Convergent Iterative Schemes for a Non–isentropic Hydrodynamic Model for Semiconductors

Pablo Amster

Depto. de Matemática,

Universidad de Buenos Aires

1428 Buenos Aires, Argentina,

email: pamster@dm.uba.ar

René Pinnau

Fachbereich Mathematik,

Technische Universität Darmstadt

D–64289 Darmstadt, Germany,

email: pinnau@mathematik.tu-darmstadt.de

Abstract

Two iterative schemes for the solution of the one–dimensional stationary full hydrodynamic model for semiconductor devices are studied. This model consists of a system of balance equations for the electron density, temperature and the electric field. The first iterative scheme relies on a decoupling of the equations in the spirit of the well–known *Gummel–iteration* for the standard drift diffusion model. Convergence is proven in the case of small deviations from the equilibrium state and high lattice temperature. Secondly, a full *Newton–iteration* is analyzed and its local second order convergence is proven.

Key words. Full hydrodynamic equations, Gummel–iteration, Newton–iteration, linearization, convergence.

AMS(MOS) subject classification. 65J15, 76N10

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1 Introduction

The ongoing miniaturization of semiconductor devices posed several challenges for numerical simulation techniques. Usually, drift diffusion models are employed, but they are not capable of resolving accurately high field phenomena such as hot electron effects, impact ionization and heat generation in the bulk material. Thus, generalizations of the drift diffusion equations were developed such as the energy transport or the hydrodynamic equations (see [MRS90, Jün01] and the references therein).

Here, we consider a *full hydrodynamic model* consisting of balance equations for the carrier density, momentum and energy, which are self–consistently coupled to Poisson's equation for the electric field. They can be derived as a moment expansion of the Boltzmann equation assuming appropriate closure conditions [GMR96]. We want to consider the one–dimensional stationary equations with non–isentropic pressure, which are stated on the bounded domain $\Omega = (0,1)$:

$$\left(\frac{m\,j^2}{n} + P(n,T)\right)_x = -q\,n\,E - \frac{m\,j}{\tau_p}, \tag{1.1a}$$

$$(a(n,T)\,T_x)_x = q\,j\,E + \frac{\tilde{w} - w_0}{\tau_w} + \left(\frac{m\,j^3}{2\,n^2} + \frac{5}{2} j\,T\right)_x, \tag{1.1b}$$

$$E_x = -\frac{q}{\epsilon_s}(n - C(x)). \tag{1.1c}$$

Here, the variables are the electron density $n(x)$, the temperature $T(x)$ and the electric field $E(x)$. The parameters are the current density j, the effective electron mass m, the elementary charge q, the relaxation times for momentum and energy τ_p and τ_w, respectively, and the semiconductor permittivity ϵ_s. The pressure function is given by $P(n,T)$ and the heat conductivity is $a(n,T)$. The density of charged background ions is denoted by $C(x)$. Further, the energy $\tilde{w} = \tilde{w}(n,T)$ can be written as

$$\tilde{w} = w_0 + \tau_w\, w(n, T - T_L),$$

where T_L denotes the lattice temperature and it holds $w(n,0) = 0$ for all $n > 0$.

The system (1.1) is supplemented with boundary conditions

$$n(0) = n_0, \quad E(0) = E_0, \quad T(0) = T_0, \quad T(1) = T_1. \tag{1.2}$$

System (1.1) has been studied analytically only recently by several authors [Yeh96, Yeh97, ZH98] employing the polytropic gas ansatz, by [DM90, DM93] for isentropic pressure functions and by [AVJM00] in the case of general pressure functions.

Generally, hyperbolic methods from computational gas dynamics are well suited for the transient simulations and the steady–state is obtained as the asymptotic large time limit. However, for the computation of current–voltage characteristics one only needs the stationary solution. This led to the development of solution methods, which work directly on the stationary equations and which proved to be one magnitude faster than the transient solvers [GJR89].

In this paper we will introduce two schemes for the numerical treatment of (1.1) and prove their convergence in the subsonic regime and for large lattice temperature. The first one is a *Gummel–type iteration*, which is robust and globally convergent. In the second approach we consider a *Newton iteration*, which exhibits the typical local second order convergence.

Especially, for semiconductor device simulations a combination of both methods proved to be well suited, i.e. employing the Gummel–type iteration to compute a good starting point for the Newton scheme. Alternatively, in [GJR89] a damped Newton–iteration was used to solve system (1.1) with a different set of variables and boundary conditions. For an excellent overview on hydrodynamical models and modern numerical approaches we refer to [AR99] and the references therein.

