Quasineutral limit of the drift-diffusion model for semiconductors with general initial data

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Abstract: The limit for vanishing Debye length (charge neutral limit) in a bipolar drift-diffusion model for semiconductors with general initial data allowing the presence of an initial layer is studied. The quasineutral limit (zero-Debye-length limit) is performed rigorously by using two different entropy functionals which yield appropriate uniform estimates. This investigation extends the results of [GLMS, GHMW] for charge neutral initial data where no initial layer occurs.
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1 Introduction and Formal Asymptotics

The scaled semiconductor drift-diffusion equations read

$$\begin{aligned} n_t^\lambda &= \mu_n div(\nabla (n^\lambda)^{\gamma_n} + n^\lambda E^\lambda) \\ p_t^\lambda &= \mu_p div(\nabla (p^\lambda)^{\gamma_p} - p^\lambda E^\lambda) \\ -\lambda^2 div E^\lambda &= n^\lambda - p^\lambda - C \end{aligned} \tag{1.1}$$

with $x \in \Omega \subset \mathbf{R}^d$, Ω bounded with smooth boundary, $t > 0$ and $E^\lambda = -\nabla\Phi^\lambda$. The unknowns $n^\lambda, p^\lambda, E^\lambda, \Phi^\lambda$ are the electron density, the hole density, the electric field and the electric potential, respectively. The given function $C = C(x)$ is the doping profile describing fixed background charges. The dimensionless positive parameters μ_n, μ_p and λ are the scaled mobilities of electrons and holes and the scaled Debye length, respectively. The constants $\gamma_n, \gamma_p > 0$ are the adiabatic or isothermal (if $\gamma_n = \gamma_p = 1$) exponents. The regime $0 < \gamma_n < 1$ (or $0 < \gamma_p < 1$) describes fast diffusion of electrons (holes), whereas $\gamma_n > 1$ ($\gamma_p > 1$) is related to slow diffusion.

We consider an insulated semiconductor modeled by the initial-boundary value problem for (1.1) subject to the boundary and initial conditions:

$$(\nabla (n^\lambda)^{\gamma_n} + n^\lambda E^\lambda)\cdot \nu = (\nabla (p^\lambda)^{\gamma_p} - p^\lambda E^\lambda)\cdot \nu = E^\lambda \cdot \nu = 0, \quad \text{on } \partial\Omega, \tag{1.2}$$

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$$n^\lambda(t=0,x) = n_0^\lambda(x), \quad p^\lambda(t=0,x) = p_0^\lambda(x), \qquad x \in \Omega, \tag{1.3}$$

where ν is a normal vector along the boundary $\partial\Omega$. The electric potential is normalized by the condition

$$\int_\Omega \Phi^\lambda dx = 0\,.$$

A necessary solvability condition for the Poisson equation (the third equation in (1.1)) subject to the Neumann boundary conditions for the field in (1.2) is global charge neutrality,

$$\int_\Omega (n^\lambda - p^\lambda - C)dx = 0.$$

Since the total numbers of electrons and holes are conserved, it is sufficient to require the corresponding condition for the initial data:

$$\int_\Omega (n_0^\lambda - p_0^\lambda - C)dx = 0. \tag{1.4}$$

We are interested in the behaviour of the solutions of the problem (1.1)–(1.4) in the vanishing Debye length limit $\lambda \to 0$.

Before stating our main results, we perform the quasineutral limit formally. Setting $\lambda = 0$ in (1.1) we obtain the system

$$\begin{aligned} n_t &= \mu_n div(\nabla n^{\gamma_n} + nE) \\ p_t &= \mu_p div(\nabla p^{\gamma_p} - pE) \\ 0 &= n - p - C, \end{aligned} \tag{1.5}$$

where $n, p, E = -\nabla\Phi$ are the formal limits of $n^\lambda, p^\lambda, E^\lambda$ as $\lambda \to 0$.

Because of the singular perturbation character of the problem (the Poisson equation becomes an algebraic equation in the limit) we cannot a priorily expect that all initial and boundary conditions hold for the limiting problem. However, by the conservation form of the continuity equations the property of zero flux through the boundary will prevail in the limit:

$$(\nabla n^{\gamma_n} + nE)\cdot\nu = (\nabla p^{\gamma_p} - pE)\cdot\nu = 0 \quad \text{on } \partial\Omega, \tag{1.6}$$

while the boundary condition for the electric field E^λ does not.

