Rigorous Derivation of a Hierarchy of Macroscopic Models for Semiconductors and Plasmas

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Abstract. A hierarchy of fluid dynamical models for semiconductors and plasmas is presented. Starting from an Euler-Poisson system, several model equations are derived by means of asymptotic analysis, for vanishing (scaled) relaxation time, electron mass or Debye length, respectively. The limiting procedure is mathematically justified. This paper is a review of recent results by the authors.

1. Introduction. For the description of physical phenomena in semiconductor and plasma devices, fluid dynamical models like the hydrodynamic (or Euler-Poisson) equations are widely used. The numerical solution of the hydrodynamic models requires a lot of computing power and special algorithms. In some situations, however, the model equations can be approximated by simpler models in the sense that a small parameter appearing in the equations—e.g. the (scaled) relaxation time, the electron mass, or the Debye length—are set equal to zero. Recently, the authors started a program to justify *rigorously* these approximate models [4,7,8,9,10].

More specifically, consider an ensemble of electrons with density n_e and charge $q_e = -1$ and positively charged particles (holes for semiconductors, ions for plasmas) with density n_i and charge $q_i = +1$. Denoting by J_e, J_i the current densities of the electrons, ions respectively, and by ϕ the electrostatic potential, the variables are supposed to satisfy the following (scaled) Euler-Poisson system:

$$\partial_t n_\alpha + \mathrm{div}\, J_\alpha = 0, \quad \alpha = e, i, \tag{1}$$

$$m_\alpha \partial_t J_\alpha + m_\alpha \mathrm{div}\,(J_\alpha \otimes J_\alpha / n_\alpha) + \nabla p_\alpha(n_\alpha) = -q_\alpha n_\alpha \nabla\phi - m_\alpha J_\alpha/\tau_\alpha, \tag{2}$$

$$-\lambda^2 \Delta\phi = n_i - n_e, \quad (t, x) \in (0, \infty) \times \mathbb{R}, \tag{3}$$

$$n_\alpha(0, x) = n_{I,\alpha}(x),\ J_\alpha(0, x) = J_{I,\alpha}(x), \quad x \in \mathbb{R}. \tag{4}$$

Here, $J_\alpha \otimes J_\alpha$ denotes the tensor product with components $J_{\alpha,i} J_{\alpha,k}$, $i, k = 1, \ldots, d$, $d \geq 1$. The physical constants are the (scaled) particle mass $m_\alpha > 0$, the relaxation times $\tau_\alpha > 0$, and the Debye length $\lambda > 0$ ($\alpha = e, i$). In semiconductor applications, the right-hand side of the Poisson equation (3) is usually replaced by $n_i - n_e + C(x)$, where $C(x)$ describes fixed charged background ions (doping profile). We take pressure functions of the form

$$p_\alpha(n_\alpha) = a_\alpha^2 n_\alpha^{\gamma_\alpha}, \qquad \gamma_\alpha \geq 1, \quad a_\alpha > 0. \tag{5}$$

Under certain conditions (see Section 2), the evolution of the particles is given by the drift-diffusion equations ($\alpha = e, i$)

$$m_\alpha \partial_t n_\alpha - \mathrm{div}\,(\nabla p_\alpha(n_\alpha) + q_\alpha n_\alpha \nabla\phi) = 0, \qquad -\lambda^2 \Delta\phi = n_i - n_e. \tag{6}$$

We usually consider these equations in a bounded domain $\Omega \subset \mathbb{R}^d$ with initial and boundary conditions ($\alpha = e, i$)

$$n_\alpha = n_{D,\alpha},\ \phi = \phi_D \quad \text{on } \Gamma_D, \qquad \nabla p_\alpha(n_\alpha) \cdot \nu = \nabla\phi \cdot \nu = 0 \quad \text{on } \Gamma_N, \tag{7}$$

$$n_\alpha(0, \cdot) = n_{I,\alpha} \quad \text{in } \Omega. \tag{8}$$

We assume that $\partial\Omega = \Gamma_D \cup \Gamma_N \in C^{0,1}$, $\Gamma_D \cap \Gamma_N = \emptyset$, $\mathrm{meas}_{d-1}(\Gamma_D) > 0$, Γ_N is open in $\partial\Omega$, and ν is the exterior normal vector.

