# Transport diffusif d’un gaz d’électrons confiné dans une nanostructure.

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# Motivation



There is a growing interest in nanoscale structure

- higher level of functionality
- higher operational speeds

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- higher operational speeds

With the decrease of channel dimensions :

- quantum effects become nonnegligible $\longrightarrow$ quantum model.

Modeling and simulation of nanotransistors is of great importance for future electronics.

# Outline



I) Introduction

- Hybrid quantum-classical modeling for an electron gas confined in a nanostructure
- Presentation of the Drift-Diffusion-Schrödinger-Poisson (DDSP) system

II) Analysis of the DDSP system : Existence, uniqueness result and long time behaviour

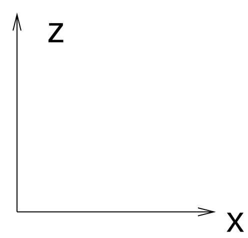
III) Numerical results : Simulation of the transport of charge carriers in a Double-Gate MOSFET

# Introduction



In nanoscale semiconductor devices, electrons might be extremely confined in one or several directions due to length scales.

- transport direction $x$
- confining direction $z$

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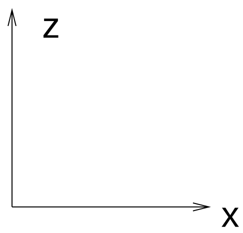


$$x \in \omega \subset \mathbb{R}^2$$
$$z \in (0, 1)$$

Two descriptions for the model :

- classical in the transport direction.
- quantum in the confining direction.
- coupled quantum/classical model when the coupling occurs in the momentum variable.

# Subband model



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

- Quantization of energy levels $\epsilon_k$.

# Subband model



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

➠ Quantization of energy levels $\epsilon_k$.

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

$$\begin{cases} -\frac{\hbar^2}{2}\frac{d}{dz}\left(\frac{1}{m_*(z)}\frac{d}{dz}\chi_k\right) + (qV + U_c)\chi_k = \epsilon_k\chi_k, \\ \chi_k[V](0) = \chi_k[V](1) = 0, \quad \int_0^1 \chi_k\chi_{k'}\,dz = \delta_{k,k'}. \end{cases}$$

$U_c$ : potential barrier.

$V$ : electrostatic potential.

# Poisson equation



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

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

where $N_D$ is a doping profile,

$N$ is the density of charge carriers,

$\varepsilon_R$, $\varepsilon_0$ are the permittivity.

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$\rho_k$ : occupation number of each state

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

# Transport direction



Classical transport equation for $x \in \omega$.

Collisions with phonons drive the electrons towards a diffusive regime.

In a kinetic regime, the transport is described by the Boltzmann equation. The diffusive regime is obtained by letting the mean free path $\eta$ going to $0$.

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Let $f_k^\eta(t,x,v)$ be the distribution function of the $k$th subband at the time $t$, the position $x$ and velocity $v$.

$$\partial_t f_k^\eta + \frac{1}{\eta}(v \cdot \nabla_x f_k^\eta - \nabla_x(\beta \epsilon_k) \cdot \nabla_v f_k^\eta) = \frac{1}{\eta^2} Q(f^\eta)_k,$$

for $\beta = 1/(k_B T)$, $k_B$ the Boltzmann constant and $T$ the temperature of the lattice.

# Transport direction

**Proposition :** For Boltzmann statistics the collision operator $Q$ in the linear BGK approximation satisfies

(i) $\displaystyle\sum_k \int_{\mathbb{R}^2} Q(f)_k\, dv = 0.$

(ii) $Q$ is a linear, self adjoint, negatif bounded operator.

(iii) Ker $Q$ = Span $\{\mathcal{M}\}$ where the Maxwellian

$$\mathcal{M}_k(t,x,v) = \frac{1}{2\pi\mathcal{Z}(t,x)} e^{-v^2/2-\beta\epsilon_k(t,x)}.$$

The repartition function is defined by

$$\mathcal{Z}(t,x) = \sum_k e^{-\beta\epsilon_k(t,x)}.$$

# Transport direction



Formally, if we assume that $f_k^\eta$ admits an Hilbert expansion $f^\eta = f^0 + \eta f^1 + O(\eta^2)$. Then

$$Q(f^0)_k + \eta Q(f^1)_k + O(\eta^2) = \eta(v\cdot\nabla_x f_k^0 - \nabla_x(\beta\epsilon_k)\cdot\nabla_v f_k^0) + O(\eta^2).$$

Thus,

$$f_k^0 = N_s \mathcal{M}_k, \ \forall\, k \geq 1,$$
$$f_k^1 = -Q^{-1}(-v\mathcal{M})_k(\nabla_x N_s + N_s \nabla_x V_s)$$

where $V_s(t,x) = -\log(\mathcal{Z}(t,x))$ is the effective potential.

# Drift-Diffusion equation



$$\partial_t f_k^\eta + \frac{1}{\eta}(v \cdot \nabla_x f_k^\eta - \nabla_x(\beta \epsilon_k) \cdot \nabla_v f_k^\eta) = \frac{1}{\eta^2} Q(f^\eta)_k.$$

By summing and integrating, we have

$$\partial_t \int \sum_k f_k^\eta \, dv + \frac{1}{\eta} \int \sum_k v \cdot \nabla_x f_k^\eta \, dv = 0.$$

Letting formally $\eta \to 0$ gives

**(DD)** $$\partial_t N_s + \mathrm{div}_x J = 0,$$

where the current $J = -\mathbb{D}(\nabla_x N_s + N_s \nabla_x V_s)$, and the diffusion matrix

$$\mathbb{D} = \sum_k \int_{\mathbb{R}^2} Q^{-1}(-v\mathcal{M})_k \otimes v \, dv.$$

In the following $\mathbb{D}$ is assumed to be given.

