GLOBAL EXISTENCE ANALYSIS FOR DEGENERATE ENERGY-TRANSPORT MODELS FOR SEMICONDUCTORS

NICOLA ZAMPONI AND ANSGAR JÜNGEL

Abstract. A class of energy-transport equations without electric field under mixed Dirichlet-Neumann boundary conditions is analyzed. The system of degenerate and strongly coupled parabolic equations for the particle density and temperature arises in semiconductor device theory. The global-in-time existence of weak nonnegative solutions is shown. The proof consists of a variable transformation and a semi-discretization in time such that the discretized system becomes elliptic and semilinear. Positive approximate solutions are obtained by Stampacchia truncation arguments and a new cut-off test function. Nonlogarithmic entropy inequalities yield gradient estimates which allow for the limit of vanishing time step sizes. Exploiting the entropy inequality, the long-time convergence of the weak solutions to the constant steady state is proved. Because of the lack of appropriate convex Sobolev inequalities to estimate the entropy dissipation, only an algebraic decay rate is obtained. Numerical experiments indicate that the decay rate is typically exponential.

1. Introduction

In this paper, we prove the global well-posedness of the energy-transport equations

$$\partial_t n = \Delta(n\theta^{1/2-\beta}), \quad \partial_t(n\theta) = \kappa\Delta(n\theta^{3/2-\beta}) + \frac{n}{\tau}(1-\theta) \quad \text{in } \Omega,\ t > 0, \tag{1}$$

where $-\frac{1}{2} \le \beta < \frac{1}{2}$, $\kappa = \frac{2}{3}(2-\beta)$, and $\Omega \subset \mathbb{R}^d$ with $d \le 3$ is a bounded domain. This system describes the evolution of a fluid of particles with density $n(x,t)$ and temperature $\theta(x,t)$. The parameter $\tau > 0$ is the relaxation time, which is the typical time of the system to relax to the thermal equilibrium state of constant temperature. The system arises in the modeling of semiconductor devices in which the elastic electron-phonon scattering is dominant. The above model is a simplification for vanishing electric fields. The full model was derived from the semiconductor Boltzmann equation in the diffusion limit using a Chapman-Enskog expansion around the equilibrium distribution [2]. The parameter β appears in the elastic scattering rate [14, Section 6.2]. Certain values were used in the physical literarure, for instance $\beta = \frac{1}{2}$ [4], $\beta = 0$ [17], and $\beta = -\frac{1}{2}$ [14, Chapter 9]. The

Date: December 15, 2014.

2010 *Mathematics Subject Classification.* 35K51, 35K65, 35Q79, 82D37.

Key words and phrases. Energy-transport equations, global existence of solutions, Stampacchia truncation, algebraic equilibration rate, semiconductors.

The authors acknowledge partial support from the Austrian Science Fund (FWF), grants P20214, P22108, I395, and W1245, and from the Austrian-French Project Amadée of the Austrian Exchange Service (ÖAD).

choice $\beta = \frac{1}{2}$ leads in our situation to two uncoupled heat equations for n and $n\theta$ and does not need to be considered. We impose physically motivated mixed Dirichlet-Neumann boundary and initial conditions

$$n = n_D,\ \theta = \theta_D \quad \text{on } \Gamma_D, \quad \nabla(n\theta^{1/2-\beta})\cdot\nu = \nabla(n\theta^{3/2-\beta})\cdot\nu = 0 \quad \text{on } \Gamma_N,\ t > 0, \tag{2}$$

$$n(0) = n_0, \quad \theta(0) = \theta_0 \quad \text{in } \Omega, \tag{3}$$

where Γ_D models the contacts, $\Gamma_N = \partial\Omega\backslash\Gamma_D$ the union of insulating boundary segments, and ν is the exterior unit normal to $\partial\Omega$ which is assumed to exist a.e.

The mathematical analysis of (1)-(3) is challenging since the equations are not in the usual divergence form, they are strongly coupled, and they degenerate at $\theta = 0$. The strong coupling makes impossible to apply maximum principle arguments in order to conclude the nonnegativity of the temperature θ. On the other hand, this system possesses an interesting mathematical structure. First, it can be written in "symmetric" form by introducing the so-called entropy variables $w_1 = \log(n/\theta^{3/2})$ and $w_2 = -1/\theta$. Then, setting $w = (w_1, w_2)^\top$ and $\rho = (n, \frac{3}{2}n\theta)^\top$, (1) is formally equivalent to

$$\partial_t\rho = \operatorname{div}(A(n,\theta)\nabla w) + \frac{1}{\tau}\begin{pmatrix} 0 \\ n(1-\theta)\end{pmatrix},$$

where the diffusion matrix

$$A(n,\theta) = n\theta^{1/2-\beta}\begin{pmatrix} 1 & (2-\beta)\theta \\ (2-\beta)\theta & (3-\beta)(2-\beta)\theta^2\end{pmatrix}$$

is symmetric and positive semi-definite. Second, system (1) possesses the entropy (or free energy)

$$S[n(t),(n\theta)(t)] = \int_\Omega n\log\frac{n}{\theta^{3/2}}dx,$$

which is nonincreasing along smooth solutions to (1). Even more entropy functionals exist; see [15] and below. However, they do not provide a lower bound for θ when n vanishes. We notice that both properties, the symmetrization via entropy variables and the existence of an entropy, are strongly related [8, 14].

Equations (1) resemble the diffusion equation $\partial_t w = \Delta(a(x,t)w)$, which was analyzed by Pierre and Schmitt [18]. By Pierre's duality estimate, an L^2 bound for $\sqrt{a}w$ in terms of the L^2 norm of $\sqrt{a}$ has been derived. In our situation, we obtain even H^1 estimates for $w = n$ and $w = n\theta$.

In spite of the above structure, there are only a few analytical results for (1)-(3). In earlier works, drift-diffusion equations with temperature-dependent mobilities but without temperature gradients [23] (also see [21]) or nonisothermal systems containing simplified thermodynamic forces [1] have been studied. Xu included temperature gradients in the model but he truncated the Joule heating to allow for a maximum principle argument [22]. Later, existence results for the complete energy-transport equations (including electric fields) have been achieved, see [11, 13] for stationary solutions near thermal equilibrium, [5, 6] for transient solutions close to equilibrium, and [7, 9] for systems with uniformly positive definite diffusion matrices. This assumption on the diffusion matrix avoids the degeneracy at $\theta = 0$. A degenerate energy-transport system was analyzed in [16], but only a simplified (stationary) temperature equation was studied. All these results give partial answers to the well-posedness problem only. In this paper, we prove for the first time a global-in-time existence result for any data and with physical transport coefficients.

Surprisingly, the above logarithmic entropy structure does not help. Our key idea is to use the new variables $u = n\theta^{1/2-\beta}$ and $v = n\theta^{3/2-\beta}$ and nonlogarithmic entropy functionals. Then system (1) becomes

$$\partial_t N(u,v) = \Delta u, \quad \partial_t E(u,v) = \kappa\Delta v + R(u,v),$$

where $N(u,v) = u^{3/2-\beta}v^{\beta-1/2}$, $E(u,v) = u^{1/2-\beta}v^{\beta+1/2}$, and $R(u,v) = \tau^{-1}N(u,v)(1-v/u)$. Discretizing this system by the implicit Euler method and employing the Stampacchia truncation method and a particular cut-off test function, we are able to prove the nonnegativity of u, v, and θ.

In the following, we detail our main results and explain the ideas of the proofs. Let $\partial\Omega \in C^1$, $\text{meas}(\Gamma_D) > 0$, and Γ_N is relatively open in $\partial\Omega$. Furthermore, let

$$n_D,\ \theta_D \in L^\infty(\Omega) \cap H^1(\Omega), \quad \inf_{\Gamma_D} n_D > 0,\ \inf_{\Gamma_D} \theta_D > 0, \tag{4}$$

$$n_0,\ \theta_0 \in L^\infty(\Omega) \cap H^1(\Omega), \quad \inf_{\Omega} n_0 > 0,\ \inf_{\Omega} \theta_0 > 0. \tag{5}$$

We define the space $H^1_D(\Omega)$ as the closure of $C_0^\infty(\Omega \cup \Gamma_N)$ in the H^1 norm [20, Section 1.7.2]. This space can be characterized by all functions in $H^1(\Omega)$ which vanish on Γ_D in the weak sense. This space is the test function space for the weak formulation of (1). Our first main result reads as follows.

Theorem 1 (Global existence). *Let $T > 0$, $d \le 3$, $-\frac{1}{2} \le \beta < \frac{1}{2}$, $\tau > 0$ and let (4)-(5) hold. Then there exists a weak solution (n,θ) to (1)-(3) such that $n > 0$, $n\theta > 0$ in Ω, $t > 0$, satisfying*

$$\begin{aligned} &n,\ n\theta,\ n\theta^{1/2-\beta},\ n\theta^{3/2-\beta} \in L^2(0,T;H^1(\Omega)) \cap L^\infty(0,T;L^2(\Omega)), \\ &\partial_t n,\ \partial_t(n\theta) \in L^2(0,T;H^1_D(\Omega)'). \end{aligned}$$

The idea of the proof is to employ the implicit Euler method with time step $h > 0$ and the new variables $u_j = n_j\theta_j^{1/2-\beta}$ and $v_j = n_j\theta_j^{3/2-\beta}$, which approximate $u = n\theta^{1/2-\beta}$ and $v = n\theta^{3/2-\beta}$ at time $t_j = jh$, respectively. We wish to solve

$$(n_j - n_{j-1}) - h\Delta u_j = 0, \quad \frac{1}{\kappa}(n_j\theta_j - n_{j-1}\theta_{j-1}) - h\Delta v_j = \frac{hn_j}{\kappa\tau}(1-\theta). \tag{6}$$

To simplify the presentation, we ignore the boundary conditions and a necessary truncation of the temperature (see Section 2 for a full proof). A nice feature of this formulation is that we can apply a Stampacchia truncation procedure to prove the strict positivity of u_j and v_j (see Step 2 in the proof of Theorem 1).

The main difficulty is to show the positivity of $\theta_j = v_j/u_j$. We define a nondecreasing smooth cut-off function ϕ such that $\phi(x) = 0$ if $x \le M$ and $\phi(x) > 0$ if $x > M$ for some $M > 0$. We use the test functions $u_j\phi(1/\theta_j)$ and $v_j\phi(1/\theta_j)$ in the weak formulation of (6), respectively, and we subtract both equations to find after a straightforward computation (see Step 3 in the proof of Theorem 1) that

$$0 = \int_\Omega \bigg(\left(1 - \frac{1}{\kappa} - \frac{h}{\kappa\tau}\right) n_j v_j \phi\left(\frac{1}{\theta_j}\right) + \frac{v_j}{\kappa} n_{j-1}\theta_{j-1}\left(\frac{1}{\theta_j} - \frac{\kappa}{\theta_{j-1}}\right)\phi\left(\frac{1}{\theta_j}\right) \\ + \frac{h}{v_j^2}\left|v_j\nabla u_j - u_j\nabla v_j\right|^2 \phi'\left(\frac{1}{\theta_j}\right) + \frac{hn_j\theta_j v_j}{\kappa\tau}\phi\left(\frac{1}{\theta_j}\right)\bigg)dx.$$

Since $\kappa > 1$, there exists $h > 0$ sufficiently small such that the first summand becomes nonnegative. The third and last summands are nonnegative, too. (Recall that we need to truncate θ_j with positive truncation.) Hence, the integral over the second term is nonpositive. Then, choosing $M \geq \kappa/\theta_{j-1}$,

$$0 \geq \int_\Omega v_j n_{j-1}\theta_{j-1}\left(\frac{1}{\theta_j} - \frac{\kappa}{\theta_{j-1}}\right)\phi\left(\frac{1}{\theta_j}\right)dx \geq \int_\Omega v_j n_{j-1}\theta_{j-1}\left(\frac{1}{\theta_j} - M\right)\phi\left(\frac{1}{\theta_j}\right)dx.$$

Because $\phi(1/\theta_j) = 0$ for $1/\theta_j \leq M$, this is only possible if $1/\theta_j - M \leq 0$ or $\theta_j \geq 1/M > 0$. Clearly, the bound M depends on j, and in the de-regularization limit $h \to 0$, the limit of θ_j becomes nonnegative only.

