Subsonic solutions to a one-dimensional non-isentropic hydrodynamic model for semiconductors

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Abstract

The one-dimensional stationary full hydrodynamic model for semiconductor devices with non-isentropic pressure is studied. This model consists of the equations for the electron density, electron temperature and electric field in a bounded domain supplemented with boundary conditions. The existence of a classical subsonic solution with positive particle density and positive temperature is shown in two situations: non-constant and constant heat conductivities. Moreover, we prove uniqueness of a classical solution in the latter case. The existence proofs are based on elliptic estimates, Stampacchia truncation methods and fixed-point arguments.

Keywords. Full hydrodynamic equations, existence, uniqueness, positive solutions, non-isentropic pressure.

1. Introduction

For the simulation of semiconductor devices usually drift-diffusion models are used. These models consist of the continuity equations expressing the conservation of mass and a drift-diffusion relation for the electron current density [M]. In order to model modern submicron devices and hot electron effects, however, more complicated model equations have to be considered, like energy-transport or hydrodynamic equations [Ju]. In this paper, we study the full hydrodynamic model consisting of the continuity equations expressing the conservation of mass, momentum and energy, coupled self-consistently to the Poisson equation for the electric field. The steady-state equations for the electron density n, the electron temperature T and the electric field E read as follows:

$$(1) \qquad \left(\frac{mj^2}{n} + P(n,T)\right)_x = -qnE - \frac{mj}{\tau_p},$$

$$(2) \qquad (a(n,T)T_x)_x = qjE + \frac{w - w_0}{\tau_w} + \left(\frac{mj^3}{2n^2} + \frac{5}{2}jT\right)_x,$$

$$(3) \qquad E_x = -\frac{q}{\epsilon_s}(n - C(x))$$

in the bounded domain $(0,1)$. Here, j denotes the (constant) electron current density, $P(n,T)$ the pressure, $a(n,T)$ the heat conductivity, and $C(x)$ the doping profile. The physical constants are the effective electron mass m, the elementary charge q, the momentum and energy relaxation times τ_p and τ_w, respectively, and the semiconductor permittivity ϵ_s. The energy $w = w(n,T)$ is written as $w = w_0 + \tau_w \widetilde{w}(n, T - T_L)$, where T_L is the lattice temperature and $\widetilde{w}$ satisfies $\widetilde{w}(n,0) = 0$ for all $n > 0$. We recall that the energy cannot be determined from the state equation [FW,R]. The equations (1)-(3) are supplemented by the boundary conditions

$$(4) \qquad E(0) = E_0, \quad n(0) = n_0, \quad T(0) = T_0, \quad T(1) = T_1.$$

Notice that we allow *general* pressure functions and heat conductivities. Often the energy equation (3) is replaced by the relation $P = n^\gamma$ with $\gamma > 1$. The corresponding model is referred to as the *isentropic* hydrodynamic model. The existence of solutions to this model has been studied in the mathematical literature since several years. Degond and Markowich proved the existence of steady-state solutions in the subsonic case [DM1,DM2]. Gamba showed existence of weak steady-state solutions in the transonic case by means of the vanishing viscosity method [G]. The transient equations are studied by several author, see e.g. Fang and Ito [FI], Jochmann [Jo] and Marcati and Natalini [MN] for $\gamma > 1$ and Poupaud, Rascle and Vila [PRV] for $\gamma = 1$.

For the full hydrodynamic model (1)-(3), usually the polytropic gas ansatz is used to get explicit expressions for the pressure and the energy:

$$(5) \qquad P(n,T) = nT, \quad w = \frac{3}{2}nT + \frac{j^2}{2n}.$$

The system of equations (1)-(3) with the relations (5) has been studied only recently. Yeh showed the existence of a unique strong solution in several space dimensions if the flow is subsonic, the ambient temperature T_L is large enough and the vorticity on the inflow boundary and the variation of the electron density on the boundary are sufficiently small [Y2]. Zhu and Hattori proved the existence of classical subsonic solutions in one space dimension for the whole space problem under the additional assumption that the doping profile is close to a constant [ZH]. The transient equations have been considered by Yeh [Y1] and Ito [I]. In the work of Ito, the energy equation has been replaced by an equation for the entropy, assuming the relations (5). No results, however, are available for the hydrodynamic equations with *general* pressure $P(n,T)$. In this paper we prove the existence of classical subsonic solutions to (1)-(4). More precisely, our first main result is as follows:

THEOREM 1 *Let the regularity assumptions (A1)-(A4) for* a, P, $\widetilde{w}$, *and* C *hold (see Section 2) and let* n_0, T_0, $T_1 > 0$. *Then there exist positive constants* j_0, δ, K, $\underline{n}$, $\overline{n}$, $\underline{T}$, *and* $\overline{T}$ *such that if*

$$|j| \leq j_0, \quad |T_0 - T_L| + |T_1 - T_L| \leq \delta \tag{6}$$

and

$$\partial_n P(\rho, \theta) \geq K \quad \text{for all } \underline{n} \leq \rho \leq \overline{n}, \ \underline{T} \leq \theta \leq \overline{T}, \tag{7}$$

there is a classical solution (n,T,E) *of (1)-(4) satisfying*

$$0 < \underline{n} \leq n(x) \leq \overline{n}, \quad 0 < \underline{T} \leq T(x) \leq \overline{T} \quad \text{for } x \in [0,1]. \tag{8}$$

The proof of this theorem is based on the Schauder fixed point theorem and on the following reformulation of (1):

$$\left(\partial_n P(n,T) - \frac{mj^2}{n^2} \right) n_x = -\left(\partial_T P(n,T) + qnE + \frac{mj}{\tau_p} \right). \tag{9}$$

The first condition in (6) corresponds to a subsonic condition. Indeed, subsonic flow is characterized by

$$\left| \frac{j}{n} \right| < \sqrt{\partial_n P/m}.$$

In the proof of Theorem 1 it is shown that $j_0 < \underline{n}\sqrt{K/m}$. Thus

$$\left| \frac{j}{n} \right| \leq \frac{j_0}{\underline{n}} < \sqrt{K/m} \leq \sqrt{\partial_n P/m}.$$

In particular, the bracket on the left-hand side of (9) is positive.

The second condition in (6) is needed to estimate T_x in the space $L^\infty(0,1)$. This bound is used in (9) in order to control the L^∞ bound on n_x. Together with the assumption (7), for given bounds for the right-hand side of (9), $|n_x|$ can be controlled. Indeed, for sufficiently large K, the variation of the electron density is small enough to get positivity of the variable.

In the case $P(n,T) = nT$, the condition (7) is equivalent to the hypothesis of sufficiently large ambient temperature which has been assumed by Yeh [Y2]. Hence, the case $P(n,T) = nT$ is included in condition (7) if T_L is sufficiently large.

In the case of constant heat conductivity $a(n,T)$, the assumption of sufficiently small differences $|T_0 - T_L|$, $|T_1 - T_L|$ can be dropped. Our second main result reads:

THEOREM 2 *Let the assumptions (A1)-(A4) hold and let* n_0, T_0, $T_1 > 0$. *Furthermore, let* $a = const$. *Then there exist positive constants* $j_0, K, \underline{n}, \overline{n}, \underline{T}, \overline{T} > 0$ *such that if* $0 < j \le j_0$ *hold, there is a classical solution* (n,T,E) *of (1)-(4) satisfying (8). Moreover, under the additional condition (A5), this solution is unique in the class of classical solutions satisfying (8).*

This paper is organized as follows. In Section 2, we make precise the assumptions (A1)-(A5) and prove Theorem 1. Theorem 2 is proved in Section 3.

2. Assumptions and proof of Theorem 1

For Theorems 1 and 2 we have supposed the following assumptions:

(A1) $P(n,T)$ is continuously differentiable in $(n,T) \in (0,\infty)^2$.

(A2) $a(n,T)$ is continuously differentiable and $a(n,T) > 0$ in $(n,T) \in (0,\infty)^2$.

(A3) $\widetilde{w}$ is continuous in both arguments, Lipschitz continuous in T, and

$$\widetilde{w}(n, T - T_L)(T - T_L) \ge 0$$

for all $(n,T) \in (0,\infty)^2$ and some $T_L > 0$.

(A4) $C \in L^1(0,1)$.

