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An Improved Wigner Monte-Carlo Technique for the Self-Consistent Simulation of RTDs

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INTRODUCTION

We present an original approach to include quantum transport in classical Ensemble Monte Carlo (EMC) simulations. The method is fully self-consistent, and includes scattering according to the Fermi Golden rule. The method is inspired by an approach suggested by Shifren and Ferry [1], with some major improvements that make possible successful comparison with other simulation techniques and experiments.

BASICS OF THE METHOD

The method takes advantage of a pseudo-particle interpretation of the Wigner function formalism. The Wigner quasi-distribution function can indeed be seen as a sum of pseudo-particles whose real and reciprocal space coordinates evolve as classical particles, and whose magnitudes (affinities) evolve according to a quantum evolution term

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

$$V_w(x,k) = \int dx' \sin(kx')\left[V\left(x+\frac{x'}{2}\right) - V\left(x-\frac{x'}{2}\right)\right]. \quad (1)$$

Such pseudo-particles are scattered as classical particles and it is possible to build an EMC-like method for quantum-transport simulation. In such a method, however, injection and boundary conditions are different from that used in classical EMC simulations. In this paper we propose an original solution for this issue that seems more suitable than Shifren's initial suggestion. Note that the pseudo-particles interpretation of this method strongly differs from Nedjalkov's [2].

RESULTS

On Fig. 1, we show J/V characteristics we got for a GaAs Resonant Tunneling Diode (RTD), for simulations with scattering activated and deactivated. On Fig. 2, the simulation with scattering deactivated is first compared with a fully self-consistent NEGF simulation and very good agreement is obtained, except for the peak current which is a little higher in the Wigner simulation. This is the first step to validate quantum mechanics handling implemented in our method.

Figs. 3 and 4 show the Wigner functions for a resonant and a non-resonant state. The population of the quasi-bound state of the RTD quantum well is clearly seen. Fig 5 shows the self-consistent potential profile for these two situations.

COMPARISON WITH EXPERIMENTS

To validate our approach of scattering handling, we compare on Table 1 peak to valley ratios of experimental RTDs [3] with values extracted from our simulations. Theses first results are encouraging, and more comparisons are underway.

CONCLUSION

We have developed a model that seems very promising to incorporate quantum mechanics effects into traditional EMC simulations. Self-consistence and scattering are included, and the method is fully compatible with classical EMC simulations.

ACKNOWLEDGEMENT

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REFERENCES

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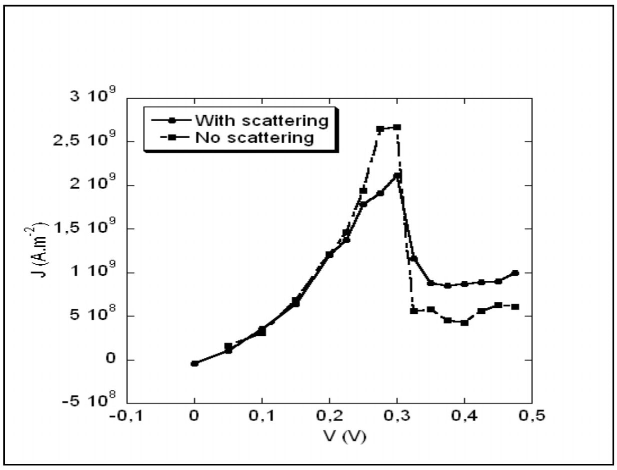

Fig. 1. J/V characteristic of a 300K GaAs RTD, with scattering activated and deactivated

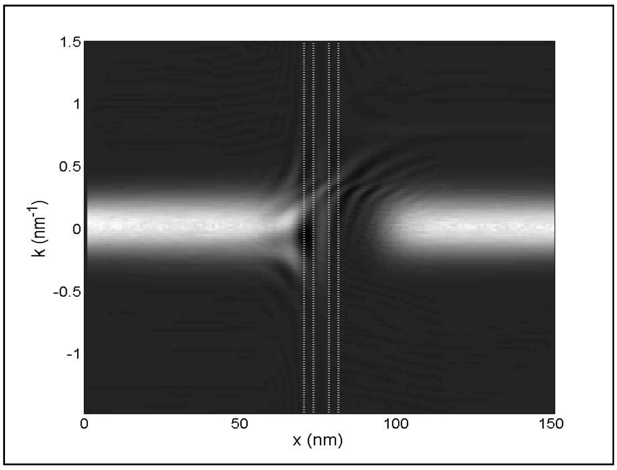

Fig. 2. Wigner function for an on-resonant state (V=0.3V)

