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On the stationary quantum drift-diffusion model*

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Abstract. A bipolar Quantum Drift Diffusion Model including generation-recombination terms is considered. Existence of solutions is proven for a general setting including the case of vanishing particle densities at some parts of the boundary. The proof is based on a Schauder fixed point iteration combined with a minimization procedure. It is proven that, contrary to the classical drift-diffusion model, vacuum can only appear at the boundary. In the case of nonvanishing boundary data, the semiclassical limit is carried out rigorously. The variational structure of the model allows to prove strong H^1 convergence of particle densities, Fermi levels and electrostatic potential.

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1. Introduction

Due to the ongoing miniaturization of electronic devices, mathematical models of ultra small semiconductors have to be capable for the descripton of quantum mechanical effects. Recently, the Schrödinger-Poisson system has gained considerable attention to describe quantum phenomena (tunneling effects, negative differential resistance in resonant tunneling diodes). Whole space problems were proven to be well-posed and the semiclassical limit has been carried out leading to collisionless kinetic models [17, 19, 13]. An important ingredient of these investigations is the introduction of the Wigner function solving a kinetic-like collisionless equation (Wigner equation) [7, 8]. Concerning the derivation and analysis of quantum mod-

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els on bounded domains, an increasing effort has been made during the very last years. First, equilibrium states of the Schrödinger-Poisson systems were analyzed by minimization techniques [21, 22, 23]. Current carrying models and absorbing boundary conditions were recently investigated [24, 2, 1, 16, 5].

The incorporation of collisions in quantum models is one of the important issues of mesoscopic semiconductor modelling. It would imply a better understanding of quantum macroscopic models (hydrodynamic, drift-diffusion). However, macroscopic "Quantum Hydrodynamic Models (QHD)", based on moment expansions, are derived from the Wigner equation or the many particle Schrödinger equation [9, 11]. Being numerically rather tractable [10, 12] the capability of QHD to simulate ultra small semiconductor devices is a field of intensive mathematical research. Also the consistency problem is of importance: It has to be expected that the solutions of QHD converge to solutions of semiclassical models as the Planck constant $\hbar$ tends to zero.

Ancona and Iafrate proposed in [4, 3] a stationary "Quantum Drift Diffusion Model (QDD)" dedicated to describe the behaviour of electrons in the vicinity of strong inversion layers. We shall extend this model to bipolar devices including generation-recombination processes. We prove the existence of solutions for fixed Planck constant in the case of vanishing particle densities at the strong inversion layer. The proof is based on a minimization argument coupled with Schauder's fixed point theorem. The essential estimates concern lower bounds away from zero in the interior of the domain. In the case of nonvanishing particle density on the boundary the semiclassical limit is performed leading to the classical drift-diffusion model.

The scaled QDD stated on a bounded domain $\Omega \subset \mathbb{R}^d$, $d = 1, 2$ or $d = 3$ reads

$$\begin{gathered}
F = V + h_N(n) - \varepsilon^2 \frac{\Delta\sqrt{n}}{\sqrt{n}}, \quad G = -V + h_P(p) - \xi\varepsilon^2 \frac{\Delta\sqrt{p}}{\sqrt{p}} \\
\vec{J_n} = \mu_n \, n \nabla F, \quad \vec{J_p} = -\mu_p \, p \nabla G \\
\nabla \cdot \vec{J_n} = R_0(n,p) R_1(F,G), \quad \nabla \cdot \vec{J_p} = -R_0(n,p) R_1(F,G) \\
-\lambda^2 \Delta V = n - p - C
\end{gathered} \tag{1.1}$$

The physical parameters of (1.1) are the scaled Planck constant ε, the scaled ratio ξ of effective electron mass and effective hole mass, the mobilities μ_n, μ_p of electrons and holes and the scaled minimal Debye length λ. All these quantities are assumed to be positive constants. $h_N(.), h_P(.)$ are the enthalpy functions of electrons and holes. Generation-recombination processes are incorporated by the algebraic functions $R_0(.,.), R_1(.,.)$. The doping profile $C = C(x)$ (x being the spatial variable) represents a fixed background charge distribution of donator and acceptor impurities. In (1.1) the electron density $n(x) \geq 0$, the hole density $p(x) \geq 0$, the electric potential $V(x)$, the Quantum Quasi Fermi Levels $F(x), G(x)$ of electrons and holes, and the current densities $\vec{J_n}(x), \vec{J_p}(x)$ of electrons and holes are unknown.

The boundary $\partial\Omega$ splits into two parts. The contact region Γ_D where charge densities, electric potential and Quantum Quasi Fermi Levels are prescribed and the isolating region Γ_N where homogeneous Neumann boundary conditions are assumed. The contact region may contain inversion layers $\Gamma_\circ$ where the charge densities vanish. This fact was pointed out by Ancona [3] as being an important issue which can be dealt with in the framework of QDD whereas it is not possible to assume vanishing charge densities within classical drift-diffusion models.

The paper is organized as follows. In section 2 existence of solutions of (1.1) involving strong inversion layers is proven. In the case of nonvanishing boundary conditions for the charge densities, the analysis can be carried out further. We prove in section 3 that in the semiclassical limit $\varepsilon \to 0$, the solutions of the QDD converge strongly to solutions of the classical drift diffusion model. We end the paper with some concluding remarks in section 4.

2. Existence of solutions

2.1. Assumptions

We shall make use of the following assumptions.

A1) $\Omega \subset \mathbb{R}^d$, $d = 1, 2$ or $d = 3$ is a bounded domain. $\partial\Omega$ is $C^{0,1}$ and piecewise regular. $\partial\Omega$ splits into disjoint sets Γ_D, Γ_N such that Γ_D has nonvanishing $d-1$-dimensional Hausdorff measure. $\Gamma_D = \Gamma_+ \cup \Gamma_\circ$. $\tilde{\Gamma}$ is the union of $\overline{\Gamma_D} \cap \overline{\Gamma_N}$ and the non regular parts of $\partial\Omega$.

A2) The enthalpy functions h_N, h_P belong to $C((0,\infty) : \mathbb{R})$, are strictly monotone increasing with

$$\lim_{u\to\infty} h_N(u) = \lim_{u\to\infty} h_P(u) = \infty$$

and the map

$$u \mapsto \sqrt{u} h_{N,P}(u)$$

belongs to $C([0,\infty) : \mathbb{R})$.

A3) R_0 belongs to $C(\mathbb{R} \times \mathbb{R} : [0,\infty))$.

A4) R_1 belongs to $C(\mathbb{R}\times\mathbb{R} : \mathbb{R})$ is monotone increasing in each argument and has the following property: Given $m, M \in \mathbb{R}, m \le M$ there exist $\overline{F}, \underline{F}, \overline{G}, \underline{G} \in \mathbb{R}$ such that $\underline{F}, \underline{G} \le m \le M \le \overline{F}, \overline{G}$ and

$$R_1(\underline{F}, \overline{G}) = R_1(\overline{F}, \underline{G}) = 0.$$

A5) The doping profile C is in $L^\infty(\Omega)$.

In assumption A1) the boundary part $\Gamma_\circ$ (which may be void) represents strong inversion layers. Γ_N is the isolating part of the boundary. The monotonicity of the enthalpy functions h_N, h_P is satisfied in the isothermal case ($h_{N,P}(u) =$

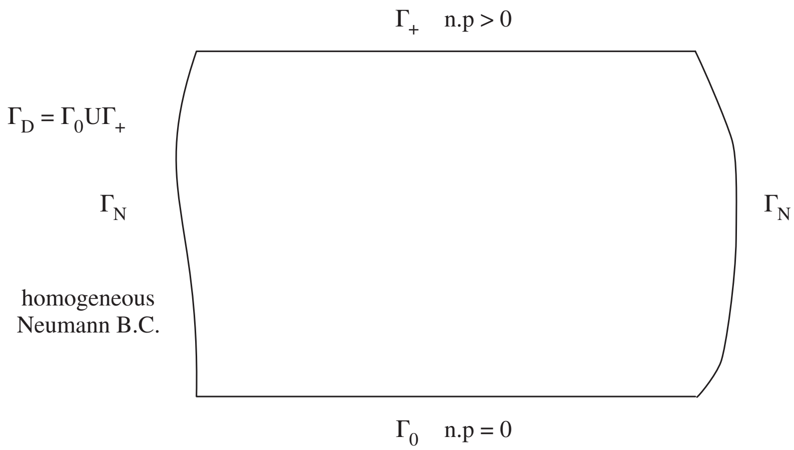

Figure 1.
The domain and the boundary conditions

$T_{n,p}u$ with $T_{n,p} > 0$) and leads to convexity properties used in the proofs. The assumptions on R_0, R_1 are trivially satisfied in case no generation-recombination processes ($R_0 = R_1 = 0$) are taken into account. In classical drift-diffusion models standard generation-recombination terms can be written as

$$R = R_0(n,p)R_1(F,G) = \frac{1}{a_0 + a_1|n| + a_2|p|}\left(\exp(F+G) - \delta^2\right)$$

with positive constants a_0, a_1, a_2, δ. We note that δ is chosen such that the generation-recombination rate vanishes in thermal equilibrium. We supply (1.1) with the following boundary conditions.

$$\begin{aligned}
&\Gamma_+ : n = n_+(x), \quad p = p_+(x), \quad V = V_{eq}(x) + V_{ext}(x), \\
&\qquad F = F_{eq} + V_{ext}(x), \quad G = G_{eq} - V_{ext}(x) \\
&\Gamma_\circ : n = 0, \quad p = 0, \quad V = V_{eq}(x) + V_{ext}(x) \\
&\Gamma_N : \nabla V \cdot \nu = \nabla F \cdot \nu = \nabla G \cdot \nu = 0.
\end{aligned} \tag{2.2}$$

We assume that n_+, p_+ are nonnegative functions of $L^\infty(\Omega) \cap H^1(\Omega)$ which are uniformly bounded away from zero. V_{eq} is the equilibrium potential and V_{ext} is the applied voltage. We assume that $V_{eq}, V_{ext} \in L^\infty(\Omega) \cap H^1(\Omega)$. The equilibrium values F_{eq}, G_{eq} of the Quantum Quasi Fermi Potentials are constant [25].