The paper is organized as follows. In Section 2 we decouple system (1.1) in a Gummel–type manner and prove the contractivity of the induced fixed point mapping. The full Newton–Iteration is considered in Section 3, where the unique solvability of the linearized system is shown which yields the local quadratic convergence of the iteration.

2 Gummel–type Iteration

In this section we decouple system (1.1) in the spirit of the well known *Gummel–iteration* for the standard drift diffusion model [Gum64]. We prove convergence of this iteration by means of Banach's fixed point principle in case of a subsonic regime and large lattice temperature.

For notational convenience we assume here and in the following section that

$$m = q = \epsilon_s = \tau_p = \tau_w = 1.$$

In [AVJM00, Theorem1] an existence result for (1.1) is given for subsonic states near the thermal equilibrium and large lattice temperature. Accordingly we assume

A.1 $a(n,T)$ is continuously differentiable and $a(n,T) > 0$ in $(n,T) \in (0,\infty)^2$.

A.2 $P(n,T)$ is continuously differentiable in $(n,T) \in (0,\infty)^2$ and there exist positive constants $\underline{n}$, $\overline{n}$, $\underline{T}$, $\overline{T}$ and K, such that

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

A.3 w is continuously differentiable and

$$w(n, T - T_L)(T - T_L) \geq 0$$

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

A.4 $C \in L^1(0, 1)$.

The proof of this theorem employs a fixed point argument based on the following reformulation of (1.1a):

$$\left(\partial_n P(n, T) - \frac{j^2}{n^2} \right) n_x = - \left(\partial_T P(n, T) + nE + j \right).$$

A compact operator $\mathcal{T} : \widetilde{B} \to \widetilde{B}$ is defined, where $\widetilde{B}$ is the closed convex set given by

$$\begin{aligned} \widetilde{B} = \big\{ (\rho, \theta) \in C^0([0, 1]) \times C^1([0, 1]) : \underline{n} \leq \rho(x) \leq \overline{n}, \\ \underline{T} \leq \theta(x) \leq \overline{T},\ |(\theta - \varphi)_x(x)| \leq M \text{ for } x \in [0, 1] \big\} \end{aligned}$$

with $\varphi(x) = T_0 + (T_1 - T_0)x$. Our aim is to prove that if we assume the additional condition

A.5 $(w(\rho, \theta_1 - T_L) - w(\rho, \theta_2 - T_L))(\theta_1 - \theta_2) \geq 0 \quad$ for all $\rho, \theta_1, \theta_2 > 0$.

then a Gummel–type iteration is applicable and convergent, i.e. we decouple the equations of system (1.1) in an appropriate way, defining a fixed point operator, and show that it is in fact a contraction. For this purpose we define the operator $\mathcal{T}$:

For any $(\rho, \theta) \in \widetilde{B}$ we set

$$E(x) = E_0 + \int_0^x (C - \rho) ds$$

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

$$\left(\partial_n P(\rho, \theta) - \frac{j^2}{\rho^2} \right) n_x = - \left(\partial_T P(\rho, \theta)\theta_x + \rho E + j \right), \qquad n(0) = n_0, \tag{2.1}$$

which is well defined for j small enough.

Finally, we set $\mathcal{T}(\rho, \theta) = (n, T)$, where T is the unique solution of the monotone problem

$$(a(n, \theta)T_x)_x = jE + w(\rho, T - T_L) + \frac{5}{2} jT_x - \frac{j^3}{\rho^3} n_x, \qquad T(0) = T_0, \quad T(1) = T_1.$$

We remark that the condition $\theta_x \in C^0([0,1])$ is not used in this definition; this allows us to extend the operator $\mathcal{T}$ to a more convenient domain:

$$B = \big\{(\rho,\theta) \in C^0([0,1]) \times H^1(0,1) : \underline{n} \le \rho(x) \le \overline{n},$$
$$\underline{T} \le \theta(x) \le \overline{T} \text{ for } x \in [0,1],\ \|(\theta-\varphi)_x\|_2 \le M\big\}\,.$$

Following the outline of the proof of [AVJM00, Theorem1], it is easy to check that $\mathcal{T}(B) \subset B$.

The main result of this section is

Theorem 2.1. *Assume* **A.1**–**A.5** *and let ∇P be Lipschitz–continuous on $[\underline{n},\overline{n}]\times[\underline{T},\overline{T}]$. Then there exist constants $j_0, \delta > 0$ such that for*

$$|j| \le j_0, \quad |T_0 - T_L| + |T_1 - T_L| \le \delta,$$

the mapping $\mathcal{T} : B \to B$ is a contraction with respect to the product norm on $C^0([0,1]) \times H^1(0,1)$.