A priori estimates which are uniform in the approximation parameter $h > 0$ are obtained by proving a discrete version of the entropy inequality [15]

$$\frac{d}{dt}\int_\Omega n^2\theta^b dx + C_1 \int_\Omega \left|\nabla\left(n\theta^{(2b+1-2\beta)/4}\right)\right|^2 dx \leq C_2, \tag{7}$$

for some $b \in \mathbb{R}$ and C_1, $C_2 > 0$. Choosing a variant of the sum of two entropies $\int_\Omega n^2(\theta^{\beta-1/2} + \theta^5)dx$, we are able to derive gradient estimates for n_j, $n_j\theta_j^{1/2-\beta}$, and $n_j\theta_j^{3/2-\beta}$ (see Step 4 of the proof of Theorem 1). Together with Aubin's lemma and weak compactness arguments, the limit $h \to 0$ can be performed.

Theorem 1 can be generalized in different ways. First, the boundary data may depend on time. We do not consider this case here to avoid too many technicalities. We refer to [7] for the treatment of time-dependent boundary functions. Second, we may allow for temperature-dependent relaxation times,

$$\tau(\theta) = \tau_0 + \tau_1\theta^{1/2-\beta}, \tag{8}$$

where $\tau_0 > 0$ and $\tau_1 > 0$. This expression can be derived by using an energy-dependent scattering rate [14, Example 6.8]. For this relaxation time, the conclusion of Theorem 1 holds.

Corollary 2 (Global existence)**.** *Let the assumptions of Theorem 1 hold except that the relaxation time is given by* (8)*. Then there exists a weak solution to* (1)-(3) *with the properties stated in Theorem 1.*

However, we have not been able to include electric fields in the model. For instance, in this situation, the first equation in (1) becomes

$$\partial_t n = \operatorname{div}(\nabla(n\theta^{1/2-\beta}) + n\theta^{-1/2-\beta}\nabla V),$$

where $V(x,t)$ is the electric potential which is a given function or the solution of the Poisson equation [14]. The problem is the treatment of the drift term $n\theta^{-1/2-\beta}\nabla V$ for which the techniques developed for the standard drift-diffusion model (see, e.g., [12]) do not apply.

Our second main result concerns the long-time behavior of the solutions.

Theorem 3 (Long-time behavior)**.** *Let $d \le 3$, $0 \le \beta < \frac{1}{2}$, $\tau > 0$, and $n_D = const.$, $\theta_D = 1$. Let (n,θ) be the weak solution constructed in Theorem 1. Then there exist constants C_1, $C_2 > 0$, which depend only on β, n_D, n_0, and θ_0, such that for all $t > 0$,*

$$\|n(t) - n_D\|^2_{L^2(\Omega)} + \|n(t)\theta(t) - n_D\|^2_{L^2(\Omega)} \le \frac{C_1}{1 + C_2 t}.$$

The proof of this theorem is based on discrete entropy inequality estimates. The main difficulty is to bound the entropy dissipation. Usually, this is done by employing a convex Sobolev inequality (e.g. the logarithmic Sobolev or Beckner inequality). However, these tools are not available for the cross-diffusion system at hand, and we need to employ another technique. Our idea is to estimate the entropy dissipation by using another entropy (choosing different values for b in the discrete version of (7)). Denoting the discrete (nonlogarithmic) entropy at time t_j by $S[n_j, n_j\theta_j]$, we arrive at the inequality

$$S[n_j, n_j\theta_j] - S[n_{j-1}, n_{j-1}\theta_{j-1}] \le ChS[n_j, n_j\theta_j]^2,$$

where $C > 0$ is independent of the time step size h. A discrete nonlinear Gronwall lemma then shows that $S[n_j, n_j\theta_j]$ behaves like $1/(hj) = 1/t_j$, and in the limit $h \to 0$, we obtain the result.

The paper is organized as follows. We prove Theorem 1 and Corollary 2 in Section 2. Section 3 is devoted to the proof of Theorem 3. The numerical results in one space dimension presented in Section 4 indicate that the existence of solutions still holds for $\beta < -\frac{1}{2}$ and $\beta > \frac{1}{2}$ and that the solutions converge exponentially fast to the steady state.

2. Global existence of solutions

We prove Theorem 1 and Corollary 2.

Step 1: Reformulation. Let $T > 0$, $N \in \mathbb{N}$, and set $h = T/N$. We consider the semi-discrete equations

$$\frac{1}{h}(n_j - n_{j-1}) = \Delta(n_j\theta_j^{1/2-\beta}), \quad j = 1, \ldots, N, \tag{9}$$

$$\frac{1}{h}(n_j\theta_j - n_{j-1}\theta_{j-1}) = \kappa\Delta(n_j\theta_j^{3/2-\beta}) + \frac{1}{\tau}n_j(1 - \theta_j) \tag{10}$$

with the boundary conditions (2). The idea is to reformulate the elliptic equations in terms of the new variables

$$u_j = n_j\theta_j^{1/2-\beta}, \quad v_j = n_j\theta_j^{3/2-\beta}.$$

Observing that $n_j = u_j^{3/2-\beta}v_j^{\beta-1/2}$ and $\theta_j = v_j/u_j$, equations (9)-(10) are formally equivalent to

$$u_j^{3/2-\beta}v_j^{\beta-1/2} - h\Delta u_j = u_{j-1}^{3/2-\beta}v_{j-1}^{\beta-1/2}, \tag{11}$$

$$u_j^{1/2-\beta}v_j^{\beta+1/2} - \kappa h\Delta v_j - \frac{h}{\tau}u_j^{1/2-\beta}v_{j-1}^{\beta-1/2}(u_j - v_j) = u_{j-1}^{1/2-\beta}v_{j-1}^{\beta+1/2}. \tag{12}$$

The boundary conditions become

$$u_j = u_D := n_D\theta_D^{1/2-\beta}, \quad v_j = v_D := n_D\theta_D^{3/2-\beta} \quad \text{on } \Gamma_D, \tag{13}$$

$$\nabla u_j\cdot\nu = \nabla v_j\cdot\nu = 0 \quad \text{on } \Gamma_N. \tag{14}$$

In order to show the existence of weak solutions to this discretized system, we need to truncate. For this, let $j\ge 1$ and let u_{j-1}, $v_{j-1}\in L^2(\Omega)$ be given such that $\inf_\Omega u_{j-1}>0$, $\inf_\Omega v_{j-1}>0$, $\sup_\Omega u_{j-1}<+\infty$, and $\sup_\Omega v_{j-1}<+\infty$. We define

$$M = \max\left\{\kappa\sup_\Omega\frac{u_{j-1}}{v_{j-1}}, \frac{1}{\inf_{\Gamma_D}\theta_D}\right\} \tag{15}$$

and $\varepsilon = 1/M$. The truncated problem reads as

$$u_j\theta_{j,\varepsilon}^{\beta-1/2} - h\Delta u_j = u_{j-1}^{3/2-\beta}v_{j-1}^{\beta-1/2}, \tag{16}$$

$$\left(1+\frac{h}{\tau}\right)v_j\theta_{j,\varepsilon}^{\beta-1/2} - \kappa h\Delta v_j - \frac{h}{\tau}u_j\theta_{j,\varepsilon}^{\beta-1/2} = u_{j-1}^{1/2-\beta}v_{j-1}^{\beta+1/2}, \tag{17}$$

where $\theta_{j,\varepsilon} = \max\{\varepsilon, v_j/u_j\}$. Note that if $u_j>0$ and $v_j/u_j\ge\varepsilon$ in Ω then (16)-(17) are equivalent to (11)-(12).

Step 2: Solution of the truncated semi-discrete problem. We define the operator $F : L^2(\Omega)\times[0,1]\to L^2(\Omega)$ by $F(\theta,\sigma) = v/u$, where $(u,v)\in H^1(\Omega)^2$ is the unique solution to the linear system

$$\sigma u\theta_\varepsilon^{\beta-1/2} - h\Delta u = \sigma u_{j-1}^{3/2-\beta}v_{j-1}^{\beta-1/2} = \sigma u_{j-1}\left(\frac{u_{j-1}}{v_{j-1}}\right)^{1/2-\beta}, \tag{18}$$

$$\sigma\left(1+\frac{h}{\tau}\right)v\theta_\varepsilon^{\beta-1/2} - \kappa h\Delta v - \sigma\frac{h}{\tau}u\theta_\varepsilon^{\beta-1/2} = \sigma u_{j-1}^{1/2-\beta}v_{j-1}^{\beta+1/2} = \sigma v_{j-1}\left(\frac{u_{j-1}}{v_{j-1}}\right)^{1/2-\beta}, \tag{19}$$

where $\theta_\varepsilon = \max\{\varepsilon,\theta\}$, with the boundary conditions

$$u = 1+\sigma(u_D-1),\ v = \sigma v_D \quad \text{on } \Gamma_D, \quad \nabla u\cdot\nu = \nabla v\cdot\nu = 0 \quad \text{on } \Gamma_N. \tag{20}$$

We have to prove that the operator F is well defined.

First, observe that (18) does not depend on v and that the right-hand side is an element of $L^2(\Omega)$. Therefore, by standard theory of elliptic equations, we infer the existence of a unique solution $u\in H^1(\Omega)$ to (18) with the corresponding boundary conditions in (20). With given u, there exists a unique solution $v\in H^1(\Omega)$ to (19) with the corresponding boundary conditions. It remains to show that u and v are strictly positive in Ω such that the quotient v/u is defined and an element of $L^2(\Omega)$.

To this end, we employ the Stampacchia truncation method. Let

$$m_1 = \min\left\{\inf_{\Gamma_D}u_D, \varepsilon^{1/2-\beta}\inf_\Omega u_{j-1}^{3/2-\beta}v_{j-1}^{\beta-1/2}\right\} > 0.$$

Note that $m_1 > 0$ because of our boundedness assumptions on $\inf_\Omega u_{j-1}$ and $\sup_\Omega v_{j-1}$. Then $(u-m_1)_- = \min\{0, u-m_1\} \in H^1_D(\Omega)$ is an admissible test function in the weak formulation of (18) yielding

$$\begin{aligned} h\int_\Omega |\nabla(u-m_1)_-|^2 dx + \sigma\int_\Omega \theta_\varepsilon^{\beta-1/2}(u-m_1)_-^2 dx \\ = \sigma\int_\Omega \big(u_{j-1}^{3/2-\beta}v_{j-1}^{\beta-1/2} - m_1\theta_\varepsilon^{\beta-1/2}\big)(u-m_1)_- dx \\ \le \sigma\int_\Omega \big(u_{j-1}^{3/2-\beta}v_{j-1}^{\beta-1/2} - m_1\varepsilon^{\beta-1/2}\big)(u-m_1)_- dx \le 0, \end{aligned}$$

taking into account $\theta_\varepsilon^{\beta-1/2} \le \varepsilon^{\beta-1/2}$ (observe that $\beta < 1/2$) and the definition of m_1. This implies that $(u-m_1)_- = 0$ and consequently $u \ge m_1 > 0$ in Ω. Defining

$$m_2 = \min\left\{\inf_{\Gamma_D} v_D, \left(1+\frac{h}{\tau}\right)^{-1} \varepsilon^{1/2-\beta} \inf_\Omega u_{j-1}^{1/2-\beta}v_{j-1}^{\beta+1/2}\right\} > 0$$

and employing the test function $(v-m_2)_- \in H^1_D(\Omega)$ in the weak formulation of (19), a similar computation as above and $\theta_\varepsilon^{\beta-1/2} \le \varepsilon^{\beta-1/2}$ yield

$$\begin{aligned} \kappa h\int_\Omega |\nabla(v-m_2)_-|^2 dx + \sigma\left(1+\frac{h}{\tau}\right)\int_\Omega \theta_\varepsilon^{\beta-1/2}(v-m_2)_-^2 dx - \frac{\sigma h}{\tau}\int_\Omega u\theta_\varepsilon^{\beta-1/2}(v-m_2)_- dx \\ = \sigma\int_\Omega \left((u_{j-1}^{1/2-\beta}v_{j-1}^{\beta+1/2} - \left(1+\frac{h}{\tau}\right)m_2\theta_\varepsilon^{\beta-1/2}\right)(v-m_2)_- dx \le 0. \end{aligned}$$

Since the integrals on the left-hand side are nonnegative, we conclude that $v \ge m_2 > 0$ in Ω. This shows that u and v are strictly positive with a lower bound which depends on ε and j. Because of $1/u \in L^\infty(\Omega)$ and $u, v \in H^1(\Omega) \hookrightarrow L^6(\Omega)$, $v/u \in W^{1,3/2}(\Omega) \hookrightarrow L^2(\Omega)$ for $d \le 3$. Hence, the operator F is well defined and its image is contained in $W^{1,3/2}(\Omega)$.

