

## High frequency resonant tunneling behavior: Testing an analytical small signal equivalent circuit with time dependent many-particle quantum simulations

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Since the pioneering work by Tsu and Esaki [1], resonant Tunneling Diodes (RTDs) have attracted a lot of attention. Their peculiar properties like Terahertz maximum operating frequency and Negative Differential Resistance (NDR), offer a wide range of applications, in either analog (frequency divider or multiplier, oscillator [2]) or digital (“multi-value” logic [3]) circuits. Recently, there is renewed interest in such devices because the progress of Silicon On Insulator (SOI) technology made it possible to build RTD devices on ultra-thin crystalline silicon with thickness lower than 10nm [4] (rather than the common III-V materials).

This work is devoted to an accurate analysis of the frequency behavior of RTDs. Such accurate analysis is a really very difficult task because one has to take into account the Coulomb correlation among electrons to assure (i) **current conservation** (the total current is the sum of the conduction plus the displacement currents due to time-dependent variations of the electric field) and (ii) **overall charge neutrality** (screening deep inside the leads assures that the total charge tends to zero). To the best of our knowledge, this is the first time that a detailed analysis of how conditions (i) and (ii) affects the relevant cut-off frequency of RTD.

We apply two different approaches. The first is a time-dependent Quantum Monte Carlo (QMC) based on many-particle Bohm trajectories [5]. This powerful simulator can include Coulomb correlations self-consistently and it has been used to extract the RTD intrinsic frequency limitation directly from the current response to a small step voltage signal. Such a rigorous approach it is used to understand the RTD behavior and to test an analytical Small Signal Equivalent Circuit (SSEC) [6] (see fig. 1) derived from a DC physics based model [7] following Liu’s approach [8].

To extract information about the different time constants associated to the several processes characterizing the electron dynamics in the RTDs, we accounted for three different conditions employed in NDR regime.

**a) Without conditions (i) and (ii):** we remove self-consistency of the Coulomb interaction in the QMC. The current in the RTD follows the voltage step with an intrinsic delay of about 0,035 ps (see fig. 2). In absence of coulomb interactions, this time is assumed to be equal to the RTD dwell time  $\tau_d$ . In the analytical model  $\tau_d = \hbar/\Gamma$  where  $\Gamma$  is the total width of the resonant level [9]. The value extracted for this structure is 0,03 ps in excellent agreement with QMC. In this case, the SSEC can be simplified by connecting in series a negative conductance  $G$  and a negative inductance  $L$  (see fig. 1 solid blue line). The resulting cutoff frequency of this simple filter is  $2\pi\tau_d = 5$  THz.

**b) With condition (i):** The potential is computed by solving the Poisson equation self-consistently with QMC. In this condition the “simulation box” is very small, thus leads are neglected. The Coulomb interaction can be modeled by a capacitance  $C$  in parallel to  $G$  (see fig. 1 dashed red line). The total capacitance  $C$  account for two contributions, the geometrical capacitance  $C_0$  and the quantum capacitance defined as  $C_q = -G\tau$ . In this case the cutoff frequency of SSEC results of 3.6 THz and it is consistent with the characteristic time (0,25 ps see fig. 3) found with QMC.

**c) With conditions (i) and (ii):** In order to ensure charge neutrality in whole device, the leads have been introduced in QMC consistently with the Poisson equation. Conversely in the small signal circuit, contacts have been included by means of a series resistance (see fig. 1 squared solid line). Thus the cut off frequency of SSEC is now 1,4 THz. This value is in very good agreement with cutoff frequency reduction obtained with QMC (see fig. 4).

We can conclude that several limitations come into play in the frequency response of an RTD, namely the intrinsic tunneling process, the transit time across the non-tunneling regions and time constant associated to the total capacitance of the structure. On the one hand the full time-dependent simulation provides a rigorous picture of the physics that governs the frequency behavior of RTD. On the other hand, our study shows that the equivalent small signal circuit is able to catch characteristic times, resulting a useful tool to design RTD.

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