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A Many-Particle Quantum-Trajectory Approach for Modeling Electron Transport and its Correlations in Nanoscale Devices

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ABSTRACT

A new approach for modeling quantum transport that explicitly takes into account the electron-electron interaction is presented. The approach is based on the computation of transport properties of many-particle systems using quantum trajectories.

INTRODUCTION

The coulomb interaction (due to the charge of the electron) and the exchange interaction (due to its fermion nature) are always present in any electron device. The role of both interactions can be obtained by directly solving the many-particle Schrödinger equation. However, due to computational limitations, its direct solution is only possible for a very limited number (N<5) of electrons. Therefore, much of our understanding of electron transport is based on a single-particle ("mean field") approximations [1]. In this conference, we will present a new approach for the modeling of quantum transport that overcomes this assumption by dealing with many-particle effects using quantum (Bohm) trajectories [2].

MANY-PARTICLE TRANSPORT PROPERTIES IN TERMS OF QUANTUM TRAJECTORIES

It is well-known that Bohm trajectories exactly reproduce the results obtained from, either the single- or many-particle Schrödinger equation [3,4]. However, the application of such trajectories to transport has been quite limited because the computation of these trajectories needs, in general, the earlier knowledge of the full wave-function.

In this conference, we show that a Bohm trajectory associated to a many-particle Schrödinger equation can be computed from a wave-function, $\Psi_b(\vec{r}_b,t)$, solution of the single-particle Schrödinger equation (with a complex unknown potential) [2]. Thus, the practical computation of Bohm trajectories in a system of N-interacting electrons can be greatly simplified. The electron-electron interaction is introduced in the computation of Bohm trajectories by taking into account the exact Coulomb force between pairs of electrons and the applied bias at the boundaries of the device. Thus, Identical bias with different lateral areas ($L_y \cdot L_z$), provide different strength of the interaction. The exchange-interaction needs the simulation of N^2 Bohm trajectories to assure the antisymmetrical behavior of the wave-function. Figs. 1, 2 and 3, show the accuracy of our approach (blue □) when compared to the exact two-particle Schrödinger solutions (red Δ).

CURRENT AND NOISE OF INTERACTING-SYSTEMS

The computational viability of the previous many-particle Bohm-trajectories formalism for is shown in Figs. 4 and 5 where $N \approx 50$ interacting-electrons are simulated. Since we are dealing with electron trajectories, most of the tools used in Monte-Carlo simulator can be directly adapted. In Fig. 4 and 5 we show how the (average) current and the (Fano factor) noise are sensible to electron-electron interactions. Such interactions provide correlations among electron dynamics that can not be simulated with independent-electron formalisms.

CONCLUSION

A new approach for modeling quantum transport that explicitly takes into account the Coulomb and exchange interactions is presented. The approach opens a new path to provide a deeper understanding of nanoscale devices, since it can directly provides information on DC, AC and noise performances of interacting-electrons phase-coherent systems [5,6].

REFERENCES

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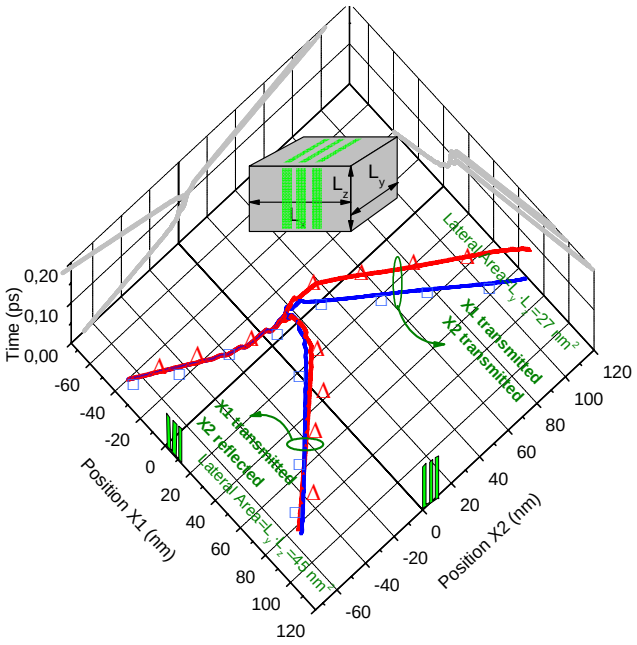

Fig. 1. Two Bohm trajectories in a two-particle configuration space (X1,X2,t) with identical initial positions but different lateral area. Only the Coulomb interaction determines (X1=trans., X2=trans.) or (X1=trans.,X2=reflc). In red (Δ), exact Bohm trajectories from a two-particle Schrödinger equation and, in blue (□), our approach. Inset: 3D device dimensions (transport in x direction). The triple-barrier region is indicated.