# The coupling



The occupation factor $\rho_k^\eta = \int_{\mathbb{R}^2} f_k^\eta \, dv$ satisfies at the limit :

$$\rho_k(t,x) = N_s(t,x) \frac{e^{-\beta\epsilon_k(t,x)}}{\mathcal{Z}(t,x)}.$$

Therefore,

$$\begin{aligned} N(t,x,z) &= \sum_{k=1}^{+\infty} \rho_k(t,x) |\chi_k(t,x,z)|^2 \\ &= \sum_{k=1}^{+\infty} N_s(t,x) \frac{e^{-\beta\epsilon_k(t,x)}}{\mathcal{Z}(t,x)} |\chi_k(t,x,z)|^2. \end{aligned}$$

And $N_s(t,x) = \displaystyle\int_0^1 N(t,x,z)\, dz$ is the surface density.

# The whole system



$$\partial_t N_s - \mathrm{div}_x \left(\mathbb{D}(\nabla_x N_s + N_s \nabla_x V_s)\right) = 0,$$

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

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$$N = N_s \sum_{k\geq 1} \frac{e^{-\beta\epsilon_k}|\chi_k|^2}{\sum_k e^{-\beta\epsilon_k}}\,; \qquad V_s = -\log\left(\sum_{k\geq 1} e^{-\beta\epsilon_k}\right).$$

# Part I
## Analysis of DDSP : Existence, uniqueness and long time behaviour

# The DDSP system



$$\partial_t N_s - \mathrm{div}_x \left(\mathbb{D}(\nabla_x N_s + N_s \nabla_x V_s)\right) = 0,$$

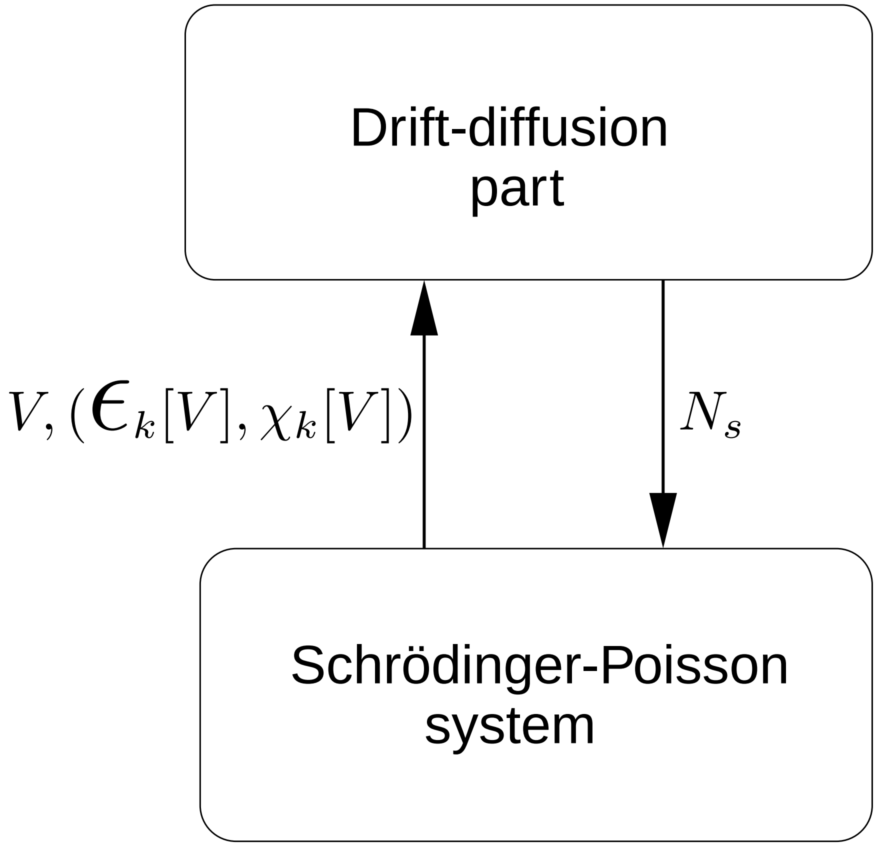
$$\begin{cases} -\dfrac{1}{2}\dfrac{d^2}{dz^2}\chi_k[V] + V\chi_k[V] = \epsilon_k[V]\chi_k[V] \\ \chi_k[V] \in H^1(0,1), \ \displaystyle\int_0^1 \chi_k[V]\chi_\ell[V]\,dz = \delta_{k\ell} \end{cases}$$

$$-\Delta_{x,z} V = N,$$

$$N = N_s \sum_{k\geq 1} \frac{e^{-\epsilon_k[V]}|\chi_k[V]|^2}{\sum_k e^{-\epsilon_k[V]}}; \quad V_s = -\log\Big(\sum_{k\geq 1} e^{-\epsilon_k[V]}\Big).$$

# Structure of the system






Analogy with the classical Drift-diffusion-Poisson model

- Entropy estimate
- Fixed point procedure
- Analysis of the Schrödinger-Poisson system

# References



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- *Vlasov-Poisson :* Ben Abdallah, Poupaud
- *Schrödinger-Poisson :* Nier
- *Vlasov-Schrödinger-Poisson :* Ben Abdallah- Méhats
- *Long time behaviour :* Arnold- Markowich- Toscani- Unterreiter, Dolbeault- Del Pino, ...
- *Spectral properties of the Hamiltonian :* Pöschel- Trubowitz

# Results



*First approach :* $\mathbb{D} = Id$

**Theorem :** Let $T > 0$ be fixed and the initial and boundary conditions smooth. The DDSP system admits a unique weak solution such that

$$N_s \in C([0,T], L^2(\omega)) \cap L^2((0,T), H^1(\omega))$$
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$(N_s^\infty, V^\infty)$ solution of the stationary problem.

