A hybrid approach for the simulation of nanoscale MOSFETs

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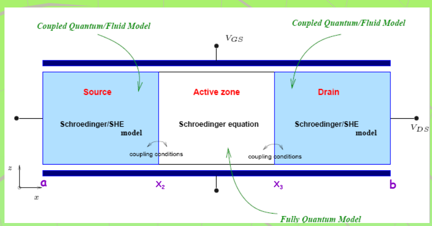
I. Motivation

Objective : Simulation of nanoscale semiconductor devices (10 nm channel-length).
Problem : Different physical phenomena occur in the different regions of the device. Quantum effects (interferences, tunneling, confinements) are localized in certain small regions, whereas in the remaining zones the transport behaves classically.
Mathematical approach : Domain decomposition methods.
Advantages of this hybrid approach :
- accurate results with inexpensive computational costs.
- comfortable inclusion of collisions in the classical zones.



II. Adiabatic quantum-fluid transport model

Purpose : Introduction of a numerically inexpensive Schrödinger/SHE model for the description of the electron reservoirs, in the time-dependent 3D case ($x \in R^2$, $z \in R$).

The electron density is given as

$$n(t,x,z) = \sum_{n\geq 1} \left(\int_{R^2} f_n(t,x,k)\, dk \right) |\chi_n(t,x,z)|^2 \,,$$

where the transversal wavefunctions χ_n are the eigenfct. of the ***1D Schrödinger operator*** in z

$$\begin{cases} -\frac{1}{2}\partial_{zz}\chi_n(t,x,\cdot) + V(t,x,\cdot)\chi_n(t,x,\cdot) = E_n(t,x)\chi_n(t,x,\cdot) \\ \int_0^1 \chi_n(t,x,z)\chi_m(t,x,z)dz = \delta_{nm}\,; \quad \chi_n(t,x,\cdot) \in H_0^1(0,1)\,. \end{cases} \qquad (1)$$

E_n: energy subbands. The distribution function f_n, associated to the n-th subband, is solution of the rescaled ***Boltzmann equation***

$$\begin{cases} \partial_t f_n + \frac{1}{\alpha}(k\cdot\nabla_x f_n - \nabla_x E_n \cdot \nabla_k f_n) = \frac{1}{\alpha^2} Q(f)_n \\ f_n(0,x,k) = f_{in,n}(x,k)\,. \end{cases} \qquad (2)$$

α: rescaled mean free path; $\mathbf{e}_n(t,x,k) = \frac{|k|^2}{2} + E_n(t,x)$: total energy; Q: elastic impurity collision op.

$$Q(f)_n(t,x,k) = \sum_{m\in N^*} \int_{R^2} \alpha_{nm} \delta(\mathbf{e}_n(t,x,k) - \mathbf{e}_m(t,x,k'))\, [f_m(t,x,k') - f_n(t,x,k)]\, dk' \,.$$

Diffusion limit $\alpha \to 0$, to get numerically cheaper methods :

Hilbert-Expansion : $f_n^\alpha = f_n^0 + \alpha f_n^1 + \alpha^2 f_n^2 + \cdots$

Inserting this Ansatz in the Boltzmann equation (2) and comparing terms of the same order in α, yields equations for f^0, f^1, f^2 :

$$Q(f^0) = 0\,, \quad Q(f^1)_n = k\cdot\nabla_x f_n^0 - \nabla_x E_n\cdot\nabla_k f_n^0\,, \quad Q(f^2)_n = \partial_t f_n^0 + k\cdot\nabla_x f_n^1 - \nabla_x E_n \cdot \nabla_k f_n^1\,. \qquad (3)$$

Properties of the collision operator enable to solve these equations. We have thus:

$$f_n^0(t,x,k) = F(t,x,\mathbf{e}_n)\,, \quad f_n^1(t,x,k) = -\vartheta_n(t,x,k)\cdot\nabla_x F(t,x,\mathbf{e}_n)\,,$$

with ϑ the unique solution in $Ker(Q)^\perp$ of $Q(\vartheta\lambda(\mathbf{e})) = -k\lambda(\mathbf{e})$.
To assure the solvability of the last equation in (3), it is necessary that ($S_{\epsilon-E_n}$: energy surface)

$$\sum_n \int_{S_{\varepsilon-E_n}} (\partial_t f_n^0 + k\cdot\nabla_x f_n^1 - \nabla_x E_n\cdot\nabla_k f_n^1)\, dN_{\varepsilon-E_n}(k) = 0\,, \quad \text{f.a.a.} \quad \varepsilon \geq E_1\,.$$

This yields, that F has to satisfy the following ***SHE model***

$$\begin{cases} \partial_t(NF) + \nabla_x\cdot J + \partial_\varepsilon(\kappa F) = 0\,, \\ J(t,x,\epsilon) = -D(t,x,\epsilon)\cdot\nabla_x F(t,x,\epsilon)\,, \end{cases} \qquad (4)$$

with the density of states N, the diffusion matrix D and the term κ given by

$$N(t,x,\varepsilon) = \sum_{n\in N^*} \int_{S_{\varepsilon-E_n}} dN_{\varepsilon-E_n}(k)\,, \quad D(t,x,\epsilon) = \sum_n \int_{S_{\epsilon-E_n}} k\otimes\vartheta_n dN_{\epsilon-E_n}(k)\,, \quad \kappa(t,x,\varepsilon) := \sum_n \partial_t E_n \int_{S_{\varepsilon-E_n}} dN_{\varepsilon-E_n}(k)\,.$$

III. The quantum/kinetic-quantum hybrid model

Purpose : Introduction of a hybrid model to describe the whole MOSFET device, in view of a numerical simulation of the stationary 2D case ($x \in R$, $z \in R$).