Standard arguments and the compact embedding $W^{1,3/2}(\Omega) \hookrightarrow L^2(\Omega)$ ensure that F is continuous and compact. When $\sigma = 0$, it follows that $u = 1$ and $v = 0$ and thus, $F(\theta, 0) = 0$. Let $\theta \in L^2(\Omega)$ be a fixed point of $F(\cdot, \sigma)$. Then $v/u = \theta$. By standard elliptic estimates, we obtain H^1 bounds for u and v independently of σ. Since u is strictly positive, we infer an L^2 bound for θ independently of σ. Thus, we may apply the Leray-Schauder fixed-point theorem to conclude the existence of a fixed point of $F(\cdot, 1)$, i.e. of a solution $(u, v) = (u_j, v_j) \in H^1(\Omega)^2$ to (16)-(17) with boundary conditions (13)-(14).

In order to close the recursion, we need to show that $\sup_\Omega u_j < +\infty$ and $\sup_\Omega v_j < +\infty$. We employ the following result which is due to Stampacchia [19]: Let $w \in H^1(\Omega)$ be the unique solution to $-\Delta w + a(x)w = f$ with mixed Dirichlet-Neumann boundary conditions and let $a \in L^\infty(\Omega)$ be nonnegative and $f \in L^s(\Omega)$ with $s > d/2$. Then $w \in L^\infty(\Omega)$ with a bound which depends only on f, Ω, and the boundary data. Since the right-hand side of (18) is an element of $L^2(\Omega)$ and $d \le 3$, we find from the above result that the solution u

to (18) is bounded. Furthermore, v solves (see (19))

$$\sigma\left(1+\frac{h}{\tau}\right)v\theta_\varepsilon^{\beta-1/2}-\kappa h\Delta v=\sigma\frac{h}{\tau}u\theta_\varepsilon^{\beta-1/2}+\sigma u_{j-1}^{1/2-\beta}v_{j-1}^{\beta+1/2}\in L^\infty(\Omega),$$

taking advantage of the L^∞ bound for u. By Stampacchia's result, $v\in L^\infty(\Omega)$. This shows the desired bounds.

Step 3: Removing the truncation. We introduce the function

$$\phi(x)=\begin{cases}0 & \text{if } x\le M,\\ 1+\cos(\pi x/M) & \text{if } M\le x\le 2M,\\ 2 & \text{if } x\ge 2M,\end{cases}$$

where we recall the definition (15) of M. In particular, $\phi\in C^1(\mathbb{R})$ satisfies $\phi'\ge 0$ in $\mathbb{R}$. Since $M\ge 1/\inf_{\Gamma_D}\theta_D$, we have $\phi(u_j/v_j)=\phi(u_D/v_D)=\phi(1/\theta_D)=0$ on Γ_D. Because ϕ' vanishes outside of the interval $[M,2M]$, it holds that $u_j\phi(u_j/v_j)$, $v_j\phi(u_j/v_j)\in H^1(\Omega)$. Consequently, $v_j\phi(u_j/v_j)$ and $\kappa^{-1}u_j\phi(u_j/v_j)$ are admissible test functions in $H^1_D(\Omega)$ for (16) and (17), respectively, which gives the two equations

$$\begin{aligned}&\int_\Omega u_j\theta_{j,\varepsilon}^{\beta-1/2}v_j\phi\left(\frac{u_j}{v_j}\right)dx+h\int_\Omega\nabla u_j\cdot\nabla\left(v_j\phi\left(\frac{u_j}{v_j}\right)\right)dx=\int_\Omega u_{j-1}^{3/2-\beta}v_{j-1}^{\beta-1/2}v_j\phi\left(\frac{u_j}{v_j}\right)dx,\\ &\frac{1}{\kappa}\left(1+\frac{h}{\tau}\right)\int_\Omega v_j\theta_{j,\varepsilon}^{\beta-1/2}u_j\phi\left(\frac{u_j}{v_j}\right)dx+h\int_\Omega\nabla v_j\cdot\nabla\left(u_j\phi\left(\frac{u_j}{v_j}\right)\right)dx\\ &\qquad-\frac{h}{\kappa\tau}\int_\Omega u_j^2\theta_{j,\varepsilon}^{\beta-1/2}\phi\left(\frac{u_j}{v_j}\right)dx=\frac{1}{\kappa}\int_\Omega u_{j-1}^{1/2-\beta}v_{j-1}^{\beta+1/2}u_j\phi\left(\frac{u_j}{v_j}\right)dx.\end{aligned}$$

We take the difference of these equations:

$$\begin{aligned}&\left(1-\frac{1}{\kappa}\left(1+\frac{h}{\tau}\right)\right)\int_\Omega u_jv_j\theta_{j,\varepsilon}^{\beta-1/2}\phi\left(\frac{u_j}{v_j}\right)dx\\ &\quad+h\int_\Omega(v_j\nabla u_j-u_j\nabla v_j)\cdot\nabla\phi\left(\frac{u_j}{v_j}\right)dx+\frac{h}{\kappa\tau}\int_\Omega u_j^2\theta_{j,\varepsilon}^{\beta-1/2}\phi\left(\frac{u_j}{v_j}\right)dx\\ &\quad+\frac{1}{\kappa}\int_\Omega u_{j-1}^{1/2-\beta}v_{j-1}^{\beta+1/2}v_j\phi\left(\frac{u_j}{v_j}\right)\left(\frac{u_j}{v_j}-\kappa\frac{u_{j-1}}{v_{j-1}}\right)dx=0.\end{aligned}\tag{21}$$

Since $\beta<1/2$, we have $\kappa=\frac{2}{3}(2-\beta)>1$. Therefore, we can choose $0<h<(\kappa-1)\tau$ which implies that $1-\kappa^{-1}(1+h/\tau)>0$, and the first integral is nonnegative. The same conclusion holds for the second integral in (21) since

$$(v_j\nabla u_j-u_j\nabla v_j)\cdot\nabla\phi\left(\frac{u_j}{v_j}\right)=\frac{1}{v_j^2}\phi'\left(\frac{u_j}{v_j}\right)|v_j\nabla u_j-u_j\nabla v_j|^2\ge 0.$$

Also the third integral in (21) is nonnegative. Hence, the fourth integral is nonpositive, which can be equivalently written as

$$\int_\Omega u_{j-1}^{1/2-\beta}v_{j-1}^{\beta+1/2}v_j\phi\left(\frac{u_j}{v_j}\right)\left(\frac{u_j}{v_j}-M\right)dx\le\int_\Omega u_{j-1}^{1/2-\beta}v_{j-1}^{\beta+1/2}v_j\phi\left(\frac{u_j}{v_j}\right)\left(\kappa\frac{u_{j-1}}{v_{j-1}}-M\right)dx.$$

Taking into account definition (15) of M, we infer that the integral on the right-hand side is nonpositive, which shows that

$$\int_\Omega u_{j-1}^{1/2-\beta} v_{j-1}^{\beta+1/2} v_j \phi\left(\frac{u_j}{v_j}\right)\left(\frac{u_j}{v_j} - M\right)_+ dx = 0,$$

where $z_+ = \max\{0, z\}$ for $z \in \mathbb{R}$, employing $\phi(u_j/v_j) = 0$ for $u_j/v_j \leq M$. Now, $\phi(u_j/v_j) > 0$ for $u_j/v_j > M$, and we conclude that $(u_j/v_j - M)_+ = 0$ and $u_j/v_j \leq M$ in Ω. Since $\varepsilon = 1/M$, this means that $v_j/u_j \geq \varepsilon$ and $\theta_{j,\varepsilon} = v_j/u_j$. Consequently, we have proven the existence of a weak solution (v_j, u_j) to the discretized problem (11)-(12) with the boundary conditions (13)-(14), which also yields a weak solution (n_j, θ_j) to (9)-(10) with the boundary conditions (2).

Step 4: Entropy estimates. Let $b \in \mathbb{R}$ and define the functional

$$\phi_b[n, n\theta] = \int_\Omega \left(f_b(n, n\theta) - f_{b,D} - \frac{\partial f_{b,D}}{\partial n}(n - n_D) - \frac{\partial f_{b,D}}{\partial(n\theta)}(n\theta - n_D\theta_D)\right) dx, \tag{22}$$

where $f_b(n, n\theta) = n^{2-b}(n\theta)^b$ and we have employed the abbreviations

$$f_{b,D} = f_b(n_D, n_D\theta_D), \quad \frac{\partial f_{b,D}}{\partial n} = \frac{\partial f_b}{\partial n}(n_D, n_D\theta_D), \quad \frac{\partial f_{b,D}}{\partial(n\theta)} = \frac{\partial f_b}{\partial(n\theta)}(n_D, n_D\theta_D).$$

The function f_b is convex if $b \geq 2$ or $b \leq 0$ since $\det D^2 f_b(n, n\theta) = b(b-2)\theta^{2(\beta-1)}$ and $\mathrm{tr} D^2 f_b(n, n\theta) = (b-1)(b-2)\theta^b + b(b-1)\theta^{b-2}$. We wish to derive a priori estimates from the so-called entropy functionals

$$S_{b_1,b_2}[n, n\theta] = \frac{1}{|b_1|}\phi_{b_1}[n, n\theta] + \frac{1}{|b_2|}\phi_{b_2}[n, n\theta].$$

The parameters (b_1, b_2) are chosen from the following set:

$$N_\beta = \left\{(b_1, b_2) \in \mathbb{R}^2 : b_1, b_2 \in N_\beta^*,\ b_1 \leq b_2,\ b_1 \leq \beta - \tfrac{1}{2},\ b_2 \geq \tfrac{5}{2} - \beta, \right\},$$

where N_β^* consists of all $b \in \mathbb{R}$ such that $(1 - 2\beta)b + 6 > 0$ and

$$4(2\beta - 1)b^3 + 4(4\beta^2 - 12\beta + 11)b^2 + (8\beta^3 - 44\beta^2 + 70\beta - 73)b - 6(2\beta - 1)^2 > 0.$$

The set of all (β, b) such that $b \in N_\beta^*$ is illustrated in Figure 1. In particular, we have $b \geq 2$ or $b \leq 0$ for all $b \in N_\beta^*$ with $-\frac{1}{2} < \beta < \frac{1}{2}$. It is not difficult to check that $(\beta - \frac{1}{2}, 5) \in N_\beta$ for all $-\frac{1}{2} < \beta < \frac{1}{2}$.

Lemma 4 (Discrete entropy inequality)**.** *Let $(b_1, b_2) \in N_\beta$. Then*

$$\begin{aligned} S_{b_1,b_2}[n_j, n_j\theta_j] &+ C_1 h \int_\Omega \left(\theta_j^{b_1+1/2-\beta} + \theta_j^{b_2+1/2-\beta}\right)|\nabla n_j|^2 dx \\ &+ C_1 h \int_\Omega n_j^2 \left(\theta_j^{b_1-3/2-\beta} + \theta_j^{b_2-3/2-\beta}\right)|\nabla \theta_j|^2 dx \\ &\leq C_2 h + S_{b_1,b_2}[n_{j-1}, n_{j-1}\theta_{j-1}], \end{aligned} \tag{23}$$

where $C_1 > 0$ depends on b and β and $C_2 > 0$ depends on τ, n_D, and θ_D. The constant C_2 vanishes if $n_D = const.$ and $\theta_D = 1$.