Remark 2.2. Subsonic flow is characterized by $|j/n| < \sqrt{\partial_n P}$ which is certainly fulfilled for $j_0/\underline{n} < \sqrt{K}$.

Proof. For $(\rho_i,\theta_i) \in B$, $i = 1,2$ and $n_i \stackrel{\text{def}}{=} (\mathcal{T}(\rho_i,\theta_i))_1$, we estimate

$$\begin{aligned}
&\int_0^1 \left(\partial_n P(\rho_1,\theta_1)(n_1)_x - \partial_n P(\rho_2,\theta_2)(n_2)_x\right)(n_1-n_2)_x\,dx = \\
&\qquad \int_0^1 \partial_n P(\rho_1,\theta_1)(n_1-n_2)_x^2\,dx \\
&\qquad + \int_0^1 \left(\partial_n P(\rho_1,\theta_1) - \partial_n P(\rho_2,\theta_2)\right)(n_2)_x(n_1-n_2)_x\,dx \\
&\qquad \ge K\|(n_1-n_2)_x\|_{L^2}^2 - L(\|\rho_1-\rho_2\|_{L^\infty} + \|\theta_1-\theta_2\|_{L^\infty})\|(n_2)_x\|_{L^2}\|(n_1-n_2)_x\|_{L^2}
\end{aligned}$$

where L is the Lipschitz constant for $\partial_n P$. Further,

$$\begin{aligned}
&\int_0^1 \left(\frac{j^2(n_1)_x}{\rho_1^2} - \frac{j^2(n_2)_x}{\rho_2^2}\right)(n_1-n_2)_x\,dx = \\
&\qquad j^2\int_0^1 \frac{(n_1-n_2)_x^2}{\rho_1^2} + j^2\int_0^1\left(\frac{1}{\rho_1^2} - \frac{1}{\rho_2^2}\right)(n_2)_x(n_1-n_2)_x\,dx \\
&\qquad \le \frac{j^2}{\underline{n}^2}\left(\|(n_1-n_2)_x\|_{L^2} + \frac{2\overline{n}}{\underline{n}^2}\|\rho_1-\rho_2\|_{L^\infty}\|(n_2)_x\|_{L^2}\|(n_1-n_2)_x\|_{L^2}\right)
\end{aligned}$$

From (2.1) and the continuity of $\partial_T P$, it is clear that $\|(n_2)_x\|_2$ is uniformly bounded for large K, which also ensures the uniform $L^\infty(0,1)$–bound on n.

Hence,

$$
\begin{aligned}
&\int_0^1 \left(\partial_n P(\rho_1,\theta_1)(n_1)_x - \partial_n P(\rho_2,\theta_2)(n_2)_x\right)(n_1-n_2)_x\,dx \\
&\qquad\qquad - \int_0^1 \left(\frac{j^2(n_1)_x}{\rho_1^2} - \frac{j^2(n_2)_x}{\rho_2^2}\right)(n_1-n_2)_x\,dx \\
&\geq \left(K - \frac{j^2}{\underline{n}^2}\right)\|(n_1-n_2)_x\|_{L^2}^2 - \widetilde{L}(\|\rho_1-\rho_2\|_{L^\infty} + \|\theta_1-\theta_2\|_{H^1})\|(n_1-n_2)_x\|_{L^2}
\end{aligned}
$$

for some positive constant $\widetilde{L} = \widetilde{L}(j,\delta,K,\underline{n},\overline{n},\underline{T},\overline{T})$. In the same way,

$$
\begin{aligned}
-\int_0^1 &\left(\partial_T P(\rho_1,\theta_1)(\theta_1)_x - \partial_T P(\rho_2,\theta_2)(\theta_2)_x\right)(n_1-n_2)_x\,dx \leq \\
&\qquad \|\partial_T P(\rho_1,\theta_1)\|_{L^\infty}\|(\theta_1-\theta_2)_x\|_{L^2}\|(n_1-n_2)_x\|_{L^2} \\
&\qquad + L(\|\rho_1-\rho_2\|_{L^\infty} + \|\theta_1-\theta_2\|_{H^1})\|(\theta_2)_x\|_{L^2}\|(n_1-n_2)_x\|_{L^2} \\
&\qquad \leq c_1(\|\rho_1-\rho_2\|_{L^\infty} + \|\theta_1-\theta_2\|_{H^1})\|(n_1-n_2)_x\|_{L^2}
\end{aligned}
$$

for some constant $c_1 > 0$. Note that $|E_1 - E_2| = |\int_0^x(\rho_1-\rho_2)ds| \leq \|\rho_1-\rho_2\|_{L^\infty}$, which implies

