HIGH FREQUENCY MODELING OF CLASSICAL AND QUANTUM NANOSCALE ELECTRON DEVICES

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One of the main interests for decreasing electron device dimensions towards nanoscale dimensions is the possibility of dealing with very short transit times, on the order of few picoseconds or less, envisaging either digital or analog THz applications [1,2]. At these frequencies, the total current depends not only on the rate of electrons crossing a particular surface (i.e. the conduction component), but also on the time-dependent variations of the electric field on that surface (i.e. the displacement current) [3,4]. Thus, the computation of THz currents is a quite difficult challenge because it needs the explicit consideration of the ("many-body" problem) Coulomb interaction among electrons.

We have recently showed a novel accurate method to solve the "many-body" problem in either classical [5] or quantum [6] scenarios. In order to improve our understanding of the total (particle plus displacement) current in nanoscale electron devices, we use our extension of the Ramo-Shockley theorem [3]. Then, the computation of the total current takes into account the whole active region (rather than just a particular surface) through the definition of a new vector function $\vec{F}_i(\vec{r})$ in the volume of the active region [4]. This new vector function provides an additional source of valuable information for understanding and predicting the behavior of THz currents. In particular, the total (particle and displacement) current through a surface "i" of volume of Fig. 1 can be written as:

$$I_i(t) = \Gamma_i^q(t) + \Gamma_i^e(t) = \sum_{a=1}^{N} \vec{F}_i(\vec{r}_a[t]) \cdot q \cdot \vec{v}_a(\vec{r}_a[t]) + \int_S \vec{F}_i(\vec{r}) \cdot \varepsilon(\vec{r}) \cdot \frac{\partial V(\vec{r},t)}{\partial t} \cdot d\vec{s} \qquad (1)$$

The first term, $\Gamma_i^q(t)$, relates the macroscopic THz current with the microscopic electron dynamics where q is the electron charge, $\vec{v}_a(\vec{r}_a[t])$ the a-electron (classical[5] or Bohm[6]) velocity and N is the number of electrons inside the whole active region. The second term, $\Gamma_i^e(t)$, provides information on the temporal variations of the scalar potential $V(\vec{r},t)$ with $\varepsilon(\vec{r})$ the (time-independent) electric permittivity.

In this work, we have simulated the electron transport trough a nanoscale resistor drawn in Fig. 1 within a time-dependent semiconductor Monte Carlo simulation of electron transport. The Coulomb interaction among electrons is computed through the novel many-particle algorithm presented in Ref. [5]. In Figs. 2,3 we show (in solid blue line) the power spectral density of the current fluctuations computed from the Monte Carlo results. In order to improve our understanding of each terms of expression (1), we have developed analytical expressions for the temporal behavior of $\Gamma_i^q(t)$ associated with a transmitted electron (see dashed red line in Fig. 4) and the term $\Gamma_i^e(t)$ associated to the temporal variations of the scalar potential $V(\vec{r},t)$ (see dashed red line in Fig. 5) and compared them with the time-dependent Monte Carlo results. We do also Fourier transform these analytical expressions to compare them with the numerical Monte Carlo results mentioned before (see Figs. 2 and 3) showing an excellent agreement.

This work is a first step towards an accurate understanding of the behavior of THz currents in nanoscale (ballistic) devices that will become a very relevant issue for next generation of THz electronics.

References:

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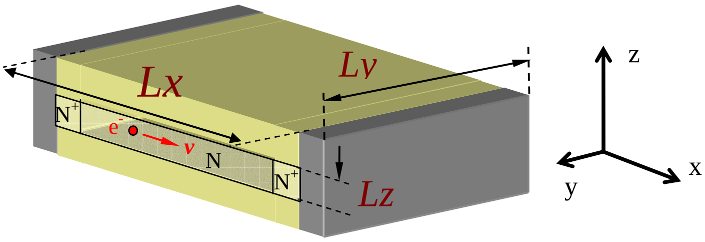

Fig.1. Schematic representation of a two-terminal nano-resistor with doping $N^+ = 2.2\cdot10^{19}$ cm^{-3} and $N = 1\cdot10^{10}$ cm^{-3}. The dimensions of the active region of the device are $Lx\cdot Ly\cdot Lz$ =20x6x6 nm. The total time-dependent current is computed through Monte Carlo simulations during 1.5 ns ($2\cdot10^6$ time steps) when a 1V bias is applied.

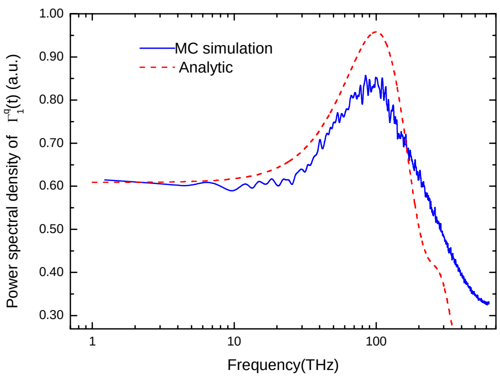

Fig.2. In solid line, power spectral density of the fluctuations of the first term of expression (1) for the device of Fig. 1. In dashed line, analytical approximation obtained from dashed line in Fig 4.

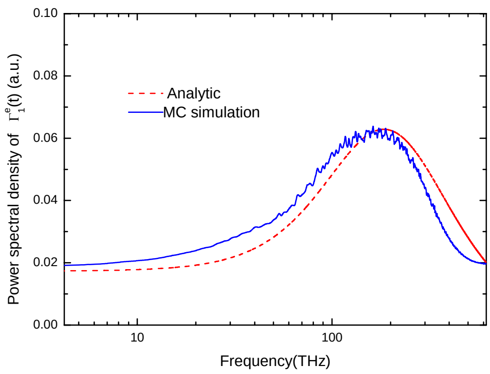

Fig.3. In solid line, power spectral density of the fluctuations of the second term of expression (1) for the device of Fig. 1. In dashed line, analytical approximation obtained from dashed line in Fig 5.

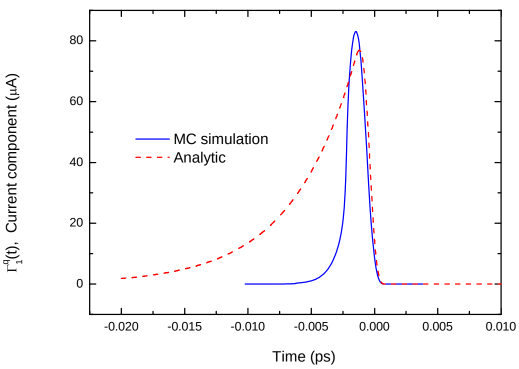

Fig.4. In solid line, zoom of the first term of the time dependent current of expression (1) for the results of Fig. 2. In dashed line, analytical approximation.

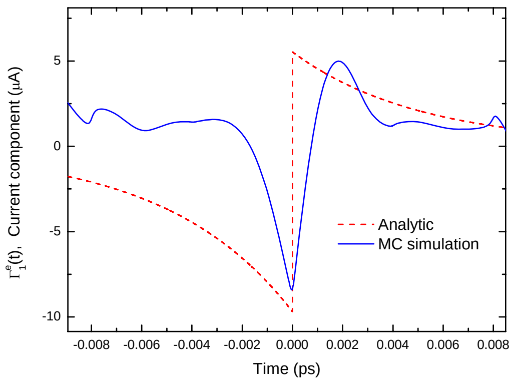

Fig.5. In solid line, zoom of the second term of the time dependent current of expression (1) for the results of Fig. 3. In dashed line, analytical approximation.