Transport of partially quantized particles

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Motivation

There is a growing interest in nanoscale structures

- higher level of functionality
- higher operational speeds

With the decrease of channel dimensions quantum effects become nonnegligible :

- tunneling effects
- interference effects
- confinements

$\Longrightarrow$ quantum models.

Motivation

The aim of this work is to describe the transport of charged particles confined in a nanotransistor.
For devices composed of semiconductors, collisions occurs in the transport.
Incorporating collisions in quantum transport equations is a great challenge whereas it is well understood for classical transport. Many approach are considered :

- Adding a collision operator in quantum transport equations.
- Localizing the region where collisions occurs and use a hydrid description.
- Decoupling the directions with a quantum description in one direction and classical in others directions.

Plan

1. Introduction and modeling
2. Results and on-going works

Plan

1 Introduction and modeling

2 Results and on-going works

Introduction

Quantum transport of electrons is described by the Schrödinger equation :

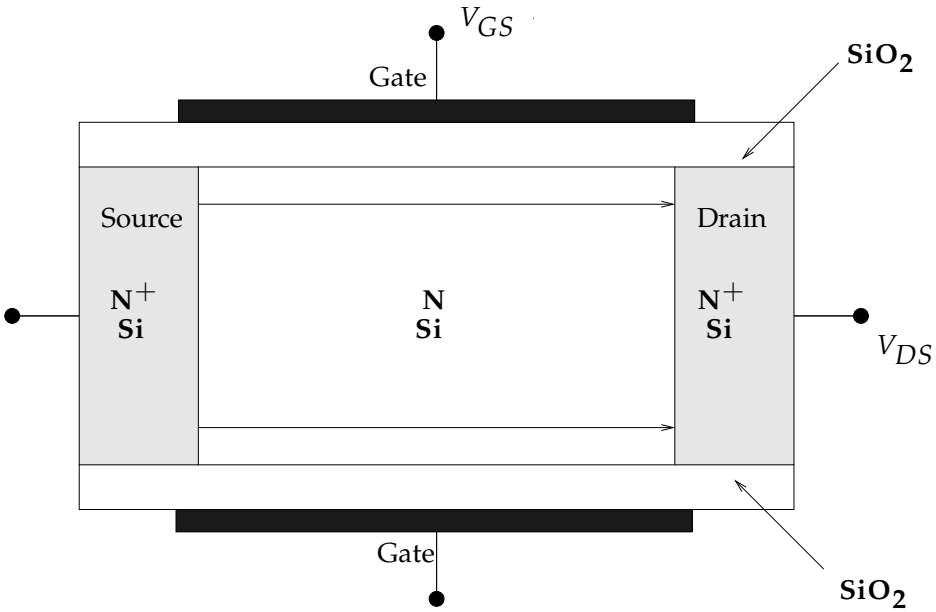
$$i\partial_t \psi = -\frac{1}{2}\Delta\psi + (V + V^{ext})\psi$$

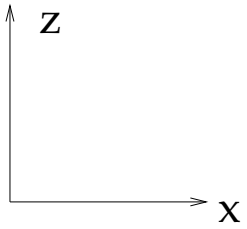
where $\psi(t,x)$ is the wave function and V the electrosatic potential and V^{ext} is an external potential.
The particle density is defined by $N = |\psi|^2$.
The selfconsistant potential V is usually computed by solving the Poisson equation

$$-\Delta V = N.$$

Introduction

In many devices, electrons might be extremely confined in one or several directions (for instance at the interface oxyde-semiconductor in nanotransistors).





$x \in \omega \subset \mathbb{R}^2$: transport direction
$z \in (0,1)$: confining direction

- Electrons are transported in the directions x parallel to the gas.
- Electrons are confined in the transverse direction z.

Semiclassical limit

The directions x parallel to the gas are semiclassical. Denoting ε the ratio between length scales in the transversal and longitudinal directions, after rescaling, we have :

$$i\varepsilon\partial_t\psi^\varepsilon = -\frac{\varepsilon^2}{2}\Delta_x\psi^\varepsilon - \frac{1}{2}\partial^2_{zz}\psi^\varepsilon + V\psi^\varepsilon.$$

The semiclassical limit is obtained by letting ε going to 0.
Formally it is natural to introduce the **subband** of the system

Subband decomposition method

Confinement in the transverse direction $z \in (0,1)$.

