BITLLES: a quantum-trajectory simulation tool for electron transport in large electronic structures

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With the aim of manufacturing smaller and faster devices, the electronic industry is today entering the nano and picosecond scales. In such particular scenarios, electron dynamics becomes affected by strongly correlated quantum dynamics, both in space and time. Thus, in order to provide an enough accurate description of the electron-electron correlations, quantum transport simulators must consider a reasonable approach to the many-particle problem. Anyway the big deal concerns the solution of the many-particle Schrödinger equation nowadays solvable only for very few degrees of freedom.

In this work we present a general purpose time-dependent 3D quantum electron transport simulator based on Bohmian trajectories that we call **BITLLES** [1-3]**.** It is based on a recently published algorithm [1] that, on the grounds of Bohmian Mechanics [2], solves the many-particle Schrödinger equation for hundreds of electrons in terms of multiple single-particle pseudo-Schrödinger equations without losing the explicit Coulomb and exchange correlations among electrons (at a level comparable to the Time Dependent Density Functional Theory) [1-4].

The code of the **BITLLES** simulator is currently made up of more than 15000 FORTRAN lines (see the algorithm in Fig.1). It has also a 3000 C++ lines for a (Windows, MAC and Linux compatible) user friendly environment to design an verify the simulated electronic structures (see Fig. 2). The computational burden associated with the solution of the self-consistent many-particle 3D Poisson-Schrödinger loops involves large simulation times. For example, one week for the complete I-V curve (DC, AC and noise) with a cluster of 24 Intel Xeon CPUs at 2.7GHz.

Same examples of the numerical viability of the **BITLLES** simulations are provided below for a Resonant Tunneling Diode (RTD). Its characteristic I-V curve with Coulomb correlations introduced at different approximation levels is plotted in Fig. 3 [3,5]. Many-particle tunneling phenomena are reveled in the (super-Poissonian) behavior of the Fano factor shown in Fig. 4 [2]. Finally, in Figs. 5 and 6 we show the transient (time-dependent) current response and its Fourier transform respectively, when a voltage step is applied in the negative differential conductance region.

References

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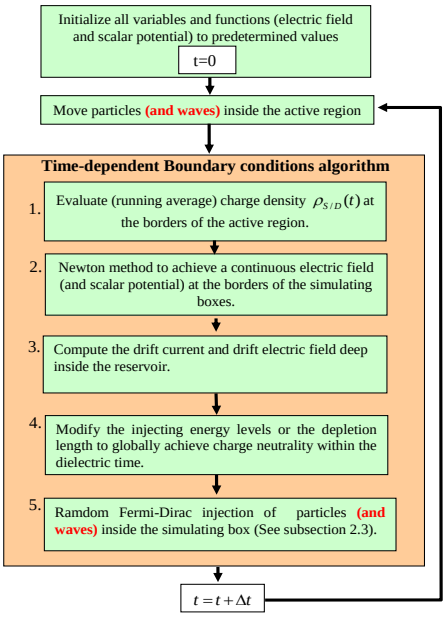

Fig. 1. General algorithm describing the fundamental routines defining the BITLLES simulator.

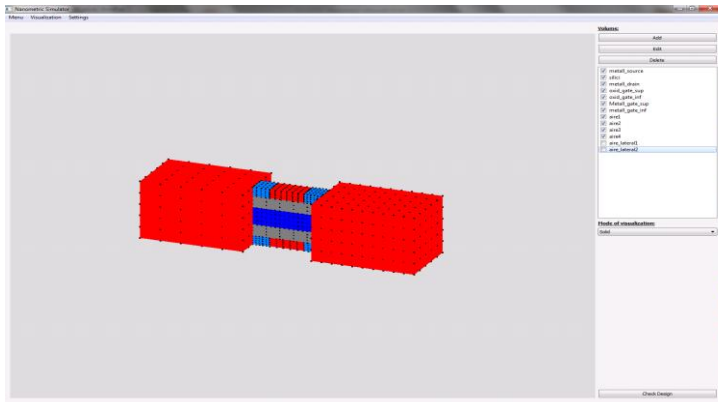

Fig. 2. Very recently BITLLES has been provided with a user friendly interface.

