Multidimensional Nanoscale device modeling: the Finite Element Method applied to the Non-Equilibrium Green's Function formalism

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Abstract— **This work deals with the modeling and the numerical simulation of quantum transport in multidimensional open nanoscale devices. The electron transport in the device is described using the Non-Equilibrium Green's Functions (NEGF) formalism and the variational form of the problem is solved using the finite element method (FEM). In this approach, the derivation of the boundary conditions at the interfaces of the device with the reservoirs, is used to calculate the self-energy functions. The FEM allows us to consider very complex geometries and non-uniform mesh, while the NEGF is a powerful formalism which will allow to include scattering in the problem. The simulations are performed by solving self-consistently the NEGF (equivalent to the open Schrödinger equation in ballistic regime) for the transport problem and the Poisson equation to account for the space charge effects.**

I. INTRODUCTION

The emergence of new simulation tools becomes critical in the exploration of quantum transport in nanoscale devices. The quantum transport modeling is usually defined by a self-consistent process between the calculation of the electron density using the NEGF formalism [1] and the calculation of the space charge effects using the Poisson's equation. The problem is solved in the device region of interest (computational domain) which is connected to the reservoirs using self-energy functions at the contacts (see Fig. 1). The discretization of the transport problem, as well as the definition of the self-energy matrices, are generally derived from the finite difference method (FDM) in uniform grids [2]. However, the modeling of multidimensionnal semiconductor devices, often requires the ability to accommodate irregular geometries.

Another approach presented in this article, consists to apply the finite element method on the variational form of the problem. One of the advantage of the finite element method which has been used extensively in engineering [3], is that the mesh can be varied to give high resolution where needed, and any kind of complex geometries can be considered. In this approach, we show that the self-energy functions are associated to open boundary conditions for the Schrödinger equation. One can show that the Schrödinger/Poisson system

is equivalent to the NEGF/Poisson system in ballistic regime [4]. However, in contrast to the Schrödinger approach, making use of the NEGF formalism will allow to include scattering processes in a direct way by using a self-energy function $[\Sigma_S]$.

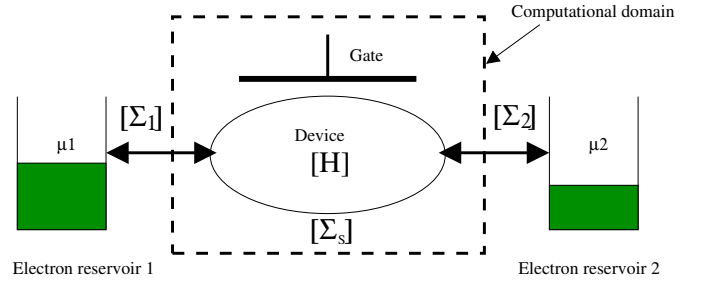## II. THE NON-EQUILBRIUM GREEN'S FUNCTION (NEGF) FORMALISM

Fig. 1. A device driven out of equilibrium by two contacts with different Fermi levels μ_1 and μ_2. $[\Sigma_1]$ and $[\Sigma_2]$ are respectively the self-energy matrices associated to the contact with the reservoir 1 and 2. A self-energy matrix $[\Sigma_S]$ can account for the scattering with the surrounding.

Denoting H the Hamiltonian of the infinite system, for a given energy E the Green's function is then defined as

$$(E - H)G(\mathbf{x}, \mathbf{x}') = \delta(\mathbf{x} - \mathbf{x}'). \tag{1}$$

It is possible to evaluate numerically the Green's function in our region of interest (computational domain) without having a deal with the entire infinite system. In this finite system, the effect of the reservoir j can be described by a self-energy function Σ_j (see Fig. 1), and the retarded Green's function is generally defined in the matrix notations by

$$[G(E)] = \left(E[S] - [H_0] - \sum_j [\Sigma_j(E)] \right)^{-1}, \tag{2}$$

where $[H_0]$ is the Hamiltonian of the isolated system, and $[S]$ is the overlap matrix of the basis functions used to discretize the

system (i.e. the identity matrix for orthogonal basis function). Denoting g_j the surface Green's function of the reservoir j then the self-energy matrices which are of the same size than $[H_0]$, are defined by

$$[\Sigma_j(E)] = [\tau_j][g_j][\tau_j^\dagger], \qquad (3)$$

where $[\tau_j]$ is a coupling matrix between the surface of the reservoir j and the whole device.