2.2. The result

The main result of this section is

2.1. *Under the assumptions of subsection 2.1 the system (1.1) with boundary conditions (2.2) possesses a solution $n, p, V, F, G \in L^\infty(\Omega) \cap H^1(\Omega)$. Furthermore, $n, p, V, F, G \in C_B(\Omega)$, $n(x), p(x) > 0$ for all $x \in \Omega$ and n, p satisfy homogeneous Neumann boundary conditions on Γ_N.*

The proof of this theorem is carried out in several steps.

Step 1: We introduce new variables which make the analysis more tractable. Given $f \in L^2(\Omega)$ we define $\Phi[f] = \Phi$ to be the (unique) H^1-solution of

$$-\lambda^2 \Delta\Phi = f, \quad \Phi = 0 \text{ on } \Gamma_D, \nabla\Phi \cdot \nu = 0 \text{ on } \Gamma_N.$$

Standard results guarantee that $\Phi[.]$ is a weakly sequentially $L^2(\Omega)$-$H^1(\Omega)$ continuous mapping. Furthermore, $\Phi[.]$ maps $L^2(\Omega)$ continuously into $L^\infty(\Omega)$. Let Φ_e be the (unique) H^1-solution of

$$-\Delta\Phi_e = 0, \quad \Phi_e = V_{eq} + V_{ext} \text{ on } \Gamma_D, \quad \nabla\Phi_e \cdot \nu = 0 \text{ on } \Gamma_N.$$

Note that Φ_e is in $L^\infty(\Omega)$. With these notations the electrostatic potential can be written as $V = \Phi[n - p - C] + \Phi_e$.

Next, we introduce $\rho = \sqrt{n}$ and $\sigma = \sqrt{p}$ as new variables. For given Quantum Quasi Fermi Potentials F, G the system (1.1),(2.2) is formally equivalent to the Euler-Lagrange equations of the functional

$$\begin{aligned} \mathcal{E}^\varepsilon(\rho, \sigma) = \varepsilon^2 \int |\nabla\rho|^2 + \xi\varepsilon^2 \int |\nabla\sigma|^2 \\ + \int H_N(\rho^2) + \int H_P(\sigma^2) + \frac{1}{2}\int |\nabla\Phi[\rho^2 - \sigma^2 - C]|^2 \\ + \int (\rho^2 - \sigma^2)\Phi_e - \int (F\rho^2 + G\sigma^2) \end{aligned} \tag{2.3}$$

where

$$H_{N,P}(s) = \int_1^s h_{N,P}(u)\, du. \tag{2.4}$$

Once ρ, σ are computed as minimizers of $\mathcal{E}^\varepsilon$ the Fermi levels F, G have to be recomputed from the current relations (second and third equation of (1.1). Hence one may wish to apply a Schauder fixed point argument to prove the existence of solutions. However, this idea meets several difficulties essentially due to the existence of *vacuum* on parts of the boundary. Vacuum in general leads to a *lack of differentiability* of the functional $\mathcal{E}^\varepsilon$ and to *degeneration* of the current relations.

Step 2: To cope with the problems mentioned above, a modified functional $\mathcal{E}_\delta$ and modified current relations are introduced.

$$\begin{aligned}\mathcal{E}_\delta(\rho,\sigma) = \varepsilon^2 \int |\nabla\rho|^2 + \xi\varepsilon^2 \int |\nabla\sigma|^2 \\ + \int H_N^\delta(\rho^2) + \int H_P^\delta(\sigma^2) + \frac{1}{2}\int |\nabla\Phi[\rho^2-\sigma^2-C]|^2 \\ + \int (\rho^2-\sigma^2)\Phi_e - \int (F\rho^2 + G\sigma^2)\end{aligned} \tag{2.5}$$

where $\delta \in (0,\infty)$ and

$$H_{N,P}^\delta(t) = \int_1^t h_{N,P}^\delta(s)\, ds. \tag{2.6}$$

with $h_{N,P}^\delta = \max\{h_{N,P}, h_{N,P}(\delta)\}$. The current relations are replaced by

$$\nabla\cdot(\mu_n[\rho^2]_\delta \nabla F) = R_0(\rho^2,\sigma^2)R_1(F,G), \tag{2.7}$$

$$\nabla\cdot(\mu_p[\sigma^2]_\delta \nabla G) = R_0(\rho^2,\sigma^2)R_1(F,G). \tag{2.8}$$

where

$$[\rho^2]_\delta = \max\{\rho^2,\delta\} \quad , \quad [\sigma^2]_\delta = \max\{\sigma^2,\delta\}.$$

For each $\delta > 0$ we define an operator T_δ on

$$\mathcal{C} = \{(F,G) \in L^2(\Omega)\times L^2(\Omega) : \underline{F} \le F \le \overline{F}, \underline{G} \le G \le \overline{G}\} \tag{2.9}$$

where $\underline{F}, \underline{G}, \overline{F}, \overline{G} \in \mathbb{R}$ are chosen such that assumption A4) of subsection 2.1 is satisfied with

$$m = \min\{F_{eq}, G_{eq}\} - \|V_{ext}\|_\infty - 1, \tag{2.10}$$

$$M = \max\{F_{eq}, G_{eq}\} + \|V_{ext}\|_\infty + 1. \tag{2.11}$$

Given $(F,G) \in \mathcal{C}$ we shall prove the existence and uniqueness of a non negative minmizer (ρ,σ) of the functional $\mathcal{E}_\delta$ in the set $(\rho_\circ,\sigma_\circ) + H_0^1(\Omega\cup\Gamma_N)$, where $\rho_\circ,\sigma_\circ \in L^\infty(\Omega)\cap H^1(\Omega)$ satisfy

$$\begin{aligned}&\text{on } \Gamma_+: \ \rho_\circ = \sqrt{n_+(x)}, \quad \sigma_\circ = \sqrt{p_+(x)}, \\ &\text{on } \Gamma_\circ: \ \rho_\circ = 0, \quad \sigma_\circ = 0.\end{aligned} \tag{2.12}$$

Then $T_\delta(F,G) = (F^*,G^*)$ is computed as a solution of

$$\nabla\cdot(\mu_n[\rho^2]_\delta \nabla F^*) = R_0(\rho^2,\sigma^2)R_1(F^*,G), \tag{2.13}$$

$$\nabla\cdot(\mu_p[\sigma^2]_\delta \nabla G^*) = R_0(\rho^2,\sigma^2)R_1(F,G^*) \tag{2.14}$$

such that the set $\mathcal{C}$ is invariant under T_δ. The existence of a fixed point (F_δ, G_δ) of T_δ follows with the aid of standard estimates from Schauder's fixed point theorem.

Step 3: We derive δ-independent estimates on $\rho_\delta, \sigma_\delta, F_\delta, G_\delta$. The most important estimates are *lower bounds* away from zero for $\rho_\delta, \sigma_\delta$ on compact subsets of $\overline{\Omega}$ not intersecting $\Gamma_\circ \cup \tilde{\Gamma}$. These estimates allow to pass to the limit $\delta \to 0$ and to finish the proof of the theorem 2.1.

2.3. Existence of Fixed Points of T_δ

In this subsection we prove that for all $\delta > 0$ and all given $F, G \in L^\infty(\Omega)$ the functional $\mathcal{E}_\delta$ possesses a unique non negative minimizer (ρ, σ) in $(\rho_\circ, \sigma_\circ) + H_0^1(\Omega \cup \Gamma_N)$.

Theorem 2.2. *Under the assumptions of subsection 2.1 and for given $F, G \in L^\infty(\Omega)$, $\delta \in (0,1]$, the functional $\mathcal{E}_\delta$ possesses a unique non negative minimizer $(\rho_\delta, \sigma_\delta)$ in $(\rho_\circ, \sigma_\circ) + H_0^1(\Omega \cup \Gamma_N)$. Additionally, $(\rho_\delta, \sigma_\delta)$ has the following properties:*

a) $\rho_\delta, \sigma_\delta$ belong to $C_B(\Omega)$.

b) There exists $D = D(\|F\|_\infty, \|G\|_\infty) > 0$ independent of δ such that

$$\|\rho_\delta\|_\infty, \|\rho_\delta\|_{H^1}, \|\sigma_\delta\|_\infty, \|\sigma_\delta\|_{H^1} \leq D.$$

c) $\rho_\delta, \sigma_\delta$ are solutions of the Euler-Lagrange equations associated with $\mathcal{E}_\delta$:

$$\begin{aligned} \varepsilon^2 \Delta \rho_\delta &= \rho_\delta \left(V_\delta + h_N^\delta(\rho_\delta^2) - F \right) \\ \xi \varepsilon^2 \Delta \sigma_\delta &= \sigma_\delta \left(-V_\delta + h_P^\delta(\sigma_\delta^2) - G \right) \\ -\lambda^2 \Delta V_\delta &= \rho_\delta^2 - \sigma_\delta^2 - C \end{aligned} \tag{2.15}$$

Furthermore, $(F, G) \mapsto (\rho_\delta, \sigma_\delta)$ is a continuous map from $\mathcal{C}$, endowed with the $L^2(\Omega) \times L^2(\Omega)$-norm, into $H^1(\Omega) \times H^1(\Omega)$.

