \((4, 1)\) point, the blue branch cannot be extended at \((2, 3)\) point because loops and double tunneling are not allowed. In the end, when all possible branches are closed, we find ourselves at the initial point and there are no directions that have not yet been explored.

When this random walk is executed, all new states are stored according to their \( N_{\text{sum}} = \sum_i (\vec{n}_i) \). Thus, when a branch attempts to create a loop, only the states with correct values of \( N_{\text{sum}} \) are checked for presence.

Lastly, using an array of all charge states, we easily compose the transition rate matrix, because each charge state has pointers to its neighbours and corresponding rates in memory. The created matrix is usually significantly sparse. Different matrix decompositions can be used for the effective solution of sparse systems of linear equations. The resulting matrix has no regular structure (unlike the single-island system, where it is tridiagonal), hence QR and LU decompositions are usually a good compromise (a more direct but less effective approach was used for the double-island system in [13]).

4. Results and discussion

Here we simplify the analysis of the double-island SET by comparing different configurations of source-CC, CC-CC and drain-CC conductance in terms of “small” and “large” values. We denote “small” values of conductance by lower-case \( g \) and “large” values by upper-case \( G \). It should be noted that even if CC-CC conductance is greater than CC-electrode conductances, the resulting CC-CC current \( I_{12} \) is a small part of the total source-drain current. It happens because the change of the electrostatic energy \( \Delta U \) for the CC-CC tunneling event is greater than the change of the electrostatic energy \( \Delta U \) for the electrode-CC tunneling event, e.g. \( \Delta U((1, 0) \rightarrow (0, 1)) > \Delta U((1, 0) \rightarrow (0, 0)) \). As a result, we distinguish different configurations
of the double-island SET by four letters: “GG ⇒ gg”, where the left values denote the first and second CC conductance with the source, the right values denote the same for the drain. All possible CC-electrode conductance cases are shown in figure 4.

In figure 5, we compare the CC-CC tunneling current dependency on the $G/g$ ratio for major configurations from the figure 4. The configuration (e) reaches its maximum at $G/g \approx 3$. Conversely, the configurations (a) and (c) do not have an extremum because the growth of the total current is suppressed by the $g$ conductances in parallel branches.

**Figure 4.** Possible symmetry configurations in terms of source-centers/centers-drain conductance for the double-island SET. The solid and dashed lines denote the $G$ and $g$ conductances respectively. The dotted lines denote the CC-CC conductance $G_{12}$.

**Figure 5.** CC-CC current divided by the source-drain current vs the $G/g$ ratio for the asymmetric double-island SET (a), (c), (e) (see figure 4). CC-CC conductance $G_{12} = 10g$. Capacitances are equal for both islands.

The experimental characteristics of the single-electron transistor in silicon with an island composed of several phosphorus dopant atoms [2] clearly revealed the splitting of the current stability diagrams ($dI/dV_T$ vs $(V_T, V_G)$). We attribute this splitting to mutual electrostatic coupling of dopants. Now we show how electrostatic coupling of CCs (e.g. dopants in silicon) and different capacitances of these CCs with the gate electrode modify the CSD
(see figure 6). For clarity of comparisons, we assume that the characteristic capacitance $C_i = C_i^S + C_i^G + \sum_{j \neq i} C_{ij} = C_S$ of every island is the same, hence the Coulomb blockade for $V_G = 0$ equals to $e/C_S$ in each case.

In the CC-CC coupling case (see figure 6(b)), the $\Delta U$ of adding electrons to CCs one by one, i.e. $(0,0,1) \rightarrow (0,1,1) \rightarrow (1,1,1)$, differs by the same amount. As a result, the areas ‘A’ and ‘B’ have the same length in terms of bias voltage. The “A” area has $\vec{n} = (0,0,1),(0,1,0),(1,0,0)$ states involved in tunneling. In the “B” one, additional $\vec{n} = (0,1,1),(1,0,1),(1,1,0)$ states are possible. Lastly, in the “C” one, $\vec{n} = (1,1,1)$ state is on.

The figure 6(a) case significantly differs from the figure 6(b) case, as the “A”, “B”, “C” areas account for states that are unique for each CC because CCs are not coupled. The “A” stands for $\vec{n} = (0,0,1)$ state, the “B” – for additional $\vec{n} = (0,1,1)$ state, and the “C” accounts for $\vec{n} = (1,1,1)$ state.

Finally, in the figure 6(c), one can distinguish areas and charge states by direct comparison with the first two CSDs. We emphasize that the three split “corners” at small $V_T$ are observed in all cases. However, only in the CC-CC electrostatic coupling case (figure 6(b)) these “corners” are identical in size and remain the same for any corresponding $V_G$.

5. Conclusion

We have developed an extensible and flexible method of single-electron transport calculation for the SET with an island composed of several CCs. For the double-island system, the CC-CC current dependency on conductance asymmetry was studied. For the triple-island system, the stability diagram splitting observed in experimental devices was confirmed and explained. It was shown that even in the case when CCs are equally electrostatically coupled to the gate electrode, the mutual capacitance of CCs results in splitting of the current stability diagrams. Thus, we have demonstrated that the simplest configurations of the double- and triple-island SET systems without a discrete spectrum of CCs can exhibit complex behaviour, which significantly depends on CC-electrodes and mutual CCs capacitances and conductances.

We believe that the proposed approach to modeling, calculation and analysis can be helpful for creation of future devices based on atomic-scale functional structures.

Acknowledgments

This work was supported by the Russian Science Foundation (grant 16-12-00072).

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