Longitudinal effective mass models for ultra-scaled confined nanostructures

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Motivations

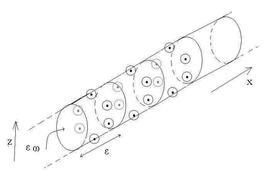
- New devices (diameter below to 3 nm) : silicon nanowires, carbon nanotubes...
- Ultra-scaled strongly confined structures exhibit electrical behavior that cannot be accounted for by using the dispersion relation of the bulk material.
- Assumption of infinite periodic structure in the wire cross section, which allow to derive the usual effective mass theorem, cannot be used anymore.

We find a longitudinal effective mass model, which consists of a device dependent Schrödinger equation for each n-th band.

- Fully quantum approaches are complex and computationally expensive.
- Boundary conditions are not easily imposed.
- Quantum models usually do not include collisions of charged particles.

We derive a nanowire classical transport model. Also, we use the quantum transport model in regions where quantum effects are strong and we couple it to the classical transport model in the rest of the device domain.

I Effective mass model



We consider the Schrödinger equation in a wire represented by $x \in \mathbb{R}$ and $z \in \epsilon\omega$:

$$\imath\hbar\partial_t\psi = -\frac{\hbar^2}{2m_e}\Delta\psi + \frac{1}{\epsilon^2}W_{\mathcal{L}}(\frac{x}{\epsilon},\frac{z}{\epsilon})\psi + V(x,\frac{z}{\epsilon})\psi,$$

$$\psi = 0 \text{ for } z \in \partial\epsilon\omega.$$

m_e : electron mass,
$W_{\mathcal{L}}$: ϵ-periodic potential generated by the lattice,
V : slowing varying (self consistent) potential,
ϵ : small parameter interpreted as the "lattice constant".

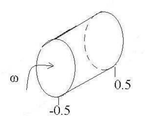
Next, the problem is rescaled. In particular, $z' = \frac{z}{\epsilon}$. For $(x, z') \in \mathbb{R} \times \omega$,

$$\imath\partial_t\psi = -\frac{1}{2}\partial_{xx}\psi - \frac{1}{2\epsilon^2}\Delta_{z'}\psi + \frac{1}{\epsilon^2}W_{\mathcal{L}}(\frac{x}{\epsilon},z')\psi + V(x,z')\psi. \quad (1)$$

Envelope function decomposition

(extending [2] to nanowires)

The orthonormal basis for the decomposition is made of generalized Bloch waves for $k = 0$, eigenfunctions in the unit cell $\mathcal{U} = (-0.5, 0.5) \times \omega$ of :



$$\begin{cases} -\frac{1}{2}\Delta\chi_n + W_{\mathcal{L}}\chi_n = E_n\chi_n. \\ \chi_n(y,z') = 0 \ \text{ on } \partial\omega, \quad \chi_n \text{ 1-periodic in } y. \\ \int_{\mathcal{U}} |\chi_n|^2 dy dz' = 1. \end{cases} \quad (2)$$

For every function $\psi \in L^2(\mathbb{R}\times\omega)$ there exists a unique sequence $\{f_n^\epsilon, ... | n \in \mathbb{N}\}$ such that the Fourier transform $\widehat{f}_n^\epsilon$ has support in $(-\pi/\epsilon, \pi/\epsilon)$ and such that

$$\psi(x,z') = \sum_n f_n^\epsilon(x)\chi_n(\frac{x}{\epsilon},z') \ . \quad (3)$$

K.p model

$$\begin{aligned}\imath\partial_t f^\epsilon_{n,kp}(t,x) &= -\frac{1}{2}\partial_{xx}f^\epsilon_{n,kp}(t,x) + \frac{1}{\epsilon^2}E_n f^\epsilon_{n,kp}(t,x) \\ &\quad - \frac{1}{\epsilon}\sum_{n'} P_{nn'}\partial_x f^\epsilon_{n',kp}(t,x) + \sum_{n'} V_{nn'}(x) f^\epsilon_{n',kp}(t,x), \end{aligned} \quad (4)$$

with the following quantities

$$V_{nn'}(x) = \int_\omega V(x,z')g_{nn'}(z')dz',$$

$$g_{nn'}(z') = \int_{-0.5}^{0.5} \chi_n\chi_{n'}dy \quad \text{and} \quad P_{nn'} = \int_{-0.5}^{0.5}\int_\omega \partial_y\chi_{n'}\chi_n dy dz'.$$

