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MATHEMATICAL MODELLING AND NUMERICAL ANALYSIS
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PARTICLE SIMULATION AND ASYMPTOTIC ANALYSIS OF KINETIC EQUATIONS FOR MODELING A SCHOTTKY DIODE (*)

by P. DEGOND (1), F. POUPAUD (2) and A. YAMNAHAKKI (3)

Abstract. — *The deterministic particle simulations of the Boltzmann Transport equation for modeling the Schottky diode problem show that the behavior of the device is entirely controlled by the non-equilibrium part of the distribution function, which is very small compared with the equilibrium part. Then, an asymptotic analysis of the problem gives us an analytical expression for the equilibrium part, and the deterministic particle method is applied to compute only the non-equilibrium (ballistic) part of the distribution function. This gives more accurate numerical results.*

Résumé. — *La simulation par la méthode particulaire déterministe de l'équation de transport de Boltzmann pour le problème de la diode Schottky montre que le comportement de ce composant est entièrement contrôlé par la partie hors-équilibre de la fonction distribution. Or celle-ci est très petite par rapport à la partie en équilibre. Une étude asymptotique de ce problème permet de donner une expression analytique de la partie en équilibre. La méthode particulaire est alors utilisée pour calculer uniquement la partie hors-équilibre (ballistique) de la fonction distribution. Cette démarche permet d'obtenir des résultats numériques plus précis.*

1. INTRODUCTION

Most numerical simulations of carrier transport in semiconductor devices are based upon drift-diffusion models (see [33], [25], [26], and references therein). However, it is well known that these equations are only valid when the carriers are in local thermo-dynamical equilibrium, which is not true when

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the electric field is large or when the active zone of the device is short. Besides, the distribution function near contacts or junctions is not an equilibrium distribution, and kinetic boundary layer phenomena may appear, which are of course not conveniently described by classical Drift-Diffusion models, [30]. To remedy to these inaccuracies, hydro-dynamical models were proposed by many authors in various forms [1], [2], [8] and [28]. However, these models require transport parameters which are not known with good accuracy (e.g. relaxation times, heat conductivities, ...). Then, the kinetic model (the Boltzmann equation) seems to give the most accurate description of the physics attainable by numerical computations.

The most widely used numerical method to simulate this kinetic model is certainly the Monte-Carlo method (see [32], [21] and references therein), but the deterministic particle method seems to be attractive in particular when one is concerned with the distribution function or transient regimes.

The aim of this work is to numerically and mathematically study the Schottky diode problem. The first part concerns the application of deterministic particle simulations of the Boltzmann Transport Equation to the Schottky diode problem. In such a device, the carrier dynamics is governed by boundary conditions which, therefore, must be accurately taken into account by the numerical method. The geometry is one dimensional in space and three dimensional with axisymetry in wave vector. The fully coupled system consisting of the Boltzmann Transport equation and the Poisson equation is solved ; the collision operator takes into account many kinds of interactions of the standard GaAs model and includes Pauli's exclusion principle. These simulations show that the behavior of the device is entirely controlled by the non-equilibrium (or ballistic) part of the distribution function, which is very small compared with its equilibrium (or Maxwellian) part. So, numerical errors round-off and truncation errors, which are small compared with the total, and thus, with the equilibrium distribution, are large compared with the non equilibrium one. Thus, the numerical results concerning the quantities which are driven by the non-equilibrium part of the distribution function (such as the current for instance) are drowned in numerical noise and are unaccessible. A remedy is found by first performing an asymptotic analysis of the problem, which allows an analytical computation of the equilibrium part of the distribution function. Then, the deterministic particle method is applied to only compute the non-equilibrium (ballistic) part of the distribution function. These computations are presented in Section 2. Section 3 contains an asymptotic analysis of the one dimensional Vlasov-Poisson system specifically designed for modeling a Schottky diode, in order to support and interpret numerical results of Section 2. The perturbation parameter appears in the boundary conditions, in close relation with the previously studied Child-Langmuir asymptotics (see [14], [15], [10], [3], [4] and reference therein). The limit Poisson problem (when the perturbation parameter is set to zero) is in the form

of an obstacle problem. On the other hand, we obtain explicit approximations of the equilibrium and non-equilibrium parts of the distribution function, and explicit formulas for the current, electric field, potential, depletion width, ...

A generalization of this asymptotic analysis to the three dimensional case can be found in [16]. A review paper which focuses more on the involved physics can be found in [5].

2. DETERMINISTIC PARTICLE SIMULATION OF THE BOLTZMANN TRANSPORT EQUATION FOR A SCHOTTKY DIODE

2.1. Introduction

The aim of this section is the numerical simulation of electron transport near a metal-N-type semiconductor contact. Due to the intrinsically kinetic character of electron transport in the depletion region of a Schottky contact it is necessary to use the Boltzmann Transport Equation. The discretization method used is the deterministic particle method. One interesting issue of such simulations is to obtain information on electron transport coefficients within the depletion layer near the junction, such as momentum or energy relaxation times. Such values of the transport coefficients are needed for instance in hydrodynamic models.

2.2. The kinetic model of the physical problem

A Schottky diode consists of a metal-semiconductor contact. At thermal equilibrium, because of different electro-chemical properties of the metal and semiconductor, a positive charge is distributed all over the depletion layer, near the semiconductor surface. This induces a potential barrier, the built-in-potential V_{bi}, which depends on the metal work function, the electron affinity of the semiconductor and the doping profile (see [34] chapter 5 for more details). When a bias is applied to the structure, the value of the built-in-potential strongly influences the current flowing through the device.

We assume the diode consists of a one-dimensional N-type semiconductor of length L in the x-direction. The distribution function f is supposed invariant under rotation of the wave vector k about the x axis. Therefore we suppose $f = f(x, k_1, k_2)$ where $x \in [0, L]$, $k_1 \in \mathbb{R}$ is the component of the wave vector parallel to the x-axis, and $k_2 \in [0, \infty]$ is the magnitude of the normal

component of the wave vector to the x-axis. The Schottky contact is put at $x = 0$ while an ohmic contact is assumed at $x = L$. Then the Boltzmann-Poisson system reads as follows :

$$\frac{\partial f}{\partial t} + v(k)\frac{\partial f}{\partial x} - \frac{q}{\hbar}E(x,t)\frac{\partial f}{\partial k_1} = Q(f)\,(x,k,t)\,,$$
$$x \in [0,L]\,, \quad k \in \mathbb{R}\times\mathbb{R}_+\,, \quad t \geqslant 0\,, \tag{2.1}$$

$$f(x,k,t=0) = f_0(x,k)\,, \quad x \in [0,L]\,, \quad k \in \mathbb{R}\times\mathbb{R}_+\,,$$

$$E(x,t) = -\frac{\partial \Phi(x,t)}{\partial x}\,, \quad x \in [0,L]\,, \quad t \geqslant 0\,, \tag{2.2}$$

$$-\Delta\Phi(x,t) = \frac{q}{\varepsilon_0\,\varepsilon_r}\,(N_D(x) - n(x,t))\,, \quad x \in [0,L]\,, \quad t \geqslant 0\,,$$

where $k = (k_1, k_2) \in \mathbb{R}\times\mathbb{R}_+$ is the wave vector, $v(k)$ is the electron velocity, given by the band diagram energy $\epsilon(k)$ according to :

$$v(k) = \frac{1}{\hbar}\nabla_k \epsilon(k)\,, \tag{2.3}$$

$\hbar$ is the Planck constant, q the absolute value of elementary charge, $E(x,t)$ the electric field, $\Phi(x,t)$ the electric potential, $N_D(x)$ the given doping profile, and $n(x,t)$ the electron density (see (2.9)). The Euclidean volume element in wave vector space is given, in this geometry, by :

$$d\Omega(k) = 2\,\pi k_2\,dk_1\,dk_2\,. \tag{2.4}$$

The boundary conditions for this problem read :

$$f(x=0,k,t) = N^0\,M(k)\,, \quad k_1 > 0\,, \quad k_2 > 0\,, \quad t \geqslant 0\,,$$
$$f(x=L,k,t) = N_D\,M(k)\,, \quad k_1 < 0\,, \quad k_2 > 0\,, \quad t \geqslant 0\,,$$
$$\Phi(0,t) = 0\,, \quad t \geqslant 0\,,$$
$$\Phi(L,t) = V_{bi} - V_A\,, \quad t \geqslant 0\,. \tag{2.5}$$

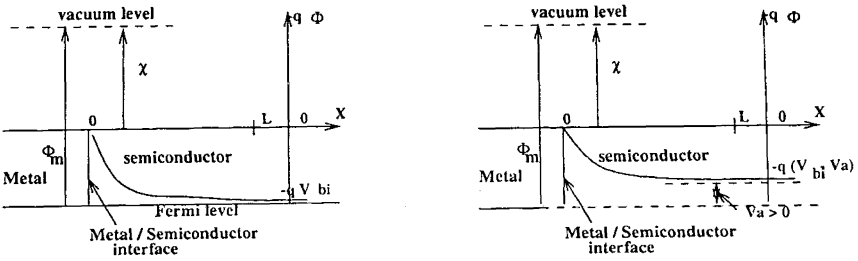
Here, we further assume that the semiconductor is non-degenerate (i.e. moderately doped) and that the injected electron distribution functions at 0 and L are at thermo-dynamical equilibrium (i.e. Maxwellians with respect to k).

$$N^0 = M_C \exp\left(-\frac{q\Phi_b}{k_B T}\right) = N_D \exp\left(-\frac{qV_{bi}}{k_B T}\right) \tag{2.6}$$

is the equilibrium density at $x = 0$, M_C the effective density of states at the conduction band, $M_C = 2\left(\frac{m^* k_B T}{2\pi\hbar^2}\right)^{\frac{3}{2}}$, (see [34]). V_{bi} is the built-in potential, which gives the potential difference between the bottom of the conduction band at $x = 0$ and $x = L$. Its definition (2.6) assumes that neutrality holds at the ohmic contact $x = L$. Φ_b is the barrier height, which depends on the metal work function Φ_m and the semiconductor electron affinity χ : $\Phi_b = \Phi_m - \chi$, (see *fig.* 1). k_B is the Boltzmann constant and $M(k)$ is the normalized Maxwellian at the lattice temperature T :

$$M(k) = C \cdot \exp\left(-\frac{\epsilon(k)}{k_B T}\right), \quad \text{where C is s.t.} \int M(k)\, d\Omega(k) = 1 .$$

V_A is the applied potential.