For the uniqueness result (see Theorem 2) we also need the assumption

(A5) $\widetilde{w}(n,T)$ is Lipschitz continuous in n and

$$(\widetilde{w}(\rho, \theta_1 - T_L) - \widetilde{w}(\rho, \theta_2 - T_L))(\theta_1 - \theta_2) \ge 0 \quad \text{for all } \rho, \theta_1, \theta_2 > 0.$$

The monotonicity of $\widetilde{w}$ imposed in (A5) (and in a weaker form in (A3)) is reasonable from physical considerations. Notice that, due to assumption (A2), the equation for the temperature is allowed to be of degenerate type.

Proof of Theorem 1: Introduce the closed convex set

$$B = \{(\rho,\theta) \in C^0([0,1]) \times C^1([0,1]) : \underline{n} \le \rho(x) \le \overline{n},\ \underline{T} \le \theta(x) \le \overline{T},$$

$$|(\theta - \varphi)_x(x)| \le M \text{ for } x \in [0,1]\}$$

where $\varphi(x) = T_1 + (T_0 - T_1)(1-x)$ and the positive constants $\underline{n}$, $\overline{n}$, $\underline{T}$, $\overline{T}$ and M are defined below. Now let $(\rho,\theta) \in B$ and define

$$E(x) = E_0 + \frac{q}{\varepsilon}\int_0^x (C-\rho)ds.$$

Further, let $n \in C^1([0,1])$ be the unique solution of the linear problem

$$\left(\partial_n P(\rho,\theta) - \frac{mj^2}{\rho^2}\right) n_x = -\left(\partial_T P(\rho,\theta)\theta_x + q\rho E + \frac{jm}{\tau_p}\right), \tag{10}$$

$$n(0) = n_0, \tag{11}$$

where we take $0 < j < \underline{n}\sqrt{K/m}$, $K > 0$ being defined below. This implies by (7) that the bracket on the left-hand side of (10) is positive.

Finally, let $T \in C^2([0,1])$ be the unique solution of the monotone problem

$$(a(n,\theta)T_x)_x = qjE + \widetilde{w}(\rho, T - T_L) + \frac{5}{2}jT_x - \frac{mj^3}{\rho^3}n_x, \tag{12}$$

$$T(0) = T_0, \quad T(1) = T_1. \tag{13}$$

The existence and uniqueness of a solution to (12)-(13) follow from standard arguments (see, e.g., [Tr]). This defines the fixed-point operator

$$S : B \to C^0([0,1]) \times C^1([0,1]), \quad S(\rho,\theta) = (n,T).$$

Since $(n,T) \in C^1([0,1]) \times C^2([0,1])$, it is easy to see that $S(B)$ is precompact. Moreover, using standard arguments, S is continuous. In order to apply the Schauder fixed-point theorem (see [GT,Tr]), it remains to prove that $S(B) \subset B$.

First we show that there exist constants $\underline{n}, \overline{n} > 0$ such that $\underline{n} \le n(x) \le \overline{n}$ for $x \in [0,1]$. Fix $0 < j \le j_1$ with arbitrary $j_1 > 0$, $0 < N < n_0$ and

$$C_1 = (|T_1 - T_0| + M)\max\{|\partial_T P(\rho,\theta)| : \underline{n} \le \rho \le \overline{n}, \underline{T} \le \theta \le \overline{T}\} + qj_1 E_\infty + j_1 m/\tau_p,$$

where $E_\infty = |E_0| + \frac{q}{\varepsilon_s}(\|C\|_1 + \overline{n})$. Here and in the following, the norm of $L^p(0,1)$ is denoted by $\|\cdot\|_p$. Then, by Assumption (7), taking $K = 2C_1/N$ and $0 < j \le j_2 := \underline{n}\sqrt{K/2m}$, we have

$$\partial_n P(\rho,\theta) - \frac{mj^2}{\rho^2} \ge K - \frac{mj_2^2}{\underline{n}^2} = \frac{K}{2},$$

and from Eq. (10) we obtain the estimate

$$|n_x| \le \frac{2}{K}\left|\partial_T P(\rho,\theta)\theta_x + q\rho E + \frac{jm}{\tau_p}\right| \le \frac{2}{K}C_1 = N.$$

Defining $\underline{n} = n_0 - N$, $\overline{n} = n_0 + N$, this implies that $\underline{n} \le n(x) \le \overline{n}$ for $x \in [0,1]$. Notice that $\underline{n} > 0$ since $N < n_0$.