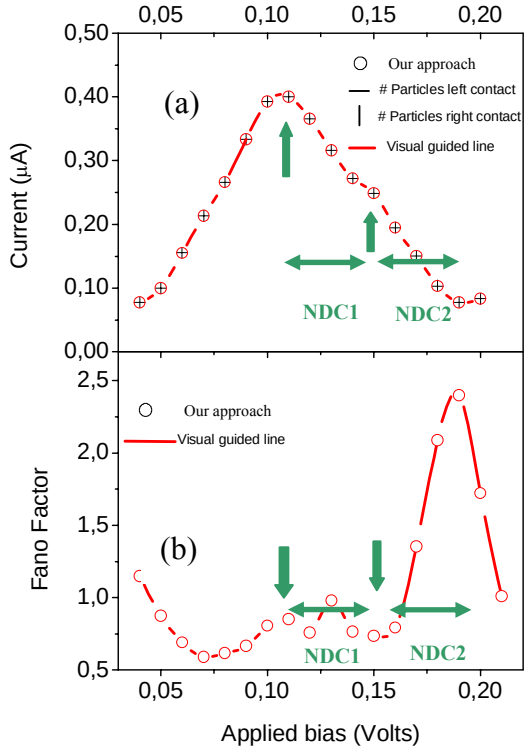

Fig. 4: Simulated (a) current and (b) noise (Fano factor) for a three barrier diode using our approach with the explicit consideration of interacting electrons. See Fig. 5. The results from our approach are obtained through the Ramo-Shockley theorem [6].

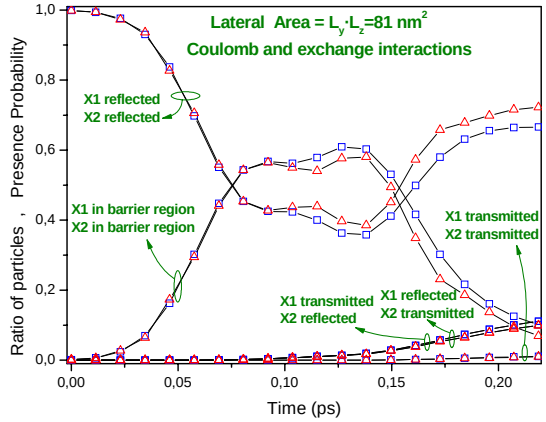

Fig. 2. In red (Δ), exact time-evolution of probability presence of a two-particle Schrödinger equation impinging in the double barrier where Coulomb and exchange interaction are considered. In blue (□), same scenario simulated with our approach.

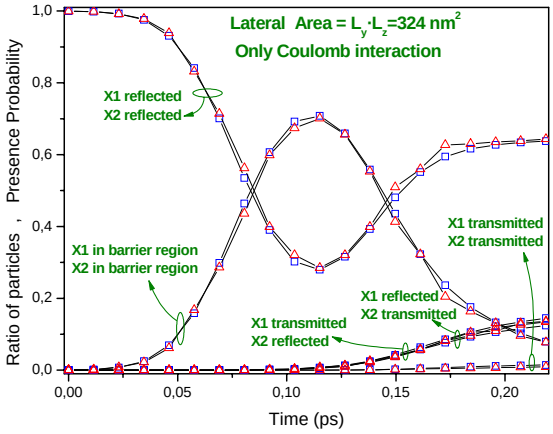

Fig. 3. Identical results of figure 2 without exchange interaction. Excellent agreement between our approach (in blue □) and two-particle Schrödinger equation (in red Δ).

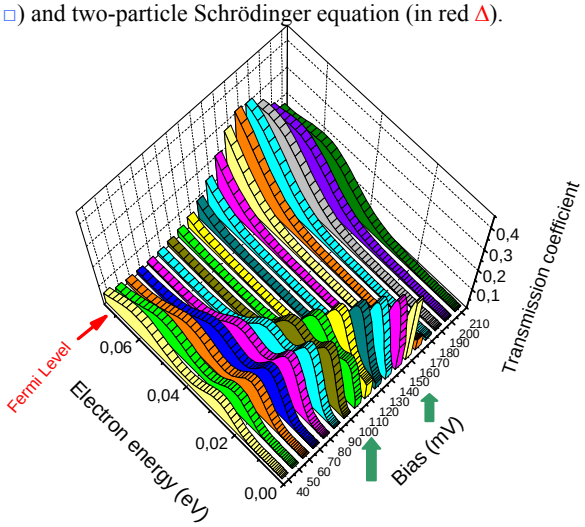

Fig. 5. The triple-barreir diode transmission coefficient of the device simulated in Fig. 4, showing the presence of two resonances (⇑) at V=0.12 V and V=0.15 V (a richer phenomenology in three-barrier than in two-barrier diodes). The electron correlations explain the different noise behavior after such resonances (**NDC1** and **NDC2**) in Fig. 4(b).