$$
-\int_0^1 (\rho_1 E_1 - \rho_2 E_2)(n_1-n_2)_x \leq c_2\|\rho_1-\rho_2\|_{L^\infty}\|(n_1-n_2)_x\|_{L^2}
$$

for some constant $c_2 = c_2(\overline{n}) > 0$. Taking the difference of

$$
\left(\partial_n P(\rho_i,\theta_i) - \frac{j^2}{\rho_i^2}\right)(n_i)_x = -\left(\partial_T P(\rho_i,\theta_i)(\theta_i)_x + \rho_i E + j\right)
$$

and testing with $(n_1-n_2)_x$ yields according to the above estimates

$$
\left(K - \frac{j^2}{\underline{n}^2}\right)\|(n_1-n_2)_x\|_{L^2} \leq (c_1+c_2+\widetilde{L})(\|\rho_1-\rho_2\|_{L^\infty} + \|\theta_1-\theta_2\|_{H^1})
$$

Choosing now $K > 0$ such that

$$
\mu \stackrel{\text{def}}{=} \frac{c_1+c_2+\widetilde{L}}{K - \frac{j^2}{\underline{n}^2}} < 1
$$

we obtain by Poincaré's inequality

$$
\|n_1-n_2\|_{H^1} \leq \frac{\mu\,\pi}{1+\pi}\left(\|\rho_1-\rho_2\|_{C^0} + \|\theta_1-\theta_2\|_{H^1}\right)
$$

Consider now $T_i \stackrel{\rm def}{=} (\mathcal{T}(\rho_i,\theta_i))_2$, and calculate

$$\int_0^1 (a(n_1,\theta_1)(T_1)_x - a(n_2,\theta_2)(T_2)_x)(T_1-T_2)_x\,dx = -j\int_0^1 (E_1-E_2)(T_1-T_2)\,dx$$
$$-\int_0^1 [w(\rho_1,T_1-T_L)-w(\rho_2,T_2-T_L)](T_1-T_2)\,dx - \frac{5}{2}j\int_0^1 (T_1-T_2)_x(T_1-T_2)\,dx$$
$$+\,j^3\int_0^1 \left(\frac{(n_1)_x}{\rho_1^3}-\frac{(n_2)_x}{\rho_2^3}\right)(T_1-T_2)\,dx$$
$$\stackrel{\rm def}{=} I_1+I_2+I_3+I_4$$

Since T_1-T_2 satisfies homogeneous boundary conditions, it is clear that $I_3=0$. Moreover, from **A.5** we get

$$\begin{aligned} I_2 &\le -\int_0^1 (w(\rho_1,T_1-T_L)-w(\rho_2,T_1-T_L))(T_1-T_2)\,dx \\ &\le c(\delta)\|\rho_1-\rho_2\|_{L^2}\|T_1-T_2\|_{L^2}, \end{aligned}$$

for some positive constant $c(\delta)$ with $c(\delta)\to 0$ as $\delta\to 0$ due to **A.3** and $w(\rho,0)=0$. Further, we easily check that

$$\begin{aligned} I_1+I_4 &\le j\big(\|E_1-E_2\|_{L^2}+c_1\|(n_1-n_2)_x\|_{L^2}+c_2\|\rho_1-\rho_2\|_{L^\infty}\big)\|T_1-T_2\|_{L^2} \\ &\le c_3\,j(\|\rho_1-\rho_2\|_{L^\infty}+\|\theta_1-\theta_2\|_{H^1})\|T_1-T_2\|_{L^2} \end{aligned}$$

for positive constants c_k, $k=1,2,3$. For the left–hand side we have:

$$\int_0^1 (a(n_1,\theta_1)(T_1)_x - a(n_2,\theta_2)(T_2)_x)(T_1-T_2)_x\,dx = \int_0^1 a(n_1,\theta_1)(T_1-T_2)_x^2\,dx$$
$$+\int_0^1 (a(n_1,\theta_1)-a(n_2,\theta_2))(T_2)_x(T_1-T_2)_x\,dx,$$

with

$$\int_0^1 a(n_1,\theta_1)(T_1-T_2)_x^2\,dx \ge \underline{a}\|(T_1-T_2)_x\|_{L^2}^2,$$

where $\underline{a}=\min_{(\rho,\theta)\in[\underline{n},\overline{n}]\times[\underline{T},\overline{T}]} a(\rho,\theta)$, and

$$\begin{aligned} &\int_0^1 (a(n_1,\theta_1)-a(n_2,\theta_2))(T_2)_x(T_1-T_2)_x\,dx \\ &\quad\le \|a(n_1,\theta_1)-a(n_2,\theta_2)\|_{L^2}\|(T_2)_x\|_{L^\infty}\|(T_1-T_2)_x\|_{L^2} \\ &\quad\quad\le L(\|n_1-n_2\|_{L^2}+\|\theta_1-\theta_2\|_{L^2})\|(T_2)_x\|_{L^\infty}\|(T_1-T_2)_x\|_{L^2} \end{aligned}$$