Simple manipulations of (1.5) give the parabolic-elliptic system (see [GLMS])

$$\begin{aligned} &(\tfrac{1}{\mu_n} + \tfrac{1}{\mu_p})p_t = div(\nabla((p+C)^{\gamma_n} + p^{\gamma_p}) + CE) \\ &-div(((\mu_n + \mu_p)p + \mu_n C)E) = div(\nabla(\mu_n(p+C)^{\gamma_n} - \mu_p p^{\gamma_p})). \end{aligned} \tag{1.7}$$

If, further, $C \equiv 0$ the limiting problem becomes

$$p_t = D div(\nabla(p^{\gamma_n} + p^{\gamma_p})), \qquad D = \frac{\mu_n\mu_p}{\mu_n + \mu_p}. \tag{1.8}$$

This fact is well-known in plasma physics, see [C, G1, G2, JP].

For general initial conditions (satisfying (1.4)) an initial time layer occurs. The solution of the corresponding layer problem determines the initial data for p by a matching principle. For more details on the formal asymptotics as well as on the history of the subject, we refer to the introduction of [GLMS].

A rigorous justification of the quasineutral limit is a longstanding challenging problem. While the status of the theory is rather advanced in certain situations (e.g., steady state problems, unipolar models), first results for time dependent bipolar models are recent. While an existence analysis of the problem (1.1)–(1.4) has been given in [Gaj] for linear diffusion ($\gamma_n = \gamma_p = 1$) and in [J] for slow diffusion ($\gamma_n,\ \gamma_p > 1$) rigorous results for the limit from (1.1)–(1.4) to (1.5), (1.6) have been derived in [G1], [GLMS], [GHMW], and [JP]. To the knowledge of the authors, no results for the fast diffusion regime are available.

The purpose of this work is an extension of the results of [G1], [GLMS], and [GHMW]. In these studies an essential assumption is the compatibility of the initial data with the limiting problem, i.e., the local charge neutrality assumption $n_0^\lambda - p_0^\lambda - C = 0$ implying the absence of an initial time layer. As a second restriction, no pn-junctions, i.e., sign changes of the doping profile C are allowed. The proofs rely on the use of an entropy functional, whose application requires the local charge neutrality of the initial data. Here, a second entropy functional is introduced, which can be used for general initial data, whose decay, however, relies on the assumption that the doping profile C is constant. Thus, we are able to remove one restriction of the earlier work (regarding the initial data), but not the other (regarding the doping profile). It will be proved that solutions of (1.1)–(1.4) converge to solutions of (1.5), (1.6) away from $t = 0$.

The paper is organized as follows: Section 2 is devoted to a priori estimates and Section 3 gives rigorous results on the quasineutral limit. Throughout this paper, we use the symbol M for various generic constants independent of the Debye length λ.

2 A Priori Estimates

The assumptions

$$\begin{gathered} C > 0\,, \qquad C = \text{const}\,, \\ \gamma_n, \gamma_p \geq 1\,, \\ n_0^\lambda, p_0^\lambda \in L^\infty(\Omega) \quad \text{uniformly in } \lambda \text{ as } \lambda \to 0\,, \qquad n_0^\lambda, p_0^\lambda \geq 0\,, \end{gathered} \tag{2.1}$$

will be used throughout this work. Existence of global solutions of (1.1)–(1.4) can then be shown (see [Gaj], [J]).

We shall need L^∞-bounds for the densities as well as boundedness away from zero (at least for the electrons, the majority carrier density).

Lemma 2.1 *Assume (2.1) and let n^λ, p^λ be a solution of (1.1)–(1.4). Then $n^\lambda, p^\lambda \in L^\infty(\Omega \times (0,\infty))$ uniformly in λ. If $n_0^\lambda \geq \delta > 0$ in Ω for some positive constant $\delta \leq C$, then $n^\lambda \geq \delta$ in $\Omega \times (0,\infty)$. If further $n_0^\lambda \geq C + \delta$, $p_0^\lambda \geq \delta$ in Ω, then $n^\lambda \geq C + \delta$, $p^\lambda \geq \delta$ in $\Omega \times (0,\infty)$.*