**Theorem :** If the boundary conditions are at thermal equilibrium. There exist $\lambda > 0$ and $C > 0$ such that for all $t \geq 0$,

$$\|N_s - N_s^\infty\|_{L^2(\omega)}(t) + \|V - V^\infty\|_{H^1(\omega)}(t) \leq Ce^{-\lambda t}.$$

# Entropy estimate



We define the relative entropy

$$
\begin{aligned}
W \quad &= \sum_k \int_\omega \left(\rho_k \log(\rho_k/\underline{\rho_k}) - \rho_k + \underline{\rho_k}\right) dx \\
&+ \frac{1}{2}\int_\Omega |\nabla_{x,z}(V - \underline{V})|^2 \, dxdz \\
&+ \sum_k \int_\omega \rho_k \left(\epsilon_k[V] - \epsilon_k[\underline{V}] - \langle |\chi_k|^2 (V - \underline{V})\rangle\right) \, dx,
\end{aligned}
$$

(underlined quantities are extension of boundary data).

**Proposition :** If $(N_s, V)$ is a weak solution of DDSP, then $\forall t \in [0,T]$, $0 \leq W(t) < C_T$. Thus,

$$
\rho_k \in L^\infty((0,T), L \log L(\omega)) \text{ and } V \in L^\infty((0,T), H^1(\Omega)).
$$

# $L^2$ estimate ( $\mathbb{D} = Id$ ) 

**Proposition :** If the initial condition $N_s^0 \in L^2(\omega)$ and if we have a weak solution $(N_s, V)$ of the DDSP system. Then we have a bound on $\|N_s\|_{L^2(\omega)}$ depending only on $T$ and on the data.

*(The fact that $\mathbb{D} = Id$ allows to use integrations by parts)*

# Schrödinger-Poisson system ( $\mathbb{D} = Id$ ) 

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

$$-\Delta_{x,z} V = N_s \sum_{k\geq 1} \frac{e^{-\epsilon_k[V]}|\chi_k[V]|^2}{\sum_k e^{-\epsilon_k[V]}}.$$

**Proposition :** Let $N_s \in L^2(\omega)$ such that $N_s \geq 0$. Then the SP system admits a unique solution $(V, (\epsilon_k, \chi_k)_{k\geq 1})$, which satisfies the estimates $\|V\|_{H^2(\Omega)} \leq C(N_s)$. Moreover, for two arbitrary data $N_s$ and $\widetilde{N_s}$, the corresponding solutions satisfy :

$$\|V - \widetilde{V}\|_{H^2(\Omega)} \leq C(N_s, \widetilde{N_s})\, \|N_s - \widetilde{N_s}\|_{L^2(\omega)}.$$

($C(N_s)$ denotes a constant depending only on $\|N_s\|_{L^2(\omega)}$.)

**Idea of the proof :** We consider the functional

$$J(V,N_s) = J_0(V) + J_1(V,N_s)$$
$$= \frac{1}{2}\int_\Omega |\nabla_{x,z}V|^2 + \int_\omega N_s \log(\sum_k e^{-\epsilon_k[V]})\,dx.$$

$J$ is a continuous, strongly convex, coercive on $H^1(\Omega) \Rightarrow$ admits a unique minimizer.

A weak solution of the Schrödinger-Poisson system is a critical point of $J$.

# Fixed point procedure



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$$\partial_t \widehat{N_s} - \mathrm{div}_x(\nabla_x \widehat{N_s} + \widehat{N_s} \nabla_x V_s) = 0,$$

with $V_s = -\log(\sum_k \exp(-\epsilon_k[V])) \longrightarrow F(N_s) = \widehat{N_s}$.

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$F$ is a contraction on $M_{T_0} = \{n \,:\, \|n\|_T \leq 2\|F(0)\|_1\}$ for $T_0$ small enough and

$$\|n\|_T^2 = \max_{0\leq t\leq T} \|n(t)\|^2_{L^2(\omega)} + \int_0^T \|n(t)\|^2_{H^1(\omega)}\, dt.$$

Entropy $\Rightarrow$ extend to $[0, T]$.$\square$

# Existence results ( $\mathbb{D} \neq Id$ )



For $\mathbb{D} \neq Id$

$$\partial_t N_s - \text{div}_x(\mathbb{D}(\nabla_x N_s + N_s \nabla_x V_s)) = 0,$$

coupled to the Schrödinger-Poisson system.

**Assumption :** $\mathbb{D}$ is a $C^1$ function on $\bar{\Omega}$ into the set of $2 \times 2$ symmetric positive definite matrix such that $\mathbb{D}(x) \geq \alpha\, Id$ for $\alpha > 0$.

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**Theorem :** Let $T > 0$, the DDSP system admits a weak solution such that

$$N_s \log N_s \in L^\infty([0,T], L^1(\omega)) \text{ and } \sqrt{N_s} \in L^2([0,T], H^1(\omega)),$$

$$V \in L^\infty([0,T], H^1(\omega)).$$

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**Idea of the proof :**

- Regularize the system.
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- Regularize the system.
- Entropy estimate : with our assumption cf case $\mathbb{D} = Id$.
- Existence of solutions for the regularized system (cf case $\mathbb{D} = Id$).
- Passing to the limit in the solution of the regularized system as the regularization tends to $0$ : Aubin-Lions compactness method.

What sense can we give to $N_s \sum_k \frac{e^{-\epsilon_k}}{\mathcal{Z}} |\chi_k|^2$ for $N_s \in L \log L(\omega)$ and $V \in H^1(\Omega)$ ?

