Physica A 398 (2014) 194–198

Contents lists available at ScienceDirect

Physica A

journal homepage: www.elsevier.com/locate/physa

Electron dynamics in nanoscale transistors by means of Wigner and Boltzmann approaches

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HIGHLIGHTS

- We use the two-dimensional, time-dependent, Wigner MC method.
- We simulate the evolution of a Gaussian wave packet moving in a realistic channel potential.
- We include the kernel of a scattering center in the channel.
- We compare the Wigner results with the Boltzmann results.

ARTICLE INFO

Article history:
Received 26 September 2013
Received in revised form 3 December 2013
Available online 28 December 2013

Keywords:
Full quantum transport
Wigner equation
Boltzmann equation
Monte Carlo methods
Nanometer scaled devices
Single dopants

ABSTRACT

We present a numerical study of the evolution of a wave packet in a nanoscale MOSFET featuring an 'atomistic' channel doping. Our two-dimensional Monte Carlo Wigner simulation results are compared against classical Boltzmann simulation results. We show that the quantum effects due to the presence of a scattering center are manifestly non-local affecting the wave propagation much farther than the geometric limit of the center. In particular the part of the channel close to the oxide interface remains blocked for transport, in contrast to the behavior predicted by classical Boltzmann propagation.

1. Introduction

With shrinking transistors dimensions down to nanometric size, the device electrical behavior starts to be dominated by both the granularity of matter [1–10] and quantum mechanical effects [11,12]. In order to preserve accuracy and reliability at the nanoscale regime, device simulation approaches have, on one hand, to depart from treating the doping as a continuum, within the Poisson equation only, and, on the other hand, to improve the traditional semi-classical modeling of transport to properly take into account the particle–wave duality. The particle-based Wigner Monte Carlo (MC) approach has been recently shown to efficiently deal with the simulation of full quantum transport [13]. In particular a Wigner MC method, based on particle's sign, for stationary cases [14] has been recently generalized for time-dependent simulations [15]. This method is general enough to deal with multi-dimensional domains. In this work we apply it to simulate two-dimensional

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0378-4371/$ – see front matter
http://dx.doi.org/10.1016/j.physa.2013.12.045

electron evolution in the channel of a nanoscale MOSFET in the presence of a single discrete dopant. The evolution problem is posed by an initial condition, there are no injecting boundaries as in the stationary problems posed by boundary conditions [16].

Our simulation results are, first of all, validated against two one-dimensional (1D) benchmarks based on the ballistic Boltzmann equation for the case of a constant applied electric field and the solution of the Schrödinger equation for the case of an idealistic potential barrier. Then, two-dimensional (2D) full quantum results are compared with results of the classical Boltzmann MC approach for a realistic device potential. Due to the non-local quantum effects, the discrete scattering center affects the wave propagation even when not directly interacting with it, blocking the charge propagation in the region close to the channel interface. These results are manifestly in contrast with the behavior predicted by classical Boltzmann propagation and demonstrate the importance of full quantum approaches for studying the electron dynamics in nanoscale devices.

2. Numerical methodology

In order to obtain a realistic potential profile of a nanoscale device, we have performed three-dimensional (3D) TCAD simulations of a well-scaled 25 nm MOSFET device using the GSS 'atomistic' simulator GARAND [17]. A vertical slice of the 3D device is then extracted and used to perform a 2D Wigner simulation of the charge transport in the presence of a discrete dopant. For the sake of simplicity, we account for the long range Coulombic nature of the impurity, calculated by a self-consistent Drift–Diffusion simulation, and focus on the internal kernel modeled by a rectangular potential barrier.

Concerning the quantum transport, the GNU package Archimedes [18] has been enhanced to implement the Wigner MC method, as formulated below for an initial condition. The method can actually be included in every MC platform, since it does not depend on the particular instance of the implementation. The model, a reformulation of the density matrix formalism, reads

$$\frac{\partial f_W}{\partial t} + \frac{1}{\hbar}\nabla_{\mathbf{k}}\epsilon(\mathbf{k}) \cdot \nabla_{\mathbf{x}} f_W = Q[f_W] \tag{1}$$

where $Q[f]$ is a quasi-distribution functional defined as

$$Q[f_W](\mathbf{x}, \mathbf{k}, t) = \int \mathrm{d}\mathbf{k}' V_W(\mathbf{x}, \mathbf{k} - \mathbf{k}', t) f_W(\mathbf{x}, \mathbf{k}', t). \tag{2}$$

The function $V_W = V_W(\mathbf{x}, \mathbf{k}, t)$, known as the Wigner potential, is defined as

$$V_W(\mathbf{x}, \mathbf{k}, t) = \frac{1}{\mathrm{i}\hbar(2\pi)^d} \int \mathrm{d}\mathbf{x}' \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}'} \left(V\left(\mathbf{x} + \frac{\mathbf{x}'}{2}, t\right) - V\left(\mathbf{x} - \frac{\mathbf{x}'}{2}, t\right)\right) \tag{3}$$

where $d = 1, 2, 3$ is the dimensionality of the problem; $V = V(\mathbf{x}, t)$ is a potential defined over the spatial domain and can be time dependent.

The Monte Carlo technique exploits the semi-discrete nature of the phase-space in accordance to the principles of quantum mechanics [15]. The main purpose of this method is to evaluate an expectation value $\langle A\rangle(t)$, expressed as an iterative series, of a macroscopic physical quantity $A = A(\mathbf{x}, \mathbf{k})$, defined over the Wigner phase-space

$$\langle A\rangle = \int_0^\infty \mathrm{d}t' \int \mathrm{d}\mathbf{x}_i \sum_{\mathbf{m}'=-\infty}^{\infty} f_i(\mathbf{x}_i, \mathbf{m}') \mathrm{e}^{-\int_0^{t'} \gamma(\mathbf{x}_i(y))\mathrm{d}y} g(\mathbf{x}_i(t'), \mathbf{m}', t') \tag{4}$$

with

$$\mathbf{x}'(y) = \mathbf{x}_i(y) = \mathbf{x}_i + \frac{\hbar\mathbf{m}'\Delta\mathbf{k}}{m^*}y; \qquad \mathbf{x}' = \mathbf{x}'(t') = \mathbf{x}_i(t'); \qquad \mathrm{d}\mathbf{x}' = \mathrm{d}\mathbf{x}_i.$$

The functions $f_i = f_i(\mathbf{x}, \mathbf{m})$ and $g = g(\mathbf{x}(t), \mathbf{m}, t)$ are, respectively, the initial quasi-distribution function and the solution of the adjoint equation [14], the kernel of which reads

$$\Gamma(\mathbf{x}, \mathbf{m}, \mathbf{m}') = V_w^+(\mathbf{x}, \mathbf{m} - \mathbf{m}') - V_w^+(\mathbf{x}, -(\mathbf{m} - \mathbf{m}')) + \gamma(\mathbf{x})\delta_{\mathbf{m},\mathbf{m}'}. \tag{5}$$

Finally, the quantity $\gamma(\mathbf{x})$ is defined as

$$\gamma(\mathbf{x}) = \sum_{\mathbf{m}=-\infty}^{\infty} V_w^+(\mathbf{x}, \mathbf{m}), \tag{6}$$

where V_w^+ takes the values of V_w if $V_w > 0$ and 0 otherwise.

Then the estimator of the expectation value (which can be considered also as a functional of the solution) can be expressed as weights of values of V_w at points taken in accordance with the transition probabilities. Details of the algorithm are given in Ref. [19] as well as in Ref. [20]. We also do not consider the problem of convergency. The analysis of convergency is