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A Single Electron Device and Circuit Simulator with a New Algorithm to Incorporate Co-tunneling

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We introduce a single electron device and circuit simulator for the investigation of devices and circuits consisting of tunnel junctions, capacitors, constant voltage sources, piece wise linear voltage sources and voltage controlled voltage sources. The simulator features a new algorithm to incorporate the quantum mechanical effect of co-tunneling.

The basic simulation method is to calculate tunnel rates for all possible tunnel events starting from a particular state (charge distribution) of the circuit. These tunnel rates strongly depend on the change in free energy, of the whole circuit. Every system tends to a state of lower energy and therefore tunnel events that lower the free energy are more likely to happen. These rates in conjunction with an evenly distributed random variable are used in a Monte Carlo method to simulate the Poisson process describing the electrons tunneling through junctions [1].

$$\Delta t = \frac{\ln r}{\Gamma(\Delta E)} \tag{1}$$

Here, ΔE is the change in free energy caused by a specific tunnel event, Γ is the tunnel rate of this event, r is an evenly distributed random variable and Δt is the time between this and the last tunnel event of the same junction. Of all possible tunnel events, the one with the shortest Δt is chosen as the winner. After this event the charge distribution changes and consequently the state as well as the tunnel rates. These steps are done many times to simulate the transport of electrons through the single electron circuit.

Co-tunnel events are very rare events and are therefore difficult to simulate with a Monte Carlo technique in a reasonable amount of time. A well known variance reducing technique for such rare events is to split the state space into a domain of frequent states and a domain of rare states [2]. If the system falls into a rare state not just one trajectory but many trajectories are calculated starting from the same state and weighted accordingly less. This method is a good choice if the ratio of the probability of a rare event to the probability of the frequent events is larger than about 10^{-6}. In the case of co-tunneling the ratio very often gets much lower and thus it is very unlikely that the Monte Carlo simulator will enter the rare state domain. Therefore, this scheme will have no impact for such rare events and their associated states and is in this case a bad choice. However, in order to study, for example, error probabilities of single electron memory devices and decay processes of quasi stable states one needs to include these very rare events.

Thus, we have developed a new algorithm which can be understood as a a mixture of a Monte Carlo approach and the Master Equation method [3] used by Fonseca et. al. [4] or of a Monte Carlo approach combined with a direct calculation technique. Instead of waiting for the Monte Carlo simulator to step into the rare state domain we only use the Monte Carlo technique for the frequent state space and directly calculate the contribution of the rare states.

The first step is to simulate by the Monte Carlo technique tunnel events with a tunnel rate larger than a certain threshold. States that are visited via these events build the frequent state space. The result of this part is a list of frequent states with their associated probabilities. The same probabilities would result from the Master Equation approach, with the difference that we use a Monte Carlo method to calculate the probabilities and not the Pade algorithm to solve the Master Equation. The advantage with our method is that we get both the set of frequent states and their probabilities with one simulation run in a much simpler and clearer way.

We make the assumption, that the set of rare events which is connected with the set of frequent events via rare tunnel events, does not change the probabilities of the frequent states. This approximation is, in the here considered strongly localized electron state case (tunnel resistance $R_T \gg R_Q = \pi\hbar/2e^2 \sim 6.5\ \mathrm{k}\Omega$) very good, because the co-tunnel rates scale with $1/R_T$ and are therefore much smaller than the frequent tunnel rates. The consequence is that the probability of the rare states is much smaller than the probabilities of the frequent states. Thus, one can calculate all branches that lead from a frequent state to other states via frequent and rare tunnel events. Every event tree of a frequent state is weighted with its probability. As soon as a frequent event leads to a frequent state this branch is not followed any further, because the information is already included in the state probabilities. Otherwise we follow the branches up to a predetermined depth. See Fig. 1 and Fig. 2.

A user-friendly graphical interface with a graphical circuit editor makes it easy to design single electron devices and straight forward to look at charges and voltages at any node and currents in any branch of the network.

Fig. 3 shows the user interface of the simulator. On the left side is the object box, the two lines on the bottom are status and help line. The editor depicts a single electron transistor with several meters specifying which simulation results are of interest to the user. In Fig. 4 one can see the various simulation parameters that control the outcome of the simulation. The user can choose among different measurement modes to study the transport of single electrons or to calculate current, voltage and charge characteristics.

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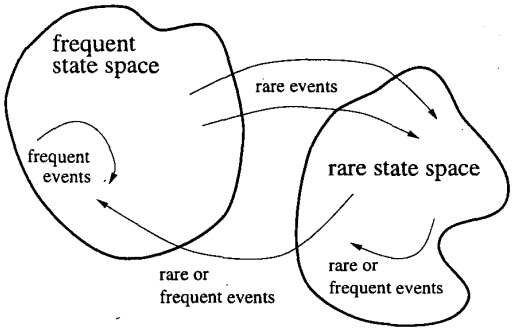

Figure 1: Frequent and rare states. The rare state space can only be reached via rare events.

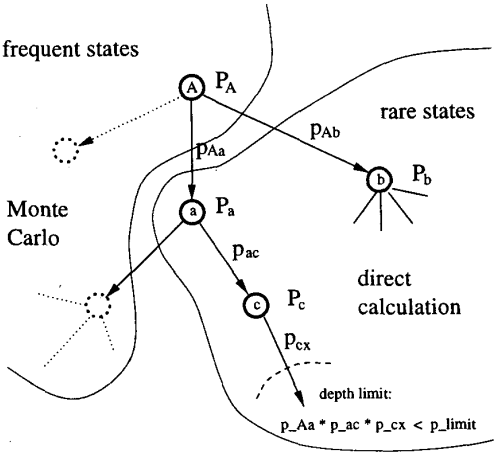

Figure 2: Calculation method to take rare states into account.

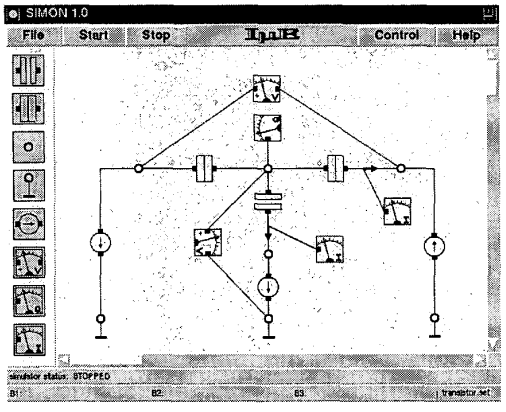

Figure 3: Graphical User Interface.

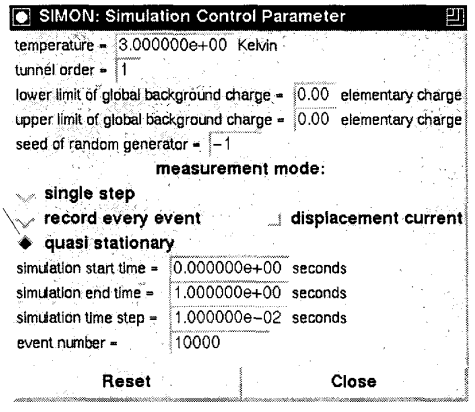

Figure 4: Simulation Parameter Window.

Acknowledgment. Our work is significantly supported by Digital Equipment Corporation at Hudson, USA.