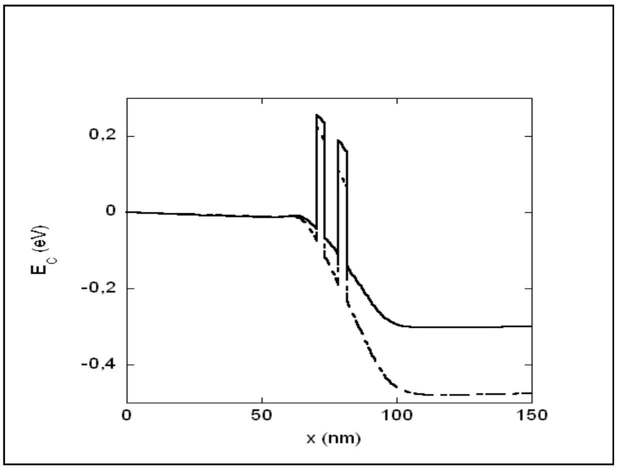

Fig. 3 Self-Consistent potential profiles of the RTD for V=0.3 (plain line) and V=0.475V (dotted line)

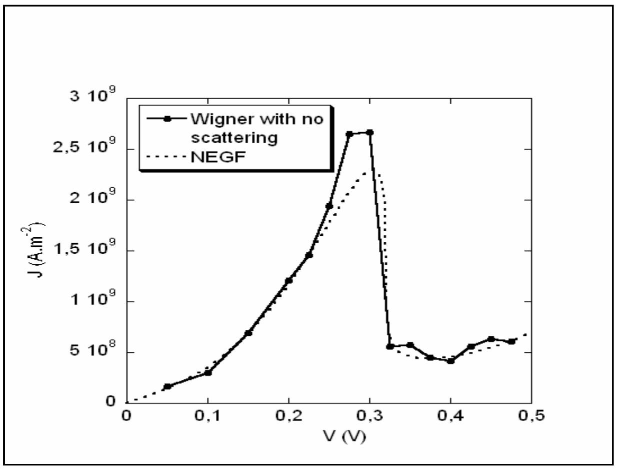

Fig. 4. Comparison of the characteristic of the RTD with scattering deactivated with a fully self-consistent ballistic NEGF calculation

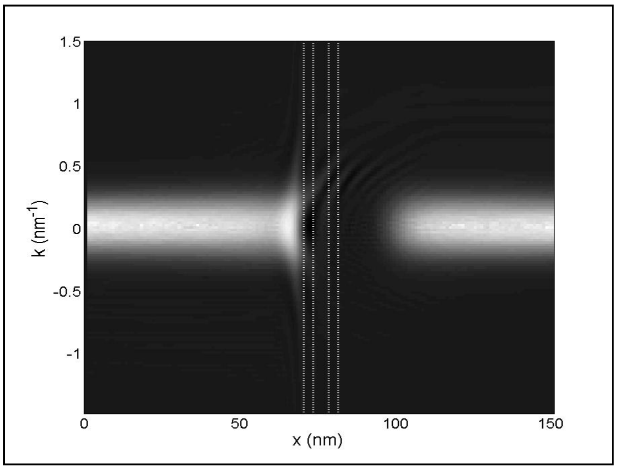

Fig. 5. Wigner function for an off-resonant state (V=0.475V)

	Exp $\frac{I_{peak}}{I_{valley}}$	Simu $\frac{I_{peak}}{I_{valley}}$
Device [3] 300K	1.3	1.25
Device [3] 77K	4.0	3.8

Table 1. Comparison of simulations and experimental results