We are interested in (1) the zero-relaxation-time limit ("$\tau_\alpha \to 0$"), (2) the zero-electron-mass limit ($m_e \to 0$), and (3) the zero-Debye-length limit ($\lambda \to 0$) in Eqs. (1)-(4) and (6)-(8). We refer to [9,10] for physical explanations of these limits.

2. Zero-relaxation-time limits. We consider this limit in Eqs. (1)-(4) in the one-dimensional case $d = 1$. The limit $\tau_\alpha \to 0$ is taken after the rescaling $t \to t/\tau$,

$J_\alpha \to \tau J_\alpha^\tau$, where $\tau = \tau_e = \tau_i$:

$$\partial_t n_\alpha^\tau + \mathrm{div}\, J_\alpha^\tau = 0, \quad \alpha = e, i, \tag{9}$$

$$m_\alpha \tau^2 \partial_t J_\alpha^\tau + m_\alpha \tau^2 \mathrm{div}\,(J_\alpha^\tau \otimes J_\alpha^\tau / n_\alpha^\tau) + \nabla p_\alpha(n_\alpha^\tau) = -q_\alpha n_\alpha^\tau \nabla \phi^\tau - m_\alpha J_\alpha^\tau, \tag{10}$$

$$-\lambda^2 \Delta \phi^\tau = n_i^\tau - n_e^\tau, \quad (t,x) \in (0,\infty) \times \mathbb{R}, \tag{11}$$

$$n_\alpha^\tau(0,x) = n_{I,\alpha}(x),\ J_\alpha^\tau(0,x) = J_{I,\alpha}(x)/\tau, \quad x \in \mathbb{R}. \tag{12}$$

THEOREM 1 *Let $T > 0$, $0 \le n_{I,\alpha}$, $J_{I,\alpha}/n_{I,\alpha} \in L^\infty(\mathbb{R})$ with compact support. Assume $\gamma_\alpha > 1$, $\alpha = e, i$. Let $(n_\alpha^\tau, J_\alpha^\tau, \phi^\tau)$ be a weak entropy solution to (9)-(12) with $\lim_{|x|\to\infty} \phi^\tau(t,x) = 0$, $t > 0$. Then, as $\tau \to 0$, up to subsequences, $(n_\alpha^\tau, J_\alpha^\tau, \phi^\tau)$ converges to $(n_\alpha, J_\alpha, \phi)$, a solution to (6), in the following sense:*

$$n_\alpha^\tau \to n_\alpha,\ \phi^\tau \to \phi \qquad \text{in } L^p_{\mathrm{loc}}((0,T)\times\mathbb{R}) \text{ strongly, for all } p \in (1,\infty),$$
$$J_\alpha^\tau \rightharpoonup J_\alpha \qquad \text{in } L^2((0,T)\times\mathbb{R}) \text{ weakly.}$$

See, e.g. [1,11] for the existence of solutions to (9)-(12). The proof of Theorem 1 is based on the construction of weak entropies and on high energy estimates and can be found in [7,8]. The case $\gamma_\alpha = 1$ is shown in [5]. For related zero-relaxation-time limits we refer to [7,8].

3. Zero-electron-mass limits. Performing formally the limit $\delta \stackrel{\mathrm{def}}{=} m_e \to 0$ in (6) gives $n_e \nabla(h_e(n_e) - \phi) = \text{const.}$ in $(0,T)\times\Omega$, where the enthalpy h_e is defined by $s h_e'(s) = p_e'(s)$, $s > 0$, $h_e(1) = 0$. The constant vanishes when we choose boundary conditions satisfying $n_{D,e} = h_e^{-1}(\phi_D)$. Then, $h_e(n_e) - \phi = 0$ after defining a reference point for the electrostatic potential. Hence, $n_e = h_e^{-1}(\phi)$ in $(0,T)\times\Omega$ and the Poisson equation in (6) has to be replaced by

