BITLLES: a quantum trajectory simulator for DC, AC, and noise with explicit Coulomb and exchange correlations among transport electrons

G. Albareda, A. Alarcón, F. L. Traversa, A. Benali, and X. Oriols

Dept. d'Enginyeria Electrònica, Universitat Autònoma de Barcelona, 08193 Bellaterra, Spain
guillem.albareda@uab.cat

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 accurate enough 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) [1-3].

The adaptation of Bohmian mechanics to electron transport leads to a quantum Monte Carlo (MC) algorithm, where randomness appears because of the uncertainties in energies, initial positions of (Bohmian) trajectories, etc [2-4]. The ability of our simulator to deal with strongly correlated systems is shown here for a Resonant Tunneling Diode (RTD). Its characteristic I-V curve with Coulomb correlations introduced at different approximation levels is plotted in Fig. 1. As it can be observed, the effect of the correlations appear not only in the magnitude of the current but also in the position and shape of the resonant region [3,5]. Many-particle tunneling phenomena are reveled in the (super-Poissonian) behavior of the Fano factor shown in Figs. 2 and 3 [2]. In Fig. 4, we show the achievement of current continuity in the computation of the AC current for the same RTD [6]. The (time-dependent) current response to a voltage step is shown in Figs. 5 and 6.

References

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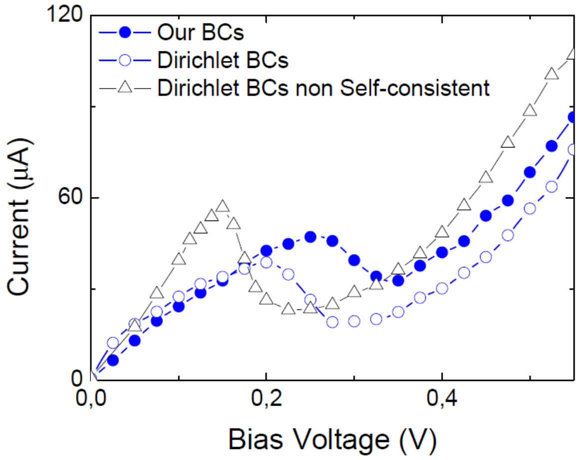

Fig. 1. DC Current for a RTD with Coulomb correlations introduced at different levels of accuracy.

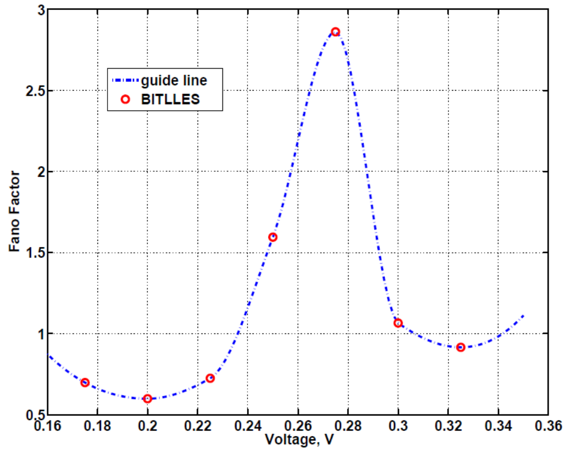

Fig. 2. Fano Factor computed for the RTD of Fig. 1 computed directly from the (time-dependent) current fluctuations.

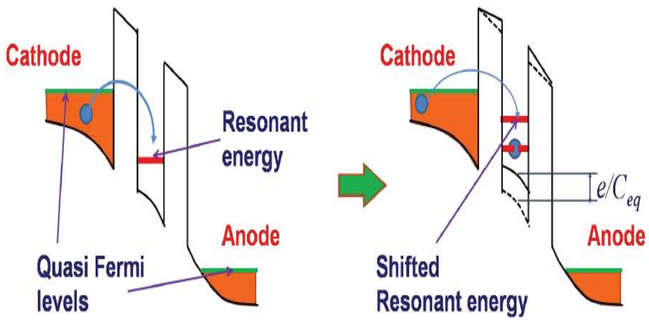

Fig. 3. RTD Band diagram. The potential deformation due to many-particle tunneling in the well is the basic mechanism of super-poissonian noise.

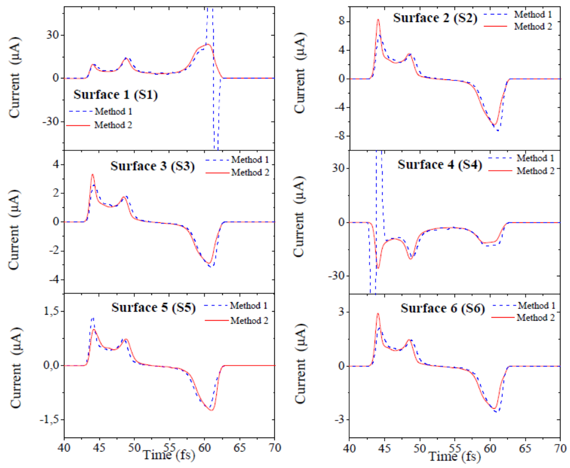

Fig. 4. Time-dependent total current computed on the six surfaces of an arbitrary parallelepiped. The sum of the current on the six surfaces is zero demonstrating the achievement of overall current continuity.

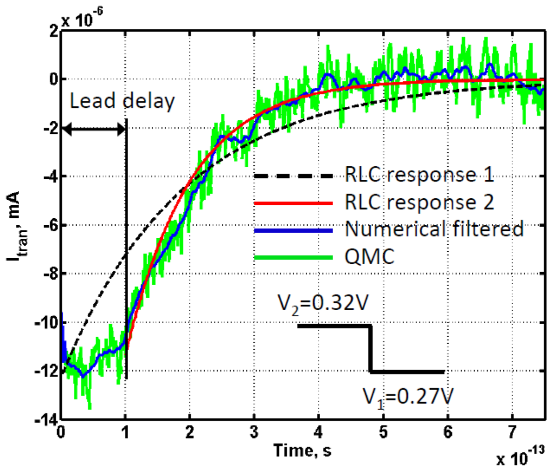

Fig. 5. Current response of the RTD to a step input voltage. Self-consistent boundary conditions including the leads are used.

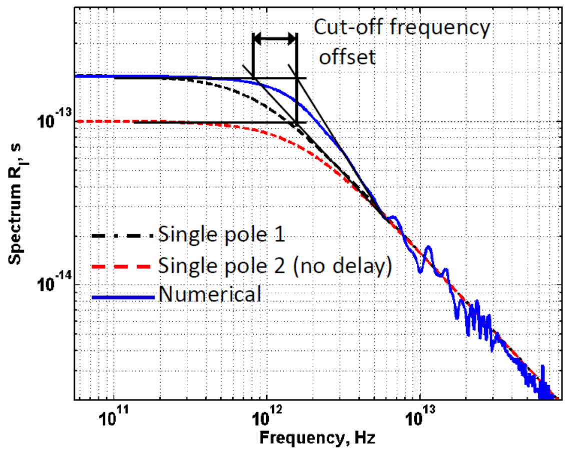

Fig. 6. Spectrum of the current response of Fig. 5. Cut off frequency and its offset due to the lead delay are pointed out.