Poster

A NOVEL APPROACH FOR MANY-ELECTRON TRANSPORT IN NANOELECTRONIC DEVICES WITH FULL COULOMB INTERACTION

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The exact computation of a system of interacting electrons is an extremely complicated issue because the motion of one electron depends on the positions of all others (i.e. particles are correlated). Thus, the prediction of the collective behaviour of many electrons is still a very active field of research in nano-electronics, quantum chemistry, nano-biology, quantum computing, etc. The accurate treatment of the electron-electron correlations in nanoelectronic devices is even a more difficult task because we deal with non-equilibrium open systems.

In this conference, we will present a novel approach for the accurate treatment of electron-electron correlations in many-electron open systems without any perturbative or mean-field approximation [1,2]. In particular, a set of $N(t)$ particles with full Coulomb interaction inside an open system is described by the following many-particle Hamiltonian [2]:

$$H(\vec{r}_1,..,\vec{r}_{N(t)},\vec{p}_1,..,\vec{p}_{N(t)},t)=\sum_{k=1}^{N(t)}\left\{K(\vec{p}_k)+q_k\cdot W_k(\vec{r}_1,..,\vec{r}_{N(t)},t)-\frac{1}{2}\sum_{\substack{j=1\\ j\neq k}}^{N(t)}q_k\cdot V(\vec{r}_k,\vec{r}_j)\right\} \quad (1)$$

where $K(\vec{p}_k)$ represents the kinetic energy of the *k*th electron, $V(\vec{r}_k,\vec{r}_j)$ refers to the exact Coulomb interaction between the *j*th and *k*th electrons, and the term $W_k(\vec{r}_1,.,\vec{r}_k,.,\vec{r}_{N(t)})$ is a particular solution of the Poisson equation taking into account all charges excepting that of the *k*th electron. Notice that the position and momentum, $\vec{r}_k$ and $\vec{p}_k$, in the Hamiltonian (1) can be either classical variables or quantum operators. Classically, the solution of the many-particle Hamiltonian (1) is obtained via a coupled system of Newton-like equations with a different electric field for each particle [2]. The quantum mechanical solution of (1) is achieved by using a quantum trajectory algorithm that includes exchange interaction [1]. The boundary conditions of the Hamiltonian (1) on the borders of the open system (in the real 3D space representation) include the Coulomb interaction between particles inside and outside of the open system [2]. The many-particle Hamiltonian provides the same electrostatic description obtained from the image-charge method, but it has the fundamental advantage that it can be directly implemented into realistic (classical or quantum) electron device simulators via a 3D Poisson solver. The merit of the quantum solution is certainly remarkable because the computational burden associated with the direct (i.e. without any approximation) solution of the many-particle wave-function is only accessible for very few (2,3..) electrons [3].

In this conference, we will show the computational viability of building a powerful time-dependent nanoscale device simulator from our many-particle algorithm [1,2]. We will present the numerical computation of the DC behaviour for a (classical) double gate field effect transistor (1D DG-FET) and a (quantum) resonant tunnelling diode (RTD). The numerical results from (1) will be compared with those computed from time-dependent mean-field algorithms showing important quantitative differences (see Figs. 1-4). We will also discuss the role of the electron-electron correlations on the frequency-dependent performance of nanaoelectronic devices and on its electric power (see Fig. 5). In particular, power consumption has been identified recently by the IRTS [4] as one of the top three overall challenges that will drive nanoelectronic industry for next years. We notice that electric power is directly proportional to the force "felt" by each electron. This force does not depend on an average (mean) electric field, but on the gradient of the term $W_k(\vec{r}_1,.,\vec{r}_k,.,\vec{r}_{N(t)})$, in (1), which

discounts the effect of the *k*th electron on itself. The mean-field approximation of the electron-electron interaction gives an important error when computing the electric power of nanoelectronic devices (the single-transistor error drawn in fig. 5 has to be multiplied by the number of transistors in present-day CPUs).