Denoting μ_j the fermi level associated to the reservoir j, the non-equilibrium density matrix is given by

$$[\rho] = \int_{-\infty}^{+\infty} \frac{dE}{2\pi} \sum_j f_{FD}(E - \mu_j)[A_j(E)], \qquad (4)$$

and one can show that

$$[A_j(E)] = [G(E)] \ [\Gamma_j(E)] \ [G^\dagger(E)], \qquad (5)$$

where Γ_j is the broadening function given by

$$[\Gamma_j] = i \left([\Sigma(E)] - [\Sigma^\dagger(E)]\right). \qquad (6)$$

The electron density n is given by the diagonal elements of the matrix density and depends on the potential U in the device (since $[H_0]$ depends on the potential U). To account for the space charge effect, the problem has to be solved self-consistently with the Poisson equation. The current density between the contacts 1 and 2, is finally given in ballistic regime by

$$I = \frac{2q}{h} \int_{-\infty}^{+\infty} dE \ T(E) \ (f_{FD}(E - \mu_1) - f_{FD}(E - \mu_2)), \qquad (7)$$

where $T(E)$ is the transmission coefficient defined by

$$T(E) = \text{Trace}[\Gamma_1 G \Gamma_2 G^\dagger]. \qquad (8)$$

To summarize, in the transport problem the NEGF formalism allows to describe the interactions of the reservoirs with the device by using self-energy functions. However, the concepts of self-energy is far more general, and a self-energy function $[\Sigma_S]$ can also be used to describe all kinds of interactions with the surroundings [2] (for example electrons-phonons or/and electrons-photons).

III. THE FINITE ELEMENT REPRESENTATION OF THE GREEN'S FUNCTION AND THE SELF-ENERGY FUNCTIONS

In contrast to the FDM, the FEM is based on the approximation of the solution of the differential equation while the original Hamiltonian operator remains unchanged. The approximate solution which is expanded in a local basis set, satisfies the differential equation only in an approximate way. In this way, the Hamiltonian operator of a closed system written in a discrete form $[H_0]$ using the FEM preserves its hermitian property even for a non-uniform mesh (the non-hermitian part of $[G]^{-1}$ comes from the self-energy matrices).

A. FEM applied to the Schrödinger equation

The stationary Schrödinger equation is defined in the multidimensional domain Ω by ($\mathbf{x} \in \Omega$)

$$H\Psi(\mathbf{x}) = E\Psi(\mathbf{x}). \qquad (9)$$

For a one band model, the Hamiltonian H is given within the effective mass approximation by

$$H = -\frac{\hbar^2}{2}\nabla\left(\frac{1}{m^*(\mathbf{x})}\nabla\right) + U(\mathbf{x}), \qquad (10)$$

where m^* is the effective mass and U is the potential energy.

Denoting $\varphi(\mathbf{x})$ an arbitrary test function in Ω, then the weak variational form of this equation is given by:

$$-\frac{\hbar^2}{2}\int_\Omega \nabla\left(\frac{1}{m^*}\nabla\Psi\right)\varphi d\Omega + \int_\Omega U\Psi\varphi d\Omega = E\int_\Omega \Psi\varphi d\Omega, \qquad (11)$$

where the equation (9) is multiplied by $\varphi(\mathbf{x})$ and integrated over Ω. The first term of this equation can be decomposed using the Green's identity such that

$$-\frac{\hbar^2}{2}\int_\Omega \nabla\left(\frac{1}{m^*}\nabla\Psi\right)\varphi d\Omega = \frac{\hbar^2}{2}\int_\Omega \frac{1}{m^*}\nabla\Psi\nabla\varphi d\Omega \qquad (12)$$
$$-\frac{\hbar^2}{2}\int_{\partial\Omega} \frac{1}{m^*}\left(\nabla\Psi \cdot \vec{\eta}\right)\varphi d_{\partial\Omega},$$