Proof Using the Poisson equation, the electron and hole equations can be written as

$$
\begin{aligned}
n_t^\lambda &= \mu_n(\Delta(n^\lambda)^{\gamma_n} + E^\lambda \cdot \nabla n^\lambda) - \tfrac{\mu_n n^\lambda (n^\lambda - p^\lambda - C)}{\lambda^2}\,, \\
p_t^\lambda &= \mu_p(\Delta(p^\lambda)^{\gamma_p} - E^\lambda \cdot \nabla p^\lambda) + \tfrac{\mu_p p^\lambda (n^\lambda - p^\lambda - C)}{\lambda^2}\,.
\end{aligned}
$$

It is easily seen that rectangles in the (n,p)-plane of the form $[\delta, \overline{p} + C] \times [0, \overline{p}]$ (with $0 \le \delta \le C$ and $\overline{p} \ge 0$) or $[\delta + C, \overline{p} + C] \times [\delta, \overline{p}]$ are invariant regions of the ODE-system for spatially homogeneous solutions. By a maximum principle argument, they are also invariant for the full PDE-system. The results of the lemma are obtained by choosing appropriate rectangles containing the initial data. ∎

Our second important tool is entropy techniques. We introduce the entropies

$$
e^\lambda(t) = \int_\Omega \left(n^\lambda \frac{(n^\lambda)^{\gamma_n - 1} - 1}{\gamma_n - 1} + p^\lambda \frac{(p^\lambda)^{\gamma_p - 1} - 1}{\gamma_p - 1} + \frac{\lambda^2}{2} |E^\lambda|^2 \right) dx + e_0 \tag{2.2}
$$

and

$$
e_1^\lambda(t) = \int_\Omega \left(\frac{n^\lambda \log n^\lambda}{\mu_n} + \frac{p^\lambda \log p^\lambda}{\mu_p} \right) dx + e_{10}, \tag{2.3}
$$

where $(\frac{A^{\gamma-1}-1}{\gamma-1})|_{\gamma=1} := \log A$ for $A > 0$ and the constants e_0, e_{10} are choosen such that the entropies are nonnegative quantities. The entropy e^λ has already been used in earlier work (see, e.g., [GHMW]). The functional e_1^λ decays only in the case C =const, considered here.

Lemma 2.2 *Assume (2.1). Then*

$$
\frac{de^\lambda}{dt} + \int_\Omega \left(\mu_n \frac{|\nabla (n^\lambda)^{\gamma_n} + n^\lambda E^\lambda|^2}{n^\lambda} + \mu_p \frac{|\nabla (p^\lambda)^{\gamma_p} - p^\lambda E^\lambda|^2}{p^\lambda} \right) dx = 0 \tag{2.4}
$$

and

$$
\frac{de_1^\lambda}{dt} + \int_\Omega \left(\gamma_n (n^\lambda)^{\gamma_n - 2} |\nabla n^\lambda|^2 + \gamma_p (p^\lambda)^{\gamma_p - 2} |\nabla p^\lambda|^2 \right) dx + \int_\Omega \frac{(n^\lambda - p^\lambda - C)^2}{\lambda^2} dx = 0 \tag{2.5}
$$

hold for solutions of (1.1)–(1.4).

Proof For (2.4), see [GHMW]. A direct calculation using (1.1) gives

$$
\frac{de_1^\lambda}{dt} + \int_\Omega \left(\gamma_n (n^\lambda)^{\gamma_n - 2} |\nabla n^\lambda|^2 + \gamma_p (p^\lambda)^{\gamma_p - 2} |\nabla p^\lambda|^2 \right) dx + \int_\Omega E^\lambda \nabla (n^\lambda - p^\lambda) dx = 0\,. \tag{2.6}
$$

Multiplying the Poisson equation by $(n^\lambda - p^\lambda - C)/\lambda^2$ and integrating with respect to x over Ω, we have

$$
\int_\Omega \frac{(n^\lambda - p^\lambda - C)^2}{\lambda^2} dx = - \int_\Omega div E^\lambda (n^\lambda - p^\lambda - C) dx = \int_\Omega E^\lambda \nabla (n^\lambda - p^\lambda) dx\,. \tag{2.7}
$$

Here we have used the assumption that the doping profile is a constant. Combination of (2.6) and (2.7) gives (2.5). ∎

Obviously, our assumptions (2.1) on the initial data are sufficient to provide boundedness of the initial value of e_1^λ uniformly in λ, leading to the following corollary of Lemma 2.2.