Proof of theorem 2.2. Set $\mathcal{M} = (\rho_\circ, \sigma_\circ) + H_0^1(\Omega \cup \Gamma_N)$. Due to $\lim_{u\to\infty} h_{N,P}^\delta(u) = \infty$ the functional $\mathcal{E}_\delta$ is bounded from below and coercive with respect to the $L^2(\Omega) \times L^2(\Omega)$ norm. Hence $\inf_{\mathcal{M}} \mathcal{E}_\delta$ exists and minimizing sequences of $\mathcal{E}_\delta$ in $\mathcal{M}$ are bounded in $L^2(\Omega) \times L^2(\Omega)$. Actually, with respect to this observation and due to the leading terms of $\mathcal{E}_\delta$ each minimizing sequence of $\mathcal{E}_\delta$ is bounded in $H^1(\Omega) \times H^1(\Omega)$ and therefore possesses subsequences weakly convergent in $H^1(\Omega) \times H^1(\Omega)$. Now the existence of minimizers of $\mathcal{E}_\delta$ follows from the $H^1(\Omega)$-weakly sequentially lower semicontinuity of $\mathcal{E}_\delta$ (which is easy to see) and the fact that $\mathcal{M}$ is $H^1(\Omega) \times H^1(\Omega)$- weakly sequentially closed. The existence of a non negative minimizer is due to the fact that, when $(\rho, \sigma) \in \mathcal{M}$ then $(|\rho|, |\sigma|) \in \mathcal{M}$ and

$$\mathcal{E}_\delta(|\rho|, |\sigma|) = \mathcal{E}_\delta(\rho, \sigma).$$

The uniqueness of the non negative minimizer follows from the pseudo convexity inequality (see [23]):

$$\mathcal{E}_\delta \left(\sqrt{\frac{1}{2}\rho_1^2 + \frac{1}{2}\rho_2^2}, \sqrt{\frac{1}{2}\sigma_1^2 + \frac{1}{2}\sigma_2^2} \right) < \frac{1}{2}\mathcal{E}_\delta(\rho_1, \sigma_1) + \frac{1}{2}\mathcal{E}_\delta(\rho_2, \sigma_2)$$

when $(|\rho_1|, |\sigma_1|) \not\equiv (|\rho_2|, |\sigma_2|)$.

Furthermore, it is readily seen that for varying $\delta \in (0,1]$, the infima of $\mathcal{E}_\delta$ in $\mathcal{M}$ range in a $\|F\|_\infty, \|G\|_\infty$-dependent compact subset of $\mathbb{R}$. This gives in connection with the previous investigations

$$\|\rho_\delta\|_{H^1(\Omega)}, \|\sigma_\delta\|_{H^1(\Omega)} \leq D'$$

where $D' = D'(\|F\|_\infty, \|G\|_\infty) > 0$ is independent of $\delta \in (0,1]$. Now assertions a),b),c) follow in analogy to the proof of Theorem 1 in [25]. The continuous dependence of $(\rho_\delta, \sigma_\delta)$ on (F,G) with respect to the specified norms is readily seen due to the pseudo convexity of $\mathcal{E}_\delta$. □

Given $(F,G) \in \mathcal{C}$, Theorem 2.2 defines $(\rho_\delta, \sigma_\delta)$ uniquely. To compute $T_\delta(F,G) = (F^*, G^*)$ we have to solve (2,13), (2.14) in $\mathcal{C}$.

Lemma 2.3. *Under the assumptions of subsection 2.1 and for given* $(F,G) \in \mathcal{C}$, $\delta \in (0,1]$, *let* $(\rho_\delta, \sigma_\delta)$ *be as in Theorem 2.2. Then the system*

$$\nabla \cdot (\mu_n[\rho_\delta^2]_\delta \nabla F^*) = R_0(\rho_\delta^2, \sigma_\delta^2) R_1(F^*, G), \tag{2.16}$$

$$\nabla \cdot (\mu_p[\sigma_\delta^2]_\delta \nabla G^*) = R_0(\rho_\delta^2, \sigma_\delta^2) R_1(F, G^*) \tag{2.17}$$

subject to the boundary conditions

$$F^* - F_{eq} - V_{ext}, G^* - G_{eq} + V_{ext} \in H_0^1(\Omega \cup \Gamma_N \cup \Gamma_\circ) \tag{2.18}$$

possesses a unique solution $(F^*, G^*) \in \mathcal{C}$ *(cf (2.9)). Furthermore, given any* $D > 0$ *the map* $(\rho_\delta, \sigma_\delta) \mapsto (F^*, G^*)$ *is continuous from*

$$\mathcal{D} = \{(\rho_\delta, \sigma_\delta) \in L^2(\Omega) \times L^2(\Omega) : \|\rho_\delta\|_\infty, \|\sigma_\delta\|_\infty \leq D\},$$

into $\mathcal{C}$, *provided both* $\mathcal{C}, D$ *are endowed with the* $L^2(\Omega) \times L^2(\Omega)$ *norm.*

Proof of Lemma 2.3. The proof is carried out by means of Schauder's fixed point theorem. (A similiar argumentation in case $R_1(F,G) = \exp(F+G) - a^2$ can be found in [18].) Given $(f,g) \in \mathcal{C}$ consider the following system of equations for f^*, g^*

$$\nabla \cdot (\mu_n[\rho_\delta^2]_\delta \nabla f^*) = R_0(\rho_\delta^2, \sigma_\delta^2) R_1(f, G), \tag{2.19}$$

$$\nabla \cdot (\mu_p[\sigma_\delta^2]_\delta \nabla g^*) = R_0(\rho_\delta^2, \sigma_\delta^2) R_1(F, g) \tag{2.20}$$

subject to the boundary conditions

$$f^* - F_{eq} - V_{ext}, g^* - G_{eq} + V_{ext} \in H_0^1(\Omega \cup \Gamma_-). \tag{2.21}$$

The right hand sides of (2.19), (2.20) belong to $L^\infty(\Omega)$. Due to the definition of $[.]_\delta$ and $\rho, \sigma \in L^\infty(\Omega)$, equations (2.19), (2.20) are uniformly elliptic. The standard theory for elliptic PDE's of order two (see e.g. [14]) provides existence and uniqueness of a solution $f^*, g^* \in C_B(\Omega) \cap H^1(\Omega)$. It is easy to see that the map $(f,g) \mapsto (f^*, g^*)$ from $\mathcal{C}$ to $H^1(\Omega) \times H^1(\Omega)$ is compact and continuous if $\mathcal{C}$ is endowed with the $L^2(\Omega) \times L^2(\Omega)$ norm. Defining

$$S(f,g) \equiv ([f^*]_{\underline{F}}^{\overline{F}}, [g^*]_{\underline{G}}^{\overline{G}})$$

where for given $k, K \in \mathbb{R}, k \leq K$

$$[.]_k^K \;:\; H^1(\Omega) \to H^1(\Omega)$$
$$\phi \mapsto [\phi]_k^K \equiv \begin{cases} K & \text{if } K \leq \phi \\ \phi & \text{if } k < \phi < K \\ k & \text{if } \phi \leq k \end{cases}$$

it is readily seen that S is a compact, continuous operator from $\mathcal{C}$ into $\mathcal{C}$. $\mathcal{C}$ being a closed, convex subset of $L^2(\Omega) \times L^2(\Omega)$, the existence of a fixed point of S follows from Schauder's fixed point theorem. Let $(F^*, G^*) = ([f^*]_{\underline{F}}^{\overline{F}}, [g^*]_{\underline{G}}^{\overline{G}} \in \mathcal{C}$ be a fixed point of S. To establish (2.19), (2.20) it remains to show that $\underline{F} \leq f^* \leq \overline{F}, \underline{G} \leq g^* \leq \overline{G}$. Since $f^* \in C(\Omega)$ the set $\{f^* - \underline{F} < 0\}$ is open and due to the definition of $\underline{F}$ (see (2.10)), each component Ω^- of $\{f^* - \underline{F} < 0\}$ does not intersect Γ^+. Hence, one gets on Ω^-

$$\nabla \cdot (\mu_n [\rho_\delta^2]_\delta \nabla [f^* - \underline{F}]) = R_0(\rho_\delta^2, \sigma_\delta^2) R_1(F^*, G), \tag{2.22}$$

subject to the boundary conditions

$$f^* - \underline{F} \in H_0^1(\Omega^- \cup (\partial\Omega^- \cap \Gamma_-)). \tag{2.23}$$

Making use of the assumed properties of R_0, R_1 (see A4)) it follows for all $x \in \Omega^-$

$$R_0(\rho_\delta^2, \sigma_\delta^2) R_1(F^*, G) = R_0(\rho_\delta^2, \sigma_\delta^2) R_1(\underline{F}, G) \leq R_0(\rho_\delta^2, \sigma_\delta^2) R_1(\underline{F}, \overline{G}) = 0,$$

which leads to $f^* - \underline{F} \geq 0$ on Ω^- by the maximum principle. This contradiction shows that $\Omega^- = \emptyset$ i.e. $f^* \geq \underline{F}$. The remaining inequalities $f^* \leq \overline{F}$, $\underline{G} \leq g^* \leq \overline{G}$ follow in analogy. This shows that (2.16), (2.17), (2.18) has at least one solution. Uniqueness of the solution follows from the assumed monotonicity of R_1, the non negativity of R_0, the continuity of each solution of (2.16), (2.17), (2.18) belonging to $\mathcal{C}$ and from the maximum principle.

