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# Identification of States and Events for the Static and Dynamic Simulation of Single Electron Tunneling Circuits

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***Abstract*—**The implementation of single-electron tunneling (SET) simulators based on the master-equation (ME) formalism requires the efficient and accurate identification of an exhaustive list of active states and related tunnel events. Dynamic simulations also require the control of the emerging states and guarantee the safe elimination of decaying states. This paper describes algorithms for use in the stationary and dynamic control of the lists of active states and events. The paper presents results obtained using these algorithms with different SET structures.

***Keywords*—**Active state**,** Coulomb blockade, Master Equation, Single electron devices

## I. Introduction

THE phenomenon of Coulomb blockade and single electron tunneling (SET) [1], together with many advances in fabrication technologies have resulted in the realization of nano-scale devices where it became possible to control and monitor the flow of single electrons through these devices. Correlated transfer of electrons in such devices has been studied, both theoretically and experimentally [2]. The operation of SET devices depends fundamentally on the behavior of discrete single electrons and the possibility to control the flow of single electrons via various junctions. This is affected by co-tunneling, thermal charge fluctuations and background charge effects.

From among the various SET circuit simulation methods that have been devised, Monte-Carlo (MC) methods are widely used in situations where individual tunnel events are traced for a long time in order to collect statistics on the behavior of the circuit[4]-[8]. The ME formalism has also been used to compute state occupancies [3]. A hybrid MC/ME technique is also described in [4]. The use of the ME approach has the advantage of being able to accurately describe the rare events, e.g. co-tunneling events.

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## II. Problem Definition and Related Techniques

Let the electronic circuit under investigation consist of a set of tunnel junctions, normal capacitors and a set of voltage sources as shown in the inset of Fig. 1. At any time $t$ during circuit operation the potential at any node in the circuit is calculated as the superposition of the potentials due to the applied voltage sources and the potentials induced by the excess charges located at various nodes of the circuit. Let $\psi(t)=\{m_1, m_2,..,m_n\}$ define the state of the circuit, where $m_i$ is the number of excess electrons at node $i$. The nodal voltages corresponding to the given state $\psi_i$ determine the electron tunneling rates between the different nodes. The transition rate from a state $\psi_i$ to a state $\psi_j$, resulting from a tunnel event from node $m$ to node $k$ is denoted by $\Gamma_{i,j}^{m,k}$. The tunneling rate across a given junction, or equivalently the rate from one state to another, is computed using the orthodox theory of tunneling [1] as:

$$\Gamma = \frac{1}{e^2 R_t} \frac{\Delta E}{1 - \exp\left( - \Delta E \big/ k_B T \right)} \tag{1}$$

where $R_t$ is the tunnel resistance of the junction and $\Delta E$ is the change in free energy due to the tunnel event. The change in the free energy, $\Delta E$, is determined by the charging energy of the electron tunneling from one node to another together with the potential profile induced by the applied sources. Circuit nodal voltage analysis is used to compute the potential profile resulting from the applied voltage sources and due to the presence of excess charges. Effects of background charges are also catered for using the same techniques [9].

The probability of finding the system in a given state is a function of the circuit topology and parameters. When the steady-state condition is established, the system could be found in a finite set of states. The probability of finding the system in any of these states is denoted by the occupancy vector $P$. Define the matrix $G$, with elements satisfying the following relations:

$$G_{i,j} = \begin{cases} -\sum_k \Gamma_{k,i} & if \ \ i = j \\ \Gamma_{i,j} & if \ \ i \neq j \end{cases} \tag{2}$$

This stationary Markov process satisfies the following Master Equation:

$$GP = 0 \tag{3}$$

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The matrix $G$ has a zero eigenvalue and equation (3) could be solved together with $1 = \sum p_i$ to find the state occupancy factors, $P$. With the set of (3) solved, various parameters of the circuit could be computed. As an example, the current across the tunnel junction between nodes $m$ & $k$ is calculated as:

$$I_{m,k} = e\sum_i p_i \sum_{j\neq i} \left(\Gamma_{i,j}^{k,m} - \Gamma_{i,j}^{m,k}\right) \quad (4)$$

where $\Gamma_{m,k}^{i,j}$ is the tunnel rate from node m to k corresponding to the state transition $\psi_i$ to $\psi_j$. Other parameters that could be computed include: the differential conductance, average excess charge or voltage at a given node in the SET structure, charge fluctuations etc.