Employing standard bounds from elliptic theory [GT83] there exist constants $c_0, c_1>0$ such that

$$\|(T_2)_x\|_{L^\infty} \le c_0 + c_1\left\| jE_2 + w(\rho_2,T_2-T_L) - \frac{j^3(n_2)_x}{\rho_2^3}\right\|_{L^2} \le r(j,\delta)$$

where $r(j,\delta) > 0$ is small for j_0 and δ small.

Hence

$$\underline{a}\|(T_1 - T_2)_x\|_{L^2} \le s(j,\delta)\left(\|n_1 - n_2\|_{L^2} + \|\rho_1 - \rho_2\|_{L^2} + \|\theta_1 - \theta_2\|_{H^1}\right),$$

and by Poincare's inequality it holds

$$\|T_1 - T_2\|_{H^1} \le s(j,\delta)\frac{1+\pi}{\underline{a}\pi}(1+\mu)(\|\rho_1 - \rho_2\|_{L^2} + \|\theta_1 - \theta_2\|_{H^1}),$$

where $s(j,\delta)$ can be made small by choosing j_0 and δ small enough.

Altogether, we have

$$\|\mathcal{T}(\rho_1,\theta_1) - \mathcal{T}(\rho_2,\theta_2)\|_{C^0\times H^1} \le \sigma\|(\rho_1,\theta_1) - (\rho_2,\theta_2)\|_{C^0\times H^1},$$

for some constant $\sigma = \sigma(j_0,\delta,K) \in (0,1)$, which yields the assertion. $\square$

Corollary 2.3. *Let the assumptions of Theorem 2.1 hold. Then the decoupling algorithm defined by the operator $\mathcal{T}$ converges for any starting value $(n^0, T^0) \in B$.*

Remark 2.4. This theorem also extends the uniqueness result in [AVJM00] as nonconstant heat conductivities are included.

3 Newton Iteration

In this section we investigate the convergence of a full Newton iteration for system (1.1). To this purpose we show the invertibility of the linearization of (1.1) in some appropriate function spaces and apply results from the well–known theory of Newton–Kantorovich [Zei86].

We employ the following assumptions

B.1 $w(n,T,j)$ is continuously differentiable in $(0,\infty)^3$ and it holds

$$w(n,0,j) = 0, \quad w_n(n,0,0) = 0, \quad w_T(n,T,j) \ge 0,$$

for all $(n,T,j) \in (0,\infty)^3$.

B.2 $P(n,T)$ is twice continuously differentiable in $(0,\infty)^2$ and there exist positive constants $\underline{n}, \overline{n}, \underline{T}, \overline{T}$ and K such that

$$P_n(\rho,\vartheta) \ge K, \qquad \text{for all } \underline{n} \le \rho \le \overline{n}, \quad \underline{T} \le \vartheta \le \overline{T}.$$

B.3 $a \in C^0([0,1])$ and there exists a positive constant $\underline{a}$ such that $a \ge \underline{a} > 0$.

B.4 $C \in C^0([0,1])$.

Remark 3.1.

a) **B.1** and **B.2** are especially fulfilled in the polytropic gas ansatz

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

b) For a smoother presentation we assume that the heat conductivity a depends only on the spatial variable (see **B.3**). Note that all forthcoming results also hold for arbitrary heat conductivities $a(n,T)$, since we control the norm $\|T_x\|_{1,\infty}$.

For notational convenience we define the Banach spaces

$$\begin{aligned} X &\stackrel{\text{def}}{=} C^1([0,1]) \times C^2([0,1]) \times C^1([0,1]), \\ Y &\stackrel{\text{def}}{=} \left[C^0([0,1])\right]^3, \end{aligned}$$

which are equipped with the canonical product norm. The norm of $C^k([0,1])$ is in the following denoted by $\|\cdot\|_{k,\infty}$.