where $\vec{\eta}$ is the normal vector exterior along the boundary $\partial\Omega$ of the domain Ω. The second term of the right side of (12) is specified on the boundary, and then contains all information about the interactions with the contacts. Assuming that the wave functions vanishes at the device boundary except in the contact regions with the reservoirs, then the integral over the entire boundary $\partial\Omega$ in (12) can be decomposed into a sum over the contacts regions so-called γ_j

$$\sum_j -\frac{\hbar^2}{2}\int_{\gamma_j} \frac{1}{m^*}\left(\frac{\partial}{\partial\eta_j}\Psi\right)\varphi d\gamma_j. \qquad (13)$$

This term will be explicitly described in the case of open boundary conditions in the next section. For the case that this boundary term is equal to zero (using homogeneous Dirichlet or Neumann boundary conditions respectively $\Psi = 0$ and $\nabla\Psi = 0$ on the frontier $\partial\Omega$), the system becomes an isolated one, and we obtain the electronic states of a closed system. In the following, we propose to solve this problem making use of the FEM in the variational form (11).

Denoting $\mathbf{u} = u_1, \ldots, u_N$ the vector of the (unknown) nodal values of Ψ corresponding to a given mesh ($u_i \equiv \Psi(x_i)$ where x_i is the position of the ith node), and $\omega_i(\mathbf{x})$ the shape functions located on each node i such that $\omega_i(x_{i'}) = \delta_{ii'}$, then the wave function can be expanded approximately in this local basis function as:

$$\Psi_h(\mathbf{x}) = \sum_{i=0}^{N+1} u_i\omega_i(\mathbf{x}) \quad (\simeq \Psi). \qquad (14)$$

The test function φ can be expanded in a similar manner (we get φ_h). Inserting the expansions for Ψ_h and φ_h into the equations (11) and (12), we obtain then a generalized eigenvalue problem in the matrix notation:

$$[H_0]\mathbf{u} = E[S]\mathbf{u}, \tag{15}$$

with

$$[H_0]_{ii'} = \frac{\hbar^2}{2} \int_\Omega \frac{1}{m^*} \nabla\omega_i \nabla\omega_{i'} d\Omega + \int_\Omega U\omega_i\omega_{i'} d\Omega, \tag{16}$$

$$[S]_{ii'} = \int_\Omega \omega_i\omega_{i'} d\Omega. \tag{17}$$

These matrices are real sparse symmetric but in the most general case $[H_0]$ will be Hermitian (as for multi-band models). Transport problems often involve several discontinuities of the potential and of the effective mass at the interface between different materials. If these quantities are defined constants by element in an appropriate mesh, then they can be treated in an exact way in the equation 16).

B. Derivation of the self-energy with the contacts

The Green's function can be considered as the wave function at $\mathbf{x}$ resulting for a unit excitation applied at $\mathbf{x}'$. We are only interested by the retarded Green's function which represents the response of the system of an impulse excitation within the device ($\mathbf{x}' \in \Omega$). Therefore, we have to define such boundary conditions which appear transparent for the outgoing waves functions from the device to the contacts.

A general form of the transparent boundary condition on the interface γ_j for the outgoing solutions of the problem is supposed to supply a relation between the normal derivatives of the solutions and their boundary values (so-called a mixed boundary condition). In the NEGF formalism, these boundary conditions on γ_j are described by the operator τ_j in (3).

We propose to define the self-energy at the contacts γ_j, when the reservoirs can be considered as semi-infinite leads. This assumption means that the potential in the reservoirs is invariant by translation along the transport direction and then the outgoing solutions are plane waves. We deal with two particular one-band problems where the dispersion relation is parabolic in the contacts. The first (case 1) is related to an one dimensional problem with two contacts. The second (case 2) deals with a two or three dimensional problem with an arbitrary number of contacts (see Fig. 2).

