Analysis of kinetic transport equations and application to MOSFETs

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INTRODUCTION

This report presents some results of kinetic tranport equations and their application to the particular case of Metall-Oxide-Semiconductor Field-Effect Transistors, that is to say MOSFETs.
The behaviour of a system of electrons in an electric potential can be described by the Quantum Vlasov Equation, that takes long range interactions between particles and quantum effects into account.
Solutions of this equation can be approximated by solutions of a classical equation obtained by the use of asymptotical developments.
Considering collisions, asymptotics also allows the derivation of a Drift Diffusion model that is usually adopted to describe the current created by charged particles in semiconductors.
In a cristal lattice, the mobile electrons initially come from the atoms of the lattice; in semi-conductors, such electrons appear at room temperature. When the electrons get free of the atoms, they leave holes ("missing electrons") in the underlying structure; these holes also contribute to the current. Free carriers doping can be realized to increase the conductivity.
Transistors are solids where the flow of current can be controlled, that means it can be switched off or amplified. In MOSFETs the conductivity of the semi-conductor is modulated by the voltage (hence "Field-Effect-Transistor") applied at the so-called gate.
Application of the previous considerations to the MOSFETs allows to compute the current circulating in the device.
An example of recent considerations of partially quantized systems combined to the drift diffusion model in semi-conductors is eventually given for MOSFETs. In fact, we show in our model that the quantum effects have no impact on the macroscopical current.

Chapter 1

Kinetic transport equations

We refer to [1] for the results of this section.

Introduction
We are interested in describing the behaviour of interacting particles (for example electrons) moving in the whole space and confronted to a potential. In order to take the quantum effects into account, we start from the Schrödinger equation and use a partial Wigner transformation in order to derive the quantum transport equations that describe the system. We omit the short range interactions (collisions) between particles, this will be introduced in chapter 3.
The equation for the whole system of particles (the so-called Quantum Liouville Equation) is not computer friendly, and we show that it can be reduced to a one particle equation (the Quantum Vlasov Equation) in an effective potential, which is itself solution of a Poisson Equation.

1.1 Quantum transport equations for N particles

Hamiltonian and density matrix
For a system of N electrons of mass m and charge $-q$ in a potential $V(x,t)$, where $x = (x_1, ..., x_N) \in \mathbf{R^{3N}}$ is the position of the ensemble, x_i is the position of the i-th electron, the Hamiltonian takes the form

$$H \;=\; -\frac{\hbar^2}{2m}\sum_{l=1}^{N}\triangle_{x_i} \;-\; qV(x,t)$$

and the Shrödinger equation for the wave function $\Psi(x_1, ..., x_n, t)$ reads

$$i\hbar\partial_t\Psi \;=\; H\Psi\ .$$

We introduce the density matrix ρ defined by

$$\rho(r,s,t) \;=\; \overline{\Psi(r,t)}\Psi(s,t)$$

(so $\rho(r,r,t) = |\Psi(r,t)|^2 = n(r,t)$ is the density of probability of finding the ensemble of particles at the position r).
Hence ρ satisfies the Heisenberg equation :

$$i\hbar\partial_t\rho \;=\; -\frac{\hbar^2}{2m}(\triangle_s\rho \;-\; \triangle_r\rho) \;-\; q(V(s,t)-V(r,t))\rho.$$

Wigner transformation
We set

$$r = x + \frac{\hbar}{2m}\eta\ , \qquad s = x - \frac{\hbar}{2m}\eta\ ,$$

and note

$$u(x,\eta,t) \;=\; \rho\left(x + \frac{\hbar}{2m}\eta, x - \frac{\hbar}{2m}\eta\right)\ .$$

We use the following definitions for the Fourier transformation $\mathcal{F}$ with respect to v :

$$\begin{aligned} \mathcal{F}g\ (\eta) \quad &:= \int_{\mathbf{R^{3N}}} g(v)e^{-iv.\eta}\ dv\ , \\ \mathcal{F}^{-1}h\ (v) \quad &:= \frac{1}{(2\pi)^{3N}}\int_{\mathbf{R^{3N}}} h(\eta)e^{iv.\eta}\ d\eta\ . \end{aligned}$$

Then the Wigner function w is defined as the inverse Fourier tranform of u with respect to η :

$$w(x,v,t) \;=\; \frac{1}{(2\pi)^{3N}}\int_{\mathbf{R^{3N}}} \rho\left(x + \frac{\hbar}{2m}\eta, x - \frac{\hbar}{2m}\eta\right)e^{iv.\eta}d\eta\ .$$

Remark that v has the dimension of velocity.

Quantum Transport Equations
Having done this, we come to the following equations for u and w :

$$\partial_t u \;+\; i\nabla_\eta.\nabla_x u \;+\; iq\frac{V(x+\frac{\hbar}{2m}\eta,t) - V(x-\frac{\hbar}{2m}\eta,t)}{\hbar}\,u \;=\; 0 \quad (1.1)$$

$$\partial_t w \;+\; v.\nabla_x w \;+\; \frac{q}{m}\theta_\hbar[V]w \;=\; 0 \quad (1.2)$$

In these equations, $x, v, \eta \;\in\; \mathbf{R^{3N}}$.
The second equation is just the Fourier transform of the first one and is called Wigner equation. The operator $\theta_\hbar[V]$ is a linear pseudo differential operator, this means that its Fourier transform acts like a multiplication operator, the multiplication function or symbol being here :

$$(\delta V)_\hbar(x,\eta,t) = im\frac{V(x+\frac{\hbar}{2m}\eta,t) - V(x-\frac{\hbar}{2m}\eta,t)}{\hbar}\ .$$

Solving the equation (1.2), we do not necessarily come to a nice Wigner function w : for example it does not necessarily stay negative for all $t \geq 0$:

this is the fact *iff* the potential V is quadratic (see [1]). Then the function w can be interpreted as a microscopic density.

Particle and current densities

From the definition of the Fourier transformation we have :

$$n(x,t) \;=\; \int_{\mathbf{R^{3N}}} w(x,v,t)\; dv$$

We also define the current density :

$$J(x,t) \;=\; -q \int_{\mathbf{R^{3N}}} v\; w(x,v,t)\; dv$$

1.2 Reduction to a one particle problem : the Quantum Vlasov Equation

The previous equations are not easily solvable because of the high number of particles that are usually involved and the difficulty to get a good model for the many-body potential.

We show in this section how to reduce the problem with N particles in a potential V to a problem with one particle in an effective potential V_{eff}, that contains the long range interactions and is solution of a Poisson Equation.

Subensembles

We will deal with subensembles of the given ensemble of N electrons. Being Fermions, the electrons obey
the Pauli principle and the function Ψ is antisymmetric :

$$\Psi(x_1,...,x_N) \;=\; 0 \qquad \text{if} \qquad x_i \;=\; x_j \qquad \text{for a couple } (i,j) \text{ with } i \neq j\;.$$

This corresponds to the fact that electrons are indistinguishable, which means the invariance under permutations of the density matrix ρ of the system. So if π is a permutation of $\{1,...,n\}$, then the symmetry property yields :

$$\rho(r_{\pi(1)},...,r_{\pi(N)},s_{\pi(1)},...,s_{\pi(N)},t) \;=\; \rho(r_1,...,r_N,s_1,...,s_N,t)$$

Because of the Schrödinger equation, the potential V has to be symmetric too whenever Fermions are considered. It has the form :

$$V(x,t) \;=\; \sum_{l=1}^{N} V_{ext}(x_l,t) \;+\; \frac{1}{2}\sum_{i,j=1}^{N} V_{int}(x_i,x_j)$$

where $V_{int}(x_i,x_j) = V_{int}(x_j,x_i)$ is the internal and V_{ext} the external potential.

We define the density matrix of a subensemble of $d \leq N-1$ electrons as :

$$\begin{aligned}&\rho^{(d)}(r_1, ..., r_d, s_1, ..., s_d, t) \\ &\quad := \int_{\mathbf{R^{3(N-d)}}} \rho(r_1, ...r_d, u_{d+1}, ..., u_N, s_1, ..., s_d, u_{d+1}, ..., u_N, t)\; du_{d+1}...du_N\end{aligned}$$

We see that the trace of $\rho^{(d)}$ now represents the electron position density of the d-particle subensemble :

$$n^{(d)}(x_1, ...x_d, t) \;=\; \rho^{(d)}(x_1, ..., x_d, x_1, ..., x_d, t)$$

This subensemble has still got the indistinguishability property.

Assumptions

We will suppose in the following that :

- ρ decays sufficiently fast to zero as $r_l, s_l \; \to \infty$
- V_{int} is of the order of magnitude $1/N$ as $N \to \infty$, so that the total potential on each particle l :

  $$V_l(x_1, ..., x_N) \;=\; \sum_{j=1}^{N} V_{int}(x_l, x_j) \;+\; V_{ext}(x_l, t)$$

  remains finite as $N \to \infty$.
- for $d << N$, we can consider that the particles in the subensemble move independantly from each other, so that we can write :

  $$\rho^{(d)}(r_1, ..., r_d, s_1, ..., s_d, t) \;=\; \prod_{i=1}^{d} R(r_i, s_i, t)$$

  with $R := \rho^{(1)}$.
  It is the so-called Hartree Ansatz.

The Quantum Vlasov Equation

We write the Heisenberg Equation

$$i\hbar\partial_t \rho \;=\; -\frac{\hbar^2}{2m}(\triangle_s \rho \;-\; \triangle_r \rho) \;-\; q(V(s,t) - V(r,t))\rho$$

with the above potential :

$$\begin{aligned}i\hbar\partial_t \rho \;&=\; -\frac{\hbar^2}{2m}\sum_{l=1}^{N}(\triangle_{s_l}\rho \;-\; \triangle_{r_l}\rho) \;-\; q\sum_{l=1}^{N}(V_{ext}(s_l,t) - V_{ext}(r_l,t))\rho \\ &\quad -\frac{q}{2}\sum_{i,j=1}^{N}(V_{int}(s_i,s_j) - V_{int}(r_i,r_j))\rho\end{aligned}$$

We set $u_l = s_l = r_l$ for $l \geq d+1$ and integrate over $\mathbf{R^{3(N-d)}}$, using the first assumption above and the indistinguishability property :

$$\begin{aligned}
i\hbar\partial_t\rho^{(d)} &= -\frac{\hbar^2}{2m}\sum_{l=1}^{d}(\triangle_{s_l}\rho^{(d)} \;-\; \triangle_{r_l}\rho^{(d)}) \\
&\quad -q\sum_{l=1}^{d}(V_{ext}(s_l,t) - V_{ext}(r_l,t))\rho^{(d)} \\
&\quad -\frac{q}{2}\sum_{i,j=1}^{d}(V_{int}(s_i,s_j) - V_{int}(r_i,r_j))\rho^{(d)} \\
&\quad -q(N-d)\sum_{l=1}^{d}\int_{\mathbf{R^3}}[V_{int}(s_l,u_*) - V_{int}(r_l,u_*)]\rho_*^{(d+1)}\,du_*
\end{aligned}$$

where

$$\rho_*^{(d+1)} = \rho^{(d+1)}(r_1,...r_d,u_*,s_1,...s_d,u_*,t)$$

For $N >> d$ and because of the second assumption, the third term of the second member can be neglected for $N \to \infty$, and the equation becomes :

$$\begin{aligned}
i\hbar\partial_t\rho^{(d)} &= -\frac{\hbar^2}{2m}\sum_{l=1}^{d}(\triangle_{s_l}\rho^{(d)} \;-\; \triangle_{r_l}\rho^{(d)}) \\
&\quad -q\sum_{l=1}^{d}(V_{ext}(s_l,t) - V_{ext}(r_l,t))\rho^{(d)} \\
&\quad -q\sum_{l=1}^{d}\int_{\mathbf{R^3}}[V_{int}(s_l,u_*) - V_{int}(r_l,u_*)]\;N\;\rho_*^{(d+1)}\,du_*
\end{aligned}$$

We now use the third assumption : we set $d=1$, and employ the Hartree Ansatz to obtain an equation for R :

$$\begin{aligned}
i\hbar\partial_t R &= -\tfrac{\hbar^2}{2m}(\triangle_s R - \triangle_r R) \;-\; q(V_{eff}(s,t) - V_{eff}(r,t))R \\
&\qquad\qquad\qquad\qquad\qquad\qquad r,s \;\in\; \mathbf{R^3}\;,\; t>0
\end{aligned}$$

The effective potential V_{eff} stands for :

$$V_{eff}(x,t) \;=\; V_{ext}(x,t) \;+\; \int_{\mathbf{R^3}} N\;R(x_*,x_*,t)V_{int}(x,x_*)\,dx_*$$

and takes the external potential and the two-body interaction into account. Multiplying the last equation by N and using the coordinate transformation like in section 1.1 :

$$r = x + \frac{\hbar}{2m}\eta\;, \qquad s = x - \frac{\hbar}{2m}\eta\;,$$

if $U(x,\eta,t) := N\;R(r,s,t)$, we come to :

$$\begin{aligned}
0 &= \partial_t U + i\nabla_\eta.\nabla_x U + iq\frac{V_{eff}(x+\frac{\hbar}{2m}\eta,t) - V_{eff}(x-\frac{\hbar}{2m}\eta,t)}{\hbar}\,U \qquad (1.3) \\
0 &= \partial_t W \;+\; v.\nabla_x W \;+\; \frac{q}{m}\theta_\hbar[V_{eff}]\,W \qquad (1.4)
\end{aligned}$$

The second equation is the inverse Fourier tranform of the first one, we have set $W := \mathcal{F}^{-1}U$, the operator $\theta_\hbar[V_{eff}]$ is defined in section 1.1 and has the symbol :

$$(\delta V_{eff})_\hbar(x,\eta,t) = im\frac{V_{eff}(x+\frac{\hbar}{2m}\eta,t) - V_{eff}(x-\frac{\hbar}{2m}\eta,t)}{\hbar} \ .$$

These are the same equations as in 1.1 but written for one particle ($x, v, \eta \ \in \ \mathbf{R^3}$) in an effective potential V_{eff} instead of V.

Particle and current densities

We can as in the preceding section write the particle density, equal to $NR(x,x,t) = U(x,\eta=0,t)$ or, by definition of the Fourier transform :

$$n(x,t) \ = \ \int_{\mathbf{R^3}} W(x,v,t) \, dv \ , \qquad x \in \mathbf{R^3}, \ \ t > 0$$

The current density is also given by :

$$J(x,t) \ = \ -q\int_{\mathbf{R^3}} \ v \ W(x,v,t) \, dv \ , \qquad x \in \mathbf{R^3}, \ \ t > 0$$

The computation of the potential V_{eff} as an integral :

$$V_{eff}(x,t) \ = \ V_{ext}(x,t) \ + \ \int_{\mathbf{R^3}} n(x_*,t) V_{int}(x,x_*) \, dx_* \tag{1.5}$$

seems to be difficult.

We now show that this integral expression can be written as a Poisson partial differential equation as soon as the two-body interaction is the usual Coulomb interaction, ie results from the Coulomb interaction field.

The Poisson Equation for the effective potential

For an interaction potential of the form :

$$V_{int}(x,y) \ = \ -\frac{q}{4\pi\epsilon_s \, |x-y|} \ , \qquad x,y \ \in \mathbf{R^3}, \ x \neq y$$

ϵ_s being the permittivity of the environment,
we obtain taking the Laplacian of (1.5) :

$$-\epsilon_s \triangle V_{eff} \ = \ -\epsilon_s \triangle V_{ext} \ - \ qn$$

and if the external potential is generated by ions of charge $+/-\ q$, then V_{eff} is solution of :

$$\epsilon_s \triangle V_{eff} \ = \ q(n-C) \tag{1.6}$$

where $C = C(x,t)$ can have positive and negative values and is the density of the background ions.

Conclusion
As a consequence, we will in the following always consider a function $w(x, v, t)$ solution of the Wigner equation and describing one particle (for example one electron) moving in an effective potential V_{eff}, re-written V and solution of a Poisson equation.
This constitutes the selfconsistent **Vlasov Poisson problem**, as the macroscopic electron density $n(x, t)$ is related to the function $w(x, v, t)$:

$$\left\{ \begin{array}{rcl} \partial_t w \ + \ v.\nabla_x w \ + \ \dfrac{q}{m}\theta_\hbar[V]w & = & 0 \\ -\epsilon_s \bigtriangleup V & = & -\epsilon_s \bigtriangleup V_{ext} \ - \ qn \\ n(x,t) & = & \displaystyle\int_{\mathbf{R^3}} w(x,v,t) \ dv \end{array} \right. \tag{1.7}$$

where $\theta_\hbar[V]$ is defined in section 1.1 and V_{ext} is the external potential supposed to be given.