Finally, the continuity of the map $(\rho_\delta, \sigma_\delta) \mapsto (F^*, G^*)$ follows from the uniform boundedness of $\rho_\delta, \sigma_\delta$ in $L^\infty(\Omega)$, the uniform ellipticity of the involved differential operators and the continuity of R_0, R_1. □

Fixed point of T_δ. We first recall $T_\delta(F,G) = (F^*, G^*) \in \mathcal{C} \cap (H^1(\Omega) \times H^1(\Omega))$ where (F^*, G^*) is defined as in Lemma 2.3. Due to Theorem 2.2 and Lemma 2.3, the map $T_\delta : \mathcal{C} \to \mathcal{C}$ is continuous and compact provided $\mathcal{C}$ is equipped with the $L^2(\Omega)$ norm. As $\mathcal{C}$ is a closed, convex subset of $L^2(\Omega) \times L^2(\Omega)$, the existence of a fixed point of T_δ follows from Schauder's fixed point theorem. □

2.4. δ-independent estimates

Throughout this subsection we assume that the assumptions of subsection 2.1 hold. Furthermore, let $\rho_\delta, \sigma_\delta, F_\delta, G_\delta, V_\delta$ be solutions of

$$\begin{aligned} \varepsilon^2 \Delta\rho_\delta &= \rho_\delta \left(V_\delta + h_N^\delta(\rho_\delta^2) - F_\delta\right) \\ \xi\varepsilon^2 \Delta\sigma_\delta &= \sigma_\delta \left(-V_\delta + h_P^\delta(\sigma_\delta^2) - G_\delta\right) \\ -\lambda^2 \Delta V_\delta &= \rho_\delta^2 - \sigma_\delta^2 - C \\ \nabla\cdot(\mu_n[\rho_\delta^2]_\delta \nabla F_\delta) &= R_0(\rho_\delta^2, \sigma_\delta^2) R_1(F_\delta, G_\delta), \\ \nabla\cdot(\mu_p[\sigma_\delta^2]_\delta \nabla G_\delta) &= R_0(\rho_\delta^2, \sigma_\delta^2) R_1(F_\delta, G_\delta) \end{aligned} \tag{2.24}$$

subject to the boundary conditions

$$\begin{aligned} \Gamma_+ \ &: \rho_\delta = \sqrt{n_+(x)}, \quad \sigma_\delta = \sqrt{p_+(x)}, \quad V = V_{eq}(x) + V_{ext}(x), \\ &\quad F_\delta = F_{eq} + V_{ext}(x), \quad G_\delta = G_{eq} - V_{ext}(x) \\ \Gamma_\circ \ &: \rho_\delta = 0, \quad \sigma_\delta = 0, \quad V_\delta = V_{eq}(x) + V_{ext}(x) \\ \Gamma_N \ &: \nabla V_\delta\cdot\nu = \nabla F_\delta\cdot\nu = \nabla G_\delta\cdot\nu = 0 \end{aligned} \tag{2.25}$$

where (F_δ, G_δ) is a fixed point of T_δ in $\mathcal{C}$ and $\delta \in (0,1]$. Due to Theorem 2.2 and Lemma 2.3 the following δ-independent estimates are available:

$$\|\rho_\delta\|_\infty, \|\rho_\delta\|_{H^1}, \|\sigma_\delta\|_\infty, \|\sigma_\delta\|_{H^1} \le D, \tag{2.26}$$

$$\underline{F} \le F_\delta \le \overline{F} \quad , \quad \underline{G} \le G_\delta \le \overline{G}, \tag{2.27}$$

where here and in the sequel D are various positive constants independent of δ. Due to the $L^\infty(\Omega)$-estimates of (2.26) it follows from Poisson's equation of (2.24) and the boundary conditions (2.25) that

$$\|V_\delta\|_\infty, \|V_\delta\|_{H^1} \le D. \tag{2.28}$$

By a slight abuse of notation let (δ) be a sequence of positive real numbers in $(0,1]$ tending to zero such that

$$\rho_\delta \to \rho_\circ, \quad \sigma_\delta \to \sigma_\circ, \quad V_\delta \to V_\circ$$

strongly in all $L^r(\Omega)$-spaces with $r \in [1,\infty)$, weakly in $H^1(\Omega)$, weak* in $L^\infty(\Omega)$ and a.e. in Ω.

Furthermore it can be assumed without loss of generality that $F_\delta \to F_\circ, G_\delta \to G_\circ$ weak* in $L^\infty(\Omega)$ with

$$\underline{F} \le F_\circ \le \overline{F} \quad , \quad \underline{G} \le G_\circ \le \overline{G}$$

as $\delta \to 0$. These types of convergence are by far sufficient to pass to the limit $\delta \to 0$ in the first three equations of (2.24):

$$\begin{aligned} \varepsilon^2 \Delta\rho_\circ &= \rho_\circ \left(V_\circ + h_N(\rho_\circ^2) - F_\circ \right) \\ \xi\varepsilon^2 \Delta\sigma_\circ &= \sigma_\circ \left(-V_\circ + h_P(\sigma_\circ^2) - G_\circ \right) \\ -\lambda^2 \Delta V_\circ &= \rho_\circ^2 - \sigma_\circ^2 - C \end{aligned} \tag{2.29}$$

subject to the boundary conditions

$$\begin{aligned} &\Gamma_+ \ : \rho_\circ = \sqrt{n_+(x)}, \quad \sigma_\circ = \sqrt{p_+(x)}, \quad V_\circ = V_{eq}(x) + V_{ext}(x), \\ &\Gamma_\circ \ : \rho_\circ = 0, \quad \sigma_\circ = 0, \quad V_\circ = V_{eq}(x) + V_{ext}(x) \\ &\Gamma_N \ : \nabla V_\circ \cdot \nu = 0. \end{aligned} \tag{2.30}$$

The main difficulty when passing to the limit $\delta \to 0$ in the current relations as well as in the boundary conditions for F_δ, G_δ is the *lack of uniform ellipticity* due to the assumed vanishing particle density on $\Gamma_\circ$.

To cope with this difficulty, we first claim that $\rho_\circ(x), \sigma_\circ(x) > 0$ for all $x \in \Omega$. Indeed, two cases are possible

- If $\lim_{u\to 0} h_N(u) \in \mathbb{R}$, *i.e.* if h_N is bounded from below then the right hand side of the first equation of (2.29) is of the form "$\rho_\circ \times L^\infty(\Omega)$-function" such that Harnack's inequality (see e.g. [14]) applies: As $\rho_\circ \ge 0$ either $\rho_\circ \equiv 0$ or $\rho_\circ(x) > 0$ for all $x \in \Omega$ must hold. As $\rho_\circ > 0$ on Γ^+, we have $\rho_\circ > 0$ in Ω.
- If $\lim_{u\to 0} h_N(u) = -\infty$ consider the set $\Omega_0 = \{x \in \Omega : \rho_\circ(x) = 0\}$. By continuity of $\rho_\circ$, this set is closed in the relative topology of Ω. On the other hand, if Ω_0 is nonvoid, choose an $x_\circ \in \Omega_0$. Then by continuity $\rho_\circ(V_\circ + h_N(\rho_\circ^2) - F_\circ) \le 0$ in an open ball B^* containing $x_\circ$ contained in Ω. Hence $\Delta\rho_\circ \le 0$ in the open set B^*. As $\rho_\circ$ assumes its non negative infimum 0 in B^* it follows that $\rho_\circ = 0$ in B^* which proves that Ω_0 is relatively open in Ω. As Ω is connected, $\Omega_0 = \Omega$ or $\Omega_0 = \emptyset$ must hold. Since $\rho_\circ > 0$ on Γ^+ it follows that $\Omega_0 = \emptyset$, i.e. $\rho_\circ > 0$ in Ω. It follows in analogy that $\sigma_\circ > 0$ in Ω.

Now let K be the closure of a smooth subdomain K° of Ω not intersecting $\tilde{\Gamma} \cup \Gamma_\circ$ (we recall that $\tilde{\Gamma}$ is the set of singular points of $\partial\Omega$). One readily verifies with the aid of the piecewise smoothness of $\partial\Omega, \partial K$ and Hopf's principle that $\inf_K \rho_\circ > 0$.