Effective mass dynamics

$$\imath\partial_t f^\epsilon_{n,em}(t,x) = -\tfrac{1}{2m_n^*}\partial_{xx}f^\epsilon_{n,em}(t,x) + \tfrac{1}{\epsilon^2}E_n f^\epsilon_{n,em}(t,x) + \sum_{n'} V_{nn'}(x) f^\epsilon_{n',em}(t,x) \quad (5)$$

where m_n^* is the n-th band effective mass given by

$$\frac{1}{m_n^*} = 1 - 2\sum_{n'\neq n}\frac{P_{nn'}P_{n'n}}{E_n - E_{n'}}.$$

Filtering the oscillations $f^\epsilon_{n,em}(t,x) = h^\epsilon_{n,em}(t,x)e^{-\imath E_n\frac{t}{\epsilon^2}}$

$$\imath\partial_t h_{n,em}(t,x) = -\frac{1}{2m_n^*}\partial_{xx}h_{n,em}(t,x) + V_{nn}(x)h_{n,em}(t,x). \quad (6)$$

II Algorithm and transport strategy

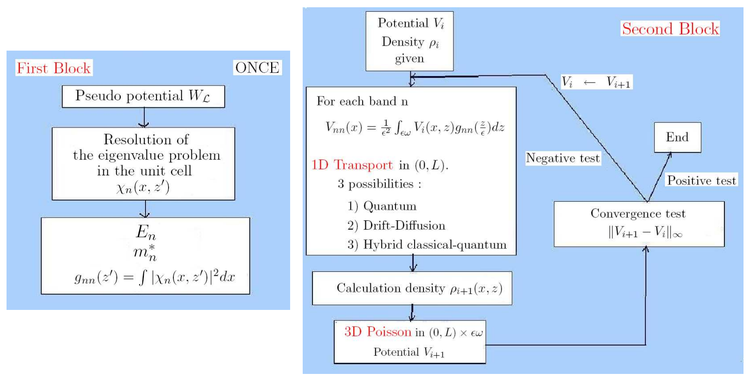


Fig - General organization of the model.

- First step : Resolution of the generalized Bloch problem (2). It is done only once for a given device.
- Second step : Coupling of 1D transport equations (including the parameters computed in the first step) and the 3D Poisson equation by means of a Gummel iterative method.

1) Quantum approach

The macroscopic charge density is given by

$$\rho(x,z) = \sum_n N_{1D}^n(x)g_{nn}(\frac{z}{\epsilon}). \quad (7)$$

N_{1D}^n is the 1D density carried by the n-th band. It is given by superimposing the densities of states injected from Source and Drain :

$$N_{1D}^n(x) = \int_{-\infty}^{+\infty}\phi_n(k)|\psi_{n,k}|^2 dk. \quad (8)$$

$\psi_{n,k}$ is the wave function solution of the stationary Schrödinger equation (resulting of (6)) with transparent boundary conditions. $\phi_n(k)$ is the reservoir statistic (we use the Boltzmann statistic).

2) Nanowire drift-diffusion model

In the classical model, the 1D density N_{1D}^n can be described by

$$N_{1D}^n(x) = \int_{-\infty}^{+\infty} N_s(x)\mathcal{M}_n(x,k)dk. \quad (9)$$

The function $\mathcal{M}_n$ is the Maxwellian

$$\mathcal{M}_n(x,k) = \frac{\hbar}{\sqrt{2\pi k_B T m_n^*}\mathcal{Z}(x)}e^{-\left(\frac{\hbar^2k^2}{2m_n^*}+E_n+V_{nn}\right)/(k_BT)} \quad (10)$$

where the repartition function $\mathcal{Z}$ is given by

$$\mathcal{Z}(x) = \sum_{n=1}^{+\infty} e^{-\left(E_n+V_{nn}\right)/(k_BT)} \ \text{ such that } \ \sum_{n=1}^{+\infty}\int_{\mathbb{R}}\mathcal{M}_n(x,k)dk = 1. \quad (11)$$

The surface density N_s satisfies the nanowire drift-diffusion equation

$$\partial_t N_s - \partial_x\Big(\mu k_B T\partial_x N_s + \mu N_s\partial_x V_s\Big) = 0 \quad \text{with} \quad V_s = -k_BT\log(\mathcal{Z}). \quad (12)$$

This equation is obtained via a diffusive limit from a set of Boltzmann equations posed on each n-th band, analogously to [3].

3) Hybrid classical-quantum model

The drift-diffusion model is used in large doped regions where the transport is expected to be classical in a highly collisional regime, whereas the fully quantum model is chosen for the active zone.