1.3 Quantum states and Wigner function

In section 1.1, we started from a state Ψ and derived the equation (1.2) for the Wigner function associated to this state.
If now we start from the equation (1.2) with an initial data w_I, we would like to know if the solution w can be associated to any state Ψ.

We consider a particle in the effective potential V and a given initial condition $w_I \in L^2(\mathbf{R^3} \times \mathbf{R^3})$. Let $\{\Psi_I^{(l)}\}$ be a complete basis of $L^2(\mathbf{R^3})$ with its usual norm, then $\{\Psi_I^{(l)}(r).\overline{\Psi_I^{(j)}(s)}\}$ is a complete basis of $L^2(\mathbf{R^3} \times \mathbf{R^3})$.

If we want w to be associated to a linear combination of states at any time, we have to require this condition for w_I.
As $w_I \in L^2 \ iff \ \mathcal{F}(w_I) = \rho_I \in L^2$, we can write :

$$\rho_I(r,s) = \sum_{l,j} \rho_{l,j} \Psi_I^{(l)}(r).\overline{\Psi_I^{(j)}(s)}$$

The $\rho_{l,j}$ are the coordinates of ρ_I in the above basis, so they are obtained by projecting ρ_I onto this base.
The solving scheme is then theoretically simple : we solve the system

$$\left\{ \begin{array}{rcl} i\hbar\partial_t \Psi^{(l)} & = & H\Psi^{(l)} \\ \Psi^{(l)}(x,0) & = & \Psi_I^{(l)}(x) \end{array} \right.$$

for every l, then define ρ by

$$\rho(r,s,t) = \sum_{l,j} \rho_{l,j} \Psi^{(l)}(r,t).\overline{\Psi^{(j)}(s,t)}$$

and come back to the Wigner function over the function u through Fourier transformation (see page 6) :

$$w(x,v,t) \;=\; \frac{1}{(2\pi)^3}\sum_{l,j}\rho_{l,j}\int_{\mathbf{R^3}}\Psi^{(l)}(x+\frac{\hbar}{2m}\eta,t).\overline{\Psi^{(j)}(x-\frac{\hbar}{2m}\eta,t)}\;e^{iv.\eta}\,d\eta$$

The theoritical solution is thus very simple, w can be associated to a pure (resp. to a mixed) state as soon as w_I is a pure (resp. mixed) state.

Chapter 2

From the Quantum Liouville Equation to the Classical Liouville Equation : the classical limit

2.1 Introduction

We want to carrry out the classical limit ($\hbar \to 0$) in the **Quantum Liouville Equation**

$$\partial_t\, w \;+\; v.\nabla_x\, w \;+\; \theta_\hbar[V]\, w \;=\; 0, \;\; x \in \mathbf{R^d},\; v \in \mathbf{R^d},\; t > 0 \tag{2.1}$$

and show that a solution of this equation can be approximated by the solution of a **Classical Liouville Equation**

$$\partial_t\, w \;+\; v.\nabla_x\, w \;+\; \nabla_x\, V \,.\, \nabla_v\, w \;=\; 0 \tag{2.2}$$

at zeroth order, while the first significant quantum corrections are of order $\hbar^2$.
We have set $q = m = 1$.

Pseudodifferential operator
The pseudodifferential operator $\theta_\hbar[V]$ (see section 1.1) has the symbol

$$(\delta V)_\hbar(x,\eta,t) = i\frac{V(x+\frac{\hbar}{2}\eta,t) - V(x-\frac{\hbar}{2}\eta,t)}{\hbar}\;.$$

It tends formally to $\nabla_x V.\nabla_v$ as $\hbar \to 0$, so we will use an expansion of a solution of (2.1) with respect to $\hbar$.
Indeed, the symbol applied to the function u, Fourier transform of w, tends

formally to $i\nabla_x V.\eta\ u$, which is the Fourier transform of $\nabla_x V.\nabla_v\ w$.

We consider the Fourier transform of (2.1) with a smooth potential V in a one-dimensional case ($d = 1$) :

$$\left\{ \begin{array}{l} \partial_t\ u\ +\ i\partial_\eta\partial_x\ u\ +\ i\dfrac{V(x+\frac{\hbar}{2}\eta\ ,t)-V(x-\frac{\hbar}{2}\eta\ ,t)}{\hbar}\ u\ =\ 0 \\ \qquad\qquad\qquad\qquad x\in\mathbf{R},\ v\in\mathbf{R},\ t>0 \\ u(x,v,0)\ =\ u_I(x,v) \qquad \text{independant of } \hbar \end{array} \right. \tag{2.3}$$

We are going to expand V and derive an Ansatz for u.

2.2 Expression of the potential term and Ansatz

Potential
For a $2N+1$-times differentiable potential V, we write as in [2] the Taylor equality of order $2N$ as follows :

$$\begin{aligned} V(x+\frac{\hbar}{2}\eta\ ,t) \quad &= \quad \sum_{j=0}^{2N-1} \frac{V^{(j)}(x,t)}{2^j\ j!}\hbar^j\eta^j \\ &\quad + \frac{\hbar^{2N}}{2^{2N}\ (2N-1)!}\int_0^\eta V^{(2N)}(x+\frac{\hbar}{2}\xi\ ,t)\ (\eta-\xi)^{2N-1}\ d\xi \end{aligned}$$

In the computation of the potential term of (2.3) the terms of magnitude $\hbar^{2k+1}$ are cancelled, and after a partial integration on the rest integral we get :

$$\begin{aligned} \frac{V(x+\frac{\hbar}{2}\eta\ ,t)\ -\ V(x-\frac{\hbar}{2}\eta\ ,t)}{\hbar} \quad &= \quad \sum_{j=0}^{N-1}\frac{V^{(2j+1)}(x,t)}{2^{2j}\ (2j+1)!}\hbar^{2j}\eta^{2j+1} + \\ +\ \hbar^{2N}\ &\underbrace{\frac{1}{2^{2N+1}\ (2N)!}\int_0^\eta [V^{(2N+1)}(x+\frac{\hbar}{2}\xi\ ,t)+V^{(2N+1)}(x-\frac{\hbar}{2}\xi\ ,t)]\ (\eta-\xi)^{2N}\ d\xi}_{=:\ I_N} \end{aligned}$$

Ansatz
As a consequence, we make the Ansatz
$u_N^\hbar(x,\eta,t) = \sum_{k=0}^{N-1}\hbar^{2k}u_k(x,\eta,t)$ that we put in equation (2.3).

Equations
Equalling the powers of $\hbar^2$, we obtain the following equations respectively for $k=0$ and $k\geq 1$:

$$\partial_t u_0\ +\ i\partial_\eta\partial_x u_0\ +\ i\eta V'(x,t)u_0\ =\ 0 \tag{2.4}$$

$$\partial_t u_k\ +\ i\partial_\eta\partial_x u_k\ +\ i\eta V'(x,t)u_k\ =\ -i\sum_{j=1}^{k}\frac{V^{(2j+1)}(x,t)}{2^{2j}\ (2j+1)!}\eta^{2j+1}u_{k-j} \tag{2.5}$$

together with the initial conditions :

$$\begin{array}{rcl} u_0(x,v,0) & = & u_I(x,v) \\ u_k(x,v,0) & = & 0 \end{array}$$

We have written (2.5) so that the second member of the equation only depends on the first $k-1$ functions u_j of the expansion. In the following paragraphs we inverse Fourier transform these equations.

2.3 Zeroth order equation

After inverse Fourier transformation of (2.4), we see that w_0 satisfies the Classical Liouville equation (see (2.2)) :

$$\partial_t w_0 \ + \ v\partial_x w_0 \ + \ V'(x,t)\partial_v w_0 \ = \ 0$$

with the initial condition (w_I is the inverse Fourier transform of u_I) :

$$w_0(x,v,0) \ = \ w_I(x,v)$$

We can "solve" it using the characteristic method :
Denoting F by
$F(a,b) \ = \ (b, V'(a))$, let us define X as the map :

$$\begin{array}{rcl} X \ : (x,v) & \longmapsto & X(x,v) \ : t \mapsto (x(t), v(t)) \\ & & \text{where } \ X(x,v) \text{ solution of } \left\{ \begin{array}{rcl} \dot{X}(t) & = & F(X(t)) \\ X(0) & = & (x,v) \end{array} \right. \end{array}$$

If w_0 is solution of the equation above, then for all (x,v), for all t, we have :

$$\frac{d}{dt} w_0(X(t),t) \ = \ 0$$

ie w_0 is constant along the characteristics, and thus :

$$\forall t, \ w_0(x(t), v(t), t) \ = \ w_I(x,v)$$

Solution w_0
Reciprocally, such a function is a solution, hence we can write the solution w_0 :

$$\forall \ x,v,t, \ w_0(x,v,t) = w_I(X(x,v)(-t))$$

This result requires some assumptions on the potential V : the characteristics should exist at any time t ! We have from [3] the following result :

Justification of the characteristics method
Let V be a potential satisfying the inequality :

$$|V'(x)| \leq C\sqrt{1+x^2}$$

for some constant C (= 1 below), then for every initial condition (x_0, v_0), the characteristics defined above exist for any time t.
Indeed, as $F(x,v) = (v, V'(x))$ is locally Lipschitz, there is a solution defined on a maximal interval $(-T_0, T_1)$. This solution $(t, X(t))$ leaves every compact subset. Let us assume $T_1 < \infty$, we come to a contradiction by showing that the solution is then bounded : let be

$$\forall\, t,\ \ N(t) = x(t)^2 \ + \ v(t)^2 \ + \ 1 \ > \ 0\ ,$$

then

$$\begin{array}{rcl}
\dot{N}(t) & = & 2x\dot{x} + 2v\dot{v} \\
 & = & 2xv + 2vV' \\
 & \leq & 2|x||v| + 2|v||V'| \\
 & \leq & 2|v|\sqrt{1+x^2} \ + \ 2|v|\sqrt{1+x^2} \\
 & \leq & 4|v|\sqrt{1+x^2} \\
 & \leq & 2(|v|^2 + (\sqrt{1+x^2})^2) \\
\Rightarrow \ \ \dot{N}(t) & \leq & 2N(t) \\
\Rightarrow \ \ N(t) & \leq & N(0)\, e^{2t} \ \leq \ N(0)\, e^{2T_1}
\end{array}$$

This is a contradiction and T_1 has to be infinite. Similarly we show $T_0 = \infty$.

2.4 Iterative computation of the k-th order terms

The inverse Fourier transform of (2.5) gives :

$$\partial_t w_k \ + \ v\partial_x w_k \ + \ V'(x,t)\partial_v w_k \ = \ -\sum_{j=1}^{k} \frac{V^{(2j+1)}(x,t)}{2^{2j}\ (2j+1)!}\, \partial_v^{2j+1}\ w_{k-j}$$

and the initial condition reads :

$$w_k(x,v,0) \ = \ 0$$

Solution w_k
Writing r_{k-1} for the second member of the equation, supposed to be known from the last $k-1$ equations, we thus have to solve the equation

$$\left\{ \begin{array}{rcl} \partial_t w_k \ + \ v\partial_x w_k \ + \ V'(x,t)\partial_v w_k & = & r_{k-1} \\ w_k(x,v,0) & = & 0 \end{array} \right.$$

which solution is given by :

$$w_k(x,v,t) \ = \ \int_0^t r_{k-1}(X(x,v)(s-t), s)\ ds \tag{2.6}$$

where X is defined as in the zeroth order case.
Indeed, introducing the characteristics as in the zeroth order, $w_k(X(x,v)(t),t)$ is now solution of

$$\frac{d}{dt} w_k(X(x,v)(t),t) \ = \ r_{k-1}(X(x,v)(t),t)$$

This gives an iterative computation of the terms of the expansion.

2.5 Conservation laws

We show that the Quantum Liouville and the classical Liouville equations preserve the L^2-norm of the solutions.

- **Quantum Liouville Equation**
  Skew-symmetry of the operator $\theta_\hbar[V]$
  If V is a real potential and

$$(f,h)_{L^2} \;:=\; \int_{\mathbf{R^2}} f\bar{g}\;dxdv\;,$$

then we have :

$$(f,\theta_\hbar[V]g)_{L^2} \;=\; -\,(\theta_\hbar[V]f,g)_{L^2}$$

Indeed, let us write $\mathcal{F}$ for the Fourier transform with respect to v (see section 1.1), and design by h^* the function

$$h^* \;: u \;\longmapsto\; h(-u)$$

for a given function h, remembering that for f and h two functions of L_2 we have :

$$\mathcal{F}(f)\star\mathcal{F}(h) \;=\; (2\pi)^d\;\mathcal{F}(f.g)$$

where $\star$ stands for the convolution of two functions, we can write :

$$\begin{aligned}
(2\pi)^d \int_{\mathbf{R}} f\;\overline{\theta_\hbar[V]g}\;dv \;&=\; \mathcal{F}(f\;\overline{\theta_\hbar[V]g})(\eta=0)\\
&=\; \mathcal{F}(f)\star\mathcal{F}(\overline{\theta_\hbar[V]g})(\eta=0)\\
&=\; \mathcal{F}(f)\star\overline{\mathcal{F}(\theta_\hbar[V]g)}^*(\eta=0)\\
&=\; \mathcal{F}(f)\star\overline{(i\frac{V(x+\frac{\hbar}{2}\eta\;,t)-V(x-\frac{\hbar}{2}\eta\;,t)}{\hbar}\mathcal{F}(g))}^*(\eta=0)\\
&=\; \int_{\mathbf{R}}\mathcal{F}(f)(-\tau).(-i)\frac{V(x-\frac{\hbar}{2}\tau\;,t)-V(x+\frac{\hbar}{2}\tau\;,t)}{\hbar}\overline{\mathcal{F}(g)}(-\tau)\;d\tau\\
&=\; \int_{\mathbf{R}}\mathcal{F}(f)(-\tau).i\frac{V(x+\frac{\hbar}{2}\tau\;,t)-V(x-\frac{\hbar}{2}\tau\;,t)}{\hbar}\mathcal{F}(\bar{g})(\tau)\;d\tau\\
(\tau\rightarrow-\tau)\quad &=\; -\int_{\mathbf{R}} i\frac{V(x+\frac{\hbar}{2}\tau\;,t)-V(x-\frac{\hbar}{2}\tau\;,t)}{\hbar}\mathcal{F}(f)(\tau)\mathcal{F}(\bar{g})(-\tau)\;d\tau\\
&=\; -\int_{\mathbf{R}}\mathcal{F}(\theta_\hbar[V]f)(\tau).\mathcal{F}(\bar{g})(-\tau)\;d\tau\\
&=\; -\mathcal{F}(\theta_\hbar[V]f)\star\mathcal{F}(\bar{g})(\eta=0)\\
&=\; -(2\pi)^d\mathcal{F}(\theta_\hbar[V]f.\bar{g})(\eta=0)\\
&=\; -(2\pi)^d\int_{\mathbf{R}}\theta_\hbar[V]f.\bar{g}\;dv
\end{aligned}$$

and the proof is completed after an integration over x.

Conservation
As a consequence, multiplying (2.1) by w and integrating over the position and velocity spaces, the gradient term vanishes after integration in x if $w \to 0$ for $x \to \infty$, and the term with the operator $\theta_\hbar[V]$ vanishes because of its skew-symmetry property :

$$\begin{array}{rcl} \partial_t \frac{1}{2} ||w||^2_{L^2(\mathbf{R^2})} \; + \; \underbrace{\int_{\mathbf{R^2}} v \, \partial_x \frac{w^2}{2} \, dxdv}_{=0} \; + \; \underbrace{\int_{\mathbf{R^2}} w \, \theta_\hbar[V] w \, dxdv}_{=0} & = & 0 \\ \Rightarrow \qquad ||w||_{L^2(\mathbf{R^2})} \; = \; c^{ste} \; = \; ||w_I||_{L^2(\mathbf{R^2})} & & \end{array}$$

- **Classical Liouville Equation**
  The conservation law for the equation (2.2) is easily seen by multiplying this equation by w and integrating over $\mathbf{R^2}$, just supposing that $w \to 0$ as $v \to \infty$.
  This means for example that the L^2-norm of the zeroth order term w_0 of the expansion is preserved.

