Multi-time measurement and displacement current in time-dependent quantum transport

X.Oriols, F.L.Traversa, G.Albareda, A.Benali, A. Alarcón, S. M. Yaro, X.Cartoixà
Dept. d'Enginyeria Electrònica, Universitat Autònoma de Barcelona (UAB)
E-mail: xavier.oriols@uab.es

INTRODUCTION

Predicting dynamic (AC, transient, noise, etc.) properties of quantum devices is much more complicated than DC ones, mainly because of two reasons. First, a multi-time measurement of the current is needed when computing dynamic properties, which implies discussing the (non-unitary) time-evolution of the quantum device each time when the current is measured. On the contrary, this issue is not relevant for the (ensemble) DC computation of the current, because only a single-time measurement is needed. Second, understanding the time-dependent behavior of electron devices implies dealing with conduction plus displacement currents. The consideration of the displacement current requires, in turn, the time-dependent solution of the many-particle Schrödinger equation. On the contrary, only the conduction current is needed for DC predictions because the displacement current is zero when averaged over a sufficiently large interval of time.

For these reasons, the proper simulation of the AC, transients and current fluctuations (correlations) of quantum devices is still a very challenging task for the scientific community, both, from a physical and computational point of view.

THE BITLLES SIMULATOR: AC, TRANSIENTS AND CURRENT FLUCTUATIONS IN QUANTUM DEVICES

Among other recent proposals for the time-dependent simulation of quantum transport, in this conference, we present the BITLLES simulator [1]. It is a general, versatile and powerful time-dependent 3D electron transport simulator based on the use of the *conditional* wave function: a many-particle wave function where some degrees of freedom are substituted by quantum (Bohmian) trajectories [2]. The adaptation of (Bohmian) *conditional* wave functions to electron transport leads to a quantum Monte Carlo algorithm, where randomness appears because of the uncertainties in energies, initial positions of the (Bohmian) trajectories, etc [2]. Next, we briefly discuss how the BITLLES tackles the two issues introduced above, showing the capabilities and numerical viability of the simulator.

The many-particle Schrödinger equation can only be solved for very few degrees of freedom. This is at the heart of most of the unsolved problems in quantum transport. We have recently shown that Bohmian trajectories allow a direct treatment of the many-particle interaction among electrons [3] with an accuracy comparable to DFT techniques. The ability of our BITLLES simulator to deal with strongly correlated systems is shown for a Resonant Tunneling Diode (RTD). Many-particle tunneling phenomena are present in the (super-Poissonian) value of the Fano factor plotted in Figs. 1 and 2. See Refs. [4] and [5].

In principle, due to the use of Bohmian trajectories, the multi-time measurement of the current is easily introduced into the BITLLES when the ammeter-system interaction is negligible, as seen in Fig. 3. In other scenarios, some (non-unitary) deformation of the wave function is required each time when the current is measured [2]. This is achieved in the BITLLES through a *weak measurement* modeling of the ammeter-system interaction [2]. In Fig. 4, we show the AC current (computed from the Ramo-Shockley-Pellegrini theorem) in the six surfaces of a parallelepiped fulfilling the current continuity requirement [6]. The (time-dependent) transient current response to a voltage step is shown in Figs. 5 and 6. See [7].

ACKNOWLEDGMENT

This work has been partially supported through MEC project MICINN TEC2009-06986.

REFERENCES

[1] *http://europe.uab.es/bitlles*
[2] X.Oriols and J.Mompart, *Applied Bohmian Mechanics: From Nanoscale Systems to Cosmology*, Editorial Pan Stanford (2012).
[3] X. Oriols, *Quantum trajectory approach to time dependent transport in mesoscopic systems with electron-electron interactions*, Phys. Rev. Let. **98**(6), 066803, (2007).
[4] G. Albareda, H. López, X. Cartoixà, J. Suñé, X. Oriols, *Time-dependent boundary conditions with lead-sample Coulomb correlations:Application to classical and quantum nanoscale electron device simulators*, Phys. Rev. B, **82**, 085301, (2010).
[5] G. Albareda, J. Suñé, and X. Oriols, *Many-particle hamiltonian for open systems with full coulomb interaction: Application to classical and quantum time-dependent simulations of nanoscale electron devices*, Phys. Rev. B. **79**, 075315, (2009).
[6] A.Alarcón and X.Oriols, *Computation of quantum electron transport with local current conservation using quantum trajectories*, Journal of Statistical Mechanics: Theory and Experiment. P01051, (2009).
[7] F.L.Traversa *et al. Time-Dependent Many-Particle Simulation for Resonant Tunneling Diodes: Interpretation of an Analytical Small-Signal Equivalent Circuit* IEEE Transaction on Electron Devices, **58**, 2104 (2011).

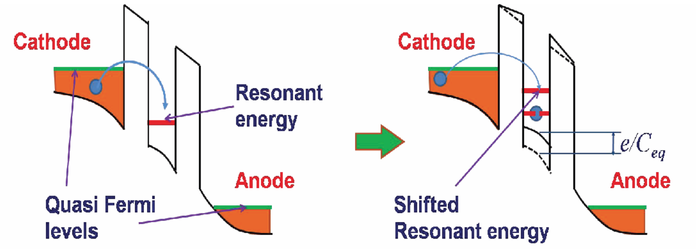


Fig. 1. RTD Band diagram. The potential deformation due to many-particle tunneling in the well is the basic mechanism of super-poissonian noise of Fig. 2.

