Quantum Correction for the Current-Based One-Particle Monte-Carlo Method

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ABSTRACT

In a previous work [1] a current-based one-particle Monte-Carlo (CBOPMC) method has been proposed, in contrast to the common OPMC method by F. Venturi et al. [2] based on densities. With the CBOPMC method one can take arbitrary generation-recombination processes into account self-consistently, which no other MC method can accomplish. This paper reports an extension of the method, where quantum potential equations [3] are included in a self-consistent way and free of the problems encountered with other MC methods [4]. Compared to MC simulators coupled with the 1D-Schrödinger equation, the CBOPMC method allows for arbitrary geometries, quantization in all directions, and tunneling. As a by-product, a model for the transport parameters in the simulated device is generated, which can be used in conventional quantum drift-diffusion simulators.

Keywords: Monte Carlo, Boltzmann equation, quantum drift-diffusion, SOI-MOSFET, generation-recombination, quantum correction, tunneling

1 INTRODUCTION

In top-of-the-art nanodevices like UTB-MOSFETs, FinFETs, or nanowire FETs, phenomena like quantum-confinement, tunneling, scattering, generation-recombination (G-R), hot electrons, and impact-ionization play an important role. Nonetheless, band-structure effects like non-parabolicity and strain are not negligible. In emerging technologies which exploit the floating-body effect, like Z-RAMs, all these effects must be considered to accurately model a device. From a theoretical point of view, the non-equilibrium Green's functions (NEGF) formalism should be able to describe such devices, but the resulting equations are still too heavy to be solved numerically for any realistic device. In a first approximation, the Boltzmann-Wigner transport equation (BWTE) could be solved, but, although progress has been achieved in the solution methods [5], it is still impracticable in concrete cases. The most complicated equation that can still be solved in a reasonable amount of time using a Monte-Carlo (MC) method is the Boltzmann transport equation (BTE), which can be coupled to some kind of quantum correction (QC).

In [1] a current-based OPMC (CBOPMC) method has been proposed, which can efficiently solve any BTE containing G-R processes. To become relevant for nanodevice simulation, this method has to be extended to take into account quantum confinement and tunneling. Two popular methods exist to model quantum effects. The first one, based on the coupling of the BTE in the transport direction with the solution of the 1D-Schrödinger-Poisson equation system in confinement direction, can be used only to describe confinement in devices where a transport direction can be well defined [6],[7]. The second one, called density gradient (DG) method [8], naturally arises from the BWTE, when all terms of order $\hbar^2$ in the derivative of the potential are considered. For TCAD applications, the second method seems to be more promising, because it can be applied to any device geometry. Furthermore, tunneling can also be described to a certain extent.

When solving the BTE using a MC method, the DG QC cannot be easily computed, because one needs to compute the first and second derivatives of the logarithm of the MC density, which is very noisy. Different approaches have been proposed to solve this problem [9], [10], [11], but all are afflicted with some inconsistencies.

In this paper, a consistent implementation of the DG QC into the CBOPMC scheme is presented. Section 2 describes the method and discusses its advantages. Section 3 addresses some implementation issues. Section 4 shows results of the application of the new method to a double-gate MOSFET. Finally, Section 5 concludes the discussion.

2 THEORY

In the following, only the equations for electrons are outlined, and only for the stationary state. The BTE with DG QC can be written as

$$\mathbf{v}(\mathbf{k})\nabla_r f(\mathbf{r},\mathbf{k}) + \frac{q}{\hbar}\nabla_k f(\mathbf{r},\mathbf{k})\cdot\nabla_r\left(\varphi(\mathbf{r}) - \Lambda_n(\mathbf{r})\right) = \int_K S(\mathbf{r},\mathbf{k},\mathbf{k}')f(\mathbf{r},\mathbf{k}')d^3\mathbf{k}', \quad (1)$$

where f is the distribution function, $\mathbf{v}$ the group velocity, φ the electrostatic potential, $S(\mathbf{r},\mathbf{k},\mathbf{k}')$ the scattering operator as defined in [12], and Λ_n is the quantum