2.6 Justification of the expansion

We want to use the Taylor expansion of V introduced in section 2.2 to show the validity of the expansion of w with respect to $\hbar$:
if $w^\hbar$ is solution of the Quantum Liouville Equation (2.1), then

$$||w^\hbar - w^\hbar_N||_{L^2} \; = \; O(\hbar^{2N})$$

The method below was found in [2].

2.6.1 Estimate

Fourier transform preserves the L^2-norm, hence we look at the equations satisfied by $u^\hbar$ and $u^\hbar_N$:

$$\left\{ \begin{array}{rcl} \partial_t \, u^\hbar \; + \; i\partial_\eta \partial_x \, u^\hbar \; + \; (\delta V)_\hbar \, u^\hbar & = & 0 \\ \partial_t \, u^\hbar_N \; + \; i\partial_\eta \partial_x \, u^\hbar_N \; + \; \Big((\delta V)_\hbar \; - \; i\hbar^{2N} \, I_N \Big) \, u^\hbar_N & = & 0 \end{array} \right.$$

where $(\delta V)_\hbar$ and I_N have been respectively defined in the introduction and in section 2.2 of this chapter.
Thus we conclude that $u^\hbar - u^\hbar_N := \omega_N$ is solution of

$$\partial_t \, \omega_N \; + \; i\partial_\eta \partial_x \, \omega_N \; + \; (\delta V)_\hbar \, \omega_N \; = \; i\hbar^{2N} \, I_N \, u^\hbar_N$$

Successive integrations by parts on I_N show that for all k :

$$I_N \; = \; \frac{1}{\hbar^{2k}} \, I_{N-k} \; ,$$

so that we can write the second member of the equation above :

$$\hbar^{2N} \rho_N \; := \; \hbar^{2N} \; i \sum_{k=0}^{N-1} \frac{1}{\hbar^{2k}} I_{N-k} \; \hbar^{2k} u_k \; = \; \hbar^{2N} \; i \sum_{k=1}^{N} I_k \; u_{N-k}$$

We set $L := \partial_t + i \partial_\eta \partial_x + (\delta V)_\hbar$. Supposing $\rho_N \in L^2$, the equation for ω_N now reads ($\mathcal{F}$ stands for the Fourier transform) :

$$\begin{array}{rrcl}
 & L\omega_N & = & \hbar^{2N} \; \rho_N \\
\Rightarrow & \mathcal{F}^{-1}(L\omega_N) & = & \hbar^{2N} \; \mathcal{F}^{-1}(\rho_N) \\
\Rightarrow & \mathcal{F}^{-1}(\omega_N).\mathcal{F}^{-1}(L\omega_N) & = & \hbar^{2N} \; \mathcal{F}^{-1}(\omega_N).\mathcal{F}^{-1}(\rho_N) \\
\Rightarrow & \int_{\mathbf{R^2}} \mathcal{F}^{-1}(\omega_N).\mathcal{F}^{-1}(L\omega_N) \; dxdv & = & \hbar^{2N} \; \int_{\mathbf{R^2}} \mathcal{F}^{-1}(\omega_N).\mathcal{F}^{-1}(\rho_N) \; dxdv \\
 & & \leq & \hbar^{2N} \; \underbrace{||\mathcal{F}^{-1}(\omega_N)||_{L^2}}_{= \, ||\omega_N||_{L^2}} \; . \; \underbrace{||\mathcal{F}^{-1}(\rho_N)||_{L^2}}_{= \, ||\rho_N||_{L^2}}
\end{array}$$

The left side of the inequality was just computed on page 18, we obtain :

$$\begin{array}{rrcl}
 & \partial_t \frac{1}{2} ||\mathcal{F}^{-1}(\omega_N)||^2_{L^2} & \leq & \hbar^{2N} \; ||\omega_N||_{L^2} \; ||\rho_N||_{L^2} \\
\Rightarrow & ||\omega_N||_{L^2} \partial_t ||\omega_N||^2_{L^2} & \leq & \hbar^{2N} \; ||\omega_N||_{L^2} \; ||\rho_N||_{L^2}
\end{array}$$

which gives after simplification, integration and because $\omega_N(x, \eta, t = 0) = 0$:

$$||\omega_N||_{L^2} \; \leq \; \hbar^{2N} \int_0^t ||\rho_N||_{L^2}(s) \; ds$$

2.6.2 Validity of the estimate

The existence and the uniform boundedness of $||\rho_N||_{L^2}$ has now to be shown, ie the existence of a constant $M(t)$ (continuous in t) independent of $\hbar$ so that :

$$||\rho_N||_{L^2} \leq M(t)$$

We write the definition of ρ_N :

$$\rho_N(x, \eta, t) = i \sum_{k=1}^{N} \frac{1}{2^{2k+1} \; (2k)!} \int_0^\eta [V^{(2k+1)}(x + \frac{\hbar}{2}\xi \; , t) + V^{(2k+1)}(x - \frac{\hbar}{2}\xi \; , t)] \; (\eta - \xi)^{2k} \; d\xi \; u_{N-k} \; .$$

Assumption on the potential
We suppose :

- The potential V belongs to C^{3N+2}

- There is a constant c with

$$\forall\, k \;=\; 1 \,...\, 3N+1\;,\; |V^{(k)}| \leq c \tag{2.7}$$

We are now delivered from the dependence of $\hbar$:

$$\begin{aligned} |\rho_N(x,\eta,t)| &\leq 2c\sum_{k=1}^{N}\frac{\eta^{2k+1}}{2^{2k+1}(2k+1)!}|u_{N-k}(x,\eta,t)| \\ &\leq 2c\sum_{k=1}^{N}\eta^{2k+1}|u_{N-k}(x,\eta,t)|\;. \end{aligned}$$

Since $\eta^{2k+1}u_{N-k} \in L^2(\mathbf{R^2})$ for $\partial_v^{2k+1}w_{N-k} \in L^2(\mathbf{R^2})$,
we should just prove that $\partial_v^{2k+1}w_{N-k}$ belongs to L^2 and its L^2-norm is bounded through a continuous function $M_{N-k}(t)$ for $k = 1...N$.

In fact, it is even possible to prove a little bit more :

Let be $\dfrac{\partial^{k+j}w_I}{\partial x^k\partial v^j} \in L^2(\mathbf{R^2})$ for $k+j \leq 3N$, then $\dfrac{\partial^{k+j}w_p}{\partial x^k\partial v^j} \in L^2(\mathbf{R^2})$ for $k+j \leq 3(N-p)$

The boundedness through functions $M_{p,k,j}(t)$ of the L^2-norm of $\dfrac{\partial^{k+j}w_p}{\partial x^k\partial v^j}$ is also obtained below in the proof of this assumption.

The assumption is proved iteratively :
We will use the following estimate for the characteristics (see justification page 21) :

$\forall\, k,j$ with $k+j \leq 3N$, $\exists\, c_{k,j}(t)$ (continuous) , $\forall\, x,v,\;\; ||\dfrac{\partial^{k+j}X}{\partial x^k\partial v^j}||_\infty \leq c_{k,j}(t)$.

Derivating the expression of w_0

$$w_0(x,v,t) = w_I(X(x,v)(-t))\;,$$

using the estimate for the characteristics and the assumption on w_I we obtain that $\dfrac{\partial^{k+j}w_0}{\partial x^k\partial v^j} \in L^2(\mathbf{R^2})$ for $k+j \leq 3N$ and the L^2-norms of these functions are bounded through (continuous) functions $M_{0,k,j}(t)$.

The regularity of w_1 is given by the formula (2.6) : it depends on the function

$$r_0 \;=\; -\frac{V^{(3)}(x,t)}{2^2\;(3)!}\;\partial_v^3\;w_0$$

so the $V^{(k)}$ being bounded, w_1 satisfies

$$\frac{\partial^{k+j}w_1}{\partial x^k\partial v^j} \in L^2(\mathbf{R^2}) \text{ for } k+j \leq 3(N-1)$$

We go on this way for higher derivatives :
We show at every step that r_{p-1} satisfies $\dfrac{\partial^{k+j} r_{p-1}}{\partial x^k \partial v^j} \in L^2(\mathbf{R^2})$ for $k+j \leq 3(N-p)$, then we use the formula (2.6) to get the same property for w_p.
We eventually come to the function w_{N-1} for which yields :

$$\frac{\partial^{k+j} w_{N-1}}{\partial x^k \partial v^j} \in L^2(\mathbf{R^2}) \text{ for } k+j \leq 3$$

Estimate of the characteristics
To show the regularity of w_k, an estimate for the characteristics has been used, ie the existence of $c_{k,j}(t)$ such as :

$$\forall x, v,\ \forall k, j \text{ with } k+j \leq 3N\ ,\ ||\frac{\partial^{k+j} X}{\partial x^k \partial v^j}||_\infty \leq c_{k,j}(t)$$

This can be proved iteratively :
The equation of the characteristics is :

$$\left\{ \begin{array}{lcl} \dot{X}(t) & = & (v(t), V'(x(t))) \\ X(0) & = & (x, v) \end{array} \right.$$

So for example $\partial_x X$ is solution of

$$\left\{ \begin{array}{lclcl} \partial_x \dot{X}(t) & = & (\partial_x \dot{x}, \partial_x \dot{v}) & = & (\partial_x v(t), \partial_x x(t) V''(x(t))) \\ & & \partial_x X(0) & = & (1, 0) \end{array} \right.$$

In the assumption (2.7) on the potential V, and doing similarly for $\partial_v X$, this leads with similar computations to page 16 to :

$$||\partial_x X|| \leq e^{at}\ \ ,\ \ ||\partial_v X|| \leq e^{at}$$

for some constant a.
Derivating the characteristics equation again we find $\partial_{xx} X$ solution of :

$$\left\{ \begin{array}{lclcl} \partial_{xx} \dot{X}(t) & = & (\partial_{xx} \dot{x}, \partial_{xx} \dot{v}) & = & (\ \partial_x v(t), \partial_{xx} x(t)\ V''(x(t)) + (\partial_x x(t))^2\ V^{(3)}(x(t))\ ) \\ & & \partial_{xx} X(0) & = & (0, 0) \end{array} \right.$$

We can there use the "variation of constant" and obtain a uniformly bounded solution.
It can be similarly done for higher and crossed derivatives.

Conclusion
As a consequence, this method shows that the expansion is valid on every

time-interval $[0,T],\ T>0$:

$$\begin{aligned}
||\rho_N||_{L^2} &\leq 2c\sum_{k=1}^{N} ||\partial_v^{2k+1} w_{N-k}||_{L^2} \\
&\leq \underbrace{2c\sum_{k=1}^{N} \underbrace{M_{N-k,0,2k+1}(t)}_{=:\, M_{N-k}(t)}}_{=:\, M(t)} \\
\Rightarrow \quad \int_0^t ||\rho_N||_{L^2}(s)\ ds &\leq \int_0^t M(s)\ ds \quad =: C(t)
\end{aligned}$$

Hence the expansion satisfies :

$$||w^\hbar - w_N^\hbar||_{L^2} \ \leq\ \hbar^{2N}\ C(t)$$

where $C(t)$ is independant of $\hbar$, continuous in t, and consequently bounded on every time-interval $[0,T],\ T>0$.

Chapter 3

Introducing collisions

3.1 Boltzmann Equations

We refer to [1] for the results of this section.

3.1.1 Introduction

Previous equations take long range interactions between particles into account, but not the short range interactions, the so-called collisions.
As will be shown in the next section, collisions allow a system that is perturbated at initial time to get back to an equilibrium state.
In the classical case, the number density $F(x, v, t)$ of particles is a positive function and takes values between 0 and 1 if the particles are electrons (because of the Pauli principle).
The idea of Boltzmann was to consider that the classical transport equation can be written as a conservation equation of the number density $F(x, v, t)$ along characteristics for particles (resp. one particle of charge q) having a convective motion caused by a potential (resp. an effective potential) V as long as collisions are neglected :

$$(\frac{dF}{dt})_{conv} \;=\; 0$$

along the caracteristics $(x(t), v(t))$ defined by :

$$\left\{ \begin{array}{rcl} \dot{x} & = & v \\ \dot{v} & = & \frac{q}{m} \nabla_x V(x,t) \end{array} \right.$$

The effect of collisions is thus supposed to balance the effect of convection :

$$(\frac{dF}{dt})_{conv} \;=\; (\frac{dF}{dt})_{coll}$$

The purpose of this section is to write an expression of the collision operator

$$Q(F) \; := \; (\frac{dF}{dt})_{coll} \, .$$

3.1.2 Collision operator

A collision is a phenomenon where particles stay at the same place but instantaneously change their velocity.
As Fermions obey the Pauli principle, an electron comes to the state (x, v) through a scattering event if it was in a state (x, v') and if there is not already an electron at the state (x, v), and it leaves its state (x, v) to go to the state (x, v') if this last state is free.
Consequently, the rate of a particle with position x at time t to change its velocity v' into v is assumed to have the form :

$$s(x, v', v)F(x, v', t)(1 - F(x, v, t))$$

where $s(x, v', v)$ is the scattering rate, and the total rate of change of F due to collisions at (x, v) takes the form :

$$Q(F)(x, v, t) \; = \; \int_{\mathbf{R^3}} [s(x, v', v)F'(1 - F) \; - \; s(x, v, v')F(1 - F')] \, dv'$$

where $F = F(x, v, t)$ and $F' = F(x, v', t)$.
This leads to the Classical Boltzmann Equation, obtained at the classical limit (chapter 2) :

$$\partial_t F \; + \; v.\nabla_x F \; + \; \frac{q}{m} \nabla_x V.\nabla_v F \; = \; Q(F)$$

with $Q(F)$ defined above. This collision operator is quadratic in F, nonlocal in velocity.
We can check the conservation property :

$$\int_{\mathbf{R^3}} Q(F)(x, v, t) \, dv \; = \; 0$$

which expresses that collisions do not destroy nor generate electrons.

3.1.3 Low densities : linear collision operator

When the particle density is very small ($F << 1$), we obtain a linear collision operator given by :

$$Q_L(F)(x, v, t) \; = \; \int_{\mathbf{R^3}} [s(x, v', v)F' \; - \; s(x, v, v')F] \, dv'$$

This operator still satisfies the conservation property.
At thermal equilibrium ($F = F_e$), the so-called "principle of detailed balance" states there is locally no scattering event. This assures the nullity of the collision operator through the condition :

$$\forall x, v, v' \ , \ \ s(x,v',v)F'_e \ - \ s(x,v,v')F_e \ = 0$$

At low densities the Maxwellian distribution at temperature T

$$M(v) \ = \ M \ exp\left(-\frac{mv^2}{2k_BT}\right) \qquad (M \text{ constant so that } \int_{\mathbf{R^3}} M(v)dv = 1)$$

can be used to describe the velocity distribution of the ensemble at thermal equilibrium; k_B is the Boltzmann constant.
So one can write $F_e = n(x,t)M(v)$ with the macroscopic density

$$n(x,t) \ = \ \int_{\mathbf{R^3}} F(x,v,t) \ dv$$

and obtain from the principle of detailed balance :

$$s(x,v',v)n(x,t)M(v') \ = \ s(x,v,v')n(x,t)M(v) \ .$$

This implies the relation :

$$\begin{aligned} s(x,v',v)M(v') \ &= \ s(x,v,v')M(v) \\ \Rightarrow s(x,v,v') \ &= \ \Phi(x,v',v)M(v') \end{aligned}$$

where Φ is symmetric in v, v', and therefore :

$$Q_L(F) \ = \ \int_{\mathbf{R^3}} \Phi(x,v',v) \ [M(v)F' \ - \ M(v')F] \ dv' \tag{3.1}$$

3.1.4 Kernel of the linear collision operator

Consequently, a function F belongs to the Kernel $Ker(Q_L)$ of this linear collision operator, ie satisfies

$$\forall x, v, t \ , \ \ Q_L(F)(x,v,t) \ = 0 \ ,$$

iff the following relation holds :

$$\begin{aligned} M(v)F(x,v',t) \ - \ M(v')F(x,v,t) \ &= \ 0 \\ \Leftrightarrow \ \frac{F(x,v',t)}{M(v')} \ &= \ \frac{F(x,v,t)}{M(v)} \end{aligned}$$

This means that F has the form :

$$F(x,v,t) \ = \ C(x,t)M(v) \ ,$$

the "constant" $C(x,t)$ (independent of v) being by definition exactly the macroscopic density $n(x,t)$.
So we have the relation :

$$F \ \in \ Ker(Q_L) \ \ \Leftrightarrow \ \ F(x,v,t) \ = \ n(x,t)M(v) \ .$$

3.1.5 Relaxation time approximation

For low densities and moreover an initial data F_I close to the equilibrium distribution, ie to a multiple of the Maxwellian, we approximate F' by $n(x, v')M(v')$ and obtain using the linearized collision operator (3.1) the relaxed collision operator :

$$Q_R(F)(x, v, t) \;=\; -\frac{1}{\tau(x, v)}\left(F(x, v, t) - n(x, t)M(v)\right) \tag{3.2}$$

where $\tau(x, t)$ stands for

$$\left(\int_{\mathbf{R^3}} s(x, v, v')\, dv'\right)^{-1} \;=\; \left(\int_{\mathbf{R^3}} \Phi(x, v', v)\; M(v')\; dv'\right)^{-1}\;.$$

It is the so-called relaxation-time and describes the average time between two consecutive collisions at (x, t).