Corollary 2.3 *Assume (2.1). Then there exists a constant M such that, for any $t > 0$,*

$$\int_0^t \int_\Omega (n^\lambda - p^\lambda - C)^2 dx ds \le M\lambda^2 .$$

The entropy e^λ, on the other hand, is not uniformly bounded initially, since $E^\lambda(t=0)$ will be $O(\lambda^{-2})$ for general initial data. Fortunately, the entropy decays sufficiently fast, such that a uniform estimate for positive times is possible. We remark that for similar situations exponential decay of E^λ (for fixed positive λ) has been shown in [ArMaTo] and in [GajGro].

Lemma 2.4 *For every $T > 0$ there is a constant $M(T)$, such that*

$$e^\lambda(t) \le \frac{M(T)}{t}, \qquad 0 < t \le T . \tag{2.8}$$

Proof Multiplying the Poisson equation by the potential Φ^λ and integrating by parts, we have, with the help of Poincare's inequality, that

$$\begin{aligned} &\lambda^2 \textstyle\int_\Omega |E^\lambda|^2 dx = - \int_\Omega (n^\lambda - p^\lambda - C)\Phi^\lambda dx \\ &\le \tfrac{\lambda^2}{2M} \textstyle\int_\Omega |\Phi^\lambda|^2 dx + \tfrac{M}{2} \int_\Omega \tfrac{(n^\lambda - p^\lambda - C)^2}{\lambda^2} dx \le \tfrac{\lambda^2}{2} \int_\Omega |E^\lambda|^2 dx + \tfrac{M}{2} \int_\Omega \tfrac{(n^\lambda - p^\lambda - C)^2}{\lambda^2} dx , \end{aligned} \tag{2.9}$$

which gives

$$\lambda^2 \int_\Omega |E^\lambda|^2 dx \le M \int_\Omega \frac{(n^\lambda - p^\lambda - C)^2}{\lambda^2} dx ,$$

where M is a constant appearing in Poincaré's inequality.

Then by using Corollary 2.3, we have

$$\lambda^2 \int_0^t \int_\Omega |E^\lambda|^2 dx ds \le M < \infty . \tag{2.10}$$

Since $e^\lambda(t)$ is a nonincreasing function (see (2.4)), we have

$$e^\lambda(t) \le \frac{\int_0^t e^\lambda(s) ds}{t}, \quad t > 0 . \tag{2.11}$$

Using the definition of $e^\lambda(t)$, Lemma 2.1, (2.10) and (2.11), we get (2.8). ■

3 The Quasineutral Limit

In this section we formulate and prove our main result. Let us start with two remarks: First, we shall justify the quasineutral limit only away from the initial time $t = 0$. This is not surprising since initial conditions are allowed not satisfying local quasineutrality. Our results show that local quasineutrality is reached within a short initial layer.

The second remark is concerned with the characteristics of slow diffusion. It is well known that in general vacuum regions may occur for the electrons if $\gamma_n > 1$ and for the holes if $\gamma_p > 1$. Our assumptions exclude an electron (majority carrier) vacuum, but allow for a hole vacuum if $\gamma_p \leq 3/2$.

Theorem 3.1 *Assume (2.1) and $n_0^\lambda \geq \delta$ in Ω for a positive λ-independent constant δ. If $\gamma_p > 3/2$, assume additionally that $n_0^\lambda \geq \delta + C$, $p_0^\lambda \geq \delta$ holds in Ω. Let $T > s > 0$ and $Q_{s,T} = (s,T) \times \Omega$. Then, as $\lambda \to 0$ the following convergences hold (after extracting subsequences):*

$$n^\lambda \to n \quad \text{strongly in } L^q(Q_{s,T})\,,\ 1 \leq q < \infty\,,$$

$$p^\lambda \to p \quad \text{strongly in } L^q(Q_{s,T})\,,\ 1 \leq q < \infty\,,$$

$$E^\lambda \rightharpoonup E \quad \text{weakly in } L^2(Q_{s,T})\,,$$

$$n^\lambda - p^\lambda - C = O(\lambda) \quad \text{in } L^2((0,T) \times \Omega)\,.$$

Furthermore, the limit (n, p, E) satisfies the system (1.5),(1.6) in $\mathcal{D}'(Q_{s,T})$.