potential (QP). The QP is defined by the following equation which contains a DG:

$$\Lambda_n(\mathbf{r}) := -\frac{\gamma_n \hbar^2}{12m}\left\{\nabla_r^2 \log\left(n(\mathbf{r})\right) + \frac{1}{2}\left(\nabla_r \log\left(n(\mathbf{r})\right)\right)^2\right\}, \tag{2}$$

where $n(\mathbf{r})$ is the density, *log* the natural logarithm, m the free electron mass, and γ_n a fit parameter. By multiplying and integrating (1) with the velocity moment of the inverse scattering operator (ISO) $S_{\mathbf{v}}^{-1}$ [13], an exact generalized drift-diffusion (GDD) equation can be written

$$q\left(\nabla_r^T\left(\mathbf{D}^T(\mathbf{r})n(\mathbf{r})\right)\right)^T - qn(\mathbf{r})\mu(\mathbf{r})\nabla_r\left(\varphi(\mathbf{r}) - \Lambda_n(\mathbf{r})\right) = \mathbf{J}_n(\mathbf{r}), \tag{3}$$

where $\mathbf{J}_n(\mathbf{r})$ is the current density, $\mu(\mathbf{r})$ the mobility tensor defined as

$$\mu_{ij}(\mathbf{r}) := \frac{q}{n(\mathbf{r})\hbar}\int_K S_{v_i}^{-1}(\mathbf{r},\mathbf{k})\partial_{k_j} f(\mathbf{r},\mathbf{k}) d^3\mathbf{k}, \tag{4}$$

and $\mathbf{D}(\mathbf{r})$ the diffusivity tensor defined as

$$D_{ij}(\mathbf{r}) := -\frac{1}{n(\mathbf{r})}\int_K S_{v_i}^{-1}(\mathbf{r},\mathbf{k}) v_j(\mathbf{k}) f(\mathbf{r},\mathbf{k}) d^3\mathbf{k}. \tag{5}$$

As soon as Λ_n is known, Eq. (1) can be solved using standard MC methods. Different methods have been developed to compute Λ_n. The simplest one consists in directly plugging the MC density n_{MC} into (1) [14]. This is, however, not optimal, because n_{MC} is usually very noisy and, therefore, difficult to differentiate numerically [4]. Ferry et al. [9] proposed to fold the electrostatic potential with a Gaussian and proved that the first term on the rhs of (2) is approximatively recovered. The second term, however, is not properly reproduced, and the two approaches result in different density profiles [15], the DG method being the nearest to the full Poisson-Schrödinger solution. Tang et al. [4], [11] derived an expression for the rhs of (2) which only depends on the electrostatic potential, but their formulation is only valid at thermodynamic equilibrium and cannot be extended to the non-equilibrium case.

The idea of the CBOPMC approach is to solve the Poisson equation coupled to (3) and (2) for given $\mu(\mathbf{r})$ and $\mathbf{D}(\mathbf{r})$. By doing so, the quantum potential Λ_n is part of the solution and its extraction is thus trivial. This approach is called MC generalised quantum drift-diffusion (MC-GQDD) method, because the equations (3) and (2) are formally analog to the usual QDD equations, the only differences being that mobility and diffusivity are tensors extracted from a frozen-field MC solution of the BTE [1] and that the Einstein relation is not assumed. The main advantage of this approach is that the QP Λ_n is a direct solution of the system of equations and, therefore, doesn't need to be extracted from the MC density n_{MC} or by any other approximative method. Another advantage is that by each iteration, the density, the electric field, and the QP are consistent. Furthermore, as the transport parameters (TPs) are generated by the MC simulation for each iteration, a transport model for the device is automatically produced.