2.a) Band diagram of the Schottky diode at equilibrium

2.b) Band diagram of the Schottky diode under forward bias

Figure 1. — Energy band diagram of the Schottky diode.

We shall only consider electrons in the Γ-valley of GaAs and intra-valley collision terms only. To be more realistic, we should perform multi-valley simulations (see [11], [17] for multi-valley simulations using the deterministic particle method). However, the purpose of this paper is more to show the practical feasibility of the method rather than to give the most accurate physical results. $Q(f)$, the intra-valley collision term, is given by :

$$Q(f)\,(x, k, t) = \int_{\mathbb{R}\times\mathbb{R}^+} [S(x, k', k) f(x, k')\,(1 - f(x, k)) - S(x, k, k') f(x, k)\,(1 - f(x, k'))]\, d\Omega(k') , \tag{2.7}$$

where $S(x, k, k')\, d\Omega(k')$ is the transition rate of the state k to the volume element $d\Omega(k')$ around the state k' at the position x. We take into account, in this model, the following elementary interactions :

◇ acoustic and piezo-electric interactions in their elastic approximation ;

◇ polar and non polar optical interactions (emission/absorption),

◇ ionized impurities interactions (its transition rate is the only one which depends on the x variable via $N_D(x)$).

$S(x, k, k')$ is the sum of all these elementary transition rates, see [32] or [12], [17], [20] for their expressions.

The energy band diagram $\epsilon(k)$ of this model is spherical, and not parabolic :

$$\epsilon(k)\,(1 + \alpha^* \epsilon(k)) = \frac{\hbar^2 k^2}{2 m^*} \tag{2.8}$$

with m^* the effective mass and α^* the non parabolicity coefficient. The density and the other macroscopic quantities are defined as follows :

• density :

$$n(x, t) = \int_{R \times R_+} f(x, k, t)\,(4\pi^3)^{-1}\, d\Omega(k)\,, \tag{2.9}$$

• mean velocity :

$$\langle v \rangle(x, t) = n^{-1}(x, t) \int_{R \times R_+} v(k) f(x, k, t)\,(4\pi^3)^{-1}\, d\Omega(k) \tag{2.10}$$

• mean energy :

$$\langle \epsilon \rangle(x, t) = n^{-1}(x, t) \int_{R \times R_+} \epsilon(k) f(x, k, t)\,(4\pi^3)^{-1}\, d\Omega(k)\,, \tag{2.11}$$

• mean internal energy :

$$e(x, t) = \langle \epsilon \rangle(x, t) - \frac{1}{2} m^* \langle v \rangle^2(x, t)\,, \tag{2.12}$$

• current density :

$$\langle j \rangle(x, t) = -qn(x, t)\langle v \rangle(x, t) + \varepsilon_0\, \varepsilon_r \frac{\partial}{\partial t}(E(x, t))\,, \tag{2.13}$$

$(4\pi^3)^{-1}$ is the density of states in k-space. We also define the total charge :

$$\rho(t) = q \int_0^L (n_D(x) - n(x,t))\, dx\,. \tag{2.14}$$

We recall that the current density is independent of x. In the numerical simulation, an average over x is computed in order to increase the accuracy. The relaxation times deduced from a kinetic model are *a priori* functions of (x,t), since the are computed from moments of the collision operator. Their expressions are given as follows (see [2], [23], [18])

- momentum relaxation time :

$$\tau_{mom}(x,t) =$$

$$-n(x,t)\langle v\rangle(x,t)\left(\int_{R\times R_+} v(k)\, Q(f)\,(x,k,t)\,(4\pi^3)^{-1}\, d\Omega(k)\right)^{-1}, \tag{2.15}$$

- energy relaxation time :

$$\tau_{ener}(x,t) =$$

$$-(W(x,t) - W_0(x,t))\left(\int_{R\times R_+} \epsilon(k)\, Q(f)\,(x,k,t)\,(4\pi^3)^{-1}\, d\Omega(k)\right)^{-1},$$

(2.16)

where $W(x,t) = n(x,t)\langle\epsilon\rangle(x,t)$ and

$$W_0 = n(x,t)\int_{R\times R_+} \epsilon(k)\, M(k)(4\pi^3)^{-1}\, d\Omega(k)\,.$$

Now, we give a brief presentation of the numerical method.

2.3. Presentation of the deterministic particle method

This numerical method has been investigated first in ([31], [9]) in the context of incompressible fluid dynamics. The application to collisional ki-

netic equation has been done in [24]. It has been used for the semiconductor Boltzmann equation in [13], [12], [11]. The distribution function is approximated, in the sense of weak solutions, by a sum of Dirac measures in the phase space (particles) :

$$f(x, k, t) \simeq f^h(x, k, t) = \sum_{i=1}^{N} \omega_i f_i(t)\, \delta(x - x_i(t)) \otimes \delta(k - k_i(t)) , \qquad (2.17)$$

where N is the number of particles, $x_i(t)$, $k_i = (k_{1,i}(t), k_{2,i}(t))$, $f_i(t)$ and ω_i are respectively the position, wave vector, weight and control volume of the i^{th} particle. They evolve in time according to :

$$\begin{aligned}
\frac{dx_i}{dt} &= v(k_i) ; & x_i(0) &= x_i^0 , \\
\frac{dk_{1,i}}{dt} &= -\frac{q}{\hbar} E_i(t) ; & k_{1,i}(0) &= k_{1,i}^0 , \\
\frac{dk_{2,i}}{dt} &= 0 ; & k_{2,i}(0) &= k_{2,i}^0 , \\
\frac{df_i}{dt} &= Q_i(t) ; & f_i(0) &= f_i^0 , \\
\omega_i(t) &= \omega_i^0 ,
\end{aligned} \qquad (2.18)$$

where $E_i(t)$ and $Q_i(t)$ are the approximations of the electric field and of the collision operator acting on the i^{th} particle. The initial x_i^0, k_i^0, f_i^0, and ω_i^0 are chosen so that

$$f_0(x, k) \simeq \sum_{i=1}^{N} \omega_i^0 f_i^0\, \delta(x - x_i^0)\, \delta(k_i - k_i^0) , \qquad (2.19)$$

the approximation (2.19) is also taken in the weak topology of measures. Possible choices of x_i^0, k_i^0, ω_i^0 and f_i^0 can be found in [31].

To define $Q_i(t)$, we introduce a cut-off function $\zeta_\alpha(x)$ such that

$$\zeta_\alpha(x) = \frac{1}{\alpha} \zeta\left(\frac{x}{\alpha}\right) ; \quad \zeta(-x) = \zeta(x) ; \quad \int \zeta(x)\, dx = 1 , \qquad (2.20)$$

where ζ is a compactly supported function, and we write

$$Q_i(t) = \sum_{j=1}^{N} [S^{\beta}(x_j, k_j, k_i) f_j(t)(1 - f_i(t))$$

$$- S^{\beta}(x_j, k_i, k_j) f_i(t)(1 - f_j(t)) \omega_j \zeta_{\alpha}(x_j - x_i)] , \qquad (2.21)$$

where S^{β} is a regularisation of the exact transition rate S, see [24], [11], [17] for a justification of this expression and [17], [20] for a presentation of a fast algorithm to compute the collision operator.

For the approximation of $E_i(t)$, we considered the classical « Particle in Cell » (PIC) method, see [22], [6], [7] and references therein for a presentation and [27], [9] for an error analysis. The approximations of the other macroscopic quantities, which depend on position and time, are defined at a fixed grid mesh points $X_m = m \Delta x$ by using a numerical quadrature and a regularisation function W, for example : $W(x) = \text{Max}(0, 1 - |x|)$ and

$$\langle v \rangle (X_m, t) \simeq n_m^{-1}(t) \sum_{i=1}^{N} \omega_i v(k_i) f_i(t) \frac{1}{\Delta x} W\left(\frac{x_j(t) - X_m}{\Delta x}\right). \qquad (2.22)$$

The numerical simulation is initialized with the stationary solution of the coupled Boltzmann-Poisson system at equilibrium :

$$f^0(x, k) = n_{eq}(x) M(k),$$

where n_{eq} is the solution of the following semi-linear elliptic problem :

$$n_{eq}(x) = N^0 \exp(\beta \Phi_{eq}) ; \quad \beta = \frac{q}{k_B T}, \qquad (2.23)$$

$$-\frac{d^2 \Phi_{eq}}{dx^2}(x) = \frac{q}{\varepsilon_0 \varepsilon_r} [N_D(x) - N^0 \exp(\beta \Phi_{eq})] ,$$

$$\Phi_{eq}(0) = 0 , \quad \Phi_{eq}(L) = V_{bi} , \qquad (2.24)$$

with N^0 given by (2.6). The time stepping procedure is detailed in [17], [20]. The computational domain is chosen rectangular. We have chosen the following boundary conditions on the wave vector : particles which leave the domain on $k_1 = k_{1,\max}$ (resp. $k_1 = -k_{1,\max}$) are re-injected, with $k_{1,i} = -k_{1,\max}$ (resp. $k_{1,i} = k_{1,\max}$) without changing neither their weights nor their positions, see [13], [11], [17] for a discussion of artificial boundary

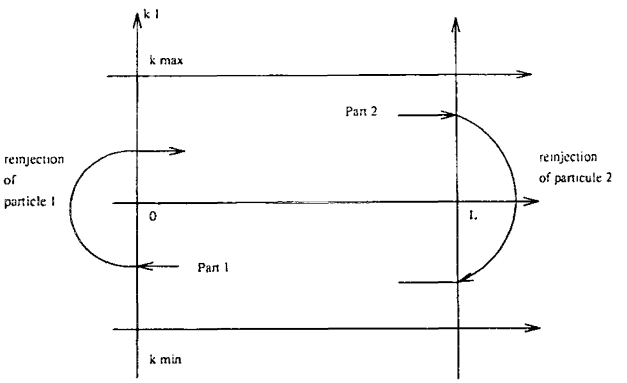


Figure 2. — Particles injection scheme in position.

conditions for particle methods. If a particle exits the domain at $x = 0$ or $x = L$, it's re-injected in the domain according to figure 2, with a weight consistent with formula (2.5). These boundary conditions are stable and have been shown to numerically preserve the total charge up to machine accuracy.