The electron density in the device is given as the superposition of mixed states

$$n^{\mathcal{A}}(x,z) := \sum_n \left(\int_{-\infty}^{\infty} f_n(x,k)dk \right) |\chi_n(x,z)|^2\,, \quad (x,z)\in I_1\cup I_3\,,$$

$$n^{\mathcal{Q}}(x,z) := \sum_n \int_0^\infty |\psi_{\epsilon,n}^+(x,z)|^2 f_n(x_2,k)dk + \sum_n \int_0^\infty |\psi_{\epsilon,n}^-(x,z)|^2 f_n(x_3,-k)dk\,, \quad (x,z)\in I_2\,.$$

Adiabatic model : The transversal direction is governed by the stationary Schrödinger operator (1), giving rise to χ_n. The distribution functions f_n are solutions of the Boltzmann equation with inflow boundary conditions (ν : absorption term)

$$\begin{cases} \frac{1}{\alpha}(k\cdot\nabla_x f_n - \nabla_x E_n\cdot\nabla_k f_n) + \nu f_n = \frac{1}{\alpha^2}Q(f)_n \quad \text{in} \quad [(a,x_2)\cup(x_3,b)]\times R \\ f_n(a,k) = F_a(\mathbf{e}_n(a,k))\,, \quad \text{for} \quad k>0 \\ f_n(b,k) = F_b(\mathbf{e}_n(b,k))\,, \quad \text{for} \quad k<0\,. \end{cases} \qquad (5)$$

Quantum model : The electron evolution in the active zone is described via the stationary 2D Schrödinger equation with open boundary conditions (QTBM)

$$-\frac{1}{2}\Delta\psi_{\epsilon,n}^\pm + V\psi_{\epsilon,n}^\pm = \epsilon\psi_{\epsilon,n}^\pm\,, \quad (x,z)\in I_2\,. \qquad (6)$$

Interface conditions : Adiabatic and quantum models are related by means of the statistics defined on the interfaces of the different zones. Let $f_n^\pm(x,\epsilon) := f_n(x, \pm\sqrt{2(\epsilon - E_n(x))})$.

$$\begin{aligned} f_n^-(x_2,\epsilon) &= \sum_l T_{l\to n}^-(\epsilon) f_l^-(x_3,\epsilon) + \sum_l R_{l\to n}^+(\epsilon) f_l^+(x_2,\epsilon)\,, \quad \epsilon > E_n(x_2) \\ f_n^+(x_3,\epsilon) &= \sum_l T_{l\to n}^+(\epsilon) f_l^+(x_2,\epsilon) + \sum_l R_{l\to n}^-(\epsilon) f_l^-(x_3,\epsilon)\,, \quad \epsilon > E_n(x_3)\,. \end{aligned} \qquad (7)$$

Reflection and transmission coefficients $T_{l\to n}^\pm$, $R_{l\to n}^\pm$ computed via the 2D wavefunctions $\psi_{\epsilon,n}^\pm$.
Coupling with Poisson equation for the electrostatic potential.

IV. Diffusion limit towards the quantum/fluid-quantum hybrid model

Purpose : Diffusion limit $\alpha \to 0$ in order to get the adequate interface conditions to couple the numerically cheaper quantum/fluid models with the fully quantum one.

Goal: Search for an $\mathcal{O}(\alpha^2)$ -approximation of the Boltzmann problem (5), (7).

Let $f_{2,n}^\alpha(x,k)$ (resp. $f_{3,n}^\alpha(x,k)$) be the distribution functions, associated to the regions (a,x_2) (resp. (x_3,b)). The same Hilbert expansion as in the time-dependent case yields :

$$f_{i,n}^0(x,k) = F_i^0(x,\mathbf{e}_n) \qquad f_{i,n}^1(x,k) = F_i^1(x,\mathbf{e}_n) - \vartheta_{i,n}(x,k)\cdot\nabla_x F_i^0(x,\mathbf{e}_n)$$

In order to obtain a second order approximation of the Boltzmann equation, F_i^0 and F_i^1 have to satisfy the following ***SHE equation***

$$\begin{cases} \nu F_i(x,\epsilon)N(x,\epsilon) + \nabla_x\cdot J_i(x,\epsilon) = 0 \\ J_i(x,\epsilon) = -D_i(x,\epsilon)\cdot\nabla_x F_i(x,\epsilon)\,. \end{cases} \quad i = 2,3 \qquad (8)$$