The resulting Boltzmann equation reads :

$$\begin{aligned} \partial_t F \;+\; v.\nabla_x F \;+\; \frac{q}{m}\nabla_x V.\nabla_v F& \\ \;=\; -\frac{1}{\tau(x, v)}\left(F(x, v, t) - n(x, t)M(v)\right)& \end{aligned} \tag{3.3}$$

In the next section we will use this equation Q_R and suppose the relaxation time to be constant.

3.2 Scaling

We use in this section the Boltzmann equation (3.3) established in the preceding section in the classical case.

3.2.1 Aria : The Boltzmann equation with relaxation time

For low densities, we have seen that we can use the linear collision operator Q_R with relaxation time τ that we assume to be constant (see (3.2) of the preceding section) :

$$Q_R(w)(x,v,t) = -\frac{1}{\tau}(w(x,v,t) - n(x,t)M(v)) \ ,$$

where $M(v)$ is the Maxwellian distribution verifying $\int_{\mathbf{R^d}} M(v)dv \ = 1$ and

$$n(x,t) = \int_{\mathbf{R^d}} w(x,v,t)dv \ .$$

Note that at any time t we have

$$\int_{\mathbf{R^d}} Q_R(w)dx \ = \ 0 \ ,$$

since no particle is created or annihilated by collisions.
So we consider the equations :

$$\begin{cases} \partial_t \, w \ + \ v.\nabla_x \, w \ + \ \nabla_x \, V \ . \ \nabla_v \, w \ = \frac{1}{\tau} \ (nM - w) \ , \ \ x \in \mathbf{R^d}, \ v \in \mathbf{R^d}, \ t > 0 \\ w(x,v,0) \ = \ w_I(x,v) \qquad \text{independant of } \tau \end{cases}$$

The initial data w_I is supposed to belong to the Schwarz space $\mathcal{S} := \mathcal{S}(\mathbf{R^d} \times \mathbf{R^d})$

3.2.2 1st variation : 1D problem in classical case

We study in this section the limit for τ going to zero in the one dimensional classical case. For a nearly close to the equilibrium initial condition, the system should go back fast to the equilibrium.
We compute the first terms of an expansion of w, and give an iterative method to compute the following terms.
We scale the time t by the relaxation time τ (s stands for "scaled" and will be immediately dropped) :

$$t_s \ = \ \frac{t}{\tau}$$

and thus consider the 1-D resulting Boltzmann equation with relaxation time :

Equation

$$\begin{aligned} \partial_t\, w \;+\; \tau(\; v\partial_x\, w \;+\; V'(x)\; \partial_v\, w \;) &\;=\; nM - w\;,\;\; x,v \in \mathbf{R},\; t>0 \quad (3.4)\\ w(x,v,0) &\;=\; w_I(x,v) \quad (3.5) \end{aligned}$$

Ansatz

We make the Ansatz

$$w^N(x,v,t) = \sum_{k=0}^{N} \; w_k(x,v,t)\; \tau^k.$$

Density

Consequently, n takes the form

$$n^N(x,t) = \sum_{k=0}^{N} n_k(x,t)\; \tau^k\;,$$

where

$$n_k(x,t) = \int_{\mathbf{R}} w_k(x,v,t)dv\;.$$

Current density

We also define the current density

$$J^N = -\int_{\mathbf{R}} v\; w^N\; dv\;\; = \sum_{k=0}^{N} J_k\; \tau^k$$

with

$$J_k(x,t) = -\int_{\mathbf{R}} v\; w_k(x,v,t)\; dv.$$

Analysis

Inserting w^N in (3.4) and equalling the powers of τ, we get the following results :

- 0th order term

  The equations for w_0 read :

  $$\left\{ \begin{array}{lcl} \partial_t w_0 &=& -w_0 \;+\; n_0\, M \\ w_0(w,v,0) &=& w_I(x,v) \end{array} \right.$$

  Density n_0

  By integration over v, we get $\;\partial_t n_0 \;=\; 0$, so

  $$n_0(x,t) = n_0(x) = n_I(x)\;(= \int w_I dv).$$

  Solution w_0

  Hence we can solve the equation for w_0 with the "variation of the constant" and find the solution :

  $$w_0(x,v,t) \;=\; n_I(x)M(v) \;+\; e^{-t}\;(w_I(x,v) - n_I(x)M(v))\;.$$

Asymptotical behaviour
It is a function of $\mathcal{S}$ for every t, and we have

$$||w_0 - n_I M||_{L^2} \ \to \ 0 \text{ as } t \ \to \ \infty.$$

The zeroth order term returns to equilibrium.

- 1st order term
  The equations for w_1 read :

  $$\begin{cases} \partial_t w_1 \ + \ v\partial_x w_0 \ + \ V'(x)\partial_v w_0 & = \ -w_1 \ + \ n_1 M \\ w_1(x,v,0) & = \ 0 \end{cases}$$

  Density n_1
  By integration over v and using that $w_0 \in \mathcal{S}$, we get for the first order density $\partial_t n_1 \ = \ \partial_x J_0 \ = \ e^{-t}\partial_x J_I$, and hence, because of $n_1(x,0) = 0$,

  $$n_1(x,t) = (1 - e^{-t})\partial_x J_I(x).$$

  Solution w_1
  Inserting this in the equation for w_1, we obtain :

  $$\begin{aligned} w_1(x,v,t) \ &= \ \partial_x J_I M \ + \ (v\partial_x \ + \ V'\partial_v)n_0 M \\ &\quad + e^{-t}\left((v\partial_x \ + \ V'\partial_v)(t(n_0M - w_I) + n_0 M) \ - (1+t)\partial_x J_I M\right) \end{aligned}$$

  Asymptotical behaviour
  We note that w_1 still belongs to $\mathcal{S}$ for good potentials, and verifies

  $$||w_1 - \partial_x J_I M \ - \ (v\partial_x \ + \ V'\partial_v)n_0 M||_{L^2} \ \to \ 0 \text{ as } t \ \to \ \infty.$$

- k-th order term, $k \geq 2$
  We have for w_k :

  $$\begin{cases} \partial_t w_k \ + \ wk \ = \ -v\partial_x w_{k-1} \ - \ V'\partial_v w_{k-1} \ + \ n_k M \ =: r_{k-1} \\ w_k(x,v,0) \ = \ 0 \end{cases} \tag{3.6}$$

  Density n_k
  The notation r_{k-1} is justified by the fact that for the density n_k, as $n_k(x,0) = 0$, we have :

  $$n_k(x,t) \ = \ \int_0^t \partial_x J_{k-1}(x,v,t)dt \ .$$

  Solution w_k
  Putting this in the equation (3.6), we find w_k as in the two first order terms :

  $$w_k(x,v,t) \ = \ e^{-t}\int_0^t e^s r_{k-1}(x,v,s)ds$$

Conclusion This gives an iterative computation of the expansion, with a leading term tending to the equilibrium distribution $n_I \ M$.

3.2.3 Variation 2 : Derivation of the Drift Diffusion Model

We still consider the (classical) Boltzmann equation :

$$\partial_t\, w \;+\; v.\nabla_x\, w \;+\; E.\nabla_v\, w \;=\; \frac{1}{\tau}(nM - w)\;,\;\; x \in \mathbf{R^d},\; v \in \mathbf{R^d},\; t > 0$$

$E(x)$ replaces ∇V.

Equation

We want to express that the collisions are leading the equation, hence we scale the time by $1/\epsilon$, with for example $\epsilon := \tau$, and come to the equation :

$$\epsilon^2\, \partial_t\, w \;+\; \epsilon\,(v.\nabla_x\, w \;+\; E.\nabla_v\, w) \;= nM - w\;,\;\; x \in \mathbf{R^d},\; v \in \mathbf{R^d},\; t > 0 \tag{3.7}$$

with the initial condition $w(x, v, 0) = w_I(x, v)$ independent of ϵ.

Ansatz

We make the Ansatz $w = \sum \epsilon^k f_k$,

Density

the density is thus $n = \int f dv = \sum \epsilon^k n_k$, $n_k = \int f_k dv$.

Other moments

We also need the first and second moments of the function w (and similarly for w_k) :

$$\begin{array}{ll} \text{the current density} & J(x,t) \;=\; -\displaystyle\int_{\mathbf{R^d}} vw\; dv \\ \text{the moment of 2nd order} & \sigma = (\sigma_{ij}(x,t))_{ij} \;=\; \left(\displaystyle\int_{\mathbf{R^d}} v_i v_j w\; dv\right)_{ij}\;. \end{array}$$

Concerning the isotropic Maxwellian Distribution M, we write $3D$ for $\int_{\mathbf{R^d}} v^2 M(v) dv$ and recall that $\int_{\mathbf{R^d}} v.\nabla_v M \;=\; -3$.

Analysis

Insertion in (3.7) leads to :

- Oth Order

  $$w_0(x, v, t) \;=\; n_0(x, t) M(v) \;\text{ with }\; n_0(x, 0) \;=\; n_I(x)$$

  So no big condition appears for n_0 in the zeroth order equation. Current of order 0 is zero :

  $$J_0(x, t) \;=\; 0\;.$$

- 1st Order

$$v.\nabla_x w_0 \;+\; E.\nabla_v w_0 \;=\; n_1 M \;-\; w_1$$

Replacing w_0 through $n_0 M$ gives an expression of w_1 :

$$w_1 \;=\; n_1 M \;-\; M v.\nabla_x n_0 \;-\; n_0 E.\nabla_v M$$

Drift diffusion current
We get a trivial equation after integrating over v, but the following current density of order 1 if we multiply by v before integrating :

$$J_1(x,t) \;=\; D\nabla_x n_0 \;-\; n_0 E$$

The first order current is the drift-diffusion current created by E and the density of order zero. The diffusion current is $D\nabla_x n_0$: by definition, diffusion takes place for heterogeneous repartition of the particles (which implies a gradient of density). The drift current is created by the motion of the electrons due to the electric field.
We get an equation for the total current using the equation of :

- 2nd order

$$\partial_t w_0 \;+\; v.\nabla_x w_1 \;+\; E.\nabla_v w_1 \;=\; n_2 M \;-\; w_2$$

By integration over v, the drift term $E.\nabla_v w_1$ vanishes (see expression of w_1 for its behaviour at $v = \infty$), and we obtain using
$\int v.\nabla_x w_1 dv \;=\; \nabla_x . \int v w_1 dv \;= \nabla_x . J_1$ the

Drift diffusion equation

$$\left\{ \begin{array}{l} \partial_t n_0 \;-\; \nabla_x . (D\nabla_x n_0 \;-\; n_0 E) \;=\; 0 \\ n_0(x,0) \;=\; n_I(x) \end{array} \right. \tag{3.8}$$

Conservation, evolution
We notice through integration of (3.8) the conservation in time of the quantity $\int_{\mathbf{R^d}} n_0(x,t)$, number of particles at the 0th order and total number of particles, since for $k \geq 1$, $n_k(x,0) = 0$ holds.

The density n_0 therefore satisfies the following equation, provided $E(x)n_0(x,t) \to 0$ as $x \to \infty$, ie for not too bad $E(x)$:

$$\frac{1}{2}\frac{d}{dt}||n_0||^2_{L^2} \;+\; D||\nabla_x n_0||^2_{L^2} \;=\; \frac{1}{2}\int_{\mathbf{R^d}} \nabla_x . E \; n_0^2 \, dx \tag{3.9}$$

This was obtained by multiplying (3.8) by n_0 and integrating over x.

- k-th order
  Iteratively we get similar equations for the w_k, but the current density at order k will now depend on the fluctuations of the current of order $k-1$:

  $$\begin{array}{rcl} \partial_t w_k \;+\; v\nabla_x w_{k+1} \;+\; E.\nabla_v w_{k+1} & = & n_{k+2}M \;-\; w_{k+2} \\ n_{k+1}M \;-\; v.\nabla_x w_k \;-\; E.\nabla_v w_k \;-\; \partial_t w_{k-1} & = & w_{k+1} \\ w_{k+2}(x,v,0) & = & 0 \end{array}$$

  As we can show iteratively, the function w_{k+1} keeps a good behaviour for infinite velocities, which leads to the equation for the density n_k and an expression of J_{k+1} :

  $$\left\{ \begin{array}{rcl} \partial_t n_k & = & \nabla_x.J_{k+1} \\ J_{k+1} & = & \nabla_x \sigma_k \;- n_k E \;-\; \partial_t J_{k-1} \end{array} \right. \tag{3.10}$$

  We used that $\int_{\mathbf{R^d}} v_i \partial_{v_j} w_k dv \;=\; 0$ for $i \neq j$,

  and $\nabla\sigma$ is the column vector (c_i) with $c_i = \sum_{j=1}^{d} \partial_{x_j} \sigma_i^j$.

In quasi stationnary cases, we can drop the correction term due to fluctuations in time of the current and get the same drift diffusion equations as in the zero-th order. In fact, this term can also be neglected in many no stationnary drift diffusion models where the fluctuation of the current occur in characteristic times that are much bigger than the relaxation time.

Conclusion
In a stationnary case, and at first order approximation, we can consider that the drift diffusion current satisfies :

$$\left\{ \begin{array}{rcl} J & = & \tau(D\nabla_x n_0 \;-\; n_0 E) \\ \nabla_x.J & = & 0 \end{array} \right. \tag{3.11}$$

3.2.4 Variation 3 : 2-D model with strong field in one direction

The aim of this section is to modelize a 2-dimensional case with strong electric field in one small direction (say y-direction). This implies big accelerations of the electrons in this direction and hence many collisions.
We still use the classical Boltzmann-type equation :

$$\begin{array}{l} \partial_t\, w \;+\; v.\nabla_{\mathbf{x}}\, w \;+\; E.\nabla_{\mathbf{v}}\, w \;=\; \frac{1}{\tau}(nM - w) \\ \mathbf{x} \;= (x,y) \in \mathbf{R^2},\; \mathbf{v} = (u,v) \in \mathbf{R^2},\; t > 0 \end{array}$$

The field E_x along the x-direction is supposed to be of order of magnitude 1, whereas E_y is of order $\frac{1}{\epsilon^2}$, so we scale as follows, with $\epsilon := \tau$:

$$t_s = \epsilon\, t,\; E_{y_s} = \frac{E_y}{1/\epsilon^2},\; y_s = \frac{y}{\epsilon^2}$$

and obtain by inserting in the equation above :

Equation

$$\epsilon^2 \partial_t w \;+\; \epsilon\,(u\partial_x w \;+\; E_x \partial_u w) \;+\; \frac{1}{\epsilon}\,(E_y \partial_v w \;+\; v\partial_y w) \;=\; nM - w$$

with the initial condition

$$w(x,v,0) = w_I(x,v) \quad \text{independent of } \epsilon.$$

Analysis
Using the current density

$$\mathbf{J}(x,y,t) = -\int_{\mathbf{R^2}} \mathbf{v}\; w(x,y,u,v,t) du dv \;=\; \Big(J^1(x,y,t), J^2(x,y,t)\Big)$$

and writing as usual $w = \sum \epsilon^k w_k$, we come for the first order terms to :

- 0th Order

$$E_y \partial_v w_0 \;+\; v\partial_y w_0 \;=\; 0 \;\text{ and }\; w_0(\mathbf{x},\mathbf{v},0) = w_I(\mathbf{x},\mathbf{v})$$

Current density
Integration over the whole velocity space and just over v gives :

$$\begin{array}{l} \partial_y J_0^2 \;=\; 0 \\ \partial_y \left(\int_{\mathbf{R}} v w_0 \; dv \right) \;=\; 0 \end{array}$$

Function w_0
For the function w_0 we conclude that it is a function of the variables

$\dfrac{v^2}{2} - V(x,y,t),\ x,\ u$ and t :

$$w_0 \ = \ w_0(\frac{v^2}{2} - V(x,y,t), x, u, t)$$

Indeed, we can introduce the characteristic curves $X(h) = (y(h), v(h))$ defined by

$$\left\{ \begin{array}{lcl} \dot{X}(h) & = & F(X(h)) \\ X(0) & = & (y_0, v_0) \end{array} \right.$$

where $F(a,b) = (b, E_y(a))$.
Then, for all x, u, t, the function $w_0(x, y(h), u, v(h), t)$ is constant along the characteristics :

$$\frac{d}{dh}(w_0(y(h), v(h))) = 0$$

and, if we introduce the potential V such as $E = \nabla_{\mathbf{x}} V$, the equation of these caracteristics is :

$$\left\{ \begin{array}{lcl} \dot{y} & = & v \\ \dot{v} & = & \frac{\partial V}{\partial y}(y(h)) \\ y(0) = y_0 & & v(0) = v_0 \end{array} \right.$$

which leads, after a short computation, to the energy conservation :

$$\frac{v^2}{2} \ - \ V(y) \ = \ c^{ste} \ = \ \frac{v_0^2}{2} \ - \ V(y_0)$$

This should be also true at $t = 0$, so we have to suppose that w_I is of the form $w_I(\dfrac{v^2}{2} - V(x,y,t), x, u, t)$.