2.4. Direct simulation

We have used a GaAs model with one valley (Γ) at 300 K. The physical and numerical parameters are chosen according to [20] and [17]. Specific values of the parameters for the Schottky diode are given in table 1. Results

Table 1. — Physical and numerical parameters.

Physical values	
Applied voltage (Volts)	0.2
Lattice temperature (K)	300.00
Device length (microns)	1.2
Doping profile (m^{-3})	$2.E+22$
Barrier height (GaAs-Aluminium contact) (volts)	0.8
Numerical values	
Time steep (ps)	0.005
Poisson meshes number	$M = 120$
Particles number	36 000
Position regularisation parameter β (μm)	0.009
Energy regularisation parameter α (meV)	4.0
Maximal parallel energy $\epsilon_1^{max} - \epsilon^0$(eV)	1.2
Maximal perpendicular energy $\epsilon_2^{max} - \epsilon^0$(eV)	0.3

are shown in figure 3 to 8. The equilibrium density (i.e. that corresponding to $V_A = 0$) is shown on figure 3 while the stationary density obtained after 2 *ps* simulation for $V_A = 0.2$ V is displayed on figure 4. The results are fairly correct in spite of a variation of 8 order of magnitudes of the density between $x = 0$ and $x = L$. The stationary density for $V_A = 0.2$ V at $x = 0$ is larger than the equilibrium density at the same point, which is a consequence of the direct biasing of the junction. The electric field (*fig.* 6) is almost linear and the electric potential (*fig.* 5) almost parabolic in the depletion region. However, the current density as a function of time (*fig.* 7) displays a chaotic behavior, with an undetermined sign and an absolute magnitude of 3 orders of magnitude above the expected one (which is about (5.10^{-4} A/cm^2 [34]). Figure 8 displays the stationary distribution function at time $t = 2$ *ps*. It is essentially Maxwellian with some numerical fluctuations, which shows that the method has only been able to capture the equilibrium part of the distribution function.

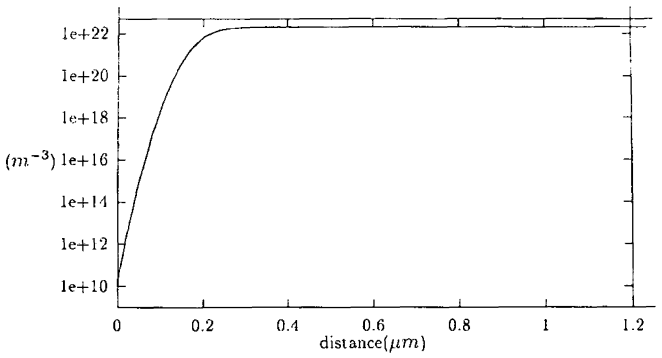


Figure 3. — Equilibrium density ($V_A = 0$) (solution of eq. (2.23)).

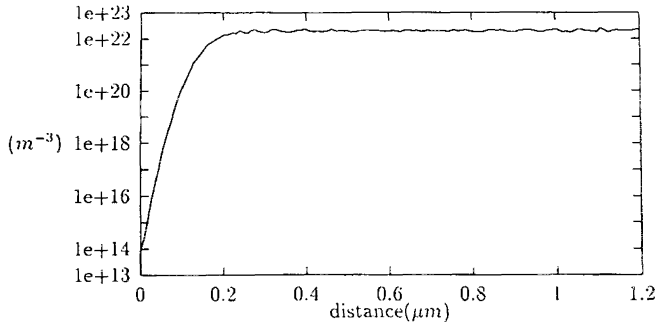


Figure 4. — Density ($V_A = 0.2$ V) at stationary state ($t = 2$ *ps*) (direct simulation).

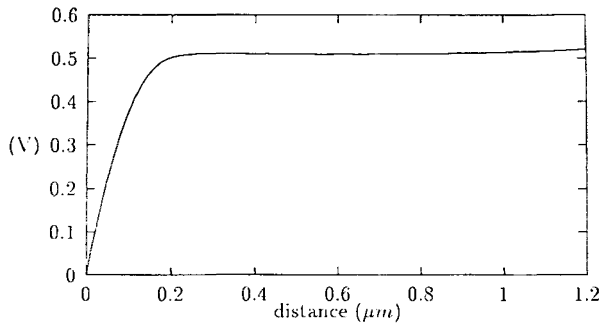


Figure 5. — Electric Potential (V_A = 0.2 V) at stationary state (t = 2 ps) (direct simulation).

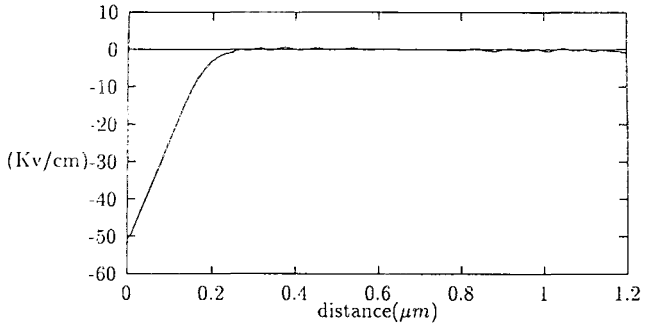


Figure 6. — Electric field (V_A = 0.2 V) at stationary state (t = 2 ps) (direct simulation).

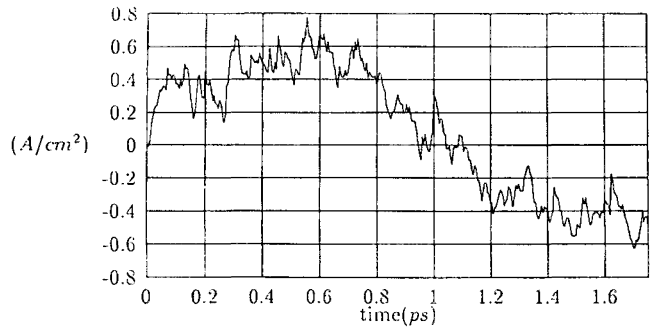


Figure 7. — Current density (V_A = 0.2 V) as a function of time (direct simulation).

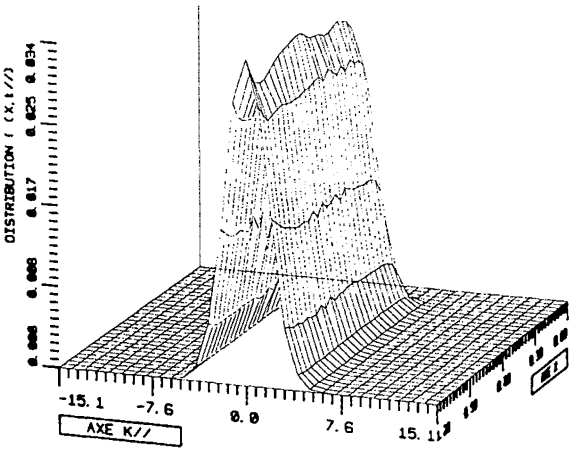


Figure 8. — Distribution function at $t = 2.\,ps$(direct simulation).

The non-equilibrium part, which determines the current is completely concealed by the numerical fluctuations. This explains why the method has been unsuccessful to capture the correct value of the current.

2.5. Decomposition in equilibrium and non equilibrium distributions and simulation of the non equilibrium distribution

In the previous subsection, we have pointed out that no information about the non equilibrium part of the distribution function (and thus, about the current) could be obtained from a direct computation of problem (2.1), (2.2), (2.5), (2.7). In this subsection, we reduce the problem to the computation of the non equilibrium distribution function.

In what follows, we assume that the electrons gas is non degenerate, i.e. the collision term Q is linearized in (2.7), we make $1 - f \approx 1$. Let

$$f^0 = N^0(x)\, M(k)\,, \quad N^0(x) = N_D \exp\left(\frac{\Phi^0(x) - \Phi(L)}{U_T}\right), \qquad (2.25)$$

where Φ^0 is solution of the following semi-linear elliptic problem :

$$-\frac{d^2\,\Phi^0}{dx^2} = \frac{q}{\varepsilon_s}\,(N_D - N^0(x))\,, \quad x \in\,]0, L[,$$

$$\Phi^0(0) = 0\,, \quad \Phi^0(L) = \Phi(L) = V_{bi} - V_A\,.$$

Then, it will be proved in the next section that $N^0(x)$ is an approximation of the stationary state carrier density (which is confirmed by a comparison

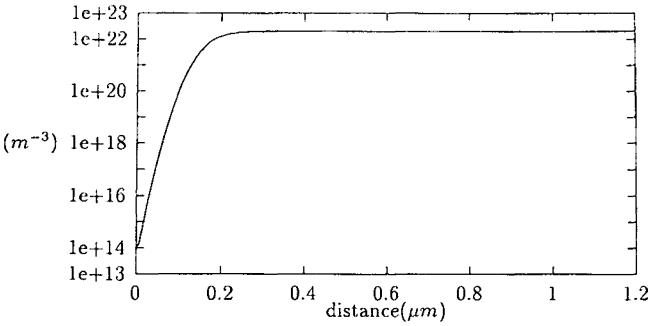


Figure 9. — Stationary state carrier density $N^0(x)$, solution of (2.25).