Energy is quantified in level ϵ_k called the *subband*.

$(\epsilon_k[V], \chi_k[V])_{k\geq 1}$ is the complete set of eigenvalues and eigenvectors of the stationary Schödinger equation :

Subband

$$\begin{cases} -\dfrac{1}{2}\dfrac{d^2}{dz^2}\chi_k + (V + V_c)\chi_k = \epsilon_k \chi_k, \\ \chi_k[V](0) = \chi_k[V](1) = 0, \quad \displaystyle\int_0^1 \chi_k \chi_{k'}\, dz = \delta_{k,k'}. \end{cases}$$

V_c : potential barrier.
V : electrostatic potential.

Semiclassical limit

Theorem [Ben Abdallah, Méhats '05]

The Wigner transform $W^\varepsilon(\psi^\varepsilon)$ of the solution of the rescaled Schrödinger equation converges weakly to

$$\sum_{k\geq 1} f_k(t,x,v)\chi_k(t,x,z)\chi_k(t,x,z')$$

where f_k is the distribution function and solves the Vlasov equation

$$\partial_t f_k + v\cdot\nabla_x f_k - \nabla_x \epsilon_k \cdot f_k = 0.$$

The charge density converges to

$$N(t,x,z) = \sum_{k\geq 1}\int_{\mathbb{R}^2} f_k\, dv\, |\chi_k(t,x,z)|^2.$$

Poisson equation

Poisson equation

$V(t,x,z)$ satisfies the Poisson equation

$$-\mathrm{div}_{x,z}(\varepsilon_R \nabla_{x,z} V(t,x,z)) = \frac{q}{\varepsilon_0}(N(t,x,z) - N_D),$$

where N_D is a doping profile,
N is the density of charge carriers,
ε_R, ε_0 are the permittivity.

The density is defined by

$$N(t,x,z) = \sum_{k=1}^{+\infty} \int_{\mathbb{R}^2} f_k(t,x) |\chi_k[V](z)|^2 \, dv.$$

Models

Schrödinger-Poisson 3D model

$$\Big\downarrow \text{ semiclassical limit}$$

classical/quantum coupled model :

$$\begin{cases} \text{Vlasov 2D,} \\ \text{Schrödinger 1D,} \\ \text{Poisson 3D.} \end{cases}$$

It justifies the use of classical/quantum coupled models where the coupling occurs in the momentum variable :

- classical in the longitudinal direction x,
- quantum in the transversal direction z.

Hierarchy of models

In semiconductors, collisions govern the motion of particles. Heuristically we can introduce collisions in the transport direction by adding a collision operator. At a kinetic level, we obtain then the Boltzmann equation for semiconductors :

Semiconductor Boltzmann transport equation

$$\partial_t f_k + (v \cdot \nabla_x f_k - \nabla_x \epsilon_k \cdot \nabla_v f_k) = Q(f)_k \,.$$

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Collisions drive the charged carriers towards a diffusive regime. In analogy with the classical case, we use then macroscopic models :

- Drift-diffusion coupled to Schrödinger-Poisson (**DDSP**),
- Energy-Transport (**ET**) coupled to Schrödinger-Poisson,
- Spherical Harmonic Expansion (**SHE**) coupled to Schrödinger-Poisson.

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Existence results

Existence for DDSP

The DDSP system admits a unique weak solution. Moreover, it converges exponentially fast towards its equilibrium as $t \to +\infty$.