- 1st order

  $$n_0 M - w_0 \ = \ v \partial_y w_1 \ + \ E_y \partial_v w_1$$

  Current density
  Integration over the velocity space before multiplication by $\mathbf{v}$ gives a similar result to the 0th order case :

  $$\partial_y \ J_1^2 \ = \ 0 \ .$$

  Because of the form of w_0, we have

  $$\int_{\mathbf{R}} v w_0 \ dv \ = \ 0$$

so that :

$$\begin{aligned} \mathbf{J_0} &= \begin{pmatrix} \int_{\mathbf{R^2}} uw_0 \, dudv \\ 0 \end{pmatrix} \\ &= \begin{pmatrix} 0 \\ -n_1 \, E_y \end{pmatrix} + \partial_y \begin{pmatrix} \int_{\mathbf{R^2}} uv \; w_1 dudv \\ \int_{\mathbf{R^2}} v^2 \; w_1 dudv \end{pmatrix} \end{aligned}$$

- 2nd order

$$n_1 M - w_1 \;=\; u\partial_x w_0 \;+\; E_x \partial_u w_0 \;+\; v\partial_y w_2 \;+\; E_y \partial_v w_2$$

We come after integration to :

$$\partial_y J_2^2 \;=\; -\partial_x J_0^1$$

and

$$J_1 \;=\; \partial_x \begin{pmatrix} \int_{\mathbf{R^2}} u^2 w_0 dudv \\ 0 \end{pmatrix} \;+\; \partial_y \begin{pmatrix} \int_{\mathbf{R^2}} uvw_2 dudv \\ \int_{\mathbf{R^2}} v^2 w_2 dudv \end{pmatrix} \;-\; \begin{pmatrix} n_0 E_x \\ n_2 E_y \end{pmatrix}$$

- 3rd order
  Time derivative is now present :

$$n_2 M - w_2 \;= \partial_t w_0 \;+\; u\partial_x w_1 \;+\; E_x \partial_u w_1 \;+\; v\partial_y w_3 \;+\; E_y \partial_v w_3$$

which leads to :

$$\partial_t n_0 \;-\; \nabla_{\mathbf{x}} . J_1 \;-\; \partial_y J_3^2 \;=\; 0$$

(we used that $\nabla_{\mathbf{x}} . J_1 \;=\; \partial_x J_1^1 + \underbrace{\partial_y J_1^2}_{=0}$).

Remark

These results have been obtained supposing that
$w_k(\mathbf{x}, \mathbf{v}, t)$ and $\mathbf{v} \; w_k(\mathbf{x}, \mathbf{v}, t)$ tend to zero as $\mathbf{v}$ tends to infinity.

An other method

The results of the first two items ($\partial_y J_0^2 \;=\; \partial_y J_1^2 \;=\; 0$) also lead to the following considerations, where we use a partial density g defined as a partial integral of w :

$$g(\mathbf{x}, u, t) = \int_{\mathbf{R}} w(\mathbf{x}, u, v, t) dv$$

If $N(u)$ denotes $\int_{\mathbf{R}} M(u, v) dv$,
and $I(\mathbf{x}, u, t)$ the partial current in y-direction :

$$I \;=\; -\int_{\mathbf{R}} v \; w \; dv \quad \text{so that} \quad \int_{\mathbf{R}} I \; du \;=\; J^2$$

We have $\partial_y I_0 \; = \; 0$ and J_1^2 does not depend on y.
The function g satisfies the :

Equation

$$\epsilon^2 \partial_t g \; + \; \epsilon \, (u \partial_x g \; + \; E_x \partial_u g) \; - \; \frac{1}{\epsilon} \, \partial_y \, I \; = \; nN - g$$

Ansatz and assumption
We write an expansion of $g \; = \; \sum_{k \geq 0} \epsilon^k \, g_k$,
analogously of $I \; = \; \sum_{k \geq 0} \epsilon_k \, I_k$.
Let us assume that $\partial_y I_1 \; = \; 0$, then

$$\frac{1}{\epsilon} \, \partial_y \, I \; = \; \sum_{k \geq 1} \epsilon^k \partial_y I_{k+1} \; .$$

Analysis

- 0th order term
  This gives in our assumption a maxwellian distribution for the zeroth order partial density :
  $$g_0 \; = \; n_0 \, N \; .$$
- 1st order equation
  $$u \, \partial_x \, g_0 \; + \; E_x \, \partial_u \, g_0 \; - \; \partial_y \, I_2 \; = \; n_1 N - g_1$$
  which implies
  $$g_1 \; = \; n_1 N \; - \; u \, \partial_x \, g_0 \; - \; E_x \, \partial_u \, g_0 \; + \; \partial_y \, I_2$$
  Integration over u now gives, because of the form taken by g_0 :
  $$\partial_y J_2^2 \; = \; 0$$
- 2nd order equation
  It reads :
  $$\partial_t g_0 \; + \; u \, \partial_x \, g_1 \; + \; E_x \, \partial_u \, g_1 \; - \; \partial_y \, I_3 \; = \; n_2 \, N \; - \; g_2$$
  and after integration over u, also using the expression of g_1 we got in the preceding item :
  $$\partial_y \, J_3^2 \; = \; \partial_t \, n_0 \; + \; \partial_x \, (E_x \, n_0 \; - D \, \partial_x \, n_0) \; + \; \underbrace{\partial_x \partial_y \int_{\mathbf{R}} u \, I_2 \, du}_{=0 \text{ if we assume } \partial_y I_2 = 0}$$

We might compare this result to the preceding result of the third order equation on page (35) and write :

$$\partial_x J_1^1 \;=\; \partial_x \left(E_x \, n_0 \; - D \, \partial_x \, n_0 \; + \underbrace{\partial_y \int_{\mathbf{R}} u \; I_2 \; du}_{=0 \text{ if } \partial_y I_2 = 0} \right) \; .$$

Chapter 4

Semiconductors

Until now we have considered particles allowed to have every energy (every velocity) and moving in a vacuum.

In fact, in a solid at room temperature, two kinds of eletrons may exist : some with lower energy strongly hold to the nucleus, while others with higher energy are free to move and allow the solid to conduct electricity. If the conductivity of semi-conductors increases with temperature, pure semi conductors will anyway not conduct enough electricity, and (technically rather complicated) methods consist in introducing free electrons : this is called doping.

Purpose of this chapter is to understand this procedure of doping and how the equations of the previous chapters can be used and adapted.

4.1 Cristal lattices

In an ideal solid exempt of impurities, atoms are periodically disposed in a cristal lattice $\mathcal{R}$ with primitive vectors $\mathbf{a_1}, \mathbf{a_2}, \mathbf{a_3}$ that define the primitive cell :

$$\mathcal{R} \; = \; \{n_1\mathbf{a_1} + n_2\mathbf{a_2} + n_3\mathbf{a_3}, \; n_1, n_2, n_3 \; \in \mathbf{Z}\}$$

A reciprocal lattice is defined :

$$\mathcal{R}^* \; = \; \{n_1\mathbf{\hat{a}_1} + n_2\mathbf{\hat{a}_2} + n_3\mathbf{\hat{a}_3}, \; n_1, n_2, n_3 \; \in \mathbf{Z}\}$$

where $\mathbf{\hat{a}_1}, \mathbf{\hat{a}_2}, \mathbf{\hat{a}_3}$ satisfy :

$$\mathbf{a_i} \; . \; \mathbf{\hat{a}_j} \; = \; 2\pi\delta_{i,j}$$

The primitive cell $\mathcal{B}$ of the reciprocal lattice is called Brillouin zone.

Let V_L be the potential generated by the ions located at the points of $\mathcal{R}$, then V_L is periodic over the lattice, and the steady states Ψ of energies E of the electron verify :

$$H_L\Psi \; = \; (-\frac{\hbar^2}{2m}\triangle \; - \; qV_L)\Psi \; = E \; \Psi \; .$$

A theorem (called Bloch Theorem) then assures that, because of the periodicity of V_L, Ψ has the form :

$$\Psi(\mathbf{r}) \;=\; \Psi_{\mathbf{k}}(\mathbf{r}) \;=\; u_{\mathbf{k}}(r)\, e^{i\mathbf{k}.\mathbf{r}}$$

where $\mathbf{r} \in \mathbf{R^3}$, $\mathbf{k} \in \mathbf{R^3}$ and $u_{\mathbf{k}}$ is periodic over the lattice.
Inserting the Bloch Ansatz into the wave equation gives :

$$-\frac{\hbar^2}{2m}(\triangle u_{\mathbf{k}} + 2i\mathbf{k}.\nabla\, u_{\mathbf{k}}) \;+ (\frac{\hbar^2}{2m}|\mathbf{k}|^2 - qV_L(r))u_{\mathbf{k}} \;=\; E\, u_{\mathbf{k}}\ .$$

The periodicity of $u_{\mathbf{k}}$ and operator theory results now imply that for each $\mathbf{k}$, the eigenvalues E consitute an infinite sequence $E_l(\mathbf{k})$.
In fact, since $e^{i\mathbf{k}.\mathbf{r}} = 1$ for $\mathbf{k} \in \mathcal{R}^*$ and $\mathbf{r} \in \mathcal{R}$, the wave vector $\mathbf{k}$ can be taken in the cell $\mathcal{B}$.
The function E_l is called the first energy band of the cristal, and for an electron of the subband l, the velocity corresponding to the wave vector $\mathbf{k}$ is :

$$v_l(\mathbf{k}) \;=\; \frac{1}{\hbar}\nabla_{\mathbf{k}} E_l(\mathbf{k})\ .$$

This is the way the equations written for v in the previous chapters can be re-written for $\mathbf{k}$: using $v_l(\mathbf{k})$, and using functions w of $(x, \mathbf{k}, t)$ instead of (x, v, t). The principal difference is the appartenance of $\mathbf{k}$ to the bounded Brillouin zone $\mathcal{B}$ and not to the unbounded domain $\mathbf{R^3}$.

4.2 Semi conductors and doping

Definition
These bands of energy E_l are here supposed to be distinct. The valence band is the highest band of energy where the electrons are still held to the nucleus, the next band is the conduction band.
A semi conductor (like Silicium, column IV of Mendeleiev's classification, ie four electrons in the valence band) is defined by the following property : at zero Kelvin, the valence band (of maximal energy E_V) is full and the conduction band (of minimal energy E_C) is empty, but at room temperature, thermical energy (of order of magnitude k_BT, with k_B the Boltzmann constant) allows electrons to jump from the valence band to the conduction band.
The difference

$$E_g := E_C - E_V$$

is called the energy gap. So the condition reads $E_g \leq k_BT$.
We mention the two other cases : metal have already got electrons in the conduction band at zero Kelvin, isolators have a too high energy gap and no electron is in the conduction band at any T.

Holes

The jump of an electron from the valence band to the conduction band lets a hole in the valence band, that might be filled in by an electron of the subband : to these moving holes a charge $+q$ is attributed. Since they can move, they contribute to the current.

Doping

In order to increase the number of conduction electrons in the semi-conductor, new atoms (impurities) are introduced. Let us take for instance foreign atoms that have one more electron (ie column $+V$ of the classification) in the valence band than the semiconductor atoms do. These atoms build a covalent bond with the semi-conductor atoms (four electrons from the Silicium together with four from the foreign atom), but there is one electron left. The foreign atoms are chosen so that their valence electrons have an energy lightly inferior to the minimal conduction energy E_C, hence the left electron can easily jump to the conduction band at room temperature. We have obtained a $n-doped$ semi-conductor : for each foreign atom, there is one more conduction electron and the covalent bond is positive charged.
Similarly we can increase the number of conducting holes by using elements of the III-rd column and create $p-doped$ semiconductors.
In practice, the doping is large, so that almost all conduction electrons come from this doping.

4.3 Drift Diffusion - Poisson Equations

Drift diffusion model for semi-conductors contains the same equations as seen before (section 3.2.3 page 30), but written a second time for the holes. They macroscopically describe the motion of the free particles (ie electrons of the conduction band and holes of the valence band). In fact, interactions exist between holes and electrons, the so-called combination-regenerations, but they will be neglected in the next chapters.

Adding the Poisson Equation (see 1.6 page 10), we get the self consistent model for semiconductors with doping concentration C :

$$\left\{\begin{array}{rcl} \partial_t n \; - \; \nabla_x . J_n & = & 0 \\ J_n & = & D \nabla_x n \; - \; n \nabla_x V \\ \partial_t p \; + \; \nabla_x . J_p & = & 0 \\ J_p & = & D \nabla_x p \; + \; p \nabla_x V \\ \epsilon_s \triangle V & = & n - p - C \end{array}\right. \tag{4.1}$$

where the indices n and p respectively stand for electrons and holes, n and p for the electron and hole densities, ϵ_s the permittivity of the environment.

Chapter 5

From Drift Diffusion to MOSFETs Equations

In the coming two chapters, the Drift Diffusion model found in section 3.2.3 of chapter 3 is written for both holes and electrons, together with the Poisson Equation (1.6) : this leads to the system (5.1).
Global aim is the expression of the current in a MOSFET. The results below have been obtained in [1] through appropriate scaling and derivation of a quasi one dimensionnal model.

The purpose of this chapter is the obtention of the MOSFET equations through appropriate scaling from the stationary Drift Diffusion Model (without recombination rate : see [1]).

5.1 Equations and boundary conditions

5.1.1 Equations

The stationary Drift Diffusion equations are given in a domain $\Omega \subseteq \mathbf{R^d}, d = 1, 2, 3$ by :

$$\begin{array}{lcl} \nabla.\,(\epsilon\,\nabla\,V) & = & q(n-p-C) \\ \\ \nabla.\,(J_n) & = & 0 \\ J_n & = & q(D_n\,\nabla\,n - \mu_n\,n\,\nabla\,V) \\ \\ \nabla.\,(J_p) & = & 0 \\ J_p & = & q(-D_p\,\nabla\,p - \mu_p\,p\,\nabla\,V) \end{array} \tag{5.1}$$

where ϵ stands for the permittivity, V for the potential n (p) for the *electron* (*hole*) density, C for the *doping* concentration, J_n (J_p) for the *current* density associated to the electrons (holes).

D_n (D_p) and μ_n (μ_p) are the diffusion and mobility coefficients of electrons (holes) and satisfy the Einstein relations

$$D_n = \mu_n U_T, \qquad\qquad D_p = \mu_p U_T, \tag{5.2}$$

where $U_T = \dfrac{k_B T}{q}$ is the thermal voltage, $U_T \approx 0.025$ V at room temperature.

5.1.2 Boundary conditions

The boundary $\partial\Omega$ of the domain Ω is assumed to consist in a Dirichlet part $\partial\Omega_D$, corresponding to Ohmic contacts and a Neumann part $\partial\Omega_N$, corresponding to insulating or artificial surfaces.

