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A single-electron device and circuit simulator

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We introduce a single-electron device and circuit simulator, called SIMON, with the following features. Tunnel junctions, capacitors, constant voltage sources, piecewise-linear time-dependent voltage sources and voltage controlled voltage sources can be connected arbitrarily to form a single-electron device or circuit. With various parameters one controls transient and stationary simulation modes. All node voltages, node charges and currents in any branch of the network can be output to files for later post-processing. The tunnelling of single electrons is simulated with a Monte Carlo technique where the change in free energy of the whole network determines tunnel rates of possible tunnel events.

Key words: tunneling, single-electron, simulation, Monte Carlo.

1. Introduction

The field of single-electronics has advanced considerably in the last years. The basic theory and underlying physical phenomena are understood and experimentally verified. Therefore, we are now entering the engineering phase and ask questions such as: What kind of novel single-electron devices are possible? Which parameters are optimal? What are the device characteristics and error rates?

To support one in finding answers to these questions, we developed a single-electron device simulator, called SIMON. It features the arbitrary connection of tunnel junctions, capacitors, constant voltage sources, piece-wise-linear time-dependent voltage sources and voltage controlled voltage sources. All node voltages, node charges and currents in any branch of the circuit are available for output. Furthermore SIMON features two simulation modes; a transient mode and a quasi-stationary mode. Thus, SIMON is easy to use for single-electron engineering.

2. Simulation method

The circuit description, that the user specifies either with a graphic circuit editor or with a SPICE-like text file, holds the list of connections of the various elements (capacitors, tunnel junctions, voltage sources) and their parameters.

From the circuit description SIMON extracts the capacitance matrix of the network. By exploiting the symmetry of the capacitance matrix, the electrostatic energy U of the circuit can be calculated efficiently. To simulate one time step, the change in free energy for all possible tunnel events is calculated eqn (1). From

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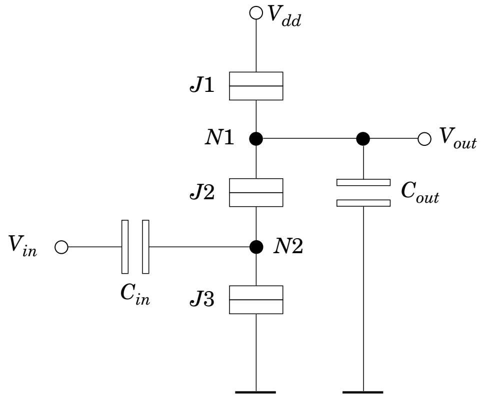

The two stable states are:

V_{in}	V_{out}	$N1$	$N2$
0	$2V_{dd}$	e	0
$2V_{dd}$	0	0	0

Fig. 1. Single-electron inverter proposed by Fukui *et al.* [5].

this free energy change a tunnel rate is derived eqn (2). From the tunnel rate using the model of a Poisson process, a concrete time interval is calculated eqn (3). Finally the event with the shortest time interval is the winner of the Monte Carlo simulation.

The Coulomb blockade is a manifestation of the tunnel rate dependence on the change in free energy. Free energy is the difference of electrostatic energy U stored in the network and work done by voltage sources W.

$$F = U - W. \tag{1}$$

Every time an electron tunnels, the state of the circuit changes. The state of the circuit is determined by the set of all node charges and node voltages. A change in state causes a change in free energy. Since the circuit will tend to a lower energy state, events that reduce the free energy will be more likely.

Once the change in free energy for all possible tunnel events is determined, the tunnel rates can be calculated by [1, 2]:

$$\Gamma = \frac{\Delta F}{q_e^2 R_T \left(1 - \exp\left(-\frac{\Delta F}{k_B T}\right)\right)}. \tag{2}$$

With this information the Monte Carlo part of the simulator is entered. Here ΔF is the change in free energy, k_B is the Boltzmann constant, T is the absolute temperature, R_T the tunnel resistance and q_e the elementary charge.