Next we prove that there exist constants $\underline{T}, \overline{T} > 0$ such that $\underline{T} \le T(x) \le \overline{T}$ for $x \in [0,1]$ by employing the Stampacchia truncation method. According to Assumption (A2) and the bounds on n and θ, there exists a constant $\alpha > 0$ such that $a(n,\theta) \ge \alpha$. Set $\overline{\theta} = \max(T_0, T_1, T_L)$ and use $(T - \overline{\theta})^+ = \max(0, T - \overline{\theta})$ as a test function in the weak formulation of (12):

$$\alpha \int_0^1 |(T-\overline{\theta})_x^+|^2 dx \le \int_0^1 (\frac{mj^3}{\rho^3}n_x - qjE)(T-\overline{\theta})^+ dx - \int_0^1 \widetilde{w}(\rho, T - T_L)(T-\overline{\theta})^+ dx$$

$$-\frac{5}{2}j\int_0^1 T_x (T-\overline{\theta})^+ dx.$$

The second term on the right-hand side is non-positive due to Assumption (A3). The last term vanishes since

$$-\frac{5}{2}j\int_0^1 T_x(T-\overline{\theta})^+ dx = -\frac{5}{4}j\int_0^1 (((T-\overline{\theta})^+)^2)_x dx = -\frac{5}{4}j\left[((T-\overline{\theta})^+)^2\right]_0^1 = 0.$$

Therefore, setting

$$C_2 = \frac{mj_2^2}{\alpha\overline{n}^3}N + \frac{q}{\alpha}E_\infty,$$

we get

$$\int_0^1 |(T-\overline{\theta})_x^+|^2 dx \le C_2 j \int_0^1 (T-\overline{\theta})^+ dx \le C_2 j \,\mathrm{meas}(T > \overline{\theta})^{1/2} \|(T-\overline{\theta})^+\|_2.$$

Using Poincaré's inequality $\|(T-\overline{\theta})^+\|_2 \le \frac{1}{\sqrt{2}}\|(T-\overline{\theta})^+_x\|_2$, we obtain

$$\|(T-\overline{\theta})^+_x\|_2 \le j\frac{C_2}{\sqrt{2}}\text{meas}(T>\overline{\theta})^{1/2}. \tag{14}$$

The imbedding $H^1(0,1)\hookrightarrow L^r(0,1)$ is continuous for any $r\le\infty$ and it is well known that for $\mathcal{U}>\overline{\theta}$ and $r>2$ the inequality

$$\text{meas}(T>\mathcal{U})^{1/r}(\mathcal{U}-\overline{\theta}) \le c\|(T-\overline{\theta})^+\|_{H^1}$$

holds [St, Ch.4]. Therefore we get from (14) and Poincaré's inequality, for another constant $c>0$, for $\mathcal{U}\ge\overline{\theta}$,

$$\text{meas}(T>\mathcal{U}) \le \frac{c}{(\mathcal{U}-\overline{\theta})^r}\text{meas}(T>\overline{\theta})^{r/2}.$$

Choosing $r/2>1$, we can apply Stampacchia's lemma [St, Ch.4]. Hence, there is a constant C_3 depending only on C_2 such that $T\le\overline{\theta}+jC_3$ in $[0,1]$. We set $\overline{T}=\overline{\theta}+j_2C_3$.

For the lower bound we set $\underline{\theta}=\min(T_0,T_1,T_L)$ and use $(-T+\underline{\theta})^+$ as a test function in the weak formulation of (12). A similar estimate as above gives

$$\|(-T+\underline{\theta})^+_x\|_2 \le jC_2'\text{meas}(-T>-\underline{\theta})^{1/2}$$

and in an analogous way we conclude the existence of a constant C_4 depending only on C_2' such that $-T\le-\underline{\theta}+jC_4$ in $[0,1]$, i.e.