At Ohmic contacts, the space charge vanishes, there is thermal equilibrium and the quasi Fermi levels ϕ_n and ϕ_p assume the values of the applied voltages :

$$\begin{array}{lcl} n - p - C & = & 0 \\ np & = & n_i^2 \\ \phi_n := V - U_T \ln\left(\frac{n}{n_i}\right) & = & U = \phi_p := V + U_T \ln\left(\frac{p}{n_i}\right) \end{array} \tag{5.3}$$

n_i is the intrinsic density of mobile carriers ($n_i \approx 10^{10} cm^{-3}$ at room temperature). We refer to [5] for the second equation.
These three conditions lead to following results for the (positive) densities n, p and for the the potential V:

$$\begin{array}{lcl} n(x) = n_D(x) & = & \frac{1}{2}\left(C(x) + \sqrt{C(x)^2 + 4n_i^2}\right) \\ p(x) = p_D(x) & = & \frac{1}{2}\left(-C(x) + \sqrt{C(x)^2 + 4n_i^2}\right) \\ V(x) = V_D(x) & = & U(x) + V_{bi}(x) \qquad\qquad \text{for } \ x \in \partial\Omega_D \end{array} \tag{5.4}$$

with $V_{bi}(x) = U_T \ln\left(\dfrac{n_D(x)}{n_i}\right)$.

Along insulating and artificial surfaces, there is no current flow and a zero electric field in the normal direction ν (unit outward normal vector to the boundary) :

$$\begin{array}{lcl} \dfrac{\partial V}{\partial \nu}(x) := \nabla\, V \cdot \nu & = & 0 \\ J_n(x) \cdot \nu & = & 0 \\ J_p(x) \cdot \nu & = & 0 \quad \text{for } \ x \in \partial\Omega_N \end{array} \tag{5.5}$$

5.1.3 With the Slotboom variables

Using the so called Slotboom variables (linear in the densities), we write :

$$n = n_i \, e^{\frac{V}{U_T}} \, u \qquad\qquad p = n_i \, e^{-\frac{V}{U_T}} \, v$$

and obtain for the current densities in (5.1), using the Einstein relations (5.2) :

$$J_n = q \, U_T \, n_i \, \mu_n \, e^{\frac{V}{U_T}} \, \nabla \, u \qquad J_p = -q \, U_T \, n_i \, \mu_p \, e^{-\frac{V}{U_T}} \, \nabla \, v$$

and thus for the equations of paragraph 5.1.1 :

$$\begin{aligned} \epsilon \, \Delta \, V &= qn_i \, (e^{\frac{V}{U_T}} u \; - \; e^{-\frac{V}{U_T}} v) \; - \; qC \\ 0 &= U_T \, n_i \, \nabla . \, (\mu_n \, e^{\frac{V}{U_T}} \, \nabla \, u) \\ 0 &= U_T \, n_i \, \nabla . \, (\mu_p \, e^{-\frac{V}{U_T}} \, \nabla \, v) \end{aligned} \tag{5.6}$$

with the boundary conditions :

Dirichlet conditions :

$$V = V_D, \;\; u = u_D, \;\; v = v_D \qquad \text{on } \partial\Omega_D \tag{5.7}$$

$$\text{with} \quad u_D = n_i^{-1} \, e^{-\frac{V_D}{U_T}} \, n_D \quad \text{and} \quad v_D = n_i^{-1} \, e^{\frac{V_D}{U_T}} \, p_D \tag{5.8}$$

Neumann conditions :

$$\frac{\partial V}{\partial \nu} \; = \; \frac{\partial u}{\partial \nu} \; = \; \frac{\partial v}{\partial \nu} \; = \; 0 \;\; \text{on } \partial\Omega_N \tag{5.9}$$

5.2 Scaling

We introduce the following scaling and bring the system of Drift Diffusion Equations (5.6), with boundary conditions (5.7), (5.8) and (5.9) into a dimensionless form. Let be

- L a characteristic length for the geometry of the transistor,
- U_T the thermal voltage seen in (5.2),
- $\widetilde{C}$ the maximal absolute value of the doping concentration ($\widetilde{C} \approx 10^{20} \; cm^{-3}$),
- $\tilde{\mu}$ a characteristic value for the mobilities μ_n and μ_p (for silicon, $\tilde{\mu}$ is of the order of 1000 $cm^2V^{-1}s^{-1}$).

We thus set (s stands for *scaled*):

$$x \; = \; L\, x_s, \qquad V \; = \; U_T\, V_s$$

$$n \; = \; \widetilde{C}\, n_s, \qquad p \; = \; \widetilde{C}\, p_s, \qquad C \; = \; \widetilde{C}\, C_s$$

$$J_n = \frac{qU_T\widetilde{C}\widetilde{\mu}}{L}\, J_{n_s}, \qquad J_p \; = \; \frac{qU_T\widetilde{C}\widetilde{\mu}}{L}\, J_{p_s}$$

$$\mu_n \; = \; \widetilde{\mu}\mu_{n_s}, \qquad \mu_p \; = \; \widetilde{\mu}\mu_{p_s}, \qquad D_n \; = \; U_T\widetilde{\mu}\mu_{n_s}, \qquad D_p \; = \; U_T\widetilde{\mu}\mu_{p_s}$$

By now the subscript s will be omitted. Introducing the parameters

$$\lambda \; = \; \left(\frac{\epsilon U_T}{q\widetilde{C}L^2}\right)^{\frac{1}{2}} \quad \text{and} \quad \delta \; = \; \left(\frac{n_i}{\widetilde{C}}\right)^{\frac{1}{2}} \tag{5.10}$$

(λ is the scaled Debye length), the Drift Diffusion problem now reads :

$$\begin{array}{lcl} \lambda^2\, \Delta\, V & = & \delta^2\, (e^V u - e^{-V} v) - \; C \\ \\ \nabla.\, (J_n) & = & 0 \\ J_n & = & \mu_n\, e^V\, \nabla\, u \\ \\ \nabla.\, (J_p) & = & 0 \\ J_p & = & -\mu_n\, e^{-V}\, \nabla\, v \end{array} \tag{5.11}$$

with the boundary conditions

$$V \; = \; V_D, \;\; u \; = \; u_D, \;\; v \; = \; v_D \qquad\qquad on\ \partial\Omega_D \tag{5.12}$$

$$\text{where } \; u_D(x) \; = \; e^{-U(x)}\;, \qquad v_D(x) \; = \; e^{U(x)} \qquad\qquad x \in \partial\Omega_D, \tag{5.13}$$

$$\begin{array}{rcl} V_D(x) & = & U(x) + \ln\left[\dfrac{C(x) + \sqrt{C(x)^2 + 4\delta^4}}{2\delta^2}\right] \\ & = & U(x) + V_{bi}(x)\;, \qquad\qquad x \in \partial\Omega_D \end{array}$$

and

$$\frac{\partial V}{\partial \nu} \; = \; \frac{\partial u}{\partial \nu} \; = \; \frac{\partial V}{\partial \nu} \; = \; 0 \qquad\qquad on\ \partial\Omega_N \tag{5.14}$$

The Slotboom variables have now taken the form :

$$u \; = \; \delta^{-2}\, n\, e^{-V} \;\; \text{and} \qquad v \; = \; \delta^{-2}\, p\, e^{V}.$$

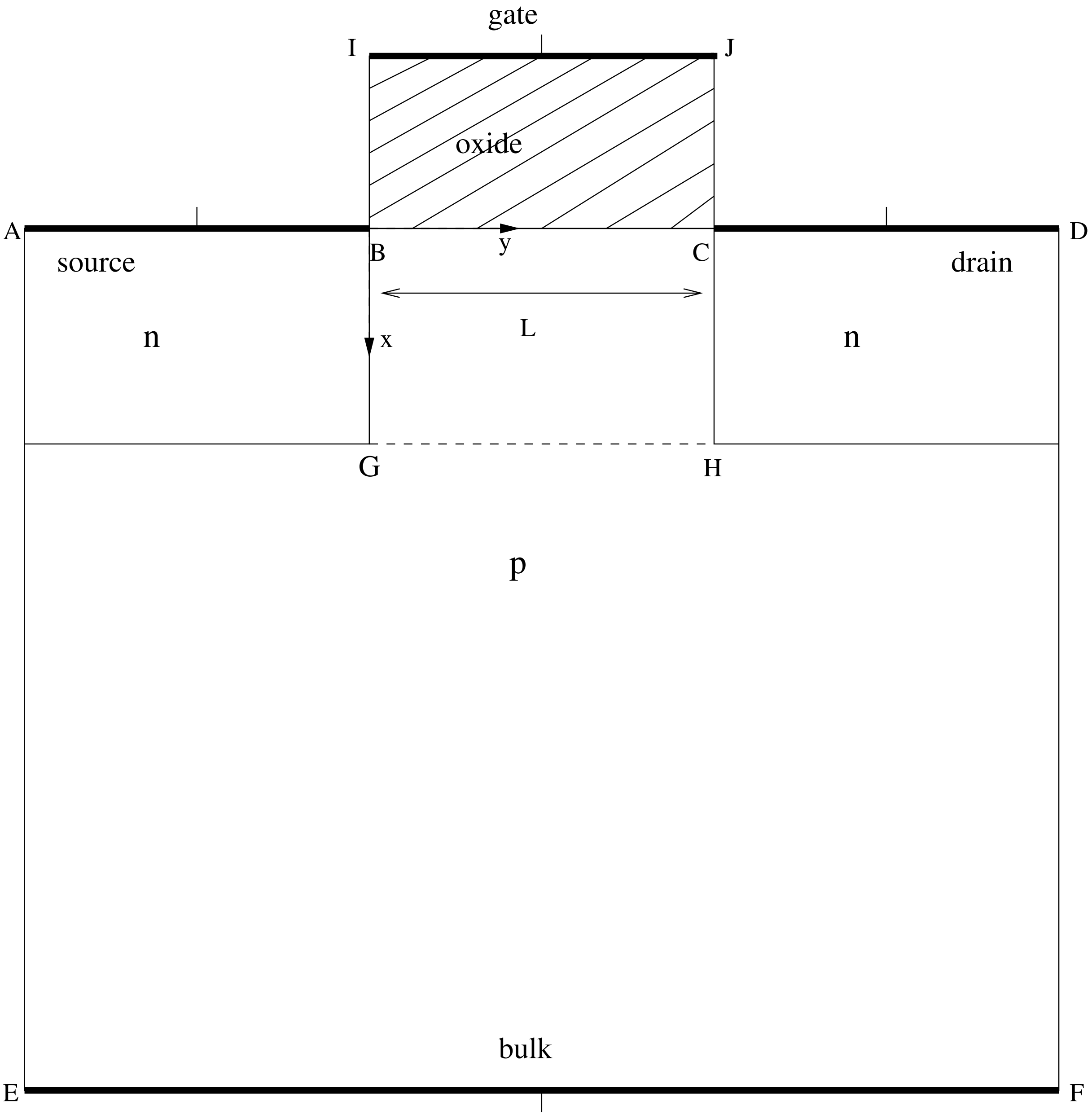

Figure 5.1: Cross section of a MOSFET

5.3 Geometry of the Metal Oxide Semiconductor Field Effect Transistor

5.3.1 Cross section of a MOSFET

see page 45

5.3.2 Explanation

A $d = 2$ dimensional model can be adopted.
The semiconductor part $ADFE$ of the MOSFET consists in three regions : *source, drain and bulk*. Each of these regions is uniformly doped, ie atoms that are positively (negatively) ionized at room temperature have been introduced in the source and drain regions (bulk region) in order to arise the number of mobile carriers : negative charged *electrons* in the so called *n-regions* let positive fixed ions, and positively charged *holes* in the *p-region* let negative fixed ions.
Bringing a n-region next to a p-region, as along BG and CH, we get opposite phenomena for the movement of the mobile carriers : electrons tend to *diffuse* from the n-region to the p-region, holes from the p-region to the n-region. However, the resulting electric field, created by the fixed ions, leads to the *drift* of mobile carriers, opposed to the diffusion. The region along the frontier with lower mobile carriers is called *pn-junction*.

In the following, the pn-junctions are assumed to be small compared to the length $L := BC$, reference length.

For positive applied bias on the gate IJ, the holes are repulsed and a *depletion* zone appears close to BC, even a *weak inversion* zone when the electron density becomes greater than the hole density, both densities remaining small for high doping. For larger applied bias, the hole density tends to zero whereas the electron density can become great : a *strong inversion* layer appears close to BC (charge can not penetrate the oxide), which may be followed by a depletion-weak inversion zone, as the potential decreases along the x-axe.

Then, applying a bias between source and drain, a current can circulate through the p-region and even become big when a strong inversion layer exists. In this case, the carriers responsible for the current flow are only the electrons (holes are not involved) : we have a so-called *n-channel* of length L.

To sum up, the gate voltage modulates the conductivity of the semiconductor, while the drain voltage controls the current flow.

5.4 MOSFET Equations and Boundary conditions

We set for the Slotboom variables, which have to be positive (see definition) :

$$u \;=\; e^{-\varphi_n} \;, \qquad\qquad v \;=\; e^{\varphi_p}.$$

So $\varphi_{n,p}$ are the quasi-Fermi levels scaled by U_T.

For example, the unscaled version for n reads : $n \;=\; n_i \; e^{\frac{V-\phi_n}{U_T}}$,
and the scaled one : $n \;=\; \delta^2 \; e^{V-\varphi_n}$.

Remembering $\varphi_n \;=\; \varphi_p \;=\; U$ the applied voltage at a Ohmic contact, we see that an equilibrium (no applied voltage : $U << U_T$) corresponds to $u \;\equiv\; v \;\equiv\; 1$.

5.4.1 Equations in the MOSFET

They simply read for the rectangle ADFE :

$$\lambda^2 \, \Delta \, V \;=\; \delta^2 \, (e^{V-\varphi_n} - e^{-V+\varphi_p}) - \; C \tag{5.15}$$

$$\begin{aligned} \nabla. \, (J_n) \;&=\; 0 \\ J_n \;&=\; -\mu_n \, e^{V-\varphi_n} \, \nabla \, \varphi_n \end{aligned} \tag{5.16}$$

$$\begin{aligned} \nabla. \, (J_p) \;&=\; 0 \\ J_p \;&=\; -\mu_p \, e^{\varphi_p - V} \, \nabla \, \varphi_p \end{aligned} \tag{5.17}$$

The oxide is free of charges, thus the potential verifies in the rectangle BCJI :

$$\Delta V \;=\; 0 \tag{5.18}$$

5.4.2 Boundary conditions

At the Ohmic contacts AB, CD and EF, we can write the Dirichlet conditions (the source is the reference voltage):

- $\varphi_n = \varphi_p = 0$ on AB
- $\varphi_n = \varphi_p = U_D$ on CD, U_D the drain-source voltage
- $\varphi_n = \varphi_p = U_B$ on EF, U_B the bulk-source voltage.

At the interface IJ, we have the condition (ideal case):

- $V(-d, y) = V_{bi} + U_G$, U_G the gate-source voltage.
- No current is assumed to be able to flow across the surfaces AE, DF, and IB, JC, so we have there homogenous Neumann conditions for the quasi Fermi levels (see (5.16) and (5.17)).

Chapter 6

A simplified model for MOSFETs

After reducing the problem on a central part of the transistor, we compute the current source-drain using a quasi-one dimensional model.

6.1 Reduction of the problem to the rectangle BCHG

We do following simplifications :
The quasi-Fermi levels corresponding to the majority carriers are constant in each $p-$and $n-$region, that means :

- $\varphi_n = 0$ in the source region, and hence on BG
- $\varphi_n = U_D$ in the drain region, and hence on CH
- $\varphi_p = U_B$ in the bulk region, and hence in BCHG

6.1.1 Rescaled equations in BCHG

We introduce the small parameter γ defined by :

$$\gamma = \frac{1}{\ln \frac{1}{\delta^2}} \quad \text{ie} \quad \delta^2 = e^{-\frac{1}{\gamma}}$$

δ has been defined in (5.10). We rescale the variables with this parameter γ :

$$W = \gamma V \,, \qquad \Phi_n = \gamma \varphi_n \,, \qquad \xi = \frac{x}{\bar{\lambda}}$$

where $\tilde{\lambda} = \dfrac{\lambda}{\sqrt{\gamma}}$.
As $\varphi_p = c^{st}$ in BCHG, the hole continuity equation is trivial, that's why we only consider the following equations :

$$\partial_\xi^2 W + \tilde{\lambda}^2 \partial_y^2 W = \exp\left(\frac{W - \Phi_n - 1}{\gamma}\right) - \exp\left(\frac{U_B - W - 1}{\gamma}\right) + 1 \quad (6.1)$$

and

$$\partial_\xi \left(\mu_n \exp\left(\frac{W - \Phi_n - 1}{\gamma}\right) \partial_\xi \Phi_n\right) + \tilde{\lambda}^2 \partial_y \left(\mu_n \exp\left(\frac{W - \Phi_n - 1}{\gamma}\right) \partial_y \Phi_n\right) = 0 \quad (6.2)$$

In the next section, we will use the smallness of $\tilde{\lambda}$ in order to derive a one-dimensional model.
We also recall that γ is a small parameter, so the discussion for the analysis of these equations in section 6.3 will be based on the sign of $W - \Phi_n - 1$ and of $U_B - W - 1$, ie the cases of small or big scaled electron-holes densities.