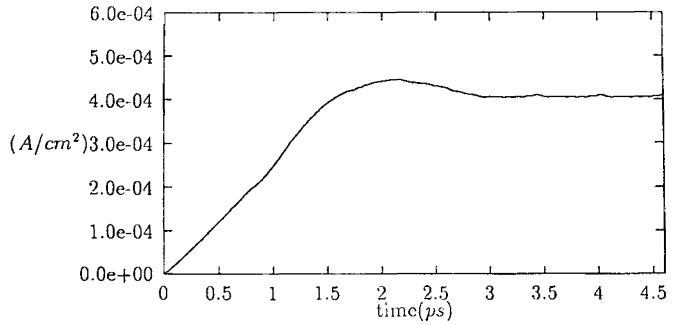


Figure 10. — Current density ($V_A = 0.2$ V) as a function of time (simulation of the non-equilibrium distribution).

between *fig.* 4 and *fig.* 10) and that f^0 is an approximation of the stationary state distribution function. Under a forward bias, we consider the distribution function $g = f^0 - f$. It satisfies the following Boltzmann-Poisson system :

$$\frac{\partial g}{\partial t} + v(k)\frac{\partial g}{\partial x} - \frac{q}{\hbar}\frac{\partial \Phi}{\partial x}\frac{\partial g}{\partial k_1} = Q(g) + r, x \in]0, L[, k \in \mathbb{R} \times \mathbb{R}_+, t > 0,$$

$$\text{with} \quad r = \frac{v(k)}{U_T} f^0\left(\frac{\partial \Phi}{\partial x} - \frac{d\Phi^0}{dx}\right),$$

$$\frac{d^2\Phi(x,t)}{dx^2} = \frac{q}{\varepsilon_s}(N^0(x) - n_g(x,t) - N_D), x \in]0, L[, t > 0,$$

$$n_g(x,t) = (4\pi^3)^{-1} \int_{R \times R_+} g(x,k,t)\, d\Omega(k), x \in]0, L[, t > 0, \quad (2.26)$$

with boundary conditions :

$$g(L, k) = 0, \text{ for } k_1 < 0, k_2 \geq 0, t > 0 ,$$

$$g(0, k) = N_0\left(\exp\left(\frac{V_A}{U_T}\right) - 1\right) M(k), \text{ for } k_1 > 0, k_2 \geq 0, t > 0 , \qquad (2.27)$$

$$\Phi(0, t) = 0, \Phi(L, t) = \Phi_L = V_{bi} - V_A, t \geq 0 ,$$

with $N_0 = N_D \exp\left(-\frac{qV_{bi}}{k_B T}\right)$. In the numerical simulation, we put $r = 0$ because it is of higher order with respect to the small parameter $\varepsilon^2 = \frac{U_T}{\Phi_L}$. It will be justified in Section 3. We have solved this system by the above described deterministic particle method with $g = 0$ as initial distribution function. Moments of g will be referred to in the subsequent discussions as « non equilibrium moments » and designed with an index g as opposed to the moments of f^0 which will be the « equilibrium moments ». The physical and numerical parameters are the same as in subsection 2.5 and are summarized in table 1. The current density (*fig.* 10) seems perfectly correct. We also remark that the total velocity (*fig.* 12) vanishes outside the depletion zone and the non equilibrium electrons velocity (*fig.* 11) is very high in this region. The energies of the two electron populations are given in figures 13 and 14. Finally, figures 15 and 16 give plots of g as a function of (x, k_1) near $k_2 = 0$ at $t = 1\ ps$ and at stationary state. At $t = 1\ ps$, the collisions had not have enough time to act, and figure 15 provides a numerical picture of the asymptotic analysis done in the following section which concerns a collisionless case. Indeed, the distribution function seems to follow a parabola like char-

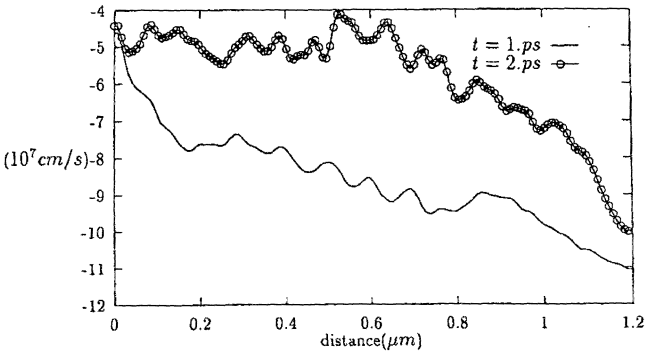


Figure 11. — Mean velocity of the non-equilibrium electrons (simulation of the non-equilibrium distribution).

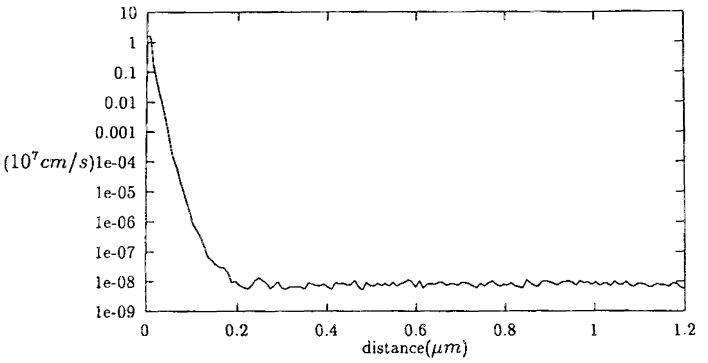


Figure 12. — Mean velocity (simulation of the non-equilibrium distribution).

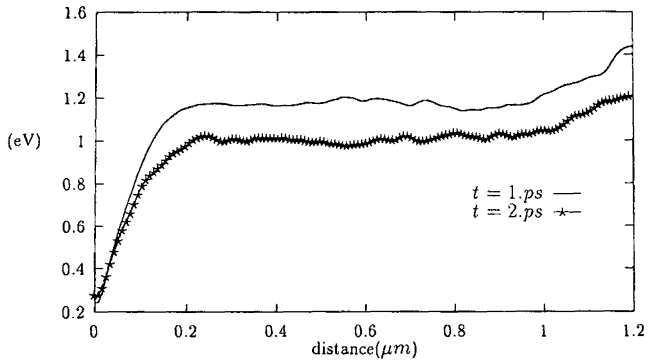


Figure 13. — Mean energy of the non-equilibrium electrons (simulation of the non-equilibrium distribution).

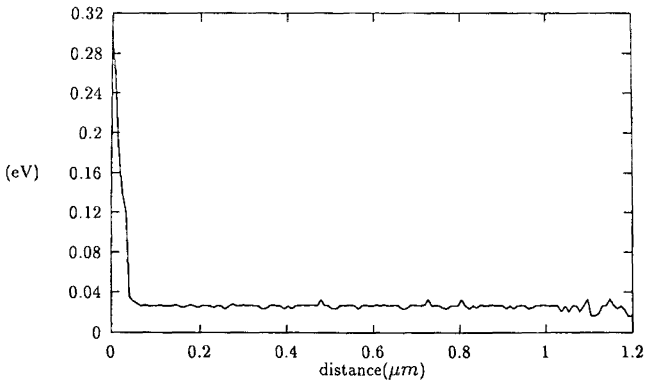


Figure 14. — Mean energy (simulation of the non-equilibrium distribution).

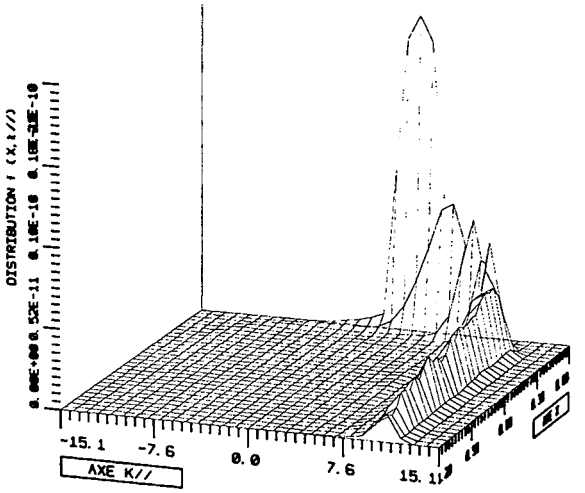


Figure 15. — The non-equilibrium distribution function at $t = 1\,ps$.

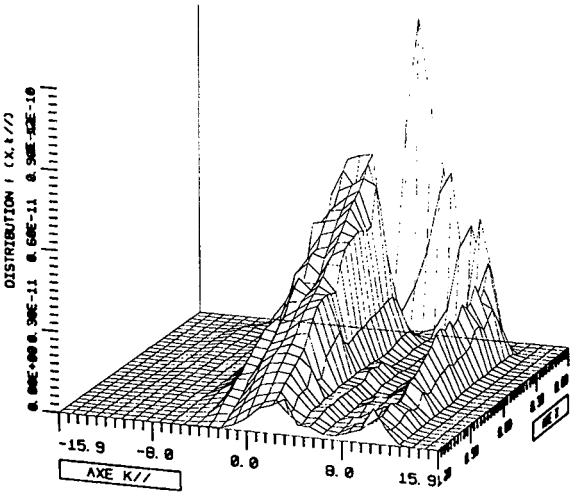


Figure 16. — The stationary state non-equilibrium distribution function (simulation of the non-equilibrium distribution).

acteristics$\left(k_1 = \sqrt{2\,\Phi(x)}\right)$, starting from the metal semiconductor contact ($x = 0$) with a zero velocity at the starting point. Once the equilibrium has been reached (*fig.* 16), the ballistic part of the distribution function is clearly visible and follows the same parabola, and the contribution of electrons which

have suffered one or more collisions appears as a thermalized part near $k_1 = 0$. This distribution function is close to the one obtained by the Child Langmuir asymptotics of the Boltzmann Transport equation in [4].

3. ASYMPTOTIC ANALYSIS OF VLASOV-POISSON SYSTEM FOR MODELING A SCHOTTKY DIODE

3.1. A simplified model

In this section, we will consider the stationary one dimensional Vlasov-Poisson system in the parabolic band approximation :

$$V\frac{\partial F(X,V)}{\partial X} + \frac{q}{m^*}\frac{d\Phi}{dx}\frac{\partial F(X,V)}{\partial V} = 0\,, \quad X \in\ ]0, L[\,, V \in \mathbb{R}$$

$$\frac{d^2\Phi}{dX^2} = \frac{q}{\varepsilon_s}(N(X) - N_D)\,, \quad X \in\ ]0, L[\tag{3.1}$$

$$N(X) = \int_{-\infty}^{+\infty} F(X,V)\,dV\,.$$

For the sake of simplicity, we neglect collisions. This is justified by the fact that the depletion zone, which is the most important region of the device, is very short and that electrons have not enough time to suffer important collisions. Boundary conditions are given as follows :

$$\Phi(0) = 0 \quad , \quad \Phi(L) = \Phi_L = V_{bi} - V_A$$

$$F(0,v) = N_D \exp\left(-\frac{V_{bi}}{U_{th}}\right)\frac{1}{\sqrt{2\pi}\,V_{th}}\exp\left(-\frac{v^2}{2V_{th}}\right)\,, \quad v > 0\,, \tag{3.2}$$

$$F(L,v) = N_D \frac{1}{\sqrt{2\pi}\,V_{th}}\exp\left(-\frac{v^2}{2V_{th}}\right) \quad , \quad v < 0\,.$$

The thermal velocity V_{th} is given by $V_{th} = \sqrt{k_B T/m^*}$. Other physical constants are defined in Section 1. We also define a characteristic velocity $V_L = \sqrt{\frac{q\Phi_L}{m^*}}$, which is the typical electron velocity when accelerated by the electric field.