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We have

$$\|\chi_k[V]\|_{L_z^\infty(0,1)} \leq C(1 + \|V\|_{L_z^2(0,1)}^{1/2}).$$

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We have

$$\|\chi_k[V]\|_{L_z^\infty(0,1)} \leq C(1 + \|V\|_{L_z^2(0,1)}^{1/2}).$$

And with the Young inequality

$$\int_\omega N_s \|V\|_{L_z^2(0,1)} dx \leq \|V\|_{H^1(\Omega)} \int_\omega (N_s \log N_s - N_s + e^{\frac{\|V\|_{L_z^2(0,1)}}{\|V\|_{H^1(\Omega)}}}) \, dx$$

Trudinger inequality : $\exists \, \gamma > 0$ such that for all $u \in H^1(\omega)$

$$\int_\omega \exp\left(\gamma \frac{u(x)^2}{\|u\|_{H^1(\omega)}^2}\right) \, dx < +\infty.$$

# Long time behaviour



We define the relative entropy

$$\begin{aligned} W^\infty(t) &= \sum_k \int_\omega (\rho_k \log(\rho_k/\rho_k^\infty) - \rho_k + \rho_k^\infty)\, dx \\ &+ \frac{1}{2}\int_\Omega |\nabla_{x,z}(V - V^\infty)|^2\, dxdz \\ &+ \sum_k \int_\omega \rho_k(\epsilon_k[V] - \epsilon_k[V^\infty] - \langle|\chi_k|^2(V - V^\infty)\rangle)\, dx. \end{aligned}$$

The relative entropy $W$ measures the distance to the equilibrium and decreases :

$$\frac{d}{dt}W^\infty(t) = D(t) = -\sum_k \int_\omega e^{-\mathbb{D}\epsilon_k} |\nabla(\log(N_s e^{V_s}))|^2\, dx.$$

Two methods :

1) For an insulating system $\Longrightarrow$ conservation of the mass.

- Logarithmic Sobolev inequality to prove

$$\frac{d}{dt}W^{\infty}(t) \leq -\lambda W^{\infty}(t)$$

(for a positive constant $\lambda > 0$) $\Longrightarrow W^{\infty}(t) \leq e^{-\lambda t} W^{\infty}(0)$.

- Csiszàr-Kullack inequality

$$\|\rho - \rho^{\infty}\|_{\ell^1(L^1(\omega))} \leq C_1 W^{\infty}(t) \leq C_1 W^{\infty}(0)\, e^{-\lambda t}.$$

# Long time behaviour



2) Non conservation of the mass (f.e. Dirichlet boundary condition) : Linearization of the entropy

$$n_s = N_s - N_s^{\infty};\ v_s = V_s - V_s^{\infty};\ v = V - V^{\infty}.$$

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➠ convergence of the relative entropy

$$\lim_{t \to +\infty} W(t) = 0.$$

Thus $\|n_s\|_{L^1(\omega)} \to 0$ and $\|v\|_{H^1(\Omega)} \to 0$ as $t$ goes to $+\infty$.

# Long time behaviour



➠ quadratic approximation of the relative entropy :

$$L(t) = \frac{1}{2}\int_\omega \frac{(n_s)^2}{N_s^\infty}\,dx + \frac{1}{2}\int_\Omega |\nabla v|^2\,dxdz$$
$$+ \int_\omega N_s v_s\,dx - \int_\Omega N v\,dxdz.$$

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**Lemma :** We have

$$\frac{1}{2}\int_\omega \frac{(n_s)^2}{N_s^\infty}\,dx + \frac{1}{2}\int_\Omega |\nabla v|^2\,dxdz \le L(t).$$

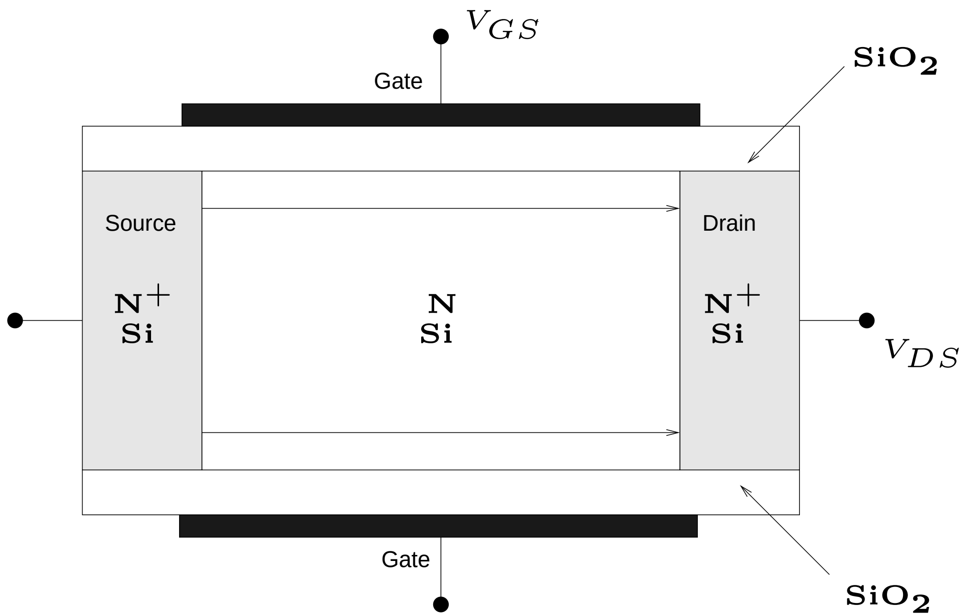
There exists $t_* > 0$ such that

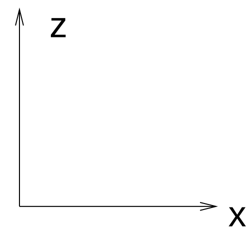
$$\forall\, t > t_*,\ \frac{d}{dt}L(t) \le -C_0 L(t).$$

# Part II
## Numerical simulations

# Simulated structure






$x = (x_1, x_2)$: transport dir.

$z$: confining dir.

Classical transport in the $x$ direction

Quantum description in the $z$ direction

➠ quantum-classical coupled system

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

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# The whole system



$$\mathrm{div}_x \left(\mathbb{D}(\nabla_x N_s + N_s \nabla_x V_s)\right) = 0,$$

$$\begin{cases} -\frac{\hbar^2}{2}\frac{d}{dz}\left(\frac{1}{m_*(z)}\frac{d}{dz}\chi_k[V]\right) + (qV + U_c)\chi_k[V] = \epsilon_k[V]\chi_k[V] \\ \chi_k[V](0) = \chi_k[V](\ell) = 0, \quad \int_0^\ell \chi_k \chi_{k'}\, dz = \delta_{k,k'}. \end{cases}$$

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

$$N = N_s \sum_{k\geq 1} \frac{e^{-\beta\epsilon_k}|\chi_k|^2}{\sum_k e^{-\beta\epsilon_k}}\, ; \qquad V_s = -\log\left(\sum_{k\geq 1} e^{-\beta\epsilon_k}\right).$$

# Numerical resolution : boundaries 

In $z = 0$ and $z = \ell$ :

Mixed boundary conditions for the potential.