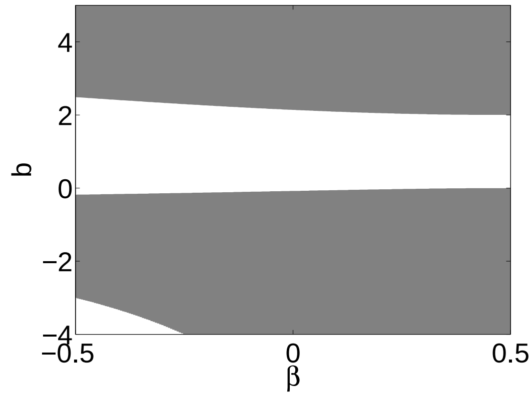

FIGURE 1. The gray regions represent all points (β, b) such that $b \in N^*_\beta$.

Proof. We abbreviate

$$f_{b,j} = f_b(n_j, n_j\theta_j), \quad \frac{\partial f_{b,j}}{\partial n} = \frac{\partial f_b}{\partial n}(n_j, n_j\theta_j), \quad \frac{\partial f_{b,j}}{\partial(n\theta)} = \frac{\partial f_b}{\partial(n\theta)}(n_j, n_j\theta_j).$$

Let $b = b_1$ or $b = b_2$. We already observed that $b \geq 2$ or $b \leq 0$. Hence, $f_b(n, n\theta)$ is convex, and using (9)-(10), we compute

$$\begin{aligned}
&\frac{1}{h}\big(\phi_b[n_j, n_j\theta_j] - \phi_b[n_{j-1}, n_{j-1}\theta_{j-1}]\big) \\
&\quad = \frac{1}{h}\int_\Omega \left((f_{b,j} - f_{b,j-1}) - \frac{\partial f_{b,D}}{\partial n}(n_j - n_{j-1}) - \frac{\partial f_{b,D}}{\partial(n\theta)}(n_j\theta_j - n_{j-1}\theta_{j-1}) \right) dx \\
&\quad \leq \frac{1}{h}\int_\Omega \left(\left(\frac{\partial f_{b,j}}{\partial n} - \frac{\partial f_{j,D}}{\partial n} \right)(n_j - n_{j-1}) + \left(\frac{\partial f_{j,b}}{\partial(n\theta)} - \frac{\partial f_{b,D}}{\partial(n\theta)} \right)(n_j\theta_j - n_{j-1}\theta_{j-1}) \right) dx \\
&\quad = -\int_\Omega \nabla\left(\frac{\partial f_{b,j}}{\partial n} - \frac{\partial f_{j,D}}{\partial n} \right)\cdot \nabla(n_j\theta_j^{1/2-\beta})dx \\
&\qquad - \kappa\int_\Omega \nabla\left(\frac{\partial f_{j,b}}{\partial(n\theta)} - \frac{\partial f_{b,D}}{\partial(n\theta)} \right)\cdot \nabla(n_j\theta_j^{3/2-\beta})dx \\
&\qquad + \frac{1}{\tau}\int_\Omega \left(\frac{\partial f_{j,b}}{\partial(n\theta)} - \frac{\partial f_{b,D}}{\partial(n\theta)} \right) n_j(1-\theta_j)dx.
\end{aligned} \tag{24}$$

We estimate these integrals term by term. First, we compute

$$\begin{aligned}
&\int_\Omega \left(\nabla\frac{\partial f_{b,j}}{\partial n}\cdot\nabla(n_j\theta_j^{1/2-\beta}) + \kappa\nabla\frac{\partial f_{j,b}}{\partial(n\theta)}\cdot\nabla(n_j\theta_j^{3/2-\beta}) \right) dx \\
&\quad = \int_\Omega \big(A\theta_j^{b+1/2-\beta}|\nabla n_j|^2 + 2Bn_j\theta_j^{b-1/2-\beta}\nabla n_j\cdot\nabla\theta_j + Cn_j^2\theta_j^{b-3/2-\beta}|\nabla\theta_j|^2 \big) dx,
\end{aligned}$$

where, taking into account that $\kappa = \frac{2}{3}(2-\beta)$,

$$A = \frac{1}{3}(-2b\beta + b + 6),$$

$$B = \frac{1}{12}(-2b\beta + b + 6)(2b - 2\beta + 1),$$
$$C = \frac{1}{6}b(4b\beta^2 - 8b\beta - 4\beta^2 + 9b + 2\beta - 6).$$

The above integrand defines a quadratic form in $\theta_j^{(b+1/2-\beta)/2}\nabla n_j$ and $n_j\theta_j^{(b-3/2-\beta)/2}\nabla\theta_j$ which is positive definite if and only if $A > 0$ and $AC - B^2 > 0$. These two conditions are equivalent to

$$(1-2\beta)b + 6 > 0,$$
$$4(2\beta-1)b^3 + 4(4\beta^2 - 12\beta + 11)b^2 + (8\beta^3 - 44\beta^2 + 70\beta - 73)b - 6(2\beta-1)^2 > 0,$$

and these inequalities define the set N_β^*. We infer that there exists a constant $C_1 > 0$ such that

$$\int_\Omega \left(\nabla\frac{\partial f_{b,j}}{\partial n} \cdot \nabla(n_j\theta_j^{1/2-\beta}) + \kappa\nabla\frac{\partial f_{j,b}}{\partial(n\theta)} \cdot \nabla(n_j\theta_j^{3/2-\beta}) \right) dx$$
$$\geq C_1 \int_\Omega \left(\theta_j^{b+1/2-\beta}|\nabla n_j|^2 + n_j^2\theta_j^{b-3/2-\beta}|\nabla\theta_j|^2 \right) dx.$$

The first two terms on the right-hand side of (24) involving the boundary contributions only are estimated by using the Young inequality with $\delta > 0$:

$$\begin{aligned}
&\int_\Omega \left(\nabla\frac{\partial f_{b,D}}{\partial n} \cdot \nabla(n_j\theta_j^{1/2-\beta}) + \kappa\nabla\frac{\partial f_{b,D}}{\partial(n\theta)} \cdot \nabla(n_j\theta_j^{3/2-\beta}) \right) dx \\
&\quad \leq \frac{1}{2\delta}\int_\Omega \left|\nabla\frac{\partial f_{b,D}}{\partial n}\right|^2 dx + \frac{1}{2\delta}\int_\Omega \left|\nabla\frac{\partial f_{b,D}}{\partial(n\theta)}\right|^2 dx \\
&\qquad + \frac{\delta}{2}\int_\Omega \big(|\nabla(n_j\theta_j^{1/2-\beta})|^2 + \kappa^2|\nabla(n_j\theta_j^{3/2-\beta})|^2 \big) dx \\
&\quad \leq \frac{1}{2\delta}\int_\Omega \left|\nabla\frac{\partial f_{b,D}}{\partial n}\right|^2 dx + \frac{1}{2\delta}\int_\Omega \left|\nabla\frac{\partial f_{b,D}}{\partial(n\theta)}\right|^2 dx \\
&\qquad + C\delta\int_\Omega \big((\theta_j^{1-2\beta} + \theta_j^{3-2\beta})|\nabla n_j|^2 + n_j^2(\theta_j^{-1-2\beta} + \theta_j^{1-2\beta})|\nabla\theta_j|^2 \big) dx,
\end{aligned}$$

where $C > 0$ depends only on β. It remains to investigate the last integral in (24) involving the relaxation term. Since $\beta < 1/2$, we have $b_1 < 0$ and $b_2 > 0$. Then

$$\begin{aligned}
&\frac{1}{\tau}\sum_{b=b_1,b_2}\frac{1}{|b|}\int_\Omega \left(\frac{\partial f_{j,b}}{\partial(n\theta)} - \frac{\partial f_{b,D}}{\partial(n\theta)} \right) n_j(1-\theta_j)dx \\
&\quad = \frac{1}{\tau}\sum_{b=b_1,b_2}\frac{b}{|b|}\int_\Omega (n_j\theta_j^{b-1} - n_D\theta_D^{b-1})n_j(1-\theta_j)dx \\
&\quad = -\frac{1}{\tau}\int_\Omega n_j^2\theta_j^{b_1-1}(\theta_j - 1)(\theta_j^{b_2-b_1} - 1)dx + \frac{1}{\tau}\int_\Omega n_jn_D(\theta_j - 1)(\theta_D^{b_2-1} - \theta_D^{b_1-1})dx.
\end{aligned}$$

Since $b_1 \le b_2$, the first expression on the right-hand side is nonpositive. The second integral is written as

$$\begin{aligned}
&\frac{1}{\tau}\int_\Omega n_j n_D(\theta_j-1)(\theta_D^{b_2-1}-\theta_D^{b_1-1})dx \\
&\qquad = \frac{1}{\tau}\int_\Omega \big((n_j\theta_j-n_D\theta_D)n_D-(n_j-n_D)n_D+n_D^2(\theta_D-1)\big)(\theta_D^{b_2-1}-\theta_D^{b_1-1})dx \\
&\qquad \le \int_\Omega g_D|n_j-n_D|dx+\int_\Omega g_D|n_j\theta_j-n_D\theta_D|dx+\int_\Omega g_D^* dx,
\end{aligned}$$

where the functions

$$g_D=\frac{n_D}{\tau}|\theta_D^{b_2-1}-\theta_D^{b_1-1}|, \quad g_D^*=n_D(\theta_D-1)g_D$$

only depend on the boundary data. Then the Young and Poincaré inequalities (with constant $C>0$) give

$$\begin{aligned}
&\frac{1}{\tau}\sum_{b=b_1,b_2}\frac{1}{|b|}\int_\Omega\left(\frac{\partial f_{j,b}}{\partial(n\theta)}-\frac{\partial f_{bD}}{\partial(n\theta)}\right)n_j(1-\theta_j)dx \\
&\qquad \le \frac{\delta}{2}\int_\Omega|n_j-nD|^2dx+\frac{\delta}{2}\int_\Omega|n_j\theta_j-n_D\theta_D|^2dx+\int_\Omega\left(g_D^*+\frac{1}{\delta}g_D^2\right)dx \\
&\qquad \le C\frac{\delta}{2}\int_\Omega\big(|\nabla(n_j-n_D)|^2+|\nabla(n_j\theta_j-n_D\theta_D)|^2\big)dx+\int_\Omega\left(g_D^*+\frac{1}{\delta}g_D^2\right)dx \\
&\qquad \le C\delta\int_\Omega\big(|\nabla n_j|^2+\theta_j^2|\nabla n_j|^2+n_j^2|\nabla\theta_j|^2\big)dx+C\delta\int_\Omega\big(|\nabla n_D|^2+|\nabla(n_D\theta_D|^2\big)dx \\
&\qquad\quad +\int_\Omega\left(g_D^*+\frac{1}{\delta}g_D^2\right)dx.
\end{aligned}$$

