Boundary conditions for nanoscale electron devices with realistic lead-sample Coulomb correlations in small simulating boxes

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Most quantum electron transport simulators use small simulation boxes implying a reduction of the degrees of freedom that are explicitly simulated. Nevertheless, the separation between the simulated degrees of freedom (electrons inside the simulation box) and those that are not simulated is always traumatic because there are correlations (interchange of energy and particles) between the active region and the leads. The importance of such correlations in electron transport was discussed in dc and ac regimes some years ago [1,2] but it has been ignored in most of the powerful quantum simulators, which have to use very small simulation boxes [3]. In this conference, we will present an accurate model of such lead-sample coulomb correlations valid for small simulating box by properly modelling the boundary conditions (BC). Instead of assuming the standard Neumann (i.e. a fixed external bias) or Dirichlet (i.e. a fixed zero electric field) BC [4], we propose an original model that does not fix the value of the scalar potential, neither the electric field nor the charge density, but just a time-dependent and self-consistent relationship between them.

As seen in figure 1, our whole BC model differentiates three regions: the two leads which are treated analytically (dotted blue), and the active region which is simulated numerically (solid yellow). Based on screening arguments, the main ingredient of our BC algorithm is imposing that the total charge in the whole system (active region, leads and reservoirs) tends (exponentially) to neutrality within the dielectric relaxation time, τ_c. This condition is equivalent to force that the (analytical) electric fields deep inside the leads (white region in figure 1) tend to its drift value, $E_{Drift} = J_x / \sigma$, within a time τ_c. Appealing to the screening theory, an exponential charge density shape between the leads and the sample can be reasonably argued. Then, the Poisson equation together with the appropriate values of the charge, $\rho(\vec{r},t)$, electric field, $\vec{E}(\vec{r},t)$, and the scalar potential, $V(\vec{r},t)$, deep inside the contacts (white region in figure 1), and in the interface of the analytic-simulated regions, are sufficient to relate this three magnitudes. In particular the scalar potential at the borders of the simulated region, V_{SD} at the source side, and V_{DD} at the drain side, can be finally written as (see figure 1),

$$V_{SD/DD}(t) = V_{SL/DL}(t) - E_{SL/DL}(t)\cdot(L_{Contact}) - \frac{\rho_{SD/DD}(t)\cdot(L_{CS/CD}(t))^2}{\varepsilon}, \qquad (1)$$

The definition of time-dependent screening lengths, $L_{CS/CD}(t)$ at source and drain sides respectively, give rise to formations of depletion regions at high bias that could not been described within an equilibrium screening theory. Even more, our model couples the scalar potential values at the borders of our sample with the injection model [5] through the self-consistent movement of the pseudo-fermi levels, in order to obtain the desired over-all charge neutrality.

In order to test our BC algorithm, in figure 2, we compare the potential energy profiles given by (i) a semi-classical many-particle Monte Carlo (MC) simulator [6] with a large 45 nm simulating box (LBMC) that includes both the leads and the active region, and (ii) the same simulator, provided with the described BC model, with a much smaller 8 nm simulating box (SBMC) that only encloses the active region. While the LBMC simulating times are around 1 day per bias point, the simulation times related to the SBMC decrease until 3 hours. The results of the SBMC are in excellent agreement with those obtained with LBMC even at high applied bias, where exists wide depletion regions. In the quantum regime, the implementation

of our BC model in a quantum trajectory simulator [6,7] is extremely important because it allows us to use small simulating boxes that make a many-particle quantum transport simulation with realistic (far from equilibrium) conditions viable. In figure 3 we compare the characteristic I-V curves for a Resonant Tunneling Diode (RTD) computed with (i) simple fixed Neumman BC and (ii) overall charge neutrality with the BC approach described here that includes the Coulomb correlations between the leads and the active region. As can be observed such correlations play an important role in the relevant parameters of the RTD even at dc regime.

As far we know, our BC approach represents the first model that allows the (computationally desirable) use of small simulating box with the (physically desirable) consideration of the meaningful Coulomb correlations between the active region and the leads. Instead of assuming standard fixed Neumann or Dirichlet BC, the model provides a time-dependent and self-consistent relationship between the value of the scalar potential, electric field and the charge density. The results are excellent without fitting parameters (See fig. 2). Our BC approach is valid for dealing with lead-sample correlations in static and also time-dependent scenarios up to times related to τ_c (i.e. $f \sim 100THz$ for highly doped contacts).

References:

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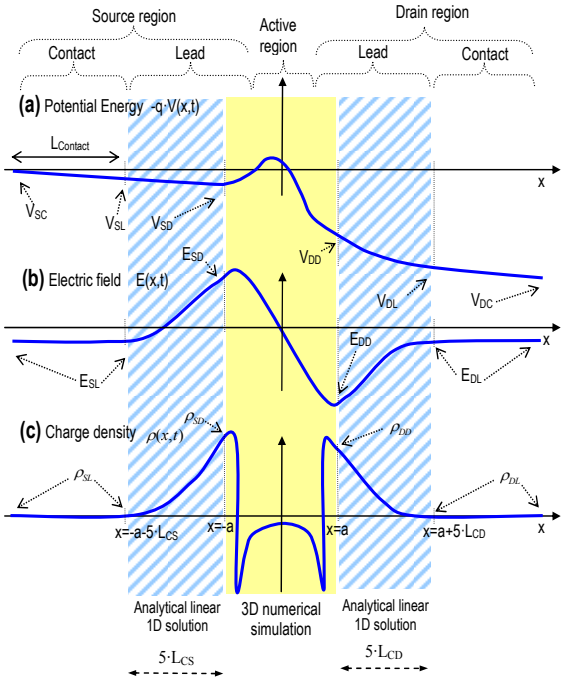

Fig. 1. Schematic description of the model. The whole system is divided into contacts (white), leads (dotted blue) and active region (yellow).

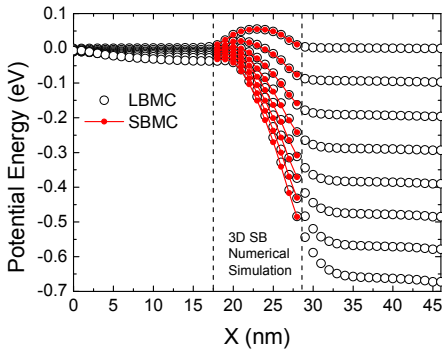

Fig. 2. Potential energy curves at different bias simulated with a LBMC that includes the whole system and a SBMC including only the active region.

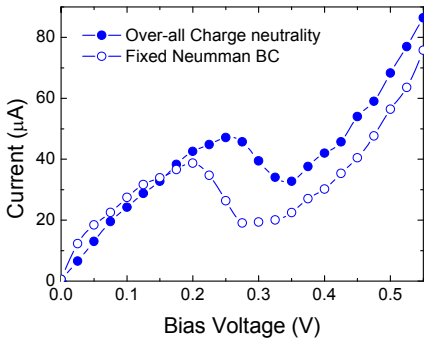

Fig. 3. I-V characteristic for a RTD, with/without including Coulomb correlations between the leads and the active region.