- Gate : ohmic contacts $\Rightarrow$ Dirichlet,
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Mixed boundary conditions for the potential.

- Gate : ohmic contacts $\Rightarrow$ Dirichlet,
- insulating frontier $\Rightarrow$ Neumann.

At the source and drain :

High dopping $N^+ \Rightarrow$ Drain and Source are equivalent to small electrons reservoirs.

- density and potential are independent of the transport direction.

# Gummel iteration



At the source :

- ➠ Schrödinger-Poisson 1D.

# Gummel iteration



At the source :

➠ Schrödinger-Poisson 1D.

No Drain-Source voltage applied : the Fermi level $\epsilon_F = \log(N_s e^{V_s})$ is constant = its values at the boundary,

➠ Schrödinger 1D – Poisson 2D.

# Gummel iteration



At the source :

- Schrödinger-Poisson 1D.

No Drain-Source voltage applied : the Fermi level $\epsilon_F = \log(N_s e^{V_s})$ is constant = its values at the boundary,

- Schrödinger 1D – Poisson 2D.

Small perturbation :

- Diagonalization of the 1D Schrödinger operator.
- Computation of the density : Drift-Diffusion 1D.
- Computation of the potential : Poisson 2D.
- Loop on the potential.

# Numerical results



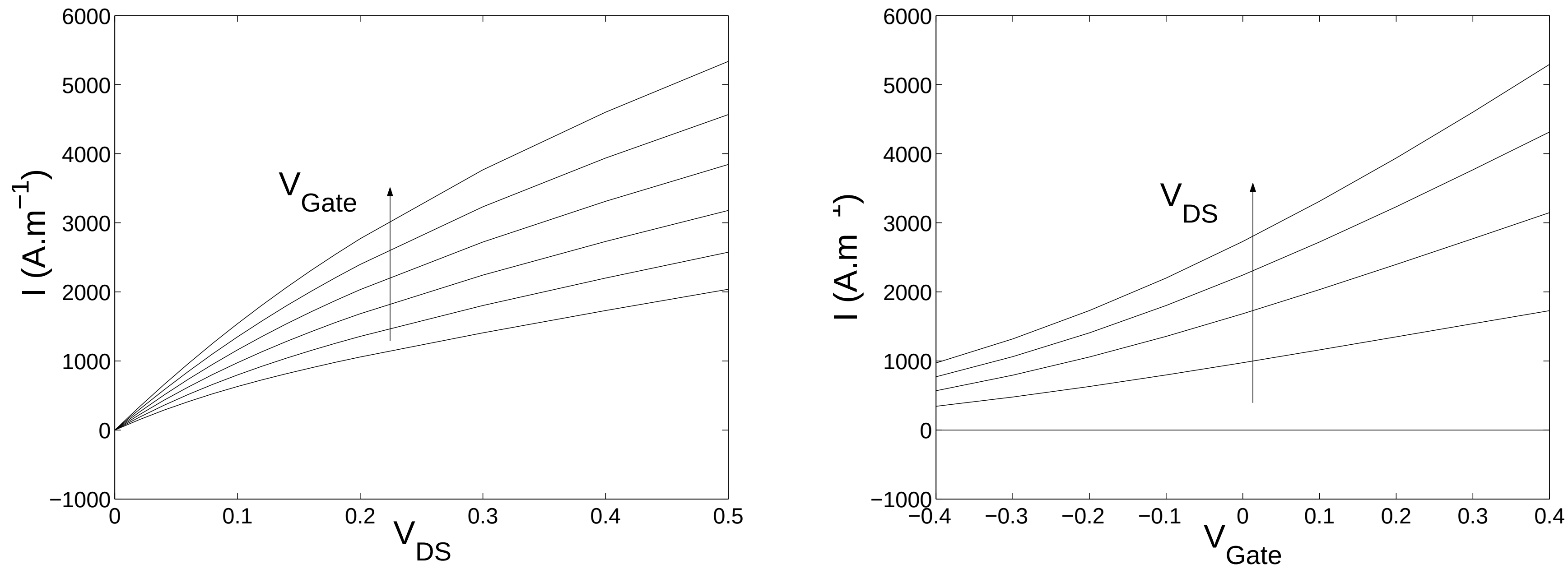



Figure 1: Left : I-V characteristics for different $V_{Gate}$; Right : charateristics current - $V_{Gate}$