Tunnelling is modelled as a Poisson process. To every possible event a duration after which an electron will tunnel is chosen randomly. From the probability distribution of the Poisson process one can deduce the following formula [3]:

$$\Delta t = -\frac{\ln r}{\Gamma(T, R_T, \Delta F)}. \tag{3}$$

Here r is an evenly distributed random number in the interval [0, 1], $\Gamma(T, R_T, \Delta F)$ is the tunnel rate depending on temperature T, the tunnel resistance is R_T and the change in free energy is ΔF. The winner is the tunnel process with the shortest time Δt. This calculation of tunnel rates, time intervals and winners is done many times to either simulate the transient behaviour of the network or to determine quasi-stationary characteristics by averaging over many events.

During the process of calculating the electrostatic energy, all node voltages and node charges are determined. The user specifies which ones are output to data files. Only the branch currents that the user is interested in are calculated and output.

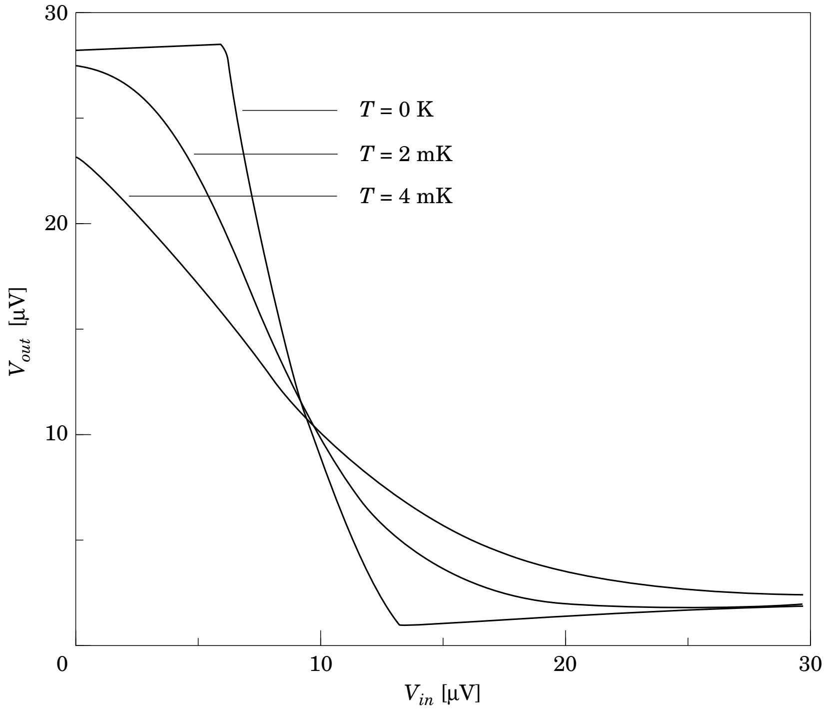

Fig. 2. Transfer characteristic of the inverter.

3. Assumptions of the model

The first significant assumption is that voltage sources are considered to have no internal resistance. Consequently, charging and discharging of capacitances occurs instantaneously.

The second assumption is that the simulator treats electrons as point charges that hope from island to island via tunnel junctions. In other words, the electron states must be localized. This requires all tunnel resistances R_T to be much larger than the quantum resistance R_q [4]

$$R_T \gg R_q = \frac{h}{q_e^2} \approx 25.8\ \mathrm{k}\Omega. \tag{4}$$

Here h is Planck's constant and q_e is the elementary charge.

4. Example

To illustrate the usage of SIMON and to show transient and quasi-stationary simulation modes we show results of a single-electron inverter proposed by Fukui *et al.* [5].

Figure 1 shows the circuit diagram of the inverter. For a low input voltage V_{in}, a positive charge sits on island N1 and zero charge on island N2 and the output voltage V_{out} is high. For high input voltage, both islands have zero charge and the output voltage is low. One can picture the transition from low input voltage to high input voltage as the lowering of the Coulomb blockade at island N2 so that the positive charge on island N1 can go via junction J2 and J3 to ground.