3.2. Scaling

Now we assume that the lattice temperature is small, or equivalently that the typical velocity of the injected electrons at the junction which is of the order of the thermal velocity V_{th} is small compared with the velocity V_L that they reach after being accelerated by the electric field :

$$\sqrt{\frac{k_B T}{m^*}} = V_{th} \ll V_L = \sqrt{\frac{q\Phi_L}{m^*}}\,. \tag{3.3}$$

Therefore, we introduce the small parameter ε by :

$$\varepsilon = \frac{V_{th}}{V_L} \ll 1 . \tag{3.4}$$

We shall use L, V_L, Φ_L and N_D as characteristic length, velocity, potential and density scales. We introduce auxiliary units of current density $\bar{J}$ and distribution function $\bar{F}$ according to

$$\bar{J} = qN_D V_L , \quad \bar{F} = \frac{N_D}{V_L} , \tag{3.5}$$

and use the following scaling :

$$\begin{aligned} &X = Lx , \quad V = V_L v , \quad \Phi = \Phi_L \varphi , \\ &F = \bar{F} f , \quad N = N_D n , \quad J = -\bar{J} j . \end{aligned} \tag{3.6}$$

With these hypotheses, the dimensionless Vlasov-Poisson system reads :

$$\begin{aligned} &v \frac{\partial f(x, v)}{\partial x} + \frac{d\varphi}{dx} \frac{\partial f(x, v)}{\partial v} = 0 , \quad x \in \,]0,1\,[\, , v \in \mathbb{R} , \\ &\frac{d^2\varphi}{dx^2} = \lambda(n(x) - 1) , \quad x \in \,]0, 1[, \\ &n(x) = \int_{-\infty}^{+\infty} f(x, v)\, dv , \quad x \in \,]0, 1[. \end{aligned} \tag{3.7}$$

The dimensionless constant λ is given by

$$\lambda = \frac{qN_D L^2}{\varepsilon_s \Phi_L} . \tag{3.8}$$

Boundary conditions then become :

$$\begin{aligned} &\varphi(0) = 0 , \quad \varphi(1) = 1 , \\ &f(0, v) = \exp\left(-\frac{\mu}{\varepsilon^2}\right) \frac{1}{\sqrt{2\pi}\varepsilon} \exp\left(-\frac{v^2}{2\varepsilon^2}\right) , \quad v > 0 , \\ &f(1, v) = \frac{1}{\sqrt{2\pi}\varepsilon} \exp\left(-\frac{v^2}{2\varepsilon^2}\right) , \quad v < 0 , \end{aligned} \tag{3.9}$$

with the following relations :

$$\varepsilon = \frac{V_T}{V_L} = \sqrt{\frac{U_T}{\Phi_L}}, \quad \exp\left(-\frac{\mu}{\varepsilon^2}\right) = \exp\left(-\frac{V_{bi}}{U_T}\right), \quad \mu = \frac{V_{bi}}{\Phi_L},$$

where the constant $\mu > 0$ is of order 1 ($\mu < 1$ under a forward bias and $\mu > 1$ under a reverse bias). Now, we are interested in the limit behavior of the distribution function, and then the density and the potential, when the parameter ε goes to zero. We use the same procedure as the 3 dimensional case [16]. However, we will obtain explicit expressions and, of course, more regularity results of the limiting problem. We introduce the functions $f_{0,\varepsilon}$ and H :

$$f_{0,\varepsilon} = n_{0,\varepsilon} \frac{1}{\varepsilon \sqrt{2\pi}} \exp\left(-\frac{v^2}{2\varepsilon^2}\right),$$

$$n_{0,\varepsilon} = \exp\left(-\frac{1 - \varphi_\varepsilon(x)}{\varepsilon^2}\right), \tag{3.10}$$

$$H(t) = \exp(-t) \quad \text{for} \quad t > 0,$$

$$H(t) = 0 \quad \text{for} \quad t < 0, \tag{3.11}$$

and we write the distribution function in the following form :

$$f_\varepsilon = f_{0,\varepsilon} + \varepsilon \max\left(\exp\left(-\frac{\mu}{2\varepsilon^2}\right), \exp\left(-\frac{1}{2\varepsilon^2}\right)\right) h_\varepsilon. \tag{3.12}$$

We will prove the two following theorems, and we will only sketch the differences with [16].

THEOREM 3.1 : *(Convergence of the equilibrium part)*
When $\varepsilon \to 0$, *the solutions* $(f_\varepsilon, \varphi_\varepsilon)$ *of problem* (3.7)-(3.9) *verify :*

$$\varphi_\varepsilon, \varphi_{0,\varepsilon} \to \varphi_0 \text{ in } W^{2,p}(0,1), p < \infty \quad \text{and in} \quad C^2([0,1[\backslash V_D),$$

$$n_\varepsilon, n_{0,\varepsilon} \to n_0 \text{ in } L^p(]0,1[), p < \infty \quad \text{and in} \quad C^1([0,1[\backslash V_D),$$

$$f_\varepsilon, f_{0,\varepsilon} \to f_0, \quad f_0(x,v) = n_0(x)\,\delta(v) \quad \text{in} \quad \mathcal{M}_b([0,1] \times \mathbb{R}) \text{ weak}^*,$$

where $\mathcal{M}([0,1] \times \mathbb{R})$ *is the space of bounded measures on* $[0,1] \times \mathbb{R}$, *and*

where V_D *is a neighborhood of* $l_D = inf\left(1, \frac{2}{\lambda}\right)$, φ_0 *and* n_0 *are defined as :*

$$n_0(x) = 0 \quad if \quad x \leqslant l_D, \qquad n_0(x) = 1 \quad if \quad x > l_D,$$

$$\varphi_0(x) = \frac{\lambda}{2} x(l_D - x) + \frac{x}{l_D}, x < l_D \quad \varphi_0(x) = 1, x \geqslant l_D$$

THEOREM 3.2 : *(Convergence of the kinetic part)*

$$h_\varepsilon \underset{\varepsilon \to 0}{\longrightarrow} h_0 = \frac{1}{\sqrt{4\pi\varphi_0}} \delta\left(v - \sqrt{2\varphi_0}\right) Sign\,(1 - \mu)$$

$$in \quad \mathcal{M}_b((0, 1) \times \mathbb{R}), \quad (3.13)$$

φ_0 *is defined in theorem* (3.1).

Moreover, the current density is given (for ε *small enough) by :*

$$j_\varepsilon = \int_{-\infty}^{+\infty} v f_\varepsilon(x, v)\, dv = \frac{\varepsilon}{\sqrt{2\pi}} \left(\exp\left(-\frac{\mu}{2\varepsilon^2}\right) - \exp\left(-\frac{1}{2\varepsilon^2}\right)\right). \quad (3.14)$$

To prove theorem (3.1), we begin by giving some uniform estimates.

3.3. Uniform estimates

Let :

$$g_{1,\varepsilon} = \frac{1}{\sqrt{2\pi}\varepsilon} H\left(\frac{v^2/2 - \varphi_\varepsilon}{\varepsilon^2}\right), \quad \rho_{1,\varepsilon} = \int_{-\infty}^{+\infty} g_{1,\varepsilon}(x, v)\, dv, \quad (3.15)$$

$$f_{1,\varepsilon} = f_{0,\varepsilon} + \left(\exp\left(-\frac{\mu}{\varepsilon^2}\right) - \exp\left(-\frac{1}{\varepsilon^2}\right)\right) g_{1,\varepsilon}, \quad n_{1,\varepsilon} = \int_{-\infty}^{+\infty} f_{1,\varepsilon}(x, v)\, dv. \quad (3.16)$$

The function $f_{1,\varepsilon}$ is non negative. Indeed $f_{1,\varepsilon} = f_{0,\varepsilon}$ if $\frac{v^2}{2} - \varphi_\varepsilon \leqslant 0$ and if $\frac{v^2}{2} - \varphi_\varepsilon \geqslant 0$, then $f_{1,\varepsilon} = \exp\left(-\frac{\mu}{\varepsilon^2}\right) g_{1,\varepsilon}$. We get :

PROPOSITION 3.1 : *There exists a solution* f^ε, φ^ε *of the problem* (3.7)-(3.9) *such that :*

$$f_{0,\varepsilon} \leqslant f_\varepsilon \leqslant f_{1,\varepsilon} \quad if \quad \mu \leqslant 1,$$

$$f_{1,\varepsilon} \leqslant f_\varepsilon \leqslant f_{0,\varepsilon} \quad if \quad \mu \geqslant 1, \quad (3.17)$$

$$\|f_\varepsilon - f_{0,\varepsilon}\|_{L^\infty(]0,1[\times\mathbb{R})} \leqslant \left(\exp\left(-\frac{\mu}{\varepsilon^2}\right) + \exp\left(-\frac{1}{\varepsilon^2}\right)\right) \frac{1}{\sqrt{2\pi}\varepsilon}, \quad (3.18)$$

$$\|n_\varepsilon - n_{0,\varepsilon}\|_{L^\infty(]0,1[)} \leqslant \left(\exp\left(-\frac{\mu}{\varepsilon^2}\right) + \exp\left(-\frac{1}{\varepsilon^2}\right)\right). \quad (3.19)$$