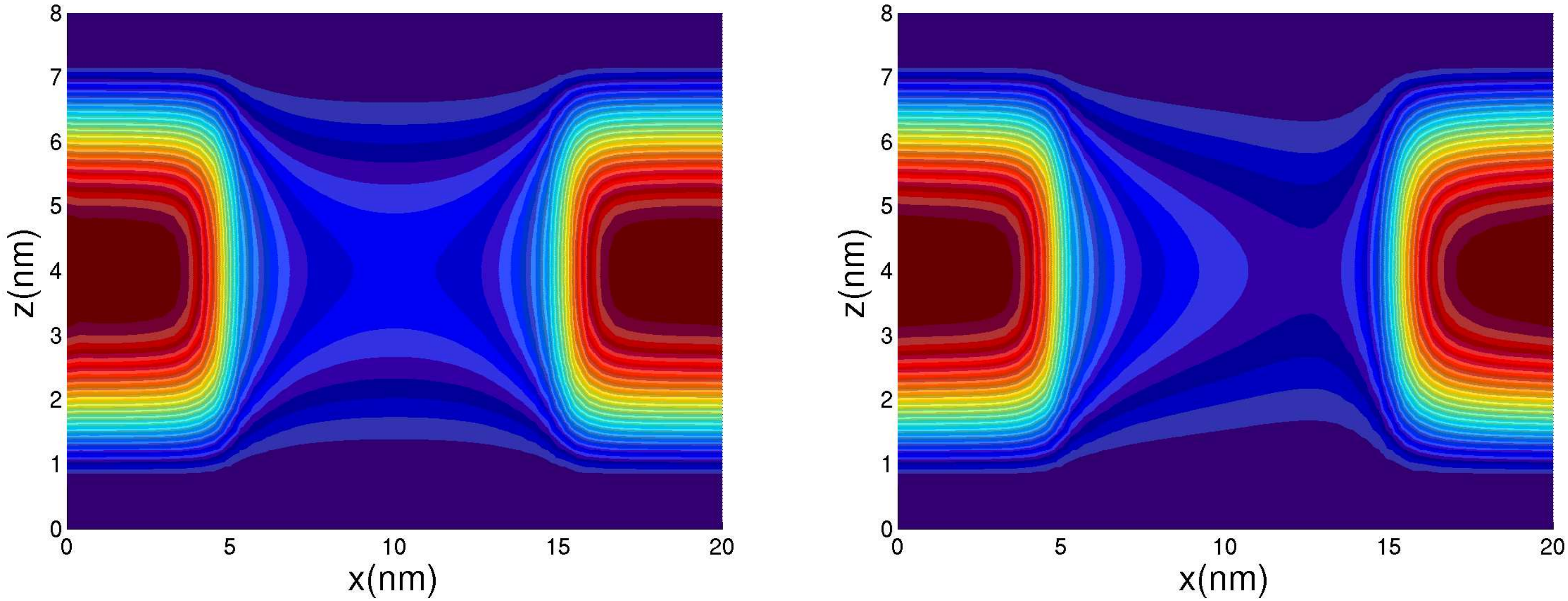



Figure 2: Evolution of the density for $V_{DS} = 0V$ (left) and for $V_{DS} = 0.2V$ (right)