The first order ***interface and boundary conditions*** are deduced immediately

$$F_2^0(x_2,\epsilon) = F_3^0(x_3,\epsilon)\,; \quad F_2^0(a,\epsilon) = F_a(\epsilon)\,; \quad F_3^0(b,\epsilon) = F_b(\epsilon)\,, \quad \forall\epsilon > E_1(x_i) \qquad (9)$$

$$\begin{cases} D_2(x_2,\epsilon)\cdot\nabla_x F_2^0(x_2,\epsilon) = D_3(x_3,\epsilon)\cdot\nabla_x F_3^0(x_3,\epsilon)\,, \quad \forall\epsilon > E_1(x_2)\,, \; \epsilon > E_1(x_3)\,, \\ J_i^0(x_i,\epsilon) = D_i(x_i,\epsilon)\cdot\nabla_x F_i^0(x_i,\epsilon) = 0\,, \quad \forall\epsilon \leq E_1(x_2) \text{ or } \epsilon \leq E_1(x_3)\,. \end{cases} \qquad (10)$$

To deduce the second order interface conditions, we have to consider the slightly changed ***boundary layer Ansatz***

$$f_{i,n}^\alpha(x,k) = F_i^0(x,\mathbf{e}_n) + \alpha\Big(F_i^1(x,\mathbf{e}_n) - \vartheta_{i,n}(x,k)\cdot\nabla_x F_i^0(x,\mathbf{e}_n) + [\theta_{i,n}(\frac{x-x_i}{\alpha},k) - \theta_i^\infty(\mathbf{e}_n)]J_i^0(x_i,\mathbf{e}_n)\Big) + \alpha^2 f_{i,n}^2(x,k) + \alpha^3 f_{i,n}^3(x,k).$$

The θ are solutions of the ***Milne problem***, involving the reflection-transmission conditions

$$\begin{cases} k\partial_\xi\theta_{i,n}(\xi,k) = Q(\theta_i)_n(\xi,k)\,, \\ \Upsilon_{2,n}^-(\epsilon) = \sum_l T_{l\to n}^-(\epsilon)\Upsilon_{3,l}^-(\epsilon) + \sum_l R_{l\to n}^+(\epsilon)\Upsilon_{2,l}^+(\epsilon) \\ \Upsilon_{3,n}^+(\epsilon) = \sum_l T_{l\to n}^+(\epsilon)\Upsilon_{2,l}^+(\epsilon) + \sum_l R_{l\to n}^-(\epsilon)\Upsilon_{3,l}^-(\epsilon)\,, \end{cases} \qquad (11)$$

where $\Upsilon_{i,n}^\pm(\epsilon) = \theta_{i,n}(0,\pm\sqrt{2(\epsilon - E_n(x_i))}) + \vartheta_{i,n}(x_i,\pm\sqrt{2(\epsilon - E_n(x_i))})D_i^{-1}(x_i,\epsilon)\,.$

We have $\theta_{i,n}(\xi,k) \to_{|\xi|\to\infty} \theta_i^\infty(\mathbf{e}_n(x_i,k))$ .With $\theta(\epsilon) = \theta_2^\infty(\epsilon) - \theta_3^\infty(\epsilon)$ the F_i^1 satisfy finally

$$F_2^1(x_2,\epsilon) - F_3^1(x_3,\epsilon) = \theta(\epsilon)J_2^0(x_2,\epsilon)\,, \quad \forall\epsilon > E_1(x_2)\,, \; \epsilon > E_1(x_3)\,, \qquad (12)$$

together with the same current condition (10) as for F_i^0. Similarly the second order boundary conditions are deduced.

Conclusion : The solution F of the SHE model (8) with transmission condition

$$F_2(x_2,\epsilon) - F_3(x_3,\epsilon) = \alpha\theta(\epsilon)J_2(x_2,\epsilon)\,, \quad \forall\epsilon > E_1(x_2)\,, \; \epsilon > E_1(x_3)\,,$$

satisfying the current condition (10), as well as adequate boundary conditions, is an $\mathcal{O}(\alpha^2)$ approximation of the average of f_i^α (over the energy surface $S_{\epsilon-E_n}$) away from the interface

$$\frac{1}{N(x,\epsilon)} \sum_n \int_{S_{\epsilon-E_n}} f_{i,n}^\alpha(x,k) dN_{\epsilon-E_n}(k)\,.$$

Project:
- Numerical discretization of these interface and boundary conditions.
- Fast approximation of the Milne problem.
- Implementation of the whole hybrid model, using the efficient SDM/WKB method [3] for the resolution of the 2D Schrödinger equation.

Acknowledgments: This work has been supported by the ACI Nouvelles Interfaces des Mathématiques MOQUA (ACINIM 176-2004), the ACI Jeunes Chercheurs (JC 1035) and the GDRE 224 GREFI-MEFI.

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