Case 1
the outgoing plane waves solutions for Ψ_j^{out} in the local coordinate η_j are given by

$$\Psi_j^{out}(\eta_j) = A_j^- \exp(ik_j\eta_j), \tag{18}$$

where k_j is the wave vector associated to lead j and A_j^-, is the unknown outgoing coefficient. At the interface $\eta_j = 0$, one can show that

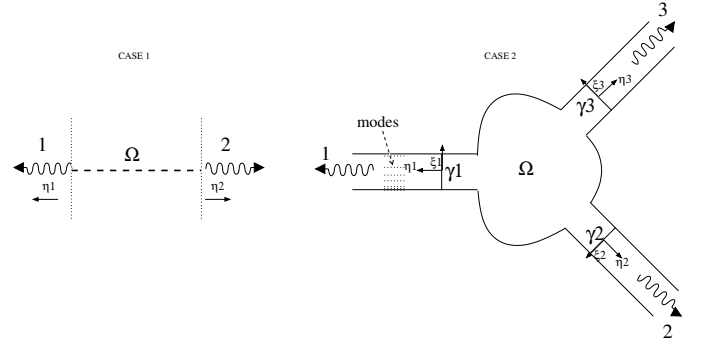$$\left.\frac{\partial}{\partial\eta_j}\right|_0 \Psi_j^{out}(\eta_j) = ik_j\Psi_j^{out}(0). \tag{19}$$

Fig. 2. Semi-infinite leads associated to a domain Ω. A 1D device is described on the left (case 1), and a 2D device on the right (case 2, which could be also interpreted as a section of a 3D device). We mention the local coordinates η_j, ξ_j associated to the lead j. The potential has an arbitrary form inside the domain Ω, but is assumed to be independent of the η_j direction in the lead j. For the case of 2D and 3D leads, one also has to account for transverse modes due to the confinement of the electrons in the direction ξ_j (where ξ_j can matched a 1D or a 2D coordinates respectively for a 2D or a 3D lead).

These boundary conditions are equivalent to those described in [5]. The boundary conditions also satisfy the following continuity relation at $\eta_j = 0$

$$\left.\frac{1}{m_j^*}\frac{\partial}{\partial\eta_j}\right|_0 \Psi_j^{out} = \left.\frac{1}{m^*}\frac{\partial}{\partial\eta_j}\right|_0 \Psi, \tag{20}$$

where m_j^* is the effective mass inside the contact j. Using the relations (19) and (20), the finite element discretization of the expression (13) can be written as $\sum_j [\Sigma_j]$, where the elements of the self-energy matrices $[\Sigma_j]$ are given by: $\forall j = 1, 2$

$$[\Sigma_j]_{ii'} = -\frac{\hbar^2}{2m_j^*} ik_j \delta_{i\in\gamma_j} \delta_{i'\in\gamma_j}. \tag{21}$$

Case 2
The outgoing plane waves solutions for Ψ_j^{out} in the local coordinates (η_j, ξ_j) of the contact j, become;

$$\Psi_j^{out}(\eta_j, \xi_j) = \sum_m A_{j,m}^- \chi_j^m(\xi_j) \exp(ik_j^m\eta_j), \tag{22}$$

where the unknown outgoing coefficients $A_{j,m}^-$, and the wave vector k_j^m, depend on the mode m which corresponds to the mth normalized eigenfunction χ_j^m in the transverse direction of lead j. ξ_j). At the interface $\eta_j = 0$, one can show that

$$\left.\frac{\partial}{\partial\eta_j}\right|_0 \Psi_j^{out}(\eta_j, \xi_j) = i\sum_m k_j^m \chi_j^m(\xi_j) \langle\chi_j^m(\xi_j)|\Psi_j^{out}(0,\xi_j)\rangle. \tag{23}$$

These conditions are equivalent to the quantum transmitting boundary conditions described in [6]. Using the relation (23) and (20) in the expression (13), the elements of the matrices $[\Sigma_j]$ are now given after discretization by: $\forall j$

$$[\Sigma_j]_{ii'} = -\frac{\hbar^2}{2}i\sum_m \frac{k_j^m}{m_j^*}\langle\chi_j^m(\xi_j)|\omega_i\rangle\langle\omega_{i'}|\chi_j^m(\xi_j)\rangle\delta_{i\in\gamma_j}\delta_{i'\in\gamma_j}, \tag{24}$$

where the effective mass in the lead j is assumed invariant along the transverse direction ξ_j.