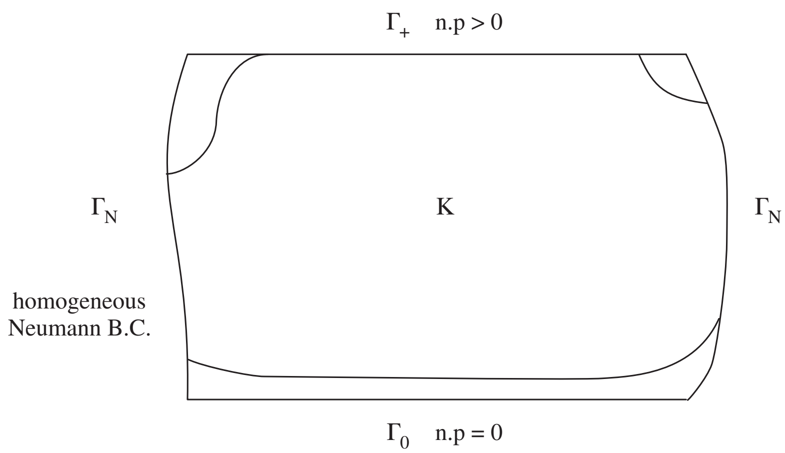

Figure 2.
The set K

Furthermore, ρ_δ can be written as $\rho_B + \tilde{\rho}_\delta$ where ρ_B is the unique (not depending on δ) harmonic extension of the boundary data and $\tilde{\rho}_\delta$ satisfies homogeneous boundary conditions on $\partial\Omega$. Analogously, we have

$$\rho_\circ = \rho_B + \tilde{\rho}_\circ.$$

It follows from a straightforward extension of Lemma A.2 of [6] that

$$||\nabla\tilde{\rho}_\delta||^2_{L^\infty(K)} \leq C(K)\left(||\Delta\tilde{\rho}_\delta||_{L^\infty(\Omega)}||\tilde{\rho}_\delta||_{L^\infty(\Omega)}\right).$$

Since the right hand side of this inequality is bounded independently of δ, then we have

$$\tilde{\rho}_\delta \to \tilde{\rho}_\circ \quad \text{strongly in } C(K)$$

Since $\rho_B \in L^\infty(\Omega)$, the sequence ρ_δ converges strongly in $L^\infty(K)$ towards $\rho_\circ$. As $\inf_K \rho_\circ > 0$ one gets for ρ_δ a uniform lower bound away from zero for all sufficiently small δ. It follows from the fourth and fifth equation of (2.24) that the $H^1(K^\circ)$-norm of F_δ is bounded for all $\delta \in (0,1]$. Hence

$$F_\delta \to F_\circ \quad \text{weakly in } H^1(K^\circ)$$

which implies

$$F_\delta \to F_\circ \quad \text{weakly in } H^1_{loc}(\Omega \cup \Gamma_+ \cup \Gamma_N).$$

Similarly, we can prove

$$G_\delta \to G_\circ \quad \text{weakly in } H^1_{loc}(\Omega \cup \Gamma_+ \cup \Gamma_N).$$

It follows from this result that F_δ and G_δ converge strongly in $L^2_{loc}(\Omega)$ which implies the almost everywhere convergence. The uniform L^∞ bounds on F_δ and G_δ imply that the convergence actually holds in $L^r(\Omega)$ for every $r < \infty$. Hence we can pass to the limit in the current relations (last two equations of (2.24)) and in the boundary conditions on $\Gamma_+ \cap \Gamma_N$ (2.25). Therefore $F_\circ$ and $G_\circ$ satisfy

$$\begin{aligned} \nabla \cdot (\mu_n \rho_\circ^2 \nabla F_\circ) &= R_0(\rho_\circ^2, \sigma_\circ^2) R_1(F_\circ, G_\circ), \\ \nabla \cdot (\mu_p \sigma_\circ^2 \nabla G_\circ) &= R_0(\rho_\circ^2, \sigma_\circ^2) R_1(F_\circ, G_\circ) \end{aligned} \tag{2.31}$$

subject to the boundary conditions

$$\begin{aligned} \Gamma_+ &: F_\circ = F_{eq} + V_{ext}(x), \quad G_\circ = G_{eq} - V_{ext}(x) \\ \Gamma_N &: \nabla F_\circ \cdot \nu = \nabla G_\circ \cdot \nu = 0 \end{aligned} \tag{2.32}$$

This finishes the proof of Theorem 2.1. □

3. The semiclassical limit $\varepsilon \to 0$

This section is concerned with the question whether solutions of the QDD converge to solutions of classical drift-diffusion models as $\varepsilon \to 0$. This question arises whenever the semiconductor device under consideration is subject to constraints close to classical settings.

3.1. Boundary conditions

Throughout section 3 it is assumed that assumptions A1)-A5) of subsection 2.1 hold.

In classical drift-diffusion models the boundary data for electrons and holes are usually assumed to be respective thermal equilibrium values. This motivates the replacement of (2.2) by

$$\begin{aligned} &\Gamma_+ : \; n = n^\varepsilon_{eq}(x), \quad p = p^\varepsilon_{eq}(x), \quad V = V^\varepsilon_{eq}(x) + V_{ext}(x), \\ &\qquad F = F^\varepsilon_{eq} + V_{ext}(x), \quad G = G^\varepsilon_{eq} - V_{ext}(x), \\ &\Gamma_\circ = \emptyset, \\ &\Gamma_N : \; \nabla V \cdot \nu = \nabla F \cdot \nu = \nabla G \cdot \nu = 0, \end{aligned} \tag{3.33}$$

where for fixed $\varepsilon > 0$ the equilibrium functions $n^\varepsilon_{eq}, p^\varepsilon_{eq}, V^\varepsilon_{eq}$ are in $C_B(\Omega) \cap H^1(\Omega)$, see [25]. Let us also recall that

$$V^\varepsilon_{eq}(x) + h_N(n^\varepsilon_{eq}(x)) - F^\varepsilon_{eq} = -V^\varepsilon_{eq}(x) + h_P(p^\varepsilon_{eq}(x)) - G^\varepsilon_{eq} = 0. \tag{3.34}$$

Furthermore standard drift-diffusion models employ additional assumptions on the enthalpy functions $h_{N,P}$. For low densities the particle pressure $P_{n,p} = \int h'_{n,p}(u)u \; du$ is assumed to be a linear function of the charge density which amounts to

$$h_{N,P}(u) = T_{n,p} \log u \quad \text{for "small" positive } u.$$

As $u \to \infty$ however asymptotic expansions of exchange-correlation terms based on Fermi Dirac statistics give [15]

$$h_{N,P}(u) = O(u^{2/3}) \quad \text{as } u \to \infty.$$

We shall therefore make use of the following additional assumptions on $h_{N,P}$:

A6) $h_{N,P}$ are locally Lipschitz continuous and

$$\lim_{u\to 0} h_{N,P}(u) = -\infty \quad , \quad \lim\inf_{u\to\infty} h_{N,P}(u)u^{-1/2-\delta} = \infty$$

for some positive δ.

Let us notice that the enthalpy functions described above satisfy the hypothesis A6). We shall assume

A7) $V_{eq}+h_N(n_{eq})-F_{eq} = -V_{eq}+h_P(p_{eq})-G_{eq} = 0, n^\varepsilon_{eq} \to n_{eq}, p^\varepsilon_{eq} \to p_{eq}, V^\varepsilon_{eq} \to V_{eq}$ strongly in $H^1(\Omega)$ and weak* in $L^\infty(\Omega)$ as $\varepsilon \to 0$ and there exists a $K > 0$ such that $K \le n^\varepsilon_{eq}, p^\varepsilon_{eq}$ for all $\varepsilon > 0$. Furthermore, $F^\varepsilon_{eq} \to F_{eq}, G^\varepsilon_{eq} \to G_{eq}$ as $\varepsilon \to 0$.

We note that all assumptions of A7) have been proven in [25].

The generation-recombination rate $R_0(.,.)R_1(.,.)$ vanishes in thermal equilibrium. Therefore it depends in general on ε. We shall assume

A8) $\lim_{\varepsilon\to 0} R^\varepsilon_0 = R_0, \lim_{\varepsilon\to 0} R^\varepsilon_1 = R_1$ locally in $C(\mathbb{R}^2)$.

In the sequel we shall employ the following notations:
For given $\varepsilon > 0$ let $\rho^\varepsilon, \sigma^\varepsilon, V^\varepsilon, F^\varepsilon, G^\varepsilon \in C_B(\Omega) \cap H^1(\Omega)$ be as in Theorem 2.1 a solution of

$$\begin{aligned}
\varepsilon^2 \Delta\rho^\varepsilon &= \rho^\varepsilon \left(V^\varepsilon + h_N\left((\rho^\varepsilon)^2\right) - F^\varepsilon\right) \\
\xi\varepsilon^2 \Delta\sigma^\varepsilon &= \sigma^\varepsilon \left(-V^\varepsilon + h_P\left((\sigma^\varepsilon)^2\right) - G^\varepsilon\right) \\
-\lambda^2 \Delta V^\varepsilon &= (\rho^\varepsilon)^2 - (\sigma^\varepsilon)^2 - C \\
\nabla\cdot\left(\mu_n (\rho^\varepsilon)^2 \nabla F^\varepsilon\right) &= R^\varepsilon_0\left((\rho^\varepsilon)^2, (\sigma^\varepsilon)^2\right) R^\varepsilon_1(F^\varepsilon, G^\varepsilon), \\
\nabla\cdot\left(\mu_p (\sigma^\varepsilon)^2 \nabla G^\varepsilon\right) &= R^\varepsilon_0\left((\rho^\varepsilon)^2, (\sigma^\varepsilon)^2\right) R^\varepsilon_1(F^\varepsilon, G^\varepsilon)
\end{aligned} \tag{3.35}$$

subject to the boundary conditions

$$\begin{aligned}\Gamma_+ :\ & \rho^\varepsilon = \sqrt{n^\varepsilon_{eq}(x)}, \quad \sigma^\varepsilon = \sqrt{p^\varepsilon_{eq}(x)}, \quad V^\varepsilon = V^\varepsilon_{eq}(x) + V_{ext}(x), \\ & F^\varepsilon = F^\varepsilon_{eq} + V_{ext}(x), \quad G^\varepsilon = G^\varepsilon_{eq} - V_{ext}(x), \\ \Gamma_N :\ & \nabla V^\varepsilon \cdot \nu = \nabla F^\varepsilon \cdot \nu = \nabla G^\varepsilon \cdot \nu = 0,\end{aligned} \tag{3.36}$$

The asymptotic result

It is the aim of the subsequent analysis to prove the following result:

Theorem 3.1. *Let the assumptions of subsection 3.1 hold. Then there exists a sequence (ε) of positive real numbers converging to zero and functions $n, p, V, F, G \in C_B(\Omega) \cap H^1(\Omega)$ satisfying*

$$\begin{aligned} 0 &= V + h_N(n) - F \\ 0 &= -V + h_P(p) - G \\ -\lambda^2 \Delta V &= n - p - C \\ \nabla \cdot (\mu_n n \nabla F) &= R_0(n,p)\, R_1(F,G)\,, \\ \nabla \cdot (\mu_p p \nabla G) &= R_0(n,p)\, R_1(F,G) \end{aligned} \tag{3.37}$$

subject to the boundary conditions

$$\begin{aligned}\Gamma_+ :\ & n = n_{eq}(x), \quad p = p_{eq}(x), \quad V = V_{eq}(x) + V_{ext}(x), \\ & F = F_{eq} + V_{ext}(x), \quad G = G_{eq} - V_{ext}(x), \\ \Gamma_N :\ & \nabla V \cdot \nu = \nabla F \cdot \nu = \nabla G \cdot \nu = 0,\end{aligned} \tag{3.38}$$

such that

$\rho^\varepsilon \to \sqrt{n}, \sigma^\varepsilon \to \sqrt{p}, V^\varepsilon \to V, F^\varepsilon \to F, G^\varepsilon \to G$ *strongly in* $H^1(\Omega)$, *weak* in* $L^\infty(\Omega)$

as $\varepsilon \to 0$.

The proof of this Theorem is carried out in several steps.
Step 1: First of all, we prove that the first three equations of 3.37 are equivalent to the minimization of

$$\begin{aligned}\mathcal{F}(n,p) = \int H_N(n) + \int H_P(p) + \frac{1}{2}\int |\nabla\Phi[n-p-C]|^2 \\ + \int (n-p)\Phi_e - \int (Fn + Gp)\end{aligned} \tag{3.39}$$

in $L^{3/2}(\Omega)\times L^{3/2}(\Omega)$. Using the regularity of unique positive minimizer (n^*, p^*) of (3.39), we construct comparison functions for $(\rho^\varepsilon, \sigma^\varepsilon)$. We recall that $(\rho^\varepsilon, \sigma^\varepsilon)$ is a solution of (3.35), (3.36) and is a minimizer of the functional

$$\begin{aligned}\mathcal{E}^\varepsilon(\rho,\sigma) = {} & \varepsilon^2 \int |\nabla\rho|^2 + \xi\varepsilon^2 \int |\nabla\sigma|^2 \\ & + \int H_N(\rho^2) + \int H_P(\sigma^2) + \frac{1}{2}\int |\nabla\Phi[\rho^2-\sigma^2-C]|^2 \\ & + \int (\rho^2-\sigma^2)\Phi_e - \int (F^\varepsilon\rho^2 + G^\varepsilon\sigma^2)\end{aligned} \tag{3.40}$$

in $\mathcal{M}^\varepsilon = \left(\sqrt{n^\varepsilon_{eq}}, \sqrt{p^\varepsilon_{eq}}\right) + H^1_0(\Omega\cup\Gamma_N)$.

Step 2: By means of the comparison functions, we derive ε independent estimates on $\rho^\varepsilon, \sigma^\varepsilon, V^\varepsilon, F^\varepsilon, G^\varepsilon$. By construction, $F^\varepsilon, G^\varepsilon$ are bounded in $L^\infty(\Omega)$ independently of ε. This fact and the growth condition on $h_{N,P}$ ensure that V^ε is uniformly bounded in $L^\infty(\Omega)$. This allows to estimate $\rho^\varepsilon, \sigma^\varepsilon$ uniformly from above and - in view of $\lim_{u\to 0} h_{N,P}(u) = -\infty$ - away from zero from below. Hence a uniform $H^1(\Omega)$-estimate on $F^\varepsilon, G^\varepsilon$ is available. The assumed $H^1(\Omega)$-convergence of the equilibrium solutions determining the boundary conditions and the comparison technique mentioned above allows to pass to the limit $\varepsilon\to 0$ then.

3.3. The limiting problem

Lemma 3.2. *Under the assumptions of subsection 3.1, let F, G be fixed in $L^\infty(\Omega)$. Then the functional $\mathcal{F}$ admits a unique non negative minimizer $(n,p)\in L^{3/2}(\Omega)\times L^{3/2}(\Omega)$. The minimizer satisfies*

$$\begin{aligned} 0 &= V + h_N(n) - F \\ 0 &= -V + h_P(p) - G \\ -\lambda^2\Delta V &= n - p - C, \quad V - V_{eq} - V_{ext} \in H^1_0(\Omega\cup\Gamma_N)\end{aligned}$$

is actually in $L^\infty(\Omega)$ and there exists $K>1$ depending on the L^∞ norms of F and G such that

$$\frac{1}{K} \le n, p \le K.$$

Moreover, if F and G are additionally in $H^1(\Omega)$, then the same holds for n and p.

Proof. It is readily seen that $\mathcal{F}$ is a srictly convex coercive lower semi continuous functional in the set of non negative pairs of functions of $L^{3/2}(\Omega)$. This implies existence and uniqueness of the minimizer (n,p).

Let us now prove that the set $\Omega_0 = \{n = 0\}$ has zero measure. We remark that

$$\frac{1}{t}\left(\mathcal{F}(n + t1_{\Omega_0}, p) - \mathcal{F}(n,p)\right) \geq 0, \quad \forall\, t \geq 0. \tag{3.42}$$

But it is easy to see that the left hand side of this inequality is equal to

$$\frac{H(t)}{t}\ \text{meas}\ (\Omega_0) + O(1), \quad \text{as}\ t \to 0^+.$$

The above expression tends to $-\infty$ whenever meas $(\Omega_0) > 0$ contradicting (3.42). Hence meas $(\Omega_0) = 0$. It follows in analogy that meas $(\{p = 0\}) = 0$.

Let us now establish the Euler-Lagrange equations satisfied by (n, p). For given $K \in \mathbb{N}$ let $\Omega_K = \{1/K \leq n \leq K\}$. Due to the positivity almost everywhere of n we have

$$\Omega = \bigcup_{K \in \mathbb{N}} \Omega_K.$$

Fix $K \in \mathbb{N}$ and let $\varphi \in L^\infty(\Omega)$ supported in Ω_K. It follows that $n + t\varphi$ is nonnegative for t small enough and the Gateaux differential of $\mathcal{F}$ at (n, p) following the direction $(\varphi, 0)$ exists and is equal to zero.

$$\mathcal{F}'(n,p)[\varphi, 0] = \int_{\Omega_K} (V + h_N(n) - F)\,\varphi = 0 \tag{3.43}$$

where V is the solution of

$$-\lambda^2 \Delta V = n - p - C, \quad V - V_{eq} - V_{ext} \in H_0^1(\Omega \cup \Gamma_N).$$

Due to the growth condition A6), we have $n, p \in L^{3/2+\delta}(\Omega)$ which immediately gives $V \in L^\infty$. Hence due to (4.3), we have

$$h_N(n) = F - V \tag{3.44}$$

almost everywhere on Ω which gives thanks to A6) the existence of $K > 1$ such that

$$\frac{1}{K} \leq n \leq K.$$

The estimate concerning p follows in the same manner. The regularity of n, p for F, G in $H^1(\Omega)$ follows from (3.44) ($h_{N,P}$ are locally Lipschitz continuous). □

3.4. End of the proof of theorem 3.1

We first prove uniform bounds on $\rho^\varepsilon, \sigma^\varepsilon, V^\varepsilon, F^\varepsilon$ and G^ε. Due to the construction of F^ε and G^ε and due to hypothesis A7) we have uniform L^∞ estimates on F^ε and G^ε. Now it is easy to see that $\inf_{\mathcal{M}^\varepsilon} \mathcal{E}^\varepsilon$ is uniformly bounded. It follows from the assumed growth conditions on $h_{N,P}$ that each term of $\mathcal{E}^\varepsilon(\rho^\varepsilon, \sigma^\varepsilon)$ is uniformly bounded. In particular,

$$||\rho^\varepsilon||_{L^{3+\delta}}, ||\sigma^\varepsilon||_{L^{3+\delta}}, ||V^\varepsilon||_{H^1} \le D.$$