Figure 2 gives the inverter characteristic for different temperatures. Figure 3 shows the input voltage V_{in} and Figs. 4 to 6 show the transient behaviour of the output voltage V_{out} that corresponds to the input voltage

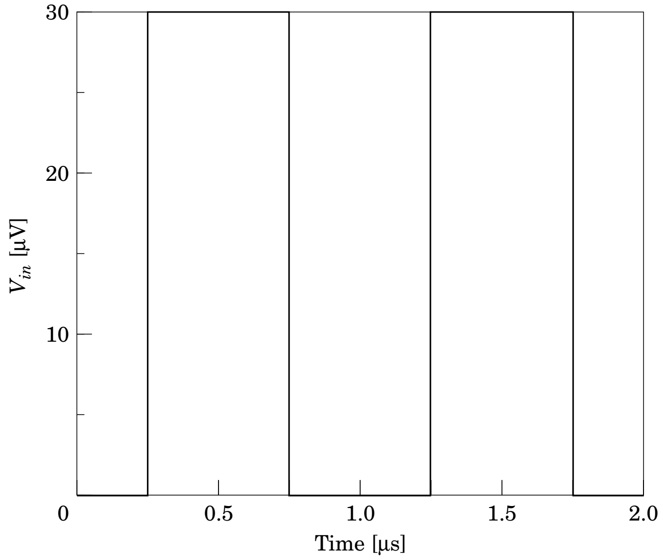

Fig. 3. Inverter input voltage.

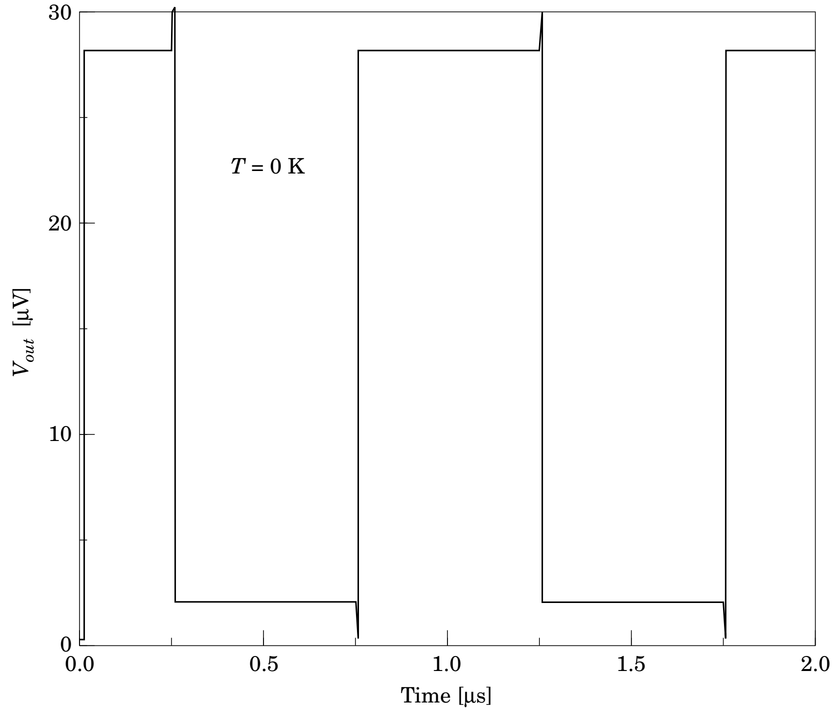

Fig. 4. Inverter output voltage for $T = 0$ K.