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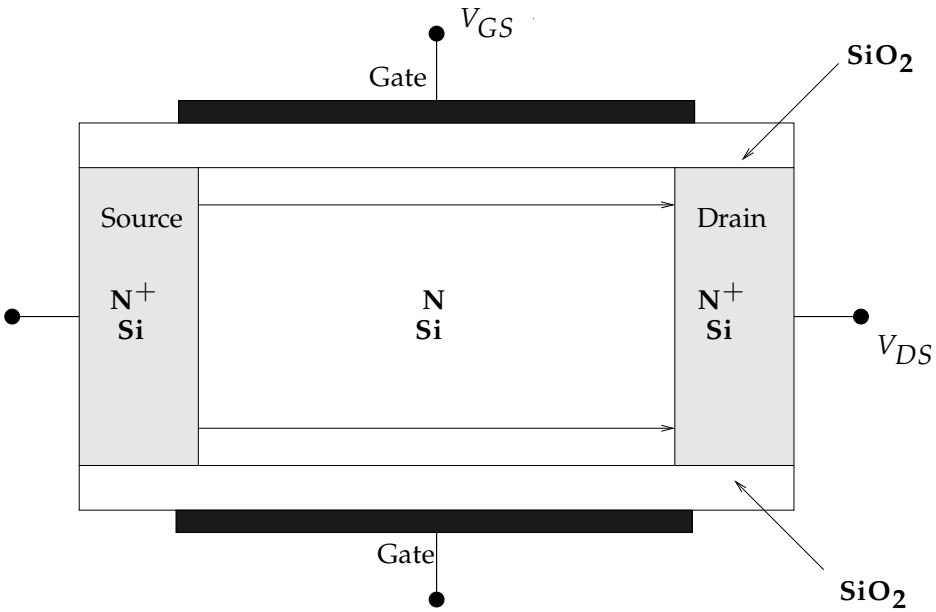
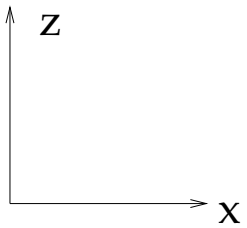
Diffusive limit

The Boltzmann-Schrödinger-Poisson system admits renormalized solutions when x lies in a bounded domain of $\mathbb{R}$. Moreover, as the mean free path goes to 0 its solutions converge towards solutions of the DDSP system.

Numerical results



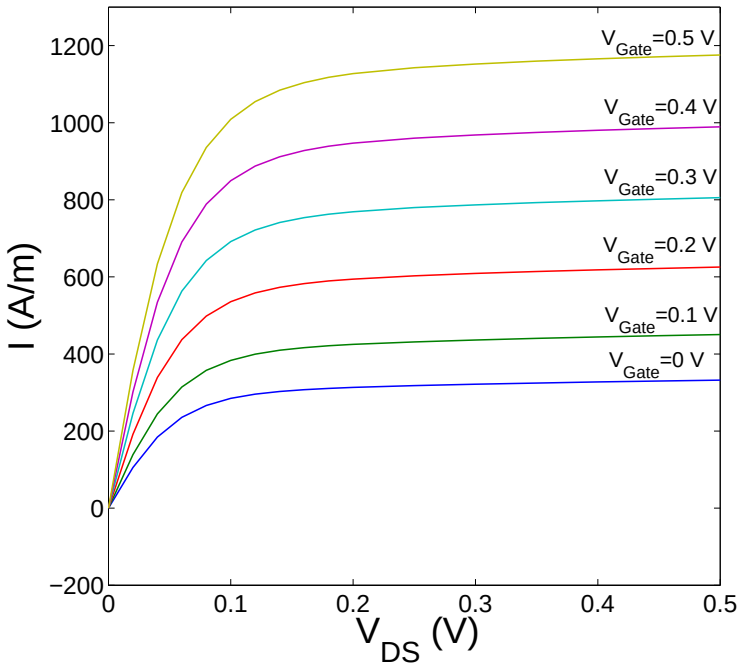


$x = (x_1, x_2)$: transport direction
z : confining direction

We will use the stationary quantum-classical coupled system $(DDSP)$ to obtain a numerical simulation of the transport of charged carriers.

Structure of Si invariant with respect to x_2 : $x = x_1$.