We introduce the operator $A : X \to Y$ which is defined by

$$A(n,T,E) \stackrel{\text{def}}{=} \begin{pmatrix} \left(\frac{j^2}{n} + P(n,T)\right)_x + n\,E + j \\ -(a\,T_x)_x + j\,E + w(n,T) + \left(\frac{j^3}{2\,n^2} + \frac{5}{2} j\,T\right)_x \\ E_x + (n - C(x)) \end{pmatrix}. \tag{3.1}$$

We set $u \stackrel{\text{def}}{=} (n,T,E)$. As mentioned in the previous section we know that in the subsonic regime there exist positive constants $j_0, \delta, \underline{n}, \overline{n}, \underline{T}, \overline{T}$ such that if

$$|j| \le j_0, \quad |T_0 - T_L| + |T_1 - T_L| \le \delta$$

and assuming **B.1**–**B.4**, the classical solution $u^* \stackrel{\text{def}}{=} (n^*, T^*, E^*) \in X$ of system $A(n^*, T^*, E^*) = 0$ satisfies

$$\underline{n} \le n^*(x) \le \overline{n}, \quad \underline{T} \le T^*(x) \le \overline{T}.$$

We consider a ball

$$B_r(u^*) \stackrel{\text{def}}{=} \{u = (n,T,E) \in X : \|u - u^*\|_X < r\}$$

around the solution u^* and choose $r < \min(\underline{n}, \underline{T})$. Then it holds $n > 0$ and $T > 0$ in $B_r(u^*)$.

For the numerical computation of $u^* = (n^*, T^*, E^*)$ we want to employ the *Newton iteration*, which is given by

1. Choose $u_0 \in B_r(u^*)$.
2. For $k = 0, 1, \ldots$ set $u_{k+1} = u_k - (A'(u_k))^{-1} A(u_k)$.

To ensure that this iteration is well defined and convergent we have to check several properties of the linearization of A. First, the reader easily verifies the differentiability of A which is stated in the following result.

Lemma 3.2. *Assume* **B.1**–**B.4**. *Then the operator $A : X \to Y$ defined by* (3.1) *is Fréchet–differentiable in $B_r(u^*)$ and the Fréchet–derivative at $u \in B_r(u^*)$ in a direction $\theta = (\theta_n, \theta_T, \theta_E) \in X$ is given by*

$$A'(u)[\theta] = \begin{pmatrix} \left(-\frac{j^2}{n^2}\,\theta_n + P_n\,\theta_n + P_T\,\theta_T\right)_x + E\,\theta_n + n\,\theta_E \\ -(a\,\theta_{Tx})_x + j\,\theta_E + w_n\,\theta_n + w_T\,\theta_T + \left(-\frac{j^3}{n^3}\theta_n + \frac{5}{2}j\,\theta_T\right)_x \\ \theta_{Ex} + \theta_n \end{pmatrix}.$$

Furthermore, there exists a constant $L > 0$ such that

$$\|A'(u) - A'(v)\|_Y \le L\,\|u - v\|_X$$

for all $u, v \in B_r(u^*)$.

Secondly, we have to show the invertibility of $A'(u)$.

Lemma 3.3. *Assume* **B.1**–**B.4**. *Then there exist constants $j_0, \delta > 0$ such that for all $u = (n, T, E) \in B_r(u^*)$ with*

$$\|T - T_L\|_{0,\infty} \le \delta$$

and if $|j| \le j_0$ then for all $f = (f_n, f_T, f_E) \in Y$ the linear system

$$A'(u)[\theta] = f \tag{3.2}$$

supplemented with boundary conditions

$$\theta_n(0) = 0, \quad \theta_E(0) = 0, \quad \theta_T(0) = 0, \quad \theta_T(1) = 0$$

has a unique solution $\theta = (\theta_n, \theta_T, \theta_E) \in X$. Furthermore, there exists a constant $M > 0$ such that

$$\left\|(A'(u))^{-1}\right\|_{Y,X} \le M \tag{3.3}$$

for all $u \in B_r(u^*)$.

For the proof of Lemma 3.3 it is most convenient to reduce the hyperbolic–elliptic system (3.2) to an elliptic equation for θ_T. To achieve this we define the matrices

$$C_1 = \begin{pmatrix} P_n - \frac{j^2}{n^2} & 0 \\ 0 & 1 \end{pmatrix}, \quad C_2 = \begin{pmatrix} \left(P_n - \frac{j^2}{n^2}\right)_x + E & n \\ 1 & 0 \end{pmatrix},$$

which only depend on the state $u = (n, T, E) \in B_r(u^*)$. Let $(\tilde{\theta_n}, \tilde{\theta_E}) \in [C^1([0,1])]^2$ denote the classical solution of the system of ordinary differential equations

$$C_1 \begin{pmatrix} \tilde{\theta_n} \\ \tilde{\theta_E} \end{pmatrix}_x + C_2 \begin{pmatrix} \tilde{\theta_n} \\ \tilde{\theta_E} \end{pmatrix} = \begin{pmatrix} -(P_T\,\theta_T)_x \\ 0 \end{pmatrix}, \tag{3.4a}$$

$$\tilde{\theta_n}(0) = \tilde{\theta_E}(0) = 0. \tag{3.4b}$$

Due to **B.2** this system is uniquely solvable for j_0 sufficiently small. This defines a solution operator $\tilde{B} : C^1([0,1]) \to [C^1([0,1])]^2$ by $\tilde{B}(\theta_T) = (\tilde{B}_1(\theta_T), \tilde{B}_2(\theta_T)) \stackrel{\text{def}}{=} (\tilde{\theta_n}, \tilde{\theta_E})$.