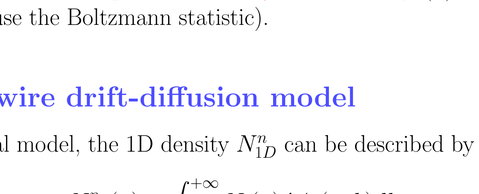


Fig - Schematic representation of hybrid model regions.

Following [1], interface conditions are obtained by imposing continuity of the current J at interfaces :

$$J(x_1) = J(x_2) := J,$$

$$e^{-\varphi(x_1)/(k_BT)} - e^{-\varphi(x_2)/(k_BT)} = \Theta_{\mathcal{Q}}J.$$

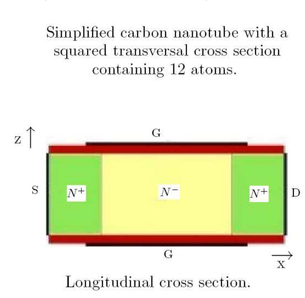
φ is the unknown electro-chemical potential and $\Theta_{\mathcal{Q}}$ is a positive coefficient depending on the reflection-transmission coefficient (quantum part). When we use the Boltzmann statistic, $\Theta_{\mathcal{Q}}$ can be computed explicitly.

III Numerical results

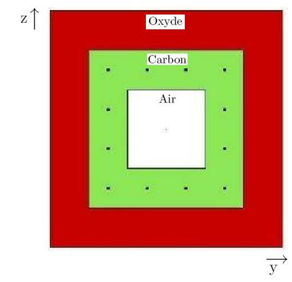
A simplified carbon nanotube as toy device

We study a carbon nanotube. The wire section (2nm) is tiny and the transport direction (channel of 10nm) is solved for a gate-all-around FET.

Simplified carbon nanotube with a squared transversal cross section containing 12 atoms.



Longitudinal cross section.



Transversal cross section with 12 atoms.

L	l	D_{N+}	D_G	N^+	N^-
30nm	2nm	10nm	20nm	1e26 m^{-3}	1e21 m^{-3}

Fig - Scheme of the toy device.

First block results

We present the first eigenstate, 2 eigs. corresponding to a multiple eigenvalue and one associated with higher energy. We recognize the 12 atom structure.

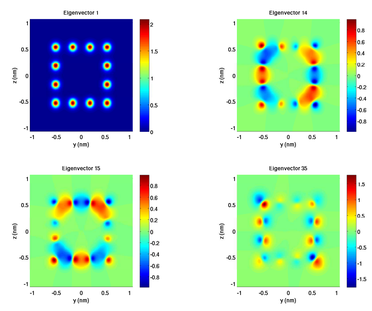


Fig - Eigenvectors χ_n at the cross section $x = 0$ for 1st, 14th, 15th and 35th mode (from left to right and top to bottom).

Second block results

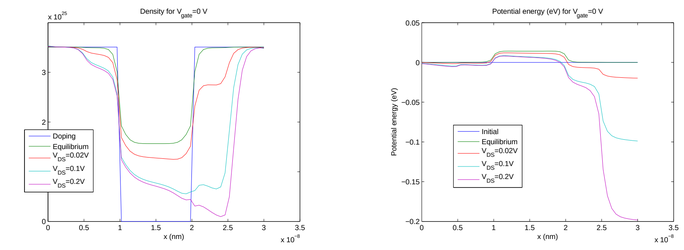


Fig - Densities (m^{-3}) in the left and potential energies (eV) in the right for different applied voltages. These 1D curves are results of an integration of 3D quantities over the 2D wire section.

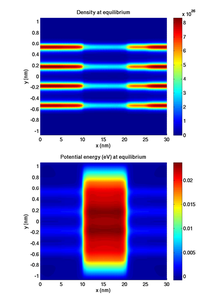


Fig - 2D slices of density (top) and potential (bottom) at equilibrium. x-axis is the transport direction. These slices cross 4 atoms.

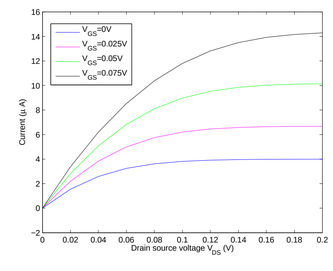


Fig - Current-voltage curves for different gate potential V_{GS} (0, 0.025, 0.05 and 0.075 V).

These curves are obtained with the hybrid approach, which improves the result quality and decreases the computational cost, compared to the fully quantum model. Even in this over simplified problem, our models are able to capture the qualitative behavior of the current for ultra-scaled confined nanostructures.

References

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