Proof: The functions $f_{0,\varepsilon}$ and $f_{1,\varepsilon}$ are solutions of the Vlasov equation (3.7). Moreover, we have

$$f_{1,\varepsilon}(0, v) = \exp\left(-\frac{\mu}{\varepsilon^2}\right) \frac{1}{\sqrt{2\pi}\varepsilon} \exp\left(-\frac{v^2}{2\varepsilon^2}\right) = f_\varepsilon(0, v)\ v > 0\ ,$$

$$f_{0,\varepsilon}(1, v) = \frac{1}{\sqrt{2\pi}\varepsilon} \exp\left(-\frac{v^2}{2\varepsilon^2}\right) = f_\varepsilon(1, v)\ v < 0\ ,$$

and $f_{0,\varepsilon} \leqslant f_{1,\varepsilon}$ for $\mu \leqslant 1$, then, these functions are respectively lower and upper-solutions of (3.7) and vice versa for $\mu \geqslant 1$. The existence of a solution of (3.7)-(3.9) such that (3.17) holds holds is guaranteed by [29]. Thus,

$$|f_\varepsilon - f_{0,\varepsilon}| \leqslant |f_{1,\varepsilon} - f_{0,\varepsilon}| \leqslant \left(\exp\left(-\frac{\mu}{\varepsilon^2}\right) + \exp\left(-\frac{1}{\varepsilon^2}\right)\right) g_{1,\varepsilon}\ . \quad (3.20)$$

The function H is bounded by 1, so (3.15) and (3.20) lead to (3.18). On the other hand, we have :

$$|n_\varepsilon - n_{0,\varepsilon}| \leqslant \int_{-\infty}^{+\infty} |f_\varepsilon - f_{0,\varepsilon}|\, dv\ ,$$

then by using (3.15) and (3.20) we obtain

$$|n_\varepsilon - n_{0,\varepsilon}| \leqslant \left(\exp\left(-\frac{\mu}{\varepsilon^2}\right) + \exp\left(-\frac{1}{\varepsilon^2}\right)\right) \rho_{1,\varepsilon}\ . \quad (3.21)$$

But,

$$\rho_{1,\varepsilon}(x) = \exp\left(\frac{\varphi_\varepsilon}{\varepsilon^2}\right) \leqslant 1 \quad \text{for} \quad \varphi_\varepsilon \leqslant 0\ , \quad (3.22)$$

and for $\varphi_\varepsilon \geqslant 0$, the change of variable $t = \dfrac{v^2/2 - \varphi_\varepsilon}{\varepsilon^2}$ yields to

$$\rho_{1,\varepsilon}(x) = \frac{1}{\sqrt{\pi}} \int_0^{+\infty} \frac{\exp(-t)}{\sqrt{t + \varphi_\varepsilon/\varepsilon^2}}\, dt\ , \quad \varphi_\varepsilon \geqslant 0\ .$$

Then, we have

$$\rho_{1,\varepsilon}(x) \leqslant \frac{1}{\sqrt{\pi}} \int_0^{+\infty} \frac{\exp(-t)}{\sqrt{t}}\, dt = 1\ , \quad \varphi_\varepsilon \geqslant 0\ , \quad (3.23)$$

The estimate (3.19) is a consequence of (3.21), (3.22) and (3.23). •

We introduce now the following elliptic problem :

$$\varphi_{0,\varepsilon}(0) = 0, \quad \varphi_{0,\varepsilon}(1) = 1,$$

$$\frac{d^2\varphi_{0,\varepsilon}}{dx^2} = \lambda\left(\exp\left(\frac{\varphi_{0,\varepsilon} - 1}{\varepsilon^2}\right) - 1\right), \quad x \in]0, 1[, \tag{3.24}$$

then, we have

PROPOSITION 3.2 : *The problem* (3.24) *has a unique solution which satisfies :*

$$1 \geq \varphi_{0,\varepsilon}(x) \geq \lambda\frac{x(1-x)}{2} + x \quad \forall x \in [0, 1], \tag{3.25}$$

$$\varphi'_{0,\varepsilon}(x) \geq 0 \quad \forall x \in [0, 1]. \tag{3.26}$$

Proof : The existence and uniqueness of solution of the problem (3.24) is classical. Then we have

$$\varphi''_{0,\varepsilon}(x) \geq -\lambda, \quad \varphi_{0,\varepsilon}(0) = 0, \quad \varphi_{0,\varepsilon}(1) = 1.$$

The maximum principle implies that $\varphi_{0,\varepsilon}$ is bounded from below as in (3.25). Now, let x_0 the point where $\varphi_{0,\varepsilon}$ matches its maximum. If we suppose that $\varphi_{0,\varepsilon}(x_0) > 1$, and $[x_0, l]$ the maximum interval in which $\varphi_{0,\varepsilon}(x) \geq 1$. Thus, $\varphi''_{0,\varepsilon}(x) \geq 0$, $\forall x \in [x_0, l]$, and $\varphi'_{0,\varepsilon}(x) \geq \varphi'_{0,\varepsilon}(x_0) = 0$, $\forall x \in [x_0, l]$. This implies that $\varphi_{0,\varepsilon}(l) \geq \varphi_{0,\varepsilon}(x_0) > 1$, and we have $l = 1$. This leads to a contradiction ($\varphi_{0,\varepsilon}(1) = 1$), and (3.25) holds.

Then, $\varphi_{0,\varepsilon}(x) \leq 1$ implies that $\varphi''_{0,\varepsilon}(x) \leq 0$ and $\varphi'_{0,\varepsilon}(1) \geq 0$. Thus, $\varphi'_{0,\varepsilon}$ is decreasing and $\varphi'_{0,\varepsilon}(x) \geq \varphi'_{0,\varepsilon}(1) \geq 0$ on [0,1]. •

Now, we have the following approximation results :

PROPOSITION 3.3 : *Let* $(f_\varepsilon, \varphi_\varepsilon)$ *be a solution of the problem* (3.1)-(3.9) *for which proposition* (3.1) *holds, then we have :*

$$|\varphi_\varepsilon(x) - \varphi_{0,\varepsilon}(x)| \leq C\left(\exp\left(-\frac{\mu}{\varepsilon^2}\right) + \exp\left(-\frac{1}{\varepsilon^2}\right)\right), \quad \forall x \in]0, 1[, \tag{3.27}$$

$$\left|\frac{d\varphi_\varepsilon(x)}{dx} - \frac{d\varphi_{0,\varepsilon}(x)}{dx}\right| \leq \frac{C}{\varepsilon^2}\left(\exp\left(-\frac{\mu}{\varepsilon^2}\right) + \exp\left(-\frac{1}{\varepsilon^2}\right)\right), \quad \forall x \in]0, 1[, \tag{3.28}$$

$$\left|n_\varepsilon(x) - \exp\left(\frac{\varphi_{0,\varepsilon} - 1}{\varepsilon^2}\right)\right| \leq \frac{C}{\varepsilon^2}\left(\exp\left(-\frac{\mu}{\varepsilon^2}\right) + \exp\left(-\frac{1}{\varepsilon^2}\right)\right), \quad \forall x \in [0, 1], \tag{3.29}$$

where the generic constants C do not depend on ε.

Proof: Let $\delta_\varepsilon = \varphi_\varepsilon - \varphi_{0,\varepsilon}$, and $r^\varepsilon = n_\varepsilon - n_{0,\varepsilon}$, then we have

$$\delta_\varepsilon(0) = \delta_\varepsilon(1) = 0,$$

$$\delta_\varepsilon''(x) = \lambda\left(\exp\left(\frac{\varphi_\varepsilon - 1}{\varepsilon^2}\right) - \exp\left(\frac{\varphi_{0,\varepsilon} - 1}{\varepsilon^2}\right)\right) + \lambda r^\varepsilon(x).$$

We obtain by multiplying by δ_ε and integrating with respect to x:

$$\int_0^1 \delta_\varepsilon'^2(x)\,dx =$$

$$-\lambda \exp\left(-\frac{1}{\varepsilon^2}\right)\int_0^1\left(\exp\left(-\frac{\varphi_\varepsilon(x)}{\varepsilon^2}\right) - \exp\left(-\frac{\varphi_{0,\varepsilon}(x)}{\varepsilon^2}\right)\right)(\varphi_\varepsilon(x) - \varphi_{0,\varepsilon}(x))\,dx$$

$$-\lambda\int_0^1 r^\varepsilon(x)\,\delta_\varepsilon(x)\,dx.$$

$$\leqslant \lambda\int_0^1 \delta_\varepsilon(x)\,dx\left(\exp\left(-\frac{1}{\varepsilon^2}\right) + \exp\left(-\frac{\mu}{\varepsilon^2}\right)\right).$$

The previous inequality holds from the exponential being a nondecreasing function and the estimate (3.19). But

$$\int_0^1 \delta_\varepsilon(x)\,dx \leqslant \left(\int_0^1 \delta_\varepsilon^2(x)\,dx\right)^{\frac{1}{2}} \leqslant \frac{1}{\pi}\left(\int_0^1 \delta_\varepsilon'^2(x)\,dx\right)^{\frac{1}{2}},$$

(π^{-1} is the Poincare constant of $]0, 1[$). This leads to

$$\left(\int_0^1 \delta_\varepsilon'^2(x)\,dx\right)^{\frac{1}{2}} \leqslant \frac{\lambda}{\pi}\left(\exp\left(-\frac{1}{\varepsilon^2}\right) + \exp\left(-\frac{\mu}{\varepsilon^2}\right)\right),$$

and according to the continuous embedding of H^1 into C^0, we obtain (3.27). From (3.19), it remains to bound $n_{0,\varepsilon} - \exp\left(\frac{\varphi_{0,\varepsilon} - 1}{\varepsilon^2}\right)$ in order to get (3.29). One can remark that

$$\left|n_{0,\varepsilon} - \exp\left(\frac{\varphi_{0,\varepsilon} - 1}{\varepsilon^2}\right)\right| \leqslant \frac{|\varphi_\varepsilon - \varphi_{0,\varepsilon}|}{\varepsilon^2}\exp\left(\frac{\sup(\varphi_\varepsilon, \varphi_{0,\varepsilon}) - 1}{\varepsilon^2}\right).$$

