Wigner Monte Carlo Approach to Quantum Transport in Nanodevices

P. Dollfus, D. Querlioz, J. Saint-Martin, V.-N. Do, A. Bournel
Institut d'Electronique Fondamentale, Univ. Paris-Sud, CNRS
Bat. 220, 91405 Orsay, France
Email : philippe.dollfus@ief.u-psud.fr

***Abstract*—The Wigner Monte Carlo approach is shown to provide an efficient way to study quantum transport in the presence of scattering and to connect semi-classical to quantum transport. The study of resonant tunneling diodes highlights the physics of the impact of scattering on resonant tunneling, and on electron decoherence and localization. The simulation of nano-MOSFET evidences a mixed regime, where both quantum transport and scattering play a significant role.**

Keywords: Tunneling, Wigner distributions, Monte Carlo methods, Quantum theory, MOSFETs, Green function, Resonant Tunneling Diodes

I. INTRODUCTION

The particle-based Monte Carlo technique has been, and is still, widely used to study the physics of transport in semiconductor devices within the semi-classical Boltzmann approximation. The extension of this method to quantum transport in nanodevices has been proposed through the Wigner function formalism. Though the Non Equilibrium Green's Functions (NEGF) formalism is now often used to simulate devices operating in the quantum regime [1-6], it remains uneasy to include realistic scattering models because of theoretical and computational difficulties. In particular, NEGF modeling cannot readily use all the work done to model scatterings in semi-classical transport situations. The Wigner quasi-distribution function (WF) can provide an original alternative to NEGF. It is defined in the phase-space as the center-of-mass Fourier transform of the density matrix of the carriers, and is most interesting because it shares many similarities with a distribution function, although it is not positive-definite [7]. In fact it tends to the Boltzmann's equation distribution function in the semi-classical limit. Besides, scattering effects can be incorporated into a WF calculation with an approach similar to that used for the Boltzmann's equation. WF thus provides a rich formalism to study the transition from semi-classical to quantum transport in nanoscaled electron devices.

Our Monte Carlo device simulator has been recently extended to include the WF evolution while maintaining full compatibility between semi-classical and quantum transport descriptions. This paper describes the main features of this approach and presents some important results regarding scattering effects in typical devices operating in quantum regime.

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II. PRESENTATION OF THE MODEL

The motion equation of the Wigner function f_w (Wigner Transport Equation, WTE) reads

$$\frac{\partial f_w}{\partial t}+\frac{\hbar k}{m^*}\frac{\partial f_w}{\partial x}=Q\,f_w+C\,f_w \tag{1}$$

where $Q\,f_w$ is the quantum evolution term resulting from the non-local effect of the potential $U\left(x\right)$, defined as

$$Qf_w\left(x,k\right)=\frac{1}{2\pi\hbar}\int dk'\,V_w\left(x,k'\right)f_w\left(x,k+k'\right) \tag{2}$$

where the Wigner potential is given by V_w

$$V_w\left(x,k\right)=\int dx'\sin\left(kx'\right)\left[U\left(x+\frac{x'}{2}\right)-U\left(x-\frac{x'}{2}\right)\right] \tag{3}$$

The term Cf_w in Eq. (1) encodes the effect of electron scattering (typically by phonons, impurities or oxide roughness) on the Wigner function. In a one-particle approach, and within an instantaneous scattering approach (that neglects quantum collision effects like collision broadening and intra-collisional field effect [8]), the collision Hamiltonian leads to the standard collision term of the Boltzmann equation of semi-classical transport [9]

$$\begin{aligned}Cf_w\left(x,k\right)=\sum_i\Big[&\int dk'f_w\left(x,k'\right)S_i\left(k',k\right)\\&-\int dk'f_w\left(x,k\right)S_i\left(k,k'\right)\Big]\end{aligned} \tag{4}$$

where *i* refers to the type of scattering mechanism and S_i is the associated scattering rate.

To solve the WTE we use the particle Monte-Carlo interpretation inspired by [10] and described in [11, 12]. The Wigner function is seen as a sum of "pseudo-particles" localized in both x and k space and weighted by a parameter called affinity. The affinity contains the quantum information on the particles and can take negative values. Such pseudo-particles have no direct physical meaning, but constitute a very ingenious way to solve the WTE: their *x* and *k* coordinates

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evolve exactly as that of classical particles, while their affinity is updated according to the Qf_w term of the WTE. Scatterings are included using the standard MC algorithm, which constitutes the strength of the method. The effect of the collision term is considered via scattering events which instantaneously change the wave-vector of pseudo-particles according to standard collision rates. This process is treated using the usual MC method, which provides a very efficient way to include scattering effects, in full analogy with semi-classical Ensemble Monte Carlo (EMC) simulations.