Numerical results



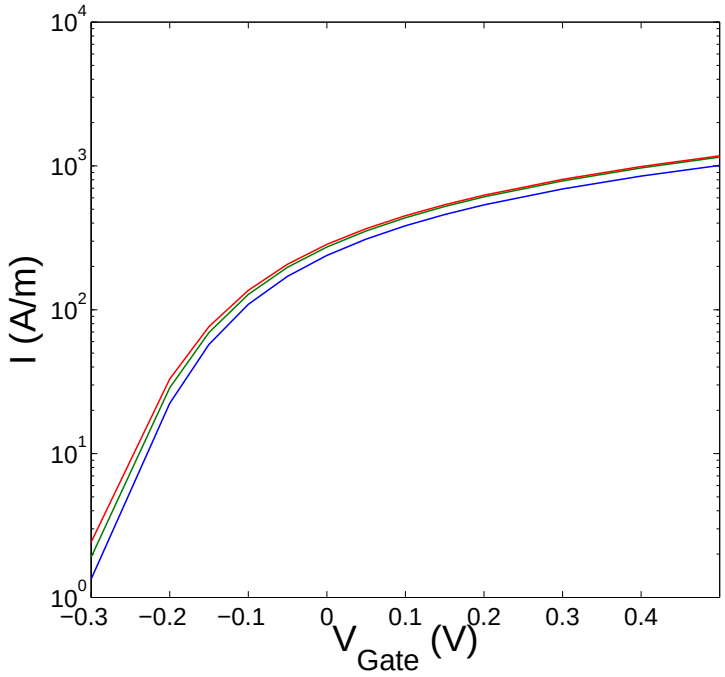
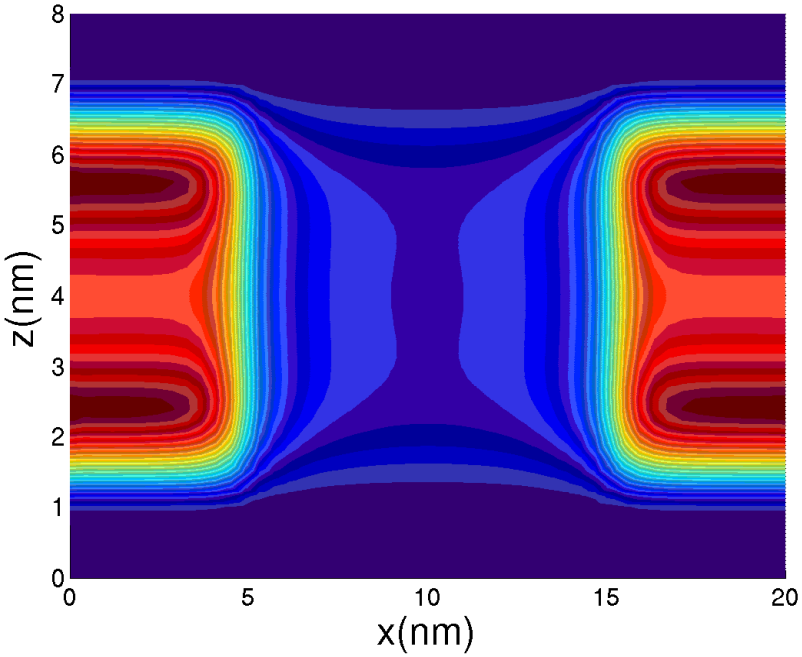


FIG.: Left : I-V characteristics for different V_{Gate} ; Right : charateristics current - V_{Gate}