By using (3.25) and (3.27), we have

$$\sup(\varphi_\varepsilon, \varphi_{0,\varepsilon}) \leq 1 + C\left(\exp\left(-\frac{1}{\varepsilon^2}\right) + \exp\left(-\frac{\mu}{\varepsilon^2}\right)\right),$$

$$\left| n_{0,\varepsilon} - \exp\left(\frac{\varphi_{0,\varepsilon} - 1}{\varepsilon^2}\right)\right| \leq \frac{C}{\varepsilon^2}\left(\exp\left(-\frac{\mu}{\varepsilon^2}\right) + \exp\left(-\frac{1}{\varepsilon^2}\right)\right) \times$$

$$\times \exp\left(C\frac{\exp\left(-\frac{\mu}{\varepsilon^2}\right) + \exp\left(-\frac{1}{\varepsilon^2}\right)}{\varepsilon^2}\right),$$

which leads to (3.29). (3.28) is then a consequence of (3.27) and (3.29). •

3.4. Asymptotic limit of the elliptic problem

This subsection concerns the passage to the limit $\varepsilon \to 0$ in the elliptic problem (3.24). The function $\varphi_{0,\varepsilon}$ remains bounded by 1 (see (3.25)), then we have

$$0 \geq \varphi''_{0,\varepsilon}(x) \geq -\lambda, \tag{3.30}$$

and $\varphi_{0,\varepsilon}$ is bounded in $W^{2,\infty}(]0, 1[)$. By using Ascoli's theorem, we have up to a subsequence :

$$\varphi_{0,\varepsilon} \to \varphi_0 \text{ uniformly in } C^1([0, 1]) \tag{3.31}$$

$$\varphi''_{0,\varepsilon} \rightharpoonup \varphi''_0 \text{ in } L^\infty(]0, 1[) \text{ weak}^* . \tag{3.32}$$

LEMMA 3.1 : *For every fixed value* $\varphi^* \in [0, 1)$, *there exist two unique real numbers* $\phi_{0,\varepsilon}(\varphi^*)$ *and* $\phi_0(\varphi^*)$ *such that :*

$$\varphi_{0,\varepsilon}(\phi_{0,\varepsilon}(\varphi^*)) = \varphi^*, \varphi_0(\phi_0(\varphi^*)) = \varphi^* \quad \textit{and} \quad \phi_{0,\varepsilon}(\varphi^*) \to \phi_0(\varphi^*). \tag{3.33}$$

Proof : It's sufficient to show that $\varphi_{0,\varepsilon}$ and φ_0 are increasing functions of x, for all x such that $\varphi_{0,\varepsilon}(x) \neq 1$ or $\varphi_0(x) \neq 1$.

If $\varphi'_{0,\varepsilon}(x) = 0$, then $\varphi'_{0,\varepsilon}(y) = 0$ on $(x, 1]$ ($\varphi'_{0,\varepsilon}$ is decreasing and $\varphi'_{0,\varepsilon}(1) \geq 0$) and $\varphi_{0,\varepsilon}(y) = \varphi_{0,\varepsilon}(1) = 1$ on $(x, 1]$. We proceed likewise for φ_0.

Now let $l_{D,\varepsilon} = \sup\{x\,;\,\varphi_{0,\varepsilon}(x) < 1\}$, and $l_D = \sup\{x\,;\,\varphi_0(x) < 1\}$, then the functions $\varphi_{0,\varepsilon}$ and φ_0 are one to one maps respectively from $[0, l_{D,\varepsilon}]$ and $[0, l_D]$ to $[0, 1)$. We note $\phi_{0,\varepsilon}$ and ϕ_0 their inverses. For $\varphi^* \in [0, 1)$, we have :

$$|\varphi_0(\phi_{0,\varepsilon}(\varphi^*)) - \varphi_0(\phi_0(\varphi^*))| = |\varphi_0(\phi_{0,\varepsilon}(\varphi^*)) - \varphi_{0,\varepsilon}(\phi_{0,\varepsilon}(\varphi^*))|$$

$$= |\varphi_0(\phi_{0,\varepsilon}(\varphi^*)) - \varphi^*| \to_{\varepsilon \to 0} 0\,,$$

by using the uniform convergence of $\varphi_{0,\varepsilon}$ to φ_0. Therefore, for ε small enough, $\varphi_0(\phi_{0,\varepsilon}(\varphi^*)) < 1$ and $\phi_0(\varphi_0(\phi_{0,\varepsilon}(\varphi^*))) = \phi_{0,\varepsilon}(\varphi^*)$. The function ϕ_0 is continuous, then

$$|\phi_0(\varphi_0(\phi_{0,\varepsilon}(\varphi^*))) - \phi_0(\varphi^*)| \to_{\varepsilon \to 0} 0,$$

which gives (3.33). •

PROPOSITION 3.4 : *The limiting potential φ_0 is given as follows*

$$\varphi_0(x) = \lambda \frac{x(l_D - x)}{2} + \frac{x}{l_D} \quad \textit{for} \quad x \leqslant l_D$$

$$\varphi_0(x) = 1 \quad \textit{for} \quad x \geqslant l_D, \textit{ where } l_D \in (0, 1]\,. \tag{3.34}$$

Proof : $l_D = \sup\{x\,;\,\varphi_0(x) < 1\}$. For every $l < l_D$, let $\phi_* \in (l, l_D)$ and $\varphi_* = \varphi_0(\phi_*)$. By using (3.33), we can obtain that, for ε small enough, $\phi_{0,\varepsilon}(\varphi_*) > l$. Thus, $\varphi_{0,\varepsilon}(x) \leqslant \varphi_*$ on $[0, l]$, the functions $\varphi_{0,\varepsilon}$ are nondecreasing. Then, we have :

$$|\varphi''_{0,\varepsilon}(x) + \lambda| = \lambda \exp\left(\frac{\varphi_{0,\varepsilon}(x) - 1}{\varepsilon^2}\right) \leqslant \lambda \exp\left(-\frac{1 - \varphi_*}{\varepsilon^2}\right), \tag{3.35}$$

and $\varphi''_{0,\varepsilon} \to -\lambda$ in $C^0(0, l)$ uniformly.

By using (3.31) and (3.32), we can conclude that :

$$\varphi_{0,\varepsilon} \to \varphi_0 \quad \text{uniformly in} \quad C^2([0, l]) \quad \forall l < l_D \tag{3.36}$$

$$\varphi''_0(x) = -\lambda \quad \text{on} \quad [0, l_D]\,, \tag{3.37}$$

but, $\varphi_0(0) = 0$ and $\varphi_0(l_D) = 1$, then (3.34) holds for $x \leqslant l_D$. The functions $\varphi_{0,\varepsilon}$ are nondecreasing, we then conclude that φ_0 is also nondecreasing from (3.31). For $x \in (l_D, 1)$, we have $1 = \varphi_0(l_D) \leqslant \varphi_0(x) \leqslant \varphi_0(1) = 1$, which ends the proof. •

PROPOSITION 3.5 : *The real number l_D is given by :*

$$l_D = 1 \quad \text{if} \quad \lambda \leqslant 2\,, \quad l_D = \sqrt{\frac{2}{\lambda}} \quad \text{if} \quad \lambda \geqslant 2\,. \tag{3.38}$$

Proof : For $x < l_D$, we have $\varphi_0'(x) = -\lambda x + \dfrac{\lambda l_D}{2} + \dfrac{1}{l_D}$. But the function φ_0 is C^1, then we have $\varphi_0'(l_D) = -\dfrac{\lambda l_D}{2} + \dfrac{1}{l_D}$. φ_0 is constant on $[l_D, 1]$, then if $l_D < 1$ we necessarily have : $\varphi_0'(l_D) = -\dfrac{\lambda l_D}{2} + \dfrac{1}{l_D} = 0$, $l_D = \sqrt{\dfrac{2}{\lambda}}$, and the condition $\lambda > 2$ holds.

On the other hand, if $l_D = 1$, then

$$\varphi_0'(x) = -\lambda x + \frac{\lambda}{2} + 1 \ \forall x \in (0, 1),$$

and φ_0 being increasing imposes that $x_0 = \dfrac{1}{2} + \dfrac{1}{\lambda} \geqslant 1$, which leads to (3.38). •

Finally, the following theorem allows us to obtain the limit behavior of $\varphi_{0,\varepsilon}$.

PROPOSITION 3.6 : *The functions $\varphi_{0,\varepsilon}$ verify :*

$$\varphi_{0,\varepsilon} \to \varphi_0 \text{ in } C^2([0, 1]\backslash V_D) \text{ uniformly for every neighborhood } V_D \text{ of } l_D\,. \tag{3.39}$$

Proof : In view of (3.36) we have only to consider the case where $l_D < 1$. We remark that $\varphi_{0,\varepsilon}'' + \lambda \geqslant 0$. If we note $\psi_\varepsilon = \lambda \exp\left(\dfrac{\varphi_{0,\varepsilon} - 1}{\varepsilon^2}\right)$, then for every $x,\ y \in\ ]l_D, 1[$

$$\int_x^y \psi_\varepsilon(z)\, dz = \int_x^y (\varphi_{0,\varepsilon}''(z) + \lambda)\, dz = \lambda(y - x) + \varphi_{0,\varepsilon}'(y) - \varphi_{0,\varepsilon}'(x)$$

$$= \lambda(y - x) + \eta_\varepsilon(x, y)\,,$$

where $\eta_\varepsilon(x, y) \to_{\varepsilon \to 0} 0$ by using (3.31).

On the other hand, the functions ψ_ε are nondecreasing (like $\varphi_{0,\varepsilon}$), then

$$(y - x)\, \psi_\varepsilon(x) \leqslant \int_x^y \psi_\varepsilon(z)\, dz \leqslant (y - x)\, \psi_\varepsilon(y)\,,$$

$$\psi_\varepsilon(x) \leqslant \lambda + \frac{\eta_\varepsilon(x, y)}{y - x} \leqslant \psi_\varepsilon(y)\,,$$

$$\text{and} \quad \lambda + \frac{\eta_\varepsilon(l_D, x)}{x - l_D} \leqslant \psi_\varepsilon(x) \leqslant \psi_\varepsilon(1) = \lambda\,, \quad \forall x \in\ ]l_D, 1[\,.$$

Thus, $\forall [a, b] \subseteq]l_D, 1[$, $\psi_\varepsilon \to \lambda$ on $[a, b]$ uniformly.

$$(\forall x \in [a, b], \lambda \leftarrow \psi_\varepsilon(a) \leq \psi_\varepsilon(x) \leq \psi_\varepsilon(1) = \lambda),$$

which leads to the uniform convergence of $\varphi''_{0,\varepsilon}$ to φ''_0 on $]l_D, 1[$.

Then, (3.36) ends the proof of (3.39). •

DEFINITION 3.1 : *l_D is called the depletion length, and the region $\{x \text{ s.t. } 0 \leq x \leq l_D\}$ is the depletion zone of the Schottky diode.*

We now are able to prove theorem (3.1) about the limiting solution of the Vlasov-Poisson problem when ε goes to zero.