Putting together the above estimations and using $\theta_j^2|\nabla n_j|^2\le C(1+\theta_j^{3-2\beta})|\nabla n_j|^2$, it follows that

$$\begin{aligned}
&\frac{1}{h}\big(S_{b_1,b_2}[n_j,n_j\theta_j]-S_{b_1,b_2}[n_{j-1},n_{j-1}\theta_{j-1}]\big) \\
&\qquad + C_1\int_\Omega\big((\theta_j^{b_1+1/2-\beta}+\theta_j^{b_2+1/2-\beta})|\nabla n_j|^2+n_j^2(\theta_j^{b_1-3/2-\beta}+\theta_j^{b_2-3/2-\beta})|\nabla\theta_j|^2\big)dx \\
&\qquad \le C\delta\int_\Omega\big((1+\theta_j^{1-2\beta}+\theta_j^{3-2\beta})|\nabla n_j|^2+n_j^2(1+\theta_j^{-1-2\beta}+\theta_j^{1-2\beta})|\nabla\theta_j|^2\big)dx+C_2,
\end{aligned} \tag{25}$$

where the constant

$$C_2=\frac{1}{2\delta}\int_\Omega\left(\left|\nabla\frac{\partial f_{b,D}}{\partial n}\right|^2+\left|\nabla\frac{\partial f_{b,D}}{\partial(n\theta)}\right|^2\right)dx+\int_\Omega\left(g_D^*+\frac{1}{\delta}g_D^2\right)dx$$

vanishes if $n_D=$ const. and $\theta_D=1$. The conditions $b_1\le\beta-1/2$ and $b_2\ge 5/2-\beta$ are equivalent to $b_1+1/2-\beta\le 0$ and $b_2+1/2-\beta\ge 3-2\beta$ as well as to $b_1-3/2-\beta\le -1-2\beta$

and $b_2 - 3/2 - \beta \geq 1 - 2\beta$. Thus, there exists a positive constant $C > 0$, which depends on b_1, b_2, and β, such that for all $\theta_j \geq 0$,

$$1 + \theta_j^{1-2\beta} + \theta_j^{3-2\beta} \leq C(\theta_j^{b_1+1/2-\beta} + \theta_j^{b_2+1/2-\beta}),$$
$$1 + \theta_j^{-1-2\beta} + \theta_j^{1-2\beta} \leq C(\theta_j^{b_1-3/2-\beta} + \theta_j^{b_2-3/2-\beta}).$$

Therefore, choosing $\delta > 0$ sufficiently small, the integral on the right-hand side of (25) can be absorbed by the corresponding integral on the left-hand side. This finishes the proof of the lemma. $\square$

Step 5: The limit $h \to 0$. We define the piecewise constant functions $n_h(x,t) = n_j(x)$ and $\theta_h(x,t) = \theta_j(x)$ for $x \in \Omega$ and $t \in ((j-1)h, jh]$, where $0 \leq j \leq N = T/h$. The discrete time derivative of an arbitrary function $w(x,t)$ is defined by $(D_h w)(x,t) = h^{-1}(w(x,t) - w(x,t-h))$ for $x \in \Omega$, $t \geq h$. Then (9)-(10) can be written as

$$D_h n_h = \Delta(n_h \theta_h^{1/2-\beta}), \quad D_h(n_h\theta_h) = \kappa\Delta(n_h\theta_h^{3/2-\beta}) + \frac{n_h}{\tau}(1-\theta_h). \tag{26}$$

The entropy inequality (23) for $(b_1, b_2) = (\beta - \frac{1}{2}, 5) \in N_\beta$ becomes, after summation over j,

$$S_{b_1,b_2}[n_h(t), n_h(t)\theta_h(t)] + C_1\int_0^t\int_\Omega \big((1+\theta_h^{11/2-\beta})|\nabla n_h|^2 + n_h^2(\theta_h^{-2} + \theta_h^{7/2-\beta})|\nabla\theta_h|^2\big)dx\,ds$$
$$\leq C_2 t + S_{b_1,b_2}[n_0, n_0\theta_0]. \tag{27}$$

We will exploit this inequality to derive h-independent estimates for (n_h) and $(n_h\theta_h)$.

Lemma 5. *There exists a constant $C > 0$ such that for all $h > 0$,*

$$\|n_h\|_{L^\infty(0,T;L^2(\Omega))} + \|n_h\theta_h\|_{L^\infty(0,T;L^2(\Omega))} \leq C, \tag{28}$$
$$\|n_h\theta_h^{1/2-\beta}\|_{L^\infty(0,T;L^2(\Omega))} + \|n_h\theta_h^{3/2-\beta}\|_{L^\infty(0,T;L^2(\Omega))} \leq C, \tag{29}$$
$$\|n_h\|_{L^2(0,T;H^1(\Omega))} + \|n_h\theta_h\|_{L^2(0,T;H^1(\Omega))} \leq C, \tag{30}$$
$$\|n_h\theta_h^{1/2-\beta}\|_{L^2(0,T;H^1(\Omega))} + \|n_h\theta_h^{3/2-\beta}\|_{L^2(0,T;H^1(\Omega))} \leq C, \tag{31}$$
$$\|D_h n_h\|_{L^2(h,T;H^1_D(\Omega)')} + \|D_h(n_h\theta_h)\|_{L^2(h,T;H^1_D(\Omega)')} \leq C. \tag{32}$$

Proof. First, we observe that there exists a constant $C > 0$, which depends only on $\beta \in (-\frac{1}{2}, \frac{1}{2})$, such that

$$1 + \theta_h^2 + \theta_h^{1-2\beta} + \theta_n^{3-2\beta} \leq C(\theta_h^{\beta-1/2} + \theta_h^5), \tag{33}$$
$$1 + \theta_h^2 + \theta_h^{1-2\beta} + \theta_n^{3-2\beta} \leq C(1 + \theta_h^{11/2-\beta}), \tag{34}$$
$$1 + \theta_h^{-1-2\beta} + \theta_h^{1-2\beta} \leq C(\theta_h^{-2} + \theta_h^{7/2-\beta}). \tag{35}$$

We claim that for $(b_1, b_2) = (\beta - \frac{1}{2}, 5)$,

$$S_{b_1,b_2}[n_h, n_h\theta_h] \geq -C + C\int_\Omega n_h^2(\theta_h^{\beta-1/2} + \theta_h^5)dx, \tag{36}$$

where $C > 0$ is a (generic) constant independent of h. Indeed, it holds $f_{b_1}(n_h, n_h\theta_h) = n_h^2\theta_h^{\beta-1/2}$ and $f_{b_2}(n_h, n_h\theta_h) = n_h^2\theta_h^5$, and the terms involving the boundary data can be estimated according to

$$\sum_{b=b_1,b_2}\int_\Omega \left|\frac{\partial f_{b,D}}{\partial n}(n_h - n_D)\right| dx \le C_\delta + \frac{\delta}{2}\int_\Omega n_h^2 dx,$$
$$\sum_{b=b_1,b_2}\int_\Omega \left|\frac{\partial f_{b,D}}{\partial(n\theta)}(n_h\theta_h - n_D\theta_D)\right| dx \le C_\delta + \frac{\delta}{2}\int_\Omega n_h^2\theta_h^2 dx,$$

where we employed the Young inequality with $\delta > 0$. We infer from (33) that

$$\frac{\delta}{2}\int_\Omega n_h^2(1+\theta_h^2)dx \le \frac{\delta}{2}C\int_\Omega n_h^2(\theta_h^{\beta-1/2} + \theta_h^5)dx,$$

and these terms can be absorbed for sufficiently small $\delta > 0$ by the corresponding terms coming from f_{b_1} and f_{b_2}. This proves (36). Now, we multiply (33) by n_h^2, integrate over Ω, and employ (36):

$$\|n_h(t)\|_{L^2(\Omega)}^2 + \|n_h(t)\theta_h(t)\|_{L^2(\Omega)}^2 + \|n_h(t)\theta_h(t)^{1/2-\beta}\|_{L^2(\Omega)}^2$$
$$+ \|n_h(t)\theta_h(t)^{3/2-\beta}\|_{L^2(\Omega)}^2 \le C\big(1 + S_{b_1,b_2}[n_h(t), n_h(t)\theta_h(t)]\big).$$

Taking into account the entropy inequality (27), estimates (28)-(29) follow.

Next, we compute, using (34)-(35),

$$\begin{aligned}|\nabla n_h|^2 &+ |\nabla(n_h\theta_h)|^2 + |\nabla(n_h\theta_h^{1/2-\beta})|^2 + |\nabla(n_h\theta_h^{3/2-\beta})|^2 \\ &\le C(1+\theta_h^2+\theta_h^{1-2\beta}+\theta_h^{3-2\beta})|\nabla n_h|^2 + Cn_h^2(1+\theta_h^{-1-2\beta}+\theta_h^{1-2\beta})|\nabla\theta_h|^2 \\ &\le C(1+\theta_h^{11/2-\beta})|\nabla n_h|^2 + Cn_h^2(\theta_h^{-2}+\theta_h^{7/2-\beta})|\nabla\theta_h|^2.\end{aligned}$$

Hence, Young's inequality gives

$$\begin{aligned}|\nabla(n_h - n_D)|^2 &+ |\nabla(n_h\theta_h - n_D\theta_D)|^2 + |\nabla(n_h\theta_h^{1/2-\beta} - n_D\theta_D^{1/2-\beta})|^2 \\ &+ |\nabla(n_h\theta_h^{3/2-\beta} - n_D\theta_D^{3/2-\beta})|^2 \\ &\le C(1+\theta_h^{11/2-\beta})|\nabla n_h|^2 + Cn_h^2(\theta_h^{-2}+\theta_h^{7/2-\beta})|\nabla\theta_h|^2 + C_D,\end{aligned}$$

where $C_D > 0$ depends on the L^2 norms of ∇n_D, $\nabla(n_D\theta_D)$, $\nabla(n_D\theta_D^{1/2-\beta})$, and $\nabla(n_D\theta_D^{3/2-\beta})$. Note that $C_D = 0$ if n_D and θ_D are constant in Ω. We integrate over $\Omega\times(0,T)$ and employ the Poincaré inequality to find that

$$\begin{aligned}\int_0^T &\big(\|n_h - n_D\|_{H^1(\Omega)}^2 + \|n_h\theta_h - n_D\theta_D\|_{H^1(\Omega)}^2 + \|n_h\theta_h^{1/2-\beta} - n_D\theta_D^{1/2-\beta}\|_{H^1(\Omega)}^2 \\ &+ \|n_h\theta_h^{3/2-\beta} - n_D\theta_D^{3/2-\beta}\|_{H^1(\Omega)}^2\big)dt \\ &\le C\int_0^T\int_\Omega\big((1+\theta_h^{11/2-\beta})|\nabla n_h|^2 + n_h^2(\theta_h^{-2}+\theta_j^{7/2-\beta})|\nabla\theta_h|^2\big)dx\,dt + TC_D \\ &\le C,\end{aligned}$$

because of the entropy inequality (27). This shows (30)-(31).

Finally, estimate (32) follows from

$$\begin{aligned}\|D_h n_h\|_{L^2(0,T;H^1_D(\Omega)')} &\le \|\nabla(n_h\theta_h^{1/2-\beta})\|_{L^2(0,T;L^2(\Omega))} \le C,\\ \|D_h(n_h\theta_h)\|_{L^2(0,T;H^1_D(\Omega)')} &\le \kappa\|\nabla(n_h\theta_h^{3/2-\beta})\|_{L^2(0,T;L^2(\Omega))}\\ &\quad + C\tau^{-1}\|n_h - n_h\theta_h\|_{L^2(0,T;L^2(\Omega))} \le C,\end{aligned}$$

using (28) and (31). □

Aubin's Lemma and Lemma 5 imply that, up to subsequences,

(37) $n_h \to n, \quad n_h\theta_h \to w \quad$ strongly in $L^2(0,T;L^2(\Omega))$,

(38) $n_h \rightharpoonup n, \quad n_h\theta_h \rightharpoonup w, \quad n_h\theta_h^{1/2-\beta} \rightharpoonup y, \quad n_h\theta_h^{3/2-\beta} \rightharpoonup z \quad$ weakly in $L^2(0,T;H^1(\Omega))$,

(39) $D_h n_h \rightharpoonup \partial_t n, \quad D_h(n_h\theta_h) \rightharpoonup \partial_t w \quad$ weakly in $L^2(0,T;H^1_D(\Omega)')$.