$$-\lambda^2 \Delta \phi = n_i - h_e^{-1}(\phi). \tag{13}$$

THEOREM 2 *Let $0 < \underline{n} \le n_{D,\alpha} \in C^0([0,T]; L^\infty(\Omega)) \cap H^1((0,T)\times\mathbb{R})$, $0 < \underline{n} \le n_{I,\alpha} \in L^\infty(\Omega)$, $\alpha = e, i$, and $\phi_D \in L^\infty((0,T)\times\mathbb{R}) \cap H^1(0,T; H^1(\Omega))$. Assume that $n_{D,e} = h_e^{-1}(\phi_D)$ and let $(n_\alpha^\delta, \phi^\delta)$ be a weak solution to (6)-(8). Then there exists a subsequence (not relabeled) converging, as $\delta = m_e \to 0$, to a solution (n_i, ϕ) to (13), (6) for $\alpha = i$:*

$$n_e^\delta \to h_e^{-1}(\phi),\ n_i^\delta \to n_i \qquad \text{in } L^p((0,T)\times\Omega) \text{ strongly, for all } p \in [2,\infty),$$
$$\phi^\delta \to \phi \qquad \text{in } L^2(0,T; H^1(\Omega)) \text{ strongly.}$$

This theorem which is also true for more general pressure functions p_α, has been proved in [10]. The proof relies on the use of an appropriate entropy inequality together with compactness-by-convexity arguments. For the existence of solutions, see [6].

For the zero-electron-mass limit in the Euler-Poisson system (1)-(4) we refer to [4].

4. Zero-Debye-length limits. Performing the limit $\lambda \to 0$ in Eqs. (6) we get formally, after some manipulations (see [9]), $n \stackrel{\text{def}}{=} n_e = n_i$ and

$$\partial_t n - \tfrac{1}{2}\Delta(p_i(n) + p_e(n)) = 0, \quad -\mathrm{div}\,(n\nabla\phi) = \tfrac{1}{2}\Delta(p_i(n) - p_e(n)). \tag{14}$$

THEOREM 3 *Let the regularity assumptions for $n_{I,\alpha}$, $n_{D,\alpha}$, and ϕ_D of Theorem 2 hold and assume $n_{I,e} = n_{I,i}$. Let $(n_\alpha^\lambda, \phi^\lambda)$ be a weak solution to (6)-(8). Furthermore, let $\omega \subset \Omega$ with $\overline{\omega} \subset \Omega$. Then there is a subsequence (not relabeled) such that, as $\lambda \to 0$,*

$$\begin{aligned} n_\alpha^\lambda &\to n && \text{in } L^p((0,T)\times\omega) \text{ strongly, for all } p \in [1,\infty), \\ \phi^\lambda &\rightharpoonup \phi && \text{in } L^2(0,T;H^1(\omega)) \text{ weakly,} \end{aligned}$$

and (n,ϕ) solves (14) and $n(0) = n_{I,e} = n_{I,i}$ in the sense of $H^{-1}(\omega)$.

We cannot expect global convergence in Ω since boundary layers may occur. However, if additionally $n_{D,e} = n_{D,i}$ holds on $(0,T)\times\Gamma_D$, then the above convergence results are global and (n,ϕ) satisfies the Dirichlet boundary conditions (7). The proof of Theorem 3 is also based on entropy estimates and appropriate compactness arguments [9].

The quasi-neutral limit $\lambda \to 0$ can also be performed in Eqs. (13), (6) for $\alpha = i$ [9]. Moreover, the limit $\lambda \to 0$ can be made rigorously for more general pressure functions and for so-called vacuum solutions (for which $n_\alpha = 0$ may occur locally), see [9]. In [3] the limit has been proved for non-vanishing doping profiles $C(x)$ in the Poisson equation (see Section 1).

In the hydrodynamic equations, the zero-Debye-length limit could be made rigorously, to our knowledge, only for *smooth* solutions to (1)-(4) (see [2]).

Acknowledgments. The authors acknowledge support from the DAAD-PROCOPE Program. The first author acknowledges support from the TMR Project "Asymptotic methods in kinetic theory" (ERB-FMRX-CT97-0157), and from the Gerhard-Hess Program of the DFG. The research of the second author was partially supported by the TMR network of the Project "Hyperbolic systems of conservation laws" (ERB-FMRX-CT96-0033).

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