In conclusion, within the effective mass approximation, a novel approach for the DC/AC current, noise, and power predictions of nanoelectronic devices with full Coulomb (and exchange) interaction will be presented. Classical and quantum examples for two different nanoelectronic devices demonstrate the computational viability of our many-particle algorithm which is able to treat electron dynamics without any (mean-field or perturbative) approximation in the description of the electrostatic and exchange interactions for a larger number (□ 50) of transport electrons [1,2].

References:

[1] X. Oriols, Phys. Rev. Lett. 98, 066803 (2007).
[2] G. Albareda, J. Suñe and X. Oriols, Phys. Rev. B, in press, (2009).
[3] "It would indeed be remarkable if Nature fortified herself against further advances in knowledge behind the analytical difficulties of the many-body problem". Max Born, 1960.
[4] International Technology Roadmap for Semiconductors, 2008 Update.

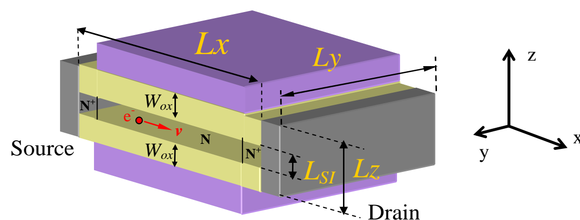

Figure 1: Schematic representation of the 1D DG-FET.

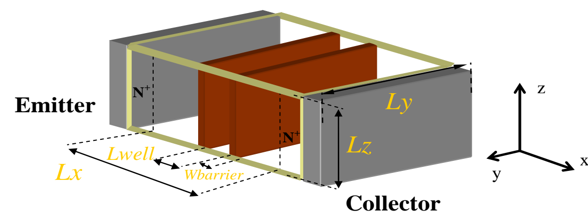

Figure 3: Schematic representation of the RTD.

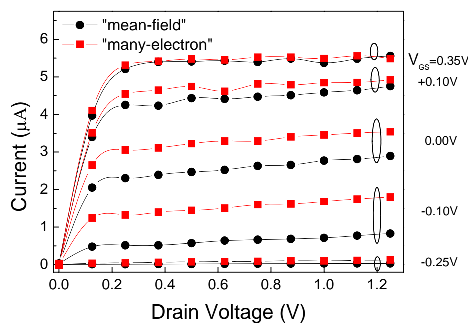

Figure 2: Average current for the 1D DG-FET of Fig. 1, using the many-electron and mean-field algorithms. The open ellipses include results with the same gate voltage indicated on the right.

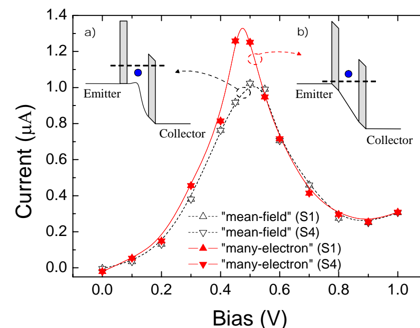

Figure 4: Average current through surfaces S1 (emitter surface) and S4 (collector surface) for the RTD of Fig. 3 as a function of bias, using the many-electron (solid symbols) and mean-field (open symbols) algorithms (lines are a visual help). Non-uniform voltages steps are used to focus on the resonant region. Insets show schematically the effect of an electron crossing an "empty" well on its own electrostatic potential using the mean-field a) or the many-electron b) approaches.

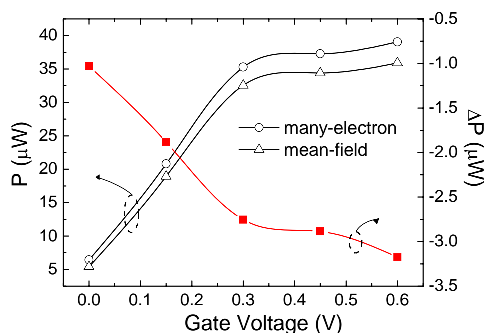

Fig. 5. Time averaged values for the electric power computed from the many-electron method and the mean-field approach in a bulk DG-FET. Differences between time averaged powers, $<P>_{\text{mean-field}}$ and $<P>_{\text{many-electrons}}$, are also presented. Results are presented per transistor.