Note that this approach strongly differs from the Wigner Monte Carlo method proposed in Ref. [13] where the quantum evolution term is described as a scattering term which induces generation and recombination of pseudo-particles.

III. RESONANT TUNNELING DIODE

We study here a Resonant Tunneling Diode (RTD), similar to that considered by Shifren et al. in Ref. [10]. A quantum well of 5 nm sandwiched between two AlGaAs barriers 0.3 eV high and 3 nm wide. The quantum well, the barriers, and 9.5 nm-thick buffer regions close to the barriers are slightly doped to 10^{16} cm^{-3} . The 50 nm-long access regions are doped to 10^{18} cm^{-3}. The temperature is 300 K. The scattering mechanisms considered are optical phonons, elastic acoustic phonons, and ionized impurities, within a single Γ band. The solution is coupled with 1-D Poisson's equation.

To check that the model handles quantum mechanics accurately, we artificially deactivate scattering in our calculation. The resulting I-V characteristic is compared on Figure 1 with the one resulting from self-consistent ballistic Green's Function calculation. A very good agreement is obtained.

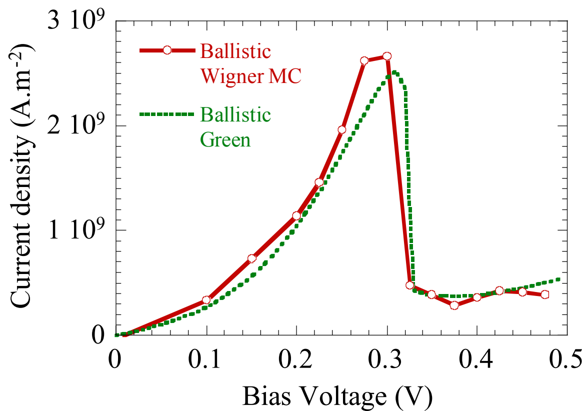

Figure 1. . I-V characteristics obtained from our model with scattering artificially deactivated (circles) compared with a fully self-consistent ballistic Green's functions simulation (dotted line)

On Figure 2, the I-V characteristics obtained from our model including scattering (squares) is compared with the ballistic simulation (circles) and with a simulation where scattering rates have been artificially multiplied by five (diamonds). It is seen that scattering effects dramatically reduce the peak-to-valley ratio and are thus essential to be considered for room-temperature simulation of RTDs.

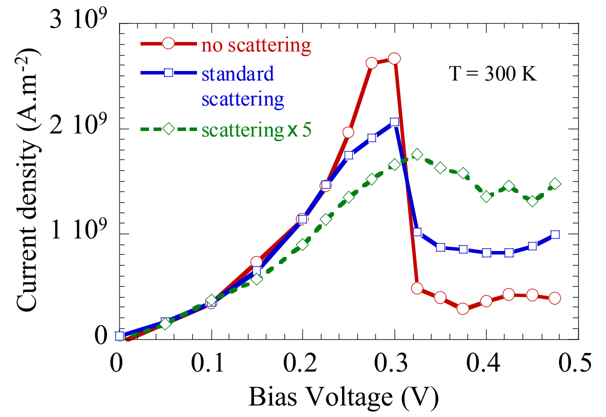

Figure 2. I-V characteristics obtained from our model with scattering artificially deactivated (empty circles), with standard scattering (squares), and scattering rates artificially multiplied by 5 (full circles)

We now compare in Table I our simulation results of peak-to-valley ratios (including scattering) with some experimental data of AlGaAs/GaAs/AlGaAs RTDs at room temperature and at 77 K [14, 15]. A good overall agreement is reached, which suggests that this method can be actually used for realistic device simulation.

TABLE I. COMPARISONS OF MEASURED AND SIMULATED PEAK-TO-VALLEY RATIOS FOR EXPERIMENTAL RTDS

	Experiment	Simulation
[14] 300 K	1.25	1.3
[14] 77 K	3.8	4
[15] 300 K	1.75	2
[15] 77 K	7	6

The Wigner function gives access to the nondiagonal terms of the density matrix (DM) which provides a clear visualization of decoherence phenomena. The coherent and the phonon-induced decoherence is highlighted in Figs. 3 (a-c) which represent the density matrix in the same scattering situations as in Fig. 2.