Proof First, Using Lemma 2.1, we have

$$n^\lambda \geq \delta\,,\ p^\lambda \geq 0\,, \qquad n^\lambda, p^\lambda \in L^\infty((0,T) \times \Omega)\,,$$

uniformly in λ, as well as $n^\lambda, p^\lambda \geq \delta$ for $\gamma_p > 3/2$. Lemma 2.2 implies

$$\frac{n^\lambda - p^\lambda - C}{\lambda}\,,\ (n^\lambda)^{\gamma_n/2-1}\nabla n^\lambda\,,\ (p^\lambda)^{\gamma_p/2-1}\nabla p^\lambda \in L^2((0,T) \times \Omega) \tag{3.1}$$

uniformly in λ. Therefore, we have

$$\nabla n^\lambda, \nabla p^\lambda \in L^2((0,T) \times \Omega) \tag{3.2}$$

uniformly in λ.

Using the equation for the entropy e^λ in Lemma 2.1 and Lemma 2.4, we get

$$\frac{\nabla(n^\lambda)^{\gamma_n} + n^\lambda E^\lambda}{\sqrt{n^\lambda}}\,,\ \frac{\nabla(p^\lambda)^{\gamma_p} - p^\lambda E^\lambda}{\sqrt{p^\lambda}} \in L^2(Q_{s,T})\,, \tag{3.3}$$

uniformly in λ. Now the L^∞-bounds (3.1) imply uniform boundedness of the current densities $\mu_n(\nabla(n^\lambda)^{\gamma_n} + n^\lambda E^\lambda)$ and $\mu_p(\nabla(p^\lambda)^{\gamma_p} - p^\lambda E^\lambda)$ in $L^2(Q_{s,T})$ and, thus,

$$n_t^\lambda, p_t^\lambda \in L^2((s,T); H^{-1}(\Omega))\,. \tag{3.4}$$

Combining (3.2) and (3.4), we obtain strong convergence of n^λ and p^λ in $L^2(Q_{s,T})$ from standard compactness results [S]. As a consequence of the L^∞-bounds we have strong convergence of n^λ and p^λ in $L^q(Q_{s,T})$ for $1 \leq q < \infty$.

Now we estimate the electric field E^λ. We multiply the Poisson equation by $(n^\lambda - p^\lambda - C)/\lambda^2$, use the equations (1.1) and obtain

$$
\begin{aligned}
&\int_s^T \int_\Omega \left[\left(\frac{(n^\lambda)^{2-\gamma_n}}{\gamma_n} + \frac{(p^\lambda)^{2-\gamma_p}}{\gamma_p} \right) (E^\lambda)^2 + \frac{(n^\lambda - p^\lambda - C)^2}{\lambda^2} \right] dx\, dt \\
&= \int_s^T \int_\Omega \left(\frac{(n^\lambda)^{3/2-\gamma_n}}{\gamma_n} \frac{\nabla (n^\lambda)^{\gamma_n} + n^\lambda E^\lambda}{\sqrt{n^\lambda}} - \frac{(p^\lambda)^{3/2-\gamma_p}}{\gamma_p} \frac{\nabla (p^\lambda)^{\gamma_p} - p^\lambda E^\lambda}{\sqrt{p^\lambda}} \right) \cdot E^\lambda \, dx\, dt \qquad (3.5) \\
&\leq \int_s^T \int_\Omega \left(\frac{(n^\lambda)^{3/2-\gamma_n}}{\gamma_n} \frac{|\nabla (n^\lambda)^{\gamma_n} + n^\lambda E^\lambda|}{\sqrt{n^\lambda}} + \frac{(p^\lambda)^{3/2-\gamma_p}}{\gamma_p} \frac{|\nabla (p^\lambda)^{\gamma_p} - p^\lambda E^\lambda|}{\sqrt{p^\lambda}} \right) |E^\lambda| dx\, dt\,.
\end{aligned}
$$

Note that by the uniform upper and lower bounds on the densities, the coefficient $(n^\lambda)^{2-\gamma_n}$ on the left hand side is bounded away from zero, and the coefficients $(n^\lambda)^{3/2-\gamma_n}$ and $(p^\lambda)^{3/2-\gamma_p}$ on the right hand side are bounded from above. Together with (3.3) we conclude

$$E^\lambda \in L^2(Q_{s,T})\,,$$

uniformly in λ, implying weak convergence of E^λ in $L^2(Q_{s,T})$. A further consequenceis the weak convergence of $n^\lambda E^\lambda$ and $p^\lambda E^\lambda$ in $L^2(Q_{s,T})$. Therefore all limits in the nonlinear terms can be performed and the proof is complete. ■

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