In order to identify the functions w, y, z appearing in (37)–(39) we show first that $n, w > 0$ a.e. in $\Omega \times (0,T)$. Let us define the discrete entropy functional:

$$\Lambda[n_h, n_h\theta_h] = \int_\Omega \left(-\log n_h - \frac{1}{\kappa}\log(n_h\theta_h) + \frac{n_h}{n_D} + \frac{1}{\kappa}\frac{n_h\theta_h}{n_D\theta_D}\right) dx, \tag{40}$$

where n_D, θ_D are the values of n_h, θ_h (respectively) on Γ_D. We point out that Λ is well defined since n_h, $n_h\theta_h$ are bounded and strictly positive. The convexity of $x \mapsto -\log x$ implies that

$$\begin{aligned}D_h\Lambda[n_h, n_h\theta_h] &\le \int_\Omega \left((D_h n_h)\left(\frac{1}{n_D} - \frac{1}{n_h}\right) + \frac{1}{\kappa}(D_h(n_h\theta_h))\left(\frac{1}{n_D\theta_D} - \frac{1}{n_h\theta_h}\right)\right) dx \qquad (41)\\ &= \int_\Omega \Big(\nabla(n_h^{\beta+1/2}(n_h\theta_h)^{1/2-\beta})\cdot\nabla(n_h^{-1}) + \nabla(n_h^{\beta-1/2}(n_h\theta_h)^{3/2-\beta})\cdot\nabla((n_h\theta_h)^{-1})\Big) dx\\ &\quad - \int_\Omega \Big(\nabla(n_h^{\beta+1/2}(n_h\theta_h)^{1/2-\beta})\cdot\nabla(n_D^{-1}) + \nabla(n_h^{\beta-1/2}(n_h\theta_h)^{3/2-\beta})\cdot\nabla((n_D\theta_D)^{-1})\Big) dx\\ &\quad + \frac{1}{\kappa}\int_\Omega \left(\frac{1}{n_D\theta_D} - \frac{1}{n_h\theta_h}\right)\frac{n_h}{\tau}(1-\theta_h)dx\\ &= \int_\Omega \Big((n_h\theta_h)^{1/2-\beta}\nabla(n_h^{\beta+1/2})\cdot\nabla(n_h^{-1}) + n_h^{\beta-1/2}\nabla((n_h\theta_h)^{3/2-\beta})\cdot\nabla((n_h\theta_h)^{-1})\\ &\quad + n_h^{\beta+1/2}\nabla((n_h\theta_h)^{1/2-\beta})\cdot\nabla(n_h^{-1}) + (n_h\theta_h)^{3/2-\beta}\nabla(n_h^{\beta-1/2})\cdot\nabla((n_h\theta_h)^{-1})\Big) dx\\ &\quad - \int_\Omega \Big(\nabla(n_h\theta_h^{1/2-\beta})\cdot\nabla(n_D^{-1}) + \nabla(n_h\theta_h^{3/2-\beta})\cdot\nabla((n_D\theta_D)^{-1})\Big) dx\\ &\quad + \frac{1}{\kappa}\int_\Omega \frac{1}{n_D\theta_D}\frac{n_h}{\tau}(1-\theta_h)dx - \frac{1}{\kappa}\int_\Omega \frac{1}{\tau\theta_h}dx + \frac{1}{\kappa\tau}\mathrm{meas}(\Omega).\end{aligned}$$

Young's inequality allows us to bound the terms on the right-hand side of (41) involving n_D, θ_D, and τ:

$$
\begin{aligned}
&-\int_\Omega \Big(\nabla(n_h\theta_h^{1/2-\beta})\cdot\nabla(n_D^{-1}) + \nabla(n_h\theta_h^{3/2-\beta})\cdot\nabla((n_D\theta_D)^{-1})\Big)dx \\
&\quad + \frac{1}{\kappa}\int_\Omega \frac{1}{n_D\theta_D}\frac{n_h}{\tau}(1-\theta_h)dx - \frac{1}{\kappa}\int_\Omega \frac{1}{\tau\theta_h}dx + \frac{|\Omega|}{\kappa\tau} \\
&\le C_D(1 + \|n_h\theta_h^{1/2-\beta}\|_{H^1}^2 + \|n_h\theta_h^{3/2-\beta}\|_{H^1}^2 + \|n_h\|_{L^2}^2),
\end{aligned}
$$

for some constant $C_D > 0$ depending on n_D, θ_D, and τ.

We need to find an upper bound for the remaining terms on the right-hand side of (41), namely:

$$
\begin{aligned}
I := \int_\Omega \Big(&(n_h\theta_h)^{1/2-\beta}\nabla(n_h^{\beta+1/2})\cdot\nabla(n_h^{-1}) + n_h^{\beta-1/2}\nabla((n_h\theta_h)^{3/2-\beta})\cdot\nabla((n_h\theta_h)^{-1}) \\
&+ n_h^{\beta+1/2}\nabla((n_h\theta_h)^{1/2-\beta})\cdot\nabla(n_h^{-1}) + (n_h\theta_h)^{3/2-\beta}\nabla(n_h^{\beta-1/2})\cdot\nabla((n_h\theta_h)^{-1})\Big)dx.
\end{aligned} \tag{42}
$$

The sum of the last two terms inside the integral on the right-hand side vanish, since

$$
\begin{aligned}
&n_h^{\beta+1/2}\nabla((n_h\theta_h)^{1/2-\beta})\cdot\nabla(n_h^{-1}) + (n_h\theta_h)^{3/2-\beta}\nabla(n_h^{\beta-1/2})\cdot\nabla((n_h\theta_h)^{-1}) \\
&\quad = -\left(\frac{1}{2}-\beta\right)n_h^{\beta-3/2}(n_h\theta_h)^{-1/2-\beta}\nabla n_h\cdot\nabla(n_h\theta_h) \\
&\qquad - \left(\beta-\frac{1}{2}\right)n_h^{\beta-3/2}(n_h\theta_h)^{-1/2-\beta}\nabla n_h\cdot\nabla(n_h\theta_h) = 0.
\end{aligned}
$$

Thus, it follows that

$$
\begin{aligned}
I &= \int_\Omega \Big((n_h\theta_h)^{1/2-\beta}\nabla(n_h^{\beta+1/2})\cdot\nabla(n_h^{-1}) + n_h^{\beta-1/2}\nabla((n_h\theta_h)^{3/2-\beta})\cdot\nabla((n_h\theta_h)^{-1})\Big)dx \\
&= -\int_\Omega \Bigg(\left(\frac{1}{2}+\beta\right)n_h^{\beta-5/2}(n_h\theta_h)^{1/2-\beta}|\nabla n_h|^2 \\
&\quad + \left(\frac{3}{2}-\beta\right)n_h^{\beta-1/2}(n_h\theta_h)^{-3/2-\beta}|\nabla(n_h\theta_h)|^2\Bigg)dx \le 0.
\end{aligned}
$$

The above relations show that

$$
\begin{aligned}
&\sup_{t\in[0,T]}\Lambda[n_h(t), n_h(t)\theta_h(t)] \le \Lambda[n_0, n_0\theta_0] \\
&\quad + C_D\big(1 + \|n_h\theta_h^{1/2-\beta}\|_{L^2(0,T;H^1(\Omega))}^2 + \|n_h\theta_h^{3/2-\beta}\|_{L^2(0,T;H^1(\Omega))}^2 + \|n_h\|_{L^2(0,T;L^2(\Omega))}^2\big),
\end{aligned}
$$

where n_0, θ_0 are the values of n_h, θ_h at initial time, respectively. The strong convergence (37) and Fatou's Lemma allow us to conclude that, for some $C > 0$,

$$
\sup_{t\in[0,T]}\Lambda[n(t), w(t)] \le C. \tag{43}
$$

From the definition (40) of Λ and (43), we deduce that

$$-\log n(x,t) - \frac{1}{\kappa}\log w(x,t) < \infty \quad \text{for a.e. } (x,t) \in \Omega \times (0,T). \tag{44}$$

Since $n, w \in L^2(0,T; L^2(\Omega))$, they are a.e. finite. This fact, together with (44), implies that $n > 0$, $w > 0$ a.e. in $\Omega \times (0,T)$.

From the convergence (37) it follows also that $n_h \to n$, $n_h\theta_h \to w$ a.e. in $\Omega \times (0,T)$. The positivity of n implies that $\theta_h = (n_h\theta_h)/n_h \to w/n$ a.e. in $\Omega \times (0,T)$. Let us define $\theta := w/n$. Since n and w are finite and positive a.e. in $\Omega \times (0,T)$, then $0 < \theta < \infty$ a.e. in $\Omega\times(0,T)$. Clearly $n_h\theta_h^{1/2-\beta} \to n\theta^{1/2-\beta}$, $n_h\theta_h^{3/2-\beta} \to n\theta^{3/2-\beta}$ a.e. in $\Omega\times(0,T)$, recalling that $\beta < 1/2$; thus from the weak convergence (38) we obtain $y = n\theta^{1/2-\beta}$, $z = n\theta^{3/2-\beta}$. These relations, together with (37)–(39), allow us to perform the limit $h \to 0$ in the equations for Dn_h, $D(n_h\theta_h)$. This finishes the proof of Theorem 1.

Step 6: Temperature-dependent relaxation times. It remains to prove Corollary 2. The proof is exactly as in Steps 1-5 except at two points. First, we need to ensure in Step 2 that $\tau(\theta)$ is bounded from below to obtain

$$\left(1 - \frac{1}{\kappa}\left(1 + \frac{h}{\tau(\theta_j)}\right)\right) \geq \left(1 - \frac{1}{\kappa}\left(1 + \frac{h}{\tau_0}\right)\right) > 0$$

for all $0 < h < (1-\kappa)\tau_0$, which is needed to estimate (21). Second, we need to pass to the limit $h \to 0$ in the relaxation time term in Step 5. This is more involved since we cannot perform the limit in $\tau(\theta_h)$. The idea is to expand the fraction $n_h/\tau(\theta_h)$ and to consider

$$\frac{n_h}{\tau(\theta_h)}(1-\theta_h) = \frac{n_h^2(1-\theta_h)}{\tau_0 n_h + \tau_1 n_h\theta_h^{1/2-\beta}}.$$

The pointwise convergences of $n_h \to n$ and $n_h\theta_h^{3/2-\beta} \to n\theta^{3/2-\beta}$ imply that

$$n_h\theta_h^{1/2} = n_h^{2(1-\beta)/(3-2\beta)}\left(n_h\theta_h^{3/2-\beta}\right)^{1/(3-2\beta)}$$

converges pointwise to $n\theta^{1/2}$ as $h \to 0$. Consequently, we have the pointwise convergence

$$\frac{n_h}{\tau(\theta_h)}(1-\theta_h) = \frac{n_h(n_h - n_h\theta_h)}{\tau_0 n_h + \tau_1 n_h\theta_h^{1/2-\beta}} \to \frac{n^2(1-\theta)}{\tau_0 n + \tau_1 n\theta^{1/2-\beta}} = \frac{n}{\tau(\theta)}(1-\theta).$$

Furthermore, by (28),

$$\sup_{(0,T)}\int_\Omega \frac{n_h^2}{\tau(\theta_h)^2}(1-\theta_h)^2 dx \leq \frac{2}{\tau_0^2}\sup_{(0,T)}\int_\Omega n_h^2(1+\theta_h^2)dx$$

is uniformly bounded such that, together with the above pointwise convergence and up to a subsequence, it follows that

$$\frac{n_h}{\tau(\theta_h)}(1-\theta_h) \rightharpoonup \frac{n}{\tau(\theta)}(1-\theta) \quad \text{weakly in } L^2(0,T; L^2(\Omega)).$$

This ends the proof.

3. Long-time behavior of solutions

We prove Theorem 3. The proof is divided into several steps.