$$T\ge\underline{\theta}-jC_4 \quad \text{in} \quad [0,1].$$

Setting $j_3=\underline{\theta}/2C_4$ and $\underline{T}=\underline{\theta}/2$, we obtain for all $0<j\le j_3$:

$$T\ge\underline{\theta}-j_3C_4=\underline{T} \quad \text{in} \quad [0,1].$$

It remains to prove that $\|(T-\varphi)_x\|_\infty\le M$ for an appropriate constant $M>0$. By elliptic estimates (see, e.g. [GT]), there exists a constant $C_5>0$ depending on the $W^{1,\infty}$ norms of n and θ (and hence, on $\overline{n},N,\overline{T}$ and $|T_1-T_0|+M$) such that

$$\|T\|_{H^2}\le C_5(M)\left\|qjE+\widetilde{w}(\rho,T-T_L)+\frac{5}{2}jT_x-mj^3\rho^{-3}n_x\right\|_2.$$

Using the Lipschitz continuity of $\widetilde{w}(\rho,\cdot)$ and the above bounds, it is clear that if j and $|T_0-T_L|+|T_1-T_L|$ are chosen sufficiently small, the L^2 norm on the right-hand side can be made arbitrarily small.

Thus there exist $j_4 \leq \min(j_1, j_2, j_3)$ and $\delta > 0$ such that for all $0 < j \leq j_4$ and $|T_0 - T_L| + |T_1 - T_L| \leq \delta$,

$$\|(T-\varphi)_x\|_\infty \leq \|T_x\|_\infty + |T_1 - T_0| \leq c\|T\|_{H^2} + \delta \leq M$$

Here we do not need to impose restrictions on $M > 0$.

We have shown that $S(B) \subset B$. Hence, Schauder's Theorem applies and we obtain a classical solution to the boundary-value problem (1)-(4).

3. Proof of Theorem 2

The proof of the existence result of Theorem 2 is similar to that of Theorem 1, except the proof of $\|(T-\varphi)_x\|_\infty \leq M$. From (12) we get the estimate

$$a\|T_{xx}\|_2 \leq qjE_\infty + c|T - T_L| + \frac{5}{2}j\|T_x\|_2 + mj^3\underline{n}^{-3}N.$$

Since $T - \varphi$ vanishes at $x = 0$ and $x = 1$, there exists $x_0 \in (0,1)$ such that $(T-\varphi)_x(x_0) = 0$. Thus

$$(T-\varphi)_x(x) = \int_{x_0}^{x} T_{xx}ds$$

and

$$\|T_x\|_2 \leq |T_1 - T_0| + \|T_{xx}\|_2.$$

We obtain

$$\left(a - \frac{5}{2}j\right)\|T_{xx}\|_2 \leq qjE_\infty + c|T - T_L| + mj^3\underline{n}^{-3}N + \frac{5}{2}j|T_1 - T_0|.$$

Taking $0 < j \leq j_5 = \min(j_1, j_2, j_3, \frac{a}{5})$ we can find a constant $M > 0$ such that

$$\|(T-\varphi)_x\|_\infty \leq c\|T\|_{H^2} + |T_1 - T_0| \leq M.$$

This proves the existence of solutions.

To prove the uniqueness of solutions, let $(n^{(1)}, T^{(1)}, E^{(1)})$ and $(n^{(2)}, T^{(2)}, E^{(2)})$ be two classical solutions of (1)-(4) satisfying (8). Then, taking the difference of the Eqs. (2) satisfied by $T^{(1)}$, $T^{(2)}$, respectively, and using $T^{(1)} - T^{(2)}$ as test function in the differnece, we obtain

$$a\int_0^1 (T^{(1)} - T^{(2)})_x^2 dx = -qj\int_0^1 (E^{(1)} - E^{(2)})(T^{(1)} - T^{(2)})dx$$

$$-\int_0^1 (\widetilde{w}(n^{(1)},T^{(1)}-T_L)-\widetilde{w}(n^{(2)},T^{(2)}-T_L))(T^{(1)}-T^{(2)})dx$$

$$+\frac{mj^3}{2}\int_0^1\left(\frac{1}{(n^{(1)})^2}-\frac{1}{(n^{(2)})^2}\right)(T^{(1)}-T^{(2)})_x dx-\frac{5}{2}j\int_0^1 (T^{(1)}-T^{(2)})_x(T^{(1)}-T^{(2)})dx$$