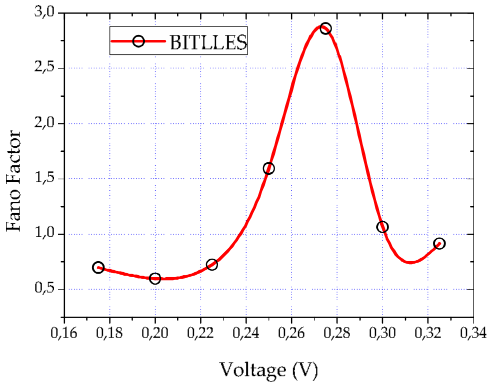


Fig. 2. Fano Factor of the RTD of Fig. 1 computed directly from the (time-dependent) current fluctuations provided by BITLLES.

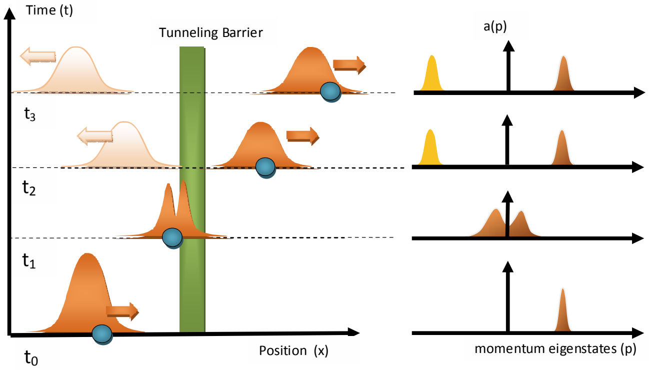


Fig. 3. (Left) Time-evolution of a (single-particle) wave-packet impinging upon a barrier. The transmitted and reflected wave-packets are spatially separated at times t2 and t3. (Right) representation of the probability of the momentum eigenstates, a(p), at different times.

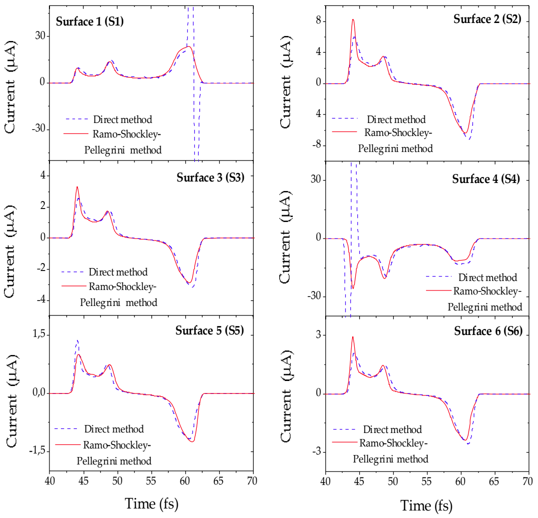
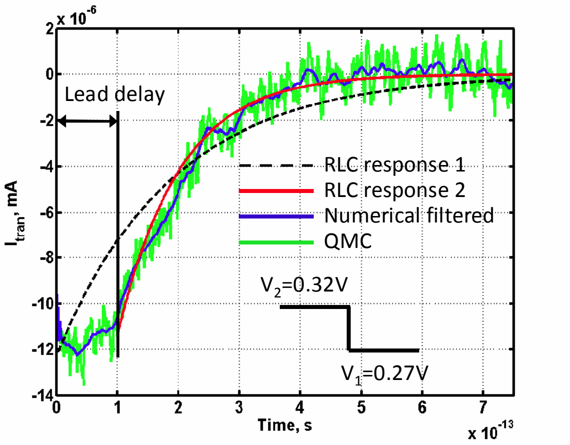


Fig. 4. Time-dependent total (conduction plus displacement) current computed on the six surfaces of an arbitrary parallelepiped. The sum of the current on the six surfaces is zero demonstrating the achievement of overall current continuity.



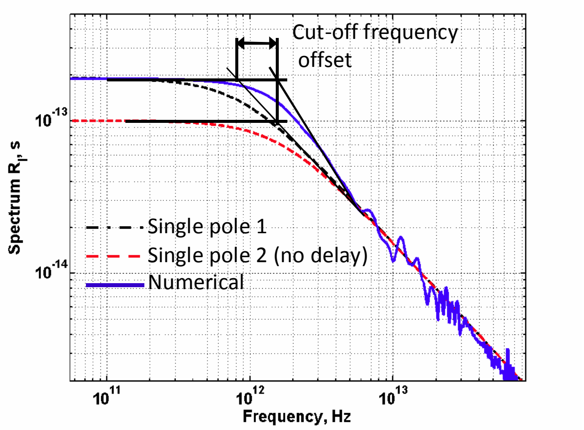


Fig. 5. Current response of the RTD to a step input voltage. Self-consistent boundary conditions including the leads are used.

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