Step 1: Let $(n_j, n_j\theta_j)$ be a solution to (26) with boundary conditions (2). We recall that both n_j and θ_j are strictly positive. Observing that the constant boundary data gives $C_2 = 0$ in (23), we obtain for $(b_1, b_2) \in N_\beta^*$,

$$\begin{aligned} S_{b_1,b_2}[n_j, n_j\theta_j] + C_1 h \int_\Omega \big((\theta_j^{b_1+1/2-\beta} + \theta_j^{b_2+1/2-\beta})|\nabla n_j|^2 \\ + n_j^2(\theta_j^{b_1-3/2-\beta} + \theta_j^{b_2-3/2-\beta})|\nabla\theta_j|^2\big)dx \le S_{b_1,b_2}[n_{j-1}, n_{j-1}\theta_{j-1}]. \end{aligned}$$

In particular, for $(b_1, b_2) = (\beta - 1/2, 5/2 - \beta) \in N_\beta^*$,

$$\begin{aligned} S_{b_1,b_2}[n_j, n_j\theta_j] + C_1 h \int_\Omega \big(1 + \theta_j^{3-2\beta})|\nabla n_j|^2 + n_j^2(\theta_j^{-2} + \theta_j^{1-2\beta})|\nabla\theta_j|^2\big)dx \\ \le S_{b_1,b_2}[n_{j-1}, n_{j-1}\theta_{j-1}], \end{aligned} \tag{45}$$

and for $(b_1, b_2) = (-3, 5) \in N_\beta^*$ (here, we need $\beta \ge 0$),

$$\begin{aligned} S_{b_1,b_2}[n_j, n_j\theta_j] + C_1 h \int_\Omega \big((\theta_j^{-5/2-\beta} + \theta_j^{11/2-\beta})|\nabla n_j|^2 \\ + n_j^2(\theta_j^{-9/2-\beta} + \theta_j^{7/2-\beta})|\nabla\theta_j|^2\big)dx \le S_{b_1,b_2}[n_{j-1}, n_{j-1}\theta_{j-1}]. \end{aligned} \tag{46}$$

Step 2: We show that the integral involving the gradient terms in (45) can be bounded from below by, up to a factor, the entropy S_{b_1,b_2}. To this end, we observe that, by the convexity of $f_b(n, n\theta) = n^{2-b}(n\theta)^b$ for $b \le 0$ or $b \ge 2$,

$$\begin{aligned} &\int_\Omega \big(f_b(n_j, n_j\theta_j) - f_b(n_D, n_D)\big)dx \\ &\quad\le \int_\Omega \left(\frac{\partial f_b}{\partial n}(n_j, n_j\theta_j)(n_j - n_D) + \frac{\partial f_b}{\partial(n\theta)}(n_j, n_j\theta_j)(n_j\theta_j - n_D)\right)dx. \end{aligned}$$

This implies that

$$\begin{aligned} \phi_b[n_j, n_j\theta_j] &\le \int_\Omega \bigg(\left(\frac{\partial f_{b,j}}{\partial n} - \frac{\partial f_{j,D}}{\partial n}\right)(n_j - n_D) \\ &\qquad + \left(\frac{\partial f_{b,j}}{\partial(n\theta)} - \frac{\partial f_{j,D}}{\partial(n\theta)}\right)(n_j\theta_j - n_D)\bigg)dx \\ &= \int_\Omega \big((2-b)(n_j\theta_j^b - n_D)(n_j - n_D) + b(n_j\theta_j^{b-1} - n_D)(n_j\theta_j - n_D)\big)dx \\ &\le C\big(1 + \|n_j\theta_j^b\|_{L^2(\Omega)}\big)\|n_j - n_D\|_{L^2(\Omega)} \\ &\quad + C\big(1 + \|n_j\theta_j^{b-1}\|_{L^2(\Omega)}\big)\|n_j\theta_j - n_D\|_{L^2(\Omega)}. \end{aligned}$$

Hence, we obtain for $(b_1, b_2) = (\beta - 1/2, 5/2 - \beta)$,

$$S_{b_1,b_2}[n_j, n_j\theta_j] \le C\phi_{b_1}[n_j, n_j\theta_j] + C\phi_{b_2}[n_j, n_j\theta_j]$$

$$\le C\big(1+\|n_j\theta_j^{\beta-1/2}\|_{L^2(\Omega)}+\|n_j\theta_j^{5/2-\beta}\|_{L^2(\Omega)}\big)\|n_j-n_D\|_{L^2(\Omega)}$$
$$+\,C\big(1+\|n_j\theta_j^{\beta-3/2}\|_{L^2(\Omega)}+\|n_j\theta_j^{3/2-\beta}\|_{L^2(\Omega)}\big)\|n_j\theta_j-n_D\|_{L^2(\Omega)}. \tag{47}$$

Noting that (again using $\beta\ge 0$)

$$n_j^2\theta_j^{2\beta-1}+n_j^2\theta_j^{2\beta-3}+n_j^2\theta_j^{3-2\beta}+n_j^2\theta_j^{5-2\beta}\le Cn_j^2(\theta_j^{-3}+\theta_j^5)$$

for some generic constant $C>0$ not depending on h, we infer from (46), after summation over j, that

$$\|n_j\theta_j^{\beta-1/2}\|_{L^2(\Omega)}+\|n_j\theta_j^{5/2-\beta}\|_{L^2(\Omega)}\le C,\quad \|n_j\theta_j^{\beta-3/2}\|_{L^2(\Omega)}+\|n_j\theta_j^{3/2-\beta}\|_{L^2(\Omega)}\le C,$$

and $C>0$ does not depend on j or h. Thus, (47) becomes, with $(b_1,b_2)=(\beta-1/2,5/2-\beta)$,

$$S_{b_1,b_2}[n_j,n_j\theta_j]\le C\|n_j-n_D\|_{L^2(\Omega)}+C\|n_j\theta_j-n_D\|_{L^2(\Omega)}.$$

Taking the square and employing the Poincaré inequality yields

$$\begin{aligned}S_{b_1,b_2}[n_j,n_j\theta_j]^2&\le C\int_\Omega\big(|n_j-n_D|^2+|n_j\theta_j-n_D|^2\big)dx\\&\le C\int_\Omega\big(|\nabla n_j|^2+|\nabla(n_j\theta_j)|^2\big)dx\le C\int_\Omega\big((1+\theta_j^2)|\nabla n_j|^2+n_j^2|\nabla\theta_j|^2\big)dx\\&\le C\int_\Omega\big((1+\theta_h^{3-2\beta})|\nabla n_h|^2+n_h^2(\theta_h^{-2}+\theta_h^{1-2\beta})|\nabla\theta_h|^2\big)dx.\end{aligned}$$

The last inequality follows from elementary estimations using the fact that $\beta<1/2$. This is the desired estimate.

Thus, it follows from (45) that

$$S_{b_1,b_2}[n_j,n_j\theta_j]+ChS_{b_1,b_2}[n_j,n_j\theta_j]^2\le S_{b_1,b_2}[n_{j-1},n_{j-1}\theta_{j-1}],$$

where still $(b_1,b_2)=(\beta-1/2,5/2-\beta)$. We employ the following lemma which is a consequence of Lemma 17 in [3].

Lemma 6. *Let (x_j) be a sequence of nonnegative numbers such that $x_j+\kappa x_j^2\le x_{j-1}$ for $j\in\mathbb{N}$. Then*

$$x_j\le\frac{x_0}{1+\kappa x_0 j/(1+2\kappa x_0)},\quad j\in\mathbb{N}.$$

Hence, with $S_0=S_{b_1,b_2}[n_0,n_0\theta_0]$,

$$S_{b_1,b_2}[n_j,n_j\theta_j]\le\frac{S_0}{1+ChjS_0/(1+2ChS_0)},$$

which can be written as

$$S_{b_1,b_2}[n_h(t),n_h(t)\theta_h(t)]\le\frac{S_0}{1+CtS_0/(1+2ChS_0)},\quad t>0. \tag{48}$$

Step 3: It remains to prove a lower bound for S_{b_1,b_2}. We employ again the convexity of f_b:

$$S_{b_1,b_2}[n_h,n_h\theta_h]\ge C\int_\Omega\lambda\big(|n_h-n_D|^2+|n_h\theta_h-n_D|^2\big)dx, \tag{49}$$

where λ is the minimal eigenvalue of the Hessian $D^2 f_{b_1}(\xi_1,\xi_2) + D^2 f_{b_2}(\xi_1,\xi_2)$ and $\xi_1 = \alpha n_h + (1-\alpha)n_D$, $\xi_2 = \alpha n_h\theta_h + (1-\alpha)n_D$ for some $0 \le \alpha \le 1$.

We recall the following results from linear algebra. If A and B are two symmetric matrices in $\mathbb{R}^{2\times 2}$ with minimal eigenvalues $\lambda_{\min}(A)$ and $\lambda_{\min}(B)$, respectively, then $\lambda_{\min}(A+B) \ge \lambda_{\min}(A) + \lambda_{\min}(B)$ (since the minimal eigenvalue is the minimum of the Rayleigh quotient). Furthermore, a simple computation shows that $\lambda_{\min}(A) = \frac12\mathrm{tr}(A) - (\frac14\mathrm{tr}(A)^2 - \det(A))^{1/2} \ge \det(A)/\mathrm{tr}(A)$. Consequently, since

$$\begin{aligned} \det(D^2 f_b(\xi_1,\xi_2)) &= b(b-2)\eta^{2b-2}, \\ \mathrm{tr}(D^2 f_b(\xi_1,\xi_2)) &= (b-1)((b-2)\eta^b + b\eta^{b-2}), \end{aligned}$$

with $\eta = \xi_2/\xi_1$, we conclude that

$$\begin{aligned} \lambda &\ge \lambda_{\min}(D^2 f_{b_1}(\xi_1,\xi_2)) + \lambda_{\min}(D^2 f_{b_2}(\xi_1,\xi_2)) \\ &\ge \frac{\det(D^2 f_{b_1}(\xi_1,\xi_2))}{\mathrm{tr}(D^2 f_{b_1}(\xi_1,\xi_2))} + \frac{\det(D^2 f_{b_2}(\xi_1,\xi_2))}{\mathrm{tr}(D^2 f_{b_2}(\xi_1,\xi_2))} \ge C\frac{\eta^{\beta-1/2} + \eta^{5/2-\beta}}{1+\eta^2}. \end{aligned}$$

Since $\beta < 1/2$, the function $x \mapsto (x^{\beta-1/2} + x^{5/2-\beta})/(1+x^2)$ has a positive lower bound. Therefore, λ is strictly positive independent of h. Going back to (49), we infer the lower bound

$$S_{b_1,b_2}[n_h, n_h\theta_h] \ge C\int_\Omega \big(|n_h - n_D|^2 + |n_h\theta_h - n_D|^2\big)dx.$$

Together with (48), this shows that

$$\|n_h(t) - n_D\|_{L^2(\Omega)}^2 + \|n_h(t)\theta_h(t) - n_D\|_{L^2(\Omega)}^2 \le \frac{S_0}{1 + C(S_0)t}, \quad t > 0.$$

In view of Lemma 5, the sequences (n_h) and $(n_h\theta_h)$ are bounded in $L^\infty(0,T;L^2(\Omega))$. Therefore, by Fatou's lemma, we obtain

$$\|n(t) - n_D\|_{L^2(\Omega)}^2 + \|n(t)\theta(t) - n_D\|_{L^2(\Omega)}^2 \le \frac{S_0}{1 + C(S_0)t}, \quad t > 0,$$

which concludes the proof.

4. Numerical experiments

In this section we present some numerical results related to (1). According to Theorem 3, the solution $(n(t), n(t)\theta(t))$ converges to $(n_D, n_D\theta_D)$ in $L^2(\Omega)$ as $t\to\infty$ if n_D, θ_D are constants and $\theta_D = 1$. We want to check this behavior in the numerical simulations if the particle density and temperature are close to zero in some point initially.

We consider system (1) in one space dimension with $\Omega = (0,1) \subset \mathbb{R}$, and we impose Dirichlet boundary conditions at $x = 0, 1$ and initial conditions (3). We choose the boundary data $n_D = \theta_D = 1$ and the initial functions $n_0(x) = \exp(-48x^2)$ for $0 \le x \le \frac12$, $n_0(x) = \exp(-48(x-1)^2)$ for $\frac12 < x \le 1$, and $\theta_0 = n_0$. Both initial functions are very small at $x = \frac12$; it holds $n_0(\frac12) = \theta_0(\frac12) = \exp(-12) \approx 6.1\cdot 10^{-6}$.