For $(f_n, f_E) \in [C^0([0,1])]^2$ we consider the system

$$C_1 \begin{pmatrix} \hat{\theta_n} \\ \hat{\theta_E} \end{pmatrix}_x + C_2 \begin{pmatrix} \hat{\theta_n} \\ \hat{\theta_E} \end{pmatrix} = \begin{pmatrix} f_n \\ f_E \end{pmatrix},$$

$$\hat{\theta}_n(0) = \hat{\theta}_E(0) = 0,$$

which is again uniquely solvable and which defines a solution operator $\hat{B}$: $[C^0([0,1])]^2 \to [C^1([0,1])]^2$ by $\hat{B}(f_n, f_E) = (\hat{B}_1(f_n, f_E), \hat{B}_2(f_n, f_E)) \stackrel{\text{def}}{=} (\hat{\theta_n}, \hat{\theta_E})$.

Altogether, any solution $\theta = (\theta_n, \theta_T, \theta_E) \in X$ of $A'(u)[\theta] = f$ fulfils

$$\theta_n = \tilde{B}_1(\theta_T) + \hat{B}_1(f_n, f_E), \quad \theta_E = \tilde{B}_2(\theta_T) + \hat{B}_2(f_n, f_E)$$

and system (3.2) can be written as

$$\begin{aligned} &- (a\,\theta_{Tx})_x + j\,\tilde{B}_2(\theta_T) + w_n\,\tilde{B}_1(\theta_T) + w_T\,\theta_T - \left(-\frac{j^3}{n^3}\,\tilde{B}_1(\theta_T) + \frac{5}{2} j\,\theta_T\right)_x \\ &\qquad = -j\,\hat{B}_2(f_n, f_E) - w_n\,\hat{B}_1(f_n, f_E) + f_T - \left(\frac{j^3}{n^3}\hat{B}_1(f_n, f_E)\right)_x \end{aligned} \tag{3.5}$$

An easy consequence of Gronwall's Lemma is the following stability estimate.

Lemma 3.4. *Assume* **B.1**–**B.4** *and let* $(\tilde{\theta_n}, \tilde{\theta_E}) \in [C^1([0,1])]^2$ *be a solution of the ordinary differential system* (3.4). *Then there exists a constant* $c = c(\|n\|_{1,\infty}, \|E\|_{1,\infty}, \underline{n}, K) > 0$ *such that*

$$\left\|\tilde{\theta_n}\right\|_{0,\infty} + \left\|\tilde{\theta_E}\right\|_{0,\infty} \le c\, \|\theta_{Tx}\|_{L^2}$$

Now we are in the position to prove the invertibility result given in Lemma 3.3.

Proof of Lemma 3.3. We show the unique solvability of (3.5) by means of the Lax–Milgram Lemma. Therefore, we define the bilinear form $b : H_0^1(0,1) \times H_0^1(0,1) \to \mathbb{R}$ by

$$b(\theta_T, \phi) = \int_0^1 a\, \theta_{Tx}\, \phi_x + \Big(j\, \tilde{B}_2(\theta_T) + w_n\, \tilde{B}_1(\theta_T) + w_T\, \theta_T\Big)\, \phi \\ + \left(-\frac{j^3}{n^3}\, \tilde{B}_1(\theta_T) + \frac{5}{2} j\, \theta_T\right) \phi_x\, dx$$

and the functional $G : H_0^1(0,1) \to \mathbb{R}$ by

$$G(\phi) \stackrel{\text{def}}{=} \int_0^1 \Big(-j\, \hat{B}_2(f_n, f_E) - w_n\, \hat{B}_1(f_n, f_E) + f_T\Big)\, \phi\, dx + \int_0^1 \frac{j^3}{n^3} \hat{B}_1(f_n, f_E)\, \phi_x\, dx$$

Then the weak formulation of the system reads: Find $\theta_T \in H_0^1(0,1)$ such that

$$b(\theta_T, \phi) = G(\phi)$$

for all $\phi \in H_0^1(0,1)$.