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To solve the Poisson equation coupled to (3) and (2), the electrostatic potential φ, the quasi-Fermi potential ψ_n, and the QP Λ_n are chosen as solution variables. The quasi-Fermi potential is unequivocally defined by the constitutive equation

$$n(\mathbf{r}) =: n_i(\mathbf{r})\exp(\beta(\varphi(\mathbf{r}) - \psi_n(\mathbf{r}) - \Lambda_n(\mathbf{r}))), \tag{6}$$

where $n_i(\mathbf{r})$ is the local intrinsic density and $\beta := \frac{k_B T}{q}$. Putting (6) in (2) gives

$$\Lambda_n(\mathbf{r}) := -\frac{\gamma_n \hbar^2 \beta}{12m}\{\Delta\left(\varphi(\mathbf{r}) - \psi_n(\mathbf{r}) - \Lambda_n(\mathbf{r})\right) + \frac{\beta}{2}\left(\nabla_r(\varphi(\mathbf{r}) - \psi_n(\mathbf{r}) - \Lambda_n(\mathbf{r}))\right)^2\}. \tag{7}$$

Eq. (7) is then solved everywhere in the device, i.e. in the semiconductor *and* insulator parts, using a finite-element method. Dirichlet boundary conditions are assumed only on semiconductor contacts, otherwise Neumann boundary conditions are used.

4 RESULTS

To demonstrate the feasibility of the method and for comparison purposes the double-gate MOSFET depicted in Fig. 1 was simulated. The I_d-V_d characteristics for a gate voltage of $V_g = 1.1\,V$ are shown in Fig. 2 in comparison to classical results from ensemble MC and results from the CBOPMC method without QC (MC-GDD). The I_d-V_d curve is hardly influenced by quantum confinement, although the internal device physics is quite different in the quantum case compared to the classical case. The differences become obvious from Figs. 3–5. Fig. 3 shows that the QP plays its role as expected in repelling the electrons from the Si-SiO_2 interface. Fig. 5 shows that the effective diffusivity in transport direction is systematically increased in the quantum case. The effective mobility in transport direction is higher in the first few nanometers of the channel and then becomes smaller as in the classical case as shown in Fig. 4. In the heavily doped regions, the TPs in the quantum and classical case are the same as expected. By construction, the new method produces two currents after each iteration. The first current originates from the frozen-field MC simulation used to compute the tensorial TPs μ and $\mathbf{D}$. The second current comes from the solution of the GQDD equation. These two currents are shown in

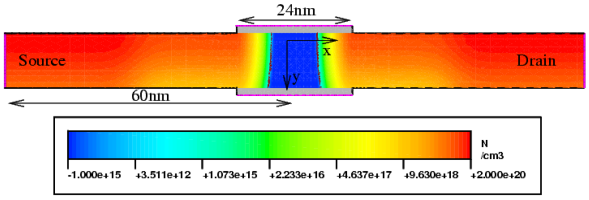

Figure 1: Double-gate MOSFET: Geometry and doping profile.

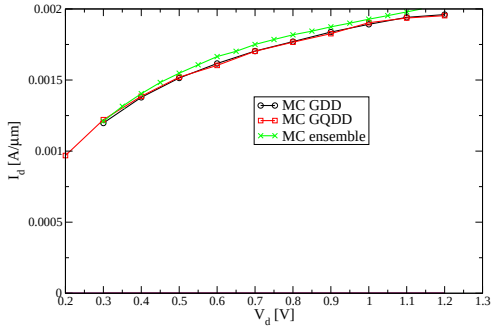

Figure 2: I_d-V_d characteristics at $V_g = 1.1\,V$.

Fig. 6 as a function of the iteration number for a chosen bias. As expected, the two currents seem to converge towards the same value, which may be interpreted as a sign for convergence. Finally, two-dimensional profiles of the TPs and of the resulting current density are shown in Figs. 7–9. The asymmetry in the TPs originates from the asymmetric doping of the device (Fig. 1). The simulation that produced these results was run in parallel using MPI-2 on 64 CPUs of type AMD Opteron(tm) 285 and took 12 hours.

