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A Hierarchy of Quantum-Classical Transport Models in the Framework of the SDM Method

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INTRODUCTION

As the channel of semiconductor devices approaches the 10 nm length-scale, quantum effects like confinement, tunneling and interference effects must be taken into account when simulating such small devices. Fully quantum models provide an accurate description in these cases, but at the expense of high computational effort [1]. An alternative approach is to treat only certain regions in the device in a quantum mechanical manner, while the rest is dealt with by classical models [2]. The advantages of these hybrid methods are low computational effort in zones where less sophisticated models are applied and high accuracy in the quantum regions.

THE SUBBAND DECOMPOSITION METHOD (SDM)

We consider the splitting-up of the device into confinement and transport directions by applying the subband decomposition approach [3]. The electron evolution in the confinement direction z is governed by the 1D Schrödinger equation

$$-\frac{\hbar^2}{2}\frac{\partial}{\partial z}\left(\frac{1}{m_z}\frac{\partial \chi_p}{\partial z}\right) - q\Phi\chi_p = \epsilon_p\chi_p\,,$$

where χ_p are the transversal wave functions and ϵ_p the eigenvalues (energy subbands). The total energy reads $E_p = \epsilon_p + \epsilon_p^{\rm kin}$. The electron evolution in the transport direction x is described by the following hierarchy of quantum, kinetic or fluid models:

- In the stationary completely quantum case, the 2D wave functions are decomposed into the transversal wave functions χ_p and the longitudinal functions φ^p, which are given by a coupled system of 1D Schrödinger equations in the transport direction x. The electron density reads then
$$n(x,z) = \sum_p \int f_{FD}(E_p)\Big|\sum_j \varphi_E^j(x)\chi_j(x,z)\Big|^2 \frac{{\rm d}k}{2\pi}\,.$$
An efficient method combining the SDM method with the WKB approximation permits to obtain accurate results with reduced simulation costs [4].
- A kinetic description for the electron distribution function is given by the Boltzmann equation
$$\frac{\partial f_p}{\partial t} + \frac{1}{\hbar}\left[\nabla_x(f_p\nabla_k E_p) - \nabla_k(f_p\nabla_x E_p)\right] = \mathcal{Q}\,,$$
where $\mathcal{Q}$ accounts for electron-phonon collisions. The electron density is written as
$$n(x,z,t) = \sum_p \rho_p(x,t)|\chi_p(z;x,t)|^2\,,$$
where $\rho_p(x,t) = (2\pi^2)^{-1}\int f_p(x,k,t)\,{\rm d}k$. The numerical treatment is realized similar as in [5] by applying shock capturing algorithms.
- In a fluid description [6], the density of electrons remains the same, but for the Boltzmann statistics the occupation factor is
$$\rho_p(x,t) = \frac{n_s(x,t)}{\sum_p e^{-\epsilon_p(x,t)}}e^{-\epsilon_p(x,t)}\,.$$
The surface density n_s satisfies the Drift-Diffusion equation
$$\frac{\partial n_s}{\partial t} - \nabla_x\cdot(D(\nabla_x n_s + n_s\nabla_x U_s)) = 0\,,$$
where the effective energy U_s generated by the electrons itselves is given by
$$U_s(x,t) = -\log\Big(\sum_p e^{-\epsilon_p(x,t)}\Big)\,,$$

These models are self-consistently coupled with the Poisson equation for the electrostatic potential. Numerical results and comparisons of the different models will be presented. Each model accounts for other specific physical phenomena, where the interest of such a comparison.

