# Current Fluctuations Originating from Non-Metallic (Physical) Leads

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## I. OVERVIEW OF THE PROBLEM

The modelization of the conductance in nanoscale systems requires the consideration of overall charge neutrality and current conservation[1,2]. Imposing overall charge neutrality assures that unbalanced charges at the borders of the active region bring about the correct voltage drop along the leads and reservoirs through the Poisson equation. In addition, the total (particle and displacement) current in the active region must be equal to the total current measured on the surface of an ammeter located far away from the active region, in the reservoir, i.e. current conservation.

### The conservation of the electrical current

The conservation of the electrical current, i.e. the total (conduction plus displacement) current computed on a surface in the simulation box is equal to the total current measured on a surface of an ammeter located far from the sample, is a necessary requirement for the prediction of ac conductances, specially at high frequencies. The explicit consideration of the displacement current assures that the total current density is a divergenceless vector. Important theoretical contributions were done by Büttiker and co-workers for predicting ac properties of mesoscopic systems within a frequency-dependent scattering matrix formalism, in weakly nonlinear regimes[1,3].

### The overall charge neutrality

The importance of overall charge neutrality, i.e. that the total charge in the whole device is zero, was clarified by the work of Landauer, Büttiker, and co-workers[4] on the "two-terminal" and the "four-terminal" conductance of ballistic devices. The well-known standard textbook expression of the dc (zero-temperature) conductance through a tunneling obstacle is known as the two-terminal equation because it is defined as the current divided by the voltage drop sufficiently far from the obstacle. However, the original formulation of the conductance proposed by Landauer[5] in 1957 was known as the four-terminal conductance because its experimental validation needs two additional voltage probes to measure the voltage drop close to the tunneling obstacle. The presence of resistances in the leads explains the difference between both expressions. The ultimate origin of such resistances is the requirement of overall charge neutrality that transforms unbalanced charges in the leads into a voltage drop via the Poisson (Gauss) equation. As a relevant example of their deep understanding of time-dependent mesoscopic scenarios, they predicted the value of the resistance in a quantum RC[6] which has been recently experimentally confirmed[7].

### Quantum transport models

Electron-transport models do include reasonable approximations that guarantee the accomplishment of the overall charge neutrality requirement. In addition, those simulators that are developed within a time-dependent or frequency-dependent framework can also assure the current conservation requirement. However, the expensive treatment of quantum and atomistic effects can only be applied to a very limited number of degrees of freedom. In fact, a very small simulation box is a mandatory requirement in modern electron transport simulators. Small means here that the leads, the spatial region separating ideal metallic conditions from the active region of the electronic device, are excluded from the simulations. For most circuit designs it can be assumed that the leads do not contribute to the electrical effects of individual components. This assumption, however, begins to break down at high frequencies and very small scales. Capacitances between the ends of the leads where they connect to the device and inductances and resistances along them can become important at high frequencies and even crucial when trying to predict the noise performance of such devices.

## II. CHALLENGES

In principle, the problem of excluding the leads from the simulation box could be solved by providing adequate boundary conditions (BCs) on each of the "open" borders of the simulation box[8]. Unfortunately, at far from equilibrium conditions, neither the charge density, the electric field nor the scalar potential have easily predictable values at the borders of the active region, specially when an external time-dependent field is being applied[9]. Among several attempts to formulate accurate BCs that reach both overall charge neutrality and current conservation none is accurate enough to capture far from equilibrium conditions. Moreover, the performance of these algorithms for time-dependent scenarios is usually even worse.

Based on the recent development of a time-dependent BCs algorithm that is able to preserve both current conservation and overall charge neutrality[10,11], in this conference we will present new insights into the time-dependent fluctuations of electrical characteristics that arise from the assumption of a more realistic contact model. We will focus, in particular, on the current fluctuations originating from finite screening lengths in molecular devices operating under the effect of an external electromagnetic field[12].

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