5 CONCLUSION

The current-based one-particle Monte Carlo method has been extended to take into account the Wigner quan-

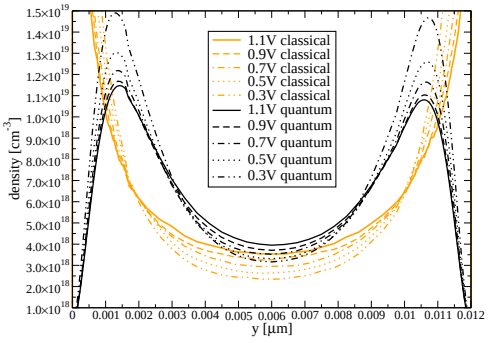

Figure 3: Profile of the density as function of y at $x = 0$.

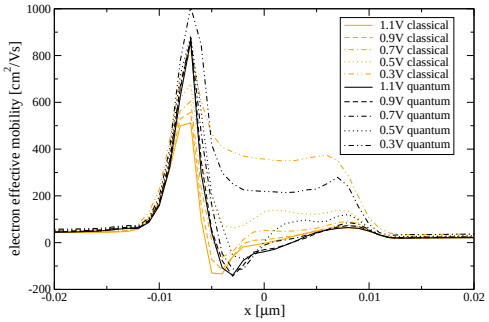

Figure 4: Effective mobility in the transport direction as function of x.

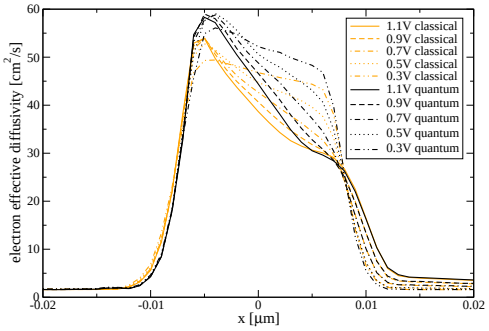

Figure 5: Effective diffusivity in the transport direction as function of x.

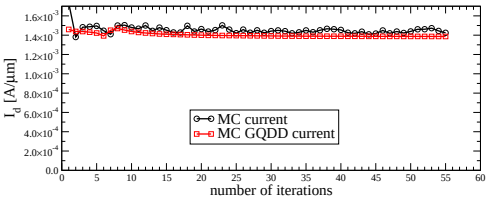

Figure 6: Comparison of the drain-current computed by Monte Carlo and computed by MC-GQDD at $V_d = 0.4\,V$.

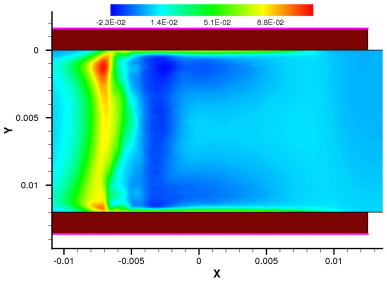

Figure 7: xx component of the mobility tensor at $V_d = 0.7\,V$.

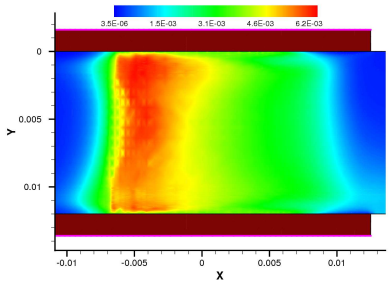

Figure 8: xx component of the diffusivity tensor at $V_d = 0.7\,V$.

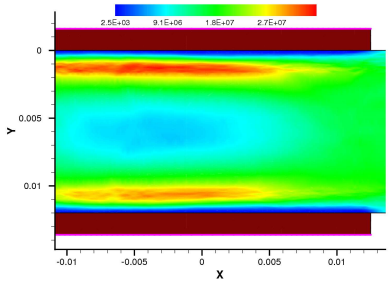

Figure 9: current density at $V_d = 0.7\,V$.

tum correction terms. Our approach has, thus, the advantages to be able to take into account self-consistently hot electron effects, generation-recombination processes as well as quantum confinement and tunneling in transport direction. Furthermore, the method is ideally parallelizable and automatically generates accurate models for the transport parameters in any devices.

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