Proof of theorem (3.1) : Proposition (3.6) and the estimates (3.27), (3.28) allow us to obtain that

$$\varphi_\varepsilon \to \varphi_0 \quad \text{uniformly in} \quad C^1(]0, 1[).$$

On the other hand, we have

$$|n_\varepsilon(x) - n_0(x)| = \left| n_\varepsilon(x) - \exp\left(\frac{\varphi_{0,\varepsilon} - 1}{\varepsilon^2}\right)\right| + \left| n_0(x) - \exp\left(\frac{\varphi_{0,\varepsilon} - 1}{\varepsilon^2}\right)\right|$$

$$= \left| n_\varepsilon(x) - \exp\left(\frac{\varphi_{0,\varepsilon} - 1}{\varepsilon^2}\right)\right| + \frac{1}{\lambda} |\varphi''_0(x) - \varphi''_{0,\varepsilon}(x)|.$$

Then Proposition (3.6) and estimate (3.29) imply that

$$n_\varepsilon \to n_0 \quad \text{uniformly in} \quad C^0(]0, 1[\backslash V_D),$$

for every neighborhood V_D of l_D.

In the same way $\varphi_{0,\varepsilon} \to \varphi_0$ uniformly in $C^2([0, 1] \backslash V_D)$. Besides, by using the estimates (3.25) and (3.29), n_ε is uniformly bounded by 2 for ε small enough.

Now, let V_D be a fixed neighborhood of l_D then :

$$\int_0^1 |n_\varepsilon(x) - n_0(x)|^p \, dx \leq \|n_\varepsilon - n_0\|_{L^\infty([0,1]\backslash V_D)} + 3 \, meas\,(V_D).$$

$$\limsup \int_0^1 |n_\varepsilon(x) - n_0(x)|^p \, dx \leq 3 \, meas\,(V_D).$$

Since V_D is an arbitrary neighborhood, this yields $n_\varepsilon \to n_0$ in $L^p(\,]0,1[\,)$ $p<\infty$. Likewise, we have $\varphi_\varepsilon \to \varphi_0$ in $W^{2,p}(\,]0,1[\,)$, $p<\infty$. On the other hand, we have

$$\left|f_\varepsilon(x,v)-n_\varepsilon\frac{1}{\sqrt{2\pi}\varepsilon}\exp\left(-\frac{v^2}{2\varepsilon^2}\right)\right| \leq |f_\varepsilon(x,v)-f_{0,\varepsilon}(x,v)|$$

$$+|n_{0,\varepsilon}(x)-n_\varepsilon(x)|\frac{1}{\sqrt{2\pi}\varepsilon}\exp\left(-\frac{v^2}{2\varepsilon^2}\right)$$

$$\leq \frac{2}{\sqrt{2\pi}\varepsilon}\left(\exp\left(-\frac{\mu}{\varepsilon^2}\right)+\exp\left(-\frac{1}{\varepsilon^2}\right)\right)$$

by using (3.18) and (3.19). Then, we easily conclude that :

$$f_\varepsilon, f_{0,\varepsilon} \rightharpoonup n_0(x)\,\delta(v) \quad \text{in} \quad \mathcal{M}_b([0,1]\times\mathbb{R}) \text{ weak}^* .$$

•

We now turn to the scaled Vlasov-Poisson problem (3.7) with boundary conditions (3.9), and to the decomposition (3.12) of the distribution function, where $f_{0,\varepsilon}$ is the equilibrium distribution (3.10) and h_ε is solution of Vlasov equation with boundary conditions

$$\begin{cases} h_\varepsilon(0,v) = \dfrac{1}{\varepsilon^2\sqrt{2\pi}}\,Sign\,(1-\mu)\left(1-\exp\left(-\dfrac{|1-\mu|}{2\varepsilon^2}\right)\right)\exp\left(-\dfrac{v^2}{2\varepsilon^2}\right), v>0 \\ h_\varepsilon(1,v) = 0, \quad v<0 , \end{cases} \tag{3.40}$$

h_ε is the kinetic part of the distribution function.

We are now interested in the proof of theorem (3.2) which concerns the limit of the correction term h_ε, because it carries all the non equilibrium dynamics. In particular, since $j_{0,\varepsilon}=\int v f_{0,\varepsilon}\,dv = 0$, the current is given by :

$$j_\varepsilon = \varepsilon \max\left(\exp\left(-\frac{\mu}{2\varepsilon^2}\right),\exp\left(-\frac{1}{2\varepsilon^2}\right)\right) jh_\varepsilon , \quad jh_\varepsilon = \int v h_\varepsilon\,dv .$$

Proof of theorem (3.2) : Let $r_\varepsilon = \dfrac{h_\varepsilon}{\alpha_\varepsilon}$, where

$$\alpha_\varepsilon = Sign\,(1-\mu)\left(1-\exp\left(-\frac{|1-\mu|}{2\varepsilon^2}\right)\right),$$

with $|\alpha_\varepsilon| \leqslant 1$ and $\alpha_\varepsilon \to_{\varepsilon \to 0} Sign\,(1-\mu)$, then r_ε satisfies Vlasov equation with boundary conditions :

$$r_\varepsilon(0, v) = \frac{1}{\sqrt{2\pi\varepsilon^2}} \exp\left(-\frac{v^2}{2\varepsilon^2}\right), \quad v > 0,$$

$$r_\varepsilon(1, v) = 0, \quad v < 0,$$

thus, for ε small enough, the explicit expression of r_ε is ([14], [19]) :

$$r_\varepsilon(x, v) = \frac{1}{\sqrt{2\pi\varepsilon^2}} H\left(\frac{\frac{v^2}{2} - \varphi_\varepsilon}{\varepsilon^2}\right) h(v),$$

H is defined by (3.11) and h is the Heaviside step function, ($h(v) = 1$, $v > 0$; $h(v) = 0$, $v < 0$).

Then, r_ε converges to $(4\pi\varphi_0)^{-\frac{1}{2}} \delta\left(v - \sqrt{2\varphi_0}\right)$ in $\mathcal{M}_b((0, 1) \times \mathbb{R})$ weak* :

Indeed, let $\psi \in C_0^0([0, 1] \times \mathbb{R})$. We have

$$\iint_{[0,1]\times\mathbb{R}} r_\varepsilon(x, v)\, \psi(x, v)\, dx\, dv =$$

$$\iint_{[0,1]\times\left\{\frac{v^2}{2} - \varphi_\varepsilon > 0\right\}} \frac{1}{\sqrt{2\pi\varepsilon^2}} H\left(\frac{\frac{v^2}{2} - \varphi_\varepsilon}{\varepsilon^2}\right) h(v)\, \psi(x, v)\, dx\, dv .$$

By using the change of variable $t = \dfrac{\frac{v^2}{2} - \varphi_\varepsilon}{\varepsilon^2}$, we have :

$$\iint_{[0,1]\times\mathbb{R}} r_\varepsilon(x, v)\, \psi(x, v)\, dx\, dv =$$

$$\frac{1}{\sqrt{2\pi}} \int_0^1 \int_0^{+\infty} \psi\left(x, \sqrt{2(t\varepsilon^2 + \varphi_\varepsilon)}\right) \frac{\exp(-t)\, dx\, dt}{\sqrt{2(t\varepsilon^2 + \varphi_\varepsilon)}}. \quad (3.41)$$

When $\varepsilon \to 0$, the Lebesgue dominated convergence theorem implies that :

$$\int_{\mathbb{R}} r_\varepsilon(x, v)\, \psi(x, v)\, dx\, dv \to \frac{1}{\sqrt{2\pi}} \int_0^1 \psi\left(x, \sqrt{2\varphi_0(x)}\right) \frac{dx}{\sqrt{2\varphi_0(x)}}.$$

Moreover, we have

$$\int_{\mathbb{R}} v r_\varepsilon(x, v)\, dv = \frac{1}{\varepsilon^2 \sqrt{2\pi}} \int_{\left\{\frac{v^2}{2} - \varphi_\varepsilon > 0\right\}} v H\left(\frac{\frac{v^2}{2} - \varphi_\varepsilon(x)}{\varepsilon^2}\right) h(v)\, dv =$$

$$\frac{1}{\sqrt{2\pi}} \int_0^{+\infty} \exp(-t)\, dt = \frac{1}{\sqrt{2\pi}},$$

which ends the proof. •

Remark 3.1

— We notice that h_ε and j_ε are positive in the reverse bias case ($\mu < 1$ or $V_A < 0$) and that h_ε and j_ε are negative in the direct bias case ($\mu > 1$ or $V_A > 0$).

— The limiting function of the non-equilibrium part h_0 is the distribution function of a mono-kinetic beam starting from the junction with velocity 0. However, the beam evolves in an uncoupled way with the electric field generated by the equilibrium part. This explains why the convergence of the non-equilibrium part is easier to obtain than the usual Child-Langmuir asymptotics [14], [15].

3.5. Comparaison with physical formulas

In physical variables, the depletion length reads :

$$L_D = L l_D = \inf\left(L, \sqrt{\frac{2\varepsilon_s \Phi_L}{qN_D}}\right) = \inf\left(L, \sqrt{\frac{2\varepsilon_s(V_{bi} - V_A)}{qN_D}}\right).$$

A formula for the depletion length is given in [34] :

$$\tilde{L}_D = \sqrt{\frac{2\varepsilon_s(V_{bi} - V_A - U_T)}{qN_D}}.$$

The difference is explained by the fact that $U_T \ll V_{bi} - V_A$ in our asymptotics. Then the values of L_D and $\tilde{L}_D$ are asymptotically equal. The other physical quantities, like the density, electric field and potential are exactly the same as the ones given in [34]. In particular, the current density becomes :

$$J = Sign(V_A)\, J_s \left|\exp\left(\frac{V_A}{U_{th}}\right) - 1\right|, \quad J_s = \frac{q}{\sqrt{2\pi}} N_D V_{th} \exp\left(-\frac{V_{bi}}{U_{th}}\right).$$

We recover a classical formula ([34], Section 5.4). The expression of the saturation current J_s corresponds to the electron flow (in either reverse or forward directions) above the barrier at equilibrium.

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