# Numerical results

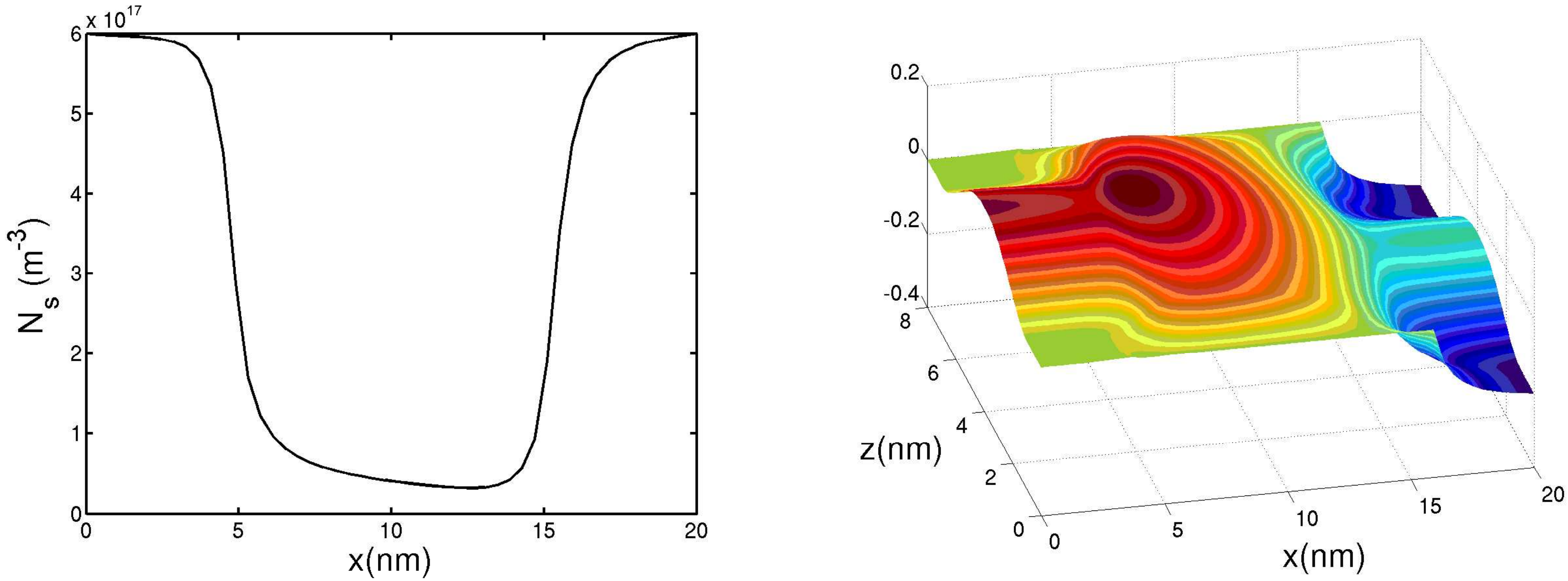


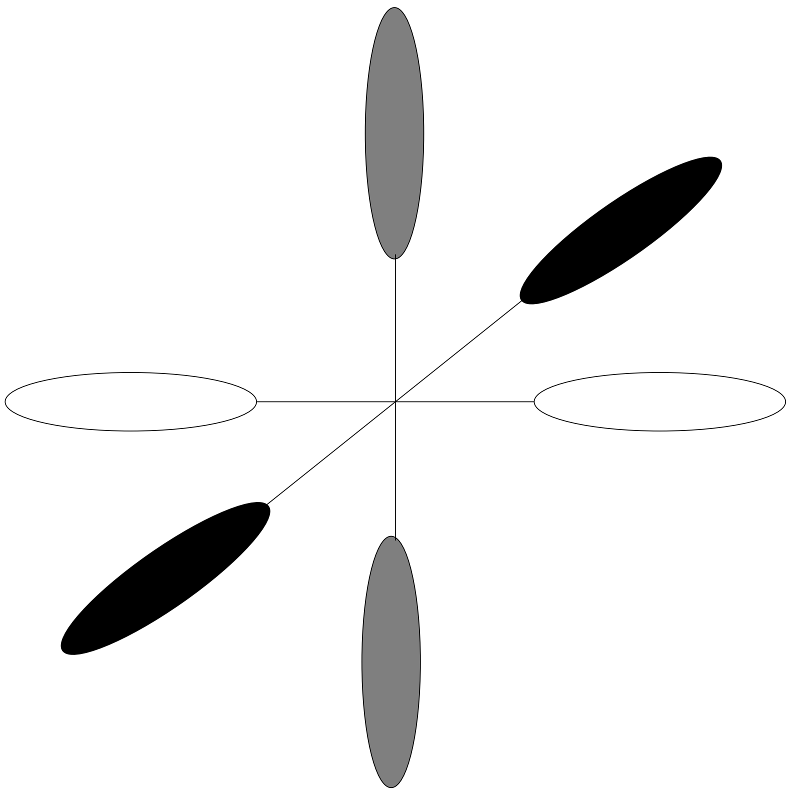

Figure 3: Left : surface density for $V_{DS} = 0.2V$; Right: Potential energy for $V_{DS} = 0.2V$

# Numerical results : 3 valleys



Anisotropics effects in silicon $\Rightarrow m_t^*$ transversal effective mass and $m_l^*$ longitudinal.

- 3 different configurations for electrons.



constant energy surface : 6 ellipsoids and 3 configurations

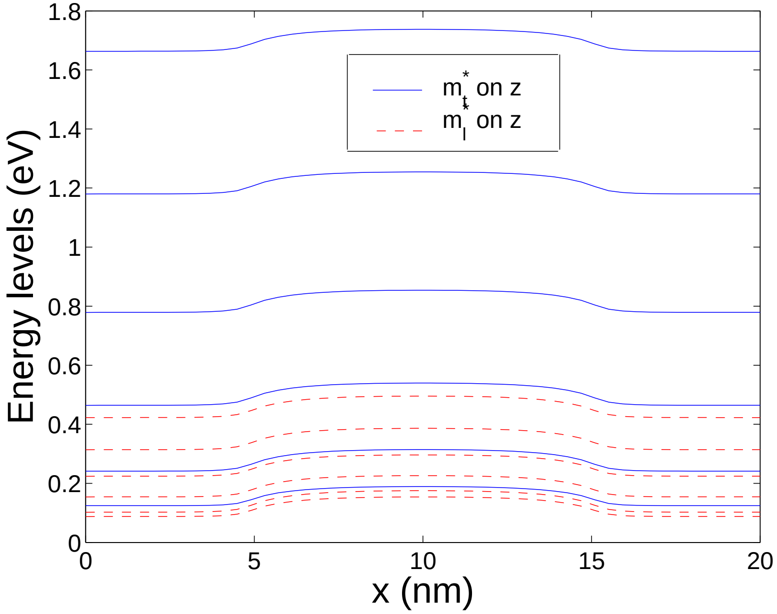
$$(m_t^*, m_t^*, m_l^*)$$

$$(m_t^*, m_l^*, m_t^*)$$

$$(m_l^*, m_t^*, m_t^*)$$

# Numerical results : 3 valleys





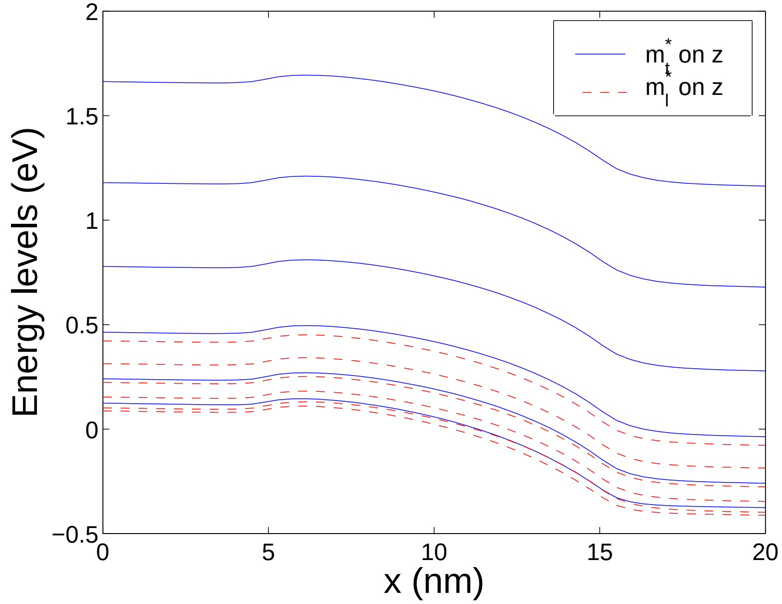




Figure 4: Energy levels $\epsilon_k(x)$ for the two values of the effective mass ($m_t^*$ in line, $m_l^*$ in dotted line) for $V_{DS} = 0V$ (left) and $V_{DS} = 0.5V$ (right)