6.1.2 Boundary conditions at the interface BC

As there is no current flow crossing BC, $J_n \cdot \nu = 0$ or :

$$\partial_\xi \Phi_n = 0 \text{ at BC.} \quad (6.3)$$

The second boundary condition on BC is :

$$\alpha \partial_\xi W = W - \gamma V_{bi} - U_G \quad (6.4)$$

where $\alpha = \dfrac{\epsilon_s d}{\epsilon_o x \tilde{\lambda}}$.

In order to get it, we compute the potential in the oxide :

The oxide thickness is small compared to the channel length : $d << L$, and L was chosen as the reference length, so that in fact : $d << 1$; setting $\eta = \frac{x}{d}$, we get from 5.18 that :

$$\partial_\eta^2 V + d^2 \partial_y^2 V = 0$$

As d tends to zero, one can write and solve the equation

$$\partial_\eta^2 V = 0 \quad (6.5)$$

knowing that, even if the Neumann conditions seem to be violated, it is possible to consider corrector layers (that reveal to be a $O(d)$) at the boundaries BI and CJ. So we suppose (6.5) to be true everywhere in BCJI and solve it :

$$V_{ox}(\eta) \ = \ V(0_+, y) - (V_{bi}(0, y) + U_G)\, \eta \ + \ V(0_+, y)$$

We used here the continuity of the potential :

$$V(0_-, y) \ = \ V(0_+, y)$$

The continuity of the electric displacement at the interface BC :

$$\epsilon_{ox} \partial_x V \ (0-, y) \ = \ \epsilon_s \partial_x V \ (0+, y)$$

gives us the boundary condition on BC :

$$\frac{\epsilon_s d}{\epsilon_o x} \partial_x V \ = \ V - V_{bi} - U_G \qquad\qquad \text{on BC}$$

which reads (6.4) in the rescaled version.

6.1.3 Boundary conditions at the interfaces BG, CH

We rescale the equations seen in the introduction :
$\Phi_n \ = \ 0$ at BG and $\Phi_n \ = \ U_D$ at CH.
The potentials along the $pn-$junctions BG and CH are left unspecified.

6.1.4 Boundary conditions at the interface GH

Firstly, we assume that no current flow occurs across GH, which leads to the boundary condition :

$$\partial_\xi \Phi_n \ = \ 0 \ \text{ at GH.} \tag{6.6}$$

It means we expect only a tangential current at the interface, but this is not necessary justified by numerical simulations.

Secondly, up to this artificial boundary the space charge is assumed to be zero, hence at the boundary : $C + p - n \ = \ 0$, or in the scaled version :

$$\exp\left(\frac{W - \Phi_n - 1}{\gamma}\right) \ - \ \exp\left(\frac{U_B - W - 1}{\gamma}\right) \ + \ 1 \ = \ 0$$

This leads to a quadratic equation for $\exp(\frac{W}{\gamma})$, from which we get the following solution :

$$W \ = \ U_B - 1 - \gamma \ \ln \frac{1}{2} \left[1 + \sqrt{1 + 4 \exp \frac{U_B - \Phi_n - 2}{\gamma}} \right] \qquad \text{on GH} \tag{6.7}$$

6.2 A quasi-one dimensional model for a formulation of the current

We get below a general 1-D formulation of the current and derive a square-root equation fot the potential W that will help us compute the current in the cases of depletion-weak inversion and strong inversion (see following section).

6.2.1 The 1-D model

Letting $\tilde{\lambda}$ go to zero in (6.1) where it appears in a quadratic way, we obtain following problem for fixed $y \in [0,1]$:

$$\partial_\xi^2 W \;=\; \exp\left(\frac{W - \Phi_n - 1}{\gamma}\right) \;-\; \exp\left(\frac{U_B - W - 1}{\gamma}\right) \;+\; 1 \tag{6.8}$$

For given Φ_n this equation combined with the boundary conditions on BC and GH ((6.4) and (6.7)) has exactly one solution

$$W \;=\; W(\Phi_n, \xi, y).$$

Doing the same for (6.2), we write :

$$\partial_\xi \left(\mu_n \;\exp\left(\frac{W - \Phi_n - 1}{\gamma}\right) \partial_\xi \Phi_n\right) \;=\; 0$$

which means, as $\partial_\xi \Phi_n \;=\; 0$ at BC (and in our assumptions also at GH, see (6.3) and (6.6)) that Φ_n does not depend on ξ :

$$\Phi_n \;=\; \Phi_n(y).$$

6.2.2 A formulation of the current

Integrating the continuity equation (6.2) over $\xi \in [0, \xi^*]$ with $\xi^* \;=\; \dfrac{BG}{\tilde{\lambda}}$ the value of ξ on GH, and using the other boundary conditions on BC and GH ((6.3) and (6.6)), the integral of the first term in (6.2) is zero and thus we obtain :

$$\int_0^{\xi^*} \partial_y \left(\mu_n \;\exp\left(\frac{W(\Phi_n, \xi, y) - \Phi_n - 1}{\gamma}\right) \partial_y \Phi_n\right) \, d\xi \;=\; 0$$

We note that $\partial_y \Phi_n$ is like Φ_n independent of ξ for $\tilde{\lambda}$ tending to zero, and set :

$$N(\Phi_n, y) \;:=\; \int_0^{\xi^*} \exp\left(\frac{W(\Phi_n, \xi, y) - \Phi_n - 1}{\gamma}\right) \, d\xi \tag{6.9}$$

so that :

$$\partial_y (\mu_n \; N(\Phi_n, y) \; \partial_y \Phi_n) \;=\; 0$$

As we considered that the holes do not contribute to the current (we set $\varphi_p = c^{st}$ in BCHG), the expression $\mu_n N(\Phi_n, y)\partial_y \Phi_n$ is exactly the (electron) current $I(y)$ at a section $y = c^{st}$, and the equation above just says it does not depend on y :

$$\begin{array}{rcl} I = c^{st} & = & \mu_n \; N(\Phi_n, y) \; \partial_y \Phi_n \\ & = & \int_0^1 \mu_n \; N(\Phi_n, y) \; \partial_y \Phi_n \; dy \end{array}$$

Remarking $\partial_y \Phi_n \; dy \; = \; d\Phi_n$ and remembering that $\Phi_n \in [0, U_D]$ for $y \in [0,1]$ (see paragraph 6.1.3), the formulation for the current reads :

$$I \; = \; \mu_n \int_0^{U_D} N(\Phi_n) \; d\Phi_n \tag{6.10}$$

6.2.3 A squareroot equation for the potential

Here $\Phi_n(y)$ and U_B are seen as parameters verifying the inequality

$$\forall \, y, \; U_B \; < \; \Phi_n(y) + 2.$$

We start from equation (6.8), multiply it with $\partial_\xi W$ and integrate over $[0, \xi^* = \frac{BG}{\tilde{\lambda}} \approx \infty]$:

$$\frac{1}{2}(\partial_\xi W)^2 \; = \; \gamma \; \exp\left(\frac{W - \Phi_n - 1}{\gamma}\right) \; - \; \exp\left(\frac{U_B - W - 1}{\gamma}\right) \; + \; W \; + \; k$$

where k is an integration constant we are determining as follows :
We introduce the notation TST (Transcendentally Small Terms), in fact $TST(\gamma)$ meaning $TST \; = \; O\left(e^{-c/\gamma}\right)$ as γ tends to zero for a positive constant c, so every $TST(\gamma)$ is small compared to any power of γ.
As a consequence, we can write :

$$W \; = \; -1 + U_B + TST \quad \text{on GH, ie for } \xi \; = \; \xi^* \approx \infty$$

Writing $\partial_\xi W(\infty) \; = \; 0$, we get the value of k :

$$k \; = \; 1 - U_B - \gamma + TST \tag{6.11}$$

Assuming W is decreasing at fixed y in BCHG, we obtain :

$$\frac{\partial_\xi W}{\sqrt{2}} \; = \; - \sqrt{\gamma \; \exp\left(\frac{W - \Phi_n - 1}{\gamma}\right) \; - \; \exp\left(\frac{U_B - W - 1}{\gamma}\right) \; + \; W \; + \; k} \tag{6.12}$$

This can be written at $\xi = 0$, using (6.4) :

$$\frac{W(0) - \gamma\, V_{bi} - U_G}{\alpha\,\sqrt{2}} = \sqrt{\gamma\ \exp\left(\frac{W(0)-\Phi_n-1}{\gamma}\right) - \exp\left(\frac{U_B-W(0)-1}{\gamma}\right) + W(0) + k} \tag{6.13}$$

We eventually remark that in this expression

$$\gamma V_{bi} = -1 + TST.$$

6.3 Computation of the potential

In this section we use the equations obtained in section 6.2.3 to compute the potential in the depletion-weak inversion case and in the strong inversion case.

We remember that the scaled densities are given by :

$$n = \exp\left(\frac{W - \Phi_n - 1}{\gamma}\right) \qquad \text{and} \qquad p = \exp\left(\frac{U_B - W - 1}{\gamma}\right)$$

6.3.1 Depletion-Weak inversion

Here is U_G supposed to be lightly greater than U_B.

Conditions on U_G

The densities n and p can be neglected (ie are $TST(\gamma)$) in all the rectangle BCHG iff $U_B - 1 < W(\xi) < \Phi_n + 1$ for all ξ.

As W is a decreasing function, it means :

$$W(0) < \Phi_n + 1 \ \text{ and } \ W(1) > U_B - 1$$

In this case $W(0)$ is solution of a simplified equation, obtained from (6.13), (6.11) and the remark at end of paragraph 6.2.3 :

$$\begin{aligned} \frac{W(0) - \gamma\, V_{bi} - U_G}{\alpha\,\sqrt{2}} &= -\sqrt{W(0) + k} \\ \approx \frac{W(0) + 1 - U_G}{\alpha\,\sqrt{2}} &\approx -\sqrt{W(0) + 1 - U_B} \end{aligned}$$

Taking the square of this equation we get :

$$W(0) = U_G - 1 + \alpha^2 - \alpha\,\sqrt{\alpha^2 + 2(U_G - U_B)}, \tag{6.14}$$

and the condition $W(0) \; < \; \Phi_n + 1$ is realised as soon as :

$$U_G \in \left[U_B, 2 + \Phi_n + \alpha \, \sqrt{2(2 + \Phi_n - U_B)} \right] \tag{6.15}$$

The right end of this intervall is thus the limit between weak inversion and strong inversion.

Potential and depletion width

Under the above assumptions, the equation (6.8) can be written :

$$\partial_\xi^2 W \; = \; 1 \quad \Rightarrow \quad W(\xi) \; = \; \frac{\xi^2}{2} + \partial_\xi W(0)\xi + W(0)$$

with $W(0) \; < \Phi_n + 1$.

As long as $W(\xi) \; > \; U_B - 1$ holds, we are in the depletion-weak inversion case, and as soon as $W(\xi)$ reaches the value $U_B - 1$, then W has to stay constant equal to this value, as there is no accumulation of holes in the semiconductor. It allows us to define the depletion width ξ_d, value of ξ after which the potential is constant.

Replacing $\partial_\xi W(0)$ and $W(0)$ in the potential above thanks to (6.13) and (6.14), we can come (neglecting the TSTs) to the following expression for the potential under ξ_d :

$$W(\xi) \; = \; \left\{ \begin{array}{ll} -1 + U_B + \frac{1}{2}(\xi - \xi_d)^2 & 0 \leq \xi \leq \xi_d \\ -1 + U_B & \xi \geq \xi_d \end{array} \right. \qquad \xi_d \; := \; -\alpha + \sqrt{\alpha^2 + 2(U_G - U_B)} \tag{6.16}$$

We note that in this case of depletion-weak inversion ξ_d and thus W are independant of Φ_n.
W is maximal for U_G equal to the right end of the interval seen in (6.15), which leads to an expression of ξ_d^{max} in the form :

$$\xi_d^{max} \; = \; \sqrt{2(2 + \Phi_n - U_B)} \tag{6.17}$$

6.3.2 Strong inversion

Here is U_G going to be strongly greater than U_B.

The electron density n is expected to be large in a some part of the rectangle BCHG, ie $W(\xi) \; > \; \Phi_n + 1$ for some ξ over a so called strong layer $[0, \xi_{inv}]$ next to the oxide. As the potential decreases we expect a depletion-weak inversion layer where n is small as in the preceding section for $\xi \in [\xi_{inv}, \xi_d]$ ending in an equipotential layer in the rest of the rectangle.

Looking at $n = \exp\left(\frac{W - \Phi_n - 1}{\gamma}\right)$, we make the Ansatz :

$$W_{inv} = 1 + \Phi_n + \gamma \ \ln \frac{1}{\gamma} \ + \gamma \ z$$

The function z is solution of a simple differential equation with boundary condition at $\xi = 0$:
Only the second exponential term (corresponding to p) is now a TST in (6.13), the first exponential (electron density) is $\exp(z(0))$, and letting γ go to zero we come to the equation :

$$\frac{2 + \Phi_n - U_G}{\alpha \sqrt{2}} = - \sqrt{(\exp(z(0)) + 2 + \Phi_n - U_B)}$$

and obtain the boundary value of z :

$$z(0) = \ln\left(\frac{(2 + \Phi_n - U_G)^2}{2 \ \alpha^2} - 2 - \Phi_n + U_B\right)$$

We move to the fast variable

$$\tau = \frac{\xi}{\gamma} = \frac{x}{\lambda \sqrt{\gamma}}, \tag{6.18}$$

write $\hat{z}(\tau) = z(\xi)$ and obtain from (6.12) the differential equation for $\hat{z}(\tau)$, letting γ tend to zero :

$$\partial_\tau \hat{z} = - \sqrt{2(\exp(\hat{z}) + 2 + \Phi_n - U_B)}$$

with the solution :

$$\hat{z}(\tau) = \ln\left((2 + \Phi_n - U_G) \sinh^{-2}\left(\sqrt{1 + \frac{\Phi_n - U_B}{2}} \tau + c\right)\right) \tag{6.19}$$

where the constant c is determined by $\hat{z}(0) = z(0)$.
As $\hat{z}(\tau)$ tends to $-\infty$ when τ tends to ∞, the potential will come under the value $1 + \Phi_n$ for a value ξ_{inv} of ξ, where the weak inversion begins. In this zone, the potential is solution of $\partial_\xi^2 W = 1$ and thus has the form

$$W_{depl}(\xi) = a + b \ \xi + \frac{\xi^2}{2}$$

The scaling shows that $\xi_{inv} << 1$ and a development of W_{inv} in terms of the slow variable ξ by zero gives :

$$\begin{aligned} W_{inv}(\xi) &= 1 + \Phi_n + \gamma \ \ln \tfrac{1}{\gamma} \ + \gamma \ \hat{z}(\tfrac{\xi}{\gamma}) \\ &= 1 + \Phi_n - \sqrt{1 + (\Phi_n - U_B)/2} \ \xi + o(\xi) + TST \end{aligned}$$

Equating the coefficients in W_{sl} and W_{depl} implies :

$$\begin{array}{rcl} W_{depl}(\xi) & = & 1+\Phi_n - \sqrt{1+(\Phi_n-U_B)/2}\,\xi + \frac{\xi^2}{2} \\ & = & -1+U_B+\frac{1}{2}(\xi-\xi_d^{max})^2 \end{array}$$

where ξ_d^{max} was given in (6.17) and is independant of U_G.