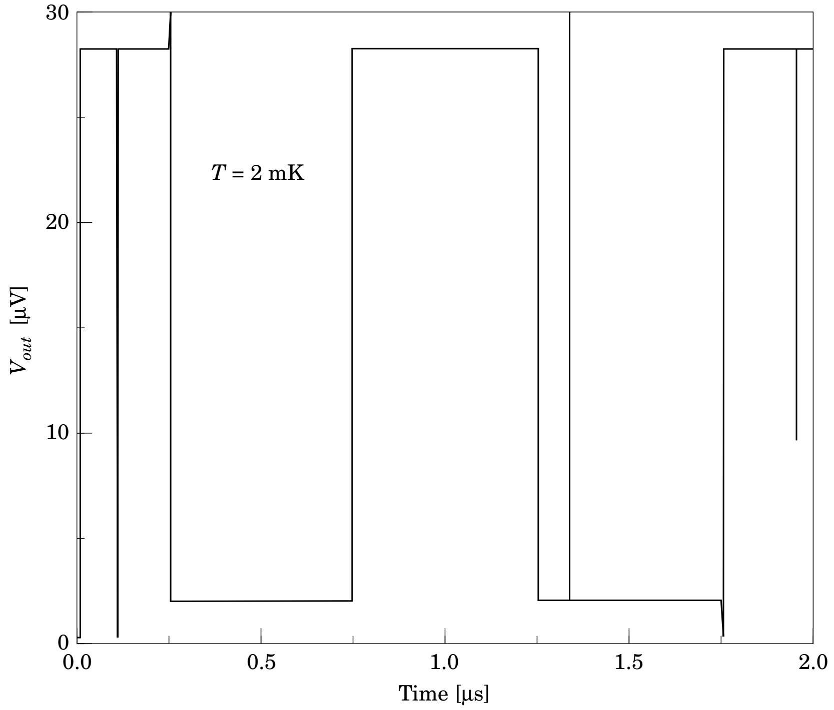

Fig. 5. Inverter output voltage for $T = 2$ mK.

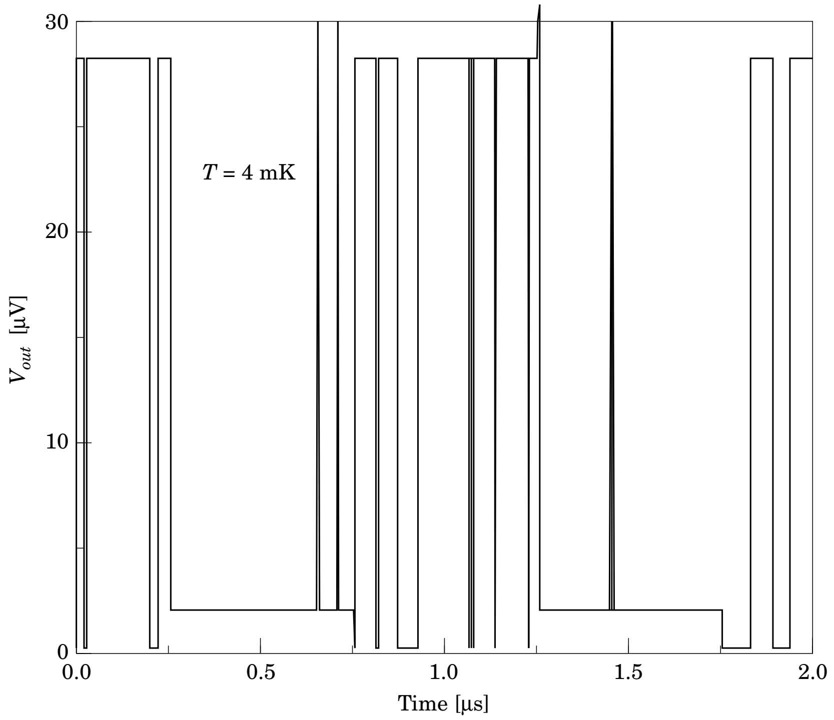

Fig. 6. Inverter output voltage for $T = 4$ mK.

of Fig. 3, for 0 K, 2 mK and 4 mK, respectively. For non-vanishing temperatures the inverter shows errors. The high output state is more error prone than the low output state (see Fig. 6).

5. Conclusion

With SIMON one has an easy to use simulation tool, which makes it possible to study a wide range of single-electron devices and circuits. The recently added graphic user interface and graphic circuit editor makes the simulator even easier to use for single-electron circuit engineering.

The two major reasons for failure of circuit designs are thermal energy and co-tunnelling [6, 7]. We are presently working to add co-tunnelling to the model used in SIMON. Once this is added, it will allow us to calculate error rates with SIMON.

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