# Numerical results : 3 valleys



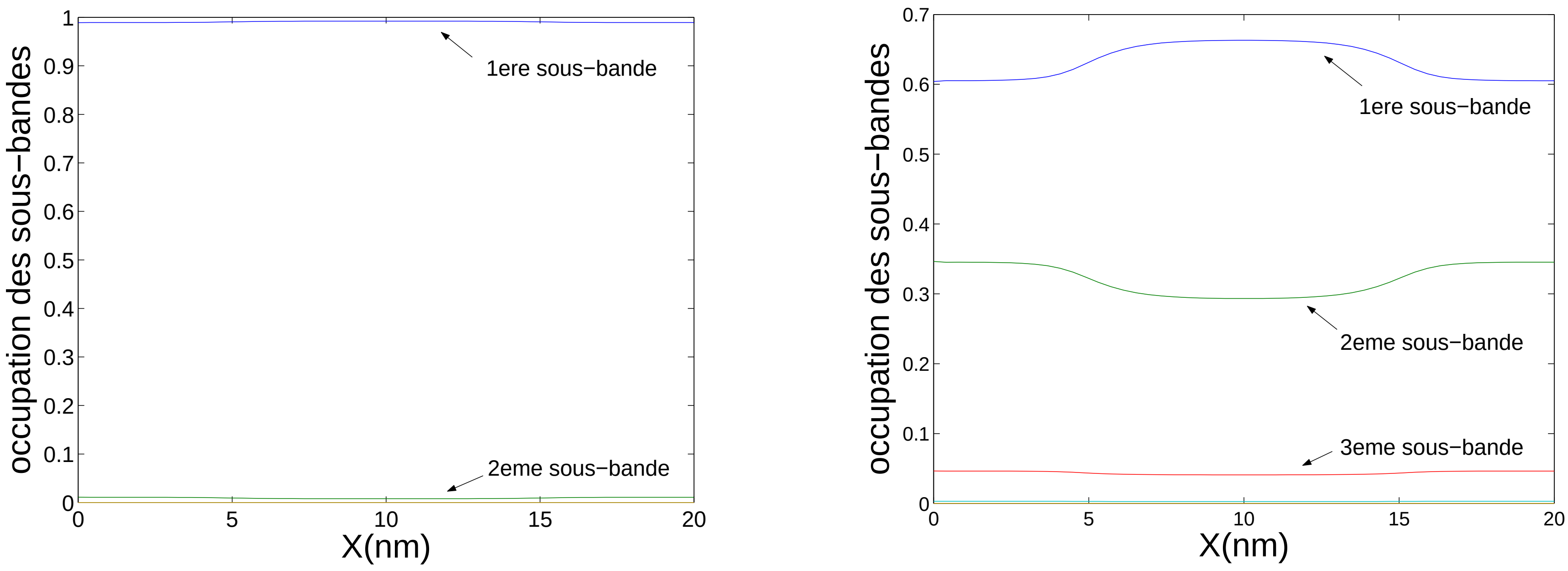



Figure 5: Effect of the effective mass on the confinement : transversal (left), longitudinal (right)

# Numerical results : 3 valleys



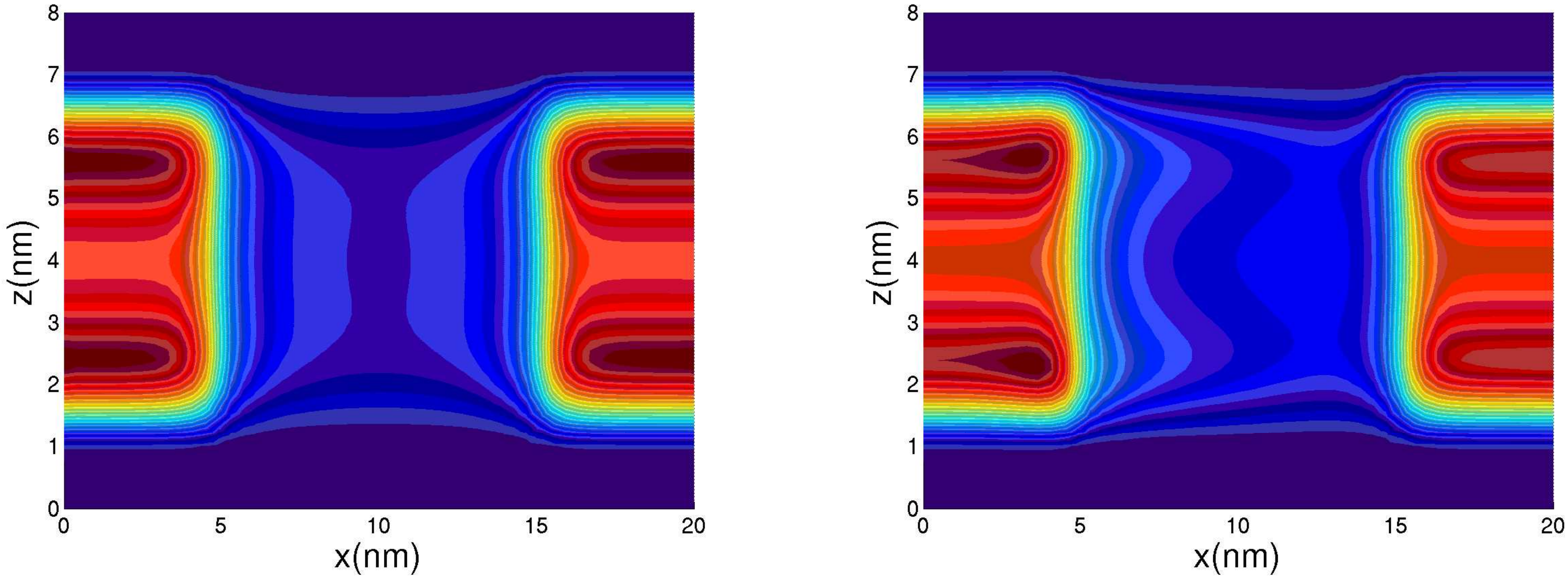



Figure 6: Left : density with $V_{DS} = V_{Gate} = 0V$ ; Right : density with $V_{DS} = V_{Gate} = 0.2V$

# Conclusion and perspectives



We introduce a hybrid coupling between a quantum and a classical model for an electron gas confined in a nanostructure. A mathematical analysis and a numerical simulation of this model was presented.

- Realize a hybrid coupling with a purely balistic model of Schrödinger type.
- Consider the Fermi-Dirac statistics.
- Take into account the dependence of the diffusion matrix in the subband energy.
- Existence results for the Boltzmann-Schrödinger-Poisson system.