Clearly, b and G are continuous

$$|b(\theta_T, \phi)| \leq c_1\, \|\theta_T\|_{H^1}\, \|\phi\|_{H^1}\,, \\ |G(\phi)| \leq c_2\, \|\phi\|_{H^1}\,,$$

where $c_i = c_i(\|n\|_{1,\infty}\,, \|T\|_{2,\infty}\,, \|E\|_{1,\infty}\,, a, \underline{n}, K) > 0$, $i = 1, 2$.

Next, we want to prove the coercivity of b.

$$\begin{aligned} b(\theta_T, \theta_T) &= \int_0^1 a\, |\theta_{Tx}|^2\, dx + j \int_0^1 \tilde{B}_2(\theta_T)\, \theta_T\, dx + \int_0^1 w_n\, \tilde{B}_1(\theta_T)\, \theta_T\, dx \\ &\quad + \int_0^1 w_T\, \theta_T^2\, dx - \int_0^1 \frac{j^3}{n^3}\, \tilde{B}_1(\theta_T)\, \theta_{Tx}\, dx + \int_0^1 \frac{5}{2} j\, \theta_T\, \theta_{Tx}\, dx \\ &\geq \underline{a}\, \|\theta_{Tx}\|_{L^2}^2 - j\, \left\|\tilde{B}_2(\theta_T)\right\|_{L^2} \|\theta_T\|_{L^2} - \|w_n\|_{L^\infty} \left\|\tilde{B}_1(\theta_T)\right\|_{L^2} \|\theta_T\|_{L^2} \\ &\quad - \frac{j^3}{\underline{n}^3} \left\|\tilde{B}_1(\theta_T)\right\|_{L^2} \|\theta_{Tx}\|_{L^2} \\ &\geq \underline{a}\, \|\theta_{Tx}\|_{L^2}^2 - c_3 \left(j + \|w_n\|_{L^\infty} + \frac{j^3}{\underline{n}^3}\right) \|\theta_{Tx}\|_{L^2}^2\,, \end{aligned}$$

where $c_3 = c_3(\|n\|_{1,\infty}\,, \|E\|_{1,\infty}\,, \underline{n}, K) > 0$. Hence, for j_0 and δ small it holds

$$b(\theta_T, \theta_T) \geq c_4\, \|\theta_T\|_{H^1}^2\,,$$

where $c_4 = c_4(\|n\|_{1,\infty}, \|T\|_{2,\infty}, \|E\|_{1,\infty}, \underline{n}, \underline{a}, K, j_0, \delta) > 0$. Note that $\|w_n\|_{L^\infty}$ is small due to **B.1** and the smallness of j_0 and δ.

Now the Lax–Milgram Lemma ensures the unique existence of a weak solution $\theta_T \in H_0^1(0,1)$ and it holds

$$\|\theta_T\|_{H^1} \leq c_4^{-1} \left(\|f_n\|_{L^2} + \|f_E\|_{L^2} + \|f_T\|_{L^2}\right).$$

Further we get from elliptic estimates [GT83]

$$\|\theta_T\|_{2,\infty} \leq c_5 \left(\|f_n\|_{0,\infty} + \|f_E\|_{0,\infty} + \|f_T\|_{0,\infty}\right)$$

and from Lemma 3.4 we deduce

$$\|\theta_n\|_{1,\infty} + \|\theta_E\|_{1,\infty} \leq c_6 \left(\|f_n\|_{0,\infty} + \|f_E\|_{0,\infty} + \|f_T\|_{0,\infty}\right),$$

where the positive constants c_5, c_6 again only depend on $\|n\|_{1,\infty}, \|T\|_{2,\infty}, \|E\|_{1,\infty}$, $\underline{n}, \underline{a}, K, j_0, \delta$. This immediately implies (3.3). $\square$

Hence, the Newton iteration is well defined and Lemma 3.2 and Lemma 3.3 are sufficient to ensure its convergence [Zei86, Proposition 5.1].

Theorem 3.5. *Assume* **B.1**–**B.4** *and let $u^* = (n^*, T^*, E^*) \in X$ be a solution of $A(n,T,E) = 0$. Then there exist constants $j_0, r, \delta > 0$ such that for all $u_\circ = (n_\circ, T_\circ, E_\circ) \in B_r(u^*)$ with*

$$|j| \leq j_0, \quad \|T_\circ - T_L\|_{0,\infty} \leq \delta$$

the sequence $(u_k)_{k\in\mathbb{N}}$ given by $u_{k+1} = u_k - (A'(u_k))^{-1}A(u_k)$ converges quadratically to u^*, i.e. there exists a constant $N = N(L, M, j_0, r, \delta) > 0$ such that

$$\|u_{k+1} - u^*\|_X \leq N \|u_k - u^*\|_X^2 .$$

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