In the ballistic case a strong coherence is observed between electrons in the quantum well and in the emitter region. Non diagonal elements are even significant between electrons in collector and emitter regions, which is a clear indication of a coherent transport regime. When including standard scattering rates the non diagonal elements strongly reduce and the coherences almost fully disappear when phonon scattering rates are multiplied by 5. In this case non-diagonal elements of the DM vanish, which indicates that the system is now in the sequential tunnelling regime. This phonon-induced transition between coherent and sequential tunnelling regimes manifests itself in the current-voltage characteristics of the RTD plotted in Fig. 2 for the three scattering situations. Phonon scattering tends to suppress the resonant tunnelling peak while the valley current increases to such a point that the negative differential conductance effect almost disappears.

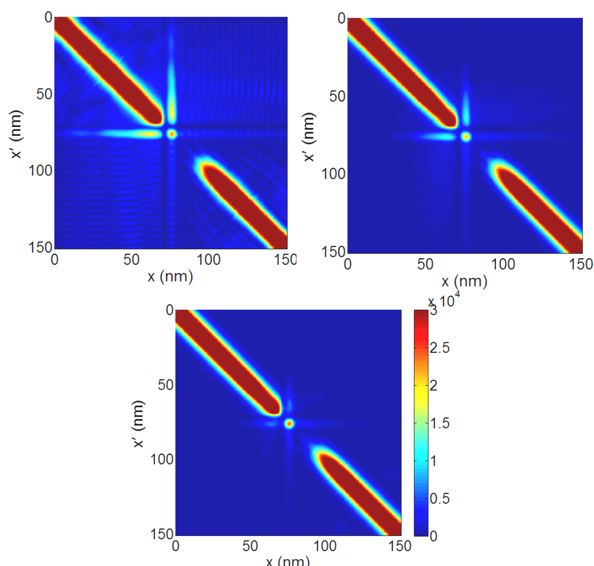

Figure 3. Density matrix of the RTD operating at peak voltage with a) no scattering, b) standard scattering rates, scattering rates multiplied by five

IV. SIMULATION OF NANOMOSFET OPERATION

We now consider the simulation of ultra-scaled end-of-roadmap double gate MOSFETs within the mode-space approximation which decouples the gate-to-gate *z* direction and the *xy* plane parallel to interfaces [12, 16-18]. A schematic of the simulated structure is presented on Figure 4.

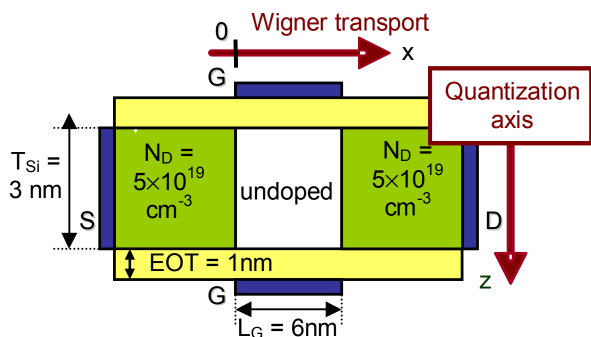

Figure 4. Simulated Double Gate MOSFET structure. Highly doped Source and Drain regions are 15 nm long.

The 1D Wigner transport equation, 2D Poisson's equation and the 1D lateral Schrödinger's equations (to compute the 2D Electron Gas subbands) are solved self-consistently, as described in [12]. It has been checked that for such a thin body transistor, the lateral wave-functions do not strongly evolve along the device, which justifies the 2DEG mode-space approach [12,19].

Figure 5 shows the drain current versus gates voltage at 300 K. They are compared with that obtained from semi-classical Boltzmann MC simulation including multi-subband description [20] to emphasize the impact of quantum transport. They are also compared with the currents resulting from a ballistic Green's function calculation (quantum transport model with no scattering) to emphasize the impact of scattering. All three models use an effective mass approach to the electronic band structure.

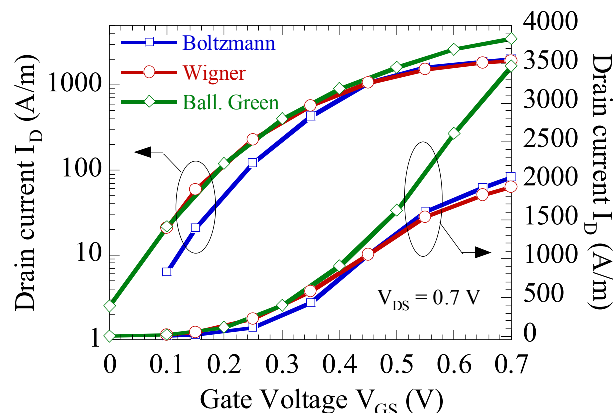

Figure 5. Drain current I_D versus gate voltage V_{GS} obtained using Wigner, Boltzmann and ballistic Green's function simulations, at high V_{DS}