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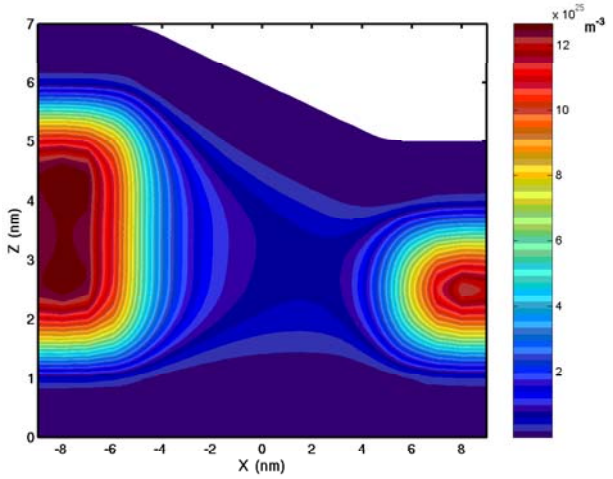

Fig. 1. Electron density for a trapezoidal MOSFET device in the quantum case for V_{DS} = 0.2 V and V_{GS} = 0.1 V.

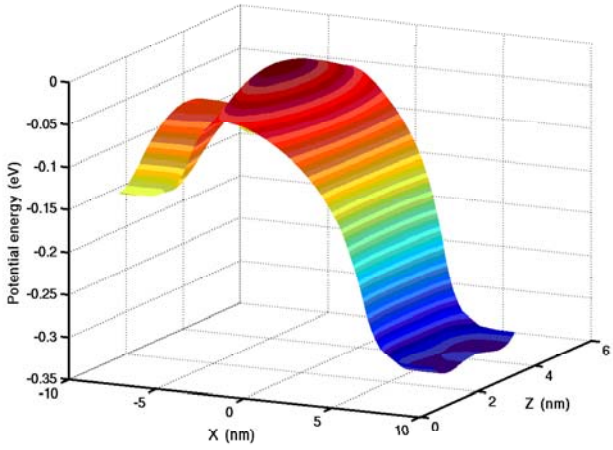

Fig. 2. Potential energy for a trapezoidal MOSFET device in the quantum case for V_{DS} = 0.2 V and V_{GS} = 0.1 V.

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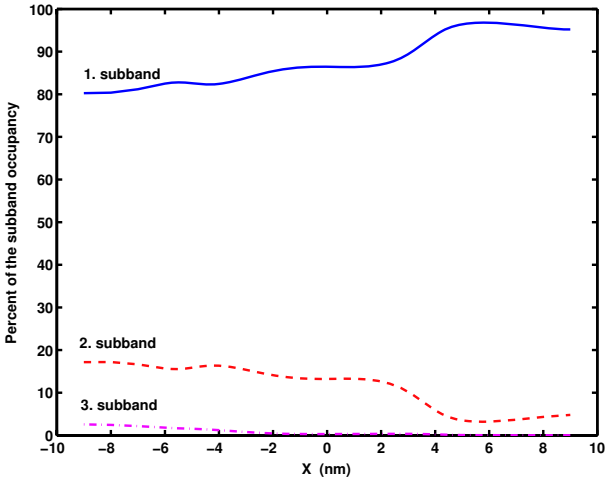

Fig. 3. Percentage of the subband occupancy for the considered trapezoidal device in the quantum case for V_{DS} = 0.2 V and V_{GS} = 0.1 V.

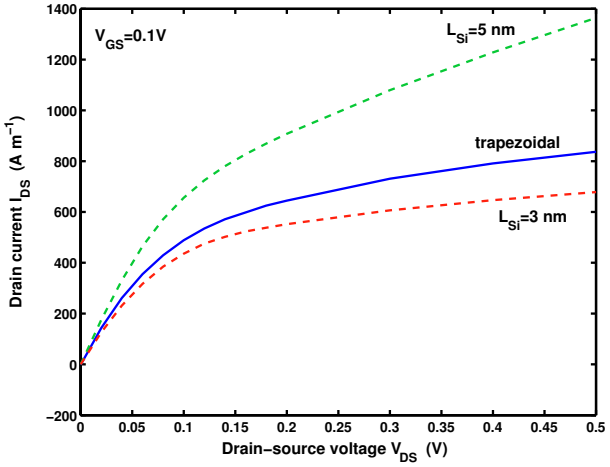

Fig. 4. Comparison of the current versus drain-source voltage characteristics in the quantum case for V_{GS} = 0.1 V for different device designs: rectangular MOSFETs (5 nm and 3 nm channel width) and a trapezoidal one.

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