This leads, together with A7) to the boundedness of $||V^\varepsilon||_{L^\infty}$. An application of the maximimum principle as in subsection 2.4 together with A7) and the uniform L^∞ bounds of $F^\varepsilon, G^\varepsilon, V^\varepsilon$ gives

$$1/K \le \rho^\varepsilon, \sigma^\varepsilon \le K \tag{3.45}$$

where $K > 1$ does not depend on ε. It follows from the current relations that

$$\int \mu_n (\rho^\varepsilon)^2 |\nabla F^\varepsilon|^2 - \int (\rho^\varepsilon)^2 \, \nabla F^\varepsilon \cdot \nabla V_{ext} = \int R_0^\varepsilon \left((\rho^\varepsilon)^2, (\sigma^\varepsilon)^2 \right) R_1(F^\varepsilon, G^\varepsilon)(F^\varepsilon - F_{eq}^\varepsilon - V_{ext})$$

$$\int \mu_p (\sigma^\varepsilon)^2 |\nabla G^\varepsilon|^2 + \int (\sigma^\varepsilon)^2 \, \nabla G^\varepsilon \cdot \nabla V_{ext} = \int R_0^\varepsilon \left((\rho^\varepsilon)^2, (\sigma^\varepsilon)^2 \right) R_1(F^\varepsilon, G^\varepsilon)(G^\varepsilon - G_{eq}^\varepsilon + V_{ext})$$

which gives in connection with (3.45), A3,A4),A8) and $V_{ext} \in L^\infty(\Omega) \cap H^1(\Omega)$, see subsection 2.1,

$$||F^\varepsilon||_{H^1}, ||G^\varepsilon||_{H^1} \le D$$

for a $D > 0$ independent of ε. We therefore have after passing to a subsequence

$$(\rho^\varepsilon)^2 \to n, \quad (\sigma^\varepsilon)^2 \to p \quad \text{weak* in } L^\infty(\Omega),$$

$$F^\varepsilon \to F, \quad G^\varepsilon \to G \quad \text{weakly in } H^1(\Omega) \text{ , weak* in } L^\infty(\Omega),$$

$$V^\varepsilon \to V \quad \text{strongly in } H^1(\Omega)$$

where clearly

$$1/K \le n, p \le K$$

and $F, G, V \in L^\infty(\Omega) \cap H^1(\Omega)$ as well as

$$-\lambda^2 \Delta V = n - p - C, \quad V - V_{eq} - V_{ext} \in H_0^1(\Omega \cup \Gamma_N)$$

and finally

$$F - F_{eq} - V_{ext} \quad , \quad G - G_{eq} + V_{ext} \in H_0^1(\Omega \cup \Gamma_N).$$

From now on the functions F and G appearing in the definition of $\mathcal{F}$ (3.39) are the weak limits of F^ε and G^ε. We shall prove now that (n,p) is nothing but the minimizer (n^*,p^*) of $\mathcal{F}$ in the set of pairs of non negative functions of $L^{3/2}(\Omega)$. Indeed it follows from Lemma 3.2 that such a minimizer of $\mathcal{F}$ exists uniquely and satisfies

$$0 = V + h_N(n^*) - F$$
$$0 = -V + h_P(p^*) - G$$

which implies, in view of A7), on one hand that $(n^*,p^*) \in (n_{eq},p_{eq}) + H_0^1(\Omega \cup \Gamma_N)$ and on the other hand that there exists a constant $K > 1$ such that $1/K \leq n^*, p^* \leq K$.

Given $\varepsilon > 0$ let

$$\mathcal{M}_\varepsilon = (\sqrt{n_{eq}^\varepsilon}, \sqrt{p_{eq}^\varepsilon}) + H_0^1(\Omega \cup \Gamma_N).$$

We note that for all $\varepsilon > 0$ the pair $\left(\sqrt{n^*} - \sqrt{n_{eq}} + \sqrt{n_{eq}^\varepsilon}, \sqrt{p^*} - \sqrt{p_{eq}} + \sqrt{p_{eq}^\varepsilon}\right)$ belongs to $\mathcal{M}_\varepsilon$. Hence due to the minimizing property of $(\rho^\varepsilon, \sigma^\varepsilon)$,

$$\limsup_{\varepsilon\to 0} \mathcal{E}^\varepsilon(\rho^\varepsilon,\sigma^\varepsilon) \leq \limsup_{\varepsilon\to 0} \mathcal{E}^\varepsilon\left(\sqrt{n^*} - \sqrt{n_{eq}} + \sqrt{n_{eq}^\varepsilon}, \sqrt{p^*} - \sqrt{p_{eq}} + \sqrt{p_{eq}^\varepsilon}\right)$$

which gives due to A7)

$$\limsup_{\varepsilon\to 0} \mathcal{E}^\varepsilon(\rho^\varepsilon,\sigma^\varepsilon) \leq \mathcal{F}(n^*,p^*). \tag{3.46}$$

On the other hand, we have

$$\mathcal{E}^\varepsilon(\rho^\varepsilon,\sigma^\varepsilon) = \mathcal{F}((\rho^\varepsilon)^2,(\sigma^\varepsilon)^2) + \varepsilon^2\int|\nabla\rho^\varepsilon|^2 + \xi\varepsilon^2\int|\nabla\sigma^\varepsilon|^2 + \int(F - F^\varepsilon)(\rho^\varepsilon)^2$$
$$+ \int(G - G^\varepsilon)(\sigma^\varepsilon)^2 + \int(\Phi_e^\varepsilon - \Phi_e^\circ)((\rho^\varepsilon)^2 - (\sigma^\varepsilon)^2)$$

The last three terms of the right hand side of the above formula tend to zero thanks to the strong convergence of $F^\varepsilon, G^\varepsilon, \Phi_e^\varepsilon$ in $L^2(\Omega)$. Therefore, it follows from the weak lower sequential semicontinuity of $\mathcal{F}$ in $L^2(\Omega) \times L^2(\Omega)$ that

$$\liminf_{\varepsilon\to 0} \mathcal{E}^\varepsilon(\rho^\varepsilon,\sigma^\varepsilon) \geq \mathcal{F}(n,p). \tag{3.47}$$

It follows from (3.46), (3.47) that actually $\mathcal{F}(n,p) \le \mathcal{F}(n^*,p^*)$ and we deduce from Lemma 3.2 and from the minimizing property of (n^*,p^*) that

$$(n^*,p^*) = (n,p).$$

This settles the algebraic relations

$$V = F - h_N(n) = h_P(p) - G.$$

Hence, we have proven that (3.41) holds in the limit and that all the boundary conditions (3.38) are satisfied. It remains now to pass to the limit in the current relations. Due to their nonlinearity, we need strong L^r convergence of ρ^ε and σ^ε.

Strong L^r convergence of densities

Due to the convexity of $H_{N,P}$ we have after a possible extraction of a subsequence

$$\lim_{\varepsilon\to 0}\int H_N((\rho^\varepsilon)^2) \ge \int H_N(n), \quad \lim_{\varepsilon\to 0}\int H_P((\sigma^\varepsilon)^2) \ge \int H_P(p).$$

Furthermore, since

$$\mathcal{F}(n,p) = \lim_{\varepsilon\to 0}\mathcal{E}^\varepsilon(\rho^\varepsilon,\sigma^\varepsilon)$$

it follows that the above inequalities are actually equalities. Applying Corollary 1 of [25] leads to the strong $L^1(\Omega)$ convergence of $(\rho^\varepsilon)^2, (\sigma^\varepsilon)^2$ towards n, p. Due to the positivity of ρ^ε and σ^ε, we have

$$\rho^\varepsilon \to \sqrt{n}, \quad \sigma^\varepsilon \to \sqrt{p} \quad \text{in } \ L^2(\Omega) \quad \text{strong.}$$

Actually, the convergence holds strongly in each $L^r(\Omega)$ because of the uniform $L^\infty(\Omega)$ estimates on ρ^ε and σ^ε. In the same spirit, we deduce from the L^2 strong convergence of $F^\varepsilon, G^\varepsilon$ and from the boundedness of their L^∞ norms, that F^ε and G^ε converge strongly in each $L^r(\Omega)$. This implies, in view of A8), that

$$R_0^\varepsilon\left((\rho^\varepsilon)^2,(\sigma^\varepsilon)^2\right) R_1^\varepsilon\left(F^\varepsilon,G^\varepsilon\right) \to R_0\left(n,p\right) R_1\left(F,G\right)$$

strongly in in all $L^r(\Omega)$ spaces, $r\in[1,\infty)$, as $\varepsilon\to 0$. This is sufficient to insure that F, G satisfy

$$\begin{cases} \nabla\cdot(\mu_n n\nabla F) = R_0\left(n,p\right) R_1\left(F,G\right), \\ \nabla\cdot(\mu_p p\nabla G) = R_0\left(n,p\right) R_1\left(F,G\right) \end{cases}$$

subject to the boundary conditions

$$F - F_{eq} - V_{ext},\, G - G_{eq} + V_{ext} \in H_0^1(\Omega\cup\Gamma_N).$$

Strong H^1 convergence of Fermi levels

We have

$$\nabla \cdot (\mu_n n \nabla F) = S$$

and

$$\nabla \cdot (\mu_n n^\varepsilon \nabla F^\varepsilon) = S^\varepsilon$$

where S and S^ε are in $L^2(\Omega)$ and S^ε converges strongly in $L^2(\Omega)$ towards S and $n^\varepsilon = (\rho^\varepsilon)^2$ is bounded in L^∞ and converges strongly to n in $L^2(\Omega)$. Multiplying the above equations by $F^\varepsilon - F$, taking the difference and integrating on Ω, we find

$$\begin{aligned}\int_\Omega n|\nabla(F^\varepsilon - F)|^2\,dx = &\int_\Omega (S^\varepsilon - S)(F^\varepsilon - F)\,dx \\ &+ (F^\varepsilon_{eq} - F_{eq}) \int_{\Gamma_+} (n^\varepsilon \nabla F^\varepsilon - n\nabla F)\cdot \nu\,ds \\ &- \int_\Omega (n^\varepsilon - n)\nabla F \cdot (\nabla F^\varepsilon - \nabla F)\,dx.\end{aligned}$$

It is readily seen that the first term of the right hand side converges to zero as ε tends to zero. Let us now prove that the second term tends to zero as $\varepsilon \to 0$. Since F^ε_{eq} tends to F_{eq}, it is sufficient to prove that $\int_{\Gamma_+} (n^\varepsilon \nabla F^\varepsilon - n\nabla F)\cdot \nu\,ds$ is bounded. For this aim, we let $\tilde{n}^\varepsilon$ be the unique harmonic function with the same boundary conditions as n^ε. Assumption A7) implies that $\tilde{n}^\varepsilon$ is bounded in H^1 as ε goes to zero. To prove that $\int_{\Gamma_+} n^\varepsilon \nabla F^\varepsilon.\nu\ ds$ is bounded, we just recall that F^ε is bounded in H^1 and that

$$\int_{\Gamma_+} n^\varepsilon \nabla F^\varepsilon.\nu\ ds = -\int_{\Gamma_+} F^\varepsilon \nabla \tilde{n}^\varepsilon.\nu\,ds + \int_\Omega \nabla \tilde{n}^\varepsilon.\nabla F^\varepsilon\,dx.$$

To deal with the third term, we notice that n^ε converges to n almost everywhere and n^ε is bounded in L^∞. Hence the Lebesgue dominated convergence theorem implies that $(n^\varepsilon - n)\nabla F$ tends to zero strongly in $L^2(\Omega)$. This implies together with the weak H^1 convergence of F^ε that the third term goes to zero in the limit.

