

## International Workshop on Computational Nanotechnology

### P:27 Do we really need the collapse law when modelling quantum transport in electron devices?

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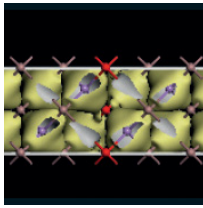
A well-known challenge in quantum theory is the description of the measurement process [1,2]. After more than one century since the birth of quantum mechanics, this fundamental problem still remains timely. In fact, our basic conception of quantum reality depends on how we ultimately solve this problem. The usual formulation of quantum mechanics (the so-called orthodox theory) argues that two fundamental laws describe the evolution of any system: (i) a unitary and linear law (given for example by the Schrödinger equation) when the system evolves without being measured and (ii) a non-unitary and non-linear law (the so-called collapse law) when it is being measured.

In principle, the correct modelling of any electron device within the orthodox theory requires including both laws. However, there is a large list of quantum transport models in the literature that do not treat explicitly the collapse law, but they only include analytical or numerical solutions of the Schrödinger (parabolic band structure) or Dirac (linear band structure) equations. Notice that it is well-known that the measurement problem cannot be generally solved in a quantum system by invoking decoherent phenomena (like phonon or impurity collisions) alone. One of the reasons that can explain why the measurement problem is usually forgotten in the quantum modelling of electron devices is that there is no such problem in classical or semi-classical modelling.

In this conference we will explain for which type of observables we can expect to induce erroneous predictions of the performance of quantum devices when neglecting the measurement problem. Based on ergodic arguments, the DC performance of quantum devices does not require the post-evolution of the system after measurement and the collapse law can be ignored (like in the successful Landauer model). However, the computation of (zero or high frequency) noise through the correlations of the measured currents at different times requires the inclusion of the collapse law (see Figs. 1 and 2). Similarly, for high frequency (AC) predictions beyond the quasi-static approximation, where a multi-time measurement of the current is necessary, the collapse law plays also a significant role (see Figs. 3).

In this conference we will also argue that there exist alternative valid theories that allow us to solve the measurement problem in a rather trivial manner [2-5]. For example, in addition to the wavefunction, Bohmian theory introduces well defined quantum trajectories in the description of a quantum state. In this way, this theory is able to solve the measurement problem without the need of invoking the collapse law. Following these ideas, the group of Dr. Oriols has developed a quantum electron transport simulator, the so-called BITLLES simulator [6], that can be used to model the DC, AC or high-frequency performance of any quantum device without the need of any further conceptual difficulty associated to the quantum measurement problem [2-4] (see Figs. 1, 2, 3).

In summary, we provide two answers to the question posed in the title. First, if you want to use the orthodox theory to provide noise and AC predictions beyond the quasi-static approximation you do effectively need the collapse law. Contrarily, the answer is no if you choose to model your quantum device with an alternative formulation of quantum mechanics. For example, within Bohmian mechanics, a general purpose simulator can be developed to provide DC, AC and noise performances of state-of-the-art nanoscale devices without the need of invoking the collapse law [2-4].



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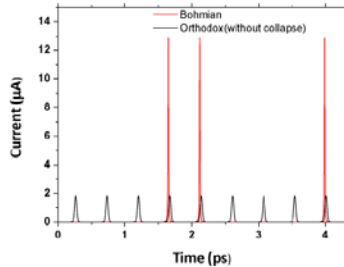


Fig1. Time dependent simulation of the electrical current measured in the collector terminal of a RTD device for a constant flux of injected electrons (all with the same energy) impinging upon a double barrier. The transmission coefficient is  $T=0.436$ . Two different models are used in the current computation: (i) (in black) we use the orthodox model without collapse law to compute quantum transport by just solving the time-dependent solution of the Schrödinger equation. (ii) in red, a Bohmian solution which uses the orthodox wave function plus trajectories that include the randomness of the measurement problem by the selection of the initial position of the trajectory that determines if the electron is either transmitted or reflected. The charge transmitted in each pulse is the average value  $qT$  (being  $q$  the electron charge) in the first model and  $q$  or  $0$  in the second one. Notice that the average results (DC current) of both models are identical.

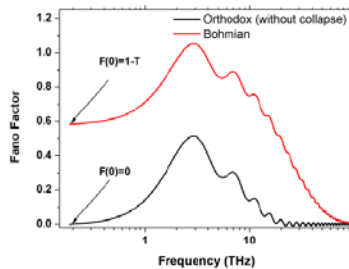


Fig.2 The noise of the electrical current corresponding to the two transport models considered in Fig 1. Fano factor,  $F(0)=S(0)/(2qI)$ , defined as the power spectral density at zero frequency  $S(0)$  divided by the average current  $I$  and the electron charge  $q$ , is plotted. The first model (black line) provides zero noise at low frequency  $F(0)=0$  since there is no randomness in its current in Fig. 1. Notice that the Schrödinger equation alone (without the collapse law) is a deterministic equation without randomness. The second model (red line) provides a Fano factor equal to  $F(0)=1-T=0.564$  due to the randomness of its current seen in Fig 1. The value corresponds to the well-known result of the fluctuations in the current due to the tunnelling barrier with transmission coefficient  $T$  (such process follows a Binomial probability distribution with probability equal to  $T$ ). Notice the differences in the spectrum of the noises of both models at either zero or high frequencies.

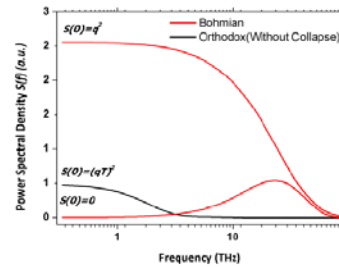


Fig.3 Power spectral density  $S(f)$  corresponding to the simulation of one single electron of figure 1 (not a constant flux) computed with the two models considered in this work. Since transmitted and reflected particles have the same description in the first model (black line) only one plot is represented. In the second model (red lines), we plot  $S(f)$  corresponding to a reflected particle and another  $S(f)$  for a transmitted one. At zero frequency, when a large flux of particles is considered, both models provide the same average value of  $S(0)$  which corresponds to the DC results. The two red lines averaged by the transmission coefficient corresponds to the black line at  $S(0)$ . However, at high frequency, important differences remain. As seen in figure 1, the result of the second model corresponds to thinner and higher current pulses that are later translated in the presence of  $S(f)$  at higher frequencies in the power spectral density.

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