The equations are discretized in time by the implicit Euler method with time step $\triangle t$ and in space by central finite differences with space step $\triangle x$. The discretized nonlinear system is solved by the Newton method. The time step is chosen in an adaptive way: It is multiplied by the factor 1.25 when the initial guess in the Newton iterations satisfies already the tolerance imposed on the residual, and it is multiplied by the factor 0.75 when the solution of the Newton system is not feasible (namely, not positive). The space step is chosen as $\triangle x = 2 \cdot 10^{-3}$ (501 grid points) and the maximal time step is $\triangle t = 2 \cdot 10^{-3}$.

Figures 2 and 3 illustrate the temporal behavior of the partical density n and the temperature θ for $\beta = -0.25$ and $\beta = 0.25$, respectively, at various small times. For larger times, the functions approach the constant steady state. The diffusion causes the singularity at $x = \frac{1}{2}$ to smooth out quickly, and the solution converges to the steady state. In Figure 4, the decay of the relative ℓ^2 difference to the steady state is illustrated in a semi-logarithmic plot. Even for $\beta < -\frac{1}{2}$ or $\beta > \frac{1}{2}$, the decay to equilibrium seems to be exponentially fast, at least after an initial phase. This may indicate that the decay rate of Theorem 3 is not optimal. Moreover, the results indicate that there may exist solutions to (1)-(3) even for $\beta < -\frac{1}{2}$ and $\beta > \frac{1}{2}$.

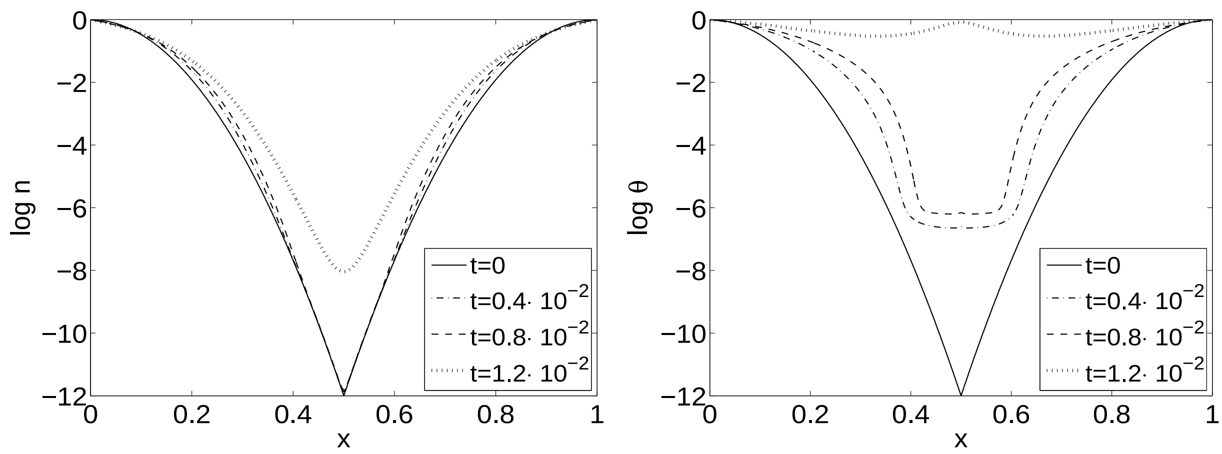

FIGURE 2. Evolution of the particle density n and the temperature θ (semi-logarithmic plot) at various times for $\beta = -0.25$.

REFERENCES

[1] W. Allegretto and H. Xie. Nonisothermal semiconductor systems. In: *Comparison Methods and Stability Theory* (Waterloo, ON, 1993), Lect. Notes Pure Appl. Math. 162, pp. 17-24. Dekker, New York, 1994.

[2] N. Ben Abdallah and P. Degond. On a hierarchy of macroscopic models for semiconductors. *J. Math. Phys.* 37 (1996), 3308-3333.

[3] C. Chainais-Hillairet, A. Jüngel, and S. Schuchnigg. Entropy-dissipative discretization of nonlinear diffusion equations and discrete Beckner inequalities. Preprint, 2013. `arXiv:1303.3791`.

[4] D. Chen, E. Kan, U. Ravaioli, C. Shu, and R. Dutton. An improved energy transport model including nonparabolicity and non-Maxwellian distribution effects. *IEEE Electr. Device Letters* 13 (1992), 26-28.

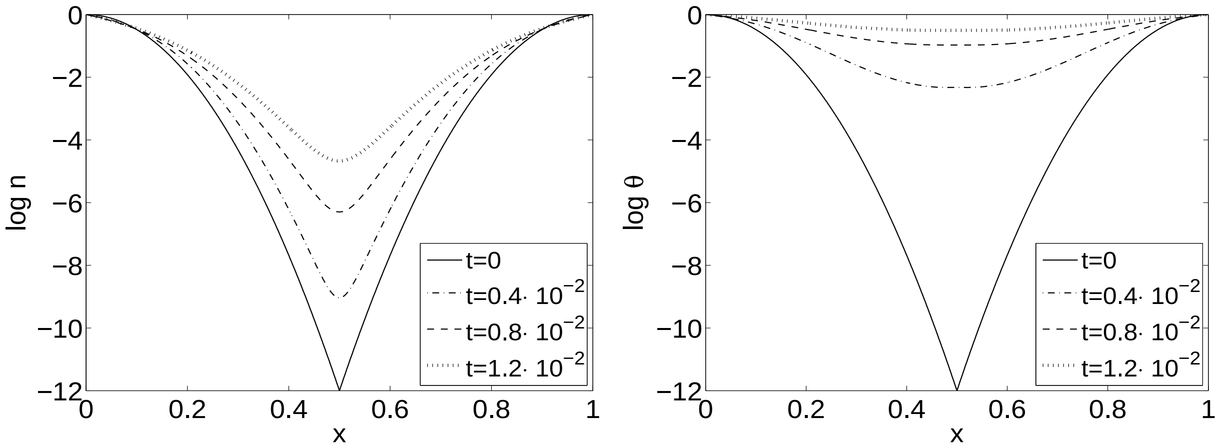

FIGURE 3. Evolution of the particle density n and the temperature θ (semi-logarithmic plot) at various times for $\beta = 0.25$.

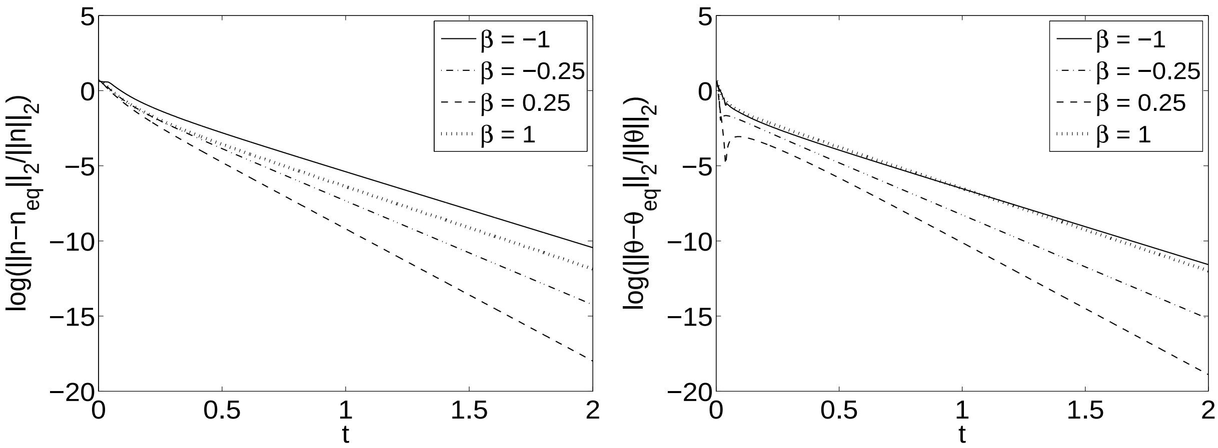

FIGURE 4. Decay of the relative ℓ^2 distance to the equilibrium functions $n_{\rm eq} = 1$ and $\theta_{\rm eq} = 1$ for various values of β (semi-logarithmic plot).

[5] L. Chen and L. Hsiao. The solution of Lyumkis energy transport model in semiconductor science. *Math. Meth. Appl. Sci.* 26 (2003), 1421-1433.

[6] L. Chen, L. Hsiao, and Y. Li. Global existence and asymptotic behavior to the solutions of 1-D Lyumkis energy transport model for semiconductors. *Quart. Appl. Math.* 62 (2004), 337-358.

[7] P. Degond, S. Génieys, and A. Jüngel. A system of parabolic equations in nonequilibrium thermodynamics including thermal and electrical effects. *J. Math. Pures Appl.* 76 (1997), 991-1015.

[8] P. Degond, S. Génieys, and A. Jüngel. Symmetrization and entropy inequality for general diffusion equations. *C. R. Acad. Sci. Paris* 325 (1997), 963-968.

[9] P. Degond, S. Génieys, and A. Jüngel. A steady-state system in nonequilibrium thermodynamics including thermal and electrical effects. *Math. Meth. Appl. Sci.* 21 (1998), 1399-1413.

[10] M. Dreher and A. Jüngel. Compact families of piecewise constant functions in $L^p(0,T;B)$. *Nonlin. Anal.* 75 (2012), 3072-3077.

[11] W. Fang and K. Ito. Existence of stationary solutions to an energy drift-diffusion model for semiconductor devices. *Math. Models Meth. Appl. Sci.* 11 (2001), 827-840.
[12] H. Gajewski and K. Gröger. On the basic equations for carrier transport in semiconductors. *J. Math. Anal. Appl.* 113 (1986), 12-35.
[13] J. Griepentrog. An application of the implicit function theorem to an energy model of the semiconductor theory. *Z. Angew. Math. Mech.* 79 (1999), 43-51.
[14] A. Jüngel. *Transport Equations for Semiconductors.* Lect. Notes Phys. 773. Springer, Berlin, 2009.
[15] A. Jüngel and P. Kristöfel. Lyapunov functionals, weak sequential stability, and uniqueness analysis for energy-transport systems. *Ann. Univ. Ferrara* 58 (2012), 89-100.
[16] A. Jüngel, R. Pinnau, and E. Röhrig. Existence analysis for a simplified transient energy-transport model for semiconductors. *Math. Meth. Appl. Sci.* 36 (2013), 1701-1712.
[17] E. Lyumkis, B. Polsky, A. Shur, and P. Visocky. Transient semiconductor device simulation including energy balance equation. *COMPEL* 11 (1992), 311-325.
[18] M. Pierre and D. Schmitt. Blow up in reaction-diffusion systems with dissipation of mass. *SIAM Review* 42 (2000), 93-106.
[19] G. Stampacchia. *Equations élliptiques du second ordre à coéfficients discontinus.* Les Presses de l'Université de Montréal, Canada, 1966.
[20] G. Troianiello. *Elliptic Differential Equations and Obstacle Problems.* Plenum Press, New York, 1987.
[21] X. Wu and X. Xu. Degenerate semiconductor device equations with temperature effect. *Nonlin. Anal.* 65 (2006), 321-337.
[22] X. Xu. A drift-diffusion model for semiconductors with temperature effects. *Proc. Roy. Soc. Edinburgh Sect. A* 139 (2009), 1101-1119.
[23] H.-M. Yin. The semiconductor system with temperature effect. *J. Math. Anal. Appl.* 196 (1995), 135-152.

Institute for Analysis and Scientific Computing, Vienna University of Technology, Wiedner Hauptstrasse 8–10, 1040 Wien, Austria
E-mail address: nicola.zamponi@tuwien.ac.at

Institute for Analysis and Scientific Computing, Vienna University of Technology, Wiedner Hauptstrasse 8–10, 1040 Wien, Austria
E-mail address: juengel@tuwien.ac.at