In the subthreshold regime (low V_{GS}) the results based on the Wigner's function are very close to the ballistic Green's function ones. However, the currents are significantly higher than that obtained using semi-classical simulation. This shows that scattering has a weak impact in this regime and that the subthreshold current is strongly enhanced by direct source-to-drain tunnelling through the high potential barrier in the channel [12]. Above the threshold (high V_{GS}), the behavior is very different. The ballistic approach strongly overestimates the current due to the efficiency of scattering and the Wigner current become similar to the current resulting from the semi-classical calculation. It is remarkable that the Wigner current is actually smaller than the semi-classical current at high V_{GS}. The quantum reflection effect due to the strong drop of the potential profile causes this current reduction [12].

Figures 6a) and 6b) compare the Wigner function f_w at high V_{GS} with the distribution function from the semi-classical calculation at the same bias. Generally, both functions exhibit the same form with two high value regions in the phase space which correspond to electrons in the source and drain regions. Besides, a long mouse tail-like curve is seen in the channel which describes the flow of ballistic carriers from S to D. However, while the distribution function remains positive-definite, there exist small domains around the tail in Fig. 4(a) where the WF oscillates and assumes negative values. This illustrates the quantum reflections and emphasizes that the Wigner function cannot be interpreted as a probability function in the presence of quantum transport, consistently with Heisenberg uncertainty principle [7, 12].

Figure 7 examines in more detail the effects of scattering above the threshold. Drain current versus gate voltage is plotted in linear scale. Ballistic Green's calculation and Wigner's calculation are plotted, as well as a Wigner's calculation where scattering has been artificially deactivated in the channel, but not in the highly-doped access regions. Comparison of Green's calculation with the two Wigner calculations shows that scattering in these access regions still has an important impact on the characteristics. Comparison of the two Wigner calculations shows that even for this 6 nm-long channel,

scattering in the channel has a small but significant impact: it reduces the transconductance $g_m = \partial I_D / \partial V_{GS}$ by 20%.

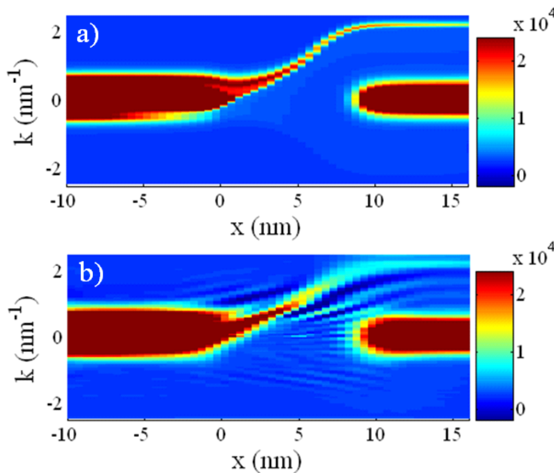

Figure 6. Cartography of a) semi-classical distribution function (Boltzmann calculation) and b) Wigner function of the first sub-band obtained for V_{GS} = 0.45 V and V_{DS} = 0.7 V

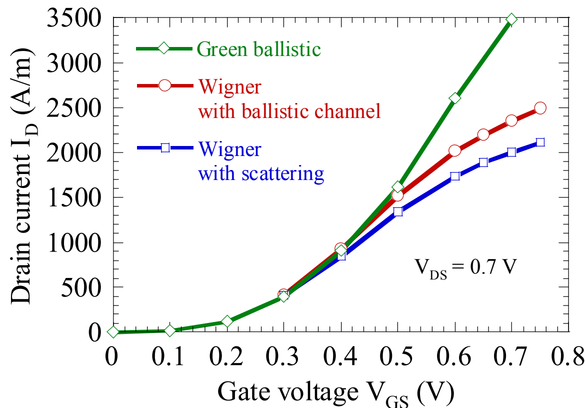

Figure 7. Room temperature current at V_{DS} = 0.7 V using Wigner including or not scattering in the channel. Comparison with Green's function calculation (no scattering anywhere).

V. Conclusion

This work examines the physics of advanced nanodevices using an original Wigner Monte Carlo simulator. Quantum transport dominates the subthreshold behavior of MOSFET, whereas scatterings have negligible impact. In contrast, quantum transport plays a moderate role above the threshold where device operation is dominated by scatterings, both in the access regions and in the channel. The study of RTDs emphasizes the role of phonon scattering in the electron localization and in the transition between coherent and sequential tunneling regimes. Our approach appears as a rich method to study the transition from semi-classical to quantum transport in nano-devices.

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