After ξ_d^{max} the potential is constant equal to U_B-1 in the rest of the rectangle. Saying that the depletion layer has to stay in the rectangle BCHG, we have the condition that ξ_d^{max} remains inferior to ξ^* for every y.
For increasing Φ_n (equal to zero at the source and to U_D at the drain), ξ_d^{max} is also increasing, and the condition reads :

$$\sqrt{2(2+U_D-U_B)} \;\leq\; \frac{BG}{\tilde{\lambda}}.$$

We sum up the results for the potential in the strong inversion case :

$$W(\xi) \;=\; \left\{ \begin{array}{ll} 1+\Phi_n+\gamma\;\ln\frac{1}{\gamma}+ & 0\leq\xi\leq\xi_{inv} \\ \quad +\gamma\;\ln\left((2+\Phi_n-U_G)\sinh^{-2}\left(\sqrt{1+\dfrac{\Phi_n-U_B}{2}}\;\dfrac{\xi}{\gamma}+c\right)\right) & \\ -1+U_B+\frac{1}{2}(\xi-\xi_d^{max})^2 & \xi_{inv}\leq\xi\leq\xi_d^{max} \\ -1+U_B & \xi\geq\xi_d^{max} \end{array} \right. \qquad (6.20)$$

The value of ξ_d^{max} is given in (6.17).

6.4 Computation of the current

We will use the formulation established in section 6.2 to compute the current in the cases of depletion-weak inversion and strong inversion. We thus need the expression of $N(\Phi_n)$ that appears in (6.10). It is defined in (6.9).

6.4.1 Expression of $N(\Phi_n)$

In the depletion-weak inversion case, we use the potential of (6.16), omit the quadratic term and integrate over $[0, \infty]$ (γ is small) :

$$\begin{aligned} N_{depl}(\Phi_n) &= \textstyle\int_0^{\xi^*} n \, d\xi \\ &\approx \textstyle\int_0^{\infty} \exp\left(\frac{W-\Phi_n-1}{\gamma}\right) \, d\xi \end{aligned}$$

$$N_{depl}(\Phi_n) = \frac{\gamma}{\xi_d} \exp\left(\frac{W(0)-\Phi_n-1}{\gamma}\right) \tag{6.21}$$

In the strong inversion case, we use the expression (6.20). In fact, we just need to compute the contribution of the strong inversion layer (integral over $[0, \xi inv]$ approximated by integral over $[0, \infty]$) and add it to the contribution of the depletion layer (6.21) with $\xi_d = \xi_d^{max}$ (integral over $[\xi_{inv}, \xi_d]$ approximated by integral over $[0, \infty]$). We obtain :

$$N_{inv}(\Phi_n) = (U_G - 2 - \Phi_n)/\alpha - \sqrt{2(2+\Phi_n-U_B)} + \gamma/\sqrt{2(2+\Phi_n-U_B)} \tag{6.22}$$

6.4.2 Currents

We use the formula (6.10) for the current, and thus have to consider three cases, depending on the value of the gate voltage U_G. The bounding values of U_G are derived from the interval (6.15). Indeed, if U_G is small enough, depletion-weak inversion prevails in the whole channel; if it is big enough, strong inversion prevails; otherwise both of these occur :

- for $U \leq U_t = 2 + \alpha\sqrt{2(2-U_B)}$ (U_t stands for *threshold voltage*), we use (6.21) and obtain :

  $$I = \mu_n \frac{\gamma^2}{\xi_d} \exp\left(\frac{W(0)-1}{\gamma}\right)(1-e^{-U_D/\gamma})$$

  So the saturation current in this subthreshold region is, for large U_D, a transcendentally small term of γ.

- for $U \geq U_t = 2 + U_D + \alpha\sqrt{2(2+U_D-U_B)}$, and so as long as the drain-source voltage verifies

$U_D \leq U_{Dsat} = U_G - 2 + \alpha^2 - \alpha\sqrt{\alpha^2 + 2U_G - 2U_B}$, we use (6.22) and obtain :

$$\begin{aligned} I \;=\; & \mu_n \left(\frac{1}{\alpha}(U_G - 2 - U_D/2)U_D \;-\; \frac{2\sqrt{2}}{3}(2 + U_D - U_B)^{3/2} \right. \\ & \left. + \frac{2\sqrt{2}}{3}(2 - U_B)^{3/2} \;+\; \gamma\sqrt{2(2 + U_D - U_B)} \;-\; \gamma\sqrt{2(2 - U_B)} \right) \end{aligned}$$

This is the *non-saturation region.*

- when the quasi Fermi level can take the value of U_{Dsat}, ie the inequalities of the two first items are not satisfied, there is a so called *pinch-off*, and (6.21) is used for $0 < \Phi_n < U_{Dsat}$ whereas (6.22) is used for $U_{Dsat} < \Phi_n < U_D$:

$$I \;=\; I_{sat} \;+\; \mu_n \frac{\gamma^2}{\xi_d} \;\exp\left(\frac{W(0) - 1}{\gamma}\right) (e^{-U_{Dsat}/\gamma} - e^{-U_D/\gamma})$$

  I_{sat} is the saturation current obtained by substituting $U_D = U_{Dsat}$ in the current of the non-saturation region. The distance of the pinch-off point to the drain is in fact very small compared to the channel length.

Chapter 7

Quantized model for MOSFETs

Miniaturization of transistors introduces quantum effects. Recent research tries to couple the classical Drift Diffusion model and a quantum description through the Schrödinger eigenvalue equation involving the quantized direction. The Poisson equation is still used to get a selfconsistent problem.

7.1 Unscaled system

For a MOSFET as pictured page 45, the *n-channel* (next to BC) is quantized in the x-direction.
We use [4] and write the unscaled sytem :

$$\left\{\begin{array}{l}
\epsilon \triangle_{x,y} V \;=\; q(n - C - p) \\[2ex]
n(x,y) \;=\; n_i \, \textstyle\sum_{p\geq 1} \exp\left(-\dfrac{\varphi_n(y) + \epsilon_p(y)}{U_T}\right) |\chi_p(x,y)|^2 \\
\quad \text{with } -\dfrac{\hbar^2}{2m}\, \partial_x^2 \,\chi_p \;-\; q\, V\, \chi_p \;=\; q\, \epsilon_p\, \chi_p \;, \qquad p \geq 1 \\
\quad \text{where } \quad \chi_p(.,y) \in H_0^1(0,d), \displaystyle\int_0^d \chi_p \chi_q \, dx \;=\; \delta_{pq}.L \\[2ex]
\nabla_y.(\underbrace{qD_n \,\nabla_y N \;-\; \mu_n \, N \,\nabla_y V_s}_{J_n}) \;=\; 0 \\
\quad \text{with } N(y) \;=\; \textstyle\int_0^L n(x,y)dx \;=\; n_i \, e^{-\varphi_n/U_T} \displaystyle\sum_{p\geq 1} e^{-\epsilon_p/U_T} \\[2ex]
\quad \text{and } V_s \;=\; -U_T \; log \left(\displaystyle\sum_{p\geq 1} e^{-\epsilon_p/U_T} \right)
\end{array}\right.$$

The quantification ($p \in \mathbf{N}$) is due to the confinement in the x-direction ($\chi_p(0,.) = \chi_p(d,.) = 0$).

Current J_n

In fact, the equation for J_n combined to the definition of V_s reduces to :

$$J_n \;=\; -\mu_n \, N \, \partial_y \phi_n \;, \qquad \partial_y J_n \;=\; 0 \;,$$

which is the equation of section 6.2.2 page 51.

Holes and doping densities

The holes desert the $n-channel$ region, so we still take for p the value (see page 47) :

$$p \;=\; n_i \, e^{(U_B - V)/U_T}$$

For the doping density we also still have :

$$C \;=\; -\tilde{C}$$

7.2 Scalings and expansion

Adimensioning

We use the scaling

$$x, y = \frac{x, y}{L}; \; V, \varphi_n, \epsilon_p = \frac{V, \varphi_n, \epsilon_p}{U_T}; \; \mu = \frac{\mu}{\tilde{\mu}}; \; J_n = \frac{J_n}{qU_T \tilde{C} \tilde{\mu}/L}$$

in order to get the following scaled equations :

- Poisson equation

$$\lambda^2 \triangle_{x,y} V \;=\; \underbrace{\delta^2 \sum_{p \geq 1} e^{-\varphi_n - \epsilon_p} \, |\chi_p|^2}_{n} \;-\; \underbrace{\delta^2 \, e^{-V + U_B}}_{p} + 1$$

  with the usual definitions $\lambda = \sqrt{\dfrac{\epsilon U_T}{q\tilde{C}L^2}}$ and $\delta^2 = \dfrac{n_i}{\tilde{C}}$.

- Schrödinger equation

$$\begin{array}{l} -\beta'^2 \partial_x^2 \, \chi_p \;-\; V \chi_p \;=\; \epsilon_p \chi_p \\ \chi_p \in H_0^{d/L} \text{ being now orthonormized} \end{array}$$

  with $\beta'^2 \;:=\; \dfrac{\hbar^2}{2mqU_TL^2}$.

- Drift Diffusion equation
  It reads :

$$\partial_y(\mu_n \, N \, \partial_y \varphi_n) \; = \; 0$$

Rescaling
We now introduce the scaling of section 6.1.1 of page 48 :

$$\begin{array}{ll} \delta^2 \; = \; e^{-\dfrac{1}{\gamma}} & \tilde{\lambda} \; = \; \dfrac{\lambda}{\sqrt{\gamma}} \\ W \; = \; \gamma V & \Phi_n, U_B, \epsilon_p \; = \; \gamma \, \varphi_n, U_B, \epsilon_p \\ \xi \; = \; \dfrac{x}{\tilde{\lambda}} & \end{array}$$

and to have the χ_p still orthonormized :

$$\chi_p \; = \; \frac{1}{\sqrt{\tilde{\lambda}}} \, \chi p_s$$

We obtain :

- for the Poisson Equation

$$\partial_\xi^2 W \; + \; \tilde{\lambda}^2 \partial_y^2 W \; = \; \frac{1}{\tilde{\lambda}} \sum_p e^{-\dfrac{\Phi_n + \epsilon_p + 1}{\gamma}} |\chi_p|^2 \; - \; e^{\dfrac{U_B - W - 1}{\gamma}} \; + \; 1$$

- for the Schrödinger equation

$$\begin{aligned} -\gamma \, \tilde{\beta}^2 \partial_\xi^2 \chi_p \; - \; W \, \chi_p \; &= \; \epsilon_p \, \chi_p \\ \int_0^{d/L\tilde{\lambda}} \chi_p \chi_q \, d\xi \; &= \; \delta_{pq} \end{aligned}$$

  with $\tilde{\beta} \; = \; \dfrac{\beta'}{\sqrt{\tilde{\lambda}}}$,

- and for the drift diffusion equation

$$\partial_y(\mu_n \, N \, \partial_y \Phi_n) \; = \; 0$$

The term in $\tilde{\lambda}^2$ in the Poisson equation will be neglected ($\tilde{\lambda} \to 0$).

Strong inversion As we are intersted in the strong inversion case, we move (similarly to the last chapter) to the fast variable

$$\tau \; = \; \frac{\xi}{\gamma}$$

and make the Ansätze :

$$\begin{aligned} W &= \Phi_n \,+\, 1 \,+\, \gamma \ln(\tilde{\lambda}) \,+\, \gamma\, z \\ \epsilon_p &= -\Phi_n \,-\, 1 \,-\, \gamma \ln(\tilde{\lambda}) \,-\, \gamma\, \lambda_p \end{aligned}$$

We have to re-re-rescale χ_p :

$$\chi_p \;=\; \frac{1}{\sqrt{\gamma}}\, \chi p_s$$

so that for the re-re-rescaled eigenfunctions :

$$\int_0^{d/L\tilde{\lambda}\gamma} \chi_p \chi_q \, d\tau \;\approx\; \int_0^{\infty} \chi_p \chi_q \, d\tau \;=\; \delta_{pq}$$

The following relations hold :

$$\begin{aligned} \partial_\xi^2 W \;&=\; \tfrac{1}{\gamma} \partial_\tau^2 z \\ n \;&=\; \sum_p e^{\lambda_p}\, \frac{|\chi_p|^2}{\gamma} \end{aligned}$$

so that the Poisson equation becomes :

$$\partial_\tau^2 z \;=\; \sum_p e^{\lambda_p} |\, \chi_p|^2 \;+\; \frac{\gamma}{\tilde{\lambda}} \exp\left(\frac{U_B - \Phi_n - 2}{\gamma} - z \right) \;+\; \gamma$$

Neglecting the last two terms (supposed to be a Transcendentally Small Term of γ), we come to the **Poisson Equation** :

$$\partial_\tau^2 z \;=\; \sum_p e^{\lambda_p}\, |\chi_p|^2$$

The **Schrödinger equation** now reads :

$$\beta^2 \partial_\tau^2 \;+\; z\, \chi_p \;=\; \lambda_p\, \chi_p$$

where β is assumed to satisfy

$$\beta \;:=\; \frac{\tilde{\beta}}{\gamma} \;=\; O(1) \quad \text{for } \gamma \to 0$$

As a consequence, we have obtained the

Drift Diffusion Schrödinger Poisson system

$$\left\{ \begin{array}{rcl} \partial_y(\mu_n\, N\, \Phi_n) &=& 0 \\ N &=& \sum_p e^{\lambda_p} \\ \beta^2 \partial_\tau^2\, \chi_p \,+\, z\, \chi_p &=& \lambda_p\, \chi_p \\ \text{with } \int_0^\infty \chi_p \chi_q \, d\tau &=& \delta_{pq} \\ \partial_\tau^2\, z &=& \sum_p e^{\lambda_p}\, |\chi_p|^2 \end{array} \right.$$

with the initial condition (see page 55)

$$\partial_\tau\ z\ (0)\ =\ \frac{2+\Phi_n-U_G}{\alpha}\ ,$$

which should be uniquely solvable for a fixed $N\ =\ \sum_p e^{\lambda_p}$.

7.3 Computation of the macroscopical current

As in the last chapter, the equation

$$\partial_y(\mu_n N \partial_y \Phi_n)\ =\ 0$$

gives the right to compute the current I through the formula :

$$I\ =\ \mu_n \int_0^1 N(\Phi_n)\partial_y\Phi_n\ dy\ =\ \mu_n \int_{\Phi_n(0)=0}^{\Phi_n(1)=U_D} N(\Phi_n)\ d\Phi_n\ ,$$

so we need to express N as function of Φ_n.
Integrating the reduced Poisson equation of the system, we have :

$$N\ =\ \sum_p e^{\lambda_p}\ =\ \partial_\tau\ z\ (\infty)\ -\ \partial_\tau\ z\ (0)$$

In the depletion zone that still follows the strong inversion zone, as seen page 56 the potential W can be written (because it is solution of the Poisson equation $\partial_\xi W\ =\ 1$) :

$$W\ =\ U_B-1+\frac{1}{2}(\xi-\xi_d)^2$$

and it is constant equal to U_B-1 for $\xi \geq \xi_d$.
The constant ξ_d is determined by the boundary value $W(0)\ =\ 1+\Phi_n$ (as $\gamma \rightarrow 0$) :

$$\xi_d\ =\ \sqrt{2(\Phi_n+2-U_B)}$$

The strong inversion layer being very small with respect to the "normal" values of ξ, we can write the following equality :

$$\partial_\tau\ z\ (\infty) =\ \partial_\xi\ W\ (0)$$

and get the value of $\partial_\tau\ z\ (\infty)$:

$$\partial_\tau\ z\ (\infty)\ =\ -\xi_d\ =\ -\sqrt{2(\Phi_n+2-U_B)}$$

Hence the total density N reads :

$$N(\Phi_n)\ =\ \frac{U_G-2-\Phi_n}{\alpha}-\sqrt{2(\Phi_n+2-U_B)}$$

which is the same as in section 6.4.1 ($\gamma \to 0$) and will lead to the same current I.

Conclusion

If the inner computations differ from the classical case when we consider the microscopical changes of the physics introduced by the quantification of one direction in a MOSFET, the macroscopical result (the current circulating through the MOSFET) remains the same.

CONCLUSION

We saw in this report how kinetic transport equations can be used to derive the computation of the current in a transistor. An appropriate Drift-Diffusion model, obtained through asymptotics, was the key to the physical description of the semiconductor.

If, at the beginning, we included the quantum effects in the equations, in fact the Drift Diffusion model was derived from the Classical Boltzmann equation. Coupling this model to a Schrödinger-Poisson system, we saw no impact on the macroscopical current in a MOSFET.

Recent research tries and use a Quantum Drift Diffusion model : the equilibrium density (that was the Maxwellian density in the classical case) is found by minimizing the "quantum entropy", defined as function of the density matrix ρ. Then, starting from the linear collision operator and the Quantum Boltzmann equation with relaxation time, the quantum drift diffusion model is obtained by a similar asymptotical method.