Numerical results



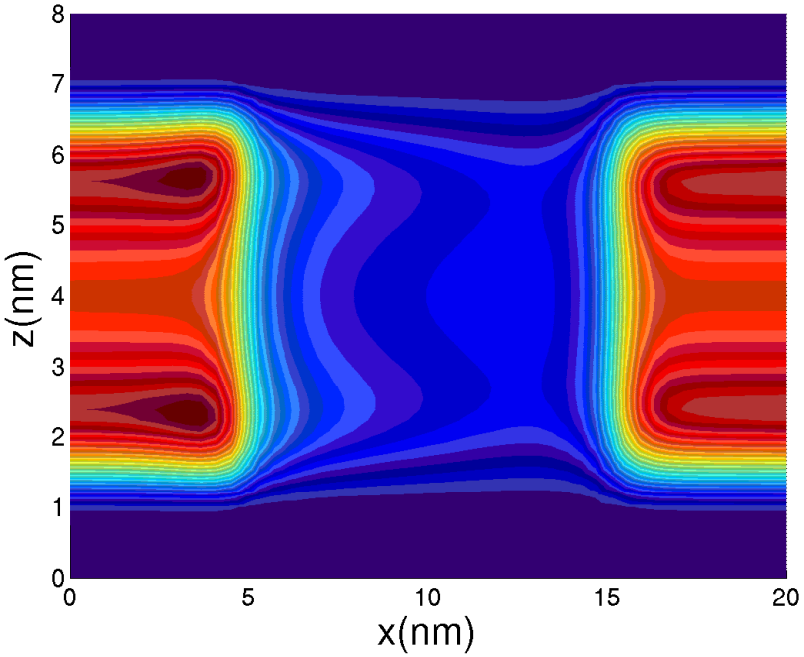
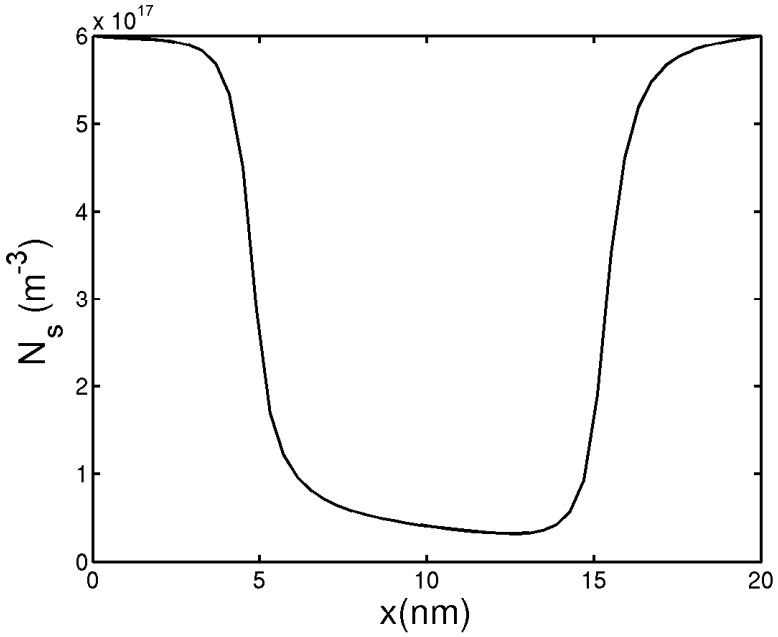


FIG.: Evolution of the density for $V_{DS} = 0V$ (left) and for $V_{DS} = 0.2V$ (right)

Numerical results



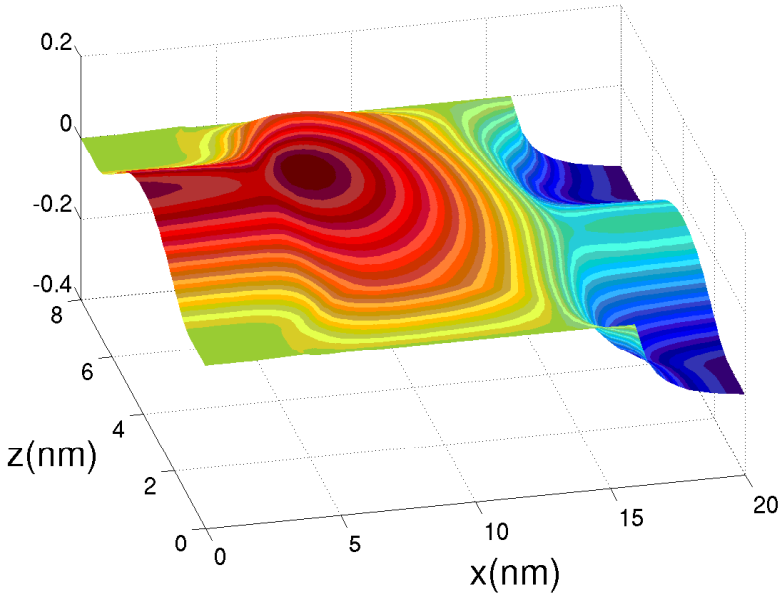


FIG.: Left : surface density for $V_{DS} = 0.2V$; Right : Potential energy for $V_{DS} = 0.2V$

On-going works and prospects

- Extension of the results for Energy-Transport coupled to Schrödinger-Poisson : temperature of the system is not constant.
- Rigorous derivation of the models : passage from the kinetic to the macroscopic models.
  $\longrightarrow$ computation of the constant in the diffusion matrix.
- Obtention of the Boltzmann-Schrödinger-Poisson model from the Schrödinger-Poisson 3D model.