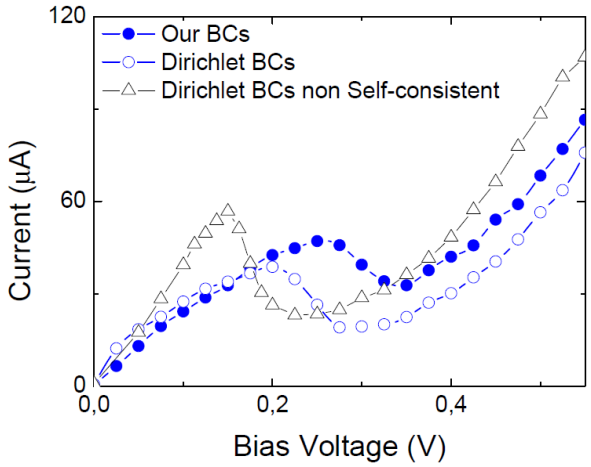

Fig. 3. DC Current for a RTD with Coulomb correlations introduced at different levels of accuracy.

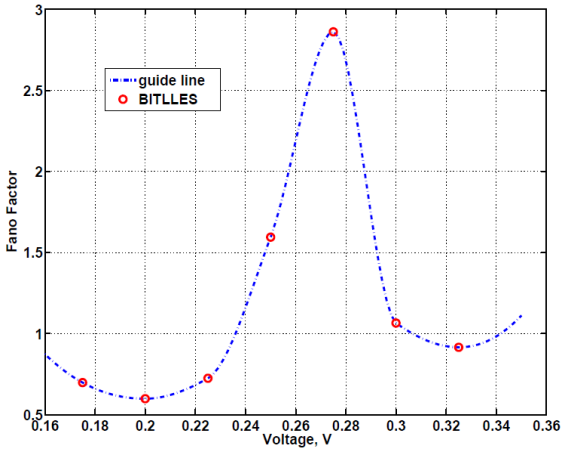

Fig. 4. Fano Factor computed for the RTD of Fig. 1 computed directly from the (time-dependent) current fluctuations.

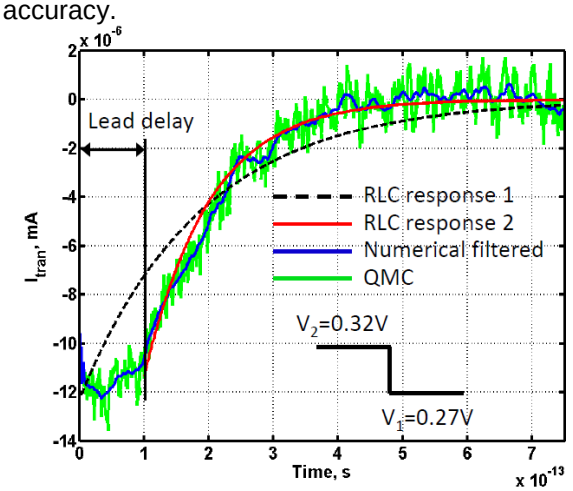

Fig. 5. Current response of the RTD to a step input voltage. Self-consistent boundary conditions including the leads are used.

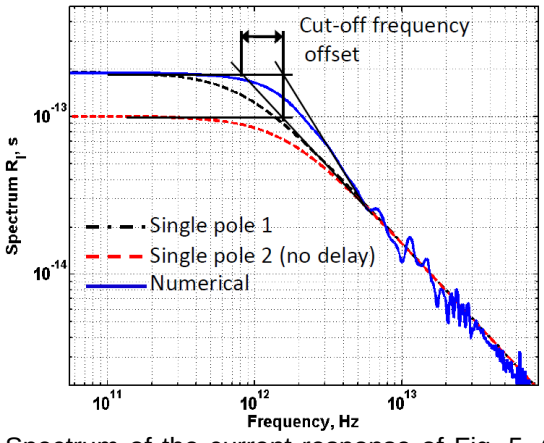

Fig. 6. Spectrum of the current response of Fig. 5. Cut off frequency and its offset due to the lead delay are pointed out.