This proves, in view of the uniform bound of n away from zero, that

$$F^\varepsilon \to F, \quad G^\varepsilon \to G \quad \text{strongly in } H^1(\Omega).$$

Using the variational structure of the problem, we are now able to prove the,

Strong H^1 convergence of densities

Given $\varepsilon > 0$ consider the following system of PDE's:

$$\begin{aligned} 0 &= W^\varepsilon + h_N((r^\varepsilon)^2) - F^\varepsilon \\ 0 &= -W^\varepsilon + h_P((s^\varepsilon)^2) - G^\varepsilon \\ -\lambda^2 \Delta W^\varepsilon &= (r^\varepsilon)^2 - (s^\varepsilon)^2 - C \end{aligned} \tag{3.48}$$

subject to the boundary conditions

$$W - V_{eq}^{\varepsilon} - V_{ext} \in H_0^1(\Omega \cup \Gamma_N). \tag{3.49}$$

We see with the aid of Lemma 3.2 that (3.48), (3,49) possesses a unique nonnegative solution $(r^\varepsilon, s^\varepsilon)$ in $L^3(\Omega) \times L^3(\Omega)$. It additionally follows from Lemma 3.2 that $r^\varepsilon, s^\varepsilon$ belong to $L^\infty(\Omega) \cap H^1(\Omega)$. Thanks to the uniform $L^\infty(\Omega)$ and $H^1(\Omega)$ bounds for $F^\varepsilon, G^\varepsilon$ and $V_{eq}^\varepsilon + V_{ext}$ we get

$$1/K \leq r^\varepsilon, s^\varepsilon \leq K \tag{3.50}$$

for a $K > 1$ independent of ε as well as

$$\|r^\varepsilon\|_{H^1}, \|s^\varepsilon\|_{H^1} \leq D$$

for a constant D independent of ε. Equations 3.48 are the Euler-Lagrange equations of

$$\mathcal{E}_{class}^{\varepsilon}(r,s) = \int H_N(r^2) + \int H_P(s^2) + \frac{1}{2}\int |\nabla\Phi[r^2 - s^2 - C]|^2 + \int (r^2 - s^2)\Phi_e^\varepsilon - \int (F^\varepsilon r^2 + G^\varepsilon s^2)$$

This observation makes it easy to verify that

$$\mathcal{E}_{class}^{\varepsilon}(r^\varepsilon, s^\varepsilon) \leq \mathcal{E}_{class}^{\varepsilon}(\rho^\varepsilon, \sigma^\varepsilon).$$

On the other hand, $(r^\varepsilon, s^\varepsilon)$ belongs to $\mathcal{M}^\varepsilon$ (see (3.34). Hence

$$\mathcal{E}^\varepsilon(\rho^\varepsilon, \sigma^\varepsilon) \leq \mathcal{E}^\varepsilon(r^\varepsilon, s^\varepsilon).$$

These two inequalities imply

$$\int |\nabla\rho^\varepsilon|^2 + \xi\int |\nabla\sigma^\varepsilon|^2 \leq \int |\nabla r^\varepsilon|^2 + \xi\int |\nabla s^\varepsilon|^2 \leq D \tag{3.51}$$

where D is independent of ε. Hence

$$\|\rho^\varepsilon\|_{H^1}, \|\sigma^\varepsilon\|_{H^1} \leq D$$

which gives

$$\rho^\varepsilon \to \sqrt{n} \quad , \quad \sigma^\varepsilon \to \sqrt{p} \quad \text{weakly in } H^1(\Omega). \tag{3.52}$$

Thanks to the Lipschitz continuity of $h_{N,P}$, the strong $H^1(\Omega)$ convergence of $F^\varepsilon, G^\varepsilon$ and V_{eq}^ε, it follows from (3.48), (3.49) that

$$(r^\varepsilon)^2 \to n \quad , \quad (s^\varepsilon)^2 \to p \quad \text{strongly in } H^1(\Omega),$$

which gives due to (3.50)

$$r^\varepsilon \to \sqrt{n} \quad , \quad s^\varepsilon \to \sqrt{p} \quad \text{strongly in } H^1(\Omega),$$

and therefore

$$\lim_{\varepsilon\to 0}\int |\nabla r^\varepsilon|^2 = \int |\nabla\sqrt{n}|^2 \quad , \quad \lim_{\varepsilon\to 0}\int |\nabla s^\varepsilon|^2 = \int |\nabla\sqrt{p}|^2.$$

It follows from (3.51) that

$$\limsup_{\varepsilon\to 0}\left(\int |\nabla\rho^\varepsilon|^2 + \xi\int|\nabla\sigma^\varepsilon|^2\right)\int|\nabla\sqrt{n}|^2 + \xi\int|\nabla\sqrt{p}|^2 \tag{3.53}$$

while the weak $H^1(\Omega)$ convergence (3.52) implies

$$\int|\nabla\sqrt{n}|^2 \le \liminf_{\varepsilon\to 0}\int|\nabla\rho^\varepsilon|^2 \quad , \quad \int|\nabla\sqrt{p}|^2 \le \liminf_{\varepsilon\to 0}\int|\nabla\sigma^\varepsilon|^2. \tag{3.54}$$

Now it is readily seen that (3.53), (3.54) together imply

$$\lim_{\varepsilon\to 0}\int |\nabla \rho^\varepsilon|^2 = \int |\nabla\sqrt{n}|^2 \quad , \quad \lim_{\varepsilon\to 0}\int |\nabla \sigma^\varepsilon|^2 = \int |\nabla\sqrt{p}|^2,$$

i.e.

$$\|\rho^\varepsilon\|_{H^1} \to \|\sqrt{n}\|_{H^1} \quad , \quad \|\sigma^\varepsilon\|_{H^1} \to \|\sqrt{p}\|_{H^1}$$

as $\varepsilon\to 0$. By the uniform convexity of $H^1(\Omega)$ and the weak convergence of (3.52) the strong convergence of $\rho^\varepsilon, \sigma^\varepsilon$ in $H^1(\Omega)$ follows. □

The following corollary asserts - roughly speaking - that the voltage-current characteristics of the QDD converge to the voltage-current characteristics of the limiting classical drift-diffusion model.

Corollary 3.3. *Under the hypotheses of Theorem 3.1, given any compact subset K of $\overline{\Omega}$ with unit outward vector $\vec{\nu}$ and any $\theta \in C^\infty(K)$,*

$$\lim_{\varepsilon\to 0}\int_{\partial K}\theta\vec{J^\varepsilon}\cdot\vec{\nu}\,ds = \int_{\partial K}\theta\vec{J}\cdot\vec{\nu}\,ds$$

where

$$\vec{J^\varepsilon} = \mu_n(\rho^\varepsilon)^2\nabla F^\varepsilon - \mu_p(\sigma^\varepsilon)^2\nabla G^\varepsilon \quad , \quad \vec{J} = \mu_n n\,\nabla F - \mu_p p\,\nabla G.$$

Proof. Since

$$\nabla\cdot\vec{J^\varepsilon} = \nabla\cdot\vec{J} = 0$$

then

$$\int_{\partial K}\theta\vec{J}\cdot\vec{\nu}\,ds = \int_K \vec{J^\varepsilon}.\nabla\theta\,dx.$$

To prove the corollary, we just recall that $\nabla F^\varepsilon, \nabla G^\varepsilon, (\rho^\varepsilon)^2$ and $(\sigma^\varepsilon)^2$ converge strongly in $L^2(\Omega)$ which implies that $\vec{J^\varepsilon}$ converges strongly in $L^1(\Omega)$. □

4. Concluding remarks

In this paper we investigated a QDD incorporating generation-recombination effects. The required structure of the generation-recombination rate R extends classical models based on mass-action laws. It should be noted that the analysis applies if no generation-recombination effects are taken into account e.g. as in [3]. The mobilities $\mu_{n,p}$ need not be constant. The analysis can be extended by assuming that they are positive continuous L^∞ functions of $x, n, p, \nabla V, \ldots$ uniformly bounded away from zero.

In our analysis, we assumed, for the sake of minimizing the already heavy notations, that electron and hole densities vanish on the *same* part of the boundary. The proof is essentially the same if one assumes that electron and hole densities vanish on *different* parts of the density. The analysis can also be carried out in the case where electrons are in a quantum regime whereas holes are considered as classical particles [3].

In the proof of the semiclassical limit (Section 3), a fundamental hypothesis is that $\lim_{u\to 0} h_{N,P}(u) = -\infty$. This prevents the appearence of vacuum in Ω for the classical drift diffusion model. In the case $\lim_{u\to 0} h_{N,P}(u) > -\infty$, it is proven in [20] that vacuum sets for the classical drift diffusion model may appear. This is in significant contrast with QDD for which we proved in section 2 that vacuum appears at most on the boundary.

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