$$= I_1+\cdots+I_4.$$

In view of Assumption (A5) (see Section 2) and Poincaré's inequality, it holds

$$I_2 \le -\int_0^1 (\widetilde{w}(n^{(1)},T^{(1)}-T_L)-\widetilde{w}(n^{(2)},T^{(1)}-T_L))(T^{(1)}-T^{(2)})dx$$

$$\le c\|n^{(1)}-n^{(2)}\|_2\|(T^{(1)}-T^{(2)})_x\|_2,$$

where $c>0$ denotes a positive generic constant. Furthermore, the first and third integral can be estimated as follows:

$$I_1+I_3 \le cj(\|E^{(1)}-E^{(2)}\|_2\|T^{(1)}-T^{(2)}\|_2+\|n^{(1)}-n^{(2)}\|_2\|(T^{(1)}-T^{(2)})_x\|_2)$$

$$\le cj\|n^{(1)}-n^{(2)}\|_2\|(T^{(1)}-T^{(2)})_x\|_2.$$

Finally, the fourth term vanishes: $I_4=0$. Therefore, we obtain

$$\|(T^{(1)}-T^{(2)})_x\|_2 \le cj\|n^{(1)}-n^{(2)}\|_2. \tag{15}$$

To derive an estimate for $n^{(1)}-n^{(2)}$, we take the difference of Eqs. (1) for $n^{(1)}$, $n^{(2)}$, respectively, integrate over $0<\xi<x$ for some $x\in(0,1]$, and multiply the resulting equation with $(n^{(1)}-n^{(2)})(x)$:

$$\left(P(n^{(1)},T^{(1)})-P(n^{(2)},T^{(2)})\right)(x)(n^{(1)}-n^{(2)})(x) \tag{16}$$

$$=-\left(\frac{mj^2}{n^{(1)}}-\frac{mj^2}{n^{(2)}}\right)(x)(n^{(1)}-n^{(2)})(x)-q\int_0^x (n^{(1)}E^{(1)}-n^{(2)}E^{(2)})d\xi(n^{(1)}-n^{(2)})(x).$$

We estimate the left-hand side by using the Lipschitz continuity of P in $[\underline{n},\overline{n}]\times[\underline{T},\overline{T}]$:

$$\left(P(n^{(1)},T^{(1)})-P(n^{(2)},T^{(2)})\right)(x)(n^{(1)}-n^{(2)})(x)$$

$$=\int_0^1 \partial_n P(\lambda n^{(1)}+(1-\lambda)n^{(2)},T^{(1)})(x)d\lambda(n^{(1)}-n^{(2)})(x)^2$$

$$+\left(P(n^{(2)},T^{(1)})-P(n^{(2)},T^{(2)})\right)(x)(n^{(1)}-n^{(2)})(x)$$

$$\ge K(n^{(1)}-n^{(2)})(x)^2-c|(T^{(1)}-T^{(2)})(x)(n^{(1)}-n^{(2)})(x)|.$$

The right-hand side of (16) is majorized by

$$cj|(n^{(1)} - n^{(2)})(x)|^2 + c\|n^{(1)} - n^{(2)}\|_1^2.$$

Therefore, we get from (16)

$$K\|n^{(1)} - n^{(2)}\|_\infty^2 \le c\|T^{(1)} - T^{(2)}\|_\infty \|n^{(1)} - n^{(2)}\|_\infty + c(j+1)\|n^{(1)} - n^{(2)}\|_\infty^2.$$

Choosing $K > 0$ large enough, we conclude, using Sobolev's inequality,

$$\|n^{(1)} - n^{(2)}\|_\infty \le c\|T^{(1)} - T^{(2)}\|_\infty \le c\|(T^{(1)} - T^{(2)})_x\|_2.$$

Hence, by (15),

$$\|(T^{(1)} - T^{(2)})_x\|_2 \le cj\|n^{(1)} - n^{(2)}\|_\infty \le cj\|(T^{(1)} - T^{(2)})_x\|_2.$$

Thus, choosing $j > 0$ small enough, we obtain $T^{(1)} = T^{(2)}$. This implies $n^{(1)} = n^{(2)}$ and $E^{(1)} = E^{(2)}$. The theorem is proved.

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