Finally, for all the cases, the self-energy matrices are complex symmetric and their elements are only non-zero for points which belong to the frontier γ_j with the contact j.

IV. THE NUMERICAL SELF-CONSISTENT ALGORITHM AND APPLICATIONS

A P^1 finite element method is used to discretize both the NEGF problem and the Poisson equation on the same mesh. Because of the highly non-linear behavior of the coupled NEGF/Poisson system, we make use of the implicit Gummel iterations. An initial guess can be derived using a Thomas-Fermi/Poisson semi-classical approach, which is solved with a Newton-Raphson method. The examples in Fig. 3 and Fig. 4 obtained with the NESSIE code, are used to illustrate respectively the electron density calculations for 3D electron waveguides devices [7] (III-V heterostructure) and for 2D nanoscale MOSFETs [8] (Si/Si02 structure).
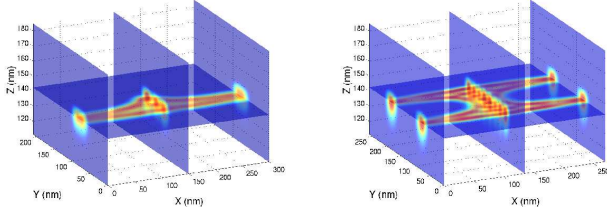

Fig. 3.   The density profile after the 3D quantum model convergence for the T-stub (left) and the directional coupler (right). The electron gas is localized a few nanometer below the AlGaAs/GaAs interface (at z=150nm) and quantum interference effects appear in the active region.
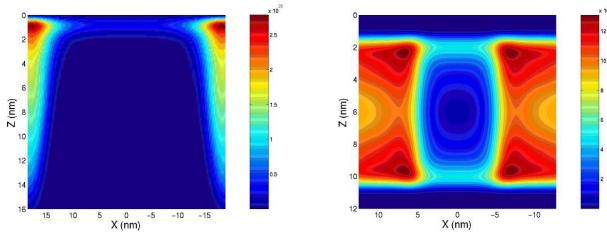

Fig. 4.   Density profile obtained at equilibrium with the 2D quantum self-consistent model for the 25nm MOSFET (left) and 10nm DG-MOSFET (right). The results show the confinement of the electrons in the channel(s).

One can show that the NEGF formalism in ballistic regime, involves the computation of a large number of independant

linear systems (only few number of column of the Green's function are required for a given energy). Therefore, for very large systems, the calculations of the electron density is extremely time consuming even with a parallel implementation, and a full-dimensional description of the transport is not often suitable to obtain the I-V curves in relevant time (however, we note the promising method [9] which is currently under study). In order to overcome these difficulties, we can apply a fast algorithm based on a subbands decomposition method which accounts for the confinement of the electrons in the structure, and then reduce the dimension of the transport problem. In practice, the method requires to subdivide the structures into a large number of (1D or 2D) slices along the transport direction. For a given potential, the method consists in solving many independent eigenvalues problems associated to each slice (see [10] for the trace minimization method). Then, the obtained multi-mode Hamiltonian reduced in this new basis function is solved using the FEM for all the energies. When all the subbands are coupled, this approach is equivalent to the full-dimensional one but having a much lower numerical cost [8] (see [11] for the uncoupled case). This approach was applied to study the coupling modes effects for the double-gate MOSFETs, and to investigate the 3D silicon nanowire transistors [12].

The FEM method applied to NEGF, can also be generalized to describe multi-band Hamiltonian where the self-energy functions need to be properly defined. For example, if we consider the spin transport properties in a device with spin "up", "down" selective contacts, the electron system can be split into two coupled subsystems composed of electrons having the same spin orientation (up,down). The FEM/NEGF technique is used to solve this two-band model for the electron-spin transport. Some obtained results with the simplified 1D problem have been shown in [13] and compared to one analytical case [14]. In order to simulate the spin-FET (as proposed in [15]), a 2D transport model for spintronics has also been implemented.

V. CONCLUSION

We have shown that the FEM can be used to discretize the NEGF formalism. This approach allows to consider non-uniform meshes and any kind of complex geometries.

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