The solution of (3) and subsequent calculation of ensemble variables would be possible only if the exact set of stationary states is known. In some studies, a superset of the states is chosen such that this set is ensured to contain all possible active states [2]. It is then left to the solution of (3) to establish the list of active states and subsequently eliminate the redundant states. It is noted that the solution of (3) constitutes an $O(n^3)$ algorithm, where $n$ is the number of states chosen for the solution; hence, the use of a superset of states could be inefficient for larger systems. In the following sections an algorithm that allows the identification of the exhaustive list of active states is presented.

Monte-Carlo simulations are extensively used in the study of SET systems to determine the stationary characteristics of such circuits [5]- [8]. When used in a typical dynamic mode, the MC technique will provide sample trace of events under the given dynamic condition. To assess the typical behavior, such simulations could be repeated a large number of times and an ensemble average behavior could then be extracted. A simulator that is commonly used, described in [6], uses the standard Monte-Carlo techniques for the static and transient simulations. However, this simulator also resorts to the direct solution of the ME in modes where the Monte-Carlo simulations would prove too expensive or inaccurate, e.g. in the simulation of the rare co-tunneling events.

## III. States and Events in Static Simulations

As mentioned earlier, building the exhaustive list of active states is an important requirement for the efficient use of the ME formalism. To identify the set of stationary active states, our simulator starts at an arbitrary initial state $\psi_0$. This initial state is added to the set of candidate active states, $S$. The algorithm then searches for all end states that may be reached starting with this state. A possible tunnel event from node m to node k would result in a change in the state of the system from state $\psi_i$ to state $\psi_j$, denoting a corresponding event by $T_{i,j}^{m,k}$. The newly identified state is added to the list $S$ while the event is added to the list of possible events, $E$. This process is repeated for all states that accumulate in the set S. By the end of this stage the set S would contain all candidate states, see Fig. 1 The algorithm *IdentifyCandidateActiveStates*() shown below provides a description of the major steps needed to find the set of all candidate states:

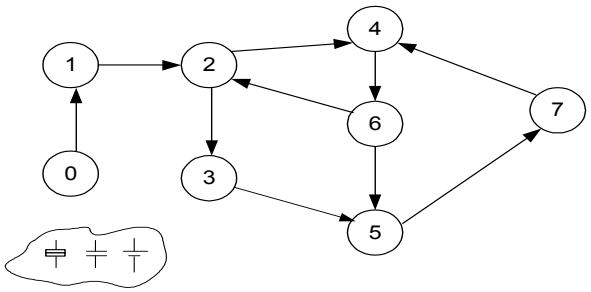



Fig.1 Illustration of a list of candidate states in static simulations

```
Algorithm IdentifyCandidateActiveStates
Initialize list of active states S={0}.
Initialize list of events E = {0}
Choose initial State ψ0
Add ψ0 to S
For each ψi in S
  For each node m in the SET circuit
    For each node k in the SET circuit and k <> m
      if m & k are connected by a tunnel junction
        Construct new state ψj using ψi and m→k event
          Calculate tunnel rate Γ(i,j)^(m,k)
          Construct T(i,j)^(m,k)
          If (Γ(i,j)^(m,k) > 0.0) then
            Add ψj to S
            Add T(i,j)^(m,k) to E
          Endif
        Endif
      EndFor
    EndFor
EndFor
```

Fig. 1 is an illustration of the working of this algorithm. The process starts with the state $\psi_0$, from which only one state, $\psi_1$, is identified and added to the list S. The second iteration also identifies another state $\psi_2$. Using $\psi_2$, two further candidate states are found linked to this state, namely $\psi_3$ and $\psi_4$. The process is repeated until no further new states are identified.

The superset of states thus identified could be safely used to solve (3) and to calculate the stationary state occupancy factors. The set of redundant states will have no contribution on the final solution and (3) will result in zero occupancy factors for these states. However, the proportion of redundant states may be high depending on the applied voltages and the initial starting state. These redundant states could be eliminated from the solution as described below.

The algorithm that decides on the active status of candidate states processes the states in the same order the states were added to the list S. In our example of Fig. 1, $\psi_0$ will be processed first, followed by $\psi_1$ etc. Each state is compared against the initial and final states of the events in $E$. A state $\psi_i$

in *S* is passive if this state does not match any of the final states $\psi_f$ of the events in *E*. In other words, once the system departs from this state it will not be possible for the system to return back to this state. This condition is expressed as:

$$\psi_i \text{ is inactive if: } \sum_j \Gamma_{i,j} > 0 \text{ and } \sum_j \Gamma_{j,i} = 0 \quad (5)$$

Once a state is deemed to be inactive, it will be removed from *S* and will have no further bearing on the status of the remaining candidate states. Also all elements of *E* where $\psi_i$ is an initial or final state shall be removed. Eventually, *S* will contain only the set of active states and the set E will contain all possible tunnel events. This reduction algorithm makes it possible to restrict the solution of (3) exclusively to the active states.

*Algorithm RemovePassiveStates*
*For each* $\psi_i$ *in S*
  *If (* $\exists T_{j,i} \in E : \Gamma_{j,i} > 0$
    →*State is active*
  *Else*
    →*State is not active*
    *Remove all events* $T_{j,i}$ *in E*
    *Remove* $\psi_i$ *from S*
  *Endif*
*EndFor*

As an illustration, and referring to Fig. 1, the state $\psi_0$ will be removed first, together with the event $T_{0,1}$, then $\psi_1$ will be removed together with the event $T_{1,2}$.

## IV. Evolution of States in Dynamic Simulations

One of the fundamental issues facing single-electronics is brought about by the stochastic nature of tunneling events. Simulations based on the ME would provide a tool suitable for assessing the transient behavior of circuits resulting from a perturbation in a given input. The operation of digital and analogue SET circuits requires the application of time-varying voltage sources at one or more nodes. Controlling the state of the single electron transistor would require applying a step voltage at the gate of the transistor. The stochastic nature of the tunnel events mean that the state of the middle node of the transistor is a function of time that could be estimated only in probabilistic terms. Ensemble Monte-Carol simulations could be used to run the simulation a large number of times then compute the ensemble averages to gain an insight of the most likely behavior. Such ensemble Monte-Carlo simulations were used e.g. in [10] to study the SET oscillations in long arrays of tunnel junctions and noise in these structures.

Time dependent solution of the dynamic ME is the alternative to using the ensemble Monte-Carlo technique. Let the SET system be described by the set of states vector *S(t)* and the probability *P(t)*. The time evolution of the state of the system and the corresponding probabilities is dependent on the current state of the system together with the corresponding tunneling rates. The tunneling rates in return are also a function of the state and the applied voltages. The time-dependent ME is expressed as:

$$\frac{dP}{dt} = G(t)P(t) \quad (6)$$

Above equation could be solved analytically for simple situations, e.g. when a step voltage is applied to the terminals of a single-electron transistor when transport is achieved via only two states. The simulator SENECA presented in [4] chooses a time step such that the external parameters of the circuit do not change during this interval, $\Delta t$. This simulator then guesses a set of states whose probabilities are expected to be greater than some threshold probability $p \geq p_{th}$; then solves the master equation for this set. Finally, the states with probabilities $p < p_{th}$ are filtered out. This algorithm could potentially get into a state where emerging states are added to the list of candidate states and immediately be removed as a result of the probability being $p < p_{th}$; thus not allowing such valid states to contribute to the transport process soon enough. In this study, a generic numerical solution is implemented. The algorithm does not make any assumptions about the applied voltages i.e. this technique will accommodate varying tunneling rates. Using first degree Taylor expansion of (5), the evolution of the state occupancies are expressed as follows:

$$P(t + \Delta t) \approx P(t) + G(t)P(t)\Delta t \quad (7)$$

With time varying voltages, the set of active states will potentially vary with time where new states will become available while other states are annihilated. The stochastic nature of the tunnel events, responsible for the creation and the annihilation, implies that there will be an equivalent relaxation or characteristic time associated with the evolution of states. This characteristic time may also vary with the varying applied voltages.It might be tempting to apply the algorithms *IdentifyCandidateActiveStates()* and *RemovePassiveStates()* at every step in order to track the evolution of states. This is not correct because some states may have high occupancy factors initially and will stay active contributing to the transport process until finally been eliminated from the lists. The application of the algorithm *RemovePassiveStates()* will remove such states immediately. Also, a possible technique is to employ a simple one-way algorithm that allows states join the active list and keep these states in the list for the entire duration of the simulation. However, this is not efficient as the probability of the exiting states decays exponentially and may therefore stay in the list far too long than numerically needed. The algorithms used in the dynamic case is designed to cater for the arriving states in one hand while continually assessing the condition for the safe removal of that states that have no or little contribution to the dynamics of the system. The algorithm presented in this paper removes a state permanently from the list *S(t)* if *(a)* the occupancy of this state becomes small enough and *(b)* the occupancy of this state is decaying, i.e. $p(t + \Delta t) < p_{th}$ *and* $\partial p / \partial t < 0$. The second condition *(b)* is imposed in order to avoid the possible removal of a growing state.

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## V. Dynamic Selection of ΔT

The time increment, $\Delta t$, should be chosen so that the simulator is able to accurately resolve the fasted process in the system on one hand while ensuring that the chosen step is not too unnecessarily too small. Referring to (2), it is noted that the largest rate would be located at the diagonal of the matrix $G(t)$. The reader is reminded that the diagonal entries of $G(t)$ correspond to the sum of all rates leaving a given state. The simulation time increment is therefore chosen as:

$$\Delta t = MIN\left( \frac{\alpha}{MAX(|G(t)|)}, \tau_{\min} \right) \quad (8)$$

where $\alpha<1$ and $\tau_{min}$ is a minimum time increment used in the simulator. In our simulations, a value of $\alpha=0.01$ is used. The dynamic algorithm starts at some known state or starts from a stationary state where the state $S(0)$ and the probabilities $P(t)$ are known.

*Algorithm DynamicSimulation*
*Pre-requisite: Initial states S(0) and occupancy vector P(0)*
*While simulation not ended*
  *Update external inputs*
  *Compute tunneling rates*
  *Compute Δt using (8) and advance time*
  *Update states & events lists S & E*
  *Compute G(t)*
  *Update occupancies using (7)*
  *For each state* $\psi_i$
    *If* $(p_i(t+\Delta t) < p_{th}(t))$ *and* $(p_i(t+\Delta t) < p_i(t))$
      *Remove state* $\psi_i$ *from S*
      *Remove events involving* $\psi_i$ *from E.*
    *Endif*
  *EndFor*
  *Renormalise P*
  *Compute required time dependent statistics*
*EndWhile*

## VI. Performance Considerations

The overall performance of the static simulator is greatly affected by the efficiency of the algorithms described in this paper. The algorithm *IdentifyCandidateActiveStates()* has an order of growth of $O\left(N_{cs} \times N_j^2\right)$ where $N_{cs}$ is the number of candidate states & $N_j$ is the number of tunnel nodes in the SET circuit. Also note that adding a new state or event to the list requires a search within the entire list to ensure the uniqueness of the state. In relatively large circuits, the choice of the initial state $\psi_0$ may have a big effect on the overall efficiency as this will determine $N_{cs}$. The algorithm *RemovePassiveStates*() is an $O\left(N_{cs} \times N_{ce}\right)$ algorithm, where $N_{ce}$ is the total number of candidate events in E. The dynamic simulations require checking and updating the lists at each step. This algorithm traverses the active list and checks whether a new state could be added. This means the algorithm inherits the order as per the *IdentifyCandidateActiveStates()*.

The number of events and states, candidate or active, strongly depends on the topology of the SET circuit and the total number of tunnel junctions and nodes in the circuit. These numbers grow very fast with the applied voltages resulting in considerable changes in the time and memory space efficiency of these algorithms.

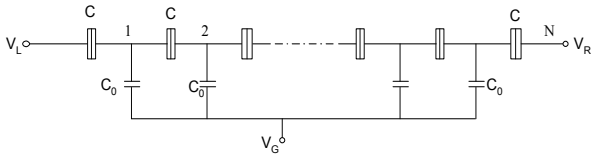



Fig. 2 An array of $N$ tunnel junctions

## VII. Results And Discussions

Validation of the simulator used in this study is provided in [11]. The effectiveness of the algorithms described above is discussed in the context of standard SET structures. First the single electron transistor, the turnstile, is considered. This structure is realized with $N=2$ in Fig. 2. The stationary conductance is computed as $\partial I / \partial V$. Fig. 3 reveals that the number of active states, together with the total number of events, increases with the applied voltage. The intuitive model for this Markovian process is a linear birth-death model. It can be shown that the number of events, $N_e$ is related to the number of states $N_s$ by the relation: $N_e = 2(N_s - 1)$, in agreement with the results shown in Fig. 3. It is also noted that the jumps in the conductance corresponds to the introduction of two additional states which is also confirmed by the corresponding steps in the I-V curves.

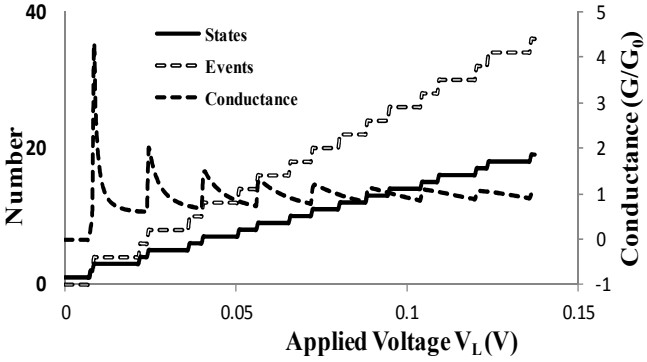



Fig. 3 Variation of active states and the corresponding events with the applied voltage $V_L$ in an inhomogeneous single-electron transistor ($N=2$, $T=0K$, $V_R=0$, $V_G=0$, $C=10^{-17}F$, $C_0=10^{-18}F$, $R_1=100k\Omega$, $R_2=1M\Omega$ *and* $G_0 = (R_1 + R_2)^{-1}$

Fig. 4 shows the variation of $N_s$ & $N_e$ against the gate voltage in a three junction system, i.e. $N=3$ in Fig. 2, at fixed source-drain voltage. It is interesting to observe the periodic oscillations of the active states, events and the resulting current with the applied gate voltage, with the period of oscillation validated as $\Delta V_G = e/C_0 = 0.16V$. The investigation of the average excess charge measured at the nodes of this circuit

reveals that exactly two additional electrons would be trapped in the circuit when the gate voltage is incremented by $e/C_0$, one electron at each node.

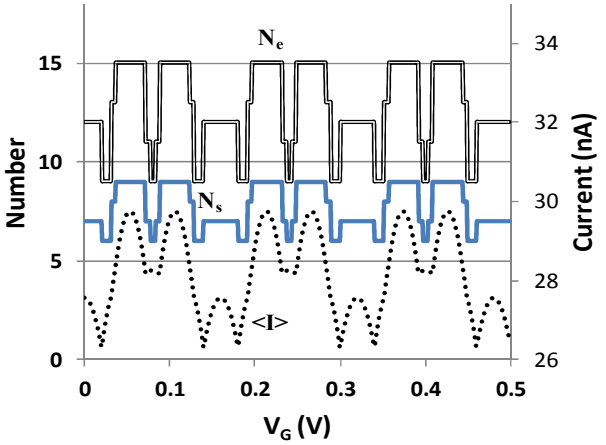



Fig. 4 Variations of the number of active states $N_s$, number of events $N_e$ and average current against the gate voltage $V_G$ in a three junction system ($N=2$, $V_L=-V_R=10mV$, $C=10^{-17}F$, $C_0=10^{-18}F$, $T=0K$, $R=100k\Omega$)

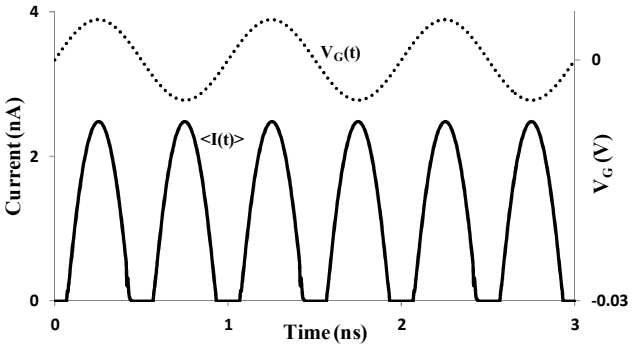



Fig. 5 Dynamic simulation of three junction system, parameters as per Fig. 3. Sinusoidal gate voltage of amplitude = $5mV$, frequency=$1GHz$ applied at $t=0$. $V_L=-V_R=7mV$

Dynamic simulations are an important technique in studying the expected behavior of SET circuits resulting from a time varying input or a perturbation in the input signal. Fig. 5 depicts the temporal behavior of the average current resulting from a sinusoidal voltage applied at the gate of a three junction system. Note that the current shown in the figure is the ensemble average current; the actual current detected across any junction will be a series of δ tunnel events. Fig. 6 shows the currents through arrays of $N=40, 60 \& 80$ junctions following a step voltage applied at the left hand side of the array. The frequency of oscillation, $f_0$, in each array if related to the steady state current Io via the fundamental relation: $I = ef_0$. Such simulations could be used to study the fluctuations across tunnel junctions.

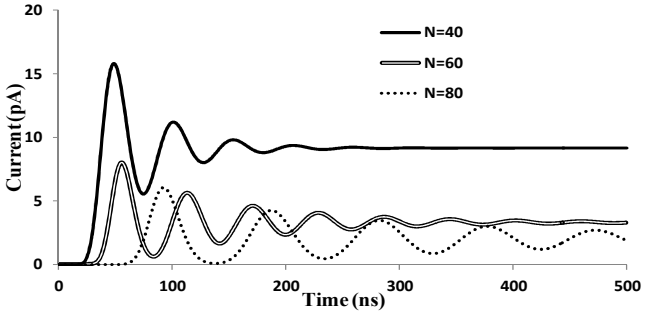



Fig. 6 Evolution of ensemble average current through arrays of *40, 60 & 80* tunnel junctions following a step change in $V_L$ 0 → *20.6mV* ($T=100mK$, $C=10^{-17}F$, $C_0=10^{-18}F$, $R=100k\Omega$)

## VIII. Conclusion

In this paper, techniques used to control and trace the states and related events in static and transient simulations of SET circuits have been presented. These algorithms were used in the simulations of various SET topologies. Simulations of circuits containing $N= 2, 3, 40, 60 \& 80$ tunnel junctions were presented, each circuit contain $2N-1$ total tunnel and normal capacitors. The efficient use of the ME formalism in the simulations of SET circuits is a viable technique for the design and optimization of SET circuits, thus the importance of the development of algorithms that would improve the efficiency and accuracy of the simulating tools.

## References

[1] K. Likharev, "Correlated discrete transfer of single electrons in ultra-small tunnel junctions", *IBM J. Res. & Dev.* Vol (32),1, pp. 144-158, 1988

[2] S. Gustavsson et. al. "Electrons in quantum dots: One by one", *J. Applied Physics*, 105, 122401, 2009.

[3] P. Heshfield, J. Davies, P. Hydgaard, C. Stanton & J. Wilkinson, "Zero-frequency current noise for the double tunnel junction Coulomb blockade", *Phys Rev B*, 47 (4), pp. 1967-1979, 1992.

[4] L. Fonseca, A. N. Korotkov and K. Likharev, "SENECA: a New Program for the Analysis of Single-Electron Devices", *VLSI Design*, Vol. 6, Nos. (1--4), pp. 57-60, 1998.

[5] V. Nguyen and V. Nguyena, "Shot noise in metallic double dot structures with a negative differential conductance", *Appl. Phys Lett*, 87, 123107, 2005.

[6] C. Wasshuber, H. Kosina & S. Selberherr, "SIMON-A simulator for single-electron tunnel devices and circuits", *IEEE Trans. Computer-Aided Design of Integrated Circuits and Systems*, 6 (9), 937-944, 2002.

[7] Y. S. Yu, J. H. OH, S. W. Hwang, and D. Ahn, "Implementation of Single Electron Circuit", *Simulation by PSPICE: KOSEC SPICE," IEIC Technical Report* vol. 100, no. 150, pp. 85-90, 2000.

[8] G. Zardalidis, and I. G. Karafyllidis, "SECS: A New Single-Electron-Circuit Simulator,", *IEEE Transactions on Circuits and Systems - I*, vol. 55, no. 9, pp. 2774-2784, 2008.

[9] S. Amakawa1 et. al, "Single-electron logic based on multiple-tunnel junctions", in *Mesoscopic Tunneling Devices*, ed. H. Nakashima, 2004.

[10] J. Bylander, T. Duty and P. Delsing, "LineWidths of Single–Electron Tunneling Oscillations: Experiment and Numerical Simulations", 24th International Conference on Low Temperature Physics - LT24. AIP Conference Proceedings, Volume 850, pp. 1442-1443 (2006).

[11] S. Babiker, "Simulation of single-electron transport in nanostructured quantum dots", *IEEE Trans. On Electron Devices*